In the Name of God, the Merciful, the Compassionate

17 th Iranian Seminar of Organic Chemistry

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Department of Organic Chemistry,
Faculty of Chemistry,
University of Mazandaran,
Babolsar, Iran

With Collaboration of Iranian Chemical Society

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به نام خداوند جان و خرد

شیمی علم اتمها ،پیوندها و مولکولهاست ، دانشی که می تواند خواص ماده ،چگونگی تغییرات و شیوه تولید آنها را از هسته اتم گرفته تا کهکشانها بررسی کند .دقت در ژرفای ماهیت این علم که کشف بخشی از راز هستی است همواره دغدغه آدمیان در طول تاریخ بشر بوده است و شاید بتوان کیمیاگری را از علوم اولیه ای دانست که بشر در فراگیری آن همت گماشت.

در این میان حضور دانشمندان ایرانی مسلمان تاثیر بسزایی در کشف شگفتیهای علم مواد داشته است ،محمد بن زکریای رازی دانشمند پرآوازه و نام آشنایی است که همواره ایرانیان به داشتن چنین فرزندی از سرزمینشان به خود بالیده اند ، هم او که دانش کیمیایی کهن را به علم شیمی نوین دگرگون ساخت ،کسی که بر این باور بود مرد فیلسوف نیز باید کیمیا بداند .

وجود رازی و دانشمندان بزرگی چون او را باید نشانگر ظرفیت استعداد ایرانی دانست که می تواند در تولید علم جهان نقش آفرینی نماید .

کشور عزیز اسلامی مان ایران پس از پیروزی شکوهمند انقلاب اسلامی ، رشد قابل توجهی در عرصه علوم پایه و طبیعی نموده است ، دستیابی به فناوریهای نوین هسته ای ،دانش سلولهای بنیادی و بسیاری موارد از این دست نمونه های هوشمندی ایرانیها در عرصه علم است.

دانشمندان ایرانی تنها با تکیه بر شعار ما می توانیم و ایمان به نعمت استعداد خدادادی و برای رضایت او و آسایش خلق وارد دنیای ناشناخته علوم می شوند و پیشرفتهای قابل توجهی را برایمان رقم زده اند .امروزه صنایع شیمیایی کشور با گسترش این علم توسعه چشمگیری یافته و کشور را صاحب خودکفایی در بسیاری زمینه ها نمود که بدون تردید این امر میسر نمی گشت مگر با همت دانشمندان و محققان این حوزه علمی .

رشته شیمی از باسابقه ترین رشته های علمی در دانشگاه مازندران است که از ابتدا به صورت مرکز تحصیلات تکمیلی راه‌اندازی شد و پس از شکل گیری دانشگاه مازندران در قالب رشته مستقل شیمی در کلیه مقاطع دانشجو پذیرفت .

حضور اعضای هیات علمی متخصص و دانشجویان پرتلاش این رشته را هم اکنون به دانشکده ای پر بار تبدیل کرده است که امروز بانی برگزاری سمیناری بین المللی در این وسعت شده است.

اینجانب ضمن گرامی داشت این رویداد فرخنده که در آغازین روزهای سال تحصیلی جدید و بهار دانش برگزار می شود امید آن دارم که میزبانان شایسته ای برای کلیه شما دانشمندان و دانش پژوهان علم شیمی کشور و جهان باشیم.

رجای واثق دارم که نتایج بحث و تبادل های علمی شما عزیزان بر غنای هر چه بیشتر این علم افزوده و موجبات رشد و تعالی کشور را رقم خواهد زد.

دکتر احمد احمد پور

سرپرست دانشگاه مازندران

In The Name of God

Wellcome Message:

It is a greet pleasure to welcome you to university of Mazandaran in Babolsar. Babolsar is a city in Mazandaran province, Iran, located on the southern coast of the Caspian sea. Since the Babol river passes through the city, both the bank of the river and the beach of the sea potentially from excellent tourist attractions in the city. Mazandaran is one of the 31 provinces of Iran which is located in the north of the country. This province enjoys a colorful historic background which extends for many centuries.In the north of the province, there is the Caspian Sea which is the largest lake in the world. However, a large part of the province is taken by the Alborz Range with its magnificent Damavand, leaving only a narrow coastal strip in the west.

The University of Mazandaran (UMZ) is the most important university in the province of Mazandaran. It was established in September 1979 by merging the former local colleges and institutions. Today, UMZ is supervised and managed by the Iranian Ministry of Science, Research and Technology (MSRT) and consists of eleven faculties, offering undergraduate courses of studies leading up to bachelor's degrees (B.A or B.Sc) in thirty nine departments. Twenty six of these programs extend to postgraduate levels of M.A, M.Sc and/or Ph.D programs and the organization still aiming to improve its well established postgraduate programs.

The University has awarded degrees to over 15000 graduates in various fields since its establishment. Many of these graduates are currently lecturing and researching at different universities and academic institutions within Iran and abroad. The chemistry faculty opened up in 1978 under the name of institute of chemistry by admitting its first PhD students and in 1982 its masters programs started. In 1986 and following the admission of BSc student, the Department had the BSc, MSc and PhD majors.

The aims of this seminar are to facilitate communication among scientists in research and teaching in various fields of organic chemistry throughout. The country both at universities and in different sectors of industries and to engage in the development and use of scientific methods in all fields of organic chemistry. I hope that the participants will enjoy the hospitality of the people of mazandaran and will have a very successful, fruitful scientific discussions and will benefit from the scientific communications of this seminar.

With best wishes
Heshmatollah Alinezhad
The Chairman of 17th Iranian Seminar of Organic Chemistry

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Abstracts

Oral Invited Presentations

Contribution of Chemistry to the Human life of Today

Junes Ipaktschi

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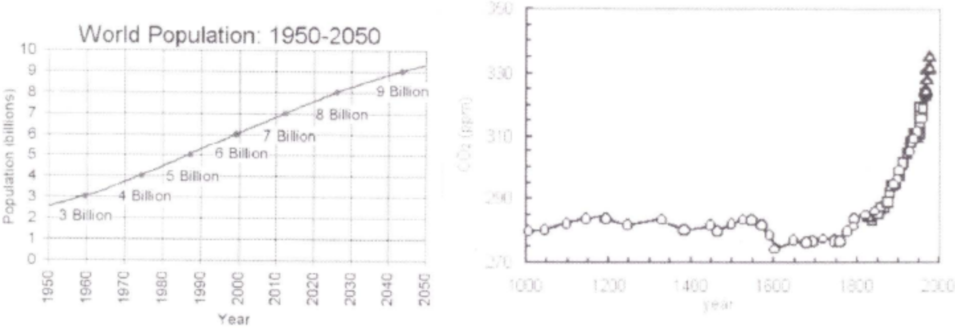
During the past five decades world population has more than doubled to more than 6.5 billion. At the same time the use of resources such as food, water and the emissions from producing goods have also increased substantially (Scheme 1).



Scheme 1: World population growth during the last decades (left) and the increase of CO_2 concentration in the atmosphere (right).

The amount and type of emissions are not only determined by the number of people living on earth, but depend also on production technologies and consumption patterns.

In this paper we discuss how chemistry can help to reduce the emission, to prevent the environment damage, and to increase the quality of life.

In the first part of the paper we will discuss the energy supply, efficient use of energy, and energy efficient production process. Further aspects of the presentation will be the environmentally friendly use of water, production of food and prevention of diseases.

Phytochemical Studies on Native and Endemic Medicinal Plants of Iran

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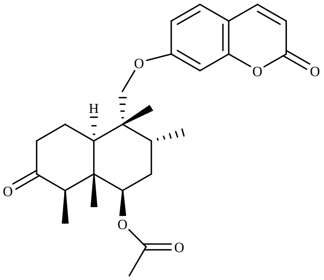
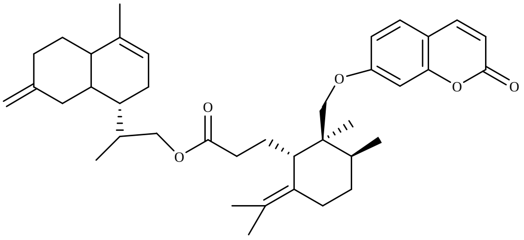
Iran is among the most geographically diverse countries in the world. This ancient nation can be divided into 12 separate geographic environments and boasts 5 major climates. This astounding diversity in geography, allows Iran to host more than 7500 species of plants, around 1800 of which are used in medicine [1,2]. Many of Iran's most precious herbal treasures are plants found nowhere else in the world [3].

In this paper our recent advances in phytochemical studies of native and endemic medicinal plants of Iran is reported. Several species from *Salvia, Thymus, Ajania, Ferula* and *Nepeta* genera have been studied. Also antimicrobial and antioxidant activities of their extracts, essential oils and active components are presented.

Recently, two new coumarin derivatives with the following structures have been isolated and identified from *Ferula pseudalliacea* for the first time.





References:

[1] Hasani-Ranjbar, S.; Larijani, B.; Abdollah, M. *Archives Med. Sci* **2008**, *4*, 285.

[2] Gorji, A. *Trends Pharmacol. Sci* **2003**, *24*, 331.

[3] Mozaffarian, V. *Encyclopedia of Iranian Plants Names,* Farhange Moaser Pub., 1996, Tehran, Iran.

Nano Silica Phosphoric Acid: an efficient and eco-friendly resin for preparations and /or functional group transformations under mild and heterogeneous conditions

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The development of environmentally benign technologies is the most challenging goal of contemporary chemistry and chemical engineering. Environmentally friendly chemical processes should be designed to use environmentally benign feeds and solvents, and utilize efficient reagent or catalyst recyclable systems. In the development of industrial processes, separation is very important. Efficient separation of reagents and catalysts to enable their reuse for subsequent cycles of reactions are also key challenges. Especially in the stream of green chemistry, separation protocols that allow for effective recovery of reagents and catalysts have been increasingly appreciated [1]. Solid acids have many advantages such as simplicity in handling, decreased reactor and plant corrosion problems and environmentally safe disposal. In addition, there is current research and general interest in heterogeneous systems because of the importance such systems have in industry and in developing technologies. Among reported solid acids, nano silica phosphoric acid [2] is used for a wide variety of reactions. It is believed that the presence of wet SiO_2 provides an effective surface area for *in situ* generation of H^+. The reactions are clean and the purification of products are straightforward. In conclusion, nano silica phosphoric acid is a good proton source from point of view of friendly using, convenience, cheapness and insolubility in all organic solvents. The cheapness and availability of the reagents, easy procedure and work-up make these methods attractive for the large scale operations. Meanwhile, nano silica phosphoric acid can serve as an efficient catalyst for some reactions. It is believed that nano silica phosphoric acid can be recycled and then be reused for two or three times. Moreover, reactions are heterogeneous and may be useful in industries [3]. In this work some applications of nano silica phosphoric acid as an efficient and eco-friendly resin in organic synthesis under mild and heterogeneous conditions are presented.

References:

[1] J. I. Yoshida, K. Itami, *Chem. Rev.,* (**2002**), 102,3693.
[2] M. A. Zolfigol, F. Shirini, K. Zamani, E. Ghofrani, S. Ebrahimi, *Phosphorus,Sulfur and Silicon and the Related Elements,* (**2004**) ,179, 2177.
[3] J. H. Clark, *Acc. Chem. Res*., (**2002**) ,35, 791.

Application of acid chlorides and hydrazonyl chlorides in multicomponent reactions

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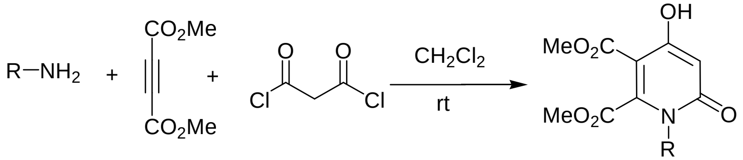
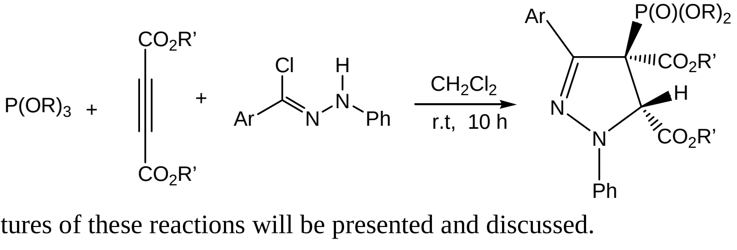
Recently, multicomponent condensation reactions have become a powerful method for the synthesis of small molecule libraries, due to the fact that products are formed in a single step by simultaneous reactions of several reagents and the molecular diversity required for such combinatorial libraries can be achieved by simply varying each component. We report a survey of our recent works on using acid chlorides or hydrazonyl chlorides in multicomponent synthesis of hetereocyclic compounds. Thus, the reaction of malonyl dichloride, alkylamines, and dimethyl acetylenedicarboxylate led to dimethyl 1-alkyl-4-hydroxy-6-oxo-1,6-dihydro-pyridine-2,3-dicarboxylates in excellent yields [1].



The 1:1 zwitterionic intermediates formed from the reaction of trialkyl phosphites with acetylenic esters were trapped by hydrazonoyl chlorides to yield dialkyl 4-(dialkoxyphosphoryl)-1-phenyl-3-aryl-4,5-dihydro-1*H*-pyrazole-4,5-dicarboxylates in good yields. This three-component synthesis of phosphorylated dihydro-1*H*-pyrazoles produces only one diasteroisomer [2].



Various features of these reactions will be presented and discussed.

References:

[1] Yavari, I.; Souri, S. *Synlett* **2007**, 2969
[2] Yavari, I.; Khalili, Gh. *Synlett* **2010**, 1862.

Metal Catalyzed Cyclization Reactions: Progress, applications and Mechanistic Studies

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Transition metals have been used for catalyzing transformations in tandem processes, and significant progress has been made in this regard. Palladium catalysts were used in different tandem reactions to construct biologically active heterocyclic compounds.

We have been interested for some time, in the development of efficient general and practical catalysts for such chemistry, especially for the synthesis of some natural products natural products. This lecture will detail our progress in this endeavor. These subjects will be discussed:

a) Novel method for the construction of 2-oxindoles using palladium catalysts.
b) Mechanistic studies of these processes. A second approach involves the preparation of potential intermediates in these processes.
c) We will also describe applications of the chemistry, with a practical emphasis on the preparation of heterocycles.

References:

[1] Tsuji, Palladium Reagents and Catalysts; John Wiely-VCH, Chichester, **2004**.

[2] De Meijere, A.; Diederich, F. Metal-Catalyzed Cross-Coupling Reactions; Wiley-VCH, Weinheim, **2004**.

[3] McGlacken, G. P.; Fairlamb, I. J.S. *Eur. J. Org. Chem.* **2009**, 4011–4029
[4] Tietze, L. F.; Brasche, G.; Gericke, K. M. *Domino Reaction in Organic Synthesis* John Wiely-VCH, Weinheim, **2006**.
[5] Bararjanian, M.; Balalaie, S.; Rominger, F.; Movassagh, B.; Bijanzadeh, H. R. *J. Org. Chem.* **2010** *75*, 2806-2812.

Synthesis of new chiral C_1- and C_2-symmetric ligands and application of them in some asymmetric reactions

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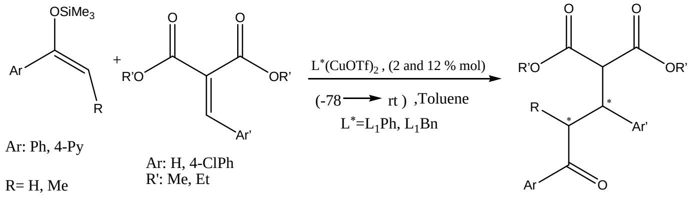
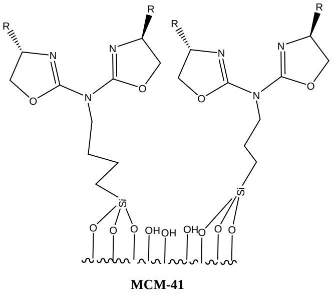
In this research, we first synthesized chiral C_2-symmetric oxazoline-based ligands, such as chiral C_2-symmetric 2,2′ bisoxazoline (1), aza bisoxazoline (2) and chiral C_1-symmetric amines (3) in high yield and enantiomeric excess, then generated the chiral complex metal of them and investigated their reactivity these chiral complexes **1-3** as homogenous catalysis in some asymmetric reactions such as Asymmetric Mukaiyama- Michael Addition (Scheme 1). Another major goal of this study was immobilizing some of the synthesized ligands on MCM-41 in a systematic approach (Scheme 2) and application of these heterogeneous catalysis in above mention asymmetric organic reactions. Furthermore, we explained various factors that affect enantioselectivity in these reactions by our working model.



Scheme1



Scheme 2

Reference

[1] Uozumi, Y.; Kato, K.; Hayashi, T. *J. Am. Chem. Soc.* **1997**, *119*, 5063.
[2] Lin, B.; Zhu, S. F.; Zhang, W.; Chen, C.; Zhou, Q. L. *J. Am. Chem. Soc.* **2007**, *129*, 5834.
[3] Lim, J., Riduan, S. N., Lee, S. and Ying Adv. Synth. Catal. **2008**, 350, 1295 – 1308.

An improved Synthesis of Oxycodone, Oxymorphone, Naltrexone and Nalmefene for Pharmaceutical Use

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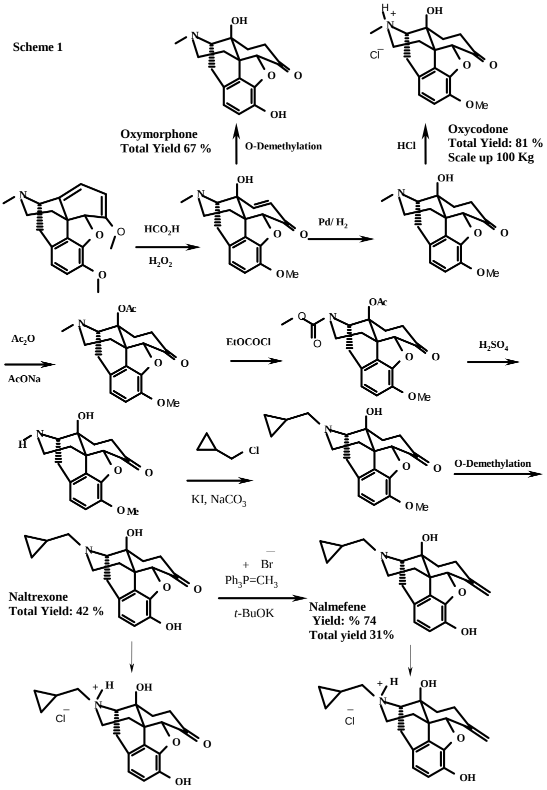
A practical method for the conversion of thebaine to oxycodone, oxymorphone, Naltrexone and nalmefene is described.[1] The procedure should allow more efficient production of opium products and may be easily modified for large-scale synthesis. Scheme 1 show the steps undertaken.



Reference

[1] Reisine, T.; Pasternak, G.; Opioid Analgesics and Antagonist. Pharmaceutical Basis of Therapeutics, 9th ed.; Hardman, J. G.; Limbird, L. E.; Molinoff, P. E.; Ruddon, R. W.; Gilman, A. G.; Eds.; McGraw-Hill: New York **1995**.

Synthesis, Characterization, Properties, Structure and Complexation of Novel Pinacolophanes, Stilbenophanes and Tolanophanes

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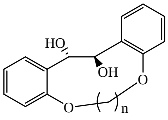
Cyclophanes represent an important class of compounds in many aspects of macrocyclic and supramolecular chemistry. The design, synthesis, Properties, Structure and complexation of pinacolophanes **1** and **2**, stilbenophanes **3** and **4**, tolanophanes **5** and **6** as macrocyclic hosts is an area of our interest in supramolecular chemistry.[1-7]

In this report, we wish to present a brief story on compounds **1–6** (n = 1-12) which has been already carried out in our lab, since 2000.



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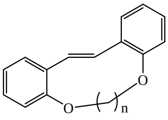

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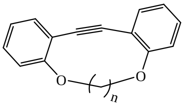

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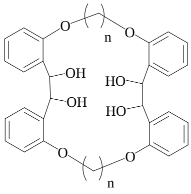

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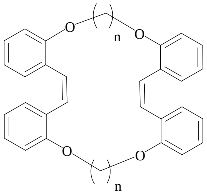

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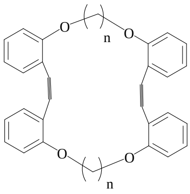

6

n = 1, 2, 3, 4, 5, 12

Reference

[1] Darabi, H. R.; Hashemi Karouei, M.; Jafar Tehrani, M.; Aghapoor, K.; Ghassemzadeh, M.; Neumüller, B. *Supramol. Chem*. **2010**, in press.
[2] Darabi, H. R.; Azimzadeh Arani, M.; Motamedi, A.; Firouzi, R.; Herges, R.; Mohebbi, A. R.;. Nasseri, S.; and Näther C. *Supramol. Chem*. **2009**, *21*, 632.
[3] Darabi, H. R.; Jadidi, K.; Mohebbi, A. R.; Faraji, L.; Aghapoor, K.; Shahbazian, S.; Azimzadeh Arani, M.; Nasseri, S. M. *Supramol. Chem*. **2008**, *20*, 327.
[4] Darabi, H. R.; Azimzadeh Arani, M.; Tafazzoli, M.; Ghiasi; M. *Monatsh Chem* **2008**, 139, 1185.
[5] Darabi, H. R.; Mirza-Aghayan, M.; Ali-Saraie, L.; Bolourtchian, M.; Neumüller, B.; Ghassemzadeh, M. *Supramol. Chem*. **2003**, *15*, 55.
[6] Darabi, H. R.; Mohebbi, A. R.; Bolourtchian, M. *Supramol. Chem*. **2003**, *15*, 465.
[7] Mirza-Aghayan, M.; Darabi, H. R.; Ali-Saraie, L.; Ghassemzadeh, M.; Bolourtchian, M.; Jalali-Heravi, M.; Neumüller, B. *Z. Anorg. Allg. Chem*. **2002**, *628*, 681.

Applications of some of the silica-based reagents in organic reactions

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Acidic catalysts have been used, mainly in industry, for producing more than 1×10 8 Mt/year of products .Among acidic catalysts, the most commonly used are HF, H_2SO_4, $HClO_4$, and H_3PO_4 . Solid acids have many advantages such as ease of handling, decreasing reactor and plant corrosion problems, and environmentally safe disposal .Also, wastes and by-products can be minimized or avoided by developing cleaner synthesis routes .On the other hand, reduction the amount of sulfuric acid /and or simplification in handling procedures is required for risk reduction, economic advantage and environment protection .Green chemistry has been defined as a set of principles that reduce or eliminate the use or generation of hazardous substances .Along this line, using solid acids such as :heteropoly acids, Nafion-H, Dowex 50, Amberlite IR-112, and Permutit-Q have attracted more attention. The importance of these catalysts is growing because of their eco-friendly nature as attention is directed toward the development of clean and green technologies for desired organic molecules to promote environmental safety.

In general, solid acid catalysts are mainly based on clay [1] and silica [2-4] .In terms of convenience, silica-based catalysts are inexpensive, easy to prepare, and insoluble in most organic solvents, which make them being recyclable from various reactions .

Herein, and because of the importance of these types of reagents, we report the applicability of some of the silica-based reagents in various organic functional group transformations either as reagent or as catalyst .

References:
[1] Bahulayan, D.; Narayan, G.; Sreekumar, V.; Lalithambika, M .*Synth .Commun* .**2002**, *32*, 3565.
[2] Zolfigol, M .A.; Shirini, F.; Ghorbani Choghamarani, A.; Mohammadpoor-Baltork, I .*Green Chem* . **2002**, *4*, 562 .
[3] Zolfigol, M .A.; Shirini, F.; Zamani, K.; Ghofrani, E.; Ebrahimi, S .*Phosphorus, Sulfur and Silicon* **2004**, *179*, 2177.
[4] Shirini, F.; Marjani, K.; Taherpour Nahzomi, H.; Zolfigol, M .A .*Phosphorus, Sulfur and Silicon* **2007**, *182*, 1245.

High activity ethylene trimerization catalyst based on new Cr-SNS ligand

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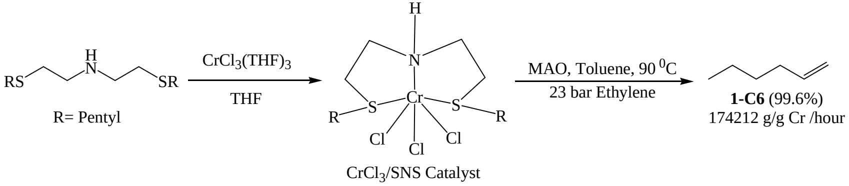
Linear α-olefins, such as 1-hexene and 1-octene, are used, among other applications, as co-monomers in the production of linear low density polyethylene (LLDPE). The conventional method of producing 1-hexene and 1-octene is by oligomerization of ethylene, which yields a wide spectrum of linear α-olefins (LAOs) [1]. A more selective route to 1-hexene is via trimerization of ethylene. In this regard, a number of trimerization catalyst systems have been developed, [2] most of them based on chromium catalysts, including the Phillips pyrrolide system, [2] the Sasol mixed heteroatomic systems, [4,5] and the BP diphosphine system [6,7] although other metals such as Ti [8] and Ta [9] have also been employed.

In this study chromium (III) complexes of tridentate SNS ligands of the form $(RSCH_2\text{-}CH_2)_2NH$ (R=alkyl, aryl) were prepared in good yield and high purity using inexpensive reagents and reacted with $CrCl_3(THF)_3$ at room temperature to give the corresponding $SNS/CrCl_3$ catalyst in high yield. An ethylene trimerization reaction at 90 °C and 23 bar ethylene, using the $SNS/CrCl_3$ complex activated by 700 equivalents of MAO, afforded 99% 1-C6. The effect of different parameters such as ethylene pressure, trimerization temperature, Al/Cr ratio, solvent and S donor substitution on 1-hexene selectivity and activity has been examined. Only 0.10 % PE was produced and the catalyst activity was about 174212 g/g Cr/h.



References

[1] Vogt D. In Applied Homogeneous Catalysis with Organometallic Compounds; Cornils B, Herrmann WA, Eds.; VCH: Weinheim, Germany, (**1996**) Vol. 1, p 245.

[2] Dixon JT, Green MJ, Hess FM, Morgan DH (**2004**) J Organomet Chem 689:3641.

[3] Freeman JW, Buster JL, Knudsen RD (**1999**) US 5856257 (Phillips Petroleum Company).

[4] McGuinness DS, Wasserscheid P, Keim W, Dixon JT, Grove JJC, Hu C, Englert U (**2003**) Chem Commun 334.

[5] McGuinness DS, Wasserscheid P, Keim W, Morgan DH, Dixon JT, Bollmann A, Maumela H, Hess FM, Englert U (**2003**) J Am Chem Soc 125:5272.

[6] Carter A, Cohen SA, Cooley NA, Murphy A, Scutt J, Wass DF (**2002**) Chem Commun 858.

[7] Agapie T, Schofer SL, Labinger JA, Bercaw JE (**2004**) J Am Chem Soc 126:1304.

[8] Deckers PJW, Hessen B, Teuben JH (**2001**) Angew Chem Int Ed 40:2516.

[9] Andes C, Harkins SB, Murtuza S, Oyler K, Sen A (**2001**) J. Am. Chem. Soc. 123:7423.

Organic Modified Gold Nanoparticles: From Synthesis to Applications

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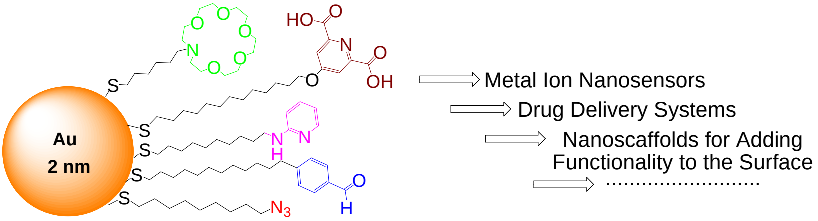
The combination of nanotechnology with chemistry is becoming increasingly important in modern science. Particularly, the design and synthesis of gold nanoparticles functionalized with targeted functional molecules, owning to their unique optical properties, have attracted much attention and been extensively used as the modern ultrasensitive detection and imaging probes.

Our group utilizes a variety of experimental techniques in our general efforts aimed at delineating the parameters that control the mechanisms and dynamics of organic reactions occurring in heterogeneous and ordered environments. In recent years, our main research interest has been directed towards incorporating solution phase reaction systems into the structure of self-assembled monolayers on gold electrode and nanoparticles (Scheme 1) [1-4].



Scheme 1.

The impetus in this area lies in the fact that organic modified nanoparticles and electrodes have important technological implications because of their enormous potential in a variety of material and device applications. Our objectives are i) to develop strategies to exploit the photo-, electro- and thermochemical reactions of these systems to serve as probes to aid in our basic understanding of the mechanistic factors that control molecular interactions and organic reactions at organized monolayer interfaces, and ii) to develop new and selective ways of adding (or removing) functionality to these monolayers.

References:

[1] Alizadeh A.; Khodaei M.M.; Karami Ch.; Workentin M.S.; Shamsipur M.; Sadeghi M., *Nanotechnology* **2010** *21*, 315503.
[2] Ismaili H.; Alizadeh A.; Snell K.E.; Workentin M.S., *Can. J. Chem.* **2009** *87*, 1708.
[3] Kell A.J.; Alizadeh A.; Yang L.; Workentin M.S., *Langmuir* **2005** *21*, 9741.
[4] Shamsipur M.; Kazemi S.H.; Alizadeh A.; Workentin M.S., *J. Electroanal. Chem.* **2007** *610*, 218.

New Sulfide, Sulfoxide, and Sulfone Monomeric Candidates For Macrocycles and Supermolecules

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The interdisciplinary nature of supermolecular and macrocyclic chemistry attracted instant and increasing attention from a variety of scientist worldwide. This area of chemistry has provided a platform for the mixing of ideas between chemists, biologists, physicists, and engineers. There are an enormous potential exists for future applications in the fields such as bio- and nanotechnology, catalysis, environmental clean-up and recovery, medicine, models for biological processes, and smart artificial systems such as photonics, molecular electronics as well as molecular machines.

In this presentation, the earliest recognized examples of such macrocycles and supermolecules as new sulfide, sulfoxide, and sulfone of dibenzo- and dinaphtho derivatives will be introduced in terms of synthesis [1], structural dynamic and properties [2], sensoring [3], host-guest systems [4], template reactions [1, 4], high performance and thermally stable materials [5], and transport membranes [6].

References:

[1] Shockravi, A,; Yousefi, A.; Bavili Tabrizi, S. ; Zakeri, M.; Abouzari-Lotf**, E.;** Sharghi ,H.; *J.Heterocyclic Chem*.; **2008**, 45, 319.

[2] Shockravi, A.; Shamsipur, M.; Fattahi, H.; Taghdiri, M.; Heidaryan, D.; Alizadeh, K.; Rostami, E.; Abbaszadeh, M.; and Yousefi, A.; *J Incl Phenom Macrocycl Chem.;* **2008,** 61:153.

[3] (a) Mashhadizadeh, M.H.; Shockravi, A.; Khoubi,Z.;Heidarian,D.;*Electroanalysis,* **2009**, 21, No. 9, 1041. (b) *J Incl Phenom Macrocycl Chem*.; DOI 10.1007/s10847-010-9770-z **2010**

[4] Rostami, E.; Shockravi, A.; Mehdipour Ataei, S.; Fattahi, H,; Heydarian, D.; Shahbanzadeh Minaee, S. Naghdi, S.; Abouzari Lotf **, E.;** Sadeghpour, M.; Hosseini, H.; Taheri, Z.; Ghorbani, S.; and Javadi, A. *Phosphorus, Sulfur, Silicon, and the Related Elements*, **2009**, 184, 2066.

[5] (a) Shockravi, A.; Abouzari-Lotf , E.; and Javadi, J. *Designed Monomers and Polymers 12, **2009**, 119–128. (b)* Shockravi, A.; Abouzari-Lotf, E.; Javadi, J. and Atabaki, F.; *European Polymer Journal*, 45, **2009**, 1599.

[6] Rahimpour, A.; Madaeni, S.S; Ghorbani, S.;Shockravi, A. and Mansourpanah, Y.; *Applied Surface Science,* **2010,** 256,1825. (b) *Journal of Membrane Science,* **2009**,*334,* 64.

Neighboring hydroxyl group participation in the diastereo selective oxidation of 2-phenylthiocyclohexanols to corresponding sulfoxides.

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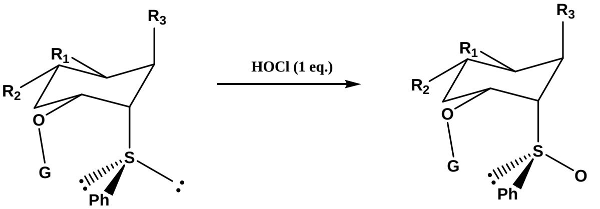
As we have reported earlier, we introduced a new, facile and rapid procedure for selective oxidation of sulfides to the corresponding sulfoxides in good yields using NaClO/H_2SO_4 in both water and 50/50 water/EtOH as solvent. [1] We have also reported that in the case of 2-phenylthio-3-aminocyclohexanoles this method was diastereoselective and for the first time we considered probable neighboring group participation. Later we have used poly (ethylene) glycol as a green and reusable solvent for these types of reactions. [2]

This work describes clearly the mechanism of diastereo selective oxidation of 2-phenylthiocyclohexanols to corresponding sulfoxides by neighboring hydroxyl group participation by hypochlorous acid. The results showed that there is a two step oxidation mechanism *via* a chlorosulfonium ion. The absolute configuration of some obtained sulfuxide was determined by X-ray crystallography.



G=H **Only one diastereoisomer**

G=Ac **1:1 mixture of diastereoisomers**

References:

[1] A. Amoozadeh and F. Nemati, Phosphorus, Sulfur, Silicon and the Relat. Elem. **2009**, 184, 2569.

[2] Amoozadeh, A.; Nemati, F. Phosphorus, Sulfur, Silicon and the Relat. Elem. **2010**, In Press.

Phytochemical Investigation of Abietanoid Quinones: Extraction , Structure Elucidation, Toward Synthesis in Laboratory

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Tehran / Iran

The rootes of Chinese sage, *Salvia miltiorrhiza* bunge (labieteae) are used to prepare an important traditional medicine in the Chinese pharmacoepia, Dan Shen.Indeed , related members of this genus are common traditional medicines throughout the world, making *Salvia* species the targets of intense phytochemical investigations. On the other hand the active constituents of these species have been reported to be several abietanoids diterpenes bearing o-quinone or p-quinones. In this report we will present results of our investigation of *Salvia* species alogwith the synthesis of some active structures.

Pyrylium salts: New strategy for synthesis and conversion

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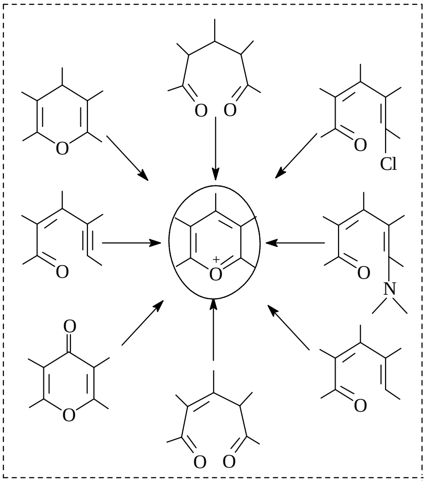
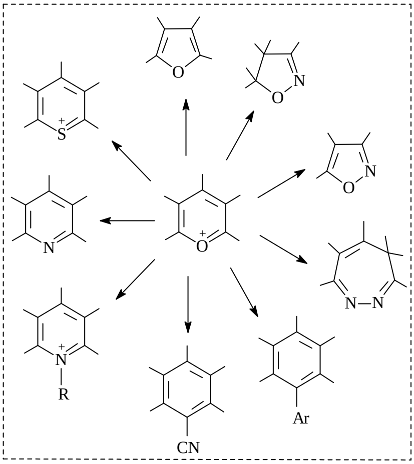
In the framework of the present "renaissance" of organic chemical synthesis, syntheses with or through heterocycles play an important part. Pyrylium salts represent, perhaps more than any other heterocyclic system, a nodal point for many synthetic routes; they can function as intermediates for an extraordinary variety of syntheses. They owe their key role both to a high formation tendency and to a high reactivity toward nucleophiles[1]

In addition to their interest for organic chemical syntheses, pyrylium salts present both theoretical and practical interest. Herein we wish to report the new method for synthesis and conversion of these salts[2].



Synthetic main routes



Schematic representation of important ring transformation

References:

[1] Balaban, A. T.**;** Fischer, G. W. *Advances in Heterocyclic Chemistry* **1982**. In: A. R. Katritzky (Ed). *Pyrylium salts: syntheses, reactions, and physical properties*. Academic Press. Inc. (London) LTD., 30-35.

[2] a) Mouradzadegun A. and Gheitasvand N., *Phosphorus Sulfur Silicon* 180 **2005**, p. 1385; b) A. Mouradzadegun A. and Dianat S. , *J. Heterocyclic Chem*., **2009,** 46, NO. 4, 778–781.

New methods for the synthesis of α- and β-functionalized phosphonates

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From organic and polymer synthesis to biology and biochemistry, phosphonate derivatives have such a wide range of properties and applications that they have stimulated an enormous amount of study for several decades [1]. In this regard, considerable attention has been focused on the synthesis of phosphonates, particularly the α- and β-functionalized analogues. Phosphonates bearing heteroatomic substituents in the α- and β-position to the phosphorus atom have shown strong activities as antibiotics, anticancer drugs and enzyme inhibitors [2]. Their activity attributed to the relative stability of the C-P bond, compared to that of the P-O bond.

Within α-functionalized phosphonates, α-hydroxyphosphonates, which are easily prepared from commercially available materials, are useful precursors for the preparation of other types of α-functionalized phosphonates. The C-P bond of α-hydroxyphosphonates and also other α-functionalized phosphonates is susceptible to the reaction conditions. Cleavage of the C-P bond in these compounds produces aldehydes or carboxylic acids. Therefore, the introduction of suitable methods for the preparation of α-functionalized phosphonates by the replacement of hydroxyl functional groups without affecting the C-P bonds in these molecules will be an important synthetic achievement in organic synthesis.

Direct phosphorus-carbon bond formation represents one of the most versatile and powerful tools for the synthesis of phosphonates. Pioneering work on P–C bond formation was carried out by Arbusov in the early 20th century, culminating in the well-known Michaelis–Arbusov reaction [3].

In the following decades the chemistry of phosphonates developed relatively slowly because of the difficulty in formation of the C–P bond.

Herein, we have reviewed our recent works on the synthesis of α- and β-functionalized phosphonates by functional group transformation or by direct phosphorus-carbon bond formation.

References:

[1] (a) Malachowski, W. P.; Coward, J. K. *J. Org. Chem.* **1994**, *59*, 7616. (b) Horiguchi, M.; Kandatsu, M. *Nature* **1959**, *184*, 901. (c) Kasting, G. B.; Francis, M. D. *J. Bone, Miner, Res.* **1992**, *7*, 513.

[2] (a) Stowasser, B.; Budt, K. H.; Jian-Qi, L.; Peyman, A.; Ruppert, D. *Tetraherdon Lett*. **1992**, *33*, 6625. (b) Smith, J. D. In The Role of Phosphonates in Living Systems; Hilderbrand, R. L., Ed.; CRC: Boca Raton, FL, 1983, pp 31-53. (c) Allen, D. W.; Anderton, E. C.; Bradley, C.; Shiel, L. E. *Polymer Degradation and Stability* **1995**, *47*, 67. (d) Catala, J. M.; Brossas, J. *Makromolekular Chemie- Makromolekular Symposia* **1993**, *74*, 147.

[3] Arbusov, B. A. *Pure Appl. Chem.* **1964**, *9*, 307.

New Approaches in Design of Solid Catalysts

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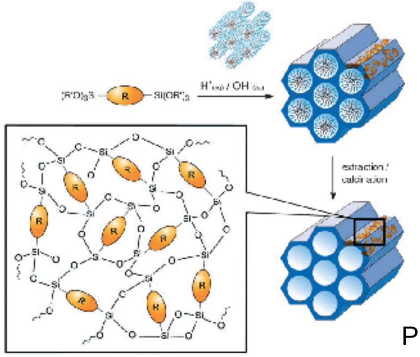
In recent years, organically functionalized ordered mesoporous silica (OMS) [1] with tunable pore structure and tailored composition have received considerable interest for broad applications. These classes of materials are mainly characterized by very large specific surface area (up to 2000 $m^2.g^{-1}$), highly ordered pore systems, and well-defined and tunable pore radius from approximately 2 to 50 nm. On the other hand, the periodic mesoporous organosilica is built from bridge organosilanes of type $(R'O)_3Si\text{-}R\text{-}Si(OR')_3$ wherein organic groups R are homogeneously distributed throughout the stable inorganic framework. [2]. In fact, these innovative area have provided a new opportunity for the design of novel nonostructured materials in which the chemical functionalities can be precisely tuned for special purpose by changing the structure, and composition of the organic groups in the framework of nanopores [3].

Herein, a brief story about this area of research has been presented and some innovation came out from our research group in the field of catalytic application of nanoporous materials (either OMS or PMO materials) in recent years will be described.



PMO Materials

References:

[1] Davis, M. E. *Nature* **2002**, *417*, 813.
[2] T. Asefa, M. J. MacLachlan, N. Coombs, G. A. Ozin, *Nature* **1999**, *402*, 867-871.
[3] (a) B. Hatton, K. Landskron, W. Whitnall, D. Perovic, G. A. Ozin, *Acc. Chem. Res.* **2005**, *38*, 305-312; (b)S. Fujita, S. Inagaki, *Chem. Mater.* **2008**, *20*, 891-908.

Quantitative Solvent-Free Organic Synthesis

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The solvent-free method in organic synthesis is one of the most interesting aspects in organic chemistry, as it fulfills the requirements of green chemistry.

Avoiding of using organic solvents in chemical industry is very attracted, in terms of environmental safety. At the same time it also lowers the costs and leads to the more economical processes.

In this lecture some of the results on solvent-free reactions, including solid-solid, solid-liquid, and solid-gas methods for both organic and inorganic synthesis will be presented. Many different types of reaction examples will be discussed. The importance of these methods is due to the high reaction yields, simplicity in the instrumental requirements as well as simple workup procedures.

Polyoxazine Modified Polyurethanes, a New Generation of Insulating Coatings with Improved Thermal and Electrical Properties

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The properties of polyurethane electrical insulators are reviewed and main advantages and drawbacks of these versatile polymers are described. The strategies for modification of polyurethanes to overcome their technical limitations are discussed. With focus on author's experiences in this field, the combination of polyoxazines (polybenzoxazine and polynaphthoxazine) moieties with polyurethanes are highlighted. In this regard, key synthetic approaches for structural design of these new materials are presented. And finally, the main determining physical, mechanical, thermal and electrical properties of these materials described in details.

References:

[1] H. Yeganeh, Mohammad Amin Shamekhi, Polym Int **2005**, 54,754.
[2] H. Yeganeh, M. Shamekhi, J Appl Polym Sci **2006**, 99,1222.
[3] H. Yeganeh, M. Atai, P. Hojati-Talemi, S. Jamshidi, Macromol. Mater. Eng. **2006**, 291, 883.
[4] H. Yeganeh, S. Jamshidi, P. Hojati Talemi, Eur. Polym. J. **2006**, 42, 1743.
[5] H. Yeganeh, H.R. Moeini, High Performance Polym. **2007**, 19,113.
[6] H. Yeganeh, P. Hojati Talemi, S. Jamshidi, J. Appl. Polym. Sci. **2007**, 103, 1776.
[7] H. Yeganeh, S. Mehdipour-Ataei, M. Ghaffari, High Performance Polym. **2008**, 20, 126.
[8] M. Jalilian, H.Yeganeh and M. Nekoomanesh Haghighi, Polym Int **2008**, 57, 1385.
[9] H. Yeganeh, M. Razavi-Nouri, M. Ghaffari, Polym. Eng. Sci. **2008**, 48, 1329.
[10] H. Yeganeh, M. Razavi-Nouri, M. Ghaffari, Polym. Adv. Tech. **2008**, 19, 1024.
[11] H. Yeganeh, M. Razavi-Nouri, M. Ghaffari, Polym. Eng. Sci. **2008** ; 48 ,1329.
[12] H. Yeganeh, M. Ghaffari, A. Jangi, Polym. Adv. Tech. **2009**, 29, 466.
[13] M. Djalilian, H. Yeganeh, M. Nekoomanesh, Polym. Adv. Tech. **2010**, 21, 118.
[14] S. Jamshidi, H.Yeganeh, S. Mehdipour-Ataei, Polym. Adv. Tech. **2010** in press
[15] S. Jamshidi, H.Yeganeh, S. Mehdipour-Ataei, Polym Int **2010** in press
[16] H.Yeganeh, A. Jangi, Polym. Int. 20**1**0 in press

Abstracts:

Poster Presentations

Preparation of tricarbonylchromium complexes of Hantzsch esters by thermal reaction from $(NH_3)_3Cr(CO)_3$

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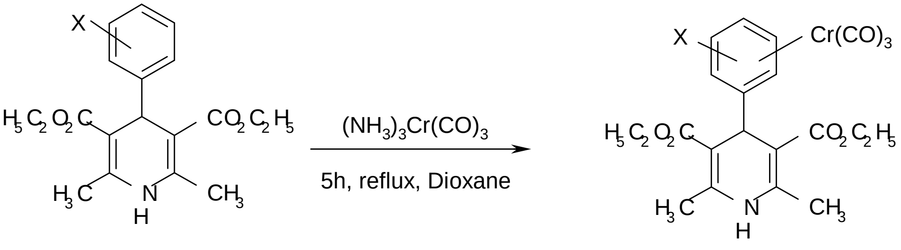
4-Aryl-1,4-dihydropyridines (Hantzsch esters) are important cardiovascular drugs which exhibit calcium channel antagonist activity [1]. Interest in the synthesis of this class of compounds continues, both to elucidate the molecular basis of action and to improve their pharmacological profile.

(Arene) chromium tricarbonyl derivatives have found wide application in synthesis [2], and more recently, in biological applications [3] as probes of drug-receptor binding. We herein report the first preparation of tricarbonylchromium 4-aryl-1,4-dihydropyridines by reaction of 4-aryl-1,4-dihydropyridines with tris(ammine) complex $[(NH_3)_3Cr(CO)_3]$ in refluxing dioxane. This procedure has such advantages as short reaction time, milder reaction conditions, and high yields. (Arene) tricarbonylchromium complexes of Hantzsch esters were obtained up to 75% yields and have been characterized by spectroscopic methods.



X = 2-OMe, 3-OMe, 2-Br,
2-Cl, 3-Cl, 4-Me

[1] Shan, R.; Velaskez, C.; Knaus, E. E. *J. Med. Chem.* **2004**, 47, 254.
[2] Collman, J. P.; Hegedus, L. Principles and Applications of Organotransition Chemistry; University Science Books: MillValley, CA, **1980;** pp 651.
[3] Gruselle, M.; Deprez, P.; Vessieres, A.; Greenfield, S.;Jaouen, G.; Larue, J. P.; Thouvenot, D. *J. Organomet. Chem.* **1989,** *359,* C53456.

Investigation catalytic activity of polyoxometalate contains cerium heteroatom in the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones

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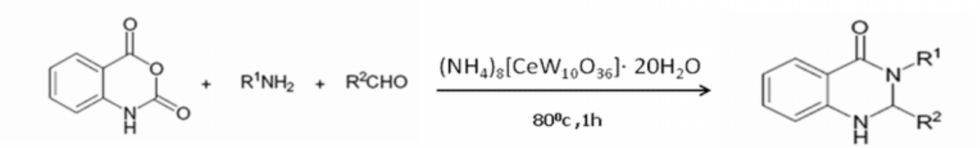
Polyoxometalates are a group of Metal-Oxygen clusters, which gain various application in many fields because of their outstanding properties such as size, mass, electron transfer and Bronsted acidity [1-2]. Metals that commonly used in these compounds are W, Mo, V, which are in highest oxidation state (d^0 & d^1) [3-4]. Due to the lack of electron in the d orbitals of these metals, they can accept electron and be as acidic and oxidative catalysts [5-6].

2,3-Dihydroquinazolin-4(1*H*)-ones are important classes of heterocycles wide rang of pharmacological and biological activities. The most general procedure for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones involves the condensation reaction of isatoic anhydride, ammonium acetate (or amines) and aldehydes in the presence of different reagents and catalysts. However, some of these methods suffer from disadvantages such as long reaction times, low yilds and tedious work-up. Therefore, introducing a new mild and procedure for the synthesis of these compounds are of practical importance [7].

In this study, a series of 2,3-dihydroquinazolin-4(1*H*)-ones have been synthesized by one-pot reaction in the presence of $(NH_4)_8[CeW_{10}O_{36}]\cdot 20H_2O$ under solvent-free condition. High yields, short reaction times, straightforward work-up, commercial availability of starting materials, low cost and relatively non-toxicity of the promoter are noteworthy advantages of thiprotocol.



Reference:

[1] Pope, M. T. *Heteropoly and Isopoly Oxometalates*; Springer-Verlag: New York, **1983**.
[2] Souchay, P. *Polyanions et Polycations;* Gauthier-Villars: Paris, **1963**.
[3] Te´ze, A.; Herve, G. *Inorg. Synth.* **1990**, *27*, 85.
[4] Mizuno, N.; Yamaguchi, K.; Kamata, K. *Coord. Chem. Rev.* **2005**, *249*, 1944.
Tangestaninejad, S.; Mirkhani,V.; Moghadam, M.; Mohammadpoor-Baltork, I.; Shams, S.; Salavati , H *Ultrason Sonochem*. ***2*008**, *15*, 438.
[5] Habibi,M ,H.; Tangestaninejad, S.; Mohammadpoor-Baltork, I.; Mirkhani,V.; Yadollahi B. *Tetrahedron Lett*. **2001**, *42*, 2851.
[6] Dabiri, M.; Salehi, P.; Baghbanzadeh, M. *Monats. Chem.* **2007**, *138*, 1191.

[4+2]Cycloaddition reactions of coumarin quinine methide with pentafulvenes.

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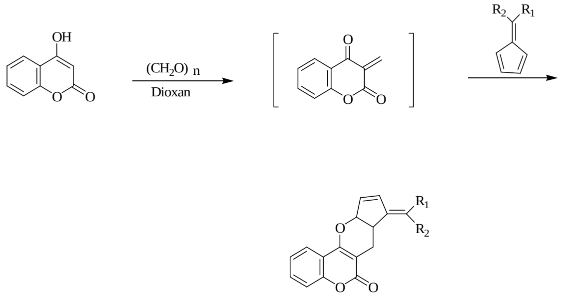
Fulvenes are both interesting and synthetically useful compounds as is evidenced by the fact that they have served as the subject of many investigations .The chemistry of pentafulvenes, their cycloaddition reaction in particular, has been the subject of extensive investigation [1]. Cycloaddition of fulvenes provide versatile and powerful approaches to various polycyclic systems and natural products [2].

A simple high yield method for the preparation of fulvenes has been reported [3,4].
the cycloaddition of o-quinone methides specially those derived from 4-hydroxycoumarin appeared attractive frome the vantage point of constructing polycyclic oxygen hetrocycles.

We have found that pentafulvenes serve as a dienophiles inverse electron demand Diels-Alder reaction with quinine methide derived from α-hydroxycoumarin leading to new pyranopyrone derivatives [2].

Structure of this compound which has been confirmed by the ^{1}H-NMR, ^{13}C-NMR,IR spectroscopy will be reported.



R_1,R_2:alkyl, aryl

References:

[1] Vijay Nair,M.V.Nandakumar,Davis Maliakal,Joseph Swaroop Mathen and Nigam P.Rath.; *Tetrahedron*. **2000**,*56*, 8001.
[2] Vijay Nair,G.N.jayan,K.V.Radhakrishnan,G.Anilkumar and Nigam P.Rath.*Tetrahedron* .**2001**,57,5807.
[3] Keith j.Stone and R. Daniel Little.Organic Chemistry.**1984**, *49*, 1849.
[4] Ihsan Erden, Christian gartner. *Tetrahedron letters*, **2009**,*50*, 2381.

Preparation of nano polyaniline by using 1-methyl-3-butyl imidazolium periodate as oxidant and solvent

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Conducting polymers have attracted a lot of interest in the past two decades primarily because these materials may possess several potential applications. Polyaniline (PANI) has been among the most studied polymers, because of its excellent environmental stability [1] and technological importance in the fields of catalysis [2], biosensors [3], batteries [4], and electronic technology [5]. Recently, polyaniline nanostructures associated with properties of technological and scientific importance have attracted considerable research interest due to their potential applications as actuators, drug delivery systems, gas sensors, biosensors, field emission displays, [6–14] electrochromic displays,[15] and organic storage batteries.[16] Polyaniline was prepared by various methods but most of them are noncontrolable concern to size distribution. Herein, we report a simple process for the synthesis of nano polyaniline by using 1-methyl-3-butyl imidazolium periodate as oxidant and solvent. Using ionic liquid as structural directing molecules has been the most economical method and bridging the gap toward practical application.

References:

[1] Chen, S. A., Fang, W. G. Electrically Conductive Polyaniline Poly(vinyl Alcohol) Composite Films – Physical Properties and Morphological Structures Macromolecules 24 1991: pp. 1242 − 1248.

[2] Malinauskas, A. Electrocatalysis at Conducting Polymers Synth. Met. 107 1999: pp. 75.

[3] McQuade, D. T., Pullen, A. E., Swager, T. M. Conjugated Polymer-Based Chemical Sensors Chem. Rev. 100 2000: pp. 2537.

[4] Novak, P., Muller, K., Santhanam, K. S. V., Haas, O. Electrochemically Active Polymers for Rechar geable Batteries Chem. Rev. 97 1997: pp. 207.

[5] MacDiarmid, A. G. Polyaniline and Polypyrrole: Where are We Headed? Synth. Met. 84 1997:pp. 27 − 34.

[6] A. G. MacDiarmid, Angew. Chem. Int. Ed. 2001, 40, 2581.
[7] J. Wang, S. Chan, R. R. Carlson, Y. Luo, G. Ge, R. S. Ries, J. R. Heath, H. R.Tseng, Nano
[8] Lett. 2004, 4, 1693.
[9] S. Virji, J. Huang, R. B. Kaner, B. H.Weiller, Nano Lett. 2004, 4, 491.
[10] J. Huang, S. Virji, B. H. Weiller, R. B. Kaner, Chem. Eur. J. 2004, 10, 1314.
[11] X. Ma, G. Li, M. Wang, Y. Cheng, R. Bai, H. Chen, Chem. Eur. J. 2006, 12, 3254.
[12] C. G. Wu, T. Bein, Science 1994, 264, 1757.
[13] J. Huang, S. Virji, B. H. Weiller, R. B. Kaner, J. Am. Chem. Soc. 2003, 125, 314.
[14] H. Liu, J. Kameoka, D. A. Czaplewski, H. G. Craighead, Nano Lett. 2004, 4, 671.
[15] S. Sukeerthi, A. Q. Contractor, Anal. Chem. 1999, 71, 2231.
[16] J. Stejshal, P. Kratochvil, S. P. Armes, S. F. Lascelles, A. Riede, M. Helmstedt, J. Prokes, I.
[17] Kivka, Macromolecules 1996, 29, 6814.
[18] C. R. Martin, Science 1994, 266, 1961.

Synthesis and characterization of new composites of poly(*o*-methoxyaniline)/silica by in situ solid-state (solvent free) polymerization in the presence of silica or silica sulfuric acid

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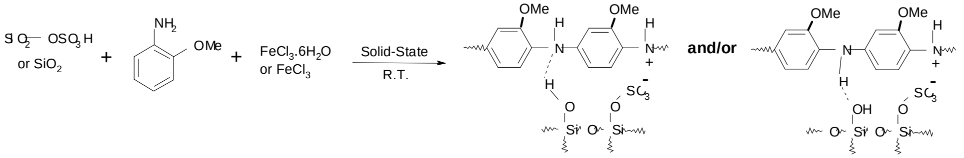
Among conducting polymers, polyaniline (PANI) has very attractive and interesting properties due to its high conductivity, good redox reversibility and stability in aqueous solutions and air for its applications and in electrochromic displays, electrocatalysis, rechargeable batteries, and sensors [1]. However, the main disadvantages of this polymer are its insolubility in common organic solvents and its infusibility. Alternative methods have been designed to improve the solubility and processability of the PANI and its synthesized derivatives [2]. Therefore, in this regard efforts have been made to synthesise functionalised polymer, copolymers or composite conducting polymeric materials. Poly(*o*-methoxyaniline) (POMA) is very similar to PANI, thus being an example of this important family of conducting polymers, they can be synthesized either chemically or electrochemically as a bulk powder or film. The solid-state reaction has many advantages: reduced pollution, low costs, and simplicity in process and handling [3,4]. These factors are especially important in industry.

In this work new POMA/Silica composites are synthesized by solid-state chemical oxidation polymerization of *o*-methoxyaniline in the presence of silica or silica sulfuric acid as dopant solid acid. Iron (III) chloride hexahydrate ($FeCl_3.6H_2O$) or iron (III) chloride anhydrous ($FeCl_3$) were used as oxidizing agent. The Fourier transform infrared (FT-IR) spectra of these polymers reveal a higher ratio of the relative intensities of the benzenoid to quinoid ring modes in composites. The composites were characterized by means of FT-IR spectra, ultraviolet visible (UV-Vis) spectrometry, scanning electron microscopy (SEM) and conductivity measurements.



References:

[1] Jamal, R.; Abdiryim, T.; Nurulla, I. *Polym. Adv. Technol.* **2008**, *19*, 1461.
[2] Abdiryim, T.; Xiao-Gang, Z.; Jamal, R. *J. Appl. Polym. Sci.* **2005**, *96*, 1630.
[3] Jamal, R.; Abdiryim, T.; Ding, Y.; Nurulla, I. *J. Polym. Res.* **2008**, *15*, 75.
[4] Modarresi-Alam, A.R.; Khamooshi, F.; et al. *Arkivoc.* **2007**, *Xvi*, 239.

Theoretical study on the stability of carbocations

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Carbocations are an important type of intermediates that are involved in many organic reactions. The significance of the carbocations as true reaction intermediates has been highlighted with the award of Nobel Prize to Professor George A. Olah in 1994 [1].The intrinsic stabilities of carbocations should be determined in the gas phase rather than in solution, because the relative stabilities of carbocations in solutions might be strongly influenced by the solvent effects due to their characteristic positive charge. The carbocation stability in the gas phase can be measured by *hydride ion affinity (HIA)*. Further insight into the aromatic character of the carbocations is provided by the magnetic properties, which can be studied computationally.

Among the carbocations, the cyclopropenyl cation, $C_3H_3^+$, is of interest to chemists because it is the smallest hydrocarbon for which the Huckel ($4n+2$) π electron rule for monocyclic ring systems is applicable. Therefore, in this research the relative aromaticity of various derivatives of this carbocation has been evaluated using nucleus-independent chemical shift (NICS) [2]. For instance, the computed NICS value in the center of the ring of $C_3H_3^+$ (-22.9) is less than those in $C_3H_2F^+$ (-26.3) and $C_3F_3^+$ (-34.8), respectively. This study has been complemented with DFT calculations to compute ^1H and ^{13}C NMR chemical shifts and provide additional insight into the ring current effects. The effects of different substituents on the aromaticity of the series have also been examined and will be reported.

References:

[1] Olah, G. A. Nobel Lecture, *Angew. Chem. Int. Ed. Engl.* **1995**, *34,* 1393.
[2] Schleyer, P. v. R.; Maerker, C.; Dransfeld, A.; Jiao. H.; Hommes, N. J. R. v. E. *J. Am. Chem. Soc.* **1996**, *118,* 6317.

Facile epoxidation of α,β-unsaturated ketones with *trans*-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane as a novel oxidant

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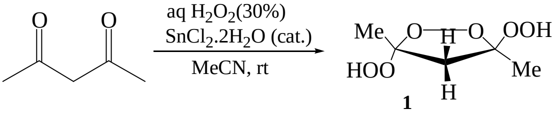
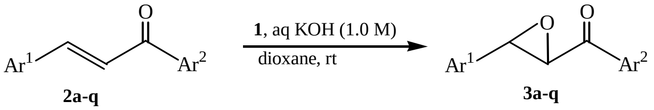
In our ongoing research on the synthesis of *gem*-dihydroperoxides [1-3], and their use in various transformations [4], we became interested to examine the oxidative ability of *trans*-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane for selective conversion of various organic groups. We have prepared this reagent via our previously reported method [4], as a white crystalline solid in high yield (85%) from the reaction of acetylacetone with aqueous (30%) H_2O_2 in acetonitrile at room temperature using a catalytic amount of stannous chloride dehydrate (Scheme **1**).



Scheme 1

Trans-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane **1** has been found to act as an efficient oxidant for selective epoxidation of *trans*-chalcones **2a-q** under the optimized conditions (rt, 1.0 M aqueous KOH in 1,4-dioxane) (Scheme **2**). The experimental results indicate that, the oxidant **1** has conveniently accomplished the conversion of all *trans*-chalcones into their corresponding epoxides **3a-q** in relatively short reaction times and excellent yields (82-96%). The structures of the products **3a-q** were fully established by analysis of their spectral (^{1}H-, ^{13}C-NMR, IR) and physical data.



Scheme 2

References:

[1] Zmitek, K.; Zupan, M.; Iskra, J. Synthetic strategies for a biologically important class of *gem*-dihydroperoxide and perketal derivatives. *Org. Biomol. Chem*. **2007**, *5*, 3895. (A review).
[2] Azarifar, D.; Khosravi, K.; Soleimani, F. *Synthesis* **2009**, 2553.
[3] Azarifar, D.; Khosravi, K.; Soleimani, F. *Molecules* **2010**, *15*, 1433.
[4] Azarifar, D.; Khosravi, K. *Eur. J. Chem*. **2010**, *1*, 15.

Catalytic oxidation of amines by hydrogen peroxide in the presence of transition metal substituted Keggin type polyoxometalate supported on Dowex

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Among a wide variety of heteropoly compounds, The Keggins are the most stable and more easily available. The Keggin heteropoly anions are typically represented by the formula $[XM_{12}O_{40}]^{x-8}$, where X is the heteroatom, x is its oxidation state, and M is the addenda atoms (usually Mo^{6+} or W^{6+})[1].

Supporting the heteropolyacids on solids with high surface area, improved their catalytic performance in various liquid-solid heterogenous reactions[2]. The supports usually used in catalysis are metal oxides, activated carbon, polymers, silica or zeolites. Important features of polymers are good mechanical properties, good thermal stability and low solubility in the environment reaction[3-4].

Catalytic oxidation of amines is an important functional transformation in organic synthesis. Amongst the possible amine oxidation products (hydroxyl, nitroso, nitro, azo and azoxy), aromatic nitroso compounds are utilized extensively as chemical feedstocks for a wide range of useful materials such as dyes, pharmaceuticals, perfumes and plastics. Oxidation of amines pose problems due to nonregioselective or over-oxidation of amines and competitive oxidation of substrates [5].

In this work, we want to report oxidation of amines with H_2O_2 in the presence of Keggin type polyoxometalate supported on polymer Dowex. Optimization of the reaction conditions such as type of solvent, amount of catalyst and amount of oxidant can be provided suitable conditions for oxidation of amines. Oxidation of various amines investigated and high to excellent yields was obtained.

References:

[1] Kozhevnikov, I. *Catalysis by Polyoxometalates;* Wiley: Liverpool. **2002**, *2* , 10.
[2] Mizuno, N.; Misono, M. *Chem. Rev.* **1998**, *98*, 199.
[3] Serp, p.; kalck, p. *Chem. Rev*. **2002**, *102,* 3085.
[4] Okuhara, T.; Mizuno, N.; Misono, M. *Adv. Catal.* **1996**, *41*, 133.
[5] Biradar,A.; Kotbagi,T.; Dongare, M.; Umbarkar, Sh. *Tetrahedron. Lett*. **2008**, *49,* 3616.

Efficient ring opening of epoxides with sodium azide catalyzed by $(TBA)_{6.75}[H_{0.5}P_2W_{17}FeO_{61}]. nH_2O$

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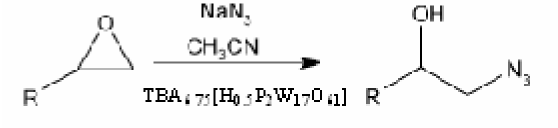
Epoxides are important intermediates in organic synthesis [1] and there are well-known carbon electrophiles capable of reacting with various nucleophiles. The azidolysis of epoxides is the most important method for preparation of azidoalcohols. The vicinal azidoalcohols are precursors of aminoalcohols [2] which are well known as •-blockers and present in various natural products and different bioactive compounds [3]. They are also useful for the synthesis of aminosugars and carbocyclic nucleosides [4].

Polyoxometalates (POMs), as metal–oxygen cluster species, have obtained extensive attention due to not only the structural diversity but also their attractive properties, such as catalytic activity, magnetism, photochemical activity and electrical chemistry [5]. The catalytic function of heteropoly compounds has been attracted much attention and both homogeneous and heterogeneous catalysis are possible. Among a wide variety of heteropoly compound, the Wells-Dawson type polyoxometalate have the large size and the high charge, so they can be used as efficient catalyst.

In this work, a Fe-substituted Wells-Dawson type polyoxometalate was synthesized and used for efficient ring opening of epoxides to the corresponding azidoalcohols. Various epoxides were converted into the corresponding azidoalcohols with sodium azide and high to excellent yields were obtained.



References:

[1] J. G. Smith. *Synthesis*, **1984**, 629
[2] S.C. Bergmeir. *Tetrahedron,* **2000**, *56*, 2561.
[3] E.F.V. Scriven.; K. Turnbull, *Chem. Rev*. **1988**, *88*, 297.
[4] J. Schubert.; R. Schwesinger.; H. Prinzbach, *Angew. Chem. Int. Ed*. **1984**, *23*, 167.
[5] C.L. Hill. *Chem. Rev*. **1998**, *98*, 1.

Solvent-free synthesis of calix [4] resorcinarenes using $Y(NO_3)_3.6H_2O$ as catalyst

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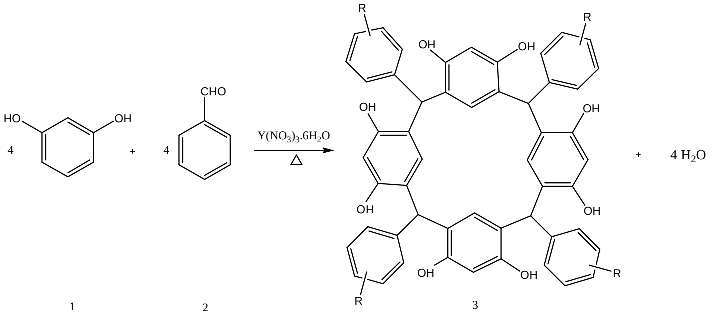
Calix [4] resorcinarenes are macrocyclic molecules with well-known cavity, consist of polar and non-polar parts [1]. They are intrinsically interesting due to their complexing abilities, conformational flexibility, and reactivity. Also, their chemistry has been applied in areas as diverse as catalysis, host-guest chemistry, selective ion transfer, sensors [2], selective receptors, as well as self-assembling molecular capsules and well-known functional nanostructures [3].

Calix [4] resorcinarenes may be prepared in high yield and purity by direct reaction of resorcinol and benzaldehyde derivatives in the presence of a catalytic amount of solid acid and at ambient temperature under solvent-free conditions. This represents a viable alternative to traditional methods. We now report the synthesis of a number of calix [4] resorcinarenes **3** (including two novel compounds) achieved under solvent-free conditions by the direct reaction of resorcinol **1** and aromatic aldehyde **2** in the presence of catalytic amounts of $Y(NO_3)_3.6H_2O$.

The solvent-free method has a good function with respect to energy usage, solvent wastes, associated hazards, reaction time, and yield. The reaction mixtures are viscous liquids or pastes even where all reagents are solids. The melt phase stiffens within minutes to yield a sticky solid wich hardens further on standing. The structure of product **3** was deduced from their IR, ^{1}H NMR and ^{13}C NMR spectral data.



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References:

[1] D. Diamond, K. Nolan, Calixarenes: designer ligands for chemical sensors, *Anal. Chem.* **2001**, *73*, 23A-29A

[2] Bohmer, V. *Angew. Chem., Int. Ed. Engl.* **1995**, *34*, 713.

[3] Rissanen, K.; Vysotsky, M. O.; Kolehmainen, E.; Bohmer, V. *Chem. Eur. J.* **2004**, *10*, 2138.

Synthesis of spirooxindole derivatives

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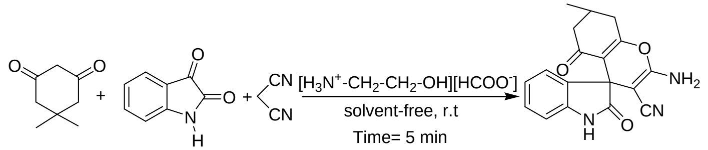
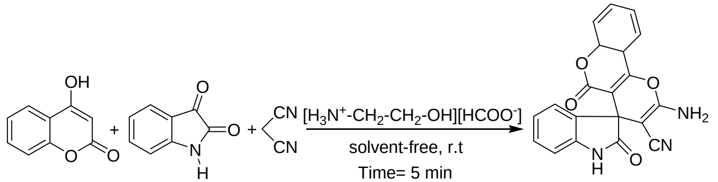
Ionic liquids (ILs) have been revealed as effective green reaction media owing to their unique properties such as tunable polarity, excellent thermal stability, immiscibility with a number of organic solvents, negligible vapor pressure, recyclability, ease of handling, environmentally benign, accelerated reaction rates, and the variety of structures available [1]. They show greater effective surface area and these unusual materials dissolve many organic and inorganic substrates. Ionic liquids (ILs) have been widely applied as catalysts or dual catalyst—solvents in green chemistry processes [2,3]. These considerations are currently driving our efforts to develop ionic liquids in organic transformations. The domino Knoevenagel condensation, conjugate addition, and cyclization for preparation of spirooxindole derivatives [4,5] in high atomic efficiency takes place in excellent yields. The recovered ionic liquid was reused for six cycles. The reaction proceeds without addition of any acid promoter. We suggested mechanism according to the literature; the formation of spirooxindole can be explained by a domino Knoevenagel condensation of isatin and malononitrile (isatylidene malononitrile), and then Michael addition of dimedone or 4-hydroxycoumarin followed by cyclization in the presence of ionic liquid as catalyst.



Yield= 66%

Found m.p= 300 °C, Lit[29]= 300 °C



Yield=59%

Found m.p= 285 °C, Lit[30]= 283-285 °C

References:

[1] Sanjay, V. Malhotra. *J. Am. Chem. Soc*. **2007**.
[2] M. Khurana, J.; Magoo, D. *Tetrahedron lett*. **2009**, *50*, 7300.
[3] Rebeiro, G.L.; Khadilkar, B.M. *Synthesis*. **2001**, 2001, 0370.
[4] Hari, G. S.; Lee, Y. R. *Synthesis* **2009**, x, 000A.
[5] Wang L.M.; Jiao, N.; Qiu, J.; Yu, J.J.; Liu, J.Q.; Guo, F.L.; Liu, Y. *Tetrahedron*. **2010**, 66, 339.

Three-Component Synthesis of Functionalized 2-oxo-2,5-dihydrothiazols

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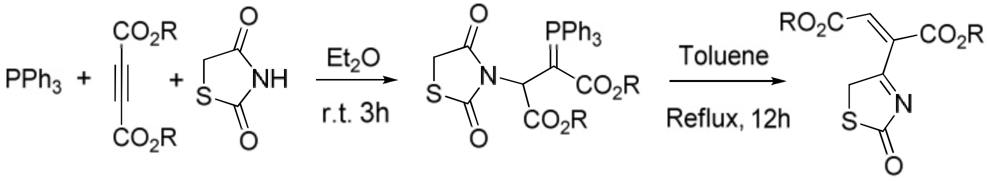
Organophosphorus compounds are widely used in organic synthesis. In recent years there has been increasing interest in the synthesis of organophosphorus compounds, that is, those bearing a carbon atom bound directly to a phosphorus atom. This interest has resulted from the recognition of the value of such compounds in a variety of biological, industrial, and synthetic uses. A large number of methods have appeared describing novel syntheses of organophosphorus compounds. The intramolecular Wittig reaction is useful in organic synthesis [1-4]. We wish to report a convenient and facile synthesis of highly functionalized 2-oxo-2,5-dihydrothiazols **5** *via* an intramolecular Wittig reaction. Thus, Ph_3P, dialkyl acetylenedicarboxylates **2**, and thiazolidine-2,4-dione **3** undergo a smooth reaction at r.t. in Et_2O to afford phosphorus ylide **4**. Compound **4** undergoes a smooth reaction in boiling toluene to produce Ph_3PO and **5** in good yields. Also, the reaction of Ph_3P with DMAD in the presence of 5-arylidenethiazolidine-2,4-dione led to **5** in good yield.



2 **3** **4** **5**

References

- [1] Becker, K. B; *Tetrahedron*, **1987**, 36, 1717.
- [2] Heron, M; *Heterocycles*, **1995**, 41, 2357.
- [3] Yavari, I; Bayat, M; *Tetrahedron*, **2003**, 59, 2001.
- [4] Zaitsev, A. B; Vasil'tsov, A. M; *Tetrahedron*, **2002**, 58, 10043.

A versatile and catalytic method for the selective oxidation of sulfides into sulfoxides and oxidation of primary and secondary alcohols into carbonyl compounds using PVP-H_2O_2, silica sulfuric acid and bromide ion as catalyst

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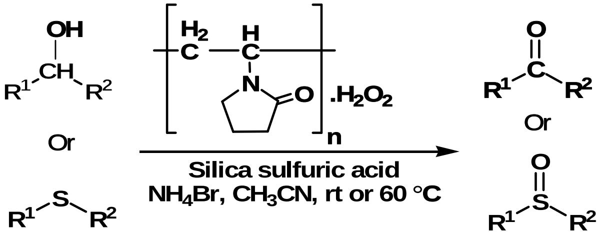
Synthetic methodology, as the building block of organic synthesis, continuously seeks for new reagents, better reaction conditions, and more efficient and selective methods. The chemoselective oxidation of sulfides to the corresponding sulfoxides is of great importance. The standing interest in the oxidation of sulfides into sulfoxides is due to its utility in different areas of chemistry such as violability as synthetic intermediates for the synthesis of chemically and biologically molecules its application in C-C bond-forming, participate in molecular rearrangements [1]. Also conversion of primary and secondary alcohols to the corresponding carbonyl compounds is essential for the preparation of fragrances and food additives as well as of many synthetic intermediates in organic chemistry [2].

Recently we have shown that bromonium ion (Br^+) can effectively apply for the oxidation of different types of organic compounds [3-4]. Therefore we wish to explore different approach for the generation of Br^+. In this research, we report a novel heterogeneous catalytic protocol for the selective oxidation of wide range of sulfides and alcohols to the corresponding sulfoxides and carbonyl compounds using supported hydrogen peroxides on the polyvinylpolypyrrolidone (PVP-H_2O_2) and silica sulfuric acid in the presence of catalytic amounts of ammonium bromide (NH_4Br) in acetonitrile at room temperature (Scheme).



Scheme

References:

[1] Satoh, T.; Kuramochi, Y.; Inoue, Y. *Tetrahedron Lett.* **1999**, *40*, 8815.
[2] Sheldon, R.A.; Arends, I. W. C. E.; Dijksman, A. *Catal. Today*, **2000**, *57*, 157.
[3] Zolfigol, M.A.; Amani, K.; Hajjami, M.; Ghorbani-Choghamarani, A.; Ayazi-Nasrabadi, R.; Jafari, S. *Catal. Commun.* **2008**, *9*, 1739.
[4] Ghorbani-Choghamarani A., Goudarziafshar H., Nikoorazm M., Yousefi S.: *Lett. Org. Chem.* **2009**, *6*, 535.

Synnthesis of stable phosphorus ylides the from reaction between N-H aromatic compound and dimethyl acetylendicarboxylate in presence of triphenyl phosphine.

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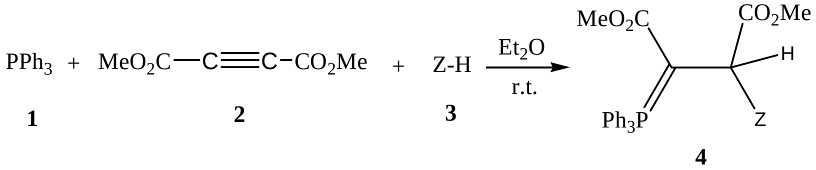
Phosphorous ylides are reactive systems, which take parting many reaction of value in orgacic synthesis[1-3]. These ylides are prepared by treatment of phosphonium salt with a base, and phosphonium salt are usually prepared from the phosphine and alkyl halide[1-3]. Phosphonium salt are also prepared by Michael addition of phosphorus nucleophiles to activated olefins among other methods[2]. We whish to describe here an efficientic synthetic route to aniline derivatives containing stable phosphorus ylides. Thus reaction of triphenylphosphine (1) with dimethyle acetylenedicarboxylates (2) in the presence of NH-aromatic compound (3) leads to the corresponding stable phosphorus ylides (4) in excellent yield . The ^{1}H , ^{13}C, and ^{31}P NMR spectra of ylide (4) is consistent with the presence of two isomers.



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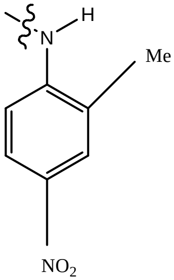
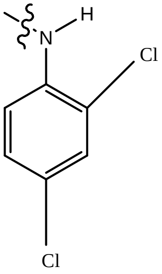
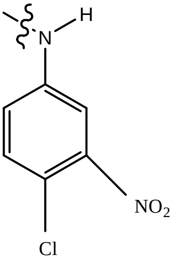
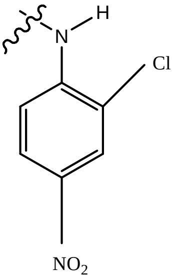
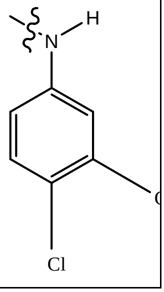
Z					

References:

[1] Yavari I and. Maghsoodlou M. T , *Tetrahedron Lett.*,**1998**, *39*, 4579 .
[2] Yavari I and. Ramazani A ,*Phosphorus, Sulfur, and Silicon*, **1997** ,*130* **,** 73.
[3] Dandia A , Khaturia S ,.Sarawgi P , and. Jain A , *Phosphorus, Sulfur, and Silicon*, **2007**,*182***,** 2529 .

Selective oxidation of alcohols by the $PhI(OAc)_2$/ $Mn(T(4-CH(CH_3)_2P)P)OAc$ /ImH catalytic system: Effect of metals, *meso*-substituents, and anionic axial ligands

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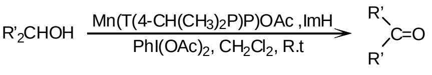
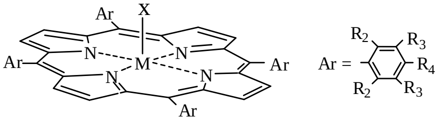
The oxidation of alcohols to the corresponding aldehydes and ketones is one of the most important functional group transformations in organic synthesis [1]. So far, many methods such as enzymatic [2] and metal free [3] oxidations have been developed for this purpose. Hypervalent iodine reagents have also received a great deal of attention due to their versatility in oxidation processes [4]. In general, pentavalent iodine reagents such as Dess–Martin periodinane and o-iodoxybenzoic acid have been widely used for efficient oxidation of alcohols to the carbonyl compounds [4,5].

In this work, we first investigated the ability of these metalloporphyrins (**Fig .1**) with different metal centers, counter ions, and *meso*-aryl substituents as catalysts in the oxidation of 4-nitrobenzyl alcohol in the presence of (diacetoxyiodo)benzene ($PhI(OAc)_2$). While the steric properties of porphyrin complexes and axial nitrogenous bases used in this study are of paramount importance in determining the overall catalytic reaction time and oxidation yield, clear evidence is provided that only the manganese porphyrins are able to catalyze oxidation of 4-nitrobenzyl alcohol, whereas the Fe, Ni and Co complexes have no acceptable catalytic activities. Manganese porphyrins with electronwithdrawing substituents on their phenyl groups are much less effective catalysts than those with electron donating substituents, so that the most efficient system that has been selected involves $Mn(T(4-CH(CH_3)_2P)P)OAc$, which was then used for oxidation of other alcohols. This method provides a cost-effective and environmentally friendly oxidation procedure due to the utilisation of less toxic $PhI(OAc)_2$.



R' = Aryl, Alkyl, H



	R_2	R_3	R_4	M	X
Mn(TPP)OAc	H	H	H	Mn	OAc
$Mn(T(4-OCH_3P)P)OAc$	H	H	OCH_3	Mn	OAc
$Mn(T(4-CH(CH_3)_2)P)P)OAc$	H	H	$CH(CH_3)_2$	Mn	OAc
Ni(TPP)Cl	H	H	H	Ni	Cl
Co(TPP)Cl	H	H	H	Co	Cl
$Fe(T(4-OCH_3P)P)Cl$	H	H	OCH_3	Fe	Cl

Fig. 1. Metalloporphyrins used in this study

References:

[1] (a) Sheldon .R.A and Koshi .J.K., Metal-Catalysed Oxidations of Organic Compounds; Academic Press: New York, **1984**; (b) Armstrong.A, *Org.Chem.*, **2003**, 99, 21.
[2] Kroutil .W, Mang .H, Edegger .K and Faber .K,. *Adv. Synth. Catal.*, **2004**, 346, 125.
[3] Adam .W, Saha-Moller .C.R. and Ganeshpure .P.A, *Chem. Rev.*, **2001**, 101, 3499.
[4] (a) Matveeva .E.D, Proskurnina .M.V. and Zefirov .N.S, *Heteroatom. Chem.*, **2006**, 6, 595; (b) Zhdankin .V.V and Stang .P.J, *Chem.Rev.*, **2002**, 102, 2523.
[5] (a) Zheng .Q.G, Chen .Z.C. and Liu .Z, *Org. Lett.*, **2003**, 5, 3321; (b) More .J.D. and Finney .N.S, *Org. Lett.*, **2002**, 4, 3001.

Synthesis of new symmetric N,N- aromatic substituted,2,5-diamino 1,3,4-thiadiazoles with one-pot reaction by use of dithiocarbamate

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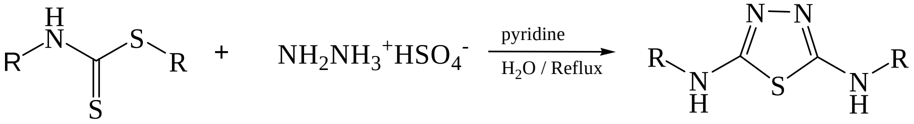
Heterocyclic compounds constitute the largest family of organic compounds, which include many of biologically material to life. Especially five-membered ring heterocyclic compounds serve as the core compound of a large number of substances that have interesting biologically activities [1].

1,3,4-thiadiazoles have been used in numerous therapeutic areas such as anti microbial, anti tumor, anti bacterial, anti convulsant and anti angiogonic activity [2-4], anti hypertensive, hypoglycemic activity [5] and are key intermediates in the preparation of various biologically compounds for example megazol, acetazolamide, anti tubercular, anti fungal, anti inflammatory, analgesic activity and lower ulcerogenic potential [6-8].

Here we are going to report a new procedure for synthesis of some 2,5-disubstituted amino-1,3,4-thiadiazoles by the reaction of easily prepared dithiocarbamates with hydrazine salt. The reaction condition is simple, efficient and gives good yields of products.



R = C_6H_5, C_6H_4Cl, C_6H_4Br, C_6H_4Me, $C_6H_3Cl_2$, C_6H_4OMe.

References:

[1] Hwang, J.; Choi, H.; Lee, D.; Gong, Y. *J. Comb. Chem.* **2005**, *7*, 816.
[2] Kaleta, Z.; Makowski, B.; Sos, T.; Dembinski, R. *Org. Lett*. **2006**, *8*, 1625.
[3] Rzeski, W. ; Matysiakb, J. ; Kandefer, M. *Bioorganic & Medicinal Chemistry.* **2007**, *15, 3201.*
[4] Turner, S.; Myers, M.; Gadie, B.; Nelson, A.; Pape, R.; Saville, J. F.; Doxey, J.; Berridge, T. *J. Med. Chem.* **1988**, *31, 902.*
[5] Oru, E.; Rollas, S.; Kandemirli, F.; Shvets, N.; Dimoglo, A.S. *J. Med. Chem.,* **2004**, *47 ,27, 6760.*
[6] Hanna, M.; Girges, M.; Rasala, D.; Gawinecki. *Drug Res.* **1995**, *45, 1074.*
[7] Mavrova, A.; Wesselinova, D.; Tsenov, Y.; Denkova, P. *European Journal of Medic Chemistry.* **2009**, *44, 63.*
[8] Aryanasab, F.; Ziyaei Halimehjani, A.; Saidi, M.R. *Tetrahedron Letters.* **2010**, *51,790.*

Esterification of free fatty acids to biodiesel by new highly Brønsted acidic ionic liquid

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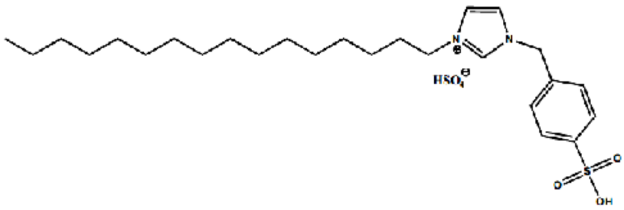
Long chain fatty acid alkyl esters can be used in the production of paints and ink additives, lubricants, solvents, plasticizers, perfumery, agro chemistry and emulsifiers in foods [1]. Also, nowadays the synthesis of biodiesel as green fuel from esterification of free fatty acids and the transesterification of vegetable oils and animal fats is a good interest, because it has high cetane number, high flashpoint and several environmental benefits such as reducing the greenhouse effect [2]. Nowadays, ionic liquids are attracting increasing attention in many fields including organic chemistry, electrochemistry, catalysis and etc. because they are recyclable, highly viscous, non-flammable and environment friendly. Also, they can be functionalized to act as acids, bases or ligands. Also, ionic liquids can serve as solvents or catalyst for esterification and transesterification reactions [3].

In this study, highly acidic ionic liquid with sulfonic acid groups synthesized and characterized with FT-IR, ^{1}H NMR, ^{13}C NMR and CHNS analyses. The esterification of oleic acid with methanol was studied using it, as catalyst. It was observed that this ionic liquid was more active than sulfuric acid at reaction condition. Further, the reaction parameters, such as reaction temperature, molar ratio, amount of catalyst and reaction time were studied and finally methyl oleate was produced with 95.1 % yield at lower time of 4.5 h. Also, we investigated the effect of length of alcohol and fatty acid's alkyl chain on the catalytic activity of ionic liquid in the esterification reaction. Although, there isn't heavy different on the activity of catalyst between the esterification of other carboxylic acids and oleic acid but result revealed that the carboxylic acids with lower number of carbon or degree of saturation had higher conversion to methyl ester. Therefore, because of its advanced character, this catalyst can be the replacement of acid catalyst in many cases of organic reactions.



References:

[1] Alípio C. Carmo Jr, Luiz K.C. de Souza, Carlos E.F. da Costa, E. Longo, José R. Zamian, Geraldo N. da Rocha Filho, *Fuel*. **2009,** *88*, 461.

[2] Bernhard M.E. Russbueldt, Wolfgang F. Hoelderich, *Appl. Catal. A: Gen*. **2009,** *362*, 47. Sikshi, S. A.; Hultin, P. G. *J. Org. Chem*. **2006**, *71*, 5888.

[3] Lei Zhang , Mo Xian a, , Yucai He , Liangzhi Li , Jianming Yang , Shitao Yu , Xin Xu, *Bioresource. Technol.* **2009**, *100* , 4368.

Chlorodiphenylphosphine/2, 3-dichloro-5, 6-dicyanobenzoquinone as a selective and efficient system for the mild ester condensation of equimolar amounts of carboxylic acids and alcohols

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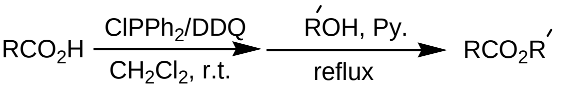
Esterification is one of the most fundamental and important reactions in organic synthesis [1]. Several bulk and fine chemicals are produced in this manner in chemical, petrochemical and pharmaceutical industries. However, in many cases of direct condensation of carboxylic acids with alcohols such as Fischer esterification, large excess amounts of either carboxylic acids or alcohols are used to give esters in high yield [2]. Also some other methods in this condensation are operated in high temperatures using Dean-Stark apparatus [3] or in acidic conditions [4]. Thus, regarding to these limitations, research towards the development of efficient, mild, within neutral media and selective methods for this transformation is an active area in organic synthesis. In continuation of our works on the new applications of trivalent phosphorus in organic synthesis [5], we now report a simple, mild, high selective and efficient ester condensation between equimolar amounts of carboxylic acids and alcohols avoiding the use of dehydrating system such as the Dean-Stark apparatus using chlorodiphenylphosphine/2, 3-dichloro-5, 6-dicyanobenzoquinone ($ClPPh_2$/ DDQ; 1.1:1.1) as a new mixed reagent in CH_2Cl_2 under neutral conditions (Scheme).



$$RCO_2H \xrightarrow[CH_2Cl_2,\ r.t.]{ClPPh_2/DDQ} \xrightarrow[reflux]{R'OH,\ Py.} RCO_2R'$$

The presented method is efficiently used for the esterification between aliphatic and aromatic carboxylic acids and primary, secondary, tertiary and benzylic as well as cyclic alcohols in a 1:1 molar ratio affording good to excellent yields of carboxylic esters. Carboxylic acids can be esterified with primary alcohols in the presence of secondary or tertiary ones or with secondary alcohols in the presence of tertiary ones with good to excellent selectivity in this method. In addition, it was found that the presented method is able to esterify of normal carboxylic acids in the presence of long chain carboxylic acids with excellent selectivity. In conclusion, the present investigation has demonstrated that the use of $ClPPh_2$/DDQ as a new mixed reagent provides a simple, mild and convenient method for selective esterification between equimolar amounts of carboxylic acids and alcohols in high yields under neutral conditions. Easy work up and availability and ease of handling of the reagent can be considered as other advantages of this method.

References:

[1] Larock, R. C. *Comprehensive Organic Transformations*, VCH, New York, **1989**.
[2] Masaki, Y.; Tanaka, N.; Miura, T. *Chem. Lett.* **1997**, 55.
[3] Chen, C.T.; Munot, Y.S. *J. Org. Chem.* **2005**, *70*, 8625.
[4] Sakakura, A.; Koshikari, Y.; Ishihara, K. *Tetrahedron Lett.* **2008**, *49*, 5017.
[5] For example: Aghapour, G.; Afzali, A. *Synth. Commun.* **2008**, *38*, 4023.

Polyamidation of bis-(4-carboxyphenyl) dimethylsilane via diisocyanate route in tetrabutylammonium bromide

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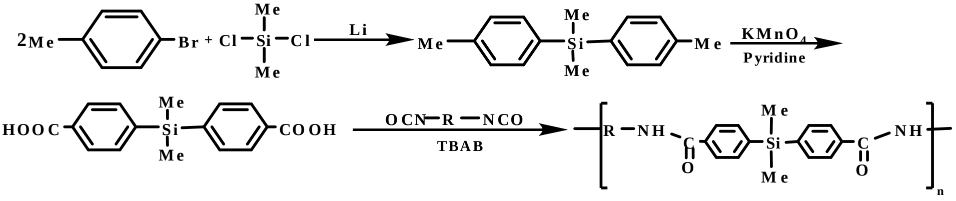
Wholly aromatic polyamides exhibit high thermal stability, good chemical resistance, and excellent mechanical properties which make them find applications in many areas [1]. However, these polymers are difficult to process due to their high glass-transition temperatures (Tg), or high melting temperatures (Tm), and insoluble nature in most organic solvents [2]. One way to overcome these difficulties is to synthesize polyamides containing silicon in the main chain. These polymers has been the subject of considerable interests such as good solubility, high thermal and thermo-oxidative stability, good flame retardency and high moisture resistance.

In fact, most preparative methods known for creating polyamide linkage are based on polycondensation reaction between diamines and diacylcholoride or direct polycondensation reaction between diamines and diacids. But, little has been reported on the synthesis of polyamides or copolyamides based on direct polycondensation reactions between diacids and diisocyanates [3-5].

In this investigation bis-(4-carboxyphenyl) dimethylsilane has been synthesized as monomer. The direct polycondensation of this diacid monomer with several aromatic and aliphatic diisocyanates, was carried out in tetrabutylammonium bromide (TBAB) as a molten ionic liquid in the presence of different catalysts in conventional heating. The resulting polyamides were characterized by FT-IR and ^{1}H-NMR spectroscopy, inherent viscosity measurements, solubility test and thermal gravimetric analysis (TG) and were obtained in high yields and moderate inherent viscosities. The main advantages of this method of polymerization is that, the use of any organic solvent was not needed throughout the whole process of polymerization; in fact, organic solvent removal is of importance to minimize economic cost and environmental impact of chemical processes. The TG results show that the presence of silane moieties in the main chain of polymer caused to increase the thermal stability of the polyamides as well as improvement of their solubility in organic solvent.



References:

[1] Cassidy, P.E.; Thermally Stable Polymers, *Marcel Dekker, New York,* **1980**.
[2] Yang, H.H.; Aromatic High-Strengh Fibers, *Wiley, New York,* **1989.**
[3] Xie, H.; Zhang, S.; Duan H. *Tet. Lett.* **2004,** *45,* 2013-2015.
[4] Peng, Y.; Song, G. *Tet. Lett.* **2004,** *45,* 5313-5316.
[5] Mallakpour, S.; Rafiee, Z. *Eur. Polym. J.,* **2007**, *43,* 1510–1515.

Engineering and characterization of collagen-based bio-nanocomposite membranes

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Preparation bio-nanocomposites with natural biopolymers, such as protein, can be achieved using a melt intercalation or a solvent intercalation method [1]. In this work, the properties of collagen hydrolysate/ poly (vinyl alcohol)/ organo-modified sodium montmorillonite **(**Na-MMT) blend were investigated by scanning electron microscopy (SEM) and Thermogravimetric Analysis (TGA).

Here we describe the modification of Na-MMT with ammonium and phosphonium salts to prepared organo-modified sodium montmorillonite**,** then using it as appliqué of collagen-based bio-nanocomposite blend and it characterized by X-RD technique.

Collagen is a group of naturally occurring proteins. It is the main protein of connective tissue and making up about 25% to 35% of the whole-body protein content.

Polyvinyl alcohol (PVA) is a water-soluble synthetic polymer. It is nontoxic, fully degradable and has high tensile strength and flexibility [2].

The PVA membrane can be modified by blending with collagen that in turn may affect the biocompatibility of the blended membrane [3]. Incorporation of organo-modified sodium montmorillonite into the biopolymer matrices results in improved mechanical properties and thermal stability of the resulting bio-nanocomposites without sacrificing biodegradability due to their nanometer size dispersion. Therefore, these bio-composite should be useful as a bioengineered material. Consequently, even though these natural polymer based bio-nanocomposite is in infancy, we hope it has a chance to be examined for its potential in the future.

References

[1] Ruixiang Zhao. Peter Torley.Peter J. Halley. *J Mater Sci* **2008**, 43,3058.

[2] First draft prepared by S.K.Saxena. *POLYVINYL ALCOHOL (PVA)* ,Chemical and Technical Assessment (CTA)© FAO **2004.**

[3] Wen-Yuan Chuang, Tai-Horng Young, Chun-Hsu Yao, Wen-Yen Chiu**,** *Biomaterials* 20 (**1999**) 1479.

The study of reaction of 5-bromo-3-(1-methylpyrrolidin-2-ylidene)-3*H*-indole with pentane-2,4-dione

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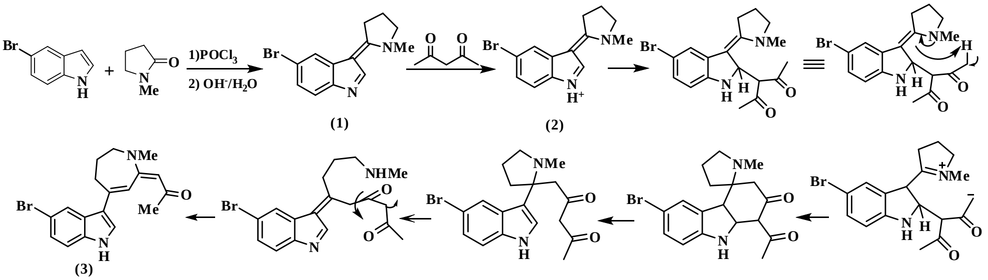
When 5-bromoindole was treated with complex formed from N-methylpyrrolidone (NMP) and phosphorous oxychloride ($POCl_3$) followed with basification of reaction mixture, 5-Bromo-3-(1-methylpyrrolidin-2-ylidene)-3*H*-indole (1) was obtained in high yield as white needle crystals.

5-Bromo-3-(1-methylpyrrolidin-2-ylidene)-3*H*-indole is a strong base and addition of a proton at the imine nitrogen produces a resonance stablised cation (2).

Herein, we report its interaction with pentane-2,4-dione. We believe that the result is the best rationalized in terms of nucleophilic addition at the imine carbon in (2). The mechanism of reaction was shown below.

It is suggested that the process is initiated by an acid-base reaction followed by nucleophilic addition to give 1-[(*E*)-4-(5-Bromo-1*H*-indol-3-yl)-1-methyl-2,5,6,7-tetrahydro-1*H*-azepin-2-ylidene]propan-2-one (3) as main product (78% yield) beside other trace products and starting compound (1).



References:

[1] Youngdale, G. A.; Anger, D. G.; Anthony, W. C. *J. Med. Chem*. **1964**, *7*, 415.
[2] Bishop, D. I.; Al-khawaja, I. K.; Joule, J. A. *J. Chem. Res (M).* **1981**, 4279.
[3] Helliwell, M. ; Aghazadeh, M. ; Baradarani, M. M. ; Joule, *J. A. Acta Cryst*. E*66*, **2010**, 01532.

Theoretical studies of free activation energies and kinetic of electron transfer of [SWCNT(5,5)-armchair-C_nH_{20}][R] (R= η^2-C_{60}Pd(dppf), η^2-C_{60}Pd(dppr) and η^2-C_{60}Pd(dppcym)$_2$, n=20-300) nanostructure complexes

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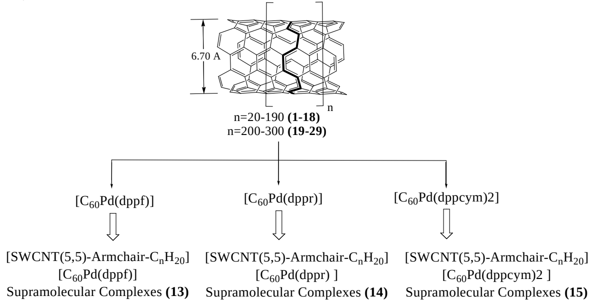
One of the most recognizable types of carbon nanotubes is the (5,5) armchair single-walled carbon nanotube. The first metal complexes containing one or several bis(triorganylphosphine)platinum fragments attached to the C_{60} core and coordinated in the olefinic η^2-mode were described in 1991.[1] Thus it became clear that fullerenes, at least the buckminsterfullerene C_{60}, can function as ligands in the reactions with transition metals. Electronic structures of exohedral palladium complexes of [60]-fullerenes with diphenylphosphinoferrocenyl, diphenylphosphinoruthenocenyl, and diphenylphosphino-cymantrenyl ligands were studied by cyclic voltammetry and semiempirical quantum_chemical calculations in 2004.[2] Probable sites of localization of electronic changes in the molecules of these complexes under electrochemical oxidation and reduction were determined before. The number of carbon atoms (n) of the SWCNTs is considered one of the most useful numerical and structural electrochemical properties for understanding the structural relationship between the structures of the unsaturated molecules η^2_C_{60}Pd(dppf), η^2_C_{60}Pd(dppr) and η^2_C_{60}Pd(dppcym)$_2$ **(10-12)** and [SWCNT(5,5)-armchair-C_nH_{20}] (n=20-190) **1-18**, to produce [SWCNT(5,5)-Armchair-C_nH_{20}][R] (R= η^2_C_{60}Pd(dppf), η^2_C_{60}Pd(dppr) and η^2_C_{60}Pd(dppcym)$_2$, n=20-300) nanostructure complexes. The relationship between this index and the first free activation energies of electron transfer ($\Delta G^{\#}_{et(1)}$), as assessed using the *electron transfer* (ET) equation on the basis of the first oxidation potentials ($^{ox}E_1$) of **A-C** for the predicted supramolecular complexes, between **1-18** and **19-29** with the metallofullerenes η^2_C_{60}Pd(dppf), η^2_C_{60}Pd(dppr) and η^2_C_{60}Pd(dppcym)$_2$ as [SWCNT(5,5)-Armchair-C_nH_{20}][R](R=η^2_C_{60}Pd(dppf),η^2_C_{60}Pd(dppr) and η^2_C_{60}Pd(dppcym)$_2$, n=20-300), are presented here. The results were extended for [SWCNT(5,5)-Armchair-C_nH_{20}][R](R= η^2_C_{60}Pd(dppf), η^2_C_{60}Pd(dppr) and η^2_C_{60}Pd(dppcym)$_2$, n=20-300).[3,4] The kinetic rate constants of the electron transfers (k_{et} , n=1,2), were also calculated.



References:

[1] T. V. Magdesieva, et al., *Russ.Chem.Bull., Int.Ed., 53(4) 2004*, 795.
[2] V. I. Sokolov, *Russ. J. Coord. Chem.*,33(10) 2007, 711.
[3] A.A. Taherpour, Chem Phys Lett , 483 (2009) 233.
[4] A.A. Taherpour, J. Phys. Chem. C, 113 (2009) 5402.

Synthesis & properties of a novel superabsorbent hydrogel based on chitosan

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Superabsorbents are three-dimensionally crosslinked hydrophilic polymers capable of swelling and retaining possibly huge volumes of water in swollen state [1]. Hydrogels are more and more attractive in biomedical fields, since they can be used as injectable scaffolds, drugs and gene carriers and smart sensors. The highly hydrated hydrogels, however, generally have low mechanical strength [2]. Chitosan, is one of the most abundant biomasses in the world. Reactive –NH_2 and –OH of chitosan are convenient for graft-polymerization of hydrophilic vinyl monomers onto it, and this is an efficient way to acquire hydrogels with novel properties [3].

In this study synthesis and optimization of a novel porous superabsorbent were presented. The chitosan-based superabsorbent were synthesized using hydrolyzed chitosan in the presence of acrylic acid, itaconic acid, N,N′methylenebisacrylamide (MBA) as a crosslinker and potassium persulfate (KPS) as initiator. Maximum capacity of swelling in de-ionized water for the fast-swelling optimized hydrogel composite was 180g/g. The effect of swelling media (salt solutions) in amount, measurement of water retention capacity (WRC) and kinetic of water absorbency was investigated. The sample was characterized by FTIR specterescopy and TGA method.

References:

[1] An Li, Junping Zhang, Aiqin Wang, *Science Direct J,* **2007,** 98, 327.
[2] Xiaohong Hu, Jie Zhou, Nan Zhang, Huaping Tan, Changyou Gao, *Science Direct J,* 2008, 352.
[3] Junping Zhang, Li Wang, Aiqin Wang, *American Chemical Society*, **2007**, *46,* 2497.

Synthesis of some thiazolo and oxathialo pyrimidine derivatives

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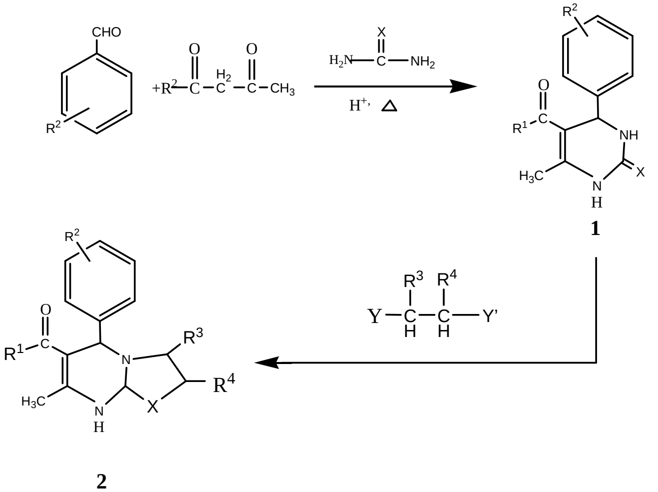
As a continuation of our work and also due to versatile biological properties of pyrimidine derivatives, we have extended the cyclocondensation reactions in order to synthesized of some thiazolo (1) and oxathialo (2) pyrimidine compounds were synthesized by a simple three component cycloaddition reactions of pyrimidine derivatives and alkyldihalides or 2-halocarboxylic acids.

All structures were confirmed by melting points, and spectroscopy data such as IR, ^{1}HNMR and ^{13}CNMR.



1

2

R^1=CH_3, OC_2H_5
R^2=H, 2-CLC_6H_4, 2-$NO_2C_6H_4$, 2MeC_6H_4, 3OH-C_6H_4, 3-BrC_6H_4
X = O, S
Y= Y′ = Br, Cl
R^3 = R^4 = H, R^3 = CH_3, R^4 = H, R^3 = H, CH_3, R^4 = COOH, COCl

Reference:

[1] Kappe, C. O. *Tetrahedron*, **1993**, 49, 6937.
[2] Foroughifar, N. Mobini Khaledi, A. Fathinejad, H. *Phosphorus, Sulfur and Silicon* **2003**, 178, 495.
[3] Baghernejad, B. *Eur. J. Chem*. **2010**, I, 54.

Synthesis, characterization and structure of DBU-hydrobromide-perbromide: a novel oxidizing agent for selective oxidation of alcohols to carbonyl compounds

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The conversions of functional groups to each other have been the center of attention in organic synthetic methodology. For instance, the selective oxidation of primary and secondary alcohols to the corresponding aldehydes and ketones is of great importance in chemistry and industry [1]. Organic tribromide salts as mild reagents are good candidates for this selective conversion, because they are not only stable, crystalline solids, and relatively soluble in most organic solvents but also can be handled more conveniently than liquid bromine and can be used successfully for this purpose.

$DBUHBr_3$ reagent was easily prepared from the reaction of DBU with molecular bromine in dry chloroform. The resulting $DBUH^+Br_3^-$ reagent has the advantages of being a non-hygroscopic and homogeneous solid which is not affected by exposure to light and moisture. It also showed a remarkable stability at room temperature for a long time. We have determined its 3D-structure by X-ray crystallography and its generality was examined in the selective oxidation of benzylic, allylic, primary and secondary alcohols into their corresponding carbonyl compounds on stirring in a mixture of dichloromethane and water at room temperature to give the corresponding products in good to excellent yields.

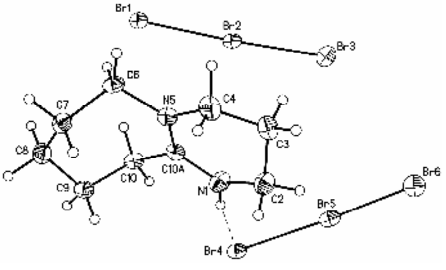
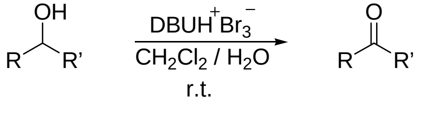


Fig. 1. Molecular structure and atomic labeling scheme (50% probability level).



References:

[1] Fey, T.; Fischer, H.; Bachmann, S.; Albert, K.; Bolm, C. *J. Org. Chem.* **2001**, *99,* 8154.

Synthesis of a novel lariat ethers containing 1,3,4-thiadiazinane-6-carboxylate or 1,3,4-thiadiazinane-6-carboxamide

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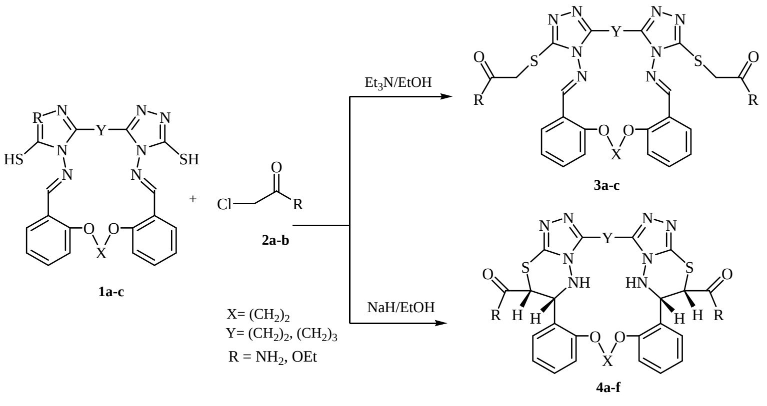
Lariat ethers are crown ethers with side-arms that contain electron-donating substituents. The donor atoms in these side-arms may cooperate with those in the macrocyclic skeleton to provide three-dimensional coordination of a ring-bound cation. The complexation behavior of lariat ethers resembles natural ionophores that transport metal ions through cell membranes [1].In several recent papers, we have reported our efforts to prepare azathia crown and lariat ethers having macrorings of various sizes and side-arms bearing a variety of donor group(s) [2, 3]. In this paper we demonstrate a novel method to introduce Lariat Ethers Containing 1,3,4-thiadiazinane-6-carboxaylate or 1,3,4-thiadiazinane-6-carboxamide.

Macrocycles **1a-c** which stimulated the authors to study their transformation into the Lariat Ethers containing amide and ester groups as side-chain. Thus, the novel lariat compounds **3a-c** and **4a-f** with neutral side-arms were prepared by reaction of corresponding azacrown macrocycles **1a-c** with chlroacetamide or chloro ethyl acetate in present of different base.



References:

[1] Gatto, V. J.; Gokel, G. W. *J. Am. Chem. Soc.* **1984,** *106*, 8240.

[2] Foroughifar, N.; Mobinikhaledi, A.; Ebrahimi, S.; Moghanian, H.; Bodaghi Fard, M. A.; Kalhor, M.; *Tetrahedron Lett.* **2009,** *50,* 836.

[3] Foroughifar, N.; Mobinikhaledi, A.; Ebrahimi, S.; *Synthesis* **2009**, 15, 2557.

Study of the effective parameters on photo-decolorization of azo dye (acid red 206) pollutant in water by UV+Fe_2O_3/ bentonite

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Organic dyes constitute one of the larger groups of pollutants in wastewater released from textile industries. Heterogeneous photo catalysis has been considered as a cost effective alternative for the purification of dye containing wastewater [1,2]. Then the photo catalytic decomposition of organic compounds in wastewater has attracted a great deal of attention .A method of supporting Fe2o3 on zeolite , without losing the photosensitization of Fe2o3 and the adsorption properties of zeolite ,is the important aspect while preparing zeolite-Based photo catalysts [3].

A first order reaction with k = 0.035min-1 was observed for the photo catalytic degradation reaction. The effects of some parameters such as pH, amount of photo catalyst, initial concentration of dye and temperature were also examined. Results show that Fe_2O_3/Bentonite is an active photo catalyst for photo degradation of AR 206 pollutant in water [4]. Based on these results, a model highlighting the photo gradation activity of immobilized [Fe_2O_3/Bentonite] which may lead to the development of an easy and effective technology in wastewater treatments is proposed.

References:

[1] Ollis, D. F. Photo catalytic Purification and Treatment of Water and Air, Elsevier, Amsterdam, 96, **1993**.

[2] Serpone, N.; Perizzetti, E. Photocatalysis-Fundamentals and lications applications, wiley/ Interscience wiley/Interscience , New York ,65, **1989**.

[3] Weiping Du, Qiong Sun, Xuejun Lv and Yiming Xu, Department of chemistry, Zhejiang university ,Hangzhou, Zhejiang,310027,china, Enhanced activity of iron oxide dispersed on bentonite for the catalytic degradation of organic dye under visible light.

[4] Jianxin Chen and Lizhong Zhua Department of Environmental Science, Zhejiang University, Hangzhou 310028, Zhejiang,330031,China,Comparative study of catalytic activity of different Fe-pillared bentonites in the presence of UV light and H_2O_2.

Melamine sulfonic acid as a recyclable catalyst for protection of carbonyl compounds to acetals and ketals under solvent-free conditions

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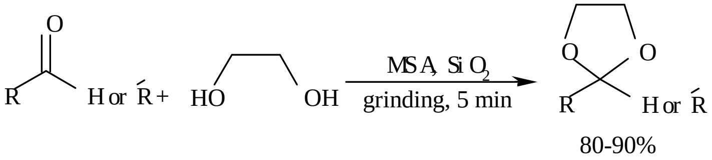
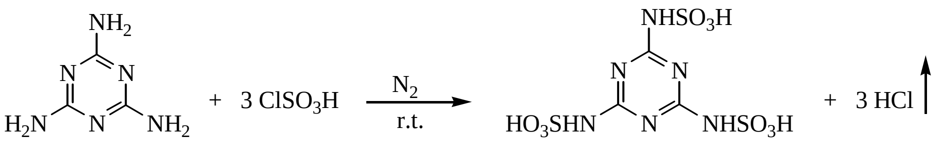
Green chemistry consists of chemicals and chemical processes designed to reduce or eliminate negative environmental impacts. The use and production of these chemicals may involve reduced waste products, non-toxic components, and improved efficiency [1].

In continuation of our researches to develop green chemistry and our new interest in developing a true catalyst using inexpensive and non polluting reagents [2], herein we report the synthesis of melamine sulfonic acid as solid acid and its application in protection of carbonyl compounds to the corresponding acetals and ketals under solvent-free conditions.



Melamine sulfonic acid was prepared by addition of chlorosulfonic acid to a suspension of melamine in CH_2Cl_2 over a period of 1 h at room temperature. Then, the mixture was shaken for 1 h, while the residual HCl was eliminated by suction. The mixture was washed with CH_2Cl_2. Finally, a white solid material was obtained in 79% yield (2.9 g).



Melamine sulfonic acid can be easily separated and reused several times without appreciable loss of activity. The availability and recoverability of the catalyst with easy procedure and work-up make this method attractive for the organic synthesis.

References:

[1] Pratt, L.R. *Chem. Rev*. **2002**, *102*, 2625.
[2] Kiasat, A.R.; Fallah-Mehrjardi, M. *J. Braz. Chem. Soc.* **2008**, *19*, 159.

Evaluation of hypericin in extract of two hypericum species(hypericum perforatum-hypericum scabrum) and Radical scavenging activity of hypericin-rich extracts of hypericum perforatum from Kashan

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Hypericum is a genus of about 400 species of flowering plants in the family Clusiaceae . Main biologically active component of this genus is hypericin. Hypericin is a naturally occurring naphthodianthrone derivative in the plant species *Hyperacid (*St. Johns wort). The hypericin concentration in the plant may vary,depending on place of growth, state of plant material (fresh or dried) before extraction and part of the plant studied.

H. perforatum is the most potent species and it is today grown and collected commercially for use in herbalism and medicine.in this study hypericin content was measured by spectrophotometry and antioxidant activity of different extracts of plants of this genus have been reported. There is no information about properties of H. perforatum from Kashan, central Iran. We are reporting radical scavenging activity of the extract of H. perforatum from Kashan. Extraction was performed after isolation of chloroform soluble compounds to rich the extract of hyperacid. Results show that hypericin-rich extract has much higher activity than the other extracts.

References:

[1] Muller, W. E. Rolli, M. Schafer, C. Hafner, U. *Pharmacopsychiatry*, **1997**, *30*, 102.
[2] Liebes, L. Mazur, Y. Freeman, D. Lavie, D. Lavie, G. Kudler, N. Mendoza, S. Levin, B. Hochster, H. Merulo, D. *Anal. Biochem*. **1991**, *195*, 77.
[3] Greeson, M. J.; Sanford, B, Monti, A. D. St. John's wort, *Psychopharmacol* **2001**, *153*, 402.

An efficient one-pot synthesis of ethyl 2-methyl-6-oxo-4-aryl-1,4,5,6-tetrahydropyridine-3-carboxylate in water as solvent

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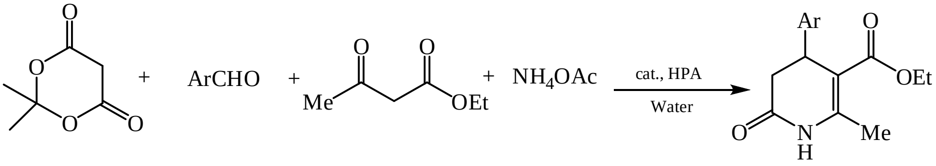
In recent years, an increasing interest has been focused on the synthesis of 1,4–dihydropyridine compounds owing to their significant biological activities, such as, calcium antagonist, antitumor, geroprotective, hepatoprotective and antidiabetic agent [1]. Thus alternative strategies for their synthesis involving different catalysts and conditions have been developed [2]. However, some methods suffer from drawbacks like some longer reaction times, unsatisfactory yields, harsh reaction conditions, and use of a large quantity of organic solvent.

The application of heteropolyacids as catalytic materials is growing continuously in the catalytic field [3]. In continuation of our investigations in the synthesis of dihydropyrimidines (DHPMs) [4], and 1,4-dihydropyridines (DHPs) [5] herein we describe a simple and efficient method for the one-pot synthesis of 4-aryl-1,4,5,6-tetrahydropyridine derivatives using heteropolyacids as catalyst in water as solvent. In this work, we introduce an efficient four-component reaction of Melderume's acid, aldehydes, ethylacetoacetate and amonium acetat in presence of tungstophophoric acid hydrate as a catalyst that provides an easy access to 4-aryl-1,4,5,6-tetrahydropyridine derivatives. This facile and efficient method affords high yields for synthesis of 1,4-dihydropyridine derivatives with short time reaction under mild conditions and friendly to the environment.



References:

[1] Shan, R.; Velazquez, C.; Knaus, E. E. *J. Med. Chem.*, **2004**, *47*, 254.
[2] (a) Hantzsch, A. *Ann. Chem.* **1882**, *1*, 215; (b) Ahluwalia, V. K.; Goyal, B.; Das, U. J. *J. Chem. Res.* **1997**, *7*, 266.
[3] Mizuno, N.; Misono, M. *Chem. Rev.*, **1998**, *98*, 199.
[4] (a) Mirza-Aghayan, M.; Bolourtchian, M.; Hoseini, M. *Synth. Commun.* **2004**, *34*, 3335; (b) Mirza-Aghayan, M., Moradi, A.; Bolourtchian, M.; Boukherroub, R. *Synth. Commun.* **2010**, *40*, 8; (c) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. *J. Iran. Chem. Soc.* **2010**, *7*, 269.
[5] Mirza-Aghayan, M.; Khoshkameh Langrodi, M.; Rahimifard, M.; Boukherroub, R. *Appl. Organometal. Chem.* **2009**, *23*, 267.

Study of the wittig reaction of[5-(5-nitrothiophen-2-yl)-1,3,4-thiadiazol-2-amine]with acetylendicarboxylate esters in the presence trimethylphosphite.

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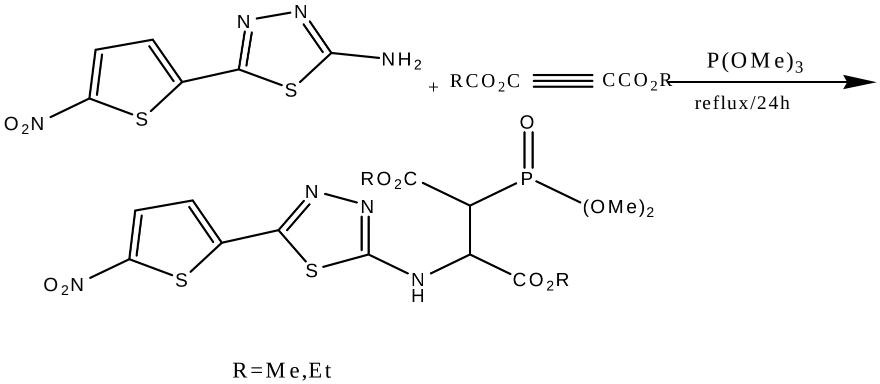
Thiadiazole is a versatile moiety that exhibits a wide variety of biological activities.Thiadiazole moiety acts as "hydrogen binding domain" and "two-electrom donor system".It also acts as a constrained pharmacophore.Many drugs containing thiadiazole nucleus are available in the market such as acetazolamide,methazolamide, sulfamethazol,etc.[1]

They are also known to possess antiviral activity and especially effective against HIV [2]. Phosphorus ylides have found use in a wide variety of reaction,especially in the synthesis of naturally occurring products,and compounds with biological and pharmacological activity.[3]

Herein we report synthesis new ylides from reaction of [5-(5-nitrothiophen-2-yl)-1,3,4thiadiazol-2-amine]with triphenyl phosphite and acetylen dicarboxylate esters under condition reflux.



References:

[1] Siddiqui,N.;AHuja,P.;AHsan,W.;Pandeya,S.N.;shamsher Alam,M.;*Journal of chemical and pharmaceutical Research.***2009**,*1(1)*,19-30.

[2] Mayekar,S.A.;Mulwad,V.V.;*Indian journal of chemistry.***2008**,*47B*,1438-1442.

[3] Heydari,R.;Hazeri,N.;Maghsoodlou,F.;Habibi Khorassani,M.S.;Barahuie,F.;Marandi,M.;*ARKIVOC* **2009** *(vii)* 86-97.

An efficient synthesis of 2-(2-oxoindolin-3-ylidene)-1,3-dithiole-4,5-dicarboxylates by a one-pot and Three-component reaction

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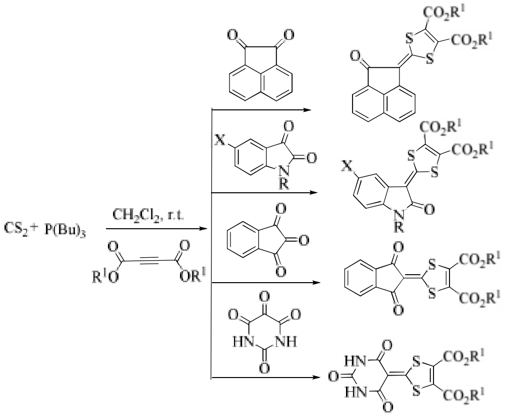
The Wittig reaction was discovered in 1953 as a new and reliable method to form carbon–carbon double bonds [1]. Oxindoles are known to possess antibacterial, antiprotozoal, and anti-inflammatory activities and are also patented as progesterone receptors agonists [2].

Derivatives of sulfur heterocycles such as thiophene and 1,3-dithiole have been widely explored as new materials because of their superconducting and optical and electronic switching properties [3]. 1,3-Dithiol-2-ylidenes have attracted much attention as building blocks for electronic materials due to their highly electron-donating properties [4, 5].

Herein we reports a mild, facile and three-component method for the synthesis of oxoindolin-ylidene-1,3-dithioles, oxoacenaphthylen-ylidene-1,3-dithioles, dioxo-inden-ylidene-1,3-dithioles and trioxotetrahydropyrimidin-ylidene-1,3-dithioles using readily available starting materials. Prominent among the advantages of this new method are operational simplicity, good yields and easy work-up procedures employed.



References:

[1] Wittig, G., Geissler, G. *Justus Liebigs Ann. Chem.* **1953**, *580*, 44.
[2] (a) Joshi, K.C.; Pathak, V. N.; Jain, S. K. *Pharmazie* **1980**, *35*, 677; (b) Bolotov, V. V.; Drugovina, V. V.; Yakovleva, L. V.; Bereznyakova, A. I. *Khim. Farm. Zh.* 1982, 16, 58; (c) Pajouhesh, H.; Parsons, R.; Popp, F. D. *J. Pharm. Sci*. **1983**, *72*, 318; (d) Popp, F. D. *J. Heterocyclic Chem*. **1984**, *21*, 1367.
[3] Marcos, C. F.; Polo, C.; Rakitin, O. A.; Rees, C. W.; Torroba, T. *Chem. Commun*. **1997**, 879.
[4] Segura, J. L.; Martin, N. *Angew. Chem., Int. Ed.* **2001**, *40*, 1372.
[5] Bryce, M. R. *J. Mater. Chem.* **1995**, *5*, 1481.

Study of three-component reaction between alkyl isocyanides, dialkyl acetylenedicarboxylates and ethyl 4-(4-aryl)-2,4-dioxobutanoate

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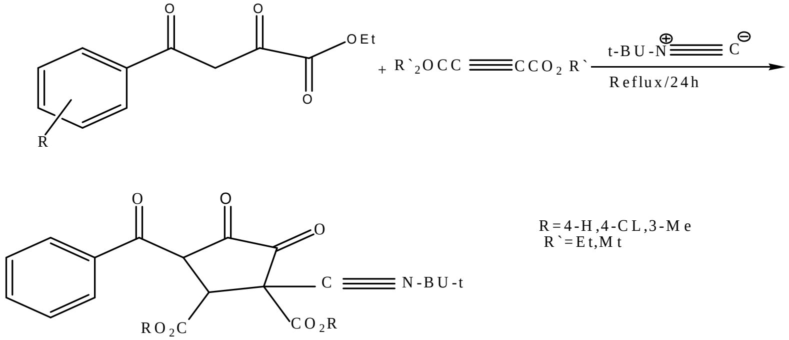
Development of simple synthetic routes for widely used organic compounds from readily available reagents is one of the major tasks in organic chemistry [1]. The increasing clinical importance of drug-resistant microbial pathogens has lent additional urgency in microbiological and antifungal research. The ability of nitroimidazoles, to act as antimicrobial and antifungal agents is well known [2,3].The resistance towards available drugs is rapidly becoming a major worldwide problem. The need to design new compounds to deal with this resistance has become one of the most important areas of research today [4]. Here we report a simple on-pot reaction between ethyl 4-(4-aryl)-2,4-dioxobutanoate and dialkyl acetylenedicarboxylates in the presence of alkyl isocyanides.



References:

[1] Laszo, P.; Organic Reactions, Simplicity and Logic, Wiley: New York, **1995**.
[2] Bock, M.; *Arzneim, Forsch.;* Drug Res. 587,**1961**.
[3] Hoffer, M.; and Grunberg, E. *J; Med.*Chem.1019, **1974**.
[4] Bhatia, S. C.; and Shanbhag, V. D.; J, Chromatogr. 325, **1984**.

Preparation and characterization of novel pyridine-based thermally stable poly(ether urea)s

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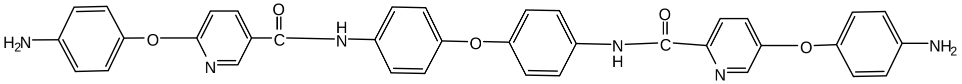
Polyureas were initially developed due to their excellent mechanical properties and outstanding resistance to hydrolysis [1]. Recently, polyureas have been reported to be used as piezoelectric and ferroelectric polymers, second-order optical non-linear polymers, lithographic matrixes, permeable membrane, biodegradable polymers, and polymer microcapsules. Potentially useful polyureas are those containing other functional groups. A wide range of commercial polymers containing urea groups, such as urea-formaldehyde, poly(amide-urea)s, poly(urethane-urea)s used as cast elastomers and poly(ether-urea-acrylate)s used as surface coatings has been reported [2,3].

The purpose of present research is preparation and characterization of polyureas with high thermal stability and also improved solubility and processability in order to increase their applications.

Nucleophilic substitution reaction of two moles of 6-chloro nicotinoyl chloride with oxydianiline (ODA) in presence of triethylamine yielded a dichloro compound (DC) in first step. In second step DC reacted with two moles of p-amino phenol to yield a diamine.



Polyureas were prepared by addition polymerization reaction of the obtained diamine with different aromatic diisocyanates including naphthalene diisocyanate (NDI), toluene diisocyanate (TDI), 4,4'-diphenylmethane diisocyanate (MDI) and para-phenylene diisocyanate (PPDI).

All the prepared polymers were characterized and their physical and thermal properties were studied. Due to especial characteristic feature of the polymers they showed nice balance of properties including improved solubility and good thermal stability. Phenylation of backbone, presence of heterocyclic pyridine ring and incorporation of ether and amide linkages were the main structural modifications to synthesize the building block for the preparation of poly(ether-urea) with improved properties.

References:

[1] Mehdipour-Ataei, S.; Sarrafi, Y.; Amiri Pirjel M. *J. Appl. Polym. Sci.***2004**, *93*, 961.
[2] Jewrajka, S. K.; Yilgor, E.; Yilgor, I.; Kennedy, J.P. *J. Polym. Sci. Part A: Polym. Chem.* **2009**, *47*, 38.
[3] Nishat, N.; Ahamad, T.; Zulfequar, M.; Hasnain, S. *J. Appl. Polym. Sci.* **2008**, *110,* 3305.

Silica gel supported ICl_3 as an efficient and reusable catalyst for the synthesis of 1, 8-dioxo-octahydroxanthene derivatives

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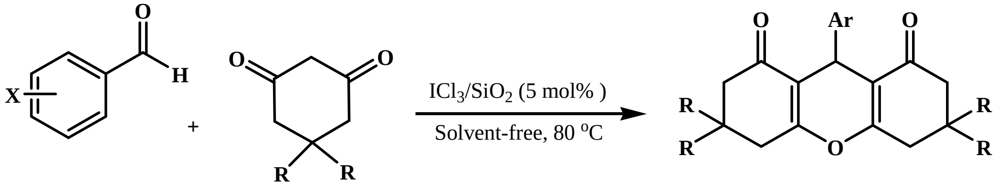
Among heterocyclic compounds containing oxygen atom, xanthene derivatives are important for different reasons such as biologic and treatment properties such as anti virus, anti phlogosis and anti bacteria [1-3].

Organic chemistry researchers from both academia and industry have started giving serious thought to the detrimental effect of non-green processes and chemicals on the environment. They have successfully developed several environmentally benign procedures to avoid, or at least minimise, these effects.

In this work, A simple, clean and cost-effective method for the synthesis of 1,8-dioxo-octahydroxanthene **3** derivatives via cyclocondensation of aldehydes **1** with dimedone or 1,3 cyclohexadion **2** in the presence of Silica gel supported ICl_3 as a highly efficient catalyst under solvent-free conditions at 80 ^oC was described.

This method is important from an environmental point of view and economic considerations, because it produces little waste, Simple preparation and stability of catalyst, simple work-up procedure and the high yields of products, short reaction times and avoiding from use of toxic organic solvents as media. Scheme of the general reaction is presented below.



1 **2** **3**

R=H, Me X=Cl, NO_2, H, Alkyl, F, Br, H

References:

[1] Lambert, R. W.; Martin, J. A.; Merrett, J. H.; Parkes, K. E. B.; Thomas, G. J. *Chem. Abstr*. **1997**, *126*, 2123.
[2] Hideo, T.; Koho, J. T. *Chem. Abstr*. **1981**, 95.
[3] Poupelin, J. P.; Saint- Rut, G. ; Foussard-Blanpin, O.; Narcisse, G. ; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.* **1978**, *13*, 67.

Preparation of selective unsymetrical benzoins

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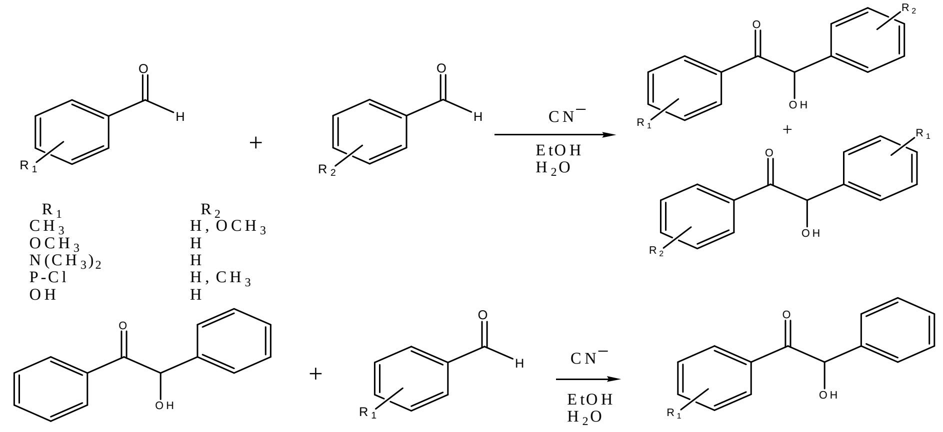
The formation of carbone_carbone bond is one of the most fundamental reaction for the construction of a molecular framework [1]. The benzoin reaction is one of the oldest reactions in organic chemistry, found serendipitously by Liebig and Wohler in 1832 [2].

α-hydroxy ketones are important building blocks for the synthesise of several drugs, natural products, auxiliaries and ligands [3-4].

We report herein a simple and rapid efficient synthesise of unsymetrical benzoins derivatives was achieved under ultrasonic irradation and microwave irradiation from the aldehyds and simple benzoins.



R_1	R_2
CH_3	H, OCH_3
OCH_3	H
$N(CH_3)_2$	H
P-Cl	H, CH_3
OH	H

References:

[1] Li-Wen Xu,a Yang Gao,a,b Jian-Jun Yin,b Lyi Lia ,Chun-Gu Xiaa, *Tetrahedron Lett*ers. **2005**, *46,* 5317.
[2] Dieter Ended , Klaus Breuer, **,** *Helveticcahimicaacta*. **1996**, *79,* 1217.
[3] Tanja Hischer,a Do¨rte Gocke,a Marı´a Ferna´ndez,b Pilar Hoyos,b Andre´s R. Alca´ntara,b Jose´ V. Sinisterra,b Winfried Hartmeiera,Marion B. Ansorge-Schumachera**,** *Tetrahedron*. **2005**, *61*, 7378.
[4] Xin Linghu, Cory C. Bausch, Jeffrey S. Johnson, *J.Am.Chem.Soc*. **2005**, *127,* 1833.

Synthesis and spectral studies on dinuclear complex of Cu(I) with PNBD Schiff base

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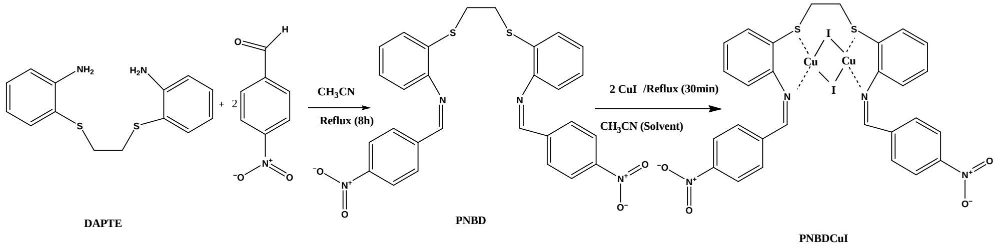
Schiff base ligands have significant importance in chemistry, especially in the development of Schiff base complexes, because Schiff base ligands are potentially capable of forming stable complexes with metal ions [1]. Thio_substituted imines are among promising organic ligands [2].

There has been a growing interest in recent years toward properties of copper(I) complexes with multidentate ligands particularly in view of their potential applications in metallosupramolecular assemblies, bioinorganic chemistry and catalysis. Many efforts have been devoted to the design and synthesis of new multidentate Schiff base ligands that are able to control the crystal structure and properties of copper(I) complexes [3].

Herein we report the synthesis of the new Schiff base ligand PNBD and also synthesis of a new copper(I) complex in which PNBD tetradentate Schiff base ligand acts as a bis-chelating ligand bridging between two copper(I) centers.



References:

[1] Naeimi, H.; Safari, J.; Heidarnezhad, A. J. *Dyes and Pigments*. **2007**, 73, 251-253.
[2] Beloglazkina, E. K.; Majouga, A. G.; Moiseeva, A. A.; Yudin, I. V.; Moiseev, F. S.; *Russ, Chem, Bull*. **2008**, 57, 358-363.
[3] Morshedi, M.; Amirnasr, M.; Salwin, A.; Woollins, J. D.; Dehno Khalaji, A. *Polyhedron*. **2009**, 28, 167-171.

Fries Rearrangement on Hydrofluorinated Silica Surface

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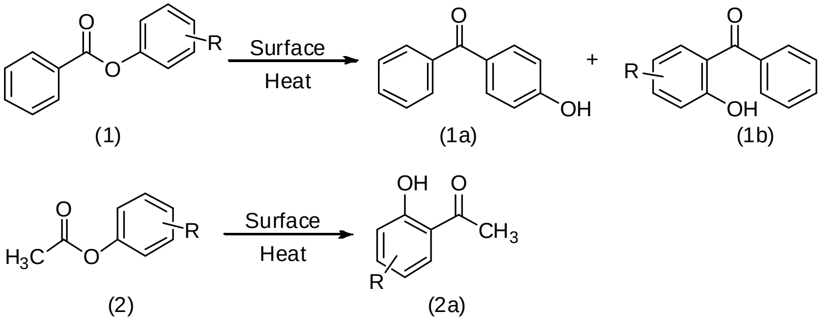
Fries Rearrangement of Aryl Esters to their corresponding hydroxy aromatic ketones is one of the most important routes in organic syntheses. The products including hydroxyacetophenones, hydroxybenzophenones and hydroxynaphthones are used as valuable intermediates in pharmaceuticals such as salbutamol, agrochemicals, flavors, fragrances, perfumes, fine chemicals and versatile building blocks for manufacturing UV stabilizers, UV absorbers in sunscreens to protect human skin against harmful UV irradiation, plastics and specialty polymers.

In order to obtain various hydroxy aromatic ketones, Fries Rearrangement of aryl esters on Hydrofluorinated Silica surface has been explored under heat in this investigation. Different analogues of aryl esters- including phenyl benzoates, phenyl acetates and naphthyl benzoates- with electron donating and electron withdrawing substituents were studied.

Herein, we report the optimized temperature and reaction time, along with excellent yields on a non-toxic, environmental-friendly surface. The corrosive property of hydrofluoric acid has been eliminated in this method. The mild reaction temperature and convenient work-up are some of its key advantages in comparison to harsh reaction condition of the previous methods.



(1a): R=H ; (1b): R= 4-Me, 4-Cl ; (2a): R= H, 4-Me, 4-Cl.

References:

[1] Fries, F.; Finck, G. *Bre.* **1908**, *41*, 4271.
[2] Collin, D. T.; Hartely, D.; Jack, D.; Lunts, L. H. C.; Press, J. C.; Ritchie, A. C.; Toon, P. *J. Med. Chem.* **1970**, *13*, 674.
[3] S. Wahie, J. J. Lloyd, P. M. Farr. *Clin. Exp. Dermatol.* **2007**, *32*, 359.
[4] Fent, K.; Kunz, P. Y.; Gomez, E. *Chimia.* **2008**, *62*, 368.

Synthesis and geometry optimization of new crown ether-containing glycoluril clips

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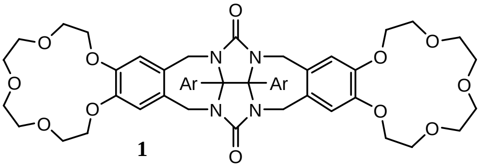
Artificial receptors are capable of mimicking of the function of cell-surface receptors. It can lead to a better understanding of the natural processes and additionally to the development of new artificial systems for use in drug delivery, catalysis, etc [1]. Glycoluril based receptors have been prepared and extensively studied in the Nolte group over the past decade. These hosts possess a well-defined cavity that allows the binding of different phenolic guests via a combination of several non-covalent interactions (H-bonding, π–π stacking, and the cavity effect) [2]. Crown ether- functionalized clip receptors are also able to bind alkaline metal ions, as well as ammonium salts, in addition to complexing neutral aromatic guests [3].

Here, we describe the synthesis and the geometry optimization of two new glycoluril based receptors with crown ether-containing aromatic side-walls (compounds **1** and **2**). The insertion of crown ether moieties, capable of additional H-bonding and electrostatic interactions, into the clip structures introduces an extra feature with potential improvement in the binding of multifunctional guests. Also, the geometry optimization studies showed these receptors have well-defined cavities and may function as hosts for neutral and cationic guests (Figure 1).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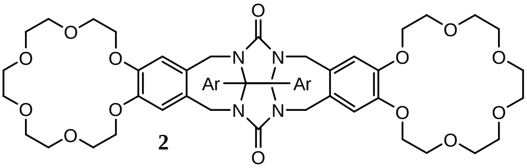
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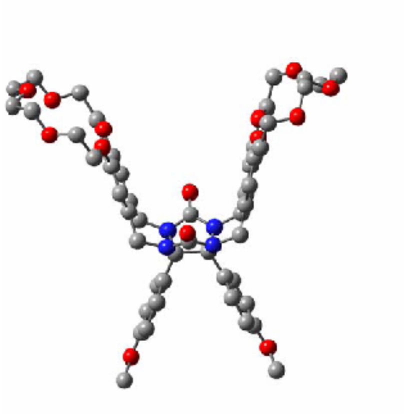

Figure 1. Computer-optimized structure of compond **1** (hydrogen atoms have been omitted for clarity)

References:

[1] Kikuchi, J. –I.; Murakami, Y. *J. Incl. Phen. Mol. Rec. Chem.* **1998**, *32*, 209.
[2] Rowan, A. E.; Elemans, J. A. A. W.; Nolte, R. J. M. *Acc. Chem. Res.* **1999**, *32*, 995.
[3] Schenning, A. P. H. J.; Escuder, B.; van Nunen, J. L. M.; de Bruin, B.; Rowan, A. E.; van der Gaast, S. J.; Feiters, M. C.; Nolte, R. J. M. *J. Org. Chem.* **2001**, *66*, 1538.

Silica-bonded *S*-sulfunic acid and silica-bonded N-propyl sulfamic acid as recyclable catalysts for the synthesis of 2-aryl-1-arylmethyl-(1*H*)-1,3-benzimidazole derivatives

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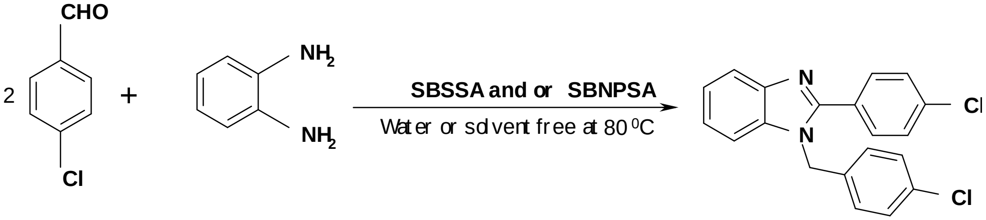
The benzimidazole nucleus is of significant importance to medicinal chemistry. Several publications report benzimidazole-containing compounds showing biological activities such as selective neuropeptide YY1 receptor antagonism [1] and as 5-lipoxygenase inhibitors for use as novel antiallergic agents [2], factor Xa (FXa) inhibitors, poly-(ADP-ribose)-polymerase (PARP) inhibitors, and human cytomegalovirus (HCNV) inhibitors [3].

2-Aryl-1-arylmethylene-(1*H*)-1,3-benzimidazoles were Synthesized by the reaction of *o*-phenylenediamines and aromatic aldehydes in the presence of silica-bonded S-sulfonic acid (**SBSSA**) and silica bonded N-propyl sulfamic acid **(SBNPSA)** in water and also under solvent-free conditions in good to excellent yields.



References:

[1] Zarrinmayeh, H.; Nunes, A. M.; Ornstein, P. L.; Zimmerman, D. A. *J. Med. Chem.* **1998** , *41*, 2709.
[2] Nakano, H.; Inoue, T.; Kawasaki, N.; Satoh, T. *Bioorg. Med. Chem*. **2000**, *8*, 373.
[3] Zhao, Z. S.; Arnaiz, D. O.; Griedel, B.; Sakata, S.; Shaw, K. J. *Bioorg. Med. Chem. Lett*. **2000**, *10*, 963.

Comparison of synthetic conditions of symmetric and asymmetric Porphyrins

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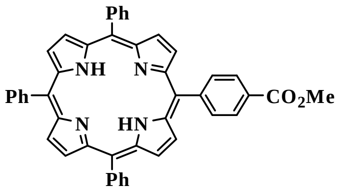
In this work, different meso-substituted porphyrins with AB_3- and A_4-porphyrin symmetry pattern have been synthesized as catalyzed by a modification of the Alder-Longo andLindsey procedures [1-3], and results have been compared. On the other hand, two synthetic methods have been compared in the formation of them. 4-(methoxycarbonyl) phenyl triphenyl porphyrin **(1)** containing two different types of mesosubstituents (A and B) can be prepared by a binary mixed aldehyde and pyrrole condensation. In this approach usually six porphyrins are formed. However, the isolation of the desired porphyrin requires slow and careful chromatography for purification, the yield is poor and obtaining pure porphyrin is not always possible. In the case of meso-tetrakis (4- (methoxycarbonyl)phenyl) porphyrin **(2)** high yields are obtained by two different methods . In one case, the mixture was oxidized with 2, 3-dichloro-5, 6- dicyano -1, 4-benzoquinone (DDQ) and in the other case was used of the clean oxidant O_2. The last synthetic pathway was advantageous mainly for an easier reaction work up and a higher yield. Such study has aimed at understanding the relationship between the Symmetry results and the yield of porphyrinand the following properties of the catalyst. We have observed that better yields are obtained in the symmetrical systems. All materials have been characterized by ^1H NMR and ^{13}C NMR spectroscopes.



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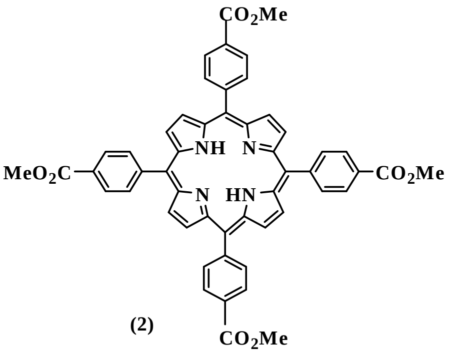

(2)

References:

[1] Adler, A. D.; Longo, F. R.; Finarelli, J. D.; Goldmacher, J.;Assour, J.; Korsakoff, L. *J. Org. Chem.***1967,** *32*, 476.

[2] Lindsey, J. S.; Wagner, R. W.; *J. Org. Chem*. **1989,** *54*, 828.

[3] Wagner, R. W.; Lindsey, D. J.; Hsu, H.C.; Schreiman, I.C.; Kearney, P.C.; Marguerettaz, A.M. *J. Org. Chem*. **1987,** *52*, 827.

One-pot synthesis and temperature dependence of NMR spectra Of ketenimine derivative of fused pyrone

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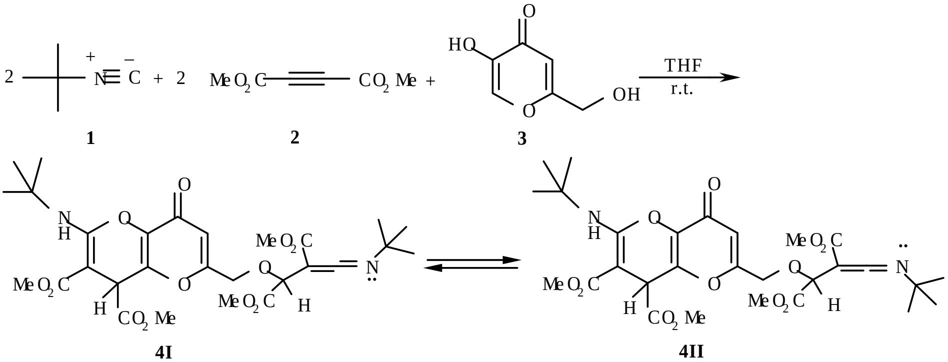
Kojic acid **3**, a γ-pyrone derivative, is a fungal metabolite produced by many species of Aspergillus and Penicillium. Kojic acid possesses both antibacterial and antifungal activities [1]. Therefore, the synthesis of kojic acid derivatives is of current interest. In this work, we studied three-component reaction of *tert*-butyl isocyanide **1,** dimethyl acetylenedicarboxylate **2** and kojic acid **3,** that leads to ketenimine derivative of fused pyrone **4**. Ketenimines generally show a bent C=C=N–R moiety. Therefore, ketenimines with different substituents at carbon atom are chiral [2]. Racemization of these stereoisomers proceed through inversion at nitrogen *via* a transition state with a linear C–C≡N–R fragment [3]. However, in solution at room temperature open chain ketenimines racemize quickly ($\triangle G^{\#}$ = 30-65 KJ mol^{-1})[4], but our studies on compound **4** that possesses ketenimine moiety with three different substituents showed compound **4** exists as two chiral rotamer **4I** and **4II** at room temperature. Barrier energy of this racemization was measured by dynamic NMR.



1 **2** **3**

4I **4II**

References:

[1] Takizawa. T.; Imai. T.; Onose. JI.; Ueda. M.; Tamura. T.; Mitsumori. K.; Izumi. K.; Hirose. M.; *Toxicological Sciences*. **2004**, *81*, 43.
[2] Runge. G.; Structural Chemistry, in *the Chemistry of ketenes, Allenes and Related Compounds*) Edited by Patai. S). Wiley, New York, **1980**.
[3] Firl. J.; Schink. K.; and Kosbahn. W.; *Chem. Lett.* **1981**, 527.
[4] Lambrecht. J.; Gambke. B.; von Seyerl. J.; Huttner. G.; Kollmannsberger-von Nell. G.; Herzberger. S and Jochims. J. C.; *Chem. Ber*. **1981**, *104*, 3751.

An efficient method for the esterification of amino acids

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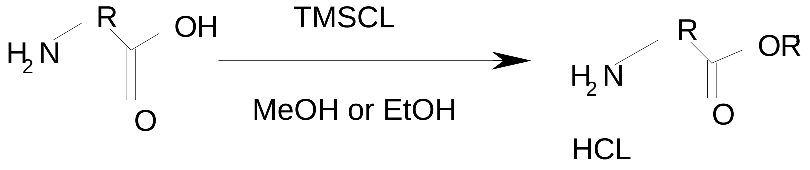
Amino acid methyl esters are important intermediates in organic synthesis, which have been used in various areas such as peptide synthesis, medicinal chemistry [1].

A variety of reagents have been reported for esterification such as thionyl chloride, 2,2-dimethoxy propane, protic acids (gaseous hydrochloric acid, sulfuric acid), TMSCL [2].

Li and Sha synthesis different amino acids methyl ester hydrochlorides with chlorotrimethylsilane. Amino acid was stirred with distilled chlorotrimethylsilane and absolute methanol at room temperature (as monitored by TLC) [3]. Then the reaction mixture was dried on arotary evaporator and recrystallized from an absolute methanol-ether mixture. We prepared amino acids methyl and ethyl ester hydrochlorides with this method, but was refluxed midly. Refluxing was improved yields. The basic and strong acidic conditions or heating are likely to affect the optical purity of chiral amino esters. The use of TMSCL/methanol or ethanol have advantageous such as easy operation, mild reaction conditions, simple workup and good to excellent yield.



R'=Me or Et

References:

[1] AL-Masoudi, N.; AL-Masoudi, I.; Saeed, B.; *Acta Pharm.* **2006**, 56, 175.
[2] Schwarz, H.; Bumpus, M.; *J. Am. Chem. Soc.* **1959**, 81, 890.
[3] Li, J.;Sha, Y.; *Molecules*. **2008**, 13, 1111.

Efficient one-pot synthesis of 2,3-dihydroquinazolin-4(1H)-ones

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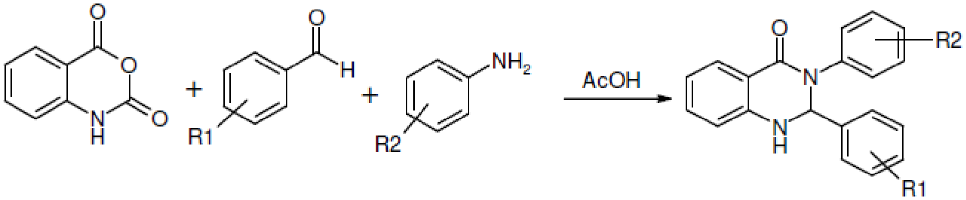
Quinazolin-4-ones are an important class of heterocycles with a wide range of pharmacological and biological activities. Various methods have already been proposed for the synthesis of these compounds (see a recent review on quinazolinones and quinazolines and references cited therein) [1]. Several synthetic methods for the preparation of 2,3-dihydroquinazolinones have been reported. Among them, the most direct procedure includes condensation of aryl, alkyl, and heteroaryl aldehydes with anthranilamide in the presence of p-toluenesulfonic acid as a catalyst [2]. The synthesis of 2,3-dihydroquinazolinones was also achieved by reductive cyclisation of onitrobenzamide or o-azidobenzamide [3].

In continuation of our interest in one-pot, muticomponent synthesis of organic compounds [4], we describe an efficient method for the synthesis of 2,3-dihydroquinazolinones through threecomponent reactions of aldehydes, amines, and isatoic anhydride using acetic acid.



This method offers some advantages in terms of simplicity of performance, low reaction times, low cost, and it follows along the line of green chemistry. The catalyst is readily available and inexpensive and can conveniently be handled and removed from the reaction mixture. We believe that this procedure is convenient, economic, and a user-friendly process for the synthesis of 2,3- dihydroquinazolinones of biological and medicinal importance.

References:

[1] Connolly, D. J.; Cusack, D.; O'Sullivan, T.P.; Guiry P. J. *Tetrahedron* **2005,** *61*, 10153.
[2] Sharma, S. D.; Kaur, V. *Synthesis* **1989**, 677.
[3] Su, W.; Yang, B.; *Aust. J. Chem*. **2002,** *55*, 695.
[4] Karimi-Jaber, Z.; Amiri, M. *Heteroatom Chem*. **2010**, *21*, 96.

Synthesis of 3- substituted thiophene-based conjugated polymers

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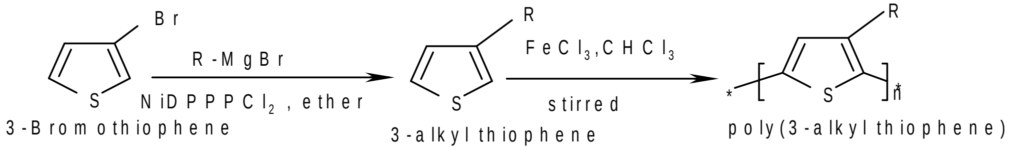
Polymers are macromolecules built up by the linking of large number of much smaller molecules. The smaller molecules that combine with each other to form polymer molecule are termed monomers, and the reactions by which they combine are termed polymerization [1] .

Conductive polymers are a class of materials with interesting properties. The polymers can be doped and become conductive, the conductivity ranging typically from (10^{-3} - 10^{-6}) times the conductivity of Cu [2]. The polymers can change colour when external parameters are changed, e.g.: doping, temperature, pressure, pH, etc.

These properties make that conductive polymers are of technological interest. Possible applications include: optical devices, electronic devices, sensors, shielding material, etc.. The 3-alkylthiophene monomer unit is asymmetric. Considering nearest neighbours only, there are thus four possible environments for a given unit in the polymer. Usually these four enchainments are indicated with: HT-HT (head-to-tail head-to-tail) for the regular enchainment, TT-HT, HT-HH and TT-HH [3].

In the course of this project, a 3-decylthiophene monomer were synthesized by coupling the grignard from 3-bromothiohene, and then this monomer were subjected to polymerization by the oxidative polymerization technique using $FeCl_3$. This polymer was also meltable thus this is processable.

This is a regioregular poly(3-decyl-thiophene-2,5-diyl). This polymer is highly soluble in chloroform, toluene, chlorobenzene, tetra-hydrofuran.



R = decyl = $CH_3CH_2(CH_2)_7CH_3$

$NiDPPPCl_2$ = dichloro-1,3-bis(diphenylphosphino)propane nickel(II)

References:

[1] Odian, G.; *Principles of Polymerization* 3 rd ed. Wiley-Interscience publication **199**3,p.1.
[2] Suigmoto, R.; Takeda, S.; Gu, H.B.; Yoshino, K., *Chem. Expres*s, **198**6, 1, 635
[3] Hoeve, W.; Wynberg, H.; Havinga, E. E.; Meijer, E. W., *J. Am. Chem. Soc.* **199**1, *11*3, 5887.

Puckering energy 1,3-Halo-1,3-dibora-cyclobot-2-ylidenes

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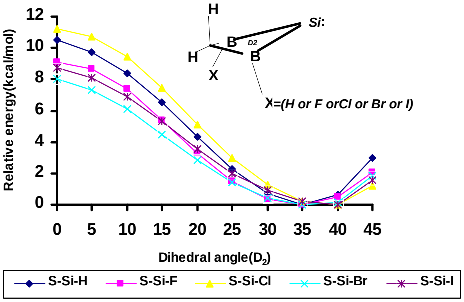
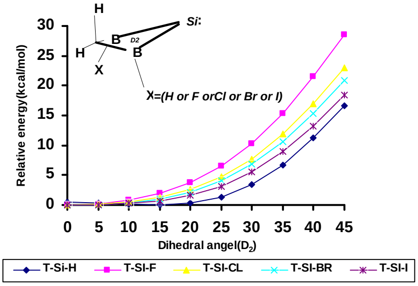
The 1,3-dibora-cyclobot-2-ylidene [1] is one of the most intriguing organoboron compounds, and its unique bonding situation has stimulated much activity in synthesis [2] and theoretical chemistry[3]. Puckering energy of 1,3-dibora-cyclobot-2-ylidene and its heavier analogues is studied in B3LYP/6-311++G** level of theory.

In order to confirm global minima, for each diboretane, energy surface studies are necessary, since puckering of 1,3-dibora-cyclobot-2-ylidene rings may alter positions of the global minima. Puckering energy surfaces are sketched for both singlet and triplet states of diboretane rings as a function of dihedral angle C-B-M-B (M=C, Si). The magnitude of puckering energy barriers for triplet states is higher than Singlet state.





References:

[1] Klusik H., Berndt A. angew.chem. 1983; 95:895; Angew. Chem., Int. Ed. Engl. 1983; 22: 877.
[2] Berndt A. angew.chem. 1993; 105:1034; Angew. Chem., Int. Ed. Engl. 1993; 32: 985.
[3] McKee ML. In*org. Chem*. **1999**; 38: 321.

New procedure for the total synthesis of cilostamide

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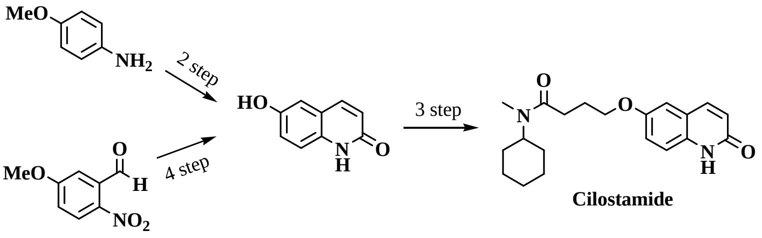
The Cilostamide is a highly functionalized compound which shows potent activity of phosphodiestrase3 inhibitory [1] lead to cardiotonic effects [2], inhibition of platelet aggregation [3] and increase in the secretion of Insulin-stimulated glucose [4]. Many procedures for the total synthesis of cilostamide have been developed.

Herein we report two procedures for the total synthesis of Cilostamide which are notable from point of view of reaction time and the yield of synthesized Cilostamide. These efficient routes to synthesis a wide range of *N*,*N*-R,R'-4-(2-oxo-1,2-dihydroquinolin-6-yloxy)butanamide, specially Cilostamide (R = methyl and R' = cyclohexyl) with emphasis on the preparation of the carbostyril (2-quinolinone) ring system is reported.

The total yields of the first procedure (47%) and of the second procedure (25%) are notable when compared with other reported methods. Although the first procedure, gives higher yield but it takes longer time (67 h for total reactions) in comparison with the second procedure (14 h for total reactions). The advantage of latter procedure, in spite of its lower yield, is less synthetic step, shorter time of total reactions and chip regents.



References:

[1] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.
[2] Phillips, P. G.; Long, L.; Wilkins, M. R.; Morrell, N. W. *Thorax*, **2000**, *55*, A35-A35.
[3] Nishikawa, M.; Komada, F.; Morita, K.; Deguchi, K.; Shirakawa, S. *Cellular Signalling*, **1992**, *4*, 453.
[4] Juan-Fita, M. J., Vargas, M. L.; Hernandez, J. *Eur. J. Pharmacol.*, **2005**, *512*, 207.

A novel one-pot method for the synthesis of 1-(3-aminoacryloyl)-3-oxo-1,3-dihydroisobenzofuran-1-yl acetate derivatives

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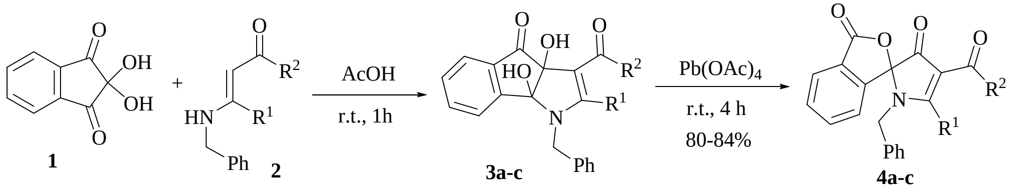
Substituted phthalides (isobenzofuran-1(3H)-ones) represent an important class of natural products that posses significant biological properties [1]. In particular, 3-substituted phthalides are vital heterocyclic motifs in many bioactive compounds such as isocoumarins, anthraquinones, anthracyclines, and several alkaloids [2]. Their notable characteristics include anti-bacterial, anti-convulsant, anti-HIV, anti-asthmatic, anti-tumor, anti-platelet activities, anesthesia prolongation, and $PGF_{2\alpha}$ inhibitory properties. Then again, the chemistry of isobenzofurans is of great importance, because of they are 10π electron systems with a quinoid nature, which makes them attractive as a unique building units for oligomeric and polymeric π-conjugated compounds [3].

As a part of our ongoing programs on the studding of oxidation of some vicinal cyclic dihydroxy compounds [4], herein we wish to report a novel one-pot and efficient procedure for synthesis of 1-(3-aminoacryloyl)-3-oxo-1,3-dihydroisobenzofuran-1-yl acetate derivatives **4** from the addition reaction of ninhydrin **1** and enaminone **2** followed by oxidative cleavage of the corresponding 3a,8b-dihydroxy-1,8b-dihydroindeno[1,2-*b*]pyrrol-4(3a*H*)-ones **2** in acetic acid and at room temperature.



All products **4** were unambiguously characterized using their spectroscopic data and CHN analysis.

References:

[1] Lin, G.; Chan, S. S.-K.; Chung, H.-S.; Li, S.-L. Chemistry and Biological Action of Naturally Occurring Phthalides. *In Studies in Natural Products Chemistry*; Atta-ur-Rahman, Ed.; Elsevier: Amsterdam, **2005**; Vol. 32, p 611.
[2] Mal, D.; Pahari, P.; De, S. R. *Tetrahedron* **2007**, *63*, 11781.
[3] Yang, H.; Hu, G.-Y.; Chen, J.; Wang, Y.; Wang, Z.-H. *Bioorg. Med. Chem. Lett*. **2007**, *17*, 5210.
[4] Mohammadizadeh, M. R.; Firoozi, N. *Tetrahedron Lett*. **2010**, *51*, 2467.

An efficient synthesis of functionalized thiochromene and S-vinyl thioether

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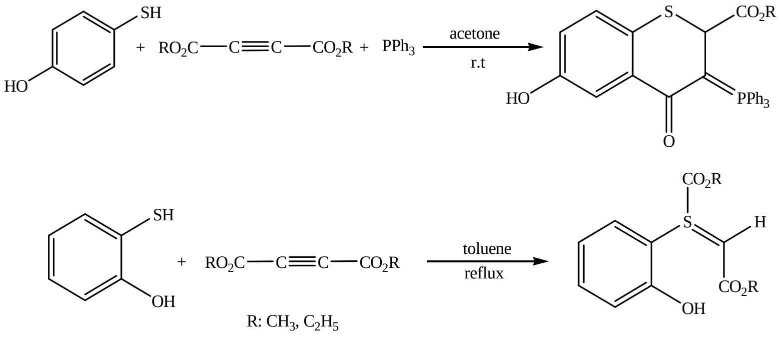
For several years, acetylenic esters have been attracting the attention of organic chemists. Acetylenic esters are reactive systems that take part in many chemical synthesis [1]. The compounds almost act as a Michael acceptor in organic reactions [2]. Michael addition of phosphorus(III) compounds such as triphenylphosphine to acetylenic esters leads to reactive 1,3-dipolar intermediate betaines which are not detected even at low temperature. These unstable species can be trapped by a protic reagent, ZH, such as methanol, amid, imide, etc. to produce various compounds e.g. ylides [3].

Herein we report an efficient synthetic route to phosphorus ylides using triphenylphosphine, dialkyl acetylenedicarboxylates and 4-mercaptophenol. We found that phosphorus ylides result from the initial addition of triphenylphosphine to the acetylenic ester and a concomitant protonation of the 1:1 adduct by 4-mercaptophenol. Then the positively charged ion is attacked by the thiophenoxy anion of the 4-mercaptophenol to form phosphorane. The functionalized thiochromene is presumably produced by intramolecular cyclization of phosphorane.

Two-component reaction of 2-mercaptophenol with dialkyl acetylenedicarboxylates was also investigated to study different reactivity of 2-mercaptophenol and 4-mercaptophenol with electron-deficient esters. The product obtained from this reaction is S-vinyl thioether.



Reference:

[1] Shaabani, A.; Teimouri, M.B.; Bijanzadeh, H.R. *Tetrahadron Lett*. **2002**, 43, 9151.
[2] Yavari, I.; Ramazani, A. *Phosph, Sulfur Silicon*. **1997**, 130, 73.
[3] Yavari, I.; Adib, m.; Hojabri, L. *Tetrahedron*. **2002**, 58, 6895.

Crosslinked poly(acrylic acid) thickener: preparation, characterization and rheological properties

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Microparticles of crosslinked poly(acrylic acid) are one of the most important water soluble polymers. This polymer is widely used as thickeners, suspending agents and viscosity modifiers. In the precipitation process, the produced polymer is non-soluble in reaction mixture whereas medium is homogeneous at initially [1]. Aqueous dispersion of carbonyl polymer was studied to determined effective parameter of increasing viscosity [2].

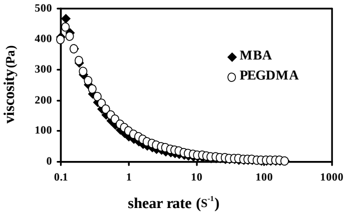
In this study, crosslinked poly(acrylic acid) were prepared by using two kind of crosslinker by precipitation polymerization method in a binary organic solvent. *N,N'*-Methylenebisacrylamide (MBA) and (polyethelne glaycol dimethacrylate, PEGDMA-330) were used as low-molecular weight and long-chain crosslinkers, respectively .

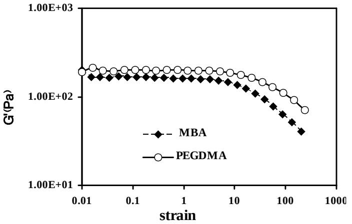
The effects of crosslinker concentration and its type on polymer properties such as swelling capacity, gel content, apparent viscosity, rheological properties (The storage modulus (G'), loss modulus (G''), the phase angle ($\tan \delta$) and rotational viscosity) and T_g were investigated.

The average molecular weight between two successive crosslinks ($\overline{M_c}$), through the Flory-Rehner equation and rubber elasticity theory was consider and the network structure of polymer was evaluated. In addition, viscosity coefficient *(m)* and flow behavior index *(n)* of power-law equation were calculated as well.

Calculated gel content and obtained swelling values observed that low-molecular weight crosslinker was more reactive than long-chain with AA. $\overline{M_c}$. Content confirmed this subject. Thus Viscosity of polymeric solution with PEGDMA was more than Viscosity of polymeric solution with MBA (fig 1).

An enhancement in G', G" and $\tan \delta$ was observed by synthesized polymer with long-chain crosslinkers (fig.2). Decreasing viscosity was observed by increasing in shear stress because of pseudoplastic model of polymer for both samples.





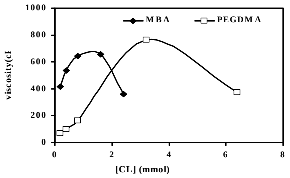


fig1. Viscosity as a function of crosslinker types

References:

[1] Bouhendi H., Haddadi-Asl V. Rafizadeh M. *Iranian poly. J.* **2009**, *18, 777.*

[2] Agarwal Y. K., Kaushik S. D. and Kumar P. C. Journal of Macromolecular Science, Part A: *Pure and Applied Chemistry* **2007,** 44, 877.

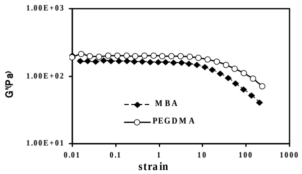


fig2. G'as a function of strain

Silica-supported $BiCl_3$ as a highly effective catalyst for the synthesis of quinoxalines

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Heterogeneous organic reactions have proven useful to chemists in the laboratory as well as in the industrial context. These reactions are affected by the reagents immobilized on the porous solid supports. Lewis acids supported on “inert” carriers have received considerable importance in organic synthesis. Indeed, these catalysts can be easily separated from the reaction products by simple filtration and quantitatively recovered in the active form. They can be recycled, making less expensive the preparation of sophisticated fine chemicals and, at the same time, avoiding contamination of the products by trace amounts of metals.

As a part of our continued interest in the development of highly expedient methods for the synthesis of heterocyclic compounds, we herein report a facile and efficient synthetic strategy for quinoxaline derivatives in excellent yield using $BiCl_3/SiO_2$ in methanol as benign solvent. Despite the use of few solid heterogeneous catalysts in literature, silica-supported heterogeneous Lewis acid catalysts, like $BiCl_3/SiO_2$, have not yet been explored with regard to the preparation of quinoxalines.

The results of TG-DTA and BET indicated that dispersed $BiCl_3$ coordinates with surface hydroxyl groups leading to formation –O-Bi-Cl as stable Lewis acid sites under the reaction condition. $BiCl_3/SiO_2$ acts as a highly efficient catalyst, even for low activity substrates, in the preparation of quinoxaline derivatives. To investigate the role of $BiCl_3/SiO_2$, the reactions were carried out in the absence or presence of silica gel. In both cases, low yield of product was obtained, which indicates that catalyst is obviously necessary for the reaction. The catalyst could be successfully recovered and recycled at least for four runs without significant loss in activity [1].

References:

[1] Darabi H. R.; Aghapoor K.; Mohsenzadeh F.; Taala F.; Asadollahnejad N.; Badiei A. R . *Catal let.* **2009**, *133,* 84.

Novel chiral poly(ester-imide)s containing different natural α-amino acids

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Optically active polymers including those bearing main or side chain amino acid units are used extensively in the pharmaceutical industry for enantioselective separation of drugs and as a biocompatible compound in dentistry, drug delivery, gene therapy and tissue engineering. Therefore, they have been the subject of intensive studies and their synthesis is a topic of current interest [1,2].

Wholly aromatic poly(ester-imide)s (PEI)s are well-known to show good physical properties. These polymers can be considered as advanced materials used in electronic devices and fiber composites due to excellent mechanical properties, improved processability, good thermal, chemical and dimensional stabilities [3]. In this paper, novel optically active PEIs, containing different amino acids in the main chain as well as in the side chain were synthesized by polycondensation of diacid monomers such as 5-(2-phthalimidyl-3-methyl butanoylamino)iso-phthalic acid and 5-(4-methyl-2-phthalimidylpentanoylamino)isophthalic acid with *N,N'*-(pyromellitoyl)-bis-L-tyrosine dimethyl ester as a phenolic diol [4-6]. The direct polycondensation reaction was carried out in a system of tosyl chloride, pyridine and *N,N*-dimethylformamide as a condensing agent under conventional heating condition. The synthesized polymers were characterized by means of FT-IR, ^{1}H-NMR, elemental and thermogravimetric analysis (TGA) technique. TGA data show that the thermally stability of the resulting polymers is rather high. This type of polymers which have both main-chain and side-chain optically active groups are expected to have the advantages of biodegradability because of the presence of amino acids as a biodegradable segment.

References:

[1] Romagnoli, B.; Harwood, LM.; Hayes, W. *Tetrahedron Lett.* **2003**, *44*, 37.
[2] Kakizawa, Y.; Harada, A.; Kataoka, K. *Biomacromolecules* **2001**, *2*, 491.
[3] Li, CH.; Chen, CC.; Chen, KM. *J. Appl. Polym. Sci*. **1994**, *52*, 751.
[4] Mallakpour, S.; Kolahdoozan, M. *Eur. Polym. J.* **2007**, *43*, 3344.
[5] Mallakpour, S.; Dinari, M. *Polym. Adv. Technol.* **2008**, *19*, 1334.
[6] Ensafi, A.A.; Mallakpour, S.; Doozande, F.; Allafchian, A.A.; Tirgir, F. *Anal Lett.* Accepted for publication, **2010**.

Direct reductive amination of aldehydes and ketones with sodium hydride as reducing agent and trimethylboraat as activator

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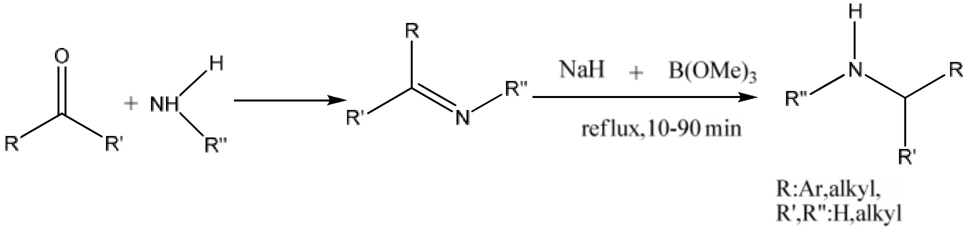
The transformation of aldehydes and ketones to amines is an important method in organic synthesis because of their versatile utility as intermediates for synthesis of pharmaceuticals[1] and agrochemicals. A simple and convenient procedure allows the reductive amination of aldehydes and ketones using sodium hydride as reducing agent and Trimethylborate as activator. The use of inexpensive reagents is the notable advantages of this method. Furthermore, due to compatibility of this reagent system with a variety of otherwise reducible functional groups, this method can provide an easy access to analogues amines bearing functional group. It is obvious that the sodium hydride alone is not reducing agent but in the presence of trimethylborate, it becomes a mild reductant.



References:

[1] G. Samuelsson, Drugs of Natural Origin, Swedish Pharmaceutical, Stockholm

[2] (a) D.B. Sharp In: P.C. Kearney and D.D. Kaufman, Editors, *Herbicides: Chemistry, Degradation, and Mode of Action*, Marcel Dekker, New York (1988), p. 301 Chapter 6. (b)H.M. Lebaron, J.E. Mcfarland and B.J. Simoneaux In: P.C. Kearney and D.D. Kaufman, Editors, *Herbicides: Chemistry, Degradation, and Mode of Action*, Marcel Dekker, New York (1988), p. 335 Chapter 7.

[3] B. T. Cho, S. K. Kang, *Tetrahedron*, **2005**, *61*, 5725.

[4] A. F. Abdel-Magid, K. G. Carson, B. D. Harris, C. A. Maryanoff, R. D. Shah, *J. Org. Chem.*, **1996**, *61*, 3849.

[5] J. W. Bae, S. H. Lee, Y. J. Cho, C. M. Yoon, *J. Chem. Soc., Perkin Trans. 1*, **2000**, 145.

Convenient one-pot selective synthesis of N1-methylated 3,4-dihydrothioxopyrimidines

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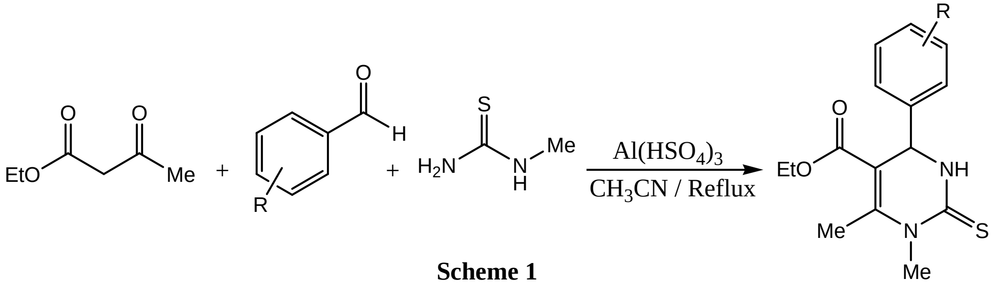
Dihydrothioxopyrimidines are potential bioactive molecules as they are structural analogs of biogenic purines and can be considered as potential nucleic acid, antibacterial and antimycobacterial activity [1, 2].

The first procedure to these compounds reported by Biginelli more than a century ago makes use of the three component, one-pot condensation of β-ketoester, an aldehyde and thiourea under strongly acidic conditions [3].

In this letter, we report a efficient method that allows the synthesis of N1-methylated 3,4-dihydrothioxopyrimidines from an aromatic aldehyde, ethyl acetoacetate, N-methylthiourea and aluminium hydrogen sulfate as catalyst in acetonitrile at reflux condition (Scheme 1).



Scheme 1

Nature of substituents on the aromatic ring did show strong effects in terms of reaction time under the reaction conditions mentioned above. When aromatic aldehydes containing electron-donating groups (such as methyl, methoxyl, or dimethylamino group) were employed, a longer reaction time was required than those of electron-withdrawing groups (such as nitro, or halides group) on aromatic rings.

Refrences:

[1] Chambhare, R. V.; Bobade, A. S.; Khadse, B. G. *Indian J Heterocycl Chem*. **2002**, *12*, 67.
[2] Chambhare, R. V.; Khadse, B. G.; Bonde, A. S. Bahekar, R. H. *Eur. J. Med. Chem*. **2003**, *38*, 89.
[3] Biginelli, P. *Gazz. Chem. Ital*. **1893**, 23, 360.

Theoritical investigation on molecular wire and Interactions of a conjugated molecular diode with a cluster of Au

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The systems being examined in this work are bis aryl substituted tetrazin and the molecule consists of three benzene rings connected to each other by an acetylene group(TFA) . All calculations were carried out using GAUSSIAN 03 program with three following steps.

step 1:a geometry optimization of diphenyltetrazine and TFA joint to Sh linkers was carried out. step 2:Then the interaction between molecules(after removal of the end H atoms of SH)with two gold (111) clusters has been studied Fig.1(a,b,c)The energy gaps for the free molecular diode decrease when an additional metal atom is added.This is due to the localization of the LUMO energy level on the metal atoms in order to understand the interactions between the metal-molecule interfaces we have carried out natural bond orbital analysis in Table.1.HOMO–LUMO gap (HLG) is a key parameter determining the conductance property[1]**.**

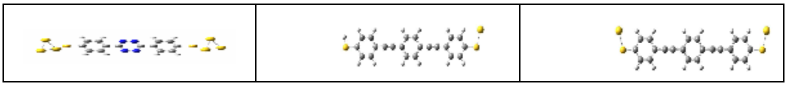
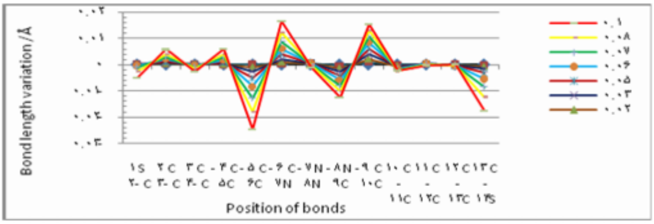


Fig.1.

Table.1.

complex	Homo$_{(ev)}$	Lumo$_{(ev)}$	HLG$_{(ev)}$
AuSWSAu	-4.90	-3.06	1.84

step 3:Then,the two terminal gold clusters were fixed in space to simulate the connection to the electrodes.The EF ranging from(0-0.103)V/A° is defined as uniform and aligned along the metal/molecules/metal inter-atomic vector , was applied to complex that can reasonably represent the working condition of the molecular wire (Fig.2). Fig.2.



References:

[1] M. A. Reed, C. Zhou, C. J. Muller, T. P. Burgin, J.M. Tour, *Science*. 279 (**1997**) 252.

A simple and efficient esterification of carboxylic acids utilizing tosyl chloride under solvent-Free conditions

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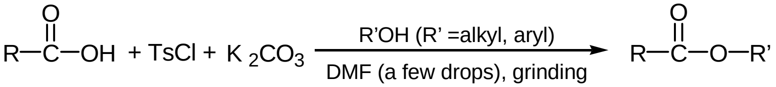
From the standpoint of elaborate complex natural product synthesis and process chemistry, direct esterification between equimolar amount of carboxylic acids and alcohols is well recognized as an important unit reaction for a wide range of organic synthesis [1]. A number of synthetic methods for the esterification have been developed [2].

Tosyl chloride/potassium carbonate combination was used successfully in anhydride, sulfonamide and alkyl tosylate preparations at solvent-free conditions [3]. Using potassium carbonate as cheap, weak basic solid support has advantages such as controlled promotion of reaction, simplicity and matches with green chemistry protocols. In order to develop the applications of $TsCl/K_2CO_3$ combination, we decided to try it for esterification of carboxylic acids with alcohols and phenols.

To a mixture of carboxylic acid, TsCl and K_2CO_3 in a mortar, alcohol (or phenol) and a few drops of DMF (as wetting agent) was added gradually and the resulting mixture was ground at room temperature for appropriate times. In very case examined, this reaction was performed successfully by using several aromatic and aliphatic and heterocycle carboxylic acids with alcohols and phenols in good to excellent yields.



$$R-\overset{O}{\overset{\|}{C}}-OH + TsCl + K_2CO_3 \xrightarrow[\text{DMF (a few drops), grinding}]{\text{R'OH (R' =alkyl, aryl)}} R-\overset{O}{\overset{\|}{C}}-O-R'$$

References:

[1] (a) Benz, G. *in Comprehensive Organic Synthesis*; Pegman: Oxford, 1991; (b) Otera, J. *Esterification*; Wiley-VCH: Weinheim**,** 2003.

[2] (a) Ziegler, F. E.; Berger, G. D. *Synth. Commun.* **1979**, *9*, 539; (b) Hajipour, A. R.; Mazloumi, Gh. Synth. Commun. **2002**, *32*, 23; (c) Tanabe, Y.; Wakasugi, K.; Iida, A. *Adv. Synth. Catal.* **2003**, *345*, 1209; (d) Khalafi-Nezhad. A; Parhami, A.; Zare, A.; Moosavi Zare, A. R. *J. Iran. Chem. Soc.,* **2008**, *5*, 413.

[3] (a) Kazemi, F.; Sharghi, H.; Nasseri, M. A. Synthesis **2004**, 205; (b) Massah, A. R.; Kazemi, F.; Azadi, D.; Farzaneh, S.; Aliyan, H.; Javaherian Naghash, H.; Momeni, A. R. *Lett. Org. Chem.* **2006**, *3*, 235; (c) Kazemi, F.; Massah, A. R.; Javaherian, M. *Tetrahedron* **2007**, *63*, 5083.

An efficient synthesis of substituted dibenzo [a,c] phenazines using Epsom salt as inexpensive catalyst

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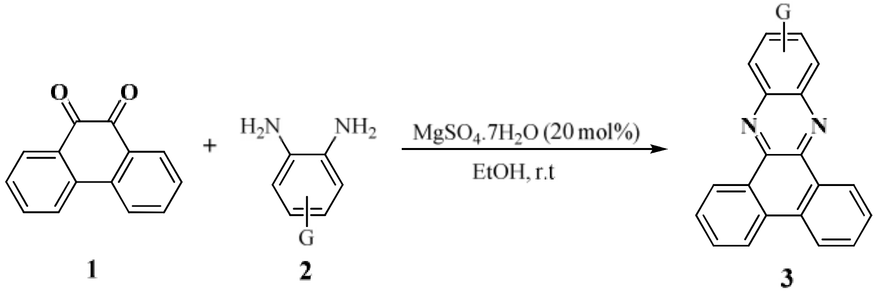
Phenazines are one of the most important classes of benzo hyterocyclic compounds which are found in structural subunits of more complex natural products [1,2]. Phenazin derivatives show a broad spectrum of biological activities such as antibacterial, antifungal, antiviral, and antitumor properties [1-3]. Thus, the synthesis of this heterocyclic nucleus has attracted much attention.

Considering that catalytic technologies play a vital role in the economic development of the chemical industries. In this research, the use of magnesium sulfate heptahydrate ($MgSO_4.7H_2O$ or Epsom salt) as an efficient catalyst for the synthesis of dibenzo [a,c] phenazines **3** based on the condensation of 9,10 phenanthrene quinine **1** and appropriated aryl 1,2 diamines **2** at room temperature was reported.

The present method has the advantages such as availability of starting materials, clean reaction, simple work-up, cheapness, short reaction times and high yields of the products. The structure of product **3** were deduced from their IR, ^{1}H NMR, ^{13}C NMR spectral data.



G= H, Ph, Cl, Me, NO_2, Br

References:

[1] Whistler, C. A. L.; Pierson, S. *J. Bacteriol.* **2003**, *185*, 3718.
[2] McDonald, M.; Mavrodi, D. V.; Thomashow, L. S.; Floss, H. G. *J. Am. Chem. Soc.* **2001**, *123*, 9459.
[3] Muller, P. K.; Krohn, K.; Muhlradt, P. F. *Infect. Immun.* **1989**, *57*, 2591.

Four-component catalyst-free reaction in the presence of water: an improved protocol for the synthesis of 6-amino-1, 4-dihydropyridine derivatives

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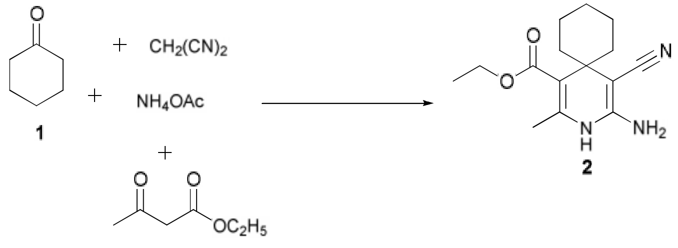
Water exhibits special properties as compared to commonly employed organic solvents. For instance, Breslow and co-worker reported acceleration of the Diels-Alder reaction "in water" with the reaction performed at very high dilution to dissolve the reactant [1], while K. Barry Sharpless and co-worker described "on water" conditions under which substantial rate acceleration was observed when the organic reactants were insoluble in the aqueous phase [2].

Dihydropyridines (DHPs) represent an important class of biologically active molecules, several of which have found use in the treatment of cardiovascular disease and hypertension. In this context, a survey of the literature has shown that 6-amino substituted 1, 4-DHPs possess neuroprotective effect against [Ca^{2+}] overload [3]. To the best of our knowledge, there are a scarce number of publications for the synthesis of these classes of compounds [4].

Herein, we report for the first time a catalyst-free four-component reaction for a combinatorial synthesis of 6-amino-1, 4-dihydropyridine framework in the presence of water at mild condition. Mild reaction conditions, operational simplicity, enhanced rates, and high isolated yield of pure products are significant advantages of this protocol.



References:

[1] D. C. Rideout, R. Breslow, *J. Am. Chem. Soc.* **1980**, *102*, 7816.
[2] S. Narayan, J. Muldoon, M. G. Finn, V. V. Fokin, H. C. Kolb, K. B. Sharpless, *Angew. Chem. Int. Ed.* **2005**, *44*, 3275-3279.
[3] R. León, C. de los Ríos, J. Marco-Contelles, M. G. López, A. G. García, M. Villarroya, *Eur. J. Med. Chem.* **2008**, *43*, 668.
[4] J. Marco-Contelles, R. León, C. de los Ríos, A. Guglietta, J. Terencio, M. G. López, A. G. García, M. Villarroya, *J. Med. Chem.* **2006**, *49*, 7607.

A green and selective synthesis of 2-aryloxazines and 2-aryltetrahydropyrimidines

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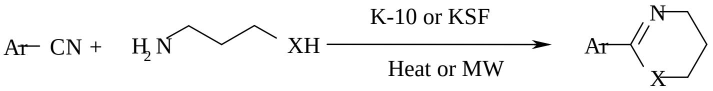
5,6-Dihydro-4*H*-1,3-oxazines and 1,4,5,6-tetrahydropyrimidines are important heterocyclic compounds, which are found in both various biologically active natural compounds and designed medicinal agents [1]. However, some of these methods are associated with certain drawbacks such as harsh reaction conditions, the use of complex or toxic reagents, low yields of the products and long reaction times [2].

Montmorillonite clays (K-10 and KSF) are environmentally friendly and economically feasible solid acids that offer several advantages such as non-corrosiveness, low cost, ease of handling and reusability [3]. The reactions catalyzed by montmorillonite clays are usually carried out under mild conditions with high yields and high selectivities and the work-up of these reactions is very simple. The combination of these solid acid catalysts with microwave irradiation provides even more benign processes. Herein we report a selective method for synthesis of 2-aryloxazines and tetrahydropyrimidines by the reaction of arylnitriles with 3-amino-1-propanol and 1,3-diaminopropane in the presence of montmorillonite K-10 and KSF under thermal conditions and microwave irradiation.



X = O, NH

References:

[1] (a) Dunbar, P. G.; Durant, G. J.; Fang, Z.; Abuh, Y. F.; El-Assadi, A. A.; Ngur, D. O.; Periyasamy, S.; Hoss, W. P.; Messer Jr. W. S. *J. Med. Chem.* **1993**, *36*, 842. (b) Bernard, T.; Jebbar, M.; Rassouli, Y.; Himdi-Kabbab, S.; Hamelin, J.; Blanco, C. *J. Gen. Microbiol.* **1993**, *139*, 126. (c) Messer, W. S. Jr.; Abuh, Y. F.; Ryan, K.; Shepherd, M. A.; Schroeder, M.; Abunada, S.; Sehgal, R.; El-Assadi, A. A. *Drug Dev. Res.***1997**, *40*, 171.

[2] (a) Karade, N.N.; Tiwari, G.B.; Gampawar, S.V.; *Synlett* **2007,** 1921. (b) Tillmanns, E.J.; Ritter, J.J. *J. Org. Chem.* **1957**, *22*, 839.

[3] Chankeshwara, S. V.; Chakraborti, A. K. *J. Mol. Catal. A: Chem.* **2006**, *253*, 198.

Coordination behavior of azines towards Fe (III), Ni (II), Co (II)

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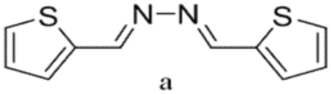
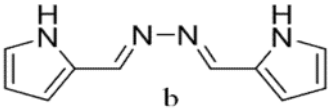
Azines constitute an important class of biologically active and stereochemically significant nitrogen donor ligands have found wide application in various fields [1-4]. Based on biologically active metal complexes, we prepared and studied some Fe (III), Ni (II) and Co (II) complexes of azines derived from heterocyclic aldehydes, with thiophene-2-aldehyde (a) and pyrrole-2-aldehyde (b).


a


b

Herein we reported the coordination behavior of Schiff bases derived from the condensation of some of the heterocydic aldehydes with hydrazine hydrate, towards Fe *(*III*)*, Ni (II), and Co (II), has been studied. The 1:2 molar reactions of MCl_2 (or MCl_3) with the Schiff bases result in colored solids. The FT-IR spectra of the ligands, exhibited ν(C=N) and ν(N–N) at ca. 1630 $cm^{-1}$and ca. 1050 cm^{-1}, respectively. The ν(C=N) shifts by ca. 20 $cm^{-1}$and ν(N–N) by ca. 10 cm^{-1} due to the bonding through the azomethine nitrogen. This feature is further supported by the appearance of ν(M–N) in the FT-IR spectra. In the spectra of the ligands, bands at ca. 3100 $cm^{-1}$and at ca. 1570 cm^{-1} are due to pyrrole or thiophene rings. FT-IR studies confirmed the formation of complexes. Also we demonstrated electronic properties for these complexes. We observed some transition states, for example band at 320 nm is due to the $\pi-\pi^*$ transition within the aromatic rings and remains almost unchanged in the spectra of the metal ions complexes.

References :

[1] Karaboek, N.; *Transition Met. Chem*. **2006**, *31*, 118.
[2] Guskos, N.; Paschalidis, D.G.; Majszczyk, J.; Typek, J.; Maryniak, M. *Mater. Sci. Poland* **2005**, *23*, 1029.
[3] Donde, R. J.; Patil, V. R.; Malve, S. P., *Acta Pot. Pharm.* **2003**, *60*, 173.
[4] Godara, M.; Maheshwari, r.; Varshney S.; Varshney, a. k. *J. Serb. Chem. Soc*. **2007**, *72*, 367.

Phytochemical composition of the essential oils from leaves, flowers, stem and root of *Phlomis herba-venti L. subsp. kopetdaghensis* and aerial parts of *Marrubium anisodon*

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The genus *Phlomis* and *Marrubium* (Lamiaceae) comprises species, which are found wild in Iran [1,2]. Several *Phlomis* species are used in herbal medicine, e.g. for treatment of respiratory tract diseases or externally for treatment of wounds [3]. Phytochemical analyses of *Marrubium* spp. have confirmed the occurence of diterpenes, caffeic acid derivatives and flavonoids [4,5].

In our research on the essential oil of the plants of Iran, we have investigated on the composition of the essential oils of *P. herba-venti* subsp. *kopetdaghensis* and *Marrubium anisodon.*

The dried leaves, flowers, stem and root of *P. herba-venti* subsp. *Kopetdaghensis* and aerial parts of *Marrubium anisodon* were separately subjected hydrodistillation using a Clevenger-type apparatus for 3-4h and oils were dried with anhydrous sodium sulfate and stored at 4°-6 °C. The oils were then submitted to GC and GC/MS analysis.

Thirteen components were identified in the oil of leaf with germacrene D (58%), α-pinene (10.4%) and bicyclogermacrene (4.4 %) as main constituents. Twenty one compounds were identified in the oil of flowers with germacrene D (48%), α-pinene (19.7%) and β-selinene (10.1%) as main components. Eighteen compounds were characterized in the oil of stem with germacrene D (57%), α- pinene (8.6%) and 2-pentadecanone (6.5%) as main constituents. In the oil of root, germacrene D (28%), α-pinene (13.6%) and spathulenol (8.6%) were found as main constituents. Fifteen components were detected in the oil of *M. anisodon*, representing 93.6% of the total oil. The major constituents were germacrene D (44.2%), β-caryophyllene (10.4%) and α-pinene (15%). All oils consist of monoterpenes, sesquiterpenes and aliphatic compounds.

References:

[1] Mozaffarian, V.; Farhang Mo’aser, Tehran, Iran, **1996**, 406.
[2] Rechinger, K. H.; *Flora Iranica*. Graz, Austria, **1982**, 150, 92.
[3] Couladis, M.; Tanimanidis, A.; Harvala, C.*; Journal of Planta Med*., **2000,** 66, 670.
[4] Bal, Y.; Kaban, S.; Kirimer, N.; *J. Essent. Oil* Res., **1999**, 11, 300.
[5] Nagy, Y.; Svajdlenka, E.; *J. Essent. Oil Res*., **1998**, 10, 585.

Mono- and bis-2-amino-4H-pyrans: Alum catalyzed three- or pseudo five-component reaction of 4-hydroxycoumarin, malononitrile and aldehydes

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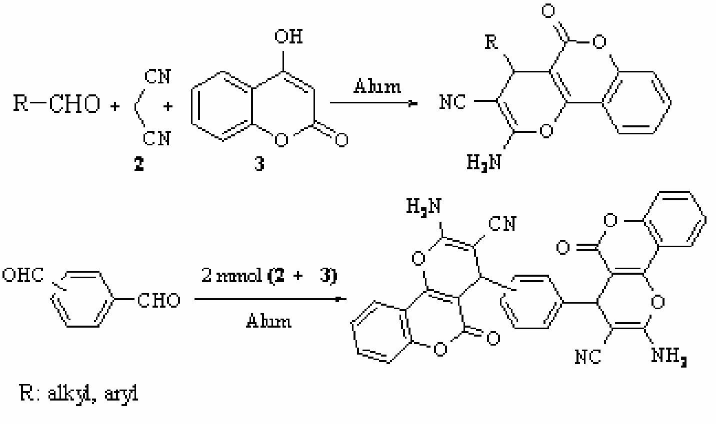
4*H*-pyran is a privileged heterocyclic ring system because many of its derivatives possess useful pharmacological activities [1]. 2-Amino-4*H*-pyran derivatives represent an important class of compounds. They are often used in cosmetics and pigments, and utilized as potentially biodegradable agrochemicals [2].

Recently, 2-amino-4*H*-pyrans were synthesized by three-component condensation reaction of aldehyde, malononitrile or ethyl 2-cyanoacetate and β-dicarbonyl compounds such as dimedone, barbituric acid or hydroxycoumarin. This condensation has been catalyzed by variety of reagents such as: HMTAB [3], TEBA [4], RE(PFO)$_3$ [5] and etc.

Thus, each of the known procedures for the synthesis of corresponding 2-amino-4*H*-pyrans has its merits; however, further studies are still necessary for the essence of facile, environmental and economical multicomponent methodology. Due to the biological activity of 4*H*-pyrans and our interest in the synthesis of heterocyclic compounds, herein, we report a simple and efficient method for the preparation of mono- and bis-2-amino-4*H*-pyran derivatives using Alum as the catalyst in the multi-component reaction of 4-hydroxycoumarin, malononitrile and aldehydes.



References:

[1] Zamocka, J.; Misikova, E.; Durinda, *J. Pharmazie*. **1991**, *46*, 610.
[2] Morinaka, Y.; Takahashi, K. *Jpn Patent* . JP52017498, **1977**.
[3] Jin, T. S.; Wang, A. Q.; Wang, X.; Zhang, J. S.; Li, T. S. *Synlett*. **2004**, 871.
[4] Shi, D. Q.; Zhang, S.; Zhuang, Q. Y.; Tu, S. J.; Hu, H. W. *Chin. J. Org. Chem*. **2003**, 23, 877.
[5] Wang, L. M.; Shao, J. H.; Tian, H.; Wang, Y. H.; Liu, B. *J. Fluor. Chem*. **2006**, 127, 97.

Synthesis of *N*, 3-diphenyl acrylamide derivatives as potential anti-oxidant agents

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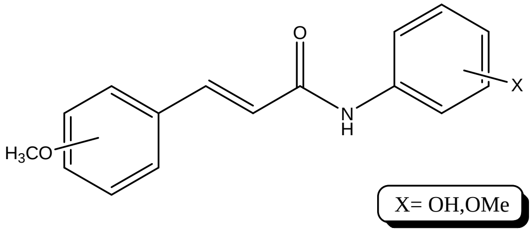
Lipid peroxidation is an important mediator of pathophysiological events in central nervous system disorders such as cerebral ischemia and trauma [1]. Lipid peroxidation is induced by free radicals with the major species of reactive oxygen species (ROS). ROS are by-products of a variety of pathways of aerobic metabolism. They are unstable and react readily with a wide range of biological substrates such as lipids, DNA and protein, resulting in cell damage [2,3].

Herein we report the synthesis of N, 3-Diphenyl acrylamide as potential anti-oxidant agents. Starting from readily available (methoxyphenyl) acrylic acid, methoxyaniline was prepared in 50% overall yield.

The purity of the synthesized compound was confirmed by chromatography. The structure of compound was characterized using IR, ^{1}HNMR and mass spectra.



Reference:

[1] Hall, E. D. In Oxygen Free Radicals in tissue Damage; Tarr, M., Samson, F., Eds.; BIrkhauser: Boston, **1993**, pp153-173.
[2] Halliwell, B.; Gutteridge, J. M. C. , Eds.; Oxford University Press, Clarendon: Oxford, **1989**; pp1-20.
[3] Roberfroid, M.; Colderon, P. B. In Free Radicals and Oxidation Phenomena in Biological systems; Roberfroid, M., Colderon, P. B., Eds.; University of Catholigue de Louvain Brussels: New York, **1995**; pp11-32.

Simple strategy for fluorination of ketamine's precursors

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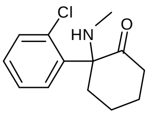
Ketamine 1 is a general, effective and short acting anesthetic drug. Which elevate blood pressure and heartbeat in the period of anesthesia. It also use in chronic pain management [1]. The medicinal chemists like to characterize drug activity of fluoro derivative of ketamine.

The first method to introduce fluorine in aromatic rings is called Balz-Schiemann reaction which aniline is converted to aryl fluoride via diazonium fluoroborate. Beside the Balz-schiemann reaction, one of the important methods is Halex (halogen-exchange) reaction. Halogen (chlorine or rarely bromine) that are activated by electron-withdrawing group, are exchange by fluoride. The usual reagent in Halex reaction is spray dried KF as a source of fluoride and phase transfer catalyst (PTC) to accelerate reaction between KF and substrate [2]. Another reagent is anhydrous tetrabutylammonium Fluoride ($TBAF_{anh}$) [3].

Preparing of 2 from fluoroaromatic precursors in a multistep reaction is a low efficient. Herein we were Fluorinated some ketamine's precursors with Halex reaction. 2-Chlorobenzoic acid, 2-chlorobenzonitrile, 2-Chlorophenyl cyclopentyl ketone, 2-Chlorophenyl cyclohexyl ketone were fluorinated by this method.The fluorination of ketamine by this method will be trend. Products were characterized by ^{1}HNMR and ^{19}FNMR.



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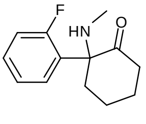

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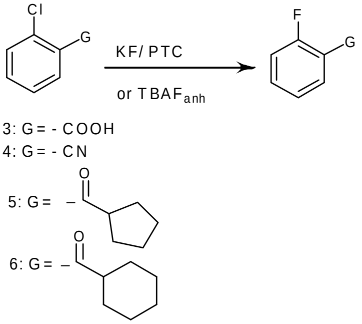

References:

[1] Visser, E.; Schug, S.A. *Biomed Pharmacother.* **2006**, *60*, 341.
[2] Sasson, Y.; Negussie, S.; Royz, M.; Mushkin, N. *Chem. Commun*. **1996**, 297.
[3] Dimagno, S. G.; Sun, H. *Angew. Chem.* **2006**, *118*, 2786.

Efficient and mild procedure for the selective nitration of phenolic compounds using supported nitric acid on polyvinylpolypyrrolidone

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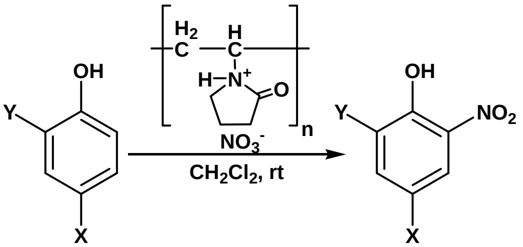
Nitration is important for two reasons: firstly, because it is the most general process for the preparation of aromatic nitro compounds; secondly, because of the part which it has played in the development of theoretical organic chemistry [1]. The nitration of phenols is a fundamental unit process of great industrial importance generating commercially valuable intermediates and there is a great need for regio-selective pollution free processes [2]. In the recent decade different procedures has been reported for the nitration of phenolic compounds [3-4], but some of these procedures are not region-selective and are the cause of environmental concerns regarding the disposal of large excesses of concentrated nitric acid and non-environmentally friendly metallic catalysts or reagents.

Therefore, designing systems, which is improved the mentioned limitations, is great of importance. Consequently, herein we report an efficient and heterogeneous procedure for the nitration of substituted phenols using supported nitric acid on polyvinylpolypyrrolidone under mild and heterogeneous conditions (Scheme 1).



Scheme 1

References:

[1] Hoggett, J.G.; Moodie, R.B.; Penton, J.R.; Schofield, K. Nitration and aromatic reactivity, Syndics of the Cambridge University Press, New York (1971).
[2] Rajagopal, R.; Srinivasan, K.V. *Synth. Commun.* **2003**, *33*, 961.
[3] Tajik, H.; Niknam, K.; Parsa, F. *J. Iran. Chem. Soc.* **2009**, *6*, 159.
[4] Yin, W.P.; Shi, M. *Arkivo* **2009**, 6.

A rapid synthesis of novel chromone-containing furopyrimidines

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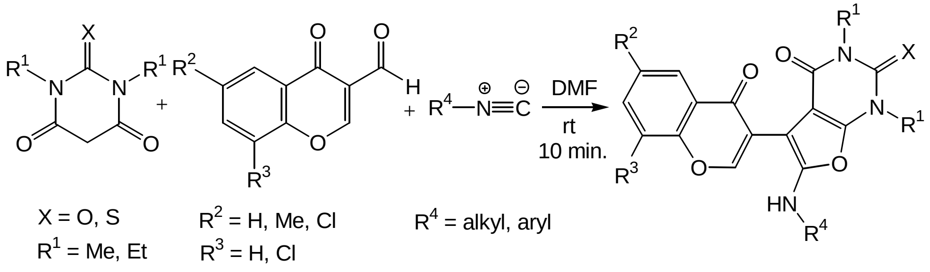
The chromone moiety forms the nucleus of a class of natural products called flavanoids and is also part of pharmacophores of various biologically active molecules, including anticancer agents such as psorospermin and pluramycin A [1-4]. Cromoglicic acid (cromolyn) is traditionally described as a mast cell stabilizer, and is commonly marketed as the sodium salt sodium cromoglicate or cromolyn sodium. This drug prevents the release of inflammatory chemicals such as histamine from mast cells and as an inhaler is used for preventive management of asthma [5,6]. On the other hand the furo[2,3-*d*]pyrimidines are an important class of annulated uracils with biological significance because of their connection with purine systems.

As part of our group's efforts to explore synthetic methodologies to access unique scaffolds or pharmaceutically related heterocycles [7,8], herein we wish to report the synthesis of a library based on the scaffold of chromone-containing furopyrimidine. Our strategy focused on the use of a one-pot three-component reaction between readily available substituted 3-formylchromones, 1,3-di-substituted (thio)barbituric acid and isocyanides.



References:

[1] Kim, M. Y.; Na, Y.; Vankayalapati, H.; Gleason-Guzman, M. *J. Med. Chem.* **2003**, *46*, 2958.
[2] Mitscher, L. A. *Chem. Rev.* **2005**, *105*, 559.
[3] Cassady, J. M.; Baird, W. M.; Chang, C. J. *J. Nat. Prod.* **1990**, *53*, 23.
[4] Kupchan, S. M.; Streelman, D. R.; Sneden, A. T. *J. Nat. Prod.* **1980**, *43*, 296.
[5] Horan, R. F.; Sheffer, A. L.; Austen, K. F. *J. Allergy Clin. Immunol.* 1990, *85*, 852.
[6] Schwartz, H. J.; Blumenthal, M.; Brady, R. *Chest* **1996**, *109*, 945.
[7] Teimouri, M. B. ; Mansouri, F. ; Bazhrang, R. *Tetrahedron* **2010**, *66*, 259.
[8] Teimouri, M. B. ; Abbasi, T. *Tetrahedron* **2010**, *66*, 3795.

Three component reaction of triphenylphosphits and dialkyl acetylenedicarboxylates with theophiline,

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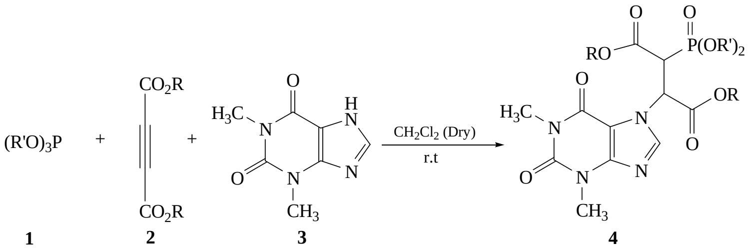
Organophosphorus compounds are important substrates in the study of biochemical processes [1]. For a long time phosphorus analogues of amino acids, in which the carboxylic acid group is replaced with phosphonate group, $P(O)(OR)_2$, have attracted particular interest in preparing analogues of numerous natural products [2]. In this area β-amido phosphonates as isosteres of β-amino acids occupy an important place and reveal diverse and interesting biological and biochemical properties [3]. There are several methods for synthesis of β-amidophosphonates. In most of them, nucleophilic trivalent phosphorus has been attached to electrophilic carbon [4].

Multicomponent reactions have proven highly efficient in the assembly of diversified molecules. Zewitterionic species often result from addition of nucleophiles to activated alkynes. Triphenylphosphine (Ph_3P) has been the most studied nucleophilic species [5].

Phosphorus ylides resulted from the three-component reaction between dialkyl acetylenedicarboxylate and theophiline in the presence of phosphits ($(R'O)_3P$) were not stable and converted to diastereoisomeric *β*-amido phosphonates. Stabilized phosphoranes were synthesized from the reaction between dimethyl acetylenedicarboxylate and theophiline in the presence of triphenylphosphine. SCF-MO calculations at B3LYP/6-311+G* level of theory indicated that (2S, 3S) and/or (2R, 3R) diastereomers of phosphonates were about 18-28 kcal/mol more stable than (2R, 3S) and/or (2S, 3R) diastereomers.



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References:

[1] R. Noyori, Asymetric Catalysis in Organic Synthesis, (John Wiley & Sons, New York, 1994).
[2] R.Engel, Synthesis of Carbon-Phosphorus Bond, (CRC Press: Boca Raton, FL, 1988).
[3] J.G. Allen, Nature, **1978**, *56*, 272.
[4] C.D. Geraldine and Q. Jean-charles, Eur. *J. Org. Chem*, **2001**, 3031.
[5] B. E. Maryanoff, and A. B. Reitz, *Chem. Rev.*, **1989**, *89*, 863.

Synthesis of (4-bromo-3-(3,4-dibromophenyl) isoxazole-5-yl)methanol

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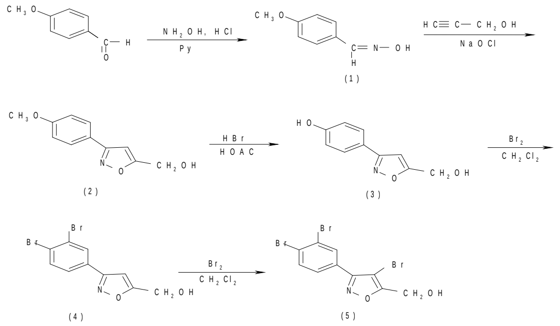
Isoxazole compounds which have various pharmacological, biological and industrial applications. Especially these compounds show the antivirus and anticancer activity [1,2]. It has been proved that they are effective in cure Parkinson and Alzheimer disease [3].

In present research four kinds of isoxazole and an oxime compound have been synthesized. At the first, 4-Methoxybenzaldehyde changed into 4-methoxybenzaldeidoxime (1) by increasing sodium hypochlorite to hydroxylamine hydrochloride in pyridine as a solvent, the compound 1 changed to nitrile oxide and [2+3] cycloaddition happened by using propargyl alcohol,as a result 3-(4- methoxy phenyl)isoxazole-5-yl)methanol (2) was prepared. At the rest of the research 4-(5- hydroxyl methyl) isoxazole-3-yl)phenol (3) was prepared by reaction of HBr and compound 2 and acetic acid. Also,(3-(3,4-dibromo phenyl)isoxazol-5-yl)methanol (4) was prepared by reaction of Br2 and compound 3 in CH2Cl2. In the final step compound (4) was added to Br2 and CH2Cl2, and (4-bromo-3-(3,4-dibromophenyl) isoxazole-5-yl)methanol (5) was prepared. The structure of synthesized compounds were confirmed by FT-IR and 1H NMR spectroscopies.



References:

[1] Shin, K.D.; Lee, M.-Y.; Shin, D.-S.;Lee,S.; Son, K.-H.; Koh, S.; Paik, Y.; Kwon, B.-M.; Han,D. C. J. *Biol. Chem.* **2005**, *280*, 41439.

[2] Sechi, M.; Sannia, L.; Carta, F.; Palomba, M.; Dallocchio, R.; Dessi, A.; Derodas, M.; Zawahir, Z.; Neamati, N. *Antiviral Chem.Chemother*. **2005**, *65*, 41.

[3] Garvey, D.; James, S.; George, P.; Mark, M.; Decker, W.; Williams, P. *J.Med. Chem*. **1994**, *37*, 8.

A mild and efficient method for the preparation of carbamyl chloride and the reaction of it with carboxylic acid.

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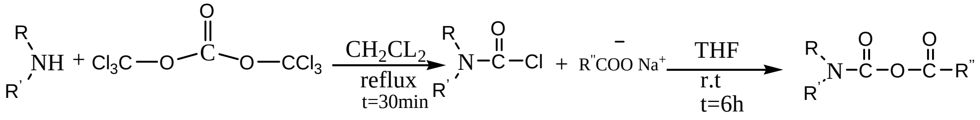
Over the last few years triphosgene [Bis(trichloromethyl)carbonat] has emerged as a versatile synthetic auxiliary for the synthesis of some important classes of organic compounds [1] this white crystaline compound has proved to be safe and advantageous in comparison with its gaseous congener, phosgene . In our recent communication [2] we wish to report the application of triphosgene as an acylating agent in the construction of carbamyl chloride from secondary amines, under very mild reaction condition. carbamyl chlorides are valuable intermediates they are useful for the preparation of various ureathan and urea . As a part of our on-going program on the synthesis and development of methodologies for carbamyl chloride, we herein report, for the first time, the reactin among carbamyl chloride and carboxylic asids, we have found that the result compounds possess potential anticancer activities and superior inhibitors of HIV[3].



R,R$'$,R$''$:alkyl,aryl

References:

[1] V. KGumaste.; B. M. Bahwal.; A.R.A.S.Deshmukh.*Tetrahedron lett*. 43, **2002**, 1345.
[2] D. Krishnasway.; B. M. Bahwal.; A. R. A. S. Deshmukh.*Tetrahedron lett*. 41, **2004**, 417.
Sikshi , S , A. ; Hultin , P. G. *J. Org. Chem* . **2006** , 71 ,5888

An Ab initio study on the thermodynamic functions of various backbone conformers for the HCO-GLY-L-ILE-GLY-NH_2 tripeptide

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Amino acid residues are the monomeric building blocks of proteins, A cogent problem is thus to build mathematical models capable of individually characterizing amino acids within peptides in order to help understand their biochemical affinities and to find similarity relationships between them [1].

Multi-dimensional conformational analysis (MDCA)-a systematic method to predict the location of all minima as input for ab initio calculations- was used to predict all topologically probable conformers.The Rama-Chandran PESs associated with a single amino acid has nine discrete possible conformations labeled as α_L, α_D, β, γ_L, γ_D, δ_L, δ_D, ε_L, ε_D [2].

Here, the conformational properties of the N- and C-terminal protected amino acids can mimic the conformational properties of polypeptides and protein segments, as these variables can be influenced by the orientation of the neighboring residues (see Fig1).

In this study, the HCO-GLY-ILE-GLY-NH_2 tripeptide was scanned about central residue, while keeping the other two residues in the β conformation and side chain dihedral angles were fixed on the gauche (-) state (χ_1, χ_2 = -60) .

We found 5 minima of the central Isoleusyn contain: $\beta_L\beta_L\beta_L$, $\beta_L\gamma_L\beta_L$, $\beta_L\alpha_D\beta_L$, $\beta_L\gamma_D\beta_L$, $\beta_L\varepsilon_D\beta_L$ and all of were optimized with frequency computation at HF/6-31G(d) level, thermodynamic properties such as: ΔE, ΔG, ΔH and ΔS Were obtained.

ΔE for five minima are : 0, 2.98, 6.80, 7.45 and 8.59, respectively.

Results show that $\beta_L\beta_L\beta_L$ conformation is the most stable among all of conformers that found.

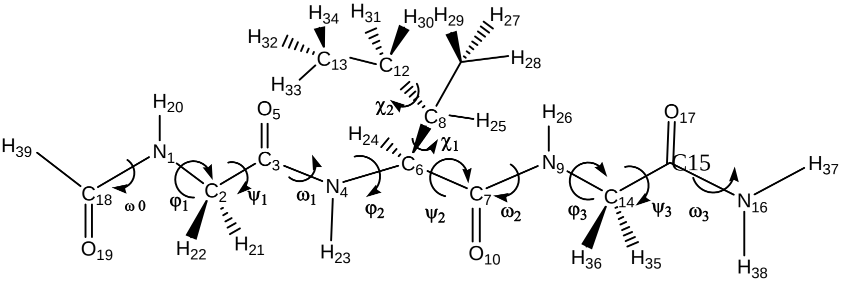

Fig1. The conformational structure of HCO-GLY-ILE-GLY-NH_2 tripeptide

References:

[1] Chass, G.A.; Sahai, M.A.; Law,J.M.S.; Csizmadia, I.G. *Quantom chem*. **2002**, *531*, 993,968.
[2] Ramachandran, G. N. *Biopolymers*. **1963**, *6*, 1494.

Puckering energy of 4-X-3-hydro,1-oxa-3-aza cyclopent-4-en-2-ylidene and their rings for M = C, Si, Ge, Sn and Pb (where X = H, F, Cl, Br and I)

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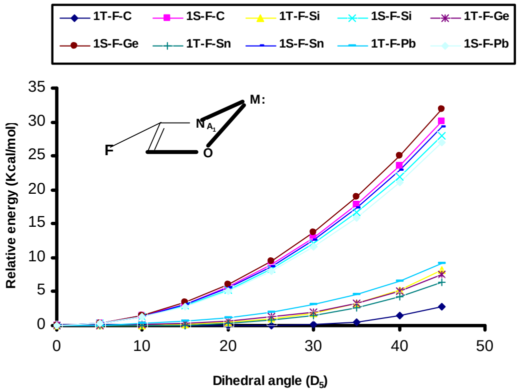
Divalent carbenes and their heavier analogues are intensely reactive, and the studies of their properties are often made through matrix isolation techniques [1]. Among the relatively more stable carbenes, the cyclic species, and their halogenated derivatives, have held a special place in the chemistry of divalent carbon intermediates.

In order to confirm global minima, for carbenes and their heavier analogues, energy surface studies are necessary [2], since puckering of cyclopent-4-en-2-ylidene rings and their heavier analogues may alter positions of the global minima. Puckering energy are presented for carbenes (which include 4-X-M-cyclopent-4-en-2-ylidene rings) as a function of dihedral angle N-M-O-C (for M = C, Si, Ge, Sn and Pb). The puckering energy appears higher for singlet states than their corresponding triplet states.



References:

[1] Gaspar, P. P. West, R. Rappoport, Z. Apeloig Y. (Eds.), Chemistry of Organic Silicon Compounds, vol. 2, Wiley, Chichester, **1997**, p. 2436.
[2] Kassaee, M. Z. Arshadi, S. Acedy, M. Vessally E. *J. Organometal. Chem.* **2005,** *690,* 3427.

Synthesis of novel spiropyrrolidines through multicomponent 1, 3 -dipolar cycloaddition reaction

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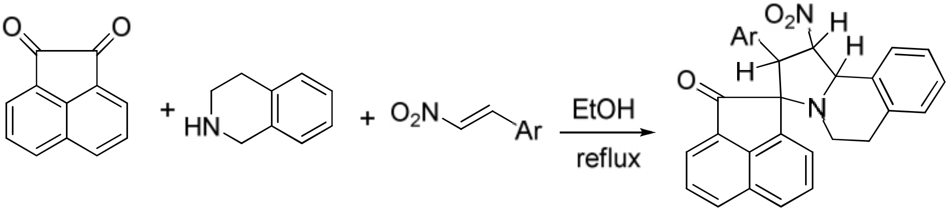
1,3-dipolar cycloaddition reaction of azomethine ylides with olefins offers a convenient one step route for the construction of a variety of complex pyrrolidine derivatives with stereogenic centers, because the reaction is usually concerted [1].

The reaction of azomethine ylides with various dipolarophiles results in highly substituted five membered nitrogen heterocycles [2]. Spiropyrrolidines have received considerable attention as a result of their biological activity, a number of which display interesting antimicrobial, antitumoral, and antibiotic properties [3].

We herein report the reaction of 1,2,3,4 tetrahydroisoquinoline with acenaphthenequinone leads to the formation of an azomethine ylide, which readily undergoes 1,3-dipolar cycloaddition with variety derivatives of nitro styrene to give a single cycloadduct, in a one pot three component process as evidenced by thin layer chromatography and mass, ^{1}H and ^{13}C NMR spectral.



References:

[1] *1,3-Dipolar Cycloaddition Chemistry*; Padwa, A., Ed.; Wiley: New York, **1984**; Vols. 1 and 2.
[2] Jayashankaran, J.; Manian, R.D.; Venkatesan, R.; Raghunathan, R. *Tetrahedron*. **2005**, 61, 5595.
[3] Kumar. S. S.; Manian, R.D.; Raghunathan, R. *Tetrahedron Letters*. **2006**, *47*, 829.

Flavonoid and an ester derivative isolated from *Galium verum* L.

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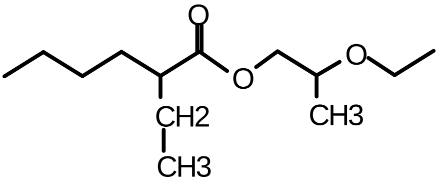
One of the most important of secondary metabolism products, occur in the plants are flavonoids. They have some very important medicine and biological especially antiradical, antioxidant and prevent cancer effects [1].

The genus *Galium* (Rubiaceae family and called Shir-Panir in Persian) is represented in Iran by about 50 species and *Galium verum* (yellow bedstraw) is one of this group plants [2].

In this study, a new ester derivative and a flavonoid have been isolated from the aerial parts of *Galium verum* and purified by column chromatography, TLC and preparative TLC techniques to yield two compounds. Those chemical structures were determined by ^{1}H-NMR, ^{13}C-NMR and IR spectroscopy techniques and were established as 2-ethoxypropyl 2-ethylhexanoate (1) and apigenin 4́- O- glycoside (2). The structure of the compounds was determined by spectroscopic techniques and by comparison with published data.



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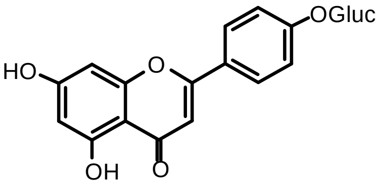

(2)

References:

[1] Picard, D. *Alt Med. Rev.*, **1996,** 1, 31 and 103.
[2] Mozaffarian, V.; *A Dictionary of Iranian Plants Names*, Farhang Moaser, Tehran, **2007**.

Preparation and characterization of some new assymmetrical Schiff bases as ligands and their complexes with Pb(II)

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Schiff base ligands have played an integral role in the development of coordination chemistry since the late nineteenth century. That metal complexes of these ligands are ubiquitous is a reflection of their facile synthesis and the accessibility of diverse structural modifications. A wide range of symmetric Schiff base ligands containing primary amine functions can be prepared in one step [1-3]. Several Schiff bases have recently been investigated as corrosion inhibitors for various metals and alloys in acid media. Due to the presence of the –C=N- group in the molecule, Schiff bases should be good corrosion inhibitors.Besides the imine group, substitution of different elements also affect the inhibition properties. Compounds containing functional groups with heteroatoms, which can donate lone pair electrons, are found to be very efficient as inhibitors against metal corrosion in many environments. Many *N*-heterocyclic compounds with polar groups and/or π-electrons are efficient corrosion inhibitors in acidic solutions. Organic molecules of this type can adsorb on the metal surface and form a bond between the *N*-electron pair and/or the π-electron cloud and the metal, thereby reducing the corrosion in acidic solutions [3-5]. The ligands L1, L2 and L3 were prepared by the condensation of 4-nitro-1,3-phenylendiamine with 2-hydroxybenzaldehyde, 5-bromo-2-hydroxybenzaldehyde and 2-nitrobenzaldehyde respectively in methanol medium. On refluxing the methanolic solution for 24 h yellow colouration were observed. The precipitates were collected by filtration and washed with methanol. All synthesized compounds were identified and confirmed by elemental analyses, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy. Lead(II) complexes with the new schiff bases ligands have been synthesized and characterized by CHN elemental analysis, IR, ^{1}H NMR, ^{13}C NMR spectroscopy.

References:

[1] A. Yamamoto, K. Morifuji, S. Ikeda, T. Saito, Y. Uchia, A. Misono, *J. Am. Chem.Soc.***1968**, *90*, 1878.
[2] J.C. Jenkins, M. Brookhart, *Organometallics,* **2003**, 22, 250.
[3] Z.Y. Yang, R. D. Yang, F.S. Li, K.B. Yu, *Polyhedron*, **2000**, *19*, 2599.
[4] S. Li, Y.G. Wang, S. Chen, R. Yu, S. Lei, H. Ma, D. Liu, *Corros. Sci.*, **1999**, *41*, 1769.
[5] S. Bilgic, N. Calıskan, *J. Appl. Electrochem.*, **2001**, *31*, 79.

Synthesis and characterization of carboxylic acid and esters labeled γ–pentamethine cyanine derivatives

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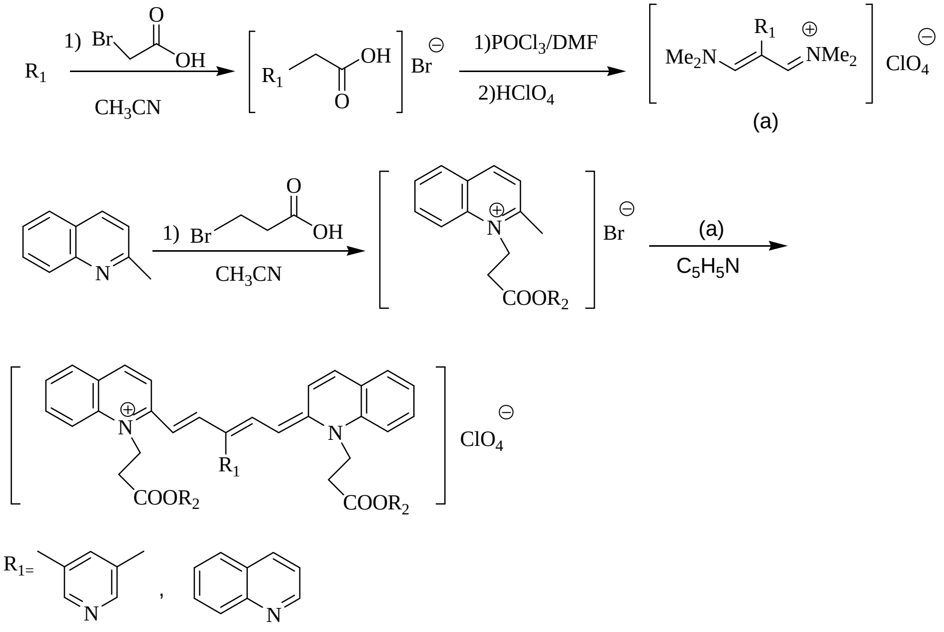
In recent years, many works have been carried out on the synthesis of cyanine dyes, among of these compounds, the pentamethine cyanin dyes are successfully used as fluorescent probes in the investigation of biological.

This work reports the synsthesis of qualidinium bromide derivatives including carboxylic acid and ester functional groups, which can react with vinamidinium salt deratives to construct different derivatives of cyanine dyes.The structure and purity of the prepared compounds, were confirmed by IR, NMR, mass spectroscopy and elemental analysis.



R_2=H,CH_3

Refrences:

[1] A. M. Mehranpour , S. Hashemina, R. Maghamifar, *Synth.Com.* **2009.**
[2] R. Knorr, J. *Org. Chem.* **1984**, *44*, 1288.

Synthesis of novel class of phosphono β-lactams

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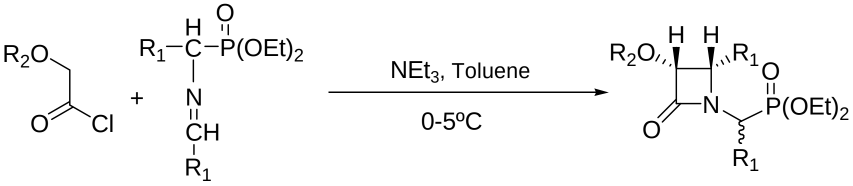
α-Functionalized phosphonics acids have attracted growing attentions because of application in the areas ofindustrial, medicinal, agricultural and synthesis intermediates. Among of α-functionalized phosphonics acids, a-amino phosphonic acids are an important class of compounds that exhibit a variety of interesting and useful properties [1].

On the other hand , the β-lactam skeleton is still hold a lot of attention due to the application in the most widely employed family of antimicrobial agents and elastease inhibitors [2].

However, In contrast to the widely studied of the synthesis of 1-aminophosphontes and β-lactam derivatives, relatively few papers heve reported on the synthesis of the compound with two functionalities in the same molecule. Thus, we decided to focus on the conjunction of two functionalities in the same mulcule that may afford powerful biological activity [3].

A novel class of β-lactam derivatives of 1-aminophosphonates is synthesized by staudinger [2+2] cycloaddition reaction of ketens with imines derived of 1-amino phosphonates.

The treatment of aromatic aldehyde with ammonia and diethyl phosphite [4] followed by reaction with ketenes, are generated from from the appropriate acyl chlorides and a tertiary amine, gives novel class of β-lactam derivatives of 1-aminophosphonates that probably afford powerful biological activity.



References:

[1] Ishiguri,Y.;Yamada,Y.;Kato,T.;Sasaki,M.;Mukai,K. Eur.Pat.Appl., EP82-301905,1982; Chem.Abstr. **1983**, *98*, 102686u.
[2] Redmore, D. *Chem. Rev*. **1971**, *71*, 315.
[3] Moonen, K.; Laureyn, I.; Stevens, C. V. *Chem. Rev*. **2004**, *104*, 6177.
[4] Kaboudin, B.; Moradi, K. *Tetrahedron Lett*. **2005**, *46*, 2989.

A facile one-pot synthesis of new [1,2,4]triazolo[5,1-*c*][1,2,4]triazin-4(8*H*)-one derivatives

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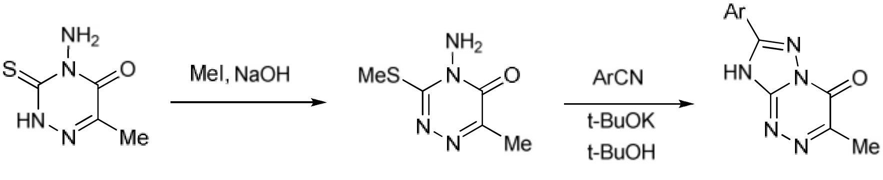
The 1,2,4-triazine ring system is a key component of commercial dyes, herbicides, insecticides and more recently pharmaceutical compositions [1,2]. Lamotrigine, a sodium channel blocker is the active component of Lamictal, which is in clinical use as an anticonvulsant therapy, contains the 1,2,4-triazine ring [3].

In connection with our interest in the synthesis of new heterocyclic compounds with potential biological activities[4, 5], we report herein the synthesis of some new [1,2,4]triazolo[5,1-*c*][1,2,4]triazin-4(8*H*)-ones **3**.

Our synthesis started from 6-methyl-4-amino-1,2,4-triazine-3-thione-5-one **1** which were converted to their thiomethyl derivatives using methyl iodide in the presence of sodium hydroxide. Reaction of the latter compounds with aryl nitriles in the presence of potassium t-butoxide in t-butanol under reflux gave the desired bicyclic products, [1,2,4]triazolo[5,1-*c*][1,2,4]triazin-4(8*H*)-ones **3**.



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References:

[1] Hurst, D. T. *Prog. Heterocyclic Chem.*, **1995**, *7*, 244.
[2] Groger, H.; Sans, J.; Gunther, T. *Chim. Oggi*, **2000**, *18*, 12.
[3] Adam, F. M.; Burton, A. J.; Cardwell, K. S.; *et. al. Tetrahedron Lett.*, **2003**, *44*, 5657.
[4] Heravi, M. M.; Montazeri, N.; Rahimizadeh, M.; *et. al. J. Heterocyclic Chem.*, **2005**, *42*, 1021.
[5] Heravi, M. M.; Montazeri, N.; Rahimizadeh, M.; Bakavoli, M.; Ghassemzadeh, M. *Monatsh. Chem.*, **2001**, *132*, 1225.

An efficient one-pot synthesis of 1,8-dioxo-octahydroxanthenes derivatives using heteropolyacid catalysts in water

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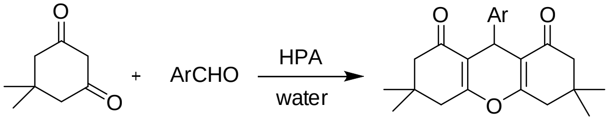
Xanthenes derivatives are important classes of organic compounds of a large number of naturally occurring, as well as synthetic derivatives, and occupy a prominent position in medicinal chemistry. Xanthene-based compounds have also been investigated for agricultural bactericide activity [1], anti-inflammatory effect [2] and antiviral activity [3]. Furthermore, these compounds have been used as dyes [4] in laser technology [5], pH-sensitive fluorescent materials for the visualization of biomolecular assemblies [6]. Thus many synthetic methods for preparing xanthenes derivatives have been reported. However, these methods are plagued by the limitation of prolonged reaction times, poor yield and side reactions of aldehydes.

The application of heteropolyacids as catalytic materials is growing continuously in the catalytic field [7]. In continuation of our investigations in organic synthesis [8], herein we describe simple and efficient protocol for the condensation reaction of aldehydes with 5,5-dimethyl-1,3-cyclohexanedione in water for the synthesis of 1,8-dioxo-octahydroxanthene derivatives using tungstophophoric acid hydrate catalyst under mild conditions. This efficient technique has the advantage to give xanthenes derivatives using a heteropolyacids catalyst in good to high yields, to be completed in short reaction times and to offer a simple product isolation procedure.



References:

[1] Hideo, T. Jpn. Tokkyo Koho JP 56005480, **1981**.

[2] Poupelin, J. P.; Saint-Ruf, G.; Foussard-Blanpin, O.; Narcisse, G.; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.* **1978**, *13*, 67.

[3] Lambert, R. W.; Martin, J. A.; Merret. J. H.; Parkes, K. E.; Thomas, G. J. PCT In. Appl. WO 97 06178.

[4] Banerjee, A.; Mukherjee, A. K. *Stain Technol*. **1981**, *56*, 83.

[5] Sirkecioglu, O.; Tulinli, N.; Akar, A. *J. Chem. Res. (s)* **1995**, 502.

[6] Knight, C. G.; Stephenes, T. *Biochem. J.* **1989**, *258*, 683.

[7] Mizuno, N.; Misono, M. *Chem. Rev.* **1998,** *98*, 199.

[8] (a) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M.; Boukherroub, R. *Synth. Commun.* **2010**, *40*, 8; (b) Mirza-Aghayan, M.; Khoshkameh Langrodi, M.; Rahimifard, M.; Boukherroub, R. *Appl. Organometal. Chem.* **2009**, *23*, 267.

Sulfonic acid functionalized ionic liquid as a recyclable and water tolerant-acidic catalyst for one-pot Friedlander quinoline synthesis

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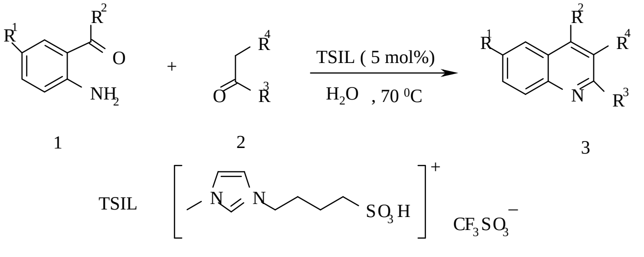
Quinolines are very important compounds partially because of their pharmacological properties which include wide applications in medicinal chemistry [1]. The Friedlander annulation is one of the simplest and most straightforward methods for the synthesis of poly substituted quinolines. This reaction is an acid or base catalyzed condensation followed by a cyclodehydration between 2-aminoaryl ketone and a second carbonyl compound including a reactive methylene group [2]. Although, modified methods employing lewis or br¢nsted acids have been reported for the synthesis of quinolines [3], the development of water stable acidic catalyst for quinoline synthesis is quite desirable.

One of the most remarkable features of ionic liquids is that the yields can be optimized by changing the anions or the cations. Recently, sulfonic acid functionalized ionic liquids were used as solvent-catalyst for several organic reactions [4]. We herein report the one pot domino approach for the synthesis of quinoline derivatives in Friedlander manner using TSIL as a catalyst. These ILs are miscible in water, and their homogeneous system is readily separated from the reaction product, combining advantages of both homogeneous and heterogeneous catalysis. In this reaction, the catalyst plays a dual role; it ensures an effective condensation and cyclization of 2-aminoaryl ketone with second carbonyl group and it also promotes the aromatization to the final product. Various types of quinolines from 2-aminoaryl ketones and *β*-ketoesters/ketones were prepared in 85-98% yields using the catalytic system of SO_3-H functionalized ionic liquid/H_2O. More importantly, the catalyst could be easily recycled for five times without loss of much activity. This would be a novel application of SO_3-H functionalized ionic liquid acting as a catalyst for the Friedlander quinoline synthesis.



References:

[1] Maguire, M. P.; Sheets, K. R.; Mcvety, K.; Spada, A. P.; Zilberstein, A. *J. Med. Chem.* **1994**, *37*,
[2] 2129.
[3] Contelles, H. M.; Mayoral, E. P.; Samadi, A.; Carreiras, M.; Soriano, E. *Chem. Rev.* **2009**, *109*, 52.
[4] Hu, Y. Z.; Zang, G.; Thummel, R. P. *Org. Lett.* **2003**, *5*, 2251.
[5] Zhao, G. Y.; Jiang, T.; Gao, H. X.; Han, B. X.; Huang, J.; Sun, D. H. *Green Chem.* **2004**, *6*, 75.

An efficient one-pot synthesis of tetrahydro-chromeno[4,3-b]chromene-6,8-dione and -dioxa-indeno[2,1-b]phenanthrene-6,8-dionederivatives under solvent free condition

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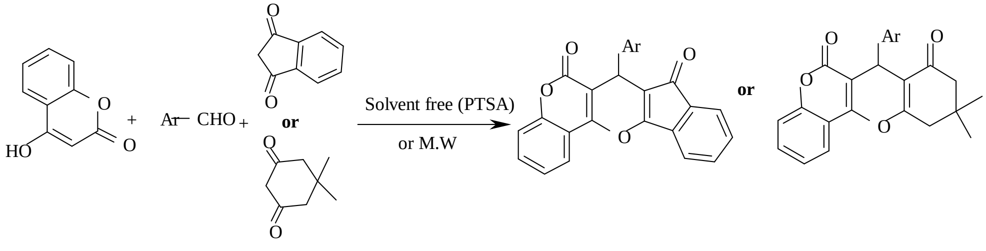
In the mainstream of current interest, multi-component processes have recently gained considerable economic and ecological interest as they address fundamental principles of synthetic efficiency and reaction design. Multi-component reactions (MCRs) have been proven to be a very elegant and rapid way to access complex structures in a single synthetic operation from simple building blocks and show high atom economy and high selectivity [1]. As a one-pot reaction, MCRs generally afford good yields and are fundamentally different from two-component reactions in several aspects [2], and permitted rapid access to combinatorial libraries of organic molecules for efficient lead structure identification and optimization in drug discovery [3].

Over the past decade, various advanced sequential MCRs have been developed where 1,3-dicarbonyl derivatives are important synthetic intermediates due to its multiple functionalities that can be involved either as nucleophilic or electrophilic species in a large variety of synthetic transformations. we have developed a solvent free, efficient and environmentally benign methodology for the synthesis of 7-(aryl)-10,10-dimethyl-7,9,10,11-tetrahydro-chromeno[4,3-b]chromene-6,8-diones, and 7-(aryl)-7H-5,13-dioxa-indeno[2,1-b]phenanthrene-6,8-diones by a one-pot, multi-component reaction.



References:

[1] Ugi, I. *Pure Appl. Chem*. **2001**, 73, 187 and references therein.
[2] Armstrong, R. W.; Combs, A. P.; Tempest, P. A.; Brown, S. D.; Keating, T. A. *Acc. Chem. Res*. **1996**, 29, 123.
[3] Tempest, P. A. *Curr. Opin. Drug Discov*. Dev. **2005**, 8, 776.

Synthesis and characterization of novel mocrocycle compound and study of liquid-liquid extraction of heavy metals with this compound

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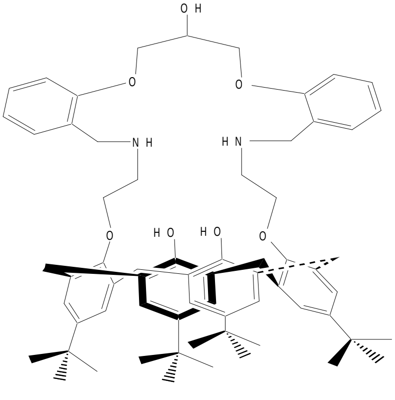
Calixarenes are macrocyclic molecules in which four phenolic unites are linked via methylene bridges at their ortho positions. Furthermore, the most significant feature of the chemistry of these molecules is their ability to bind selectively alkali and alkaline earth cations.[1,2] Recently a wide variety of calixarene derivatives with donating or nondonating side-arms attached to the lower rim have been designed and synthesized in order to alter the original cation-molecule binding ability and selectivity Indeed, calixarene derivatives with additional binding sites at the lower rim give much enhanced binding ability and altered selectivity in compare with the parent calixarenes.[3]

In the present research,we have synthesized and Characterized Mocrocyclice ligand of Calix[4]arene Reduced form adition of 1,3-diaminocalix[4]arene and dialdehid, (Scheme 1).All of the reaction products were Characterized by spectral methods .in orther to at next sextion We have studied Liquid-Liquid Extraction of Heavy metal ions with this compound.



References:

[1] Zhang, W. C., Huang, Z. T., *J. Chem. Soc. Chem.* **1997**.
[2] Gutsche. C. D., Calixarenes, Reviesed, *Royal, Soc, Chem,* Cambridge U.K. **1998** .
[3] Khandar, A. A. Hosseini- Yazdi, S. A, *Polyhedron*, **2003.**

Baker's yeast catalyzed synthesis of nitrogen heterocycles in aqueous medium

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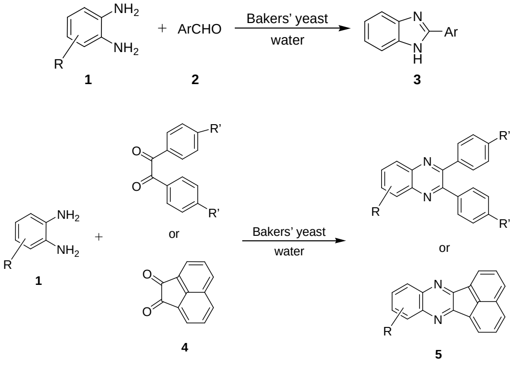
The benzimidazole moiety is found in various bioactive compounds having antiviral, antiulcer, antihypertension and anticancer properties. General methods for the synthesis of benzimidazoles involve treatment of 1,2-phenylenediamines with carboxylic acids or various derivatives under strongly acidic conditions or with aldehydes followed by oxidation [1]. Despite efficiency of some published methods, some of these suffer from one or more disadvantages such as high reaction temperature, prolonged reaction time, toxic solvents, etc. Therefore, development of mild and practical synthetic routes to 2-substituted benzimidazoles continues to attract researchers' attention.

Quinoxaline derivatives are an important class of nitrogencontaining heterocycles in medicinal chemistry. For example, quinoxaline is a part of various antibiotics such as echinomycin, levomycin, and actinoleutin that are known to inhibit growth of gram positive bacteria, and are active against various transplantable tumors [2].

Baker's yeast among microorganisms is inexpensive, versatile and its growth does not require the assistance of microbiologist [3].

Herein, we wish to report synthesis of benzimidazole and quinoxaline derivatives via reaction of 1,2-phenylenediamines with different aromatic aldehydes and 1,2-diketones using bakers' yeast at room temperature.



References:

[1] Gravatt, G.; Baguleyi,B.C.; Bigi, F.;Wilson, W.; Denny, W.A. *J. Med.Chem.* **1994**, *37*, 4338.
[2] Bailly, C.; Echepare , S.; Gago, F; Waring , M.J.; *Anti- Cancer Drug Des.* **1999**, *15*, 291.
[3] Servi, S. *Synthesis* **1990,** 1.

MCM-41-SO_3H as a mild, efficient and reusable nanoreactor for the one pot synthesis of 1,8-dioxo decahydroacridines under solvent free condition

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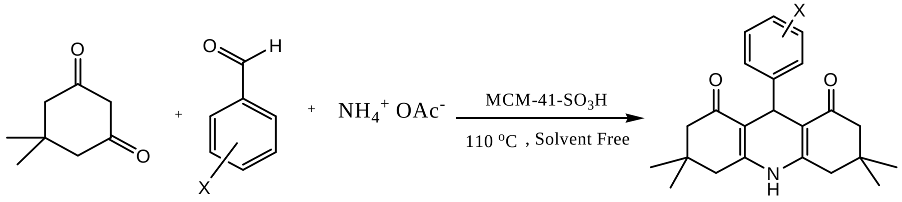
In recent years more attractive possibilities have been arisen by the development of various new silica materials with ordered structure. One of the best-known examples is MCM-41, which is a structurally well-ordered mesoporous material with a narrow pore size distribution between 1.5 and 10 nm, depending on the surfactant cation and a very high surface area up to 1500 m^2 g^{-1}.[1] Very recently MCM-41-SO_3H has been prepared and used as a Brønsted acid, by our research group for some acid catalyzed reactions. We have employed MCM-41-SO_3H as an effective nanocatalyst in the one-pot multicomponent synthesis of 1,8-dioxo decahydroacridines which are well known polyfunctionalized 1,4-dihydropyridine derivatives that are widely prescribed as calcium ß-blockers and used for the treatment of hypertension and defibrillation. In addition acridines are important compounds reported to possess antitumour, cytotoxic, anticancer, antimicrobial, anti-MDR, antibacterial and fungicidal activity. Reportedly, the conventional synthesis of 1,4-dihydropyridine derivatives was performed in organic solvent such as HOAc, CH_3CN, DMF, and water .[2] We have developed a simple and efficient methodology for the high-yielding synthesis of 1,8-dioxo decahydroacridines by one-pot three-component coupling of dimedone, aromatic aldehydes and ammonium acetate in the presence of MCM-41-SO_3H as catalyst under the solvent-free conditions. This catalyst is highly efficient, easily available, economical, operationally simple, and requires mild reaction conditions. Also the products were formed in excellent yields with short reaction times. This method offers several advantages, such as omitting toxic solvents, very simple work-up procedure and needs no chromatographic methods for purification of the products. The starting materials are also inexpensive and commercially available.



References:

[1] W. Zhang, T. R. Pauly, T. J. Pinnavaia, *Chem. Mater.* **1997**, *9*, 2491.
[2] T. S. Jin, J. S. Zhang, T. T. Guo, A. Q. Wang, T. S. Li, *Synthesis*, **2004**, 2001.

Cobalt (II) chloride accelerated one-pot three-component synthesis of α-aminophosphonates under solvent-free conditions at room temperature

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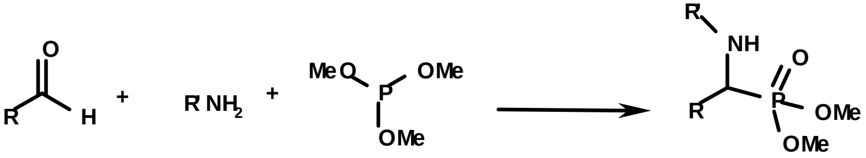
The synthesis of α-aminophosphonates as naturally occurring α-aminoacids has attracted a significant interest by organic chemists in recent years. They have been attracting a good deal of attention ever since the first compounds with a phosphorus–carbon bond were detected among natural products. One-pot three-component condensation of aldehydes, amines, and dimethylphosphite or trimethylphosphite is the most convenient method for the preparation of these compounds. In this context some methods and catalysts have been reported [1-3]. Although, these approaches are satisfactory for synthesis of α-aminophosphonate, the harsh reaction conditions, expensive reagents, use of toxic organic solvents and long reaction times limit the use of these methods.

Due to extending our interest in the development of practical, safe, and environmentally friendly procedures for several important organic transformations [4] we now describe a simple, general and efficient protocol for the synthesis of α-aminophosphonates *via* three-component reactions of aldehydes, amines, and trimethyl phosphite using catalytic amounts of cobalt chloride under solvent-free conditions at room temperature.



This method offers some advantages in term of simplicity of performance, solvent free condition, and low reaction time. Several examples illustrating this novel and general method for the synthesis of α-aminophosphonates are carried out. The structures of all products were confirmed using physical and spectral (NMR and IR) data.

References:

[1] Hosseini-Sarvari, M. *Tetrahedron* **2008**, *64*, 5459.
[2] Ranu, B. C.; Hajra, A. *Green Chem.* **2002**, *4*, 551.
[3] Kaboudin, B.; Sorbiun, M. *Tetrahedron Lett*. **2007**, *48*, 9015.
[4] Karimi-Jaber, Z.; Amiri, M. *Heteroatom Chem*. **2010**, *21*, 96.

Volatile compounds identification in rice (*Oryza sativa* L.) using $F_{2:3}$ families

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Rice is a major food commodity throughout the world. Scented or aromatic rice is popular in Asia and has gained wider acceptance in Europe and the United States and because of their aroma, flavour and texture, aromatic varieties fetch a higher price in the rice market than do the non-aromatic rice varieties. Because of the economic and culture impact of aromatic rice and need to enhance their productivity without sacrificing their quality traits, plant breeders and food chemists have been interested in determining the volatile compounds associated with aromatic rice. Yajima et al [3] and Kim [2] identified over 100 compounds using cooked rice, which included hydrocarbons, alcohols, aldehydes, ketones, acids, esters, phenols, pyridines, pyrazines and other compounds. Kim [2] reported that hydrocarbon compounds were not significantly different between aromatic and non-aromatic rices but aromatic rice had higher levels of alcohol, aldehydes and ketones, acids and other compounds. There is a blend of various volatiles which imparts pleasant odor to raw or cooked non-aromatic or aromatic rice. A population of F3 families of rice derived from the cross between aromatic MousaTarom and high product 304 varieties analyzed for their aromatic and volatile compounds. The gas chromatography (Shimadzu GC-17A) analysis was conducted with fused silica capillary DBX-5 column (95% phenyl and 5% polydimethyl siloxane); 0.25 mm internal diameter, 0.25 µm film thickness, and 30 m length .

Ground samples were prepared by grinding of 20 g portions of rice grains in a household coffee grinder for 30 s. About 0.7 g of each sample in a 10 ml vial with aluminum cap equipped with silicon septum was heated at 50oC for 15 min using ultra-sonic bath after adding 300 µl double distilled water, and the headspace gas was introduced into the commercial PDMS fiber for HS-SPME (head space- solid-phase micro extraction) for 30 min [1]. The desorption was conducted at 260oC for 2 min. The column temperature was programmed by holding at 40oC for 30 minutes and then increased to 200oC at rate of 4oC/min and then increased to 270oC at rate of 35oC/min and holding at this temperature for 3 min. The flow rate (1mL/min) of the carrier gas, helium (99.999% purity), was split 1:1 (by volume) at the end of the capillary. The ion source and the GC-MS transfer line temperature was 260°C. Mass spectrometry (MS) was performed by means of an MS- QP5050A in tandem with the capillaries described above [1]. 14 volatile compounds were identified in the present study which included benzene acetic acid, beta-elemene, camphene, camphor, butyl-cyclobutane, cyclopropane, d-Limonene, heptadecane, hexadecane, isobornyl acetate, nonyl aldehyde, pentadecane, silicate anion tetramer, and tetradecane.

References:

[1] Ghiasvand, A.R.; Setkova, L.; Pawliszyn J. *Flavour Fragr. J.* **2007**, 22, 377.
[2] Kim, C. Y. Ph.D. thesis submitted to Hungnam National University, Aejeon, Korea. **1999**, 112.
[3] Yajima, I.; Yanai, T.; Nakamura, M. *Agric Biol. Chem.* **1978**, 42, 1229.

Facile, convenient and regioselective direct *ortho* acylation of phenols and naphthols catalyzed by Alumina supported- Lewis acids under free solvent and microwave conditions

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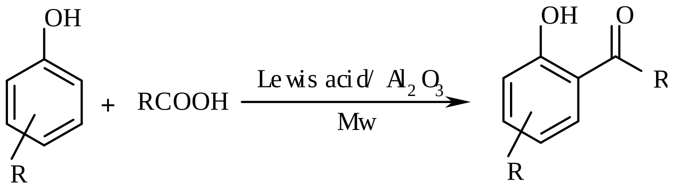
Acylation is one of the fundamental reactions in organic chemistry and can be carried out by wide variety of reagents [1]. Acyl groups play an important role in the chemistry of biomolecules [2], they are fragments of important natural products, such as; peptides [2,3] or modified peptide bond isoesters and also they serve as protecting groups. Ortho-hydroxyarylketones, as a variety of compounds with acyl group, are also important synthetic intermediates in the synthesis of biologically active compounds such as; chalcones, flavanones, naphthoquinones and pesticides.

Lewis acids have been used as catalysts for an enormous variety of organic reactions, including electrophilic additions to C-C multiple bonds, hydroborations, and acylation of aryl compounds.

In this research, we examined the ortho-acylation of hydroxyaryl compounds with organic acids, in the presence of alumina supported-Lewis acids under microwave irradiation and atmospheric pressure conditions. The acylation were performed without solvent and short reaction times to efford the corresponding ortho-acylated hydroxyaryl compounds in high yields.



References:

[1] M.A. Ogliaruso, J.F. Wolfe, in: S. Patai (Ed.), *In the Chemistry of Acid Derivatives*: Supplement B, Part 1, Interscience, Chichester **1979**, pp.267–490.
[2] R.J. Simmonds, *Chemistry of Biomolecules*: An Introduction, The Royal Society of Chemistry, Cambridge **1992.**
[3] J.H. Clark, A. R´Enson, K. Wilson, *Catal. Lett*. **1999**, 61, 51.

Using of lipase as a biocatalyst in esterification reaction

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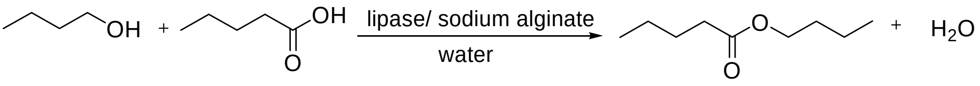
Lipases are ubiquitous enzymes which are found in most organisms from the microbial, plant and animal kingdom [1]. The high versatility of lipases, recognized as the most important group of biocatalysts in biotechnology [2] allows their applications in different industries like food, detergent, pharmaceutical, leather, textile, cosmetic and paper [3]. This group of enzymes is a powerful tool for catalyzing not only hydrolysis, but also esterification and transesterification reactions involving water insoluble esters [4]. Esterification reaction is one of the most applicable reactions in organic chemistry.

Herein, we have reported preparation of n- butyl pentanoat by using n- butanol and pentanoic acid and lipase as catalyst [5]. This reaction is free of any organic solvent and lipase was immobilized on a polymer and can be recovered and recycled for 10 times.

Determination of the best conditions for this reaction (such as temperature, volume of acid and alcohol and concentration of enzyme) is one of the aimes of this research work.



References:

[1] Jaeger, KE.; Ransac, S.; Bijkstra, BW.; Colson, C.; van Heuvel, M.; Misset, O. *FEMS Microbiol Rev*. **1994**, *15*, 29.
[2] Hasan, F.; Shah, A.; Hameed, A. *Enzyme MicrobTechnol*. **2006**, *39*, 235.
[3] Houde, A.; Kademi, A.; Leblanc, D. *Appl Biochem Biotechnol.* **2004**, *118*, 155.
[4] Brockman, H.; Momsen, W.; Tsujita, T. *JAOCS.* **1988**, *65*, 891.
[5] Jane, E.S.; Silva and Paulo, C.; Jesus. *Annals of the Brazilian Academy of Sciences*. **2003**, *75*(2), 57.

Synthesis and characterization of photoactive polyamides bearing triaryl imidazole pendent

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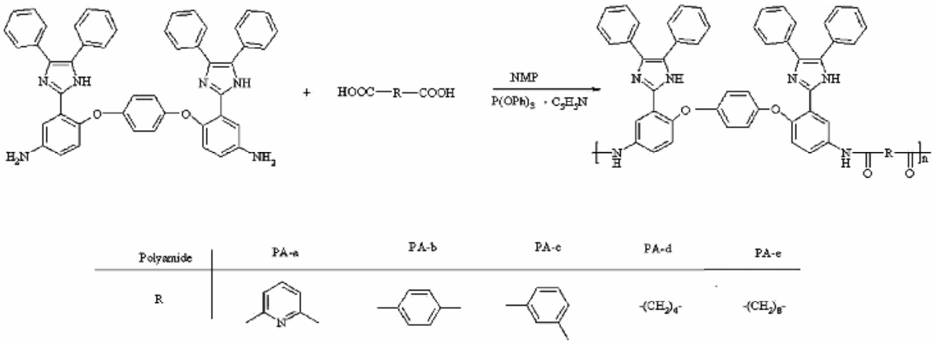
A new symmetrical diamine containing triaryl imidazole pendent group was successfully synthesized by the nucleophilic substitution reaction of hydroquinone with 2-(2-chloro-5-nitrophenyl)-4, 5-diphenyl-1H-imidazole (I). A series of polyamides (PAs) were prepared from the diamine monomer and various dicarboxylic acids via phosphorylation polyamidation. These PAs are readily soluble in many organic solvents; their inherent viscosities ranged from 0.58 to 0.89 dL/g and gave tough and flexible films by solution-casting. They had useful levels of thermal stability associated with relatively high T_gs (186-278 °C), 10% weight loss temperatures in excess of 355 °C, and char yields at 600 °C in air up to 67%. All the polymers emitted in dilute (0.2 g/dL) DMAc solution (425-495), with photoluminescence (PL) quantum yields in the range 0.14-0.28. The chemiluminescence activity of polyamides was studied in the presence of peroxyoxalate[1-3].



References:

[1] Ghaemy, M.; Barghamadi, M. *J. Appl .Polym.Sci.* **2008**, *110*, 1730.
[2] Ghaemy, M.; Alizadeh, R.; Behmadi, H. *Eur. Polym. J.* 2009, *45*, 3108.
[3] Ghaemy, M.; Barghamadi, M. *J. Appl .Polym.Sci.* **2009**, *114*, 3464.

Unexpected synthesis of *N*-methylbenzo[d]isoxazolium hydroxides under microwave irradiation conditions

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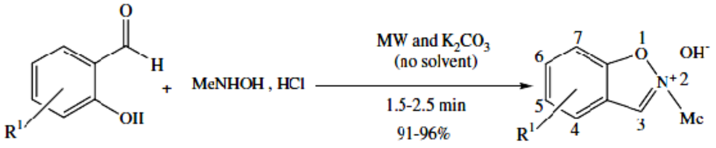
The early reports of the application of commercial microwave (MW) ovens for the synthesis of small organic molecules appeared in 1986 [1]. MW heating, along with solventless system, has been widely used for many organic reactions in our laboratory. Nitrones have a positive charge on the nitrogen atom which can be delocalized between the nitrogen atom and the α-carbon atom. The extent of the delocalization is naturally influenced by substituents on the α-carbon and the nitrogen. They behave as electrophiles toward organometallics and as 1,3-dipoles in cycloadditions.

In our continuing interest in the development of solvent-free systems for the sake of environmentally benign chemical transformations, we explored the use of microwave-assisted synthesis of nitrones through K_2CO_3 catalyzed condensation reaction of monosubstituted hydroxylamines with salicylaldehydes under solventless conditions [2].

In this article, we wish to disclose our results for a new, efficient, and expeditious cyclization of (Z)-N-methyl-C-(2-hydroxyphenyl)- nitrones, as an intermediate to N-substituted benzo [d]isoxazolium hydroxides , in excellent yields. The formation of these fused isoxazolium salts is very interesting from a biological and chemical point of view.

Our approach is based on the condensation reaction of N-methylhydroxylamine and N-enylhydroxylamine with 2-hydroxybenzaldehyde derivatives in the presence of potassium carbonate.



References:

[1] Giguere RJ, Bray TL, Duncan SM,Majetich, G. *Tetrahedron Lett* **1986,** *27*, 4945.
[2] Valizadeh H, Gholipur H, Zarrebin R, Amiri M, Sabzi, M. *Phosphorus Sulfur* **2008,** *183*, 1552.
[3] Zaho Q, Han F, Romero, DL. *J Org Chem* **2002,** *67*, 3317.

Synthesis and characterization of some water-soluble derivatives of phenanthroline and investigation of their interaction with anionic surfactant

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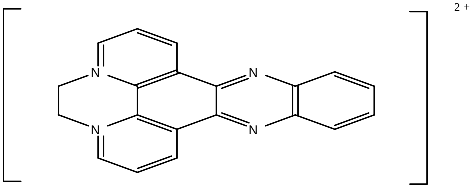
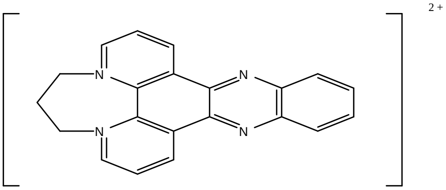
Dipyrido-[2,3-a:2',3'-c]-phenazine (dppz) is known to act as a ligand in a number of transition metal complexes. These complexes were found to show high binding affinity to the biological structures such as DNA and antitumor applications [1]. Whereas as a planar aromatic molecule dppz itself is virtually insoluble in aqueous solution and so is not convenient for biological issues. Recently some water-soluble derivatives of dppz have be obtained through diquaternization of pyridyl nitrogens with 1,2-dibromoethane which leads to eldppz [2]. The present work is aimed to modify the procedure and to obtain other water-soluble derivatives of dppz. So, dicationic propylene substituted dppz has been synthesized as different salts {[pldppz](ClO_4^{-})$_2$ and [pldppz](PF_6^{-})$_2$} , *via* a modified procedure in good yield. All compounds were characterized by UV-Vis, FT-IR and NMR spectroscopy. Beside synthetic issues a further aim of this work is to study the interaction of these compounds with micelles, as simplest models of cell membranes. Several spectral methods, such as Uv-Vis, Fluorescence and RLS (Resonance Light Scattering) have been exploited for investigation interaction of eldppz and pldppz with SDS [3].



ethylene-bipyridyldiylium- Phenazine (eldppz)



propylene-bipyridyldiylium- Phenazine (pldppz)

References:

[1] Phillips, T.; Haq, I..; Meijer, A. J. H.; Adams, H.; Thomas, J. A. *Biochemistry-us*. **2004,** *43,* 13657.
[2] Phillips, T.; Rajput, C.; Twyman, L.; Haq, I.; Thomas, J. A. *Chem. Commun*. **2005,** *12*,4327.
[3] Scolaro, L. M.; Donato, C.; Romeo, R. *Inorg. Chim. Acta.* **2000,** *300***,** 987.

Synthesis of dialkyl 2-alkanoyloxy (or benzoyloxy)-3- [alkylimino(1*H*-pyrrol-2-yl)methyl]succinates and 2,5-diaminofurans derivative via an isocyanide-based four- component reaction

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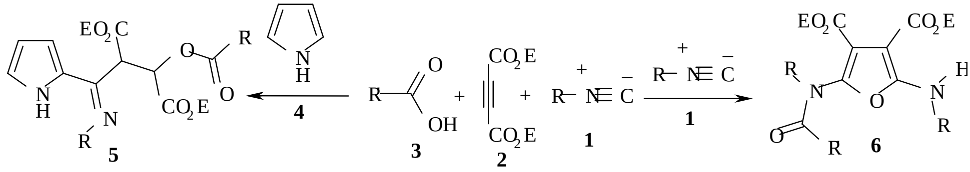
A multicomponent reaction (MCR) is a process in which three or more easily accessible components are combined together in a single reaction vessel to produce a final product displaying features of all inputs and thus offers greater possibilities for molecular diversity per step with a minimum of synthetic time and effort. MCRs constitute an especially attractive synthetic strategy since they provide easy and rapid access to large libraries of organic compounds with diverse substitution patterns [1].

A large and important class of MCRs are the isocyanide based multicomponent reactions (IMCRs), first of them was introduced in 1921 by Passerini. One of the most utilized multicomponent reactions is Ugi reaction. Synthesis of α-acylamino amides is achieved by reacting aldehydes, primary amines, carboxylic acids and isocyanides. Recently, three-component reaction between isocyanides, electron-deficient acetylenic esters and organic compounds containing at least one acidic NH, OH or CH group have been reported [2].

In the course of our works on the reaction between isocyanids and acetylenic esters [3], here we wish to report the four component reaction between cyclohexyl isocyanide, acetylenic esters, carboxylic acids and pyrrole. Thus, the reaction between isocyanide **1**, dialkyl acetylenedicarbixylate (DAAD) **2**, carboxylic acid **3** and pyrrole **4** leads to tetraaddacts **5** in good yields. Also four-component reaction between two equivalents of an isocyanide **1**, DAAD and aliphatic carboxylic **3** acids at room temperature leads to 2,5-diaminofuran **6** derivatives in good yields.



References:

[1] Domling, A. *Chem. Rev*. **2006**, 106, 17.
[2] Yavari, I.; Djahaniani, H.; Nasiri, F. *Tetrahedron* **2003**, 59, 9409.
[3] Anary-Abbasinejad, M.; Mosslemin, M. H.; Anaraki-Ardakani, H.; Tahan, S. *J. Chem. Res.* **2006**, 306.

Selective recognition of ATP in water

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Among many phosphate anions, adenosine triphosphate (ATP) is a multifunctional nucleotide that is most importantas a molecular currency of intracellular chemical energy transfer [1,2].

We have recently introduced a Calixarene Dimers as Host Molecules for oligophosphates, which can bind these molecules in polar solvents such as methanol [3]. In order to obtain extremely powerful binders, which can complex ATP in water, we have synthesized a new generation of water soluble Calix[4]arene – dimer according to the following reactions.

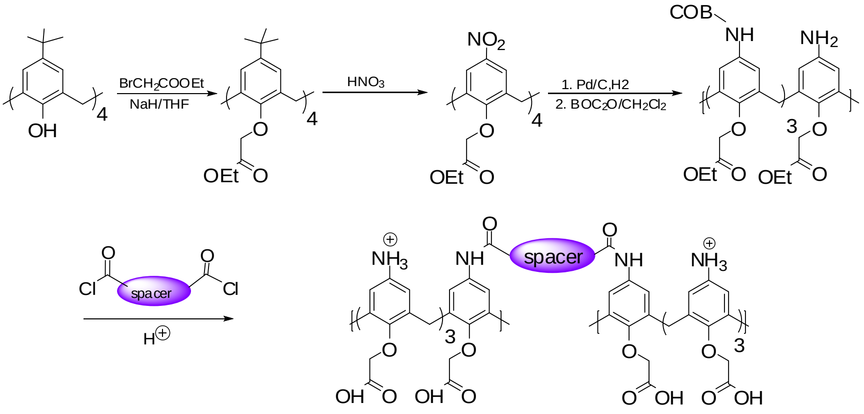

Fig. 1: Synthesis of Calix[4]arene – Dimer

The first binding experiments showed that the synthesized Dimer can bind selectively ATP in water.

References:

[1] Prakash P., Neelakandan.; Hariharan, M.; Ramaiah, D.; *Org. Lett.*, **2005**, *7*, 5765.
[2] Amilan Jose, D.; Mishra, S.; Ghosh, A.; Shrivastav, A.; Mishra, S.; Amitava, D.; *Org. Lett.*, **2007**, *9*, 1979.
[3] Zadmard, R.; Taghvaei-Ganjali, S.; Gorji, B.; Schrader, T.; *Chem. Asian J.* **2009**, *4*, 1458.

[Omim]Cl ionic liquid as the catalyst for synthesis of quinoxalinone derivatives

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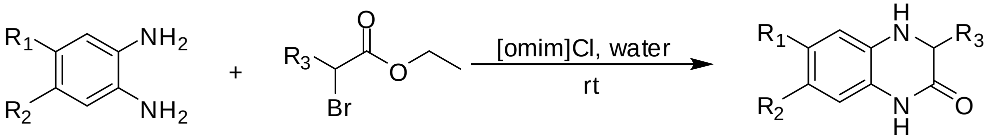
Within the family of biologically active heterocyclic templates, the quinoxalin-2-ones moiety has received much attention in recent years as an important pharmacophore unit in numerous biologically active compounds. Such compounds are reported to possess diverse biological activities including inhibition of aldose reductase and kinases. Moreover, the quinoxalinone skeleton is also used as an intermediate in designing novel quinoxalinone derivatives with the potential of biological properties such as anticancer, antimicrobial, antifungal, antithrombotic, and anxiolytic activities [1-3].

In present work, we have investigated the use of 1-methyl-3-octylimidazolium chloride ionic liquid as catalyst and water as solvent for the facile homogenous synthesis of a series of substituted quinoxalinones by the nucleophilic displacement reactions between *o*-phenylenediamines and ethyl 2-bromoalkanoates without the use of any base or any other additives. The reaction was found to proceed under mild conditions at room temperature with excellent yields (85-97%). The ionic liquids were recycled and reused for at least six times without significant loss of activity. The effect of temperature was also investigated. No by–products were observed as monitored by the ^{1}H NMR and GC spectra of the products.



Reference:

[1] Sanna, P.; Carta, A.; Loriga, M.; Zanetti, S.; Sechi L. II Farmaco. **1999,** *54,* 161.
[2] Carta, A.; Sanna, P.; Gherardini, Laura.; Usai, Donatella.; Zanetti, Stefania. II Farmaco. **2001,** *56,* 933
[3] Honore, T.; Drejer, J. Science. **1988,** *241,* 701.

Reaction of 2-nitro trans-cinnamaldehyde with acetylenic esters in the presence of triphenylphosphine

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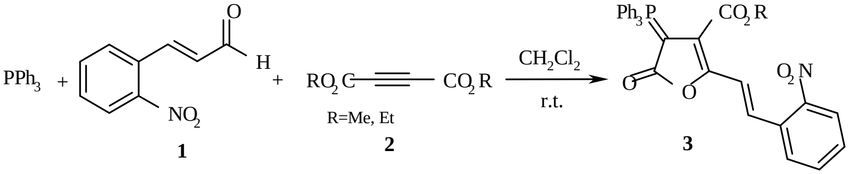
In recent years, there has been increasing interest in the synthesis of organophosphorus compounds, that is, those bearing a carbon atom bond directly to a phosphorus atom. A large number of methods have appeared describing novel syntheses of organophosphorus compounds [1-3]. Here we report a simple, one-pot, three-component synthesis of methyl 2- [(E)- 2-(2-nitrophenyl)vinyl]-5-oxo-4-(phosphoranylidene)-4,5-dihydrofurun-3-crboxylate **3**. Thus, the reaction of triphenylphosphine and *trans*- 2- nitro cinnamaldehyde **1** in the presence of dialkyl acetylenedicarboxylate **2** leads to compound **3**.



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The structures of **3a-b** were assigned on the basis of their elemental analysis and ^{1}H, ^{13}C NMR and Mass spectra data as well as from the IR spectra.

References:

[1] Hudson, H. R. *The Chemistry of Organophosphorus Compounds: Primary, Secondary and Tertiary Phosphines and HeterocyclicOrganophosphorus (III) Compounds*. Wiley, New York, **1990**, *Vol.* I, PP 386-472.
[2] Engel, R. *Synthesis of Carbon-Phosphorus Bonds,* CRC Press, Boca Raton, FL, **1998.**
[3] Cadogan, J. I. G. *Organophosphorus Reagents in Organic Synthesis,* Academic Press, New York, **1979.**

Trimerization reaction of benzylnitrile

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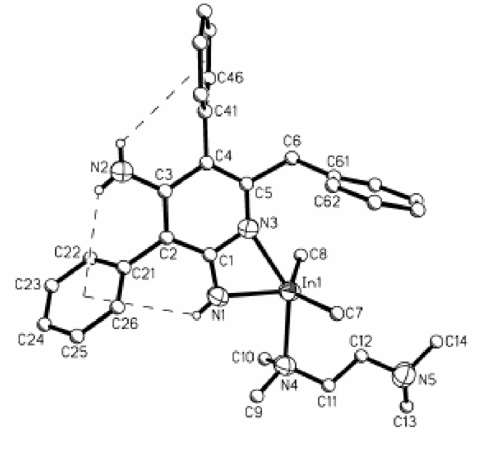
In previous works it was been able to elucidate the reaction between the metalanes MMe_3 (M = Al, Ga, In) and acetonitrile [1-3]. In the case of Al, Ga, and in, the generation of a six membered heterocycle with evolution of methane was observed.

In this work the reaction of phenylacetonitrile with $InMe_3$ in boiling toluene in a molar ratio of 3:1 leads to a trimerization of the nitrile with evolution of methane. The presence of CsF accelerates the reaction.

The six methylene protons from the three benzylnitrile molecules undergo different reaction pathways. One proton was abstracted for the formation of methane, three protons were used in hydrogen shifts for the generation of NH_2 and NH functions, and two protons are still present in a methylene group. All carbon atoms of the pyridine ring are substituted.



References:

[1] Kopp, M. R,; Neumueller, B. *Z. Anorg. Allg. Chem.* **1999**, *625*, 739.
[2] Kopp, M. R,; Kraeuter, T. ; Dashti-Momertz, A. ;Neumueller, B. *Organometallics*. **1998**, *17*, 4226.
[3] Kopp, M. R,; Neumueller, B. *Z. Anorg. Allg. Chem.* **1999**, *625*, 1246.

Silica gel factionluzed by pipyrazin solfunic acid as an efficient catalyst for the formylation and acetylation of alcohols under heterogeneous conditions

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O-Formylation and *O*-Acetylation could be the method of choice for protecting an alcoholic group in a complex synthetic sequence [1]. Although various formylation and acetylation reagents have been reported previously, there are still serious limitations for the preparation of formats or acetates due to the drastic reaction conditions, the use of uncommon reagents, formation of undesirable or toxic by-products, and the application of expensive catalysts for preparation of formylating agents and thermal instability of the reagents.

In this article we prepared Silica gel factionluzed by pipyrazin solfunic acid, and used as a recyclable catalyst for the formylation and acetylation of alcohols. These reactions were accomplished by the mixing of hydroxyl groups with ethyl formate or ethyl acetate in the presence of this catalyst at room temperature in good to excellent yields.

$$\mathrm{ROH} + \mathrm{CH_3CO_2Et} \text{ or } \mathrm{HCO_2Et} \xrightarrow[\text{RT}]{\text{Silica gel factionluzed by pipyrazin solfunic acid}} \mathrm{CH_3CO_2R} \text{ or } \mathrm{HCO_2R}$$

References:

[1] Iranpoor, N.; Firouzabadi, H.; Jamalian, A.; *Tetrahedron Lett.***2005**, *46, 7963.*

Synthesis and characterization of poly (4-vinyl pyridine)-$AlPO_4$ nanocomposite as a new organic-inorganic hybrid catalyst and it's application in the basic reaction

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The Knoevenagel condensation is a C=C double bond formation reaction between carbonyl compounds and active methylene compounds and widely employed to synthesize intermediates of fine chemicals. In the Knoevenagel subset the nucleophile is generated by a base reacting with a relatively acidic methylene group. The homogeneous reactions suffer disadvantages in separation and regeneration. The replacement of liquid base by solid heterogeneous base catalysts, enable the easy separation and recycling of the catalyst from the reaction mixture [1]. Design and preparation of organic–inorganic hybrid catalysts based on molecular sieves have been gaining large interest, which are achieved by functionalizing the porous system [2].

AlPOs are the porous analogues of aluminum phosphate and are built from alternating AlO_4^- and PO_4^+ tetrahedra. Some of these materials have the framework topologies of known zeolites, but many have novel Structures, in some cases, such as VPI-5, $AlPO_4$-11, -14, -15,-17, -21 [3,4].

In this work, we wish to report the synthesis of poly (4-vinyl pyridine)-$AlPO_4$ nanocomposite by in situ polymerization of 4-vinyl pyridine (4VP) in the presence of AlPOs. Aluminophosphate molecular sieves were synthesized from aqueous hydrothermal systems with various reactions gel mixture and in the presence of organic amine templating agents. The large surface area of $AlPO_4$ causes this novel compound to act as an efficient basic catalyst. The basic catalytic activity of this novel organic-inorganic hybrid was tested for Knoevenagel condensation reaction in water as solvent. The Catalysts were characterized by XRD, XRF, SEM, FT IR, BET and TPD techniques. The effect of reaction temperature, reaction time, amount of catalyst, solvent, different aldehydes, acidic methylene reagents and molar ratio of Al/P for synthesis of $AlPO_4$ was investigated.

In different basic catalyst tested, excellent yields (100%) and short reaction time (10 min) at room temperature was achieved. It was observed that the activity of the catalyst just decreased to 90% after performing five regeneration processes.

References:

[1] Climent, M.J.; Corma, A.; Iborra, S.; Velty, A. *J. Mol. Catal .A.* Chem. **2002**, *182*, 327.
[2] Wight, A.P.; Davis, M.E. *Chem. Rev*. **2002**, *102*, 3589.
[3] Pastore, H.O.; Coluccia, S.; Marchese, L. *Annu. Rev. Mater. Res.* **2005**, *35*, 351.
[4] Jiang, F.Y.; Tang, Z.K.; Zhai, J.P.; Ye, J.T.; Han, J.R. *Micropor. Mesopor. Mater.* **2006**, *92*, 129.

Substituent study on 1, 3-D.C. of substituted nitrones with ethylene: a Hammett study via DFT

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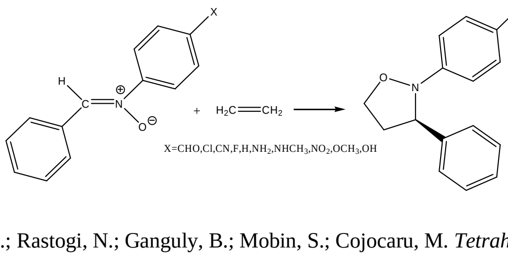
1,3-Dipolar cycloadditions offer suitable one-step routes for the production of a variety of five-membered heterocycles [1]. High stereospecificity/stereoselectivity associated with these reactions makes them synthetically significant [2]. 1,3-dipolar cycloaddition (1,3-D.C.) reaction of nitrones with alkenes is one of the most valuable reactions in organic synthesis since the hetero-atoms such as nitrogen and oxygen are pharmacologically important [3]. In this research we extended our studies to discover the effect of substituent on the 1,3-D.C. reaction of substituted nitrones with ethylene by applying the Hammett equation. Originally, Hammett study was based on ionizations of m- and p-XC6H4Y, where'log $k/k_o=\rho\sigma$' was introduced as 'the Hammett equation'. In this equation k_o is the rate constant for X=H and k is the rate constant for the group X, ρ is a constant for a given reaction under a given set of conditions, and σ is a constant characteristic of the group X. The structures of reactants, TSs and products were optimized using B3LYP method and 6-31+G* basis set with Gaussian 03 computational package. To confirm the nature of the stationary species and evaluate the activation energy barriers, frequency calculations were carried out. For minimum state structures, only real frequency values and for the transition states, only a single imaginary frequency value was accepted. The Berny algorithm method was used to locate the TSs. The following equation shows our results of a linear regression for log (k_X/k_o) versus Hammett σ_p constant.

$$\log\frac{k_x}{k_o} = 1.2173\sigma_p + 0.0421 \quad \text{and} \quad R^2=0.9657$$

The Hammett ρ value of 1.2173 was obtained in the reaction of nitrones with ethylene. The correlation coefficient between log (k_x/ko) and σ_p □is 0.9657. Positive Hammett ρ value indicates that the electron withdrawing groups moderately increase the rate of this reaction.



References:

[1] Namboothiri, I.; Rastogi, N.; Ganguly, B.; Mobin, S.; Cojocaru, M. *Tetrahedron.* **2004**, *60*, 1453.
[2] Sridharan, V.; Muthusubramanian, S.; Sivasubramanian, S.; Polborn, K. *Tetrahedron*. **2004**, *60*, 8881.
[3] Phomkeona, K.; Takemoto, T.; Ishima, Y.; Shibatomi, K.; Iwasa, S.; Nishiyama, H. *Tetrahedron.* **2008**, *64*, 1813.

Substituent effect on Baeyer–Villiger oxidation of substituted benzaldehydes with ethaneperoxidacid: A Hammett study via DFT

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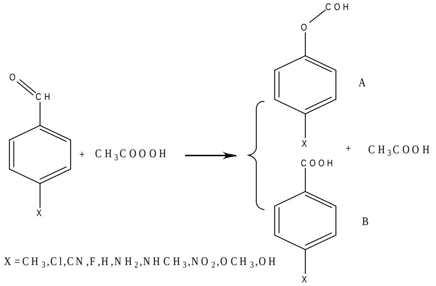
In the presence of acid catalysts, peroxy compounds are capable of oxidizing ketones by insertion of an oxygen atom into one of the carbon-carbon bonds at the carbonyl group [1]. The reaction is called the Baeyer–Villiger oxidation, and became one of the most well-known and widely applied reactions in organic synthesis [2]. The mechanism involves a sequence of steps that begins with addition to the carbonyl group, followed by peroxide bond cleavage with migration to oxygen [3].

In this research we extended our studies to discover the effect of substituent on the Baeyer–Villiger oxidation reaction of substituted benzaldehydes with ethaneperoxic acid by applying the Hammett equation. Originally, Hammett study was based on ionizations of m- and p-XC6H4Y, where'log $k_x/k_o=\rho\sigma$' was introduced as 'the Hammett equation'. In this equation k_o is the rate constant for X=H, k is the rate constant for the group X, ρ is a constant for a given reaction under a given set of conditions, and σ is a constant characteristic of the group X. The structures of reactants and products were optimized using B3LYP method and 6-311++G** basis set with Gaussian 03 software. To confirm the nature of the stationary species and evaluate the thermodynamic parameters, frequency calculations were carried out. The following equation, show our results of a linear regression for log(k_x/ko) versus Hammett σ constant.

$$\log\left[\frac{k}{k_o}\right]_A = 2.22\sigma - 0.697 \text{ and } R^2=0.92 \quad \& \quad \log\left[\frac{k}{k_o}\right]_B = 0.41\sigma - 0.035 \text{ and } R^2=0.87$$

The Hammett ρ values of 2.22 and 0.41 were observed for product A and B, respectively. The correlation coefficient between log(k_x/ko) and σ are 0.92 and 0.87, in the channel A and B. Positive Hammett ρ value indicates that the electron withdrawing groups moderately increase the rate of this reaction.



References:

[1] Brink, G.-J. ten.; Arends, I. W. C. E.; Sheldon, R. A. *Chem. Rev*. **2004**, *104*, 4105.
[2] Meneses, L.; Araya, A.; Pilaquinga, F.; Fuentealba, P. *Chemical Physics Letters*. **2008**, *460*, 27.
[3] Carey, F.A.; Sundberg, R.J. Advanced Organic Chemistry, Fifth Edition, Part B.

Synthesis and characterization of lower rim C-silylated calix[4]arene

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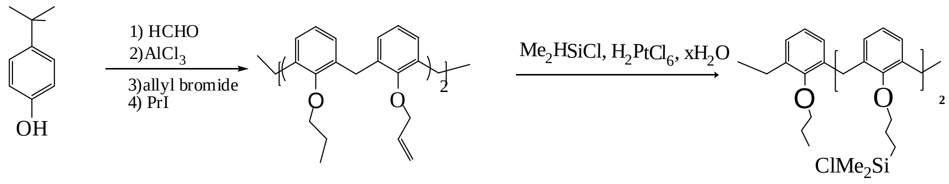
In the last two decades, interest in calixarenes in analytical and separation chemistry have been increased because of their ability to form reversible complexes with neutral as well as charged molecules [1].

Calixarenes substituted with silyl groups have potential for the recognition of anionic spices.

In the literature a few C-silylated calixarenes, specially in cone conformastion, which has a great and suitable cavity for molecular recognition, have been reported, thus in this work, we have synthesized and fully characterized a new C- silylated calix[4]arene , which has silyl –group at the lower rim [2]. For silylating of calix[4]arene we have used catalytic hydrosilylation according to the following methods [3].



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All of the molecules (2-6) were characterized with the common methods in organic chemistry (1H-NMR, ^{13} C- NMR, Ms, ...).

References:

[1] Gutsche, C. D. In *Calixarenes, Monographs in SupramolecularChemistry*; Stoddart, J. F., Ed.; Royal Society of Chemistry: Cambridge, **1989**; Vol. 1.

[2] Billo, F.; Musau, R. M.; Whiting, A. *ARKIVOC* **2006**, 199.

[3] Magdalena ´Sliwka-Kaszy´nska, K. Jaszczołt,D.Witt, J. Racho´n, Journal of Chromatography A **2004**, *1055*, 21.

A simple synthesis of ferrocenyl bis-amides by a Ugi four-component reaction

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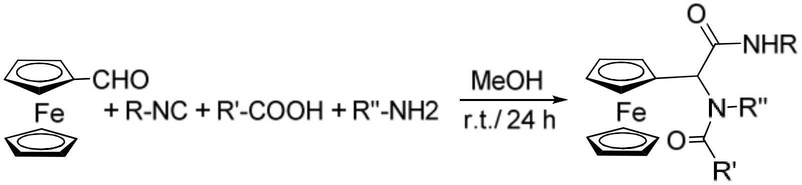
Ferrocene derivatives are characterized by their ability to make metal-centred redox systems to generate oxidized or reduced form of different properties, therefore they have been widely employed in various fields such as: molecular recognition as biosensors [1], in asymmetric catalysis [2], in polymer science as redox active polymers and dendrimers [3], in nonlinear optics [4], in synthesis of complex photochemical systems [5] and in pharmacology [6]. Successful attempts of the synthesis of amino acids bearing ferrocene moiety have been also performed [7]. Ferrocenyl amino acids found their application in food chemistry as a possible substitute for phenylalanine in the commercial sweetener aspartame [8].

The reactions using ferrocenecarboxaldehyde as starting material have recently attracted the interest of the synthetic community because the formation of different ferrocene derivatives can be expected depending on the specific conditions and structure of the building blocks [9].

Considering the above reports, the development of new and simple synthetic methods for the efficient preparation of the new ferrocene derivatives will be a beneficial and interesting challenge. In this paper, we report an efficient synthesis of ferrocenyl bis-amides by an Ugi four-component reaction using ferrocenecarboxaldehyde.



References:

[1] Constable, E. C. *Angew. Chem. Int. Ed. Engl.* **1991**, *30*, 407.
[2] Richards, C. J. ; Locke, A. J. *Tetrahedron: Asym.* **1998**, *9*, 2377.
[3] Hudson, R. D. A. *J. Organomet. Chem.* **2001**, *637*, 47.
[4] DiBella, S. *Chem. Soc. Rev.* **2001**, *30*, 355.
[5] Ferry-Forgues, S.; Delaraux-Nicot, B. *J. Photochem. Photobiol. A: Chem.* **2000**, *132*, 137.
[6] Top, S.; Vessieres, A.; Cabestaing, C.; Laios, L.; Leclerq, G.; Prorot, C.; Jaouen, G. *J. Organomet. Chem.* **2001**, *637*, 500.
[7] Schlögl, K. *Monatsh. Chem.* 1957, *8*, 601.
[8] H. Brunner, W. König, B. Nuber, *Tetrahedron: Asym.* **1993**, *4*, 699.
[9] Yousefi, R.; Azizi, N.; Saidi, M. R. *J. Organomet. Chem.* **2005**, *690*, 76.

Synthesis of fully functionalized dipeptide-bound chitosan *via* six-component reaction

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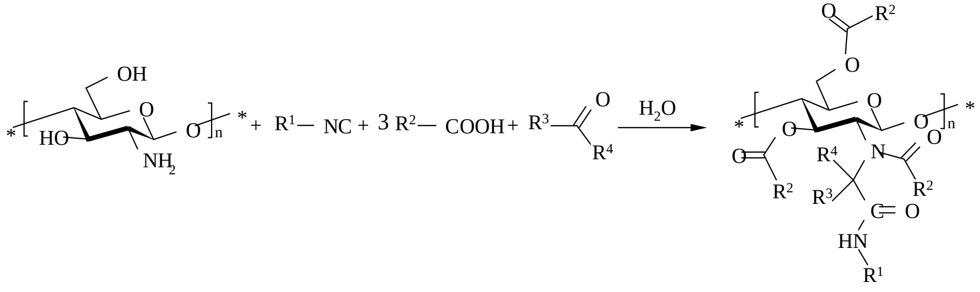
Chitosan, a natural linear biopolyaminosaccharide is obtained by alkaline deacetylation of chitin, which is the principal component of protective cuticles of crustaceans such as crabs, shrimps, prawns, lobsters [1]. It displays interesting properties such as biocompatibility, biodegradability and its degradation products are non-toxic, non-immunogenic and non-carcinogenic [2]. Therefore, chitosan has prospective applications in many fields such as biomedicine, waste water treatment, functional membranes and flocculation [3]. Recently, much attention has been paid to utilize chitosan in biomedical applications, for example, as a wound dressing, skin grafting template, hemostatic agent, hemodialysis membrane and drug delivery vehicle, etc also after chemical modification [4].

In connection with our recent interest aimed at the development of efficient protocols for the preparation of biologically active molecules via isocyanide-based multicomponent reactions [5,6], in this report the efficient synthesis of some novel fully functionalized dipeptide-bound chitosans *via* six-component simultaneously Ugi reaction/estrification is described.



References:

[1] Ravi Kumar, M. N. V.; Muzzarelli, R. A. A.; Muzzarelli, C.; Sashiwa, H.; Domb, A. J. *Chem. Rev.* **2004**, *104*, 6017.
[2] Sashiwa, H.; Aiba, S. *Prog. Polym. Sci.* **2004**, *29*, 887.
[3] Jayakumar, R.; Prabaharan, M.; Reis, R. L.; Mano, J. F. *Carbohydrate Polymers* **2005**, *62*, 142.
[4] Agnihotri, S. A.; Aminabhavi, T. M. *J. Control. Release* **2004**, *96*, 245.
[5] Teimouri, M. B.; Tayyebi, A. *J. Chem. Res.* **2010**, 178.
[6] Teimouri, M. B.; Mansouri, F. *J. Chem. Res.* **2010**, 330.

Synthesis of pH sensitive nano colloidal polyaniline in presence of ultrasonic irradiation

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Polyaniline (PANI) is well-studied and is the preeminent electrically conducting organic polymer with the potential of a variety of applications such as in batteries, microelectronics, antistatic coatings, sensors, and actuators [1]. Notwithstanding the immense potential, the applications remain quite below the potential due to its poor solubility in most organic solvents and insolubility in water [2]. The preparation of colloidal PANI is one of the attractive alternatives to overcome its poor processability due to its insolubility in common organic solvents and water [3]. In this work, primarily nano polyaniline was synthesized by chemical oxidative polymerization under ultrasonic irradiation in an inert atmosphere.

The estabilized Polyaniline particles system is based on poly (styrene–alt–maleic anhydride) (PSMA) copolymer and its derivatives. therfore, nano colloidal Polyanilines were prepared by enzymatic polymerization of using hydrolyzed PSMA, PSMA was reformed by isopropylamine, or PSMA was reformed by poly (ethylene glycol) (PEG) as the steric stabilizers and ammonium persulfate, oxidant and HCl as dopant in presence of ultrasonic irradiation.

As can be seen in the (fig.1) the nano particles of Polyaniline colloidal were obtained in this work.

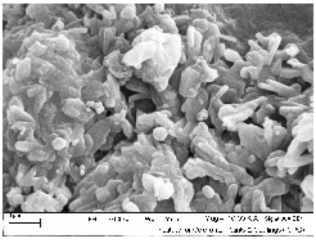

Fig .1 SEM images of nano Polyaniline colloidal

References:

[1] Arizmendi, L.; Del-Angel, M.; and Romero-Garcia, J. *Langmuir.*, **2007**, *23*, 8.
[2] Li, G.; Martinez,C.; Semancik, S. *JACS.*, **2005**, *127*, 4903.
[3] Sarma, T.K.; Chattopadhyay, A. *J. Phys. Chem. A.*, **2004,** *108*, 7837.

Simple and catalyst-free three-component method for the synthesis of spiro[indenopyrazolopyridine-indoline]diones

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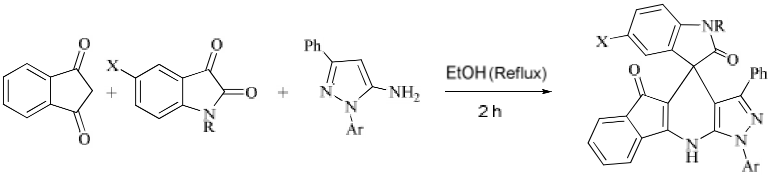
In the past few years, combinatorial methods using multi-component reactions have been closely examined as a fast and convenient solution for the synthesis of diverse classes of compounds [1]. Multi-component reactions (MCRs) have been steadily gaining importance in synthetic organic chemistry [1, 2].

Indole and indoline fragments are important moieties of a large number of natural biologically active compounds [3], and some of indolines, spiro-annulated with heterocycles in the 3-position, have shown high biological activity [4].

In the current work, we have elaborated a new multi-component reaction which gives wide access to spiro[indeno[1,2-*b*]pyrazolo[4,3-e]pyridine-indoline]diones production via three-component reaction of pyrazol-5-amines with 1,3-indandione and isatins. The advantages of this procedure are mild reaction conditions, high yields of products, operational simplicity and easy work-up procedures.



References:

[1] (a) Tietze, L. F. *Chem. Rev.* **1996**, *96*, 115; (b) Dömling, A. *Chem. Rev.* **2006**, *106*, 17.

[2] (a) Dömling, A.; Ugi, I. *Angew. Chem., Int. Ed.* **2000**, *39*, 3168; (b) Ugi, I. *Angew. Chem., Int. Ed. Engl.* **1982**, *21*, 810.

[3] Sundberg, R. J. *The Chemistry of Indoles*; Academic: New York, NY, **1996**.

[4] (a) Joshi, K. C.; Chand, P. *Pharmazie* **1982**, 37; (b) Da-Silva, J. F. M.; Garden, S. J.; Pinto, A. C. *J. Braz. Chem. Soc.* **2001**, *12*, 273; (c) Abdel-Rahman, A. H.; Keshk, E. M.; Hanna, M. A.; El-Bady, Sh. M. *Bioorg. Med. Chem.* **2004**, *12*, 2483. (d) Zhu, S.-L.; Ji, S.-J.; Yong, Z. *Tetrahedron* **2007**, *63,* 9365.

The synthesis and characterization of 5-(bromomethyl)-4-bromo-3-(3-bromo-4-methoxyphenyl)-isoxazole

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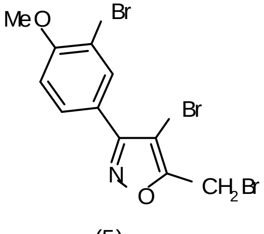
Isoxazole derivatives have been used as key intermediates in organic syntheses and investigated intensively for the last several years because of their biological activities [1]. In spite of this wide spectrum of properties, the number of tri-substituted isoxazoles by different functional groups, useful as scaffolds in the synthesis of many differently tri-substituted isoxazole, is scarce [2].

This present research work describes the synthesis of new compound of isoxazole family. First, 4-methoxybenzaldehyde (**1**) was transformed to 4-methoxybenzaldoxime (**2**) by using NH_2OH in pyridine. The in situ generated nitriloxide from reaction between **2** and NaOCl, was reacted with propargyl alcohol to produce 3-(4-methoxyphenyl)-5-hydroxymethyl isoxazole (**3**) in a cycloaddition procedure. Then, twice bromination of compound **3** with bromine in CH_2Cl_2 produced 3-(3-bromo-4-methoxyphenyl)-4-bromo-5-hydroxymethyl isoxazole (**4**). The required bromo-derivative of the synthesized isoxazole (**5**) was obtained from reaction of (**4**) and PBr_3-mediated bromination in high yield.

The structure of all the synthesized compounds was characterized and confirmed by FT-IR and NMR spectroscopy techniques.



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References:

[1] Lee, Y.; Kim, B. H. *Med. Chem. Lett.* **2002**, *12*, 1395.
[2] Ruano, J.; Fajardo, C.; Martin, M. R. *Tetrahedron* **2005**, *61*, 4363.

New silane-containing aromatic polyimides with reduced dielectric constant

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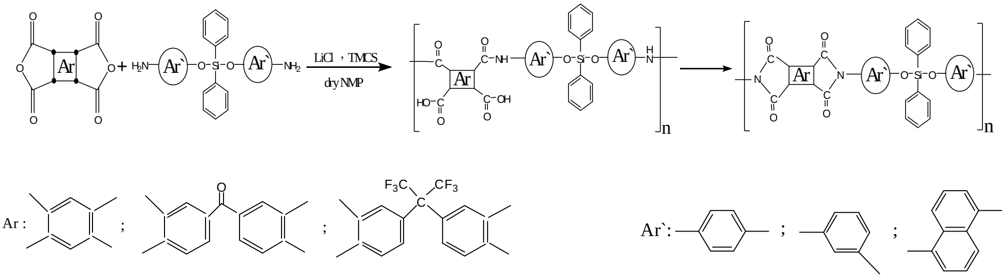
Recently rapid developments in the area of thermo-resistant engineering plastics have been observed. Polyimide (PI) materials have attracted attentions due to their high thermal stability, solvent resistance, good mechanical strength, excellent dimensional stability, low coefficient of friction, low dielectric constant, and resistance to creep and wear [1-2]. However, they are generally insoluble and infusible. The main structural modifications to attain processable polyimides have been carried out by introducing flexible spacers and also bulky substitutes such as pendent aryl rings into their backbone [3-4]. In this study, three silane diamines were prepared by the reactions of 4-aminophenol, 3-aminophenol, and 5-amino-1-naphthol with dichlorodiphenylsilane in the presence of triethylamine. The related silane-containing polyimides were prepared by two-step polycondensation reactions of these diamines with three different aromatic dianhydrides. Incorporation of bulky groups and also low-polarizing siloxane units into the polymer backbones effectively improved the solubility of related thermally stable polyimides and decreased the dielectric constant of them, whereas avoid of weak linkages and incorporation of aromatic structures led to high thermal stability of the polyimides. Structure-property relations of the prepared polyimides were also studied.



References:

[1] Liaw, D.; Lin, S.; *J Polym Sci Part A: Polym Chem*. **2002**, *40*, 2066.
[2] Mehdipour-Ataei, S.; Sarrafi, Y.; Hatami, M.; Akbarian-Feizi, L.; *Eur Polym J*. **2005**, *41*, 491.
[3] Ghosh, M.K.; Mittal, K.L.; Polyimides: Fundamentals and Applications. New York: Marcel Dekker, Inc., 1996.
[4] Sroog, C.E.; Endrey, A.L.; Abramo, S.V.; Berr, C.E.; Edwards, W.M.; Olivier,K.L.; *J Polym Sci Part A: Polym Chem.* **1965**, *3,* 1373.

Synthesis and evaluation of six novel antibacterial fibers disperse dyes based on sulfonamides

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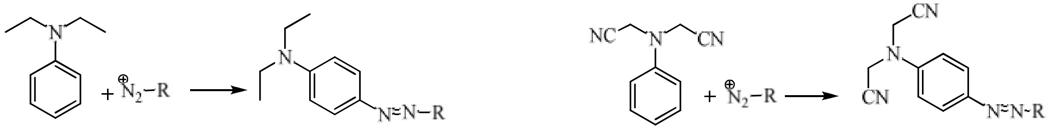
Bacteria are microorganism that grows up in humidity conditions causing many problems. One of the methods to terminate growing of them is the use of antibacterial agents. Sulfonamides are the chemicals that imparting antibacterial properties to a media where they apply. In order to combine the strength of antibacterial activities of sulfonamides and their capability of being diazotized, three novel antibacterial azo desperse dyes based on sulfonamides were synthesized and evaluated. To do this, three sulfonamides viz. amino-N-(4-methyl-2-pyrimidinyl) benzene sulfonamide (sulfadiazine (SFD)), 4-amino-N-(4-dimethyl-2-pyrimidinyl)benzene sulfonamide(sulfamerazine (SFMr)) and 4-amino-N-(4,6-dimethyl-2-pyrimidinyl)benzene sulfonamide (sulfadimidine (SFDd)) were diazotized [1] using HCl and $NaNO_2$ to produce diazonium salts The resultant diazonium salts were then coupled with the coupling component such as N, N-diethyl aniline and N, N-dicyano ethyl aniline to produce the dyes [2]. The synthesized dyes were filtered off, purified and characterized by ^{1}HNMR, FT-IR and Uv-Vis spectrophotometer. The results from spectral data are strongly indicating that the research work was successful. The novel dyes were then applied on cellulosic fabric by conventional method and finally their antibacterial activity assessments were carried out by AATCC 147 test procedure [3]. Bathochromic shift and solvatochromic shift were examined for above-mentioned dyes [4]. The synthesis route for the dyes is shown in the following.



R = SFD,SFMr,SFDd

Reference:

[1] Nagaraja, P.; R. Sunitha, K.; A. Vasantha, R .*J. Pharmaceutics & Biopharmaceutics*., **2002**, 53, 187.
[2] R. Maradiya, H. *J. Saudi chemical Society***, 2010**, 14, 77.
[3] Kawabata, A.; A. Tailor, J.*J. Carbohydrate Polymers*, **2007**, 67, 375.
[4] R. Kaafarani, B.; Wex, B.; Strehmel, B. *J. Photochem. Photobiol. Sci*., **2002**, 1, 942.

Synthesis and evaluation of three novel antibacterial azo reactive dyes based on sulfonamides

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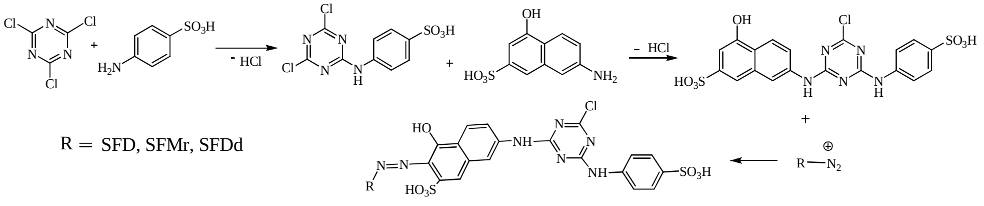
Bacteria are microorganism that grows up in humidity conditions causing many problems. One of the methods to terminate growing of them is the use of antibacterial agents. . In order to combine the strength of antibacterial activities of sulfonamides and their capability of being diazotized, three novel antibacterial azo reactive dyes based on sulfonamides were synthesized and evaluated. To do this, three sulfonamides viz. amino-N-(4-methyl-2-pyrimidinyl) benzene sulfonamide (SFD), 4-amino-N-(4-dimethyl-2-pyrimidinyl)benzene sulfonamide (SFMr) and 4-amino-N-(4,6-dimethyl-2-pyrimidinyl)benzene sulfonamide (SFDd) were diazotized [1] to produce diazonium salts. A coupling component was prepared by the condensation of 6-amino-1-hydroxynaphtalene-3-sulfonic acid (J-acid); 2, 4, 6-trichloro-1, 3, 5-triazine (cyanuric chloride) as a reactive group and 4-aminobenzene sulfonic acid (sulfanilic acid) in two separate steps [2]. The resultant diazonium salts were then coupled with the coupling component to produce the dyes. The synthesized dyes were filtered off, purified and characterized by ^{1}HNMR, FT-IR and Uv-Vis spectrophotometer. The results from spectral data are strongly indicating that the research work was successful. Dyes were then applied on cellulosic fabric by conventional method and their antibacterial activity assessments were carried out by AATCC 147 test procedure [3]. The synthesis route for the dyes is shown in the following.



Reference:

[1] Nagaraja, P.; R. Sunitha, K.; A. Vasantha, R .*J. Pharmaceutics & Biopharmaceutics,* **2002**, 53, 187.
[2] Mokhtari, J.; A.S. Philips, D.; A. Tailor, J.*J. Dyes & Pigments,* **2004**, 63, 51.
[3] Kawabata, A.; A. Tailor, J.*J. Carbohydrate Polymers,* **2007**, 67, 375.

Synthesis of xanthenediones in the presence of modified montmorillonite catalyst

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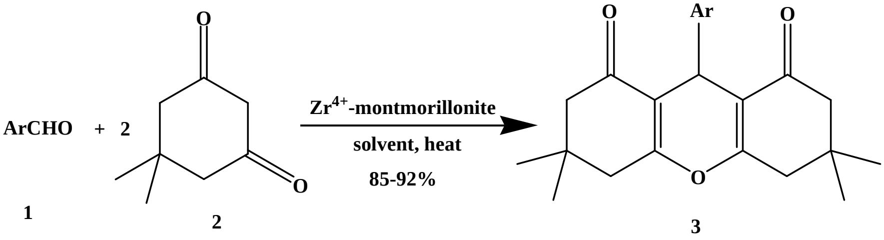
Xanthenes are known for possessing various biological properties including anti-bacterial, anti-viral and anti-inflammatory activities. In particular, xanthenedione derivatives constitute a structural unit in several natural products, and they are valuable synthons because of the inherent reactivity of the inbuilt pyran ring [1].

Xanthene derivatives are also very useful and important organic compounds widely used as dye, in laser technologies and fluorescent materials for visualization of biomolecules [2].

On the other hand, solid acids have opened new perspectives in synthetic organic chemistry not only in terms of yield and selectivity, but also concerning the work-up, recyclability, and mild reaction conditions. Specially, montmorillonite K10 and KSF clays are most attractive over classical acids because of their reusability, environmental compatibility, low cost, nontoxicity, and operational/experimental simplicity. Cation exchanging on montmorillonite with transition metal ions can result in a change in acidities [3].

At present research work we have developed an efficient one-pot three-component reaction for the synthesis of xanthenedione derivatives by the reaction of aryl aldehydes and dimedone in the presence of zirconium modified montmorillonite K10 catalyst in lower reaction times and higher yields (85-92%) (Scheme 1).



Scheme 1

In this presentation various aspects of this new method will be discussed.

References:

[1] Song, G.; Wang, B.; Luo, H.; Yang, L. *Catal. Common.* **2007**, *8*, 673.
[2] Varma, R.S. Tetrahedron 2002, 58, 1235.
[3] Ballini, R.; Fiorini, D.; Victoria, G. M.; Palmieri, A. *Green Chem.* **2003**, *5*, 475.

Synthesis and characterization of nickel nanoparticle-poly(vinyl amine)/SBA-15 composite and it's application for reduction of nitro compounds

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The reduction of nitro and carbonyl compounds is very important in organic synthesis both from the academic and industrial view points. Hydrogen transfer reduction is safer, highly selective and eco-friendly compared to the commonly used reduction processes which involve hazardous molecular hydrogen or Fe/HCl. A wide variety of soluble metal complexes have been reported for this purpose. However, it has been observed that controlling the reduction rates is quite difficult with these highly active homogeneous catalysts. On the other hand, the use of heterogeneous catalysts offers several advantages over homogeneous systems with respect to easy recovery and recycling of catalysts as well as minimization of undesired toxic wastes [1].

Noble metal nanoparticles are attractive for catalysis because of their size effects. There are various liquid phase methods for preparing nanoparticles such as the chemical reduction, sol-gel, reversed micelle, hot-soap, pyrolysis, and spray pyrolysis methods [2]. However, having very active surface atoms could often lead to aggregation of the naked nanoparticles and decreases in catalytic activity and selectivity. Recently, many stabilizing methods like dispersion of metal nanoparticles in organic functional polymers have been developed to solve the problem [3].

In this work, nickel nanoparticles were prepared from $NiCl_2$ in the presence of poly vinyl amine grafted to mesoporous silica with $NaBH_4$ as reducing agent, after mixing the metal solution with the organic-inorganic hybrid composite. The catalyst was characterized by FT-IR, XRD, SEM, TEM, TG and BET techniques.

In the presence of this catalyst, the aromatic nitro compounds are quantitatively reduced by $NaBH_4$ to form the corresponding amines under atmospheric pressure in aqueous medium. Catalysis was due to the efficient nanoparticle mediated electron transfer from BH_4^- ion to the nitro compounds [4]. The effect of $NiCl_2$ concentration, $NaBH_4$ concentration, mesoporous silica content and reducing agent contents for nitro compounds reduction are also investigated. The catalyst showed excellent yield (100 %) in a short time (2 min), with excellent recycling capability.

References:

[1] Chen, Y.; Qiu, J.; Wang, X.; Xiu, J. *J. Catal.* **2006**, *242*, 227.
[2] Dur´an Pach´on, L.; Rothenberg, G. *Appl. Organomet. Chem*, **2008**, *22*, 288.
[3] Manian Manesh, K.; Gopalan, A. I.; Lee, K. P.; Komathi, S. *Catal. Commun*, **2010**, *11* 913.
[4] Pradhan, N.; Pal, A.; Pal, T. *Coll. Surf. A: Physicochem. Eng. Asp.* **2002**, *196*, 247.

Configurational analysis of some functionalized azo compounds through *Ab initio* calculations and experimental results

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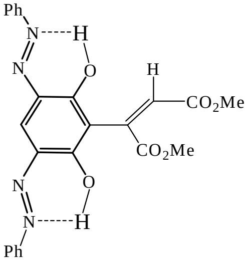
Azoaromatic compounds have been widely used as dyes and pigments in a variety of industrial and chemical synthetic products [1-3].

Also, they play an important role in other practical applications such as biological reactions [4], optical storage technology and photo electronic effects [5].

We have reported a simple and efficient reaction for the synthesis of the multifunctionalized azo structures (1 and 2) and the characterization of the synthesized azo pigments has been described by different spectroscopic techniques. The influence of the substituents on the data of them has been described. Also, theoretical calculations are expected in principle to produce many properties and structural features can be obtained with an accuracy that is competitive with experiment. Ab initio calculations at the HF/6-311G* level of theory provide a picture of the cis and trans configurations of several azo derivatives from both structural and energetic points of view. Twenty five forms were studied by computational methods and we found that the possibility of hydrogen bonding in these molecules is the most important factor for the stability of them.



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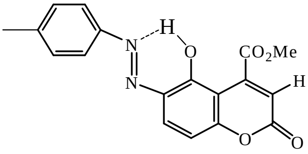

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References:

[1] Koh, J.; Greaves, AJ. *Dye and Pigments*. **2001**, 50, 13.
[2] Gur, M.; Kocaokutgen, H.; Tas, M. *Dye and Pigments.* **2007**, 72, 101.
[3] Pearce, CI.; Lloyd, JR.; Guthrie, JT. *Dyes and Pigments.* **2003**, 58, 179.
[4] Kondil, SS. *Transition Met. Chem.* **1998**, 23, 461.
[5] Katz, HE.; Singer, KD.; Sohn, JE.; Dirk, CW.; King, LA.; Gordon, HM. *J. Am. Chem. Soc*. **1987**, 109(21), 6561.

A new four-component method for the synthesis of spiroindenopyridine-indolines

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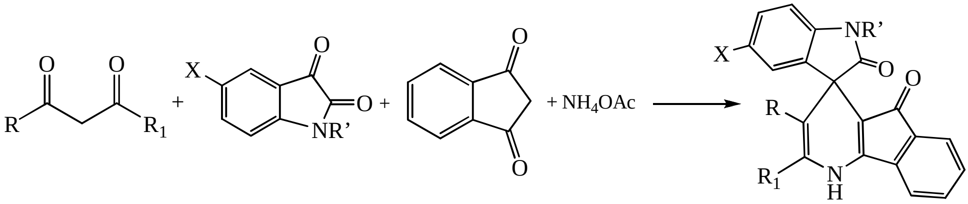
Indenopyridine derivatives represent important biological and medicinal scaffolds. The indenopyridine skeleton is present in the 4-azafluorenone group of alkaloids, represented by its simplest member onychnine [1].

Indole and indoline fragments are important moieties of a large number of a variety of natural products and medicinal agents,5 and some of indolines, spiro-annulated with heterocycles in the 3-position, have shown high biological activity [2,3].

Multicomponent reactions (MCRs), in which multiple reactions are combined into the synthetic operation have been used extensively to form carbon-carbon bonds in the synthetic chemistry [4]. Such reactions offer a wide range of possibilities for the efficient construction of highly complex molecules in a single procedural step, thus avoiding the complicated purification operations and allowing savings of both solvents and reagents.

Herein we reports a mild, facile and four-component method for the synthesis of spirooxindols fused diindenopyridine using readily available starting materials. Prominent among the advantages of this new method are operational simplicity, good yields and easy work-up procedures employed.



References:

[1] Zhang, J.; El-Shabrawy, A.-R. O.; El-Shanawany, M. A.; Schiff P. L.; Slatkin, D. J. *J. Nat. Prod.* **1987**, *50*, 800.
[2] Joshi, K. C.; Chand, P. *Pharmazie* **1982**, 37.
[3] Da-Silva, J. F. M.; Garden, S. J.; Pinto, A. C. *J. Braz. Chem. Soc.* **2001**, *12*, 273.
[4] Tietze, L. F.; Modi, A. *Med. Res. Rev.* **2000**, *20*, 304.

Synthesis of magnetic nanoparticle- supported reusable catalyst and their application in organic synthesis

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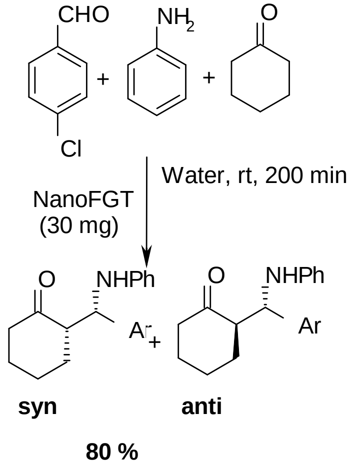
A simple and novel nanoparticle-supported and magnetically recoverable organocatalyst has been developed, which is readily prepared from inexpensive starting materials in a truly sustainable manner; which catalyzes the Mannich reaction in pure water. The present methodology offers several advantages such as excellent yields, simple procedure, short reaction times and milder conditions with very small amount of catalyst. It was found that both the diastereoselectivity and the rate of the reaction were improved with this organocatalyst in water.



References:

[1] K. Manabe, Y. Mori, S. Kobayashi, *Tetrahedron* 2001, 57, 2537.

[2] N. Azizi, L. Torkiyan, M.R. Saidi, *Org. Lett.* 2006, 8, 2079.

Corrosion performance of steel coated with co-polyamides and polyaniline

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The corrosion performance of steel coated with co-polyamide polymers and polyaniline in neutral salt spray (NSS) and accelerated corrosion testing is presented [1]. A coating of the nylon polymer on steel is not sufficient to prevent corrosion in a chloride medium, the underlying steel showing signs of corrosion after only three days in the NSS environment [2]. Open-circuit potential measurements indicate the steel is corroding forming soluble ferrous and ferric oxy-complexes. Polyaniline by itself is also insufficient in inhibiting corrosion on steel [3]. A synergy exists between an under-layer of polyaniline and a top layer of the nylon coating in minimizing corrosion.

Table 1: Results from NSS studies

Days in NSS cabinet	Co-polyamide coating only	PANi:co-polyamide coating
Day 1	No signs of corrosion	No signs of corrosion
Day 2	Very slight signs of corrosion	No signs of corrosion
Day 3	Slight signs of corrosion	No signs of corrosion
Day 4	Slight signs of corrosion	No signs of corrosion
Day 5	Corrosion	No signs of corrosion
Day 6	Corrosion	No signs of corrosion
Day 7	Corrosion	No signs of corrosion
Day 8	Bad corrosion	No signs of corrosion
Day 9	Bad corrosion	No signs of corrosion
Day 10	Severe corrosion	No signs of corrosion
Day 11	Severe corrosion	No signs of corrosion
Day 12	Severe corrosion	No signs of corrosion
Day 13	Severe corrosion	No signs of corrosion
Day14	Severe corrosion	No signs of corrosion

References:

[1] A.G. MacDiarmid and N. Ahmad, *US Patent* , **1997**, 5, 645.
[2] M.E. Leyva, G.M.O. Barra, B.G. Soares, *Synth. Met.* **2001**, 123, 443.
[3] A. Gabriel, N.J. Laycock, H.N. McMurray, G. Williams, A. Cook, *Electrochem. Solid State Lett*. **2006**, 9, B57.

Facile and efficient synthesis of functionalized thiopyran derivatives

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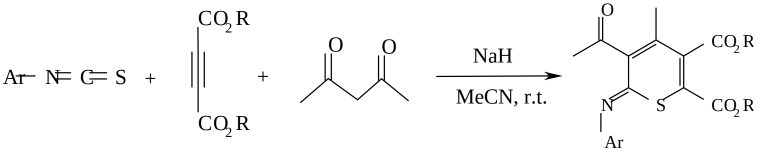
Substituted thiopyrans attracted much attention because of their pharmaceutical activities such as anti-inflammatory [1], anti-bacteria [2], anti-hyperplasia [3], antipsychiatric [4], analgesics and anti-cancer activities [5]. Hence, the development of new and facile synthetic method for the preparation of thiopyrans is considered to be of great significance. Limited procedures have been reported for the preparation of iminothiopyrans, namely the addition of arylethylidene malononitriles to dimethyltrithiocarbonateand the reaction of substituted 1,3-butadiene with isothiocyanates .

We present herein our results involving synthesis of thiopyran derivatives, using commercially available starting materials in excellent yields. Thus, the reaction of aryl isothiocyanates **1**, activated acetylenes **2** with 1,3-dicarbonyl **3**, in acetonitril at room temperature, produced derivatives **4** in good yields.



1 **2** **3** **4**

References:

[1] Rogier, D. J. J.; Carter, J. S.; Talley, J. J. *Chem Abstr* **2001**, *135*, 107252.
[2] Brown, M.J.; Carter, P. S.; Fenwick, A. E.; Fosberry, A. P. *Bioorg Med Chem Lett* **2002**, *12*, 3171.
[3] Quaglia, W.; Pigini, M.; Piergentili, A.; Giannella, M.; Gentili, F. *J Med Chem* **2002**,*45*,1633.
[4] Van Vliet, L. A.; Rodenhuis, N.; Dijkstra, D.; Wikstrom, H.; Pugsley, T. A. *J Med Chem* **2000**, *4 3*, 2871.
[5] Wang, W.; Li, H.; Wang, J.; Zu, L. S. *J Am Chem Soc* **2006**, *128*, 10354.

Room-temperature synthesis of mono arylidines of cyclic ketones with primary amines under solvent-free conditions

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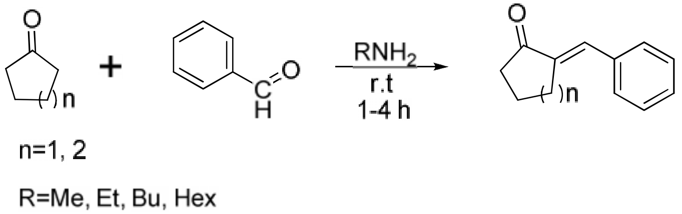
On "green chemistry" front, acceleration of chemical reactions caused by addition of substoichiometric quantities of organic compounds containing no metal in their structures, termed as organocatalysis, has increasingly gained popularity among synthetic organic chemists in recent years [1].

Monoarylidenes of cyclic ketones are of great importance in synthetic organic chemistry since they are found as a key component in many natural and biologically active compounds [2]. In addition, they could serve as convenient precursors for other nucleophylic synthetic transformations [3]. Several strategies are offered so far for the preparation of these compounds. However, many of them usually incorporate more than one step reaction or need the use of commercially unavailable starting materials.

In the framework of our ongoing program on the study of aldol condensation reactions [4] and in continuation of our previous investigations on the development of environmentally safe organic transformations [5], we would like to herein report a novel and high yield room-tempearture synthesis of the title compounds which is applicable to the reaction of cyclic ketones with both aromatic and aliphatic aldehydes.



References:

[1] MacMillan, D. W. C. *Nature* **2008**, *455*, 304.
[2] Das, U.; Doroudi, A.; Das, S.; Bandy, B.; Balzarini, J.; De Clercq, E.; Dimmock, J. R. *Bioorg. Med. Chem.* **2008**, *16*, 6261.
[3] Caruana, P. A.; Frontier, A. J. *Tetrahedron* **2007**, *63*, 10646.
[4] Abaee, M. S.; Mojtahedi, M. M.; Sharifi, R.; Zahedi, M. M.; Abbasi H.; Tabar-Heidar, K. *J. Iran Chem. Soc.* **2006**, 3, 293.
[5] Mojtahedi, M. M.; Abaee, M. S.; Hamidi, V. *Catal. Commun.* **2007**, *8*, 1671.

Synthesis of quinoxaline derivatives *via* reaction of Aryl-1,2-diamines with1,2-diketones using $CdCl_2.6H_2O$ as an efficient, mild and reusable catalyst

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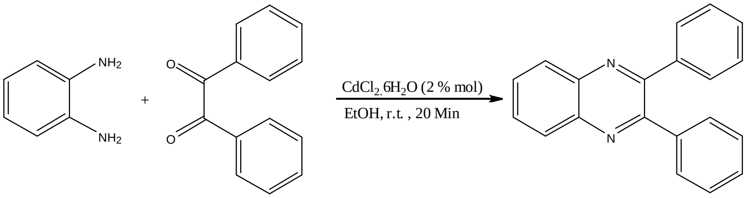
Quinoxaline derivatives are an important class of nitrogen containing heterocycles in medicinal chemistry [1-3]. Forexample, quinoxaline is a part of various antibiotics such asechinomycin, levomycin, and actinoleutin that are known toinhibit growth of gram positive bacteria [2], and are activeagainst various transplantable tumors [3]. Several kinds of synthetic routes toward quinoxalines have been developed,inclding the condensation of aryl-1,2-diamines with a 1,2-diketones[4], heteroannulation of nitroketene N,S-aryliminoacetals with $POCl_3$ [5], andformation of α-hydroxy ketones *via* a tandem oxidationprocess using $Pd(OAc)_2$ or $RuCl_2$-$(PPh_3)_3$-TEMPO [6] as well as MnO_2 [7].Cadmium II Chloride hexahydrate [$CdCl_2.6H_2O$] efficiently catalyzes the reaction of aryl-1,2-diamineswith 1,2-diketones in EtOH at room temperature to afford quinoxaline derivatives as biologically interesting compounds. Ease of recycling of the catalyst is one of the most advantages of the proposed method.



References:

[1] a) Jaso, A.; Zarranz, B.; Aldana, I.; Monge , A. *Eur. J. Med. Chem*. **2005**, *48*, 2019.; b) Carta, A.; Paglietti, G.; Nikookar, M. E. R.; Sanna, P.; Sechi, L.; Zanetti, S. *Eur. J. Med. Chem*. **2002**, *37*, 355.
[2] Dell, A.; William, D. H.; Morris, H. R.; Smith, G. A.; Feeney, J.; Roberts, G. C. K. *J. Am. Chem. Soc*. **1975**, *97*, 2497.
[3] Bailly, C.; Echepare, S.; Gago, F.; Waring, M. *J. Anti-Cancer Drug Des*. **1999**, *15*, 291.
[4] Heravi, M. M.; Bakhtiari, K.; Tehrani, M. H.; Javadi, N. M.; Oskooie, H. A. *ARKIVOC xvi*. **2006**, *16.*
[5] Venkatesh, C.; Singh, B.; Mahata, P. K.; Junjappa, H. *Org. Lett*. **2005**, *7*, 2169.
[6] Robinson, R. S.; Taylor, R. J. K. *Synlett.* **2005**, 1003.
[7] Raw, S. A.; Wilfred, C. D.; Taylor, R .J. K. *Org. Biomol. Chem*. **2004**, *2*, 788.

The estimation of the optimal geometry of the drug – nanoparticle complexes, the determination of the binding energy of the complexes

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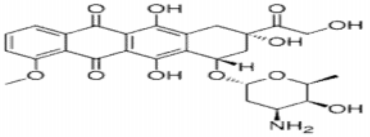
Doxorubicin is a drug used in cancer chemotherapy. It is an anthracycline antibiotic, closely related to the natural product daunomycin, and like all anthracyclines it works by intercalating DNA. It is commonly used in the treatment of a wide range of cancers, including hematological malignancies, many types of carcinoma, and soft tissue sarcomas. In this report the physicochemical properties of doxorubicin and complexes of this drug with nano particles are investigated by computational methods. For large reactive systems, the calculation of energies can be simplified by treating the active part with a high-level quantum mechanicalQMab initio or density functional approach and the environment with a less sophisticated semiempiricalSE approach, as an improvement over the widely used hybrid quantum mechanical/molecular mechanicalQM/MM methods. One such method is the original ‘‘Our-own-N-layer Integrated molecular OrbitalMolecular MechanicsONIOM’’ approach [1,2].



Doxorubicin

Docking of ligands to receptors, coupled with appropriate binding energy estimates [3], is a powerful technique used in structure- based drug design. Doxorubicn, nanoparticles and complexes of doxorubicin with nanoparticles were optimized. Then the binding energy and physic chemical properties were calculated.

Table. 1. Binding energy of doxoRubicin to is butyle cyano(ev)

n	2	3	4	5	6
Binding energy(ev)	-0.206763	-0.26203	-0.21757	-0.22097	-0.21524

Table. 2. Dipole moment of complex doxorubicin and doxorubicin and nano particla

unit	**Complex doxorubicin** (debye)	**doxorubicin** (debye)	**Nano particla= iso butyle cyano acrylat** (debye)
n=2	4.4660	4.9424	6.794
n=3	5.9312	5.2771	5.7639
n=4	9.2904	4.736	6.0935
n=5	9.2494	4.7063	6.787
n=6	8.4256	4.6921	5.6347

Table. 3. Geometric parameters for non-classical H bonds for molecule

n	2	3 5	4 6
Angle O…H…N	141.2626	137.9516	175.3288

Reference:

[1] M. Svensson, S. Humbel, R. D. Froese, T. Matsubara, S. Sieber, and K. Morokuma, J. Phys. Chem. 100, 19357, 1997.
[2] T. Vreven, K. Morokuma, J. Comput. Chem. 21, 1419, 2000.
[3] J. D. Holt, T. T. S. Kuo, G.E. Brown. Phys. Rev. C **2004,** *69*, 034329.

Synthesis and evaluating some new mono-and bis azodyes, pigmenets and related complex, based of 2,3 and 4-aminopyridine

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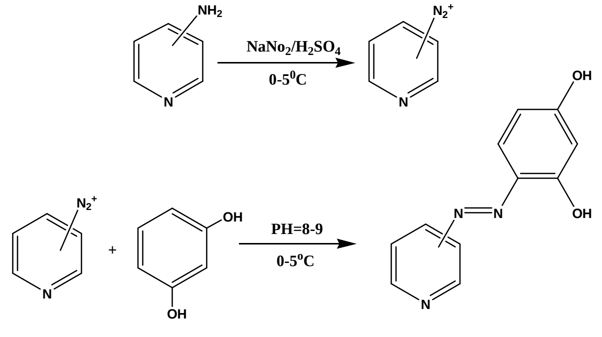
Some pyridine derivatives possess biological and pharmacological properties. Interesting activities of report pyridine have stimulate chemists to develop the chemistry of these compound [1-2]. Some azo pyridine derivatives also find application in dyes and related complex. Metal complexes of monoazo compounds are principally useful as trivalent chromium and cobalt complexes for dyeing of protein and polyamide fibers [3]. Metal-complex dyes are very versatile in terms of applications. Virtually all substrates, apart from a few synthetic fibers,
can be dyed and printed with this class of dyes. Countless shades from greenish yellow to deep black can be generated, depending upon the metal, the dye ligands, and the combination of dye ligands in mixed complex dyes [4]. In this research a number of new azo dyes were synthesized. These syntheses were started by coupling resorcinol with diazotized pyridine derivatives. We used two of the synthesized dyes as ligands for preparing some new metal complexes. The effect of substituents, pH and diffrents solvents on their absorption maxima (λ_{max}) was evaluated. The structure of all synthesis compound were confirmed by IR, ^{1}H-NMR,^{13}C-NMR,UV- Vis,Mass spectroscopy and elemental analysis.



$NH_{2=}$*o,m,p*

References:

[1] Zollinger, H. Diazo chemistry I: Aromatic and heteroaromatic compounds. Weinheim: VCH; **1994**.
[2] Fraser, W. Li, S.; Meade, T. *J. Am. Chem. Soc.***1999**, *121*, 1413.
[3] Cavalla.J.; Dolby. L.; Hofer.; M. Chasin, *US Patent*, **1997**, *665*, 737.
[4] Wojciech K.; Magdalena. M.; Joanna. K.; Ryszard. T. *Dyes and Pigments*. **2007**, *74*, 9.

Synthesis of nanocrystalline cellulose supported nickel or copper catalyst and its applications in coupling reactions

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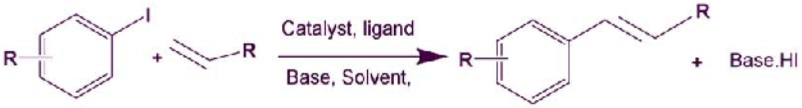
Heterogeneous catalysis for the synthesis of fine chemicals is particularly attractive as it allows production and ready separation of large quantities of products with the use of a small amount of catalyst [1].

In recent years, the emphasis of science and technology is shifting more towards environmentally friendly
and sustainable resources and processes, in this regard biopolymers are attractive candidates to explore for supported catalysis.

Nanocrystalline cellulose supported methal catalysts was prepared and applied for the Heck and Sonogashira coupling reactions by treating aryl iodides with alkenes or phenylacetylene, to afford corresponding coupled products in good to excellent yields. The catalyst was recovered
by simple filtration and reused for several cycles [2].



R: COOEt , Ph , COOH , …

References:

[1] Sheldon, R. A.; Bekkum, H.V.; Fine Chemicals through Heterogeneous Catalysis, Wiley-VCH, Weinheim, **(2001)**.

[2] Reddy, K. R. Kumar, N. S. Reddy, P. S. Sreedhar, B. Kantam, M. *J. Mol. Catal. A,* **2006,** *252,* 12.

Preparation of chelating polymers based on poly(vinyl acetate-alt-maleic anhydride) in nano scale for refining of industrial waste water

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Recently, the removal and recovery of heavy metal ions from industrial wastewater has been a significant concern in all academic and industrial branches owing to economic and environmental factors [1,2]. The alternative poly(vinyl acetate-alt-maleic anhydride) copolymer was prepared by free radical polymerization of vinyl acetate and maleic anhydride in presence of benzoyl peroxide as initiator. Then the series of chelating polymers network in nano scale were synthesized by reaction of poly(vinyl acetate-alt-maleic anhydride) with 1,2-diaminoethane, 1,3-diaminopropane and 1,6-diaminohexane in presence of ultrasonic irradiation. The obtained chelating polymers were characterized by FT-IR analysis and scanning electron microscopy (SEM), XRD and difrancial scaning calorimetric(DSC). The investigation of heavy metal ions (Cu(II), Ni(II), Cr(II), and Co(II)) adsorption by obtained chelating polymers from aqueous solutions were carried out[3,4]. The amount of remaining metals ions in aqueous solutions were determined by spectrophotometric determination.

References:

[1] Shin,D.H.; Ko,Y.G.; Choi,U.S. and Kim,W.N. *Polyme Adv Technol*.**2004** , *15*, 459.
[2] Rivas,B.L.;Jara,M.;Pereira,E.D. *J. Appl. Polym. Sci*. **2003**,*89*,2852.
[3] Iemma, F.; Cirillo, G.; Spizzirri, U.G.; Puoci,F.;Parisi,O.I.; Picci,N. *Eur polymer J.* **2008**,*44*, 1183.
[4] Shukla, S.R.;Pai ,R.S.; Shendarkar, A.D. *Sep Purif Technol.* **2006**, *47*, 141.

P_2O_5/SiO_2 catalyst for the synthesis of 2-arylbenzimidazole under heterogeneous and solvent-free conditions

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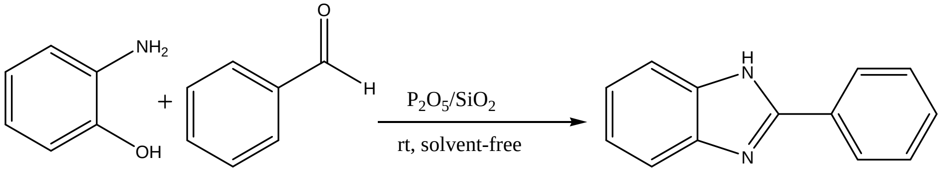
The benzimidazole moiety is found in various bioactive compounds having antiviral, antiulcer, antihypertension and anticancer properties.[1] General methods for the synthesis of benzimidazoles involve treatment of 1,2-phenylenediamines with carboxylic acids or various derivatives under strongly acidic conditions or with aldehydes followed by oxidation.[2-3]

Phosphorus pentoxide/silica gel is an inexpensive, heterogeneous and commercially available catalytic system which has been used in several transformations.

We have observed that benzimidazoles can be synthesized efficiently by treatment of 1,2-phenylenediamine with aldehydes in the presence of P_2O_5/SiO_2 as an efficient, low cost and heterogeneous catalytic system in the absence of solvent at room temperature.

Several aldehydes underwent the above conversion to form a series of benzimidazoles(Scheme 1).



In conclusion, P_2O_5/SiO_2 has been employed here for the first time as a mild and efficient reagent for the convenient preparation of benzimidazoles in high yields from 1,2-phenylenediamine and a wide variety of aldehydes.

References:

[1] (a) Gravatt, G. L.; Baguley, B. C.; Wilson, W. R.; Denny, W. A. *J. Med. Chem.* **1994**, *37*, 4338; (b) Tuncbilek, M.; Kiper, T.; Altanlar, N. *Eur. J. Med. Chem*. **2009**, *44*, 1024.

[2] (a) Middleton, R. W.; Wibberley, D. G. J. *Heterocycl. Chem*. **1980**, 17, 1757; (b) Dudd, L. M.; Venardou, E.; Garcia-Verdugo, E.; Licence, P.; Blake, A. J.; Wilson, C.; Poliakoff, M. *Green Chem*. **2003**, *5*, 187.

[3] (a) Lombardy, R. L.; Tanious, F. A.; Ramachandran, K.; Tidwell, R. R.; Wilson, W. D. *J. Med. Chem.* **1996**, *39*, 1452; (b) Beaulieu, P. L.; Hache, B.; von Moos, E. *Synthesis*. **2003**, 1683.

Electrophilic addition of hydrogen fluoride and water to asymmetric olefins: A DFT study

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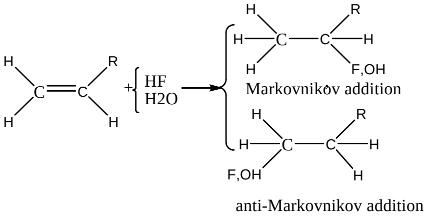
The addition of hydrogen halides and water to asymmetrically substituted alkenes leads to two products. The major product is predicted by the empirical Markovnikov rule [1], which states when water or hydrogen halide are added to an asymmetric alkene, the major product is resulted from the addition of acidic proton to the double bond carbon that attached to more hydrogen atoms, while the hydroxyl group or halide ion add to the other double bond carbon. This arrangement creates a more stable carbocation intermediate. In this research, we extended the last studies considering the effects of the electron-donating and electron-withdrawing substituent groups in the addition of hydrogen fluoride or water to asymmetric olefins by calculating the activation energy for the transition states [2].



$$\text{Ea for HF} = \begin{cases} 37.42 \text{ for R=F} \\ 17.37 \text{ for R=NHNH2} \\ 47.92 \text{ for R=NO2} \end{cases} \qquad \text{Ea for H2O} = \begin{cases} 46.75 \text{ for R=F} \\ 25.46 \text{ for R=NHNH2} \\ 54.53 \text{ for R=COF} \end{cases}$$

$$\text{Ea for HF} = \begin{cases} 49.69 \text{ for R=F} \\ 50.51 \text{ for R=NHNH2} \\ 41.93 \text{ for R=NO2} \end{cases} \qquad \text{Ea for H2O} = \begin{cases} 58.35 \text{ for R=F} \\ 63.14 \text{ for R=NHNH2} \\ 40.67 \text{ for R=COF} \end{cases}$$

The structures of reactants, TSs and products were optimized using B3LYP method and 6-311G** basis set with Gaussian 03 computational package. To confirm the nature of the stationary species and evaluate the activation energy barriers, frequency calculations were carried out. For the minimum state structures and the transition states were accepted only real frequency values and a single imaginary frequency value, respectively. The Berny algorithm method was used to locate the TSs. The activation energies in the two possible channels indicate that the alkenes with resonance electron-donating substituent groups (F and $NHNH_2$) prefer to give Markovnikov products while the alkenes with electron-withdrawing substituent groups (COF and NO_2) prefer to give anti-Markovnikov product. The latter can be understood because the electron-withdrawing groups distort toward themselves the pi electron cloud and then lead to anti-Markovnikov addition. In these reactions, the entropies of activation are negative (about -37 kcal/mol.K) and confirm the associative reaction.

References:

[1] Markovnikov, V. *Liebigs Ann.Chem.*, **1870**, *228*, 153.
[2] Meneses L. et al. *Chemical physics letters*, **2007**, *446*, 170.

A novel one-pot synthesis of 7-iminotetrahydropyrimidopyrimidins under catalyst free conditions in water

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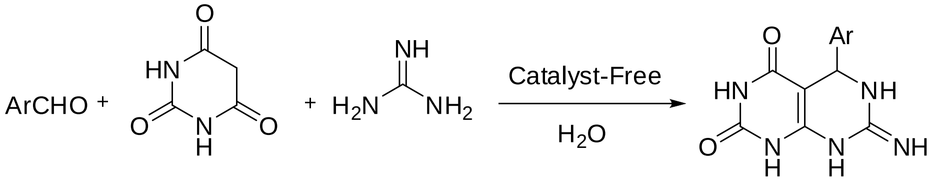
Dihydropyrimidin-2(1*H*)-ones (DHPMs) possess significant therapeutic and pharmacological properties. Certain DHPMs have shown to act as calcium channel blockers, α-1a-adrenergic receptor antagonists, mitotic kinesin inhibitors, antihypertensive agents, neuropeptide Y (NPY) antagonists, antiviral and antibacterial agents [1]. Therefore, this heterocyclic nucleus has gained a great importance and several modified procedures of the original Biginelli protocol for obtaining dihydropyrimidinones have recently been reported [2].

In continuation of our investigations in the Biginelli reaction [3], herein we introduce a new three-component reaction of aldehydes **1a-j**, barbituric acid **2** and guanidine **3** that provides an easy access to 7-iminotetrahydropyrimidopyrimidins **4a-j** building blocks under catalyst free condition in water. This enviromental friendly reaction has also the adavantages of catalyst free conditions, short reaction times and simplicity of operation.



1a-j **2** **3** **4a-j**

References:

[1] (a) Kappe, C. O. Eur, J. Med. Chem. **2000**, *35*, 1043; (b) McDaniel, M. P.; Collins, K. S.; Benham, E. A. Journal of Catalysis **2007**, *252*, 281.
[2] (a) Ranu, B. C.; Hajira, A.; Jana, U. *J. Org. Chem*., **2000**, 65, 6270; (b) Yadav, J. S.; Reddy, B. V.
[3] S.; Srinivas, R.; Venugopal, C.; Ramalingam, T. Synthesis, **2001**, 1341.
[4] (a) Mirza-Aghayan, M.; Bolourtchian, M.; Hoseini, M. *Synth. Commun*., **2004**, *34*, 3335; (b) Mirza- Aghayan, M.; Moradi, A.; Bolourtchian, M.; Boukherrob, R. *Synth. Commun*., **2010**, *40*, 8; (c) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. *J. Iran. Chem. Soc.* **2010**, *7*, 269; (d) Mirza-Aghayan, M.; Baie Lashaki, T.; Rahimifard, M.; Boukherroub, R.; Tarlani, A. A. *submitted for publication*, (e) Mirza-Aghayan, M.; Baie Lashaki, T.; Boukherroub, R. *submitted for publication*.

Boric acid (H_3BO_3) catalyzed three-component reaction of aldehydes, amines and cyanides: a high yielding synthesis of *α*-aminonitriles under solvent-free conditions

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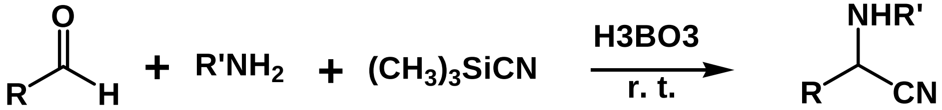
α-Aminonitriles are not only versatile intermediates for the synthesis of α-aminoacids and various nitrogen containing heterocycles such as imidazoles and thiadiazoles but also exhibit a valuable dual reactivity, which has been utilized in a broad range of synthetic applications [1].

The Strecker reaction provides one of the most important methods for the synthesis of α-aminonitriles. Numerous modifications have been made to the original Strecker reaction, using a variety of cyanating agents such as hydrogen cyanide, sodium or potassium cyanide, Bu_3SnCN, bis(dialkylamino)cyanoboranes, diethylphosphorocyanidate, and trimethylsilyle cyanide (TMSCN).

TMSCN is a safer, more effective, and more easily handled anion source compared to others. The efficiency of the reaction has been increased by the use of catalysts [2-3]. Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for one-pot multi-component reactions [4], we would like to introduce the first procedure for boric acid promoted combination of aldehydes, amines, and TMSCN leading to the synthesis of a-aminonitriles under solvent-free conditions at room temperature.



This method offers some advantages in terms of simplicity of performance, low reaction times, solvent-free condition, low cost, and it follows along the line of green chemistry. The catalyst is readily available and inexpensive and can conveniently be handled and removed from the reaction mixture.

References:

[1] Gonzalez-Vera, J. A.; Garcia-Lopez, M. T.; Herranz, R. *J. Org. Chem.* **2005**, *70*, 3660.
[2] Mojtahedi, M. M.; Abaee, M. S.; Abbasi, H. *J. Iran. Chem. Soc.*, **2006**, *3*, 93.
[3] Reddy, B. M.; Thirupathi, B.; Patil, M. K. *J. Mol. Catal. A: Chem.* **2009**, *307*, 154.
[4] Karimi-Jaberi, Z. Amiri, M. *Heteroatom Chem.* **2010**, *21*, 96.

Comparative study of microwave effect on antioxidant activity of *Mentha spicata*

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Mentha is one of the most known medicinal plants with different uses in medicins and foods. Considering different biological activity of this plant especially antioxidant activity, optimization of methods to improve biological quality of its extracts is very important. In spite of recent reports about useful applications of microwave-assisted extractions from plants as a rapid and easy method, it is predicted that these irradiations could damage structure of some useful and bioactive components in plants. In this study, effect of time duration of irradiation on antioxidant activity of extracs from Mentha spicata is investigated and compared to soxhlet method. Results show that in spite of predictions, antioxidant activity of the extracts exhibit no considerable difference.

References

[1] S. Hemwimon, P. Pavasant, A. Shotipruk, *Sep.Purif. Technol*. **2007**, *54*, 44-50
[2] C. Proestos, M. Komaitis, *LWT-Food Sci. Technol*. **2008** , *41*, 652-659.
[3] Camel, V. *Trends in Analytical Chemistry*. **2000** , *19*, 229-248.
[4] Pathirana, C. L., & Shahidi, F. *Food Chemistry*. **2005** , *93*,47-56.

An efficient one-pot synthesis of dimethyl 5-cyano-4-(alkyllamino)-1,2,5,6-tetrahydro-6-oxo-1-arylpyridine-2,3-dicarboxylate derivatives

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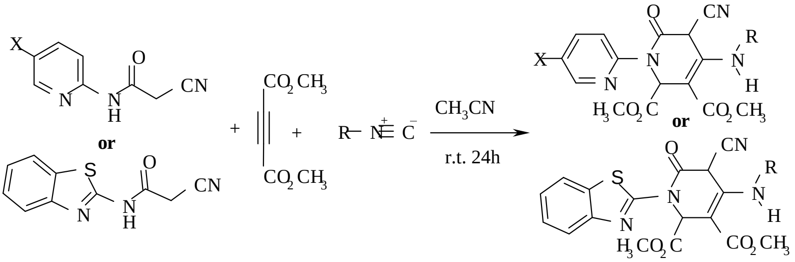
Modern synthetic design demands high efficiency in terms of minimization of synthetic steps together with maximization of complexity [1]. One of the ways to fulfill these goals is the development and use of multicomponent reactions (MCRs) which consist of several simultaneous bond-forming reactions and allow the high efficient synthesis of complex molecules starting from simple substrates in a one-pot manner [2].

Because of the unique reactivity of the isocyanide functional group, isocyanide-based MCRs (I-MCRs) are among the most versatile, in terms of the number and variety of compounds which can be generated. A recently developed class of I-MCRs is the reaction of isocyanides with electron-deficient acetylens in the presence of an electrophile. Addition of isocyanides to acetylene diester is well known to produce a reactive zwitterionic intermediate, which further reacts with different electrophiles to afford a wide veriety of carbo- and heterocycles [3].

Here we report a three-component reaction between isocyanides and dimethyl acetylenedicarboxylate and 2-cyano-N-arylacetamides to produce dimethyl 5-cyano-4-(alkyllamino)-1,2,5,6-tetrahydro-6-oxo-1-arylpyridine-2,3-dicarboxylate derivatives in high yields.



References:

[1] Trost, B. M. *Science* **1991**, 254, 1471.
[2] Bienayme, H.;.Hulme, C.; Oddon, G.; Schmidt, P.; *Chem.sEur. J*. **2000,** 6, 3321.
[3] Anary-Abbasinejad, M.; Mosslemin, M. H.; Anaraki-Ardakani, H. *Synlett* **2009**, 16, 267

Synthesis of C-3 substuted 7-(2-(1H-indol-3-yl) acetamido)-8-oxo-5-thia-1-azabicyclo [4.2.0] oct-2-ene-2-carboxylic acids as a new β-lacam antibiotics

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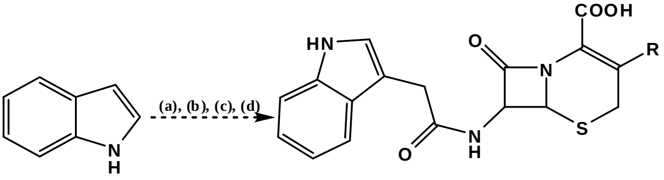
Indole fragment is featured widely in a wide variety of pharmacologically and biologically active compounds [1].for example bis indole and their derivatives are found in bio active metabolites of terrestrial origin [2].

Cefalosporins as semi synthetic β-lacam antibiotics and have wide spectrum antibacterial effects.

In this work we studied the reaction of activated indoleacetic acid, which was synthesized by Manich reaction between indole and diethyl amine followed by its reaction with different β-lacam intermediate such as 7-AVCA, 7-ANCA and 7-ADCA. (scheme1) [3].



R=H, methyl, vinyl

(a)CH_2O/ Et_2NH/CH_3COOH/30-40°C, (b)NaCN/ reflux/ H_3O^+,
(c) $SOCl_2$/ CCl_4, (d)Piv-Cl/ CH_2Cl_2/TEA/ B-lacam

scheme1

Products characterized by infra red spectra were determined on KBr plate using a BRUKER FT- IR spectrometer and ^{1}H-NMR, ^{13}C-NMR were obtained in $CDCl_3$ and DMSO-d_6 on BRUKER 300MHz spectrometer.

References:

[1] Sundberg, R, J.The chemistry of indoles; Academic press: New York, **1996,** p113
[2] Nagamitsu. M.; Heike K., Akira W.; Makoto K. *Organic Geochemistry*. ***2006****, 37, 12.*
[3] Larock, R. C.; *Comperhensive organic transformation*. Wiley-VCH, New York, **1999.**

A novel multi-component synthesis of 1,2-disubstituted pyrrolo[2,3-b]quinoxalines through Sonogashira Coupling reaction

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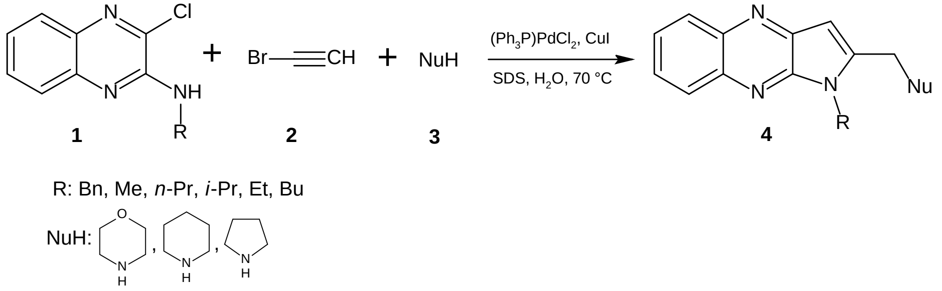
Multi-component reactions (MCRs) are powerful tools in the modern drug discovery process and allow the fast, automated, and high throughput generation of organic compounds [1].

The Pd-catalyzed cross-coupling reactions of aryl halides or triflates with terminal alkynes, commonly referred to as Sonogashira reactions, are powerful, versatile and popular tools for selective construction of new C-C bonds[2].

Herein, we report a novel multi-component synthesis of 1,2-disubstituted pyrrolo[2,3-b]quinoxalines through palladium catalyzed reaction. The reaction of 2-alkylamino-3-chloroquinoxaline **1** with propargyl bromide **2** and cyclic secondary amines **3** in the presence of $PdCl_2(PPh_3)_2$, CuI and SDS in water led to the formation of new 1,2-disubstituted pyrrolo[2,3-b]quinoxalines **4**.



References:

[1] Weber, L.; *Curr. Med. Chem. 2002, 9, 1241–1253.*

[2] Chinchilla, R.; Najera, C. *Chem. Rev.* **2007**, *107*, 874.

Synthesis and characterization of novel biologically and optically active copolymers derived from poly (vinyl alcohol)

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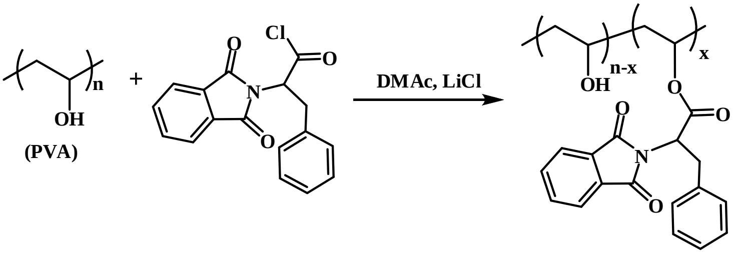
Over the last few years, the need of polymers and copolymers with more complex architecture for specific applications leads to the development of chemical modification of industrial synthetic polymers [1]. Poly (vinyl alcohol) (PVA) is the most commercially important water soluble plastic in use. PVA find wide use in industries such as the medical, packaging, paper and building industries because of its extraordinary properties, which include excellent mechanical and thermal properties, oxygen barrier properties, oil and solvent resistance, water solubility, biodegradability and biocompatibility [2]. In order to improve the desired properties for advanced applications PVA can be modified with a series of long-chain aliphatic carboxylic acids, acid chlorides and crosslinking with difunctional hardeners such as dianhydrides [3,4].

In this present study for the first time we wish to report the successful modification of PVA with optically and biologically active group containing L-phenylalanine amino acid. The resulting copolymers were characterized by FT-IR and ^{1}H-NMR spectroscopy, specific rotation, elemental and thermogravimetric analysis techniques.



References:

[1] Mallakpour, S. E.; Hajipour, A.; Khoee, S. *Polym. Int*. **1998**, *47*, 193.
[2] Finch, C. *Poly (vinyl alcohol); Properties and Applications*. John Wiley and Sons: Vannessa, G.; Jacobs, D. **2005**.
[3] Ciminez, V; Mantecon, A.; Cadiz. V. ***J.** Appl. Polym. Sci*. **1996**, *59*, 425.
[4] Haralabakopoulos, A.; Tsiourvas, D.; Paleos, C. *J. Appl. Polym. Sci*. **1998**, 69, 1885.

Chemical composition and antibacterial activity of the essential oil from aerial parts of *Thecocarpus meifolius* Boiss. a species endemic to Iran

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The genus *Thecocarpus* , family Umbelliferae,is represented in the flora of Iran by only one species,*T.meifolius* Boiss .This plant growing wild in Isfahan,Fars and Chaharmahal-Bakhtiarie provinces of Iran[1].

No studies on the chemical composition or oils of *Thecocarpus* species have previously been reported.

Microwave extraction of essential oil from aerial parts of *T.meifolius*, endemic to Iran,were analyzed by GC and GC/MS.The aerial parts of the plant were collected from Chaharmahal-Bakhtiarie in July 2009.

Forty-four components in the oil of *T.meifolius*, which represented about 92.4% of the total oil, were identified.The oil of *T.meifolius* consisted of two monoterpene hydrocarbons (0.7%), one oxygenated monoterpene (0.7%), thirteen sesquiterpene hydrocarbons (22.8%), eighteen oxygenated sesquiterpenes (57.7%) and ten nonterpenoid compounds (10.5%).The major component of this oil was spathulenol (30.8%).Other notable constituents were caryophyllene oxide (8.9%) and germacrene D(6.0%). As can be seen from the above information ,the oil of the plant was rich in regard to sesquiterpenes (80.5%).The monoterpene freaction was relatively small, representing only 1.4% .

Antibacterial activity was measured using the growth inhibitory zones.The oil of the plant was moderate active against Gram positive and Gram negative bacteria.

Reference

[1] Mozaffarian,V.A Dictionary of Iranian Plant Names. Farhang Moaser Publishers, Tehran . Iran . **1996** . 544.

Synthesis and characterization of 2, 6-bis (4-acetylphenoxy) pyridine and conjugated aromatic polymers based on this monomer and also studies of solubility, photophysical and thermal properties of synthetic polymers

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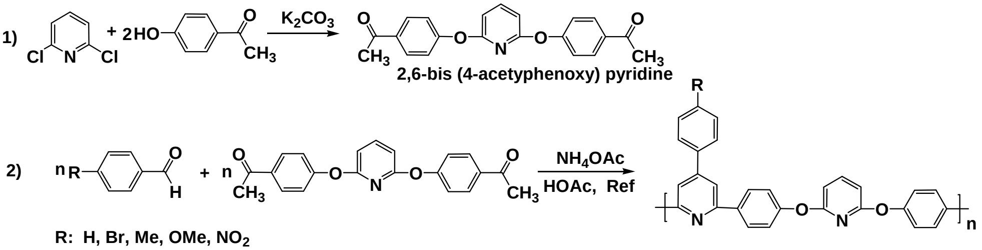
Light-emitting diodes (LEDs) are currently dominated by inorganic-based semiconductors. However, their applications are severely limited by their fabrication approaches, which are not amenable to large flat panel displays. The first demonstration of efficient polymeric light-emitting diodes (PLEDs) in 1990 stimulated intense interests in display applications for conjugated fluorescent polymers [1]. In comparison to conventional LEDs, PLEDs offer a wide variety of advantages, such as their facile processabilities and consequent ready fabrication into large flat panel displays.

Poly(2,5-pyridinediyl) (PPy) and its derivatives, with electronaccepting nature is a family of promising conjugated polymers because of their high luminescence, excellent electron transporting behaviour and their general resistance to oxidation [2].

In this work in the first stage we synthesized and characterized the 2, 6-bis (4-acetylphenoxy) pyridine monomer according to the procedure was described in the scheme 1. and the new conjugated polymer with used the modified Chichibabin [3] method were synthesized(scheme 2). All of the new polymers were fully characterized by FT-IR,^{1}H-NMR spectroscopies and elemental analysis. The physical properties, such as optical, solubility and thermal stability of the polymers were studied. All of these new polymers show excellent thermal stability and very good solubility in polar aprotic solvents.



References:

[1] Leclerc, M. *J. Polym. Sci., Part A: Polym. Chem.* **2001**, *39*, 2867.
[2] Horsburgh, L. E.; Monkman, A. P.; Samuel, I. D. W. *Synth. Met.* **1999**, *101*, 113.
[3] Weiss, M. *J. Am. Chem. Soc.* **1952**, *74*, 200.

Studies on the optically active, biodegradation and biocompatibility of new poly(ester-amide)s derived from Tyrosine

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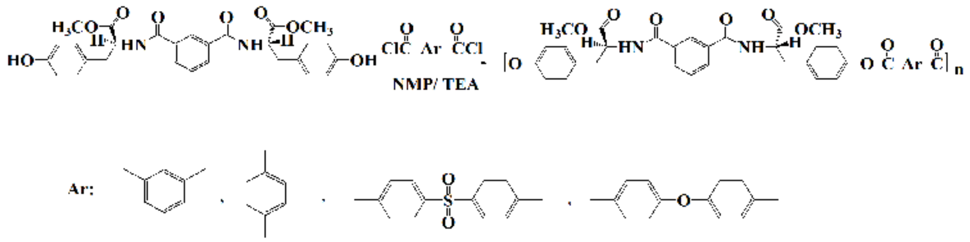
Polyesters have found a wide range of applications, such as drug controlled release carriers, green plastics as wrapping materials because of their biodegradability and biocompatibility [1,2,3]. Polyamides have excellent mechanical and processing properties in comparison with polyesters, and moreover, they could be easily modified. Therefore, the combination of these two classes of polymers would produce a new family of polymeric materials, poly(ester amide)s (PEAs). PEAs have both ester and amide blocks on their backbones and are regarded as promising biodegradable materials, as they combined good mechanical, thermal and processing properties of polyamides and the biodegradability of polyesters [4].

In this work, s-tyrosine methyl ester was synthesized from s-tyrosine [5]. Then a novel optically active diol was synthesized from this methyl ester. A number of novel PEAs were synthesized by polycondensation of this diol with different diacid chlorides. All of the above polymers were characterized by means of FT-IR spectroscopy, specific rotation, ^{1}H-NMR and typical ones by elemental and thermogravimetric analysis.



References:

[1] Uhrich, K. E.; Cannizzaro, S. M.; Langer, R. S.; Shakesheff, K. M. *Chem. Rev.* **1999**, *99*, 3181.
[2] Chiellini, E.; Solaro, R. *Adv. Mater.* **1996**, *8*, 305.
[3] Mallakpour, S.; Hashemi, E. *Polym. Bull.* **2010**, *in press*.
[4] Garg, P.; Keul, H.; Klee, D.; Moeller, M. *Macromol .Chem. Phys.* **2009**, *210,* 1754.
[5] Nagai, A.; Ishikawa, J.; Kudo, H.; Endo, T. *J. Polm. Sci. Part A: Polym. Chem*. **2004,** *42*, 1143.

Preyssler-type heteropoly acid: A new, mild and efficient catalyst for protection of carbonyl compounds

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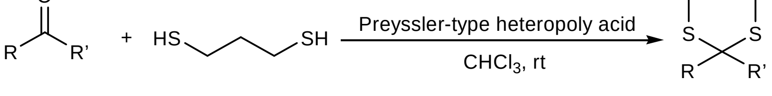
The protection of carbonyl compounds as dithioacetals is an important sequence in multi step preparation of many important organic compounds including multifunctional complex molecules [1].

Moreover, the electrophilic properties of carbonyl group in aldehydes and ketones can be a good choice to be attacked by a nucleophile at the site. Thus, one of the most popular methods for protection of carbonyl groups is to convert them into their corresponding dithioacetals.[2]

There are many methods in the literature for the protection of carbonyl compounds as dithioacetals using various catalysts or stoichiometric reagents [2]. However, most of these procedures have some restrictions such as low yields of the products, long reaction times, harsh reaction conditions, difficulties in work-up and the requirement for an inert atmosphere. Therefore, the search for alternative methods that can overcome these drawbacks is desirable.

On the other hand, precise control of the acidity in a small-scale reaction with usual corrosive any strong acid is extremely difficult. Considering the reversible nature of some processes in organic syntheses, low yield in reaction with pervious usual strong liquid acid is expected. So Preyssler-type heteropoly acid ($H_{14}NaP_5W_{30}O_{110}$) has been introduced as an efficient alternative. The advantages of Preyssler acid as a solid acid catalyst may include large number of balanced protons, strong acidity, high hydrothermal stability, and wide pH range stability in solution [3].

In this work, we wish to report a simple and easy method for chemoselective thioacetalization of various aromatic and aliphatic aldehydes and ketones using Preyssler-type heteropoly acid as a new and efficient catalyst.



References:

[1] Kunz, H. Waldmann, H. *Comprehensive Organic Synthesis*, eds. B.M. Trost and I. Fleming, Pergamon, New York, **1991**, Vol. 6, pp 677–681.
[2] Sartori, G. Ballini, R. Bigi, F. Bosica, G. Maggi R. Righi, P. *Chem. Rev.*, **2004**, *104*, 199.
[3] Kim, H. Jung, J.C. Park, D.R. Lee, J. Cho, K.M. Park, S. Lee S. H. Song, I. K. *Korean J. Chem. Eng.*, **2008**, *25*, 231.

Using new vinamidinium salts derivatives to the synthesis of new cyclam derivatives

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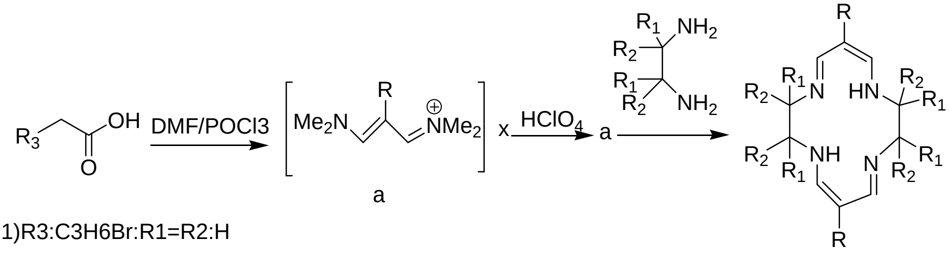
Derivatives of cyclam (1,4,8,11-tetraazacyclotetradecane) are of considerable intrest in bio inorganic chemistry.biology and medicine.Some derivatives of cyclam represent a new entity of low molecular weight molecules that inhibit human immunodeficiency virus(HIV) [1].

This work reports the synthesis of three novel cyclam derivatives via vilsmeier reaction to constract the vinamidinium salt and 1,2-diamin derivatives to synthesis of desired cyclam [2-4].



1)R3:C3H6Br:R1=R2:H

2)R3:C3H6Br:R1=R2:Me

3)R3:C3H6Br:R1:H,R2:Me
4)X=$Cl^{\ominus}$, $ClO_4^{\ominus}$

References:

[1] Clercq, E. D, *Molecular Pharmacology* **2000**, *57*, 833.
[2] Collman, J. P.; Brauman, J. I.; Collins, T. J.; Iverson, B. L.; Long, G.; Pettman, R. B.; Sessler, J. L.; Walters, M. A.; *J.* Am. *Chem. Soc*. **1983,** 105, 3038.
[3] Eric l. S.,Charles A.; Johnson I, Michael M.Haley, *Chem. Rev*. **2006**, 106, 5344.
[4] Reiner S., Hans-Gert K., Diana K., Jrg B., Karl-Heinz S., Elisabeth V., Eckard B., Michael K., Herbert de G. *Inorg. Chem*., **2007**, 46 (26), 11416.

One-pot synthesis through the reaction of Ethyl 3-oxo 3-phenyl propanoate and deravitives with di methyl acetylene dicarboxylate in the presence of $P(OPh)_3$

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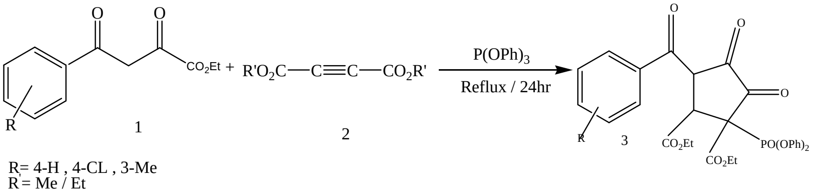
New or improved methods for phosphonate synthesis continue to attract much attention because phosphonates present biologically important properties and serve as natural products, analogues of phosphates, phosphonopeptides, aminoacid analogues and pro drugs. It appears that they have an important role in the therapeutic behavior of anti cancer and anti-HIV drugs [1].

α-Amino phosphonic acid and phosphonates are biologically attractive peptide mimics of α-amino acids. Because they have intriguing biological activities such as anti-HIV, protease inhibitory, and antibacterial activities [2].

There have been many studies on reactions between trivalent phosphorus nucleophiles and α,β-unsaturated carbonyl compounds in the presence of a proton source such as an alcohol or a CH-acid [3].

We report here an efficient synthetic route to phosphoruse ylides using triphenylphosphite, acetylene dicarboxylate and Ch-acids. Thuse, reaction of CH-acids 1 with acetylene dicarboxylate esters 2 in the presence of triphenylposphite leads to phosphorous ylides 3 in excellent ylids.



References:

[1] Maghsoodlou, M. T.; Hazeri, N.; Habibi-Khorassani, S. M. ; Saghatforoush, L.; Rofouei, M. K.; Rezaie, M. *ARKIVOC*, **2006**, (xiii) 117.
[2] Akiyama, T.; Morita, H.; Bachu, P.; Mori, K.; Yamanaka, M.; Hirata, T. *Tetrahedron*, **2009**, 65, 4950.
[3] Yavari, I.; Alizadeh, A.; Anary-Abbasinejad. M. *Tetrahedron Letters*, **2003**, *44*, 2877.

Synthesis of 3,6-diaryl-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines as novel cAMP-specific phosphodiesterase inhibitors

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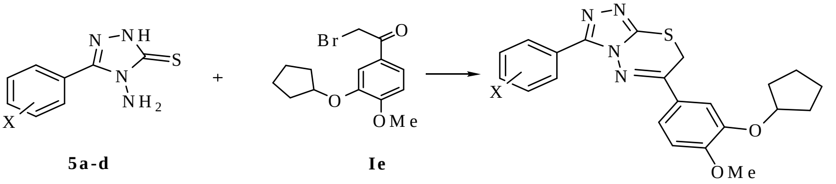
The enzyme phosphodiesterase-4 (PDE4) plays a key role in many physiological or pathological process in mammalian organs, where its inhibition increases cyclic adenosine monophosphate (cAMP) causing benefits in many diseases or conditions. Thus, the design of novel, potent and selective second generation of PDE-4 inhibitors with reduced side effects represent a critical need in the pharmaceutical industry [1,2].

A novel series of PDE4 inhibitors, 6-(3-(cyclopentyloxy)-4-methoxyphenyl)-3-aryl-7H-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazine, while aryl= (2-methoxyphenyl in 6a), (3-methoxyphenyl in 6b), (p-Tolyl in 6c), and (Phenyl in 6d) were developed and examined for their safety and efficacy. Initial structure activity relationship (SAR) highly suggests that these compounds are among the cathecol diether class of PDE4 inhibitors.



5a-d **Ie**

6a-d
6a: X =2-OMe
6b: X =3-OMe
6c: X =4-Me
6d: X =H

The concentrations of extracellular cAMP and cyclic guanosine monophosphate (cGMP) were determined using enzyme-linked immunoassay technique. Results show that all compounds cause a significant increase in the concentration of cAMP, while the concentration of cGMP stays approximately unchanged. Results indicate that presence of a non bulky 3,4-functionality located at the 5 position of the 3,6-dihydro-2H-1,3,4-thiadiazine ring but not the phenyl ring attached at the 3 position of the 1,2,4-triazole is important. The precise function of 6-(3-(cyclopentyloxy)-4-methoxyphenyl)-3-aryl-7*H*-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazines needs further investigation by biochemical assays for ascertaining the selectivity of these compounds to inhibit different subtypes of cAMP-PDE.

References:

[1] Burnouf, C.; Pruniaux, M.P.; Szilagyi, C.M. In: Bristol JA (Ed.), *Annu Rep Med Chem*, Academic Press, San Diego, **1998**, pp. 91.
[2] Souness, J.E.; Aldous, D.; Sargent, C. *Immunopharmacology* **2000**, 47, 127.

Synthesis of an anticorrosion coating composition by aniline-formaldehyde and melamine-formaldehyde resins

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The use of Intrinsically Conducting Polymers (ICPs) [1] as coating material to protect various metals against corrosion received substantial attention in recent years [2]. ICPs, because of their unique properties, have found a wide range of applications. An important and promising example of such applications is to protect against corrosion [3]. It has been proven that conducting polymers such as polyaniline (PINi) is applicable as coating to protect certain metals against corrosion [4]. The use of polyaniline as coating material however, provides some restrictions. Aniline coating properties have been addressed in this work to introduce a new and more resistive coating. In pursue of this, two methods of synthesis were employed (a) To add melamine-formaldehyde resin into a previously homogenized solution of cross-linked aniline-formaldehyde resin. Under oxidizing condition Sodium Dodecyl Sulphate (SDS) as dispersing agent was used. The reaction underwent under reflux condition between 55 to 65 degree centigrade for approximately 3 to 5 hours. (b) To add methyl methacrylate monomer as initiator into a previously homogenized solution of aniline-formaldehyde resin. The selection of this monomer provides flexible coating product. With the use of aniline as monomer and melamine-formaldehyde dispersed by SDS, the polymerization reaction proceeded in the range of temperature and time similar to those noted in method (a). Optimization of the two methods were conducted with respect to changes in molar ratio of the reactants, temperature and time to achieve a product with substantial resistant against heat and oxidizing conditions. Electrical conductivity data of resin was measured using a four-probe method. Thermal study of the coating product was carried out using Thermo-Gravimetric Analyses (TGA). Further study of the coating polymer conducted using Differential Scanning Calorimetry (DSC) and salt spray test to shows high resistance under salt spray solution after 36 days. The cross-cut test approved adhesion requirements of the resin onto the substrate and Scanning Electron Microscopy (SEM) was employed to study the type of surface morphology of the final polymer.

Reference

[1] S. Sathiyanarayanan, corrosion protection of iron by benzoate doped polyaniline containing coating, progress in organic coatings, 64, 2009, 460.
[2] E. Armelin, polyaniline, polypyrrole and poly(3,4-ethylenedioxythiophene) as additives of organic coatings to prevent corrosion, surface & coatings technology, 203, 2009, 3763-3769.
[3] H. Tang, a study on mechanism of corrosion protection of polyaniline coating and its failure, corrosion science, 49, 2007, 4232.
[4] V.-T. Truong, corrosion protection of magnesium by electroactive polypyrrole/paint coatings, Synthetic metals. 110, 2000, 7.

A novel study on the synthesis, characterization and morphology of a composite of polyaniline and silica in a solvent-free process

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Conducting polymers have attracted significant attention in recent decades because of their potential applications in various fields [1-4]. Among these polymers, polyaniline (Pani) is unique because of its high electrical conductivity, good environmental stability and ease of preparation [5].

PANI in association with inorganic fillers, otherwise known as a composite material, can further improve its inherent properties. Thus far, inorganic fillers or additives have been used intensively for many reasons such as for the enhancement of surface hardness, decreasing shrinkage, increasing resistance against flame, providing colors, improving appearance, changing thermal and electrical conductivity, and most importantly, for the reduction of the product cost without losing the desired properties of the components. Silicon dioxide particles, for example, constitute one of the common fillers in composite materials such as plastics and films. They not only lower the cost, but also improve the tensile strength and stiffness of the base resin, leading to composites of improved performance; the filler must be well dispersed into the matrix to avoid flaws of weak cohesion [6].

In the current paper which has been followed the solid-state reactions [7], the new composite of polyaniline was synthesized by chemical oxidative polymerization of aniline as a monomer, $FeCl_3.6H_2O$ as an oxidation and doping agent and also silica to be second phase of this polymer. The composite showed the properties of semi-conductive polymers. The whole of processes have done in room temperature. Doped composite was characterized by using FT-IR, UV-Vis and four-probe conductivity measurement; furthermore, morphological studies have operated by SEM.

$$\text{Silica + Aniline + } FeCl_3.6H_2O \longrightarrow$$

References:

[1] MacDiarmid, A.G.; Mu, S.L.; Somasiri, M.L.D.; Wu, W. *Mol. Cryst. Liq. Cryst*. **1985**, *121*, 187.
[2] Kitani, A.; Kaya, M.; Sassaki, K.J. *J. Electrochem. Soc*. **1986**, *133*, 1069.
[3] Pei Q.; Bi, X. *J. Appl. Polym. Sci*. **1989**, *38*, 1819.
[4] Athawale, A.A.; Kulkarni, M.V. *Sensors and Actuators B*. **2000**, *67*, 173.
[5] Genies, E.M.; Boyle, A.; Lapkowski, M.; Tsintavis, C. *Synth. Met*. **1990**, *36*, 139.
[6] Shui, M.; Yuanlong, R.; Pu, B.; Li, J.J.; Colloid Interface Sci. **2004**, *273*, 205.
[7] Modarresi-Alam, A.R.; Khamooshi, F.; etal. *Scientia Iranica* **2008**, *15*, 452.

Free-solvent synthesis of hydrophobically modified corn starch in water

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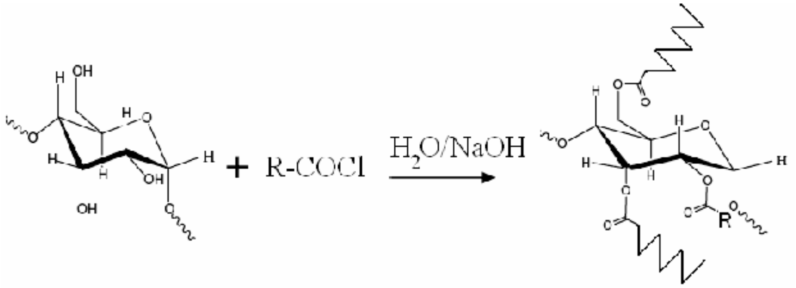
Chemical modification of starch has been widely studied for producing hydrophobic and water-resistant material by way of chemical reaction with hydroxyl groups in the starch molecule [1, 2]. In this paper an efficient method for synthesizing hydrophobically modified starch without using organic solvents is described. Starch esterification was performed with long chain fatty acid chlorides (C_8, C_{12}, C_{16}) in two steps, in the first step, starch dispersed in the reaction medium was alkali treated and the second, esterification. The chemical structural characteristics of the obtained products were investigated using spectroscopy methods.



This reaction is simple and convenient methods for esterification of starch and have several benefits in comparison to previous classic methods [3] including: a) utilizing water as green solvent instead of organic solvents b) the reaction time is very short and is completed just during several minutes c) the hydrophobically modified products are precipitated from water and are separated without need to any non solvent.

References:

[1] Kapusniak, J.; Siemion, P. *Journal of Food Engineering*. **2007**, *78*, 323.
[2] Chi, H.; Xu, K.; Wu, X.; Chen, Q.; Xue, D.; Song, C. *Food Chemistry*. **2008**, *106*, 923.
[3] Fang, J. M.; Fowler, P. A.; Tomkinson, J.; Hill, C. A. S. *Carbohydrate Polymers*. **2002**, 47, 245.

Fluorinated imidazolium salts

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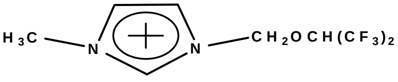
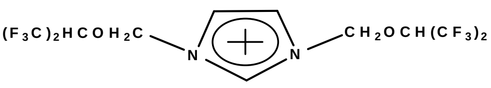
A search in the literature indicates that the number of imidazolium-based salts containing fluoroanions is much greater than those containing fluorocations since the former can be easily obtained by the anion exchange process[1], as mentioned earlier. The synthesis of each of the fluoroalkylated imidazolium salts needs its own specific strategy and has some difficulties. For this reason, imidazolium salts containing fluoroanions such as $(FH)_nF^-$, BF_4^-, PF_6^-, $N(SO_2CF_3)_2^-$, $OSO_2CF_3^-$, AsF_6^-, SbF_6^-, NbF_6^- have been comprehensively reviewed[2]. In the fluorous imidazolium cations, fluoroalkyl segment are directly or indirectly, by (CH2)n spacers, attached to one or both imidazole nitrogen atoms[3,4].

A review on the fluorinated imidazolium cations indicated no report on the insertion of CH2OCH spacer between the imidazole and fluorinated segment. Such an insertion would result in the formation of a-ammonium ether, as shown in Fig. 2. Here, we report the first synthesis of fluorous imidazolium salts (**1a**) and (**1b**) involving one or two $-CH_2OCH(CF_3)_2$ groups attached to the imidazole nitrogen atoms. These products were characterized by ^{1}HNMR and ^{13}CNMR and^{19}FNMR and FTIR spectroscopy. Also, the X-ray single crystal data obtained for (**1b**) is presented.



1 a



2 b

References:

[1] D. Fang, J. Cheng, K. Gong, Q.Shi, Xin-Li Zhou, Zu-Liang Liu, *J. Fluorine Chem.* , **2008**, *129*, 108.
[2] K. Matsumoto, R. Hagiwara, *J. Fluorine Chem.* , **2007**, *128* , 317.
[3] V.V. Rudyuk, D. V. Fedyuk, L. M. Yagupolskii, *J. Fluorine Chem.* , **2004**, *125*, 1465.
[4] R. P Singh, S. Manandhar, J. M Shreev, *Tetrahedron Lett.* , **2002**, *43*, 9497.

Synthesis and characterization structure of new formazane dye with quinoline moiety

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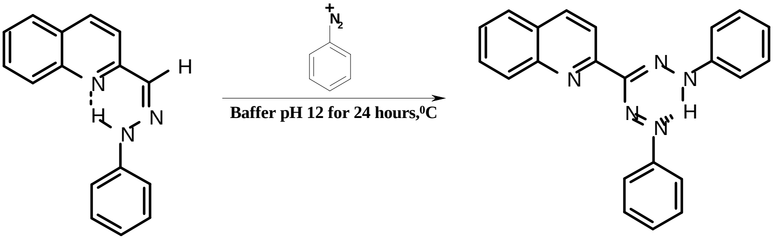
Azo compounds are highly colored and have been used as dyes and pigments for a long time. They have been receiving much attention and have been widely used in many practical applications such as coloring fibers, photoelectronic applications, printing systems, optical storage technology, textile dyes as well as in many biological reactions and in analytical chemistry [1].

These compounds began to be widely studied in the 1940s and 1950s. Because of the uniqueness of the reactions that involve them, as well as their suspected biochemical usefulness. Closely related molecules have been developed which will penetrate various plant and animal tissues, react with enzyme to produce formazans. Such compound from distinct class with characteristic properties, their structure was first elucidated by Bamberger and von pechmman, who was first agreed to call them formazyl compounds [1-3].

Formazans are usually produced by the reaction of an aldehyde arylhydrazone with a diazonium salt in basic solution. Many macro cyclic formzans have been synthesized and their applications in selective metal extraction and determination were studied. Several studies on the synthesis of complexes.



References:

[1] Kulkarni S S and Jianjing C, *J Med Chem.*, **2003**, *46*, 2589.
[2] Desai K G and Desai K R, *Indian J Chem.*, **2005**, *44(*B), 2097.
[3] Sikshi, S. A.; Hultin, P. G. *J. Org. Chem.* **2006**, *71*, 5888.

Poly(acrylamide-co-itaconic acid)/laponite superabsorbent composites: Synthesis, swelling behavior and thermal stability

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Superabsorbents are type of hydrogels capable to swell and absorb a large amount of water. While the shapes of hydrogels do not change extensively during swelling, because of highly swelling capacity of superabsorbent hydrogels, their shape will extensively change. Because of their excellent response to changing environment conditions such as temperature, pH, and solvent composition, hydrogels have been attracting in many industrial applications. Superabsorbents with high swelling capacity are of special interest as potential water retainer systems for agriculture fields [1].

The higher production cost and low gel strength of these hydrogels, however, restrict their application widely. To improve these limitations, inorganic compounds with low cost can be used. The introduction of inorganic fillers to a polymer matrix increases its strength and stiffness properties. It has been reported that the type of dispersion of clay in composites determines the properties of polymer composites. Among these materials, superabsorbents composites are a class of crosslinked polymers as they can be synthesized through insertion of water soluble polymers into clay particles through polymerization of hydrophilic monomers in the presence of clay powder [2]. In the present study, we attempted to synthesize a novel superabsorbent composite using acrylamide (AAm) and itaconic acid (IA) monomers as well as laponite clay in the presence of APS and TEMED as the initiator and the catalyst, respectively. In this work, the superabsorbent composites were prepared in the absence of any organic crosslinker. The effect of reaction variables on the equilibrium swelling capacity and also, the thermal stability of the samples were determined.

References:

[1] Mark, H. F. *Encyclopedia of Polymer Science and Technology,* Vol. 2, Hydrogels, by Jay Friedrich Künzler, Bausch and Lomb Inc., John Wiley & Sons, Inc., **2004**, 691-722.
[2] Peng Li, Nam Hoon Kim, David Hui, Kyong Yop Rhee, Joong Hee Lee. *Applied Clay Science* 2009**,** *22*, 414.

Synthesis of some new 2-amino, 2- alkyl amino and 2- thioalkyl -4, 5- diaryl imidazole derivatives

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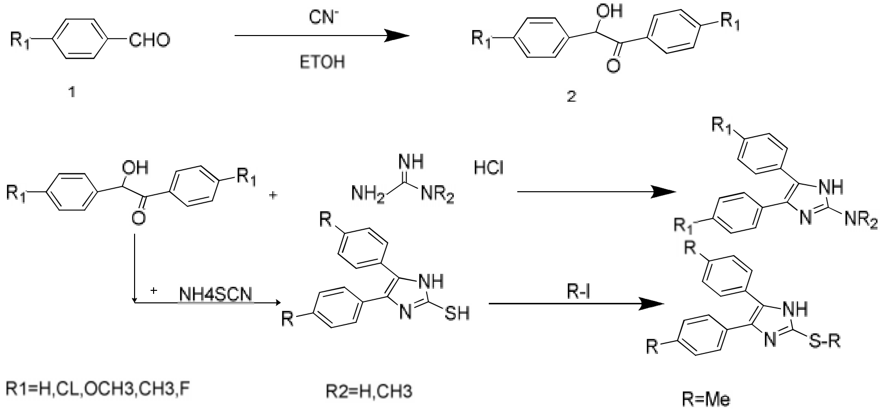
Diaryl heterocyclic derivatives showed anti inflammatory properties that are referred to cyclooxygenase (COX) enzyme inhibition. The inhibition of COX enzyme causes to reduce inflammatory factors such as prostaglandins[1].In such inflammatory nervous disorders such as Alzheimer and dementia, the inflammation was occurred on the neurons in central nervous system (CNS)[2]. In the present study some diaryl imidazole compound were synthesized.

Starting from guanidine hydrochloride (2), reaction with benzoine (1), 2- amino-4, 5 diaryl imidazoles were prepared. In the other hand reaction of benzoine (1) with ammonium thiocyanate gave 4,5-diaryl imidazoles 2-tione. The alkylation's of the last compound with methyl iodide gave 2- methyl thio -4,5 –diaryl imidazole. The reaction was optimized and the yield of reaction was studied. The structures of synthesized compounds were confirmed by ^{1}HNMR and Mass spectra.



References:

[1] Praveen Rao, Amini M, Habeeb AG,Knaus E.E, Med. Chem. Lett .2003, 13: 2205.
[2] Broe AG, Grayson DA, Creasy EM, Warte LM, 2000, 57 (11): 1586.
[3] M.Salami, M.Gharemani, N.Naderi, M.Amini, F.Salami, M.Amanlou, K.Abdi, R.Salehi, A.shafiee, acta phamacol. Sin. 2007, 28(8), 1254.

Synthesis of 1-phenyl imino(1H,3H) thiazolo [3,4-a]benzimidazole derivatives

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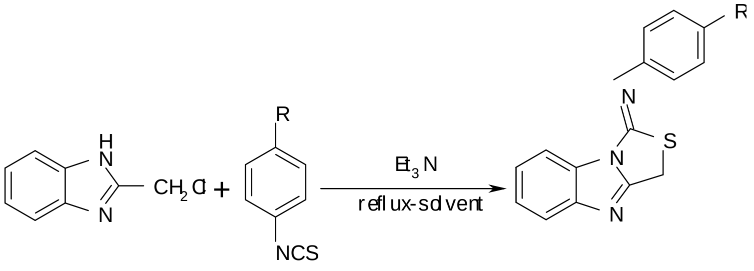
In several papers reported a series of 1-aryl-(1H,3H)thiazolo [3,4-a] benzimidazole which proved to highly active as HIV-1 NNRTIs.Extensive structure-activity relationship(SAR) studies have been performed within this family of compounds and it has been observed that specific requirements exist with regard to the structural determints for optimum anti-HIV activity [1].

In this article, we report synthesis 1-phenyl imino (1H,3H) thiazolo [3,4-a] benzimidazole derivatives from the reaction of 2-Chloromethylbenzimidazole with several aryle isothiocyanates [2].

In the rayl isothiocyanates C=S and C=N sites are reactive center and substituents on aryl isotjiocyante had a large influence on the competition between the alternative reaction site [3].
NNRTIs : non-nucleosides reverse transcriptase.



R: H, CH_3, NO_2

References:

[1] A .Rao, A.; Chimirri, E. D.; Dercq, A. M.; Monforte, P.; Monforte, C.; Pannecouque and Zappala, M. *IL Farmaco*. **2002**, *57*, 819.
[2] Phillips, A. *J. Chem. Soc.* **1928**, 2393.
[3] Butler, R. N.; Grogan, D. C.; Mc. Donald, P. D.; Burke, L. A. *J. Chem. Soc., Perkin Trans. 1*, **1997**, 3587.

Solvent free nucleophilic addition of primary amines to dimethyl (*E*)-2-(2-nitrophenoxy)-2-butenedioate

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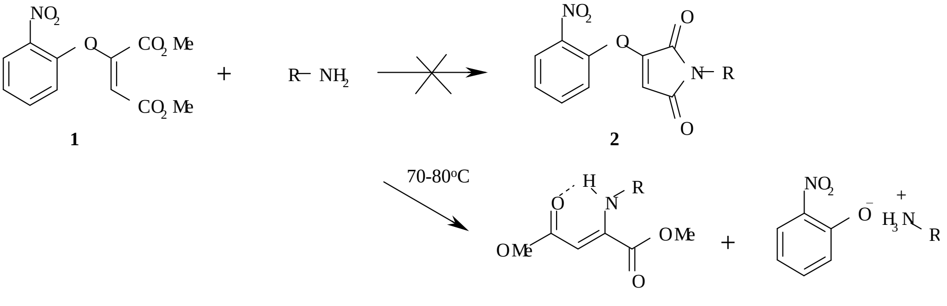
Nucleophilic addition to benzene derivatives with electron withdrawing groups on the *ortho* and *para* position relative to leaving group is an important strategy to synthesis of substituted benzenes [1]. We have recently developed a general method for the preparation of dimethyl (*E*)-2-phenoxy-2-butenedioate from the reaction of various substituted phenols with dimethyl acetylenedicarboxylate in the presence of a catalytic amount of trimethylamine solution [2]. We envisioned that an addition of primary amines to dimethyl (*E*)-2-(2-nitrophenoxy)-2-butenedioate **1** should give the malimide derivatives **2** [3]. Unexpectedly, however, this reaction afforded enaminocarbonyl compounds **3** and quaternary ammonium salt **4** quantitatively under solvent free conditions at 70-80°C. The structures of **3** and **4** were deduced by ^{1}H, ^{13}C NMR, and IR spectroscopy.



1 **2** **3** **4**

References:

[1] Citterio, A. *Org. Synth.* **1984**, *62,* 67.
[2] Nasiri, F.; Atashkar, B. *Monatsh Chem.* **2008**, *139*, 1223.
[3] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62,* 6968.

N-Methyl pyrrolidinium hydrogen sulfate an efficient acid catalyst for the three-component synthesis of α -amino nitriles ,coumarins and amidoalkyl naphthols

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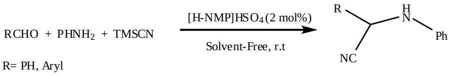
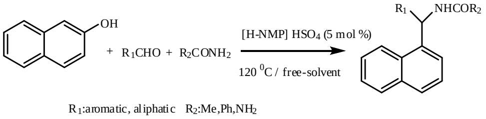
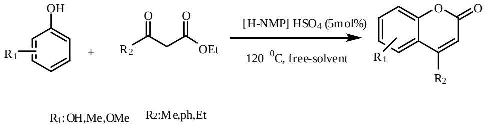
Multi-component reactions (MCRs) are very important and as they can produce the target products in one pot without isolating the intermediates and reducing the reaction times and energy have attracted more interest in modern organic syntheses. α–Amino nitriles are important intermediates for prepation of α-amino acids [1]. The strecker reaction is one of the general method in synthesis of α-aminonitriles [2]. The coumarins are heterocyclic organic compounds [3], Pechmann reaction is a well-known simple method for synthesize of coumarins from phenols and β-ketoesters in the presence of an acid catalyst. Interestingly the 1-amidomethyl-2-naphthols can be converted to important biologically active 1-aminomethyl-2-naphthol derivatives by an amide hydrolysis reaction [4].

herein we wish to report an efficient and green method for the synthesis of α-aminonitrils , coumarins and amidoalkyl-2-naphtols employing Brönsted acidic ionic liquid [H-NMP][HSO_4] as novel catalyst under solvent -free conditions were prepared using this methodology as shown belowin. good to excellent yields with short reaction times Simple work-up and reusability of the catalyst are advantages of this method. The products were characterized by spectral data (IR, ^{1}H and ^{13}C NMR) and with comparison of their physical data (m.p) with the literature data.







References:

[1] Dyker ,G. *Angew.Chem., Int. Edn* **1997**, *36*, 1700**.**
[2] Strecker,A. *Ann. Chem. Pharm.* **1850**, *75*, 27.
[3] Costova, I N.; Nikolov, N M.; Chipilska, L N . *J Ethnopharm* . **1993**, *39*, 205**.**
[4] Shen, A. Y.; Tsai, C. T.; Chen, C. L. *Eur. J. Med. Chem.* **1999**, *34*, 877.

H_2O_2-$SOCl_2$ As an efficient system for the oxidation of organonitrogen compounds

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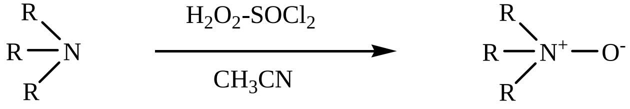
The development of simple, efficient, environmentally-benign and economically viable chemical processes or methodologies for widely used organic compounds is in great demand. Oxidation of organonitrogen compounds is importantm both from industrial and synthetic viewpoints as *N*oxides obtained by oxidation of tertiary nitrogen compounds find wide application as oxidants, and offer functional group manipulation and structural modification possibilities not accessible by other methods [1].

The search for general, efficient syntheses of *N*-oxide compounds under mild conditions is of continuing interest for organic chemists. A variety of catalytic methods are reported in the literature for the oxidation of tertiary nitrogen compounds to N-oxides [2]. However, most of these methods are deficient in some respects, such as low yields, difficult accessibility, drastic reaction conditions which effect substituents. In continuation of our studies on oxidation [3], we report herein a new and simple method for the oxidation of a variety of tertiary nitrogen compounds to N-oxides in near quantitative yields using H_2O_2 as oxidant and $SOCl_2$ as the promoter (Scheme 1).



Scheme 1.

References:

[1] (a) Rheenen, V. Van; Cha, D. Y.; Hartley, W. M. *Org. Synth. Coll. Vol.* 6 **1988**, 342; (b) Schroder, M. *Chem. Rev.* **1980**, 80, 187.
[2] (a) Zhu, Z.; Espenson, J. H. J. Org. Chem. 1995, 60, 1326; (b) Jiao, Y.; Yu, H. Synlett 2001, 1, 73.
[3] (a) Bahrami, K. *Tetrahedron Lett.* **2006,** *47*, 2009; (b) Khodaei, M. M.; Bahrami, K.; Shiekh Arabi, M. *J. Sulfur Chem.* **2010,** *31*, 83.

Efficient iodination of aromatic compounds using polymer supported ICl_2^-

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Halogenation of organic substrates is an important reaction for the preparation of pharmaceutical and agrochemicals [1]. Iodine-substituted aromatic compounds have found wide applications in medicine and biochemistry. Iodo-arenes and vinyl iodides are important synthetic intermediates in various cross-coupling reactions, especially for carbon-carbon and carbon-heteroatom bond formations [2].

On the other hand, the use of polymeric reagents as participants in organic synthesis has emerged as an attractive approach in both fundamental and biological fields in recent years [3,4]. Although there are several polymeric halogenating reagents, only a few reports on iodinating reagents are found in literature. Since the iodine molecule is the least reactive among the halogens towards electrophilic substitution processes, most of the synthetic effort has been placed in converting molecular iodine into a more active species [3].

Herein we report the preparation of poly [1,4-phenylen diamine-co-pyridine 2,5-dicarboxylic acid] dichloroiodate as a polymeric iodinating reagent, and use of this polymeric reagent for the iodination of active aromatics such as amines and phenols. The spent reagents after completion of reactions were easily removed by filtration and were regenerated for further use. Easy work-up and high yields are other advantages of using this polymeric reagent.

References:

[1] Seevers, R. H.; Counsell, R. E. *Chem. Rev.* **1982**, *82*, 575.
[2] Diederich, F.; Stang, P. J. *Metal-Catalyzed Cross-coupling Reactions,* Wiley-VCH: New York, **1997**.
[3] Sumi Mita, S.; Sreekumar, K. *Macromol. Chem. Phys.* **1997**, *198*, 1611.
[4] Tamami, B.; Parvanak Borujeni, K. *Iranian Polymer Journal* **2009**, *18*, 191.

Synthesis and evaluating some new mono and bis azo dyes and pigment

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Azo compounds and their complexes with transition metals have attracted much attention, in part because of their physicochemical properties and applications in many important areas. They are highly colored and have been studied widely because of their excellent thermal and optical properties in applications such as optical data storage, photoswitching, non-linear optics and photochromic materials, dyes, chemical analysis and pharmaceuticals .Furthermore, azo compounds are known to be involved in a number of biological reactions such as inhibition of DNA, RNA and protein synthesis, carcinogenesis, and biological activity against bacteria and fungi [1-2]. Heterocyclic amines have been used extensively in the preparation of disperse dyes. These dyes show outstanding discharge-ability on polyester [3].

A series of some new mono and bis azo dyes from aniline derivatives as bisazo components has been synthesized by the coupling reactions whit resorcinol. In this effort,Different azo deyes were synthesized, separated and charactrized, and then The condensation was buffered with sodium bicarbonate at a reaction temperature of less than 10°c. The structure of the compounds confirmed by FT-IR, ^{1}H-NMR,^{13}C-NMR,UV spectra.

References:

[1] Wang S, Shen S, Xu H. Synthesis, spectroscopic and thermal properties of a series of azo metal chelate dyes. Dyes Pigments **2000**;*44*(3): 195.
[2] Abe T, Mano S, Yamada Y, Tomotake A. Thermal dye transfer printing with
[3] Process Research laboratory, Glenmark Research Centre, T.T.C. Industria Area, Mahape, Navi, Mumbai400709 India

Novel periodic mesoporous silica chlorides (PMSCl) with 2D P_6mm hexagonal structures: efficient catalysts for the Beckmann rearrangement

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Since the first reports on surfactant–templated mesoporous materials appeared in the past decade, a wide variety of these materials, which possess uniform channels with large pore size (2 – 40nm), high surface area (up to 2000 $m^2.g^{-1}$), and tuneable structure have been synthesized [1].

Herein we described a novel route for the synthesis of a family of ordered mesoporous chlorinated silica (namely SBA-Cl-1 and SBA-Cl-2) with 2D P_6mm hexagonal structures and tunable wt% of chlorine by treating SBA-15 with thionyl chloride. Owing to high surface area, high mesopores volume, and tunable wt% of chlorine content, these *nano-silica-chlorides* could be considered as very promising materials in catalysis, and also in the preparation of new highly loaded stationary phase for various types of chromatographic techniques.

Encouraged by high surface area, high chlorine content of the surface, and highly stable and ordered structures of SBA-Cls, we speculated whether these materials might also be suitable catalysts (or reagents) in some organic tranformations. Along the line of this hypothesis, we were also interested to study the catalytic performance of SBA-Cls in the Beckmann rearrangement. The Beckmann rearrangment is a common organic transformation to convert ketoxime into amides [2]. We demonstrated that these materials are effective catalysts for the Beckmann rearrangements of various types of ketoximes.

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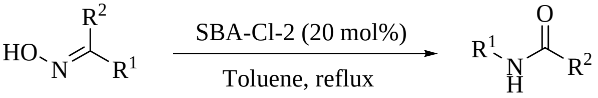

References:

[1] (a) Kresge, C. T.; Leonowicz, M. E.; Roth, W. J.; Vartuli, J. C.; Beck, J. S. *Nature* **1992**, *359*, 710. (b) Zhao, D.; Feng, J.; Huo, Q.; Melosh, N.; Fredrickson, G. H.; Chmelka, B. F.; Stucky, G. D. *Science* **1998**, *279*, 548.

[2] (a) Marthala, V. R. R.; Jiang, Y.; Huang, J.; Wang, W.; Gläser, R.; Hunger, M. *J. Am. Chem. Soc.*, **2006**, *128*, 14812. (b) Marthala, V. R. R.; Rabl, S.; Huang, J.; Rezai, S. A. S.; Thomas, B.; Hunger, M. *J. Catal.*, **2008**, *257*, 134. (c) Palkovits, R.; Schmidt, W.; Ilhan, Y.; Erdem-Senatalar, A.; Schüth, F. *Micropor. Mesopor. Mater.*, **2009**, *117*, 228.

Alumina-supported manganese porphyrin: An efficient catalyst for aromatization of Hantzsch 1,4-dihydropyridines and epoxidation of alkenes with (MCPBA)

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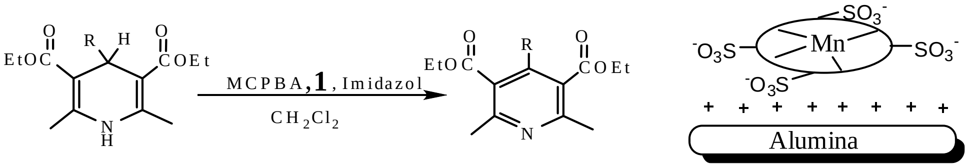
Today the development of an efficient model system resembling the activity of cytochrome P-450 has been one of the areas of most intense research activity [1−2]. Many metalloporphyrin complexes, mainly iron and manganese, proved to be able to catalyze oxidation reactions [3−4]. High yields and rates have been obtained with these biomimetic systems, making them useful for complete conversion of various substrates and potentially useful preparative oxidations in organic chemistry [5−6].

In this work aromatization of 1,4-dihydropyridines and epoxidation of a wide range of alkenes have been performed by Meta-Chloroperoxybenzoic Acid (MCPBA) as an oxidizing agent in CH_2Cl_2 in the presence of the catalytic amount of anionic porphyrin-5,10,15,20-(*p*-sulfonatophenyl)-porphyrinatomanganese(III) acetate (Mn(TSPP)OAc) supported on alumina (**1**) and imidazole. These procedures offers several advantages including low loading of catalyst, high yields and short reaction time.



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References:

[1] M.J. Coon and R.E. White, Dioxygen Binding and Activation by Metal Centers, T.G. Spiro, Ed., pp.73, Wiley: New York, **1980**.
[2] R.E. White and M. Coon, *J. Annu. Rev. Biochem*. **1980**, 49, 315.
[3] A.J. Appelton, S. Evans and J.R. Lindsay Smith, *J. Chem. Soc*. **1996**, 2, 281.
[4] P. Ho_man, A. Robert and B. Meunier, *Bull. Soc. Chim. Fr*. **1992**, 129, 85.
[5] A. Maldotti, C. Bartocci, G. Varani, A. Molinari, P. Battioni and D. Mansuy, *Inorg. Chem*. **1996**, 35, 1126.
[6] D. Dolphin, T.G. Traylor and L.Y. Xie, *Acc. Chem. Res*. **1997**, 30, 251.

Synthesis of mono- and bis photocromism compounds

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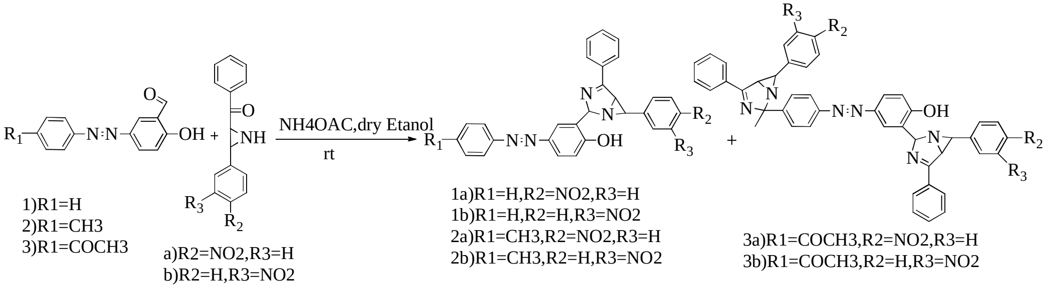
Photochromism is defined as the reversible conversion induced by light of substance (photochromism) into product that differing in absorption spectrum (color) and internal energy, dielectric constant and other physicochemical parameters. Photochromic materials are used widely. Photochromism has attracted considerable attention because of its potential application to molecular devices, such as optical memories and switches. Among various photochromic compounds, 1,3-diazabicyclo[3.1.0]hex-3-ene derivatives are the subject of intense research due to their photochromic behavior even in the crystalline state. Molecules which show photochromic reactivity in the crystalline state are rare. In recent years, they are being considered as extremely promising systems to store information [1- 3].

In this effort, for first time different azo deyes such as **1**-**3** were synthesized, separated and charactrized, and then was reacted with various ketoaziridins **a** and **b** in the present of excess ammonium acetate in the dry ethanol as solvent at room temperature in the required time. The desired compounds content in their structure one **1a**-**2b** and two molecules of ketoaziridine **3a**-**3b** were synthesized and characterized by TLC, m.p., IR, ^{1} H NMR, ^{13}CNMR, and UV-Vis spectra.



References:

[1] H. Kiyani, N. O. Mahmoodi, K. Tabatabaeian, M. Zanjanchi, *J. Phys. Org. Chem.*, **2009**, *22*, 559.
[2] H. Kiyani, N. O. Mahmoodi, K. Tabatabaeian, M. Zanjanchi, *Mendeleev Commun.* **2009**, *4*, in press.
[3] N. O. Mahmoodi, K. Tabatabaeian, M. Arvand, H. kiyani and B. Sharifzadeh, Russian Journal of Organic Chemistry has been accepted for publication **2010**,*46*, No.6.

A green synthesis of functionalized 1,3-dithiolanes

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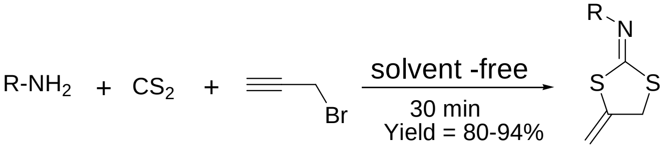
2-Iminium-1,3-dithiolanes are important in crop protection against herbicides. Several methods for the synthesis of these thiolanes have been developed amongst which the most widely used methods include the reaction of *vic*-dithiocyanates in refluxing hydrochloric acid, by the reaction of *vic*-dithiols and cyanogen chloride, acid-catalyzed cyclization of propargyl, allylic, or β-hydroxy alkyl esters of dithiocarbamic acids, photolysis of chlorinated *S*-allyl dithiocarbamate compounds, and by the iodocyclization of S-allyl dithiocarbamates [1-4]. We report herein the synthesis of 2-iminium-1,3-dithiolane derivatives under mild conditions by reacting aliphatic and aromatic amines with CS_2 and propargyl bromide without any catalyst and solvent. This procedure avoids the difficulties of other methods such as toxicity of cyanogen chloride, the corrosiveness of mineral acids and low yield of products. Various features of this reaction will be presented and discussed.



References:

- [1] Maxwell, R. J.; Silbert, L. S. *J. Org. Chem*. **1977**, *42*, 1515.
- [2] Addor, R. W. *J. Org. Chem*. **1964**, *29*, 738.
- [3] Kennard, K. C.; Vanallan, J. A. *J. Org. Chem*. **1959**, *24*, 470.
- [4] Halimehjani, A. Z.; Maleki, H.; Saidi, M. R. *Tetrahedron Lett*. **2009**, *50*, 2747.

Solvent-free ring-opening of epoxybis(silane) with aromatic thiols catalyzed by $MgBr_2 \cdot OEt_2$

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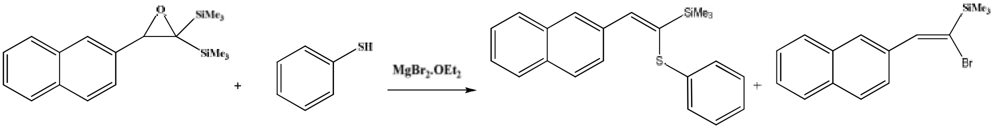
α-Ring opening of *α,β*–epoxybis(silanes) has been observed under both nucleophilic and electrophilic conditions. They undergo regio- and stereospecific *α*-opening by a variety of nucleophiles which experience syn or anti *β*-elimination providing a convenient route to a number of heterosubstituted olefins of known stereochemistry. Ring opening of epoxybis(silane) with thiols is an important method in organic synthesis. In recent years, magnesium bromide ethyl etherate ($MgBr_2 \cdot OEt_2$) has found many applications as a mild Lewis-acid to ease various synthetic organic transformations. Ring opening of *α,β*-epoxybis(silanes) with thiophenol under magnesium bromide ethyl etherate catalysis affords formation of thiovinylsilane at room temperature. Nucleophilic attack of the thiols and subsequently Peterson olifination occures and gives the corresponding thiovinylsilane. This process is highly regioselective for the bis(silyl)-substituted carbon.

The results of ^{1}HNMR. ^{13}CNMR, FT-IR, GCmass spectra and CHNS has confirmed the formation of these products.



Refrences:

[1] Hodgson,D.M.Cominaa,P.J. and Drew,M.G.*J.Chem.Soc.Perkin Trans.* **1997,** *1,* 2279.
[2] Cuadrado, P. and Gonzalez-Nogal,A.M.*Tetrahedron Lett,* **2000,** 1111.
[3] Mojtahedi, M.; Bolourtchian, M.; Abbasi. H., *Phosphorus, Sulfur, and Silicon,* **2007,** *182,* 905.
[4] K.D. Safa, Kh.Ghorbanpour, A.Hassanpour, Sh.Tofangdarzadeh. *Journal of Organometallic Chemistry* **2009,** *694,* 1907.

Triplet germylenes *vs.* triplet silylenes *vs.* triplet carbenes: Theoretical predictions

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Divalent carbenes, silylenes and germylenes are of considerable interest in organic and organometallic chemistry [1]. However, there are some differences in the electronic ground states and the atomic properties of these Group 14 elements [2]. In this study, singlet and triplet Group 14 divalents, with H-M-X and MX_2 formulae, are compared and contrasted at QCISD(T)/6-311++G** and B3LYP/6-311++G** levels (M = Ge, Si, C, and X = H, Li, Na, K). Among these 42 species, 6 novel ground state triplet germylenes, H-Ge-X and GeX_2, are encountered which appear more stable than their corresponding singlet minima (X = Li, Na, K). All H-M-X and MX_2 angles (Φ) emerge wider in triplet species compared to their corresponding singlet states. All triplet X-*M*-X species appear more linear than their corresponding triplet H-M-X, for M = Ge, Si, but not C.

As the electro-positivity of X increases, the M-X bond distances in all species lengthen, while their singlet-triplet energy separations ($\Delta E_{s\text{-}t}$) decrease. The $\Delta E_{\text{LUMO-HOMO}}$ for singlet HMX and MX_2 species appear inversely proportional to the size of X, showing a trend of K > Na > Li, for M = Ge and Si, but not for C. So, for M = C, not only the size trend fails, but the relative sensitivity to X also diminishes. Interestingly, for singlet MX_2 species, linear correlations are found between the $\Delta E_{\text{LUMO-HOMO}}$ and their corresponding $\Delta E_{s\text{–}t,X}$, merely for M = Ge, but not C and not even for Si!(Fig. 1).

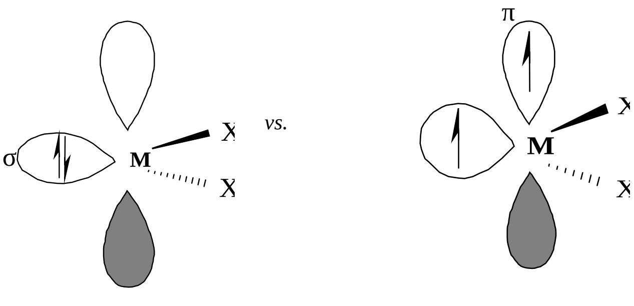

Fig. 1. The highest occupied molecular orbitals (HOMO) for the singlet ($\sigma^2\pi^0$) states of divalents (MX_2) and the singly occupied molecular orbitals (SOMO) for the corresponding triplet ($\sigma^1\pi^1$) states.

References:

[1] Nemirowski, A.; Schreiner, P.R.; *J. Org. Chem.* **2007,** *72*, 9533.
[2] Kassaee, M.Z;. Buazar, F.; Soleimani-Amiri, S.; *J. Mol. Struct. (THEOCHEM)* **2009**, *899*, 46.

Synthesis and characterization of polymers based on poly(styrene-co-maleic anhydride) with 9-anthracene methanol.

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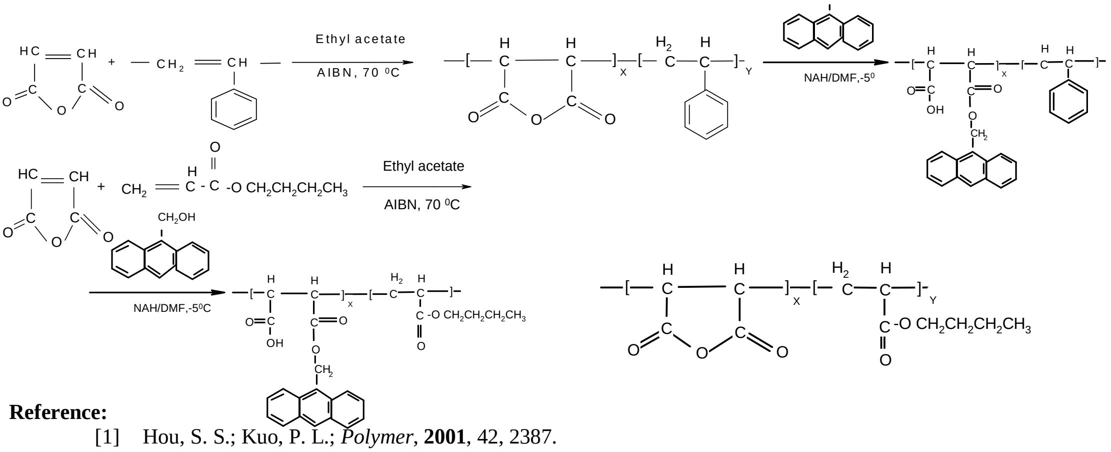
In this work the compolymers of maleic anhydride(MAN) with different monomers such as 4-metoxy styrene, 4-methyl styrene ,were synthesized by free radical polymerization method in ethyl acetate solution using azobis (iso butyronitrile) (AIBN) as initiator at 70±1°C [1].

The structure and compositions of the copolymers were determined by ^{1}H-NMR and permeation chromatography respectively [2].

The, copolymers of MAN have been modified by incorporation of highly sterically hindered demanding 9-anthracene methanol through the MAN motieties. The structure of all the polymers was characterized by FT-IR, ^{1}H-NMR spectroscopic techniques[4]. It was found that these polymers with 9-anthracene methanol groups in polymer side chains leads to an different in the rigidity and glass transition temperature of polymer as shown by dynamic mechanical thermal analysis(DMTA)[3]. The results show that, with the incorporation of the 9-anthracene methanol group in the polymer side chains, a series of novel modified polymer are obtained.

Figure shows the synthesis route of copolymers.



Reference:

[1] Hou, S. S.; Kuo, P. L.; *Polymer*, **2001**, 42, 2387.

[2] Chitanu, G.; Bumbu, G. G.; Stoleriu, A.; carpov, A.; vasile, C.; Anghelescu- Dogaru, A.; Rinaudo, M.; *Polymer Degradation and stability*, **1999**, 65, 75.

[3] Dincer, S.; Koseli, V.; kesim, H.; Rzaew, Z. M. O.; piskin, E.; *European polymer Journal* , **2002**, 38, 2143.

[4] Al- sabagh, A.M.; Noor El- Din, M.R.; Morsi, R.E.; Elsabee, M.Z.; *journal of petroleum science and Engineering*, **2009**, 65, 139.

Synthesis of (4-oxo-1,3-thiazinan-5-yl)acetic acids from isothiocyanates, alkylamines, and ithaconic anhydride

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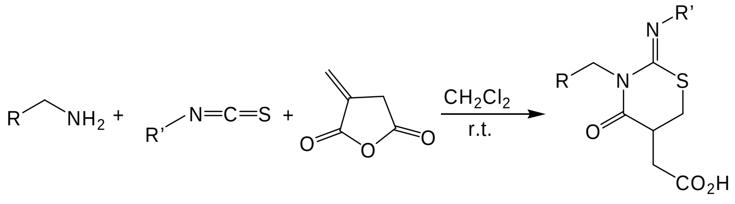
Polyfunctionalized heterocyclic compounds play important roles in the drug discovery process. Analysis of drugs in late development or on the market shows that 68% of them are heterocycles. Therefore, it is not surprising that research in the field of synthesis of heterocyclic compounds has received special attention [1]. Multicomponent reactions (MCRs), because of their productivity, simple procedures, convergence, and facile execution, are one of the best tools in combinatorial chemistry [2]. Therefore, the design of novel MCRs has attracted great attention from research groups working in various areas such as drug discovery, organic synthesis, and material science. As a result, the number of new MCRs in recent years is growing rapidly [3].

Herein, we report a three-component synthesis to (4-oxo-1,3-thiazinan-5-yl)acetic acids. The reaction of primary amines with phenylisothiocyanate and benzoylisothiocyanate in the presence of itaconic anhydride (dihydro-3-methylenefuran-2,5-dione, proceeded smoothly in CH_2Cl_2 and was complete within 2-5 h. The ^1H- and ^{13}C-NMR spectra of the crude products clearly indicated the formation of (4-oxo-1,3-thiazinan-5-yl)acetic acids in good yield.



R = Alkyl, Benzyl R' = Phenyl, Benzoyl Yield: 56-85%

References:

[1] A. Dömling, I.Ugi, *Angew. Chem., Int. Ed. Engl.* **2000**, *39*, 3168.
[2] N. K. Terrett, *Combinatorial Chemistry*; Oxford University Press: New York, **1998**.
[3] R. V. A. Orru, M. Greef, *Synthesis* **2003**, 1471.

A novel catalytic method for synthesis of HNIW (CL-20)

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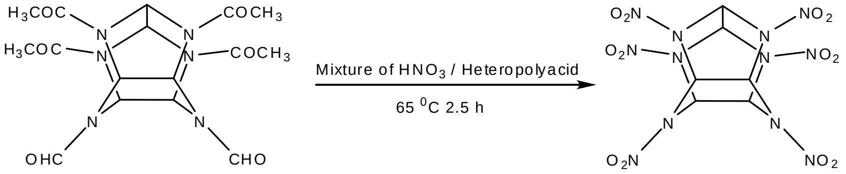
Hexanitrohexaazaisowurtzitane (HNIW or Cl-20) is a high-energetic material with a cage structure [1]. It is considered as the most powerful explosive. It is usually prepared via nitration of precursors with concentrated nitric and sulfuric acids [2]. We report herein for the first time the use of an efficient catalytic and mild reaction condition for nitration of 2,6,8,12-tetraacetyl-4,10-diformyl-2,4,6,8,10,12-hexaazaisowurtzitane (TADFIW). It has been well documented that heteropolyacids (HPAs) are an efficient and green catalysts. So we use it as nitric acid activator. This strategy gave us a milder condition for nitration reaction. Also we could run reactions in reasonably lower temperature. All these modifications gave us excellent results. By the use of new nitrating agents, the reaction eliminated the use of concentrated sulfuric acid and was environmental friendly. Meanwhile, the effects of the reaction temperature, time and other factors on the yield were analyzed. The structure and purity of the compounds were characterized by elemental analysis, HPLC, IR, ^{1}HNMR.



Nitration of TADFIW to HNIW by HNO_3/Heteropolyacids (HPAs)

References:

[1] P. Karakaya, M. Sidhoum, C. Christodoulatos, S. Nicolich, W. Balas, J. Hazard. Mater. **2005**, *B120*, 183.
[2] S. Jin, Q. Shu, S. Chen, Y. Shi, Propellants, Explosives, Pyrotechnics, **2007**, *32*, 468.

Efficient cyanosilylation of aldehydes and the preparation of dihydropyrimidinones using benzyl DABCO bromide

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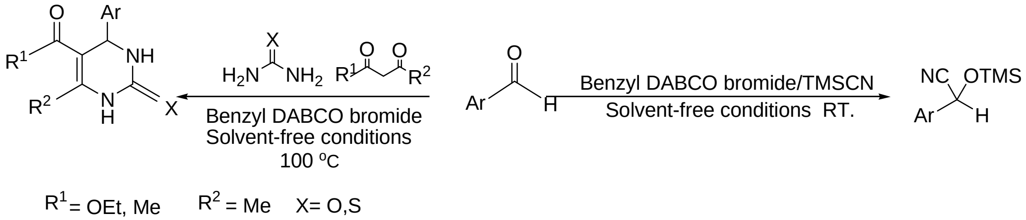
Organocatalysis is currently being vigorously pursued because of its attractive features such as the metal-free conditions, experimental simplicity and the ease to recover the organocatalysts [1]. A number of the applications of organocatalysts have been developed [2]. Here we report application of benzyl DABCO bromide as an organocatalyst for cyanosilylation of aldehydes and the preparation of dihydropyrimidinones.

Cyanosilylation of aldehydes was achieved by a simple mixing of aldehyde, trimethylsilyl cyanide (TMSCN) in the presence of benzyl DABCO bromide under solvent-free conditions at RT (Scheme). A wide range of aldehydes were subjected to cyanosilylation. However the reaction failed in the case of ketones, probably due to steric reasons.



Scheme

3,4-Dihydropyrimidinones (DHPMs) and their sulfur analogs have attracted considerable interest [3]. They are normally prepared using Biginelli reaction [4]. We report here benzyl DABCO bromide catalyzed the preparation of dihydropyrimidinones through a three-component reaction under solvent free conditions (Scheme). Benzaldehyde, β-keto esters or β-diketone and urea or thiourea reacted in the presence of benzyl DABCO bromide under solventless conditions at 100 °C within 50 min to furnish 3,4-dihydropyrimidin-2-(1*H*)-ones. Under the optimized reaction condition, similar condensations using various aldehydes were investigated. Aromatic aldehydes having electron-donating as well as electron-withdrawing substituents underwent the conversion smoothly.

In conclusion we have demonstrated a safe and simple method for the cyanosilylation of aldehydes and the preparation of dihydropyrimidinones under solvent free conditions at room temperature using benzyl DABCO bromide. It is also worthwhile to note that the catalyst is inexpensive and easily prepared.

References:

[1] Dalko, P. I. Moisan, L. *Angew. Chem., Int. Ed.* **2004**, *43,* 5138.
[2] Kobayashi, S. Tsuchiya Y. Mukaiyama, T. *Chem. Lett.* **1991**, 537.
[3] For a review, see: Kappe, C. O. *Acc. Chem. Res.* **2000**, *33*, 879.
[4] Biginelli, P. Gazz. *Chim. Ital.* **1893**, *23*, 360.

Synthesis of anti-corrosion inorganic-organic ($SrCrO_4$/poly o-phenylenediamine) nano capsules by green chemistry

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Corrosion of metals is one of the main destruction processes resulting in huge economic losses, especially in the aerospace, and automotive. The corrosion phenomenon is particularly important for the alkaline-acid sections of the oil industry, namely, the atmospheric distillation plants, pipelines, vacuum vessels, hydrodesulfuration plants, and catalytic reactors. Polymer or sol-gel coatings are normally applied on the metal surface providing a barrier for permeation of corrosive species. However, when the barrier is damaged and the corrosive agents penetrate the metal surface the coating system cannot stop the corrosion process. So far, the most effective anticorrosion coatings for active protection of metals are chromate-containing systems [1].

The drawback of chromates is their superior oxidation properties, which make them environmentally unfriendly. The hexavalent chromium species can be responsible for several diseases including cancer, which is the main reason for banning Cr^{6+}- containing anticorrosion coatings in Europe in 2007 [2].

One of the possible solutions to achieve active corrosion protection is to introduce an environmentally friendly corrosion inhibitor directly into the coating, providing release of the inhibitor and termination of the corrosion propagation at already damaged corrosion defects. To overcome this unavoidable problem, the streamline is the use of corrosion inhibitors (CI), which can significantly diminish the corrosion rate. As an inhibitor, strontium chromate is added into organic coatings to protect corrosion of iron, zinc, aluminum and their alloys [3,4]

Here, for making a high efficiency and safe corrosion inhibitor, $SrCrO_4$ nanoparticles were synthesized in brine medium. It is proposed that great attraction between $Si^{2+}$and Cl^- of brine cause a barrier for aggregation of nano particles [5]. Then a coating of poly o-phenylenediamine was prepared by oxidation polymerization with the help of urea-hydrogen peroxide.

Finally, corrosion inhibition of this nano capsule was studied by wheel test at Iranian oil company. This research has been done with cooperation of National Iranian South Oilfields Company.

References:

[1] Twite, R.L.; Bierwagen, G.P., *Prog. Org. Coat.* **1998,** *33,* 91.
[2] Khramov, A.N.; Voevodin, N.N.; Balbyshev, V.N.; Donley, M.S., *Thin Solid Films,* **2004,** 549.
[3] Yang, D.; Qi, L., *J. MA, Adv*. **2002,** *14*, 1543.
[4] Prosek, T.; Thierry, D., *Prog. Org. Coat.* **2004,** *49***,** 209.
[5] Wang, W.; Xu, C.; Zhen, L.; shao, W.; Yang, L., *Materials Letter.* **2007,** *61,* 3146.

Modification technique of polyacrylonitrile (PAN) fiber by chelating ligand for adsorption and removal of heavy metals from environment samples

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There are many techniques of modified fibers, which have large specific surface areas and high adsorption rates, have attracted great attention in heavy metal removal from wastewater in recent decades [1]. In this work a chelating fiber containing monoamide ligands was prepared via the stepwise modification of acrylic fibers, polyacrylonitrile (PAN), with iminodiaceticacid (IDA). First stage of modification was performed through hydrolysis in a base and at second step, carboxylic acid groups have been converted in to acid chloride groups by using thionyl chloride. Finaly, functionalization of PAN fibers was continued by iminodiaceticacid [2].

The fiber structure was investigated by different experiment techniques of characterization such as fourier transform infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), scaning electron microscopy (SEM) was also investigated in this study [3,4]. The polyacrylonitrile –monoamide (PAN-MA) was examined as chelating material in a series of batch adsorption experiment for removal Sm (Samarium) ion. The ion adsorption of PAN-MA was determined with the ICP method. PAN-MA show adsorption metal ions more than usual fiber because of the modification.

References:

[1] Chen, J. P.; Wang, L. *Chemosphere* **2004,** *54,* 397.
[2] Deng, S.; Bai, R.; Chen, J. P. *Colloid Interface Sci.* **2003**, *260*, 265.
[3] Liu, R. X.; Zhang, B.W.; Tang, H. X.; *React. Funct. polym*. **1999**, *39*, 71.
[4] Marie, J. R., E.; Ronald, D.N.; Per, M. C. *Langmuir* **2002**, *18***,** 1604.

One pot multi-component synthesis of octahydroquinazolinone and 3,4-dihydropyrimidin-2(1H)-ones and their corresponding 2-(1H)thiones

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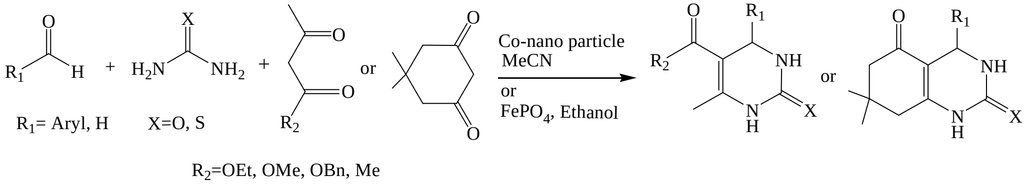
Dihydropyrimidinones (DHPMs) are an important class of heterocyclic compounds having important biological activities. They are reported to serve as the integral backbones of several calcium channel blockers, antihypertensive agents and α1-1-a-antagonists [1].

Octahydroquinazolinone derivatives have attracted considerable attention since they exhibit potent antibacterial activity against Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa, and calcium antagonist activity [2].

Many synthetic methods for preparing these compounds have been reported, many of these methods involve expensive reagents, strongly acidic conditions, long reaction times, high temperatures and stoichiometric amounts of catalysts, and give unsatisfactory yields. Therefore, the discovery of a new and an inexpensive catalyst for the preparation of these compounds under neutral and mild conditions is of prime importance [3].

Herein we wish to report a simple and efficient method for the synthesis of 1,2,3,4-tetrahydropyrimidine-5-carboxylate and 3,4,7,8-tetrahydroquinazoline. The reaction in the presence of Co-nano particle in refluxing acetonitrile and using Iron(III) phosphate in refluxing ethanol gave the corresponding dihydropyrimidinone and octahydroquinazolinone. This one-pot synthesis is novel in the sense that it preserves the simplicity of multi component one-pot reaction and improves the yields.



References:

[1] Wang, M.; Jiang, Heng.; Wang, Zh. *J. Chem. Research*. **2005**, 691.
[2] Hassani, Z.; Islami, M. R.; Kalantari M. *Bioorg. Med. Chem. Lett.* **2006**, *16*, 4479.
[3] Shaabani, A.; Bazgir, A.; Teimouri, F. *Tetrahedron Lett*. **2003**, *44*, 857.

Synthesis of palladium-nanocatalysts supported on carbon nanotubes and their application for cross-coupling reactions

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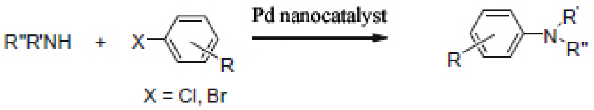
Aromatic amines are important substructures commonly used in synthetic pharmaceutical compounds, in xerographic, agrochemicals and photographic materials or in conducting polymers [1]. These materials have been prepared by Ullmann type reactions, which involve the coupling of amines with arylhalides, traditionally. Despite these copper promoted reactions that require high temperatures [2], palladium catalysts have developed for Buchwald–Hartwig amination reactions as a powerful synthetic method for the formation aromatic amines in mild conditions [3].

In this work four types of hybrid nanomaterials containing aromatic ligands π- stacked and wrapping dendrimeres on carbon nanotube as palladium nanocatalyst were prepared. Warpping and π-stacking of polymers which are able to support metal nanoparticles to CNTs not only improves their solubility and dispersability but lead to new hybrid nanostuctures suitable for chemical catalysis. All hybrid nanomaterials were able to support palladium nanoparticles. Variety of amines through cross coupling reactions (Buchwald reaction) catalyzed by these systems was synthesized and characterized (Scheme 1).

Yield and mild condition for preparation of amines showed that synthesized hybrid nanomaterials are promising systems in order to use in cross coupling reactions in high scale.



Scheme 1

References:

[1] Wolfgang Kleist.; Sandra S. Pröckl .; Markus Drees.; Klaus Köhler.; Laurent Djakovitch. *Journal of Molecular Catalysis A: Chemical* **2009 ,***303* 15.
[2] Mayur J. Bhanushali, Nitin S. Nandurkar, Malhari D. Bhor, Bhalchandra M. Bhanage *Journal of Molecular Catalysis A: Chemical 259* **2006** 46.
[3] R. Rama Suresh, K. C. Kumara Swamy *Tetrahedron Letters 50* **2009,** *6004.*

Synthesis of 3,4-dihydropyrimidin-2(1H)-ones and their sulfur derivatives with H_2SO_4 supported on charcoal

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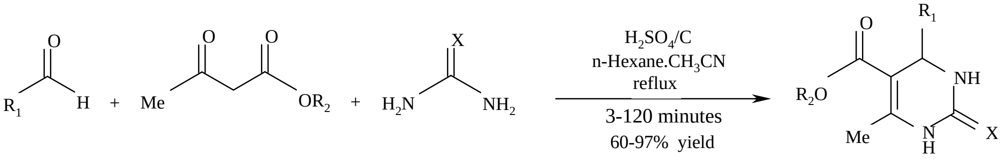
Biginelli reaction, first reported in 1893 [1], is a one-pot three component condensation of ethyl acetoacetate with benzaldehyde and urea in the presence of Bronsted acid giving 3,4-dihydropyrimidin-2 (lH)-ones. Because of the presence of dihydropyrimidone moiety in some bioactive natural products there has been increasing interest to synthesis multi-functionalized dihydropyrimidin-2(lH)-one scaffolds of promising pharmacological activity [2,3].

The literature review shows that a variety of reagents/catalysts have been reported for the synthesis of Biginelli 3,4-dihydropyrimidones. However, most of the reported methods suffer from disadvantages such as low yield of the products, long reaction times, expensive reagents/catalysts and harsh reaction conditions. In this context and in order to overcome these shortcomings, herein, we wish to report H_2SO_4 supported on charcoal as a fast and efficient promoter for three-component condensation of Biginelli 3,4-Dihydropyrimidin-2(1H)-ones (thiones). The obtained results show that this method provides an efficient and much improved modification of original Biginelli reaction, in terms of excellent yields, short reaction times and simple work-up procedure.



R_1: PH-Y, R_2: Et, Me, X: O,S

References

[1] P. Biginelli, Gazz. *Chim. Ital*. **1893**, *23*, 360.
[2] C.O. Kappe, *Tetrahedron* **1993**, *49*, 6937**.**
[3] A.D. Patil, N.V. Kumar, W.C. Kokke, M.F. Bean, A.J. Freyer, C.D. Brosse, S. Mai, A. Truneh, D.J. Faulkner, *J. Org. Chem*. **1995**, *60*, 1182.

Synthesis and characterization of new composites of poly(*o*-Toluidine) and polyaniline with silica sulfuric acid by solid-state method

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Polyaniline (PANI) is a very important polymer owing to its diversified chemistry and interesting physical properties [1]. Preparation of composites of conducting polymer (PANI) has been considered to provide a suitable solution to the processibility problem [2-3] and in addition, it has been found that ring-substituted (alkyl and alkoxy) and *N*-alkyl substituted PANI are more soluble than unsubstituted PANI. Therefore, many studies have been devoted to the synthesis of soluble PANI derivatives [4].

One way of making composites involves synthesizing the conductive polymer inside the matrices of conventional polymers (for example, inorganic polymers such as silica) or incorporating the inorganic component into the conducting PANI matrix using chemical or electrochemical polymerization [5].

In continuation of our recent works on the application of heterogeneous reagents and solid acids for the development of useful synthetic methodologies, herein we wish to report a new application for silica sulfuric acid (SSA) as solid acid [6-7].

In the present paper, new composite of poly(*o*-toluidine) (POT) with silica sulfuric acid was directly synthesized by using a solid-state polymerization method in present of iron (III) chloride hexahydrate as oxidant in chemical polymerization of *o*-toluidine and so on polyaniline emeraldine base (PA-EB) doped with SSA in solid state to preparation of the composite . The composites were characterized by Fourier transform infrared (FT-IR) spectra, ultraviolet visible (UV-Vis) spectrometry and conductivity measurements. Scanning electron microscopy (SEM) was done to study the morphology of composites.

References:

[1] Mishra, A.K.; Tandon, P., *J. Phys. Chem*. B. **2009**, *113*, 9702.
[2] Paul, D.R.; Robeson, L.M., *Polymer nanotechnology: Nanocomposites, Polymer*. **2008**, *49*, 3187.
[3] Pud, A.; Ogurtsov, N.;, Korzhenko, A.; Shapoval, G., *Prog. Polym. Sci*., **2003**, *28*, 1701-1753.
[4] Jamal, R.; Abdiryim, T.; Nurulla. I., *Polym. Adv. Technol*. **2008**; *19*: 1461.
[5] Modarresi-Alam, A.R. et al. *Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications, Ottawa, Ontario, Canada, 4-6 August* **2010**.
[6] Modarresi-Alam, A.R.; Khamooshi, F.; et al *Scientia Iranica* **2008**, *15*, 452.
[7] Modarresi-Alam, A.R.; Khamooshi, F., et al, *ARKIVOC* **2007**, *xvi*, 238.

Synthesis and characterization of some new polyaspartimide

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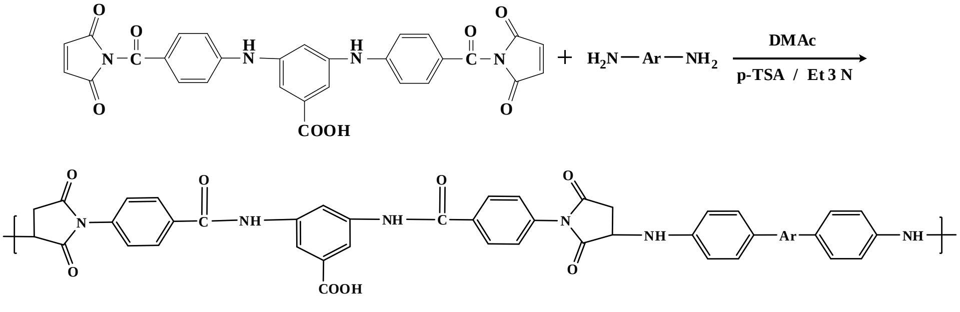
Research on thermostable polymers has involved structures with high resonance energies with strong chemical bonds. The compounds investigated contain double bond rings conjugated with heteroatoms; these polymers are resistance to high temperatures and are widely used in the field of aeronautics, and some composite organic matrix pieces used in this domain must retain their properties in continuous service at temperatures higher than 200 °C [1].

Bismaleimides (BMI) are interesting materials with good thermal stability and wide application from their synthesis polymers and resins. Various applications of polyaspartimide indicate good thermal stability, chemical behavior and thermomechanical properties of these type polymers [2].

Some high thermal resistance polyaspartimides were synthesized via Michael addition reaction between equimolar of various aromatic diamines with the new synthesis bismaleimide as monomer which prepared from 3, 5-diaminobenzoic acid and 4-maleimidobenzoic acidchloride [3, 4]. The monomer completely characterized by FT-IR, ^{1}H NMR, ^{13}C NMR and elemental analysis. In the polymer synthesis, *p*-toluenesulfonicacid and N, N-dimethylacetamide was used as a catalyst and as a solvent (scheme 1). The polymers are soluble in highly polar solvent such as DMF, DMSO, DMAc. All polymers were characterized by fourier transformed infrared, proton nuclear magnetic resonance spectroscopy, elemental analysis, thermal gravimetric analysis and differential scanning colorimetry. Thermal analyses indicate that the polymers are fairly heat stable. Used condition for polymers preparation showed below schematically.



(Scheme 1)

References:

[1] Grenier-Loustalot, M. F. *Eur. Polym. J.* **1998,** *34,* 95.
[2] Sava, M. *J. Appl. Polym. Sci.* **2009,** *112,* 1399.
[3] Wang, C. S.; Lin, C.H. *Polym.* **1999**, *40*, 5665.
[4] Wu, C. S.; Liu, Y. L.; Chiu, Y.S. *Polym.* **2002,** *43,* 1773.

Investigation on benzylic rearrangement on the surface and under microwave irradiation

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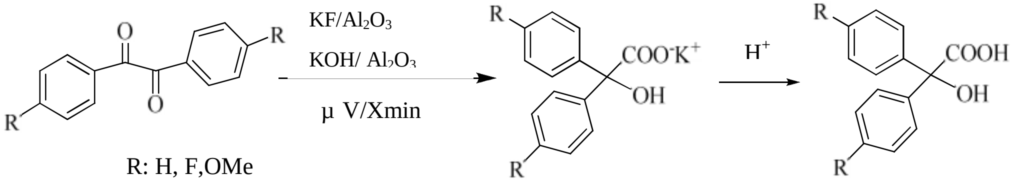
Benzyls (1, 2-diphenyl-1, 2-ethanedions) are organic compounds with the chemical formula of $(C_6H_5CO)_2$. This compound are useful intermediates in organic syntheses. Rearrangement of Benzyls to their corresponding Benzylic Acids analogues under basic condition is one of the most interesting reactions in organic chemistry. Benzyls undergo this rearrangement in the presence of basic solvents such as water and ethanol. The mechanism of this endodermic reaction is also very interesting [1], [2].

Benzylic rearrangement accomplishes under heat, after 2 hours in the presence of basic solvents such as water AND ethanol with the yield of 88.9%. The reaction yield is 91% with refluxing solvent, under heat and in the same reaction time [3]. Initially, the effective reaction condition under pressure was investigated. The solvent-free rearrangement was studied afterwards under microwave irradiation and shorter reaction time.

Finally, the rearrangement was monitored on two basic surfaces of KOH/Alumina and KF/Alumina. Various benzyl analogues with different electron-donating and electron-withdrawing substituent's at Para- location were studied on this investigation. Different amounts of KOH/Alumina and KF/Alumina basic surfaces were also applied under various microwave irradiation times. That the modified time of microwave irradiation was 4 minutes and the modified amount of basic surface was 4 gr per each 0.01 mol of benzyl substituent's.



Reference:

[1] K.Narang, *Trans. Met. Chem*, **1997**, *22*, 333.
[2] Maruyama.T, *J. Chem. Soc. Perkin Trans.1*, **1995**, *7*, 733.
[3] Jackman.M, *J. Am. Chem. Soc.* **1948,** *70*, 497.

An eco-friendly procedure for the synthesis of 2-phosphonomethylmalononitriles

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Phosphonates exhibit a wide range of notable biological properties which expand their applications as enzyme inhibitors, metabolic probes [1], peptide mimetics [2], antibiotics, and pharmacologic agents [3] besides to their traditional roles as intermediates in organic synthesis [4].

Water is a desirable solvent for reasons of cost, safety and environmental impact [5]. However; organic solvents are still used instead of water for mainly two reasons. First, most organic substrates are not soluble in water and as a result, water cannot function as a reaction medium. Second, many reactive substrates, reagents and catalysts are sensitive towards water and are decomposed or deactivated in aqueous media. A possible way to improve the solubility of substrates is the use of surface active reagents that can form micelles [6] or vesicular structures in aqueous media.

Herein we report a new, one-pot and convenient method for the synthesis of a variety of 2-phosphonomethylmalononitriles in aqueous micellar solution. The method offered several advantages such as using a safe, cheap and environmentally benign reaction media, short reaction times, good to high yields and lack of possible side reactions.

References:

[1] (a) Allen, M. C.; Fuhrer, W.; Tuck, B.; Wade, R.; Wood, J. M. *J. Med. Chem.* **1989**, *32*, 1652. (b) Patel, D. V.; Rielly-Gauvin, K.; Ryono, D. E. *Tetrahedron Lett*. **1990**, *31*, 5587. (c) Stowasser,B.; Budt, K. H.; Li, J. Q.; Peyman, A.; Ruppert, D. *Tetrahedron Lett*. **1992**, *33*, 6625.
[2] Kafarski, P.; Lejczak, B. *Phosphorus, Sulfur, Silicon Relat. Elem*. **1991**, *63*, 193.
[3] (a) Baylis,E. K.; Campbell, C. D.; Dingwall, J. G. *J. Chem. Soc., Perkin Trans. 1* **1984**, 2845. (b) Atherton, F. R.; Hassal, C. H.; Lambert, R. W. *J. Med. Chem*. **1986**, *29*, 29.
[4] Maryanoff, B. E.; Reitz, A. B. *Chem. Rev*. **1989**, *89*, 863.
[5] (a) Li, C. J.; Chan, T. H. *Organic Reaction in Aqueous Media*, John Wiley & Sons: New York, **1997** (b) *Organic Reaction in Wate;* Grieco, P. A., Ed.; Blackie Academic and Professional: London, **1998.**
[6] (a) Fendler, J. H.; Fendler, E. J. *Catalysis in Micellar and Macromolecular System*, Academic Press: London, **1975**. (b) *Mixed Surfactant System*; Holland, P. M.; Rubingh D. N. Eds.; American Chemical Society, Washington DC, **1992**.

Synthesis and analgesic effects of new pyrrole derivatives of phencyclidine in mice

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Phencyclidine (1-[1-phenylcyclohexyl]piperidine, CAS 956-90-1, PCP, **I**) and many of its analogues have shown pharmacological effects [1-3]. In this paper, some new Pyrrole derivatives of **I**, (1-[1-phenylcyclohexyl]pyrrole, **II** and 1-[1-[4-methylphenyl][cyclohexyl]]-pyrrole, **III**) and intermediates were synthesized and the acute and chronic pains of II and III were examined on mices using tail immersion (as a model of acute thermal pain) and formalin (as a model of acute and chronic chemical pain) tests and the results are compared to PCP and control groups.

The results indicated that **III** produces higher analgesic effects in tail immersion test compared to the PCP and control groups, with a marked and significant increase in tail immersion latency for all doses. The formalin test showed that **III** is effective in acute chemical pain (phase I, 0-5 min. after injection) in doses 1 and 5 mg/kg and also chronic pain (initial-phase II, 15-40 min. after injection) will be significantly attenuated by this compound compared to PCP and saline (control) in dose of 1, 5 and 10 mg/kg.

It is concluded that, substitution of Pyrrole aromatic ring instead of piperidine in PCP molecule could be effective in acute thermal (in all doses) and chronic (doses of 1 and 5 mg/kg) pains and it could also effective in acute chemical pain compared to the PCP and control.

References:

[1] Ahmadi A, Mahmoudi A. Synthesis and Biological Properties of 2- Hydroxy-1- (1-Phenyltetralin) Piperidine and some of its Intermediates as Derivatives of Phencyclidine. *Arzneim-Forsch/Drug Res*. **2005**; *55* (9): 528.

[2] Ahmadi A, Shafiezadeh M, Fathollahi Y. Synthesis with improved yield and study on analgesic effect of 2-hydroxyphencyclidine. *Arzneim-Forsch/Drug Res.* **2005**; *55*: 172.

[3] Ahmadi A, Khalili M, Abbassi S, Javadi M, Mahmoudi A, Hajikhani R. Synthesis and Study on Analgesic Effects of 1-[1-[4-methylphenyl][cyclohexyl]-4-piperidinol and 1-[1-[4-methoxyphenyl] [cyclohexyl]]-4-piperidinol as Two new Phencyclidine Derivatives. *Arzneimittelforschung.* **2009**; *59*(4):202.

Synthesis of functionalized benzo[*g*]chromene derivatives

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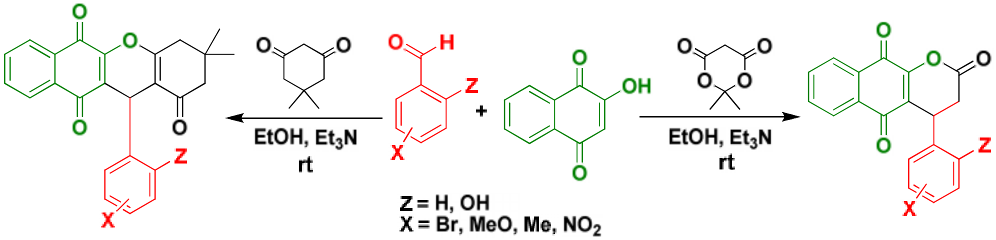
Naturally occurring benzo[*g*]chromenes show a broad spectrum of biological activities including anti cancer, anti-inflammatory, antimalarial, and pesticides activities. This moiety is core fragment of different natural products including pyranokunthone B, lambertellin, *β*-lapachone and *α*-xiloidone. Because of the broad pharmacological activities of benzo[*g*]chromenes, different synthetic methods have been introduced by research groups. A semi synthetic method has been introduced by Machado *et al*. Wei and coworkers reported the synthesis of chromene derivatives in acetic acid media using microwave irradiation [1-4].

As a part of our continuing interest in the development of new synthetic methods in heterocyclic compounds [5-6], here in, we report new methods for the synthesis of benzo[*g*]chromene derivatives via reaction between an aldehyde, Meldrum's acid or dimedone, and 2-hydroxynaphthalene-1,4-dione in the presence of a catalytic amount of triethylamine in EtOH at room temperature.

Products are separated from the reaction media with a simple filtration and no more purification is needed.



References:

[1] Brown, P. M.; Krishnamoorthy, V.; Mathieson, J. W.; Thomson, R. H. *J. Chem. Soc. C.* **1970**, 109.
[2] Kesteleyn, B.; De Kimpe, N.; Van Puyvelde, L. *J. Org. Chem.* **1999**, *64*, 1173.
[3] Machado, T. B.; Pinto, A. V.; Pinto, M. C. F. R.; Leal, I. C. R.; Silva, M. G.; Amaral, A. C. F.; Kuster, R. M.; Netto-dosSantos, K. R. *Int. J. Antimicro. Ag.* **2003**, *21*, 279.
[4] Wei, P.; Zhang, X.; Tu, S.; Yan, S.; Ying, H.; Ouyang, P. *Bioorg. Med. Chem. Lett.* **2009**, *19*, 828.
[5] Shaabani, A.; Ghadari, R.; Sarvary, A.; Rezayan, A. H. *J. Org. Chem.* **2009**, *74*, 4372.
[6] Shaabani, A.; Ghadari, R.; Ghasemi, S.; Pedarpour, M.; Rezavan, A. H.; Sarvary, A.; Ng, S. W. *J. Comb. Chem.* **2009**, *11*, 956.

Preparation of trisubstituted imidazoles in the presence of sulfuric acid ([3-(3-silicapropyl)sulfanyl]propyl)ester and silica bonded N-propyl sulfamic acid under solvent-free conditions

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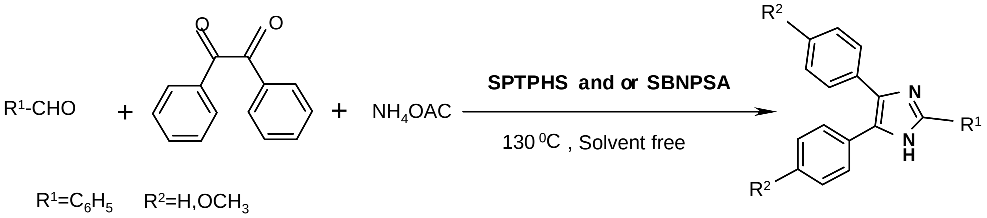
The imidazole moiety is present in wide naturally occurring molecules [1] and pharmaceutically active compounds.[2] Among these, 2,4,5-trisubstituted imidazoles are of great interest because of their chemical and biological activities, making them common structures in numerous synthetic compounds [2] and therapeutic agents [3].

Trisubstituted imidazoles have been synthesized in high yields in the presence of sulfuric acid ([3-(3-silicapropyl)sulfanyl]propyl)ester **(SPTPHS)** and Silica bonded N-propyl sulfamic acid **(SBNPSA)** as catalysts. The reaction was carried out at 130°C under solvent-free conditions. The reaction work-up is simple and the catalyst is easily separated from the products by filtration.



References:

[1] Choudhary, D.; Paul, S.; Gupta, R.; Clark, J. H. *Green Chem.* **2006**, *8*, 479.
[2] Ferreira, P.; Phillips, E.; Rippon, D.; Tsang, S. C. *Appl. Catal. B*: *Environmental* **2005**, *61*, 206.
[3] Karimi, B.; Khalkhali, M. *J. Mol. Catal. A*: *Chem.* **2005**, *232*, 113.

Preparation of amidoalkyl naphthols by a three-component reaction catalyzed by ZnO as a solid heterogeneous catalyst under solvent-free conditions

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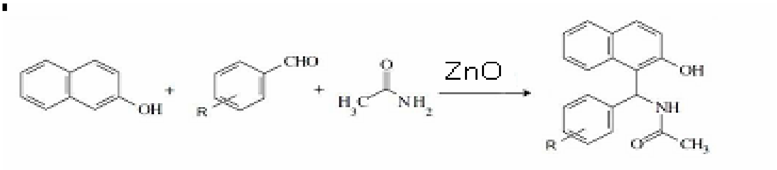
An efficient method for the preparation of amidoalkyl naphthols using a multi-component, one-pot condensation reaction of 2-naphthol, aldehydes and acetamide in the presence of Zinc Oxide under solvent-free conditions is described.

Multicomponent reaction (MCR) condensations involve three compounds reacting in a single event, but consecutively to form new products, which contains the essential parts of all the starting materials [1]. The developing of new MCRs, and improving known multi-component reactions are an Amidoalkyl Naphthols area of considerable current interest [2]. One such reaction is the synthesis of Amidoalkyl Naphthols. The prevalence of in natural products and pharmacologically active compounds has instituted a diverse array of synthetic approaches to these heterocycles [3].

There are several methods for the synthesis of highly substituted Amidoalkyl Naphthols [4] Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for several important organic transformations [5] in this paper we report a simple and environmentally benign methodology for the synthesis of tetrasubstituted Amidoalkyl Naphthols via direct four-component condensation reaction between aldehydes, 2-naphthol, benzaldehyde and acetamide using catalytic amounts of ZnO under solvent-free conditions.



References:

[1] Domling, A.; Ugi, I. *Angew Chem Int Ed* **2000**, *39*, 3168.
[2] Eilbracht, P.; Barfacker, L.; Buss, C.; Hollmann, C.; Kitsos-Rzychon, B. E.; Kranemann, C. L.; Rische, T.; Roggenbuck, R.; Schimdt, A. *Chem Rev* **1999**, *99*, 3329.
[3] Sisko, J. *J Org Chem* **1998**, *63*, 4529.
[4] Katritzky, A. R.; Boulton, A.J. (Eds.), *Advances in Heterocyclic Chemistry; Academic: New York,* **1980**; Vol. 27.
[5] Karimi-Jaberi, Z. Amiri, M. *Heteroatom Chem.* **2010**, *21*, 96.

Condensation of indole with various carbonyl compounds and synthesis of acylals from aldehydes using polystyrene-supported $FeCl_3$

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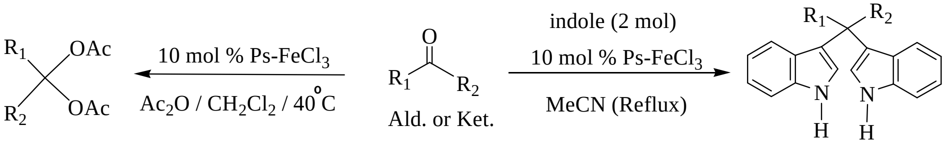
Indole and its corresponding compounds have been identified as an important category of heterocyclic compounds in medicinal chemistry. Among different indole derivatives, bis-indolylmethanes are known as a privileged group because of their representation in natural products and extensive applications in pharmaceuticals. Synthetically, the reaction of indole with aldehydes or ketones produces azafulvanium salts, which further react with another indole molecule to form bis-indolylmethanes [1]. A great number of catalysts have been reported in the literature for the preparation of bis-indolylmethanes in which protic acids as well as Lewis acids are employed. Although these methods were appropriate, many of them are associated with several drawbacks, including the requirement of large or stoichiometric amount of catalysts due to their deactivation by the nitrogen-containing reactants, exhausting work-up, and environmental pollution.

Acylals have attracted great interest in organic synthesis for the protection of carbonyl groups because of their remarkable stability in basic and neutral reaction media as well as towards aqueous acids [2]. Generally, acylals can be prepared from aldehydes by treatment with acetic anhydride in the presence of proton acids or Lewis acids. However, most of the reported methods suffer from one or more disadvantages such as: strongly acidic or oxidizing conditions, poor selectivity, tedious work-up, environmental pollution, and the use of moisture-sensitive or unreusable catalysts.

In a continuation of our ongoing program to develop environmentally benign methods using heterogeneous catalysts [3], herein we now wish to report that cross-linked polystyrene supported $FeCl_3$ (Ps-$FeCl_3$) is an effective and highly chemoselective heterogeneous catalyst for the efficient electrophilic substitution of indole with a variety of carbonyl compounds and for acetylation of aldehydes with acetic anhydride.



References:

[1] Sundberg, R. J. The Chemistry of Indoles, Academic Press: New York, **1996**.

[2] Greene, T. W.; Wuts, P. G. M. Protective Groups in Organic Synthesis, 3rd ed., John Wiley: New York, **1999**.

[3] Parvanak Borujeni, K.; Tamami, B. *Catal. Commun.* **2007**, *8*, 1191.

Synthesis and investigation of thermal and optical properties of new photochromic azo schiff Bases

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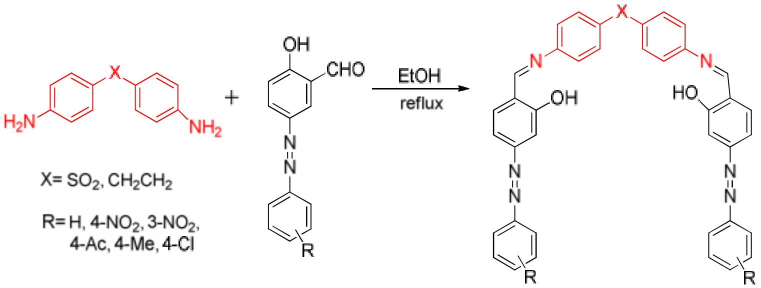
Azo compounds are very important molecules and have attracted much attention in both academic and applied research due to their versatile application in various fields, such as dyeing textile fiber, biomedical studies and advanced application in organic synthesis and high technology areas such as laser, liquid crystalline displays, electro-optical devices and ink-jet printers [1].

There is considerable interest in Schiff base ligands and their complexes due to their antitumor activities. In recent years, organic materials with second-order nonlinear optical properties have been extensively studied for use in photonic devices, such as high speed photonic switching, electro-optic modulators, components of optical communication systems and others [2]. *o*-Hydroxy Schiff bases exist as enol, keto or enol/keto mixtures. N-Substituted *o*-hydroxylimines have been reported to display thermochromism and photochromism in the solid state by H-atom transfer from the hydroxyl O-atom to the N-atom [3]. Azo–azomethines have been extensively used as dyestuffs for wool, leather and synthetic fabrics. Azo–azomethines also used in photonic devices, electrooptic modulators and as well as components of optical communication systems of their second order nonlinear optical properties [4].

According to the above facts, we decided to synthesize a new Photochromic azo Schiff base and investigation of their Thermal and Optical Properties. For this propose synthesis, separation, purification and characterization of twelve new azo Schiff Bases was preformed. The structure of final compounds was identified by by TLC, m.p., IR, ^{1} H NMR, ^{13}CNMR, and UV-Vis spectra.



References:

[1] Nishihara, H. *Bulletin of the Chemical Society of Japan* **2004**, *77*, 407.
[2] Iijima, T.; Jojima, E.; Antonov, L.; Stoyanov, St.; Stoyanova, T. *Dyes Pigments* **1998**, *37*, 81.
[3] Odabasoglu, M.; Albayrak, C.; Buyukgungor, O. *Acta Crystallogr.* **2004**, *E60*, o142.
[4] Ogawa, K.; Harada, J. *J. Mol. Struct.* **2003**, *647*, 211.

A novel synthesis of 6, 8-dimethyl-(3 or 4)-arylpyrimido[4, 5-c]pyridazine-5, 7(*6H, 8H*)-diones as new potential monoamine oxidase inhibitors

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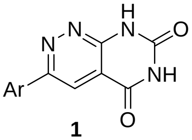
Pyridazine derivatives and heterocyclic annelated pyridazines continue to attract attention due to their wide variety of interesting biological activities.[1] The synthesis and utility of many pyridazine derivatives as analgesics, insecticidals, [2] fungicidals,[3, 4] cardiotonics,[5] have been reported. Very recently, we have reported the synthesis of 3-arylpyrimido[4, 5-c]pyridazine-5, 7(6*H*, 8*H*)-diones **1** and their sulfur analogues **2** as potential monoamine oxidase inhibitors.[6]



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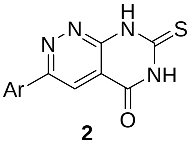
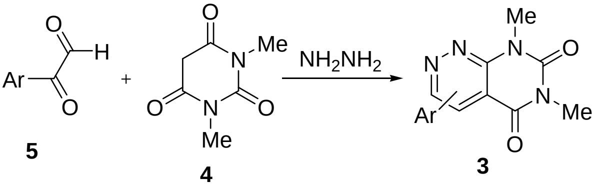


2

At this stage, we report novel synthesis of 6, 8-dimethyl-(3 or 4)-arylpyrimido[4, 5-c]pyridazine-5, 7(*6H, 8H*)-diones **3** which may have better MAO inhibitory effects. The method used in this communication has the advantage of utilizing 1, 3-dimethylbarbituric acid as reagent, possibly offering broader applications and milder conditions for construction of new pyrimidopyridazine derivatives.



References:

[1] Quintela, J. M.; Veiga, M. C.; Conde, S.; Peinador, C. *Monatsh Chem*. **1996**, *127*, 739.
[2] Numata, T.; Ogura, T.; Hirat, K.; Kudo, M. *Jpn Kokai Tokyo Koho Jp*, **1989**, *63*, 159, 372 [*Chem. Abstr. 110*, 75538].
[3] Yoshioka, H.; Obato, Fujii, T. K.; Fukuda, Y.; Ooka, A. *Eur. Pat. Appl. Ep*. **1989**, *283*, 271.
[4] Matolesy, G. World Rev Pest Contr, **1971**, *10*, 50 [*Chem. Abstr.* **1972**, *76*, 820315].
[5] Okujima, H.; Naeimatsu, A.; Kobayashi, M.; Funlya, R.; Kitada, K. *Jpn Kokai Tokyo Jp*, **1989**, *63*, 215, 672 [*Chem. Abstr.* **1989**, *110*, 75541].
[6] Rimaz, M.; Khalafy, J.; Noroozi Pesyan, N.; Prager, R. H. *Aust. J. Chem.* **2010**, *63*, 507.

Synthesis and characterization of novel thermally stable aromatic poly(amide-imide)s based on L-aspartic acid and various aromatic diamines

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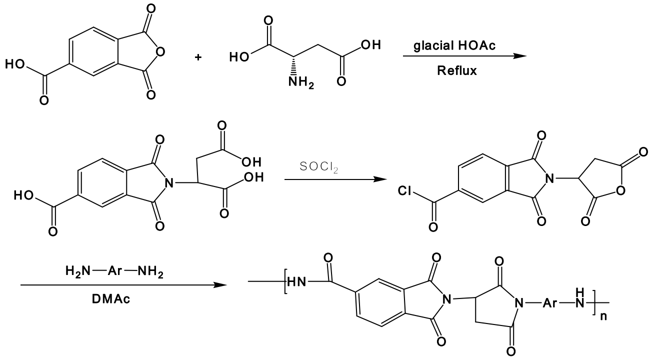
Aromatic polyamides indicate a number of useful properties such as high thermal stability, chemical resistance, low flammability, and excellent mechanical properties. Meanwhile, incorporation of imide groups in the backbone of polyamides improves their thermal properties [1-3]. Natural amino acids are used in polymer synthesis to create some new semi-crystalline optically active polymers [4-6].

In this research a new triacid was synthesized from L-aspartic acid and trimellitic anhydride in glacial acetic acid at 1:1 molar ratio. Subsequent transformation of this triacid to 2-(2,5 dioxo-tetrahydrofuran-3-yl)-1,3-dioxoisoindoline-5-carbonyl chloride were carried out using thionyl chloride. Solution polymerization was carried out in DMAc, using 2-(2,5 dioxo-tetrahydrofuran-3-yl)-1,3-dioxoisoindoline-5-carbonyl chloride and different diamines [3]. These poly(amide-imide)s were characterized by ^{1}HNMR, FT-IR spectroscopy and CHN analysis. The FT-IR spectrum of the following polymers showed characteristic bands at 3372 cm^{-1} (N-H stretching of amide group), two bands at 1723 and 1780 cm^{-1} (corresponding to the cyclic imide group), and a broad band at 1682 cm^{-1} (corresponding to amide carbonyl groups). These polymers are organosoluble in polar aprotic solvents and are thermally stable.



References:

[1] Behniafar, H.; Banihashemi, A . *Eur. Polym. J.* **2004**, *1409*, 1415.
[2] Yganeh, H.; Tamami, B.; Ghazi, I. *Ir. Polym. J.* **2005**, *277*, 285.
[3] Banihashemi, A.; Vakili, M.R.e-*Polym*. **2007**, *no*.008.1.
[4] Hajipour, A. R.; Zahmatkesh, S.; Banihashemi, A.; Rouho, A. *E. Polym. Bulletin*. **2007,** *145*, 159.
[5] Hajipour, A. R.; Zahmatkesh, S.; Zarei, A.; Khazdooz, L.; Rouho, A. E. *Eur. Polym. J*. **2005**, *2290*, 2296.
[6] Mallakpour, SH.; Rafimanzelat, F. *Eur. Polym. J.* **2005**, *2945*, 2955.

P_2O_5/Al_2O_3 As an efficient heterogeneous catalyst for environmentally friendly greener synthesis of 1, 8-dioxo-octahydroxanthenes

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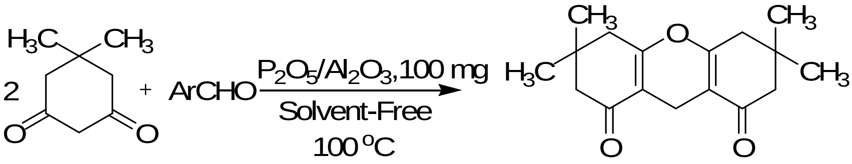
Xanthene's derivatives are parent compounds of a large number of naturally occurring and synthetic derivatives, and occupy a prominent position in medicinal chemistry [1,2]. Therefore, the discovery of a new and efficient catalyst with high catalytic activity, short reaction time, recyclability and simple work-up for the preparation of 1,8-dioxo-octahydroxanthene derivatives under mild and practical conditions is of prime interest. The aim of the present study was to utilize the P_2O_5/Al_2O_3 as an inexpensive catalyst for the synthesis of 1,8-dioxo-octahydroxanthene derivatives *via* the condensation reaction of various aromatic aldehydes with dimedone under solvent-free thermal conditions (Scheme).

Various 1,8-dioxo-octahydroxanthene derivatives were prepared from different aromatic aldehydes and 5,5- dimethyl-1,3-cyclohexanedione (dimedone) in the presence of the catalyst. The aromatic aldehydes containing both electron-donating and electron-withdrawing groups afforded the corresponding products in high yields. The catalyst was easily separated in simple work-up and was recycled several times without loss of reactivity under the described reaction conditions.



References:

[1] Wang, H. K.; Morris-Natschke, S. L.; Lee, K. H. *Med. Res. Rev.* **1997**, *17*, 367.
[2] Rukavishnikov, A. V.; Smith, M. P.; Birrell, G. B.; Keana, J. F. W.; Griffith, O. H. *Tetrahedron Lett.* **1998**, *39*, 6637.

Extraction of Eugenol from cloves and preparation of their dimmer derivatives

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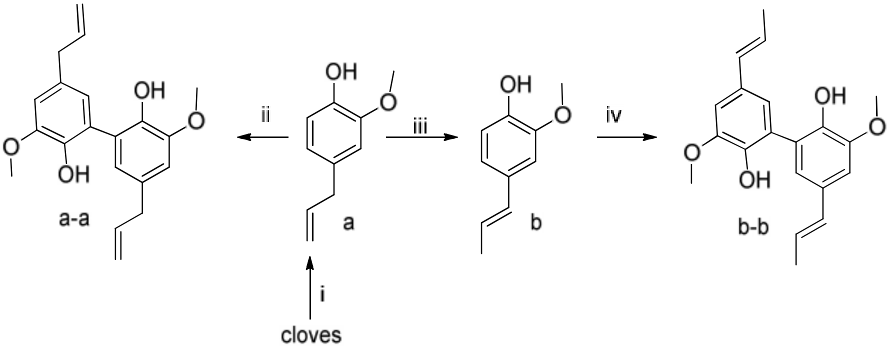
Eugenol is a long-known natural product occurring in essential oils from clove, cinnamon, piment, oil of bay, laurel, basil and nutmeg. Together with other spice constituents, eugenol is under detailed investigation for its biological effects in the human body. With the best of our knowledge there is not any report regarding of extraction, isomerization and dimmerization of this antiseptic drug in Iran. Here we reported the extraction of eugenol from cloves and isomerization and dimmerization in the presence of new set of reagents.

There are several reagents that transfer the eugenol to it isomerizes form. Here we report a new set of reagent such as KF, Al_2O_3, and ethylene glycol in mw condition.

Oxidative coupling reactions of phenols with $FeC1_3$, are faster and more efficient in the solid state than in solution. This procedure was applied in the eugenol for preparation of biseugenol **aa** and bis isoeugenol **bb**. The final product was isolated purified and characterized. The coupling reactions of **a** and **b** by irradiation with ultrasound also are in the development [1,2].



i) extraction from petrolum ether; ii & iv) $FeCl_3$, $6H_2O$; iii) KF, Al_2O_3, ethylene glycol mw

References:

[1] Belletire, J.L; Mahmoodi, N.O, *Journal of Natural Products* **1992,** 55, 194-206.
[2] Lawless, J. *The Encyclopedia of Essential Oils*; Thorsons: London, UK, **2002**; p. 48, 53, 55, 69, 81, 82, 84, 168.

Three-component synthesis of polyfunctional ketenimines

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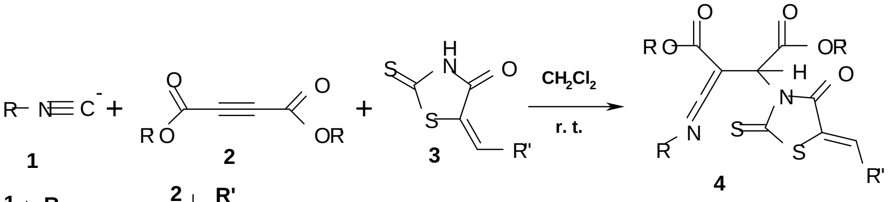
Multicomponent reactions (MCRs), with three or more reactants combine in a one-pot procedure to give a single product, have become increasingly popular during the last decade [1]. They are economically and environmentally advantageous because multi-step syntheses produce considerable amounts of waste mainly due to complex isolation procedures often involving expensive, toxic, and hazardous solvents after each step. MCRs are finding increased use in the discovery process for new drugs and agrochemicals [2]. MCRs that involve isocyanides are by far the most versatile reactions in terms of scaffolds and number of accessible compounds [3].

Benzylidene derivatives of rhodanine are of great interest for the synthetic organic chemists because of the broad biological activities shown by these compounds [4].

Herein we report a one-pot three-component reaction of alkyl isocyanides (**1**), dialkyl acetylenedicarboxylates (**2**) and 5-(4-dimethylaminobenzylidene)rhodanine (**3**), which affords highly functionalized ketenimines (**4**) in moderate to excellent yields (scheme 1). The structure of compounds **4a-4d** was deduced from their ^{1}H NMR, ^{13}C NMR, IR and Mass analyses.



1	R
a	t-Bu
b	Cy

2	R'
a	Me
b	Et
c	t-Bu

R"= PhN(CH$_3$)$_2$

4	R	R'	Yeild (%)
a	t-Bu	Me	95
b	t-Bu	Et	>98
c	t-Bu	t-Bu	>98
d	Cy	Me	60

References:

[1] Dömling, A.; Ugi, I. *Angew. Chem., Int. Ed.* **2000**, *39*, 3169.
[2] Heck, S.; Domling, A. *Synlett.* **2000**, 424.
[3] Zhu, J. E. *J. Org. Chem.* **2003**, 1133.
[4] Insuasty, B.; Gutiérrez, A.; Quiroga, J.; Abonia, R.; Nogueras, M.; Cobo, J.; Svetaz, L.; Raimondi, M.; Zacchino, S. *Arch. Pharm. Chem. Life Sci.* **2010**, *343*, 48.

Bench scale synthesis of 2-chloro-2-(difluoromethoxy)-1,1,1, trifluoroethane from Isoflurane

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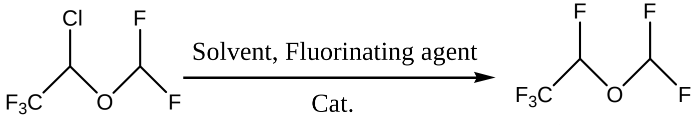
Desflurane (2,2,2-trifluoro-1-fluoroethyl-difluoromethyl ether) is a highly fluorinated methyl ethyl ether used for maintenance of general anesthesia. Together with Sevoflurane, it is gradually replacing Isoflurane (2-(difluoromehyl)-1,1,1,2-tetrafluoroethane) for human use, except in the third world where its high cost precludes its use.

Different methods for the synthesis of Desflurane have been introduced in the literature among which fluorination of Isoflurane is the most, cited method. [1-3]

In the current research, different fluorinating reagents such as KF, $NaBF_4$, BF_3OEt_2, ([MPIM][BF4] and [MPIM][F]), have been applied under different reaction conditions in the presence or absence of catalysts such as 18-Crown-6 , 15-Crown-5 and KI . The influence of solvents such as DMSO PEG-400 and CH_3CN, pressure and temperature on the yield of the reaction and byproducts were evaluated. The reaction was also carried out under solvent-free condition and the results were compared. After optimization of the reaction condition, KF and 18-Crown-6 were selected as fluorinating agent and catalyst and the reaction was scaled up under high pressure at 185°C in DMSO as solvent for 6 hour to obtain crude Desflurane. Finally, fractional distillation was performed on the reaction mixture involving both Desflurane and unreacted Isoflurane to get 98% pure Desflurane in 51% yield.



(Isoflurane) (Desflurane)

References:

[1] Charles, F.; Cicco, US Patent, 5056924, **1991**
[2] Donald, F.; Halpern, Mark L. Robin, US Patent, 4874901, **1989**
[3] Leonid, A.; Rozov, Ralph A. Lessor, US Patent, 6800786, **2004.**

An efficient synthesis of substituted 1,8-naphthyridines catalyzed by Mgo

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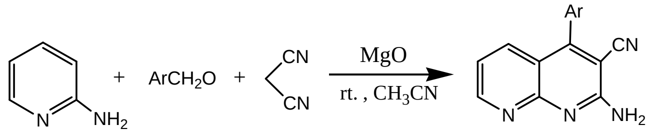
The synthesis of 1,8-naphthyridines and their derivatives is of high interest in organic chemistry due to their wide range of biological activities such as chemotherapeutic agents (e.g., cancer) and anti-infectives (e.g., AIDS). Some 1,8-naphthyridines have been reported to act as growth regulators, fungicides, bactericides, herbicides, insecticides, and nemathocides [1-5].

An efficient and environmentally friendly multicomponent synthesis of benzo(*b*)-1,8-naphthyridines catalyzed by MgO in CH_3CN. Equimolar amounts of substituted aromatic 2-aminopyridine **1** reacted with aldehydes **2** and mononitrile **3** in presence of MgO catalyst to give the corresponding substituted naphthyridine in high yields. All three reactants were used in the molar ratio 1:1:1 in each experiment.

The method is very simple and affords a variety of different substituted naphthyridine derivatives. Most importantly, aromatic aldehydes carrying either electron-donating or electron-withdrawing substituents reacted very well in good to excellent yields.

This reaction offers several advantages that include high yields, the ability to produce compounds in parallel, its novelty and its enviromentally friendly status.



1 2 3 4

References:

[1] Litvinov, V. P.; Roman, SV.; Dyachenko, VD.; *Russ Chem Rev*. **2000**, 69, 201.
[2] Barlin, G. B.; Tan, W-L.; Aust *J Chem*, **1984,** 37, 1065.
[3] Ramesh, D.; Sreenivasulu, B.; *Indian J Heterocyclic*, **2006**, 15, 363.
[4] Barbara, B.; Teresa, Z.; *Arkivoc*, **2001**, VI, 77.

Synthesis of silylethers by chlorosilanes in the presence of ferric hydrogensulfate under mild condition reaction

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The protection of hydroxyl groups as a silylethers is widely used in the chemistry of drugs, steroids, sugars and novel products synthesis. This derivative is also applicable to increase volatility for analysis in liquid or gas chromatography and mass spectrometry. So far different type of reagent and catalysts was reported for this purpose and often for trimethylsilylation of alcohols and phenols [1-2] and among them hydrogensulfate salts promoted trimethylsilylation of alcohols with hexamethyldisilazane (HMDS) in solutions and under solvent-free conditions under reflux conditions [3-4].

In this paper we wish to report a convenient methods not only for preparation trimethylsilylethers of alcohols ,phenols and drugs,but also synthesis kind of silylethers (trimethylsilylethers ,triethylsilylethers and t-butyldimethylsilylethers) by chlorosilanes in the presence of $Fe(HSO_4)_3$ as a cheep, available, not toxis and commerichal catalyst in very mild condition reaction. Synthesized silylethers were characterized by GC, FT-IR and H-NMR spectra.

$$\mathrm{ROH} \xrightarrow{\text{A or B}} \mathrm{ROSiR'_3}$$

A) $Fe(HSO4)_3$ /R'_3SiCl /solvent ,rt
B) Fe $(HSO4)_3$/R'_3SiCl / solvent-free, rt

(R= R or Ar)

Reference:

[1] Amantini D. , Fringuelli F., Pizzo F., Voccarol , *J. Org. Chem.* **2001,** *66*, 6743.
[2] Nishiguchi I,Kita Y,Watanabe M, Ishino Y,OhnoT,,Maekawe H , *Synlett*, **2000**, 1025.
[3] Shirini F ,Zolfigol M.A and Abri A , *Montsh. Chem.* **2008**, *139*, 17.
[4] Shirini F, Zolfigol M. A, Abedini M, *Phosphorus, Sulfur and Silicon and the Related Elements*, **2005,** *180*, 2299.

Efficient method for the synthesis of pyrimidoquinolines

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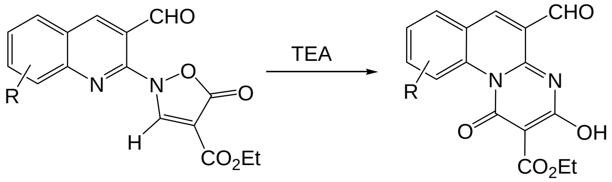
The development of new methods for the synthesis of nitrogen-containing heterocycles is of extreme importance in organic chemistry. In between of these compounds pyrimidoquinolines are important because of their biological properties, which are known to depend mainly on the nature and position of substituents and include anticancer [1], antimalarial [2], antimicrobial [3], anti-oxidant and anti-inflammatory activities [4,5].

In the present work, a series of new heterocyclic compounds, involving pyrimidoquinolines were successfully synthesized via rearrangements of *N*-quinolinyl isoxazol-5(2H)-ones, substituted on *N*-2 with 2-chloroquinoline derivatives, in the presence of mild base-catalysed triethylamine under reflux conditions, through intramolecular cyclization. This method has the advantages of short synthetic route.



R = H , Me , OMe

This paper shows a new and facile synthetic pathway to the pyrimidoquinoline system allowing a large substitution patterns. Furthermore, starting from suitable substrate, the synthesis of other heterocyclic compounds is possible, which may have pharmaceutical applications.

References:

[1] Dlugosz, A.; Dus, D. *Farmaco.* **1996**, *51*, 364.
[2] Joshi, A. A.; Viswanathan, C. L. *Anti-Infect. Agent. Med. Chem.* **2006**, *5*, 105.
[3] El-Sayed, O. A.; Al-Bassam, B. A.; Hussein, M. E. *Arch. Pharm. Pharm. Med. Chem*. **2002**, *335*, 403.
[4] El-Sayed, O. A.; Al-Turki, T. M.; Al-Daffiri, H. M.; Al-Bassam, B. A.; Hussein, M. E. *Boll. Chim. Farm*. **2004**, *143*, 227.
[5] El-Gazzar, A. B. A.; Hafez, H. N.; Nawwar, G. A. M. *Eur. J. Med. Chem.* **2009**, *44*, 1427.

One pot aza Micheal synthesis of new derivatives of γ- lactams

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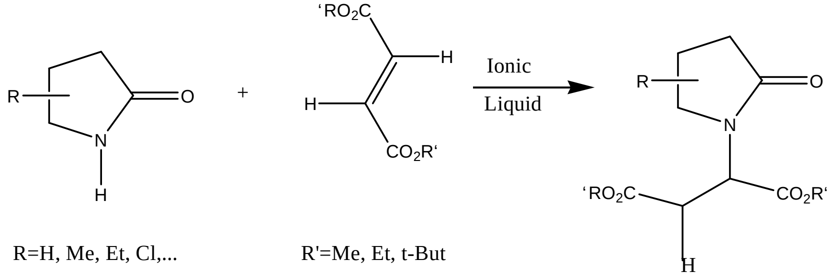
γ-Lactams and their derivatives have shown a broad spectrum of biological activities such as antibiotics, antibacterial, and antifungi [1-3]. In this paper we have investigated the synthesis of new derivatives of γ-lactams in solvent and solventless ionic liquids conditions .We have used substituted γ-lactams **1** and fumaric esters **2** in azamicheal reaction. The structure of compounds **3** were deduced from its elemental analyses and its IR, ^{1}H and ^{13}C-NMR spectra. This facile and efficient method affords high yields for synthesis of γ-lactams derivatives with short time reaction and environmentally friendly conditions.



R=H, Me, Et, Cl,...
1

R'=Me, Et, t-But
2

3

References:

[1] Gavrilyuk, J.I.; Wuellner, U.; Barbas, C.F., *Bioorganic & Medicinal Chemistry Letters.*, **2009,** *19*, 1421.
[2] Kamimura, A. ; Nagata, Y. ; Kadowaki, A. ; Uchidaa, K. ; Unoc, H., *Tetrahedron* **2007,** *63*, 11856.
[3] Lubben, M. ; Feringa, B.L., *Tetrahedron: Asymmetry* **1991,** *2(8)*, 775.

Synthesis of new derivatives of spiro-oxindoles using modified montmorillonite as catalyst

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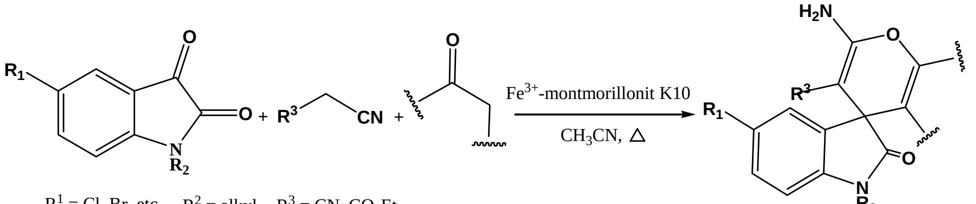
Compounds with an indole moiety exhibit antibacterial and antifungal activities [1]. Furthermore, it has been reported that spiroindoline derivatives have highly enhanced biological activity [2]. The spiro-oxindole system is the core structure of many pharmacological agents and natural alkaloids [3]. On the other hand in recent years, the use of solid acidic catalysts, such as montmorillonite clays, has received considerable attention in different areas of organic synthesis, because of their environmental compatibility, reusability, operational simplicity, nontoxicity, noncorrosiveness, low cost, and easy isolation [4].

At present study due to our continued interest in the development of efficient and environmentally friendly procedures for the synthesis of heterocyclic compounds [5], we studied the reaction of isatin derivatives, malononitrile, and different carbonyl compounds in the presence of modified montmorillonite K10 catalyst in acetonitrile. This reaction furnished the desired spiro-oxindole products in high yields (85-95%) and short reaction times.



R^1 = Cl, Br, etc. R^2 = alkyl R^3 = CN, CO_2Et

In this presentation various aspects of this protocol will be discussed.

References:

[1] Sundberg, R. J. The Chemistry of Indoles; Academic: New York, NY, 1996.
[2] Da-Silva, J. F. M.; Garden, S. J.; Pinto, A. C. *J. Braz. Chem. Soc.* **2001**, *12*, 273.
[3] Dandia, A.; Singh, R.; Khaturia, S.; Merienne, C.; Morgant, G.; Loupy, A. *Bioorg. Med. Chem.* **2006**, *14*, 2409.
[4] Vaccari, A., *Catal. Today* **1998**, *41*, 53; Gil, A.; Gandia, L. M.; Vicente, M. A. *Catal. Rev.* **2002**, *42*, 145.
[5] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K. *Molecules* **2009**, *14*, 1468; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *Heterocycles* **2008**, *75*, 2825; Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N. O.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49*, 1450.

Novel pH-sensitive carriers containing naproxen pendant groups for colon-specific drug delivery

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The carboxyl group of naproxen was converted into vinyl ester group by reacting naproxen with vinyl acetate in the presence of mercuric acetate as a catalyst. Cubane-1, 4-dicarboxylic acid (CDA) was covalently linked with 2-hydroxyethyl methacrylate (HEMA) is the cross-linking agent (CA). Methacrylic-type polymeric prodrugs were synthesized by free radical copolymerization of methacrylic acid, vinyl ester derivative of naproxen (VN) and polyethylene glycol monomethacrylate (PEGMA) in the presence of cubane crosslinking agent. The structure of the VN was characterized and confirmed by FT-IR, ^{1}H-NMR and ^{13}C-NMR spectroscopy. The composition of the cross-linked three-dimensional polymers was determined by FTIR spectroscopy.

The hydrolysis of drug polymer conjugates was carried out in cellophane membrane dialysis bags and the in vitro release profiles were established separately in enzyme-free simulated gastric and intestinal fluids (SGF, pH 1 and SIF, pH 7.4). Detection of hydrolysis solution by UV spectroscopy at selected intervals showed that the drug can be released by hydrolysis of the ester bond between the drug and polymer backbone in low rate [1]. Drug release studies showed that the increasing content of MAA in the copolymer enhances hydrolysis in SIF. The results suggest that these polymeric prodrugs could be useful for release of naproxen in controlled release systems [2].

References:

[1] Mahkam, M.; *J. Bioact.comp. Polym***, 2004**, *19*, 209.
[2] Kopecek, J.; Kopeckova, P.; Brondsted,H.; Rihoa, B.; Yeh,P, Y.; Ikesue, K.; *J Control. Rel.* **1992,** *19*,121.

A fructose-selective fluorescence sensor

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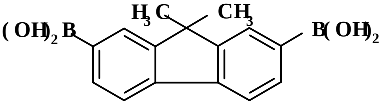
Saccharides play very important roles in a wide range of biological processes and as biomarkers [1], a great deal of effort has been directed towards investigating ways to achieve selective recognition of various carbohydrates using small molecule sensors [2]. In the search for small molecules sensors for biologically important saccharides, the boronic acid group plays an especially important role as a key recognition moiety [3]. The ability of boronic acids to reversibly interact with diol-containing saccharides allows the boronic acid moiety to be used in carbohydrate recognition and sensing. In using the boronic acid moiety for carbohydrate sensor design it is especially important to have boronic acid receptor compounds that change their fluorescent properties upon binding [4].

We synthesized 9,9-dimethylfluorene-2,7-diboronic acid (**1**) and 9,9-dimethylfluorene-2-boronic acid (**2**) and its binding properties toward glucose, fructose, sorbitol, melibiose and saccharose have been studied using fluorescence analysis.

Results shown that, these synthesized boronic acids can be used selectively for fructose recognition.



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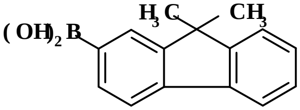

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References:

[1] Wells,L.; Vosseller,K. Hart GW. *Science*. **2001**, *291*, 2376.
[2] Fang, H.; Kaur, G.; Wang, B. *J Fluoresc*. **2004**, *14*, 481.
[3] Shinkai, S.; Takeuchi, M. *Biosens Bioelectron*. **2004**, *20*, 1250
[4] Lin N, Yan J.; Huang, Z.; Altier, C.; Li, M.; Carrasco, N.;, Suyemoto, M.; Johnston, L.; Wang, S.; Wang, Q.; Fang, H.; Caton-Williams, J.; Wang, B. *Nucleic Acids Res* .**2007**, *35*, 1222.

Synthesis of azo dyes based on 1-and 2-naphthol using silicagel supported $HClO_4$ / wet-SiO_2 in the presence of $NaNO_2$ in mild and heterogeneous conditions.

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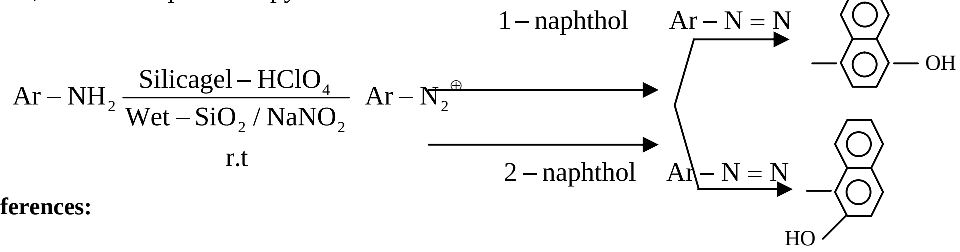
Azo dyes are the largest group of aqueous pigments that makes up 35% of global production of color. So azo dyes are used very widely. It is worth noting that different azo dyes compounds show activities against heart disease and Alzheimer's. [1] Considering that the synthesis of some azo dyes based on 1-naphthol and 2-naphthol requires some special conditions such as low temperature and concentrated liquid acids, in addition to high costs it leads to corrosion of reactors and equipment. There fore, the use of solid acid beds can be an appropriate solution to resolve these problems. It is expected that the reaction to be performed with more efficiency, less by products, lower cost ,time and desired bed can also be used repeatedly. [2] As we know, working with liquid acids comes with many problems specially when applied to industrial scale. While the solid acid beds not only have a very good ability to do similar reactions but also they are free from some side problems such as corrosion and undesirable environmental effects. [3].

In this case it is not require providing special cold condition. The reaction easily takes place in room temperature and resulting diazonium salt can remain on the solid substrate for a long time (even several days) This project focuses on the effect of perchloric acid embedded silicagel solid bed on production of azo dyes in wet silicagel in the presence of sodium nitrite as diazotization reagent of aromatic amines products are verified by IR, ^{1}H-NMR, ^{13}C-NMR spectroscopy data.



References:

[1] Dabbgh, H. A, Teimouri,A, Najafi Chermani, A. *Dyes and Pigment*, **2007**, *73*,239-244.
[2] Towns, A.D. *Dyes and Pigment*, **1999**, *42(1)*, 3-28.
[3] (a) Zollinger, H. **2003**, Color chemistry. Switzerland: Verlag Helvetica Chimia Acta, 3rd ed.

Efficient synthesis of bis(substitued) benzylidene cycloalkanones and hexahydro-4-phenylquinazoline-2(3*H*)-thione derivatives

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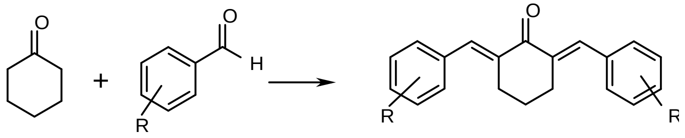
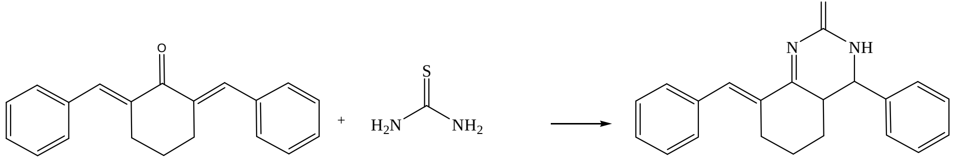
Aldol-condensation reactions are important synthetic reactions and in classical methods, they were performed in the presence of strong acids or bases. Due to the importance of methylene structural unit which are found in many naturally occurring compounds and antibiotics and the use of α,α'-bis(substitued) benzylidene cycloalkanones as precursors for synthesis of bioactive pyrimidine derivatives, condensation of cyclopentanone and cyclohexanone with aldehydes and ketones were of special interest. For this purpose, some catalytic procedures are reported [1-2].

Condensation of nitrogen-containing binucleophilic agents with α,β-unsaturated ketones is one of the most suitable synthetic pathways to five-, six- and seven-membered partially hydrogenated heterocyclic compounds-potential pharmaceutically active analogs of natural compounds [3].

Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for several important organic transformations [4], we describe an efficient method for cross aldol condensation of cyclic ketones with aldehydes using catalytic amounts of p-toluenesulfonic acid under solvent-free conditions for the synthesis of α,ά-bis(substituted benzylidene) cycloalkanones and their reaction with thiourea to synthesis 8-benzylidene-hexahydro-4-phenylquinazoline-2(3*H*)-thione derivatives.





References:

[1] Iranpoor, N.; Kazemi, F. *Tetrahedron* **1998**, *54*, 9475.
[2] Daskiewicz, J. B.; Comte, G.; Barron, D. *Tetrahedron Lett.* **1999**, *40*, 7095.
[3] Temple, C.; Coburn, W. C.; M. C. Thorpe, Montgomery, J.A. *J. Org. Chem.* **1965**, *30*, 2395.
[4] Karimi-Jaberi, Z.; Amiri, M. *Heteroatom Chem.* **2010**, *21*, 96.

Comparison catalytic activity between two photocatalytic thin glass films of TiO_2/SiO_2 towards degradation of organo phosphorous pollutants.

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This study demonstrated an effective and reliable method for degradation of organo pesticide by nano TiO_2 / SiO_2 coated films [1]. Two types of TiO_2 films, i.e., nano TiO_2 / SiO_2 and nano TiO_2 / SiO_2 / Nd were prepared by a sol gel dip- coating methods which, Titanium tetra isopropoxide and Neodmium nitrate were as the raw materials [2]. The photocatalytic activities were investigated by UV-induced degradation of organo pesticide as a model of organic pollutant in aqueous solutions [3]. Complete decomposition was happened after irradiation. In the other words, the photocatalytic degradation pathways on the nano TiO_2 coated films were discussed [4].

In this research we prepared two different photocatalysts, Ti O_2 thin glass films without dopant metal ion and TiO_2 / SiO_2 / Nd thin films coated on glass that they characterized by TEM, SEM, XRD and BET measurement .Their photocatalytic activities were compared by degradation of Malathion and Diazinon, as source of organo phosphorous pesticides under high pressure Mercury lamp within two hours. Concentration of the pesticides determined with UV-Vis spectroscopy. The results showed that the degradation process in the presence of nano-composite of TiO_2 / SiO_2 / Nd had good efficiency with compare of that nano-composite of TiO_2 / SiO_2.The results and grafts will be presented and discussed later.

References:

[1] Devipliya, S; Yesodharan S, *sola Energy Material & solar cells*, **2005**, *86*, 309.
[2] Abroomand Azar, P; Moradi Dehaghi, S; Samadi, S, *Asian J. of Chem***.,** **2010**, *22*, 9314.
[3] Senthilnathan, J.; Ligy, P, *J. of Environmental science and health*, **2009**, B, 44, *3*, 262.
[4] Sojic, D.; Despotovic, V. N.; Abazovic, N. D.; Comor, M. I. Abramovic, B. F, J. of Hazardous materials**, 2010**, Article in press.

A cost effective synthesis of *1,8*-dioxo-dioxodecahydroxanthene using metal hydrogen sulfate as a ryclable catalyst

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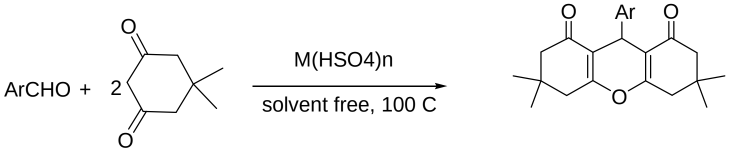
Xanthene derivatives is a very important class of compounds widely used as leuco-dye, in laser technology and in fluorescent materials. Furthermore, these compounds have recently received great attention because of the wide range of their therapeutic and biological properties such as antibacterial, antiviral and anti-inflammatory activities [1,2].

In recent years inorganic solid inorganic acidic salts such as metal hydrogen sulfates play a prominent role in organic synthesis under heterogeneous conditions along this line, using $Mg(HSO_4)_2$, $Fe(HSO_4)_2$, $Al(HSO_4)_3$, $KHSO_4$ which are low in toxicity, highly stable toward humidity, recyclable and air stable have received more attention. The importance of these solid inorganic acid catalysts is growing because of their safe and eco-friendly nature as attention is directed toward the development of clean and green technologies for important organic molecules to promote environmental [3,4].

In this reaserch we introduced a new method for the preparation of 1,8 dioxo xhanthene derivatiry by mixing dimedone and derivatiry, an aldehyde and ammounts of metal hydrogen sulfates such as [$Mg(HSO_4)_2$, $Al(HSO_4)_3$, $KHSO_4$, $FeHSO_4$] as catalyst. We accomplished this reaction under solvent-free conditions and also in good to excellent yields.



Scheme 1

Reference:

[1] Zhang, Z.; Lui, Y. *Catal. Commun*. **2008,** *9*, 1715.
[2] Kantevari, S.; Bantu, R.; Nagarapu, L. *J. Mol. Catal. A***. 2007**, *269*, 53.
[3] Shirini, F.; Zolfigol, M. A.; Abri, A. R. *Lett. Org. Chem***. 2006**, *3*, 292.
[4] Zolfigol, M.A.; Niknam, K.; Shirini, F.; Mohammadpoor-Baltork, I.; Ghorbani Choghamarani, A. Baghbanzadeh, M*. JICS*. **2006**, *3, 1*, 73.

Employment of Fischer indole synthesis in the preparation of biindoles

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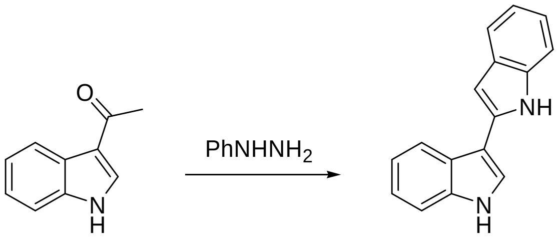
Indole-unit is present actively in the structure of many valuable natural products and also biological active man-made compounds. Therefore many methods were reported for the synthesis and functionalization of such compounds [1-3]. One of the oldest and most reliable methods for synthesizing substituted indoles is the Fischer indole synthesis developed in 1883 by Emil Fischer [4].

In the base of our knowledge this versatile method was not used for the synthesis of biindolyl compounds. We wish by using such procedure to provide a new access to the preparation of biindoles. For example 3-acetylindole reacted with phenylhydrazine and yielded 2,3'-biindolyle **1**.



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References:

[1] Shiri, M.; Zolfigol, M. A.; Kruger, H. G.; Tanbakouchian, Z. *Chem. Rev.* **2010**, *110*, 2250.
[2] Humphrey, G. R.; Kuethe, J. T. *Chem. Rev.* **2006**, *106*, 2875.
[3] Cacchi, S.; Fabrizi, G. *Chem. Rev.* **2005**, *105*, 2873.
[4] Fischer, E.; Jourdan, F. *Ber.* **1883**, *16*, 2241.

Synthesis of bis[1,2,4]triazolo[4,3-b:1',5'-d][1,2,4]triazines: Derivatives of a new heterocyclic ring system

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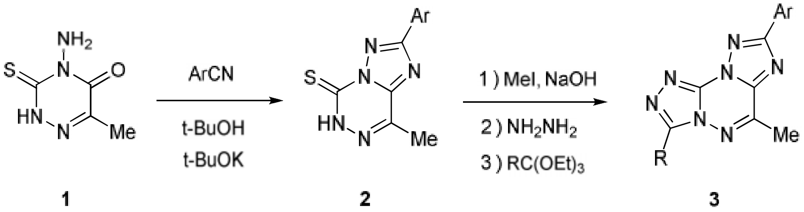
Triazolotriazines as potential biologically active heterocycles have been the subject of recent studies. Literature reports had already established triazolotriazines as antimicrobial [1] and antifungal [2] agents with potential application as enzyme inhibitors [3]. Moreover, some of these compounds have been identified as selective adenosine A (2a) receptor antagonists [4-6].

In connection with our interest in the synthesis of new heterocyclic compounds with potential biological activities, we have recently reported a convenient synthesis of new 1,2,4-triazolo[1,5-d][1,2,4]triazine-5-thiones **2** via cyclocondensation of 6-methyl-4-amino-1,2,4-triazine-3-thione-5-one **1** with aryl nitriles in the presence of potassium t-butoxide in t-butanol under reflux [7]. In continuation of this work, herein we wish to report a new route for the synthesis bis[1,2,4]triazolo[4,3-b:1',5'-d][1,2,4]triazines **3**, a novel heterocyclic ring system, through heterocyclization of suitably functionalized triazine **1** with aryl nitriles followed by methylation, nucleophilic displacement with hydrazine, and finally cyclocondensation with orthoesters.



References:

[1] Abdelall, M. M. *Phosphorus, Sulfur Silicon Relat. Elem.*, **2009**, *184*, 2208.
[2] El-Sharief, A. M. S.; Ghorab, M. M.; El-Gaby, M. S. A.; et. al. *Heteroatom Chem.*, **2002**, *13*, 316.
[3] Bojack, G.; Earnshaw, C. G.; Klein, R.; Lindell, S. D.; et. al. *Org. Lett.*, **2001**, *3*, 839.
[4] Vu, C. B.; Pan, D.; Peng, B.; Sha, L.; et. al. *Bioorg. Med. Chem. Lett.*, **2004**, *14*, 4831.
[5] Peng, H. R.; Kumaravel, G.; Yao, G.; et. al. *J. Med. Chem.*, **2004**, *47*, 6218.
[6] Kumaravel, G.; Engber, T.; et. al. *Abstracts of Papers of the Am. Chem. Soc.*, **2006**, *231*, 174.
[7] Heravi, M. M.; Montazeri, N.; Rahimizadeh, M.; et. al. *J. Heterocyclic Chem.*, **2005**, *42*, 1021.

Highly efficient bromination of aromatic compounds with bromide catalyzed by iodic acid or periodic acid in water

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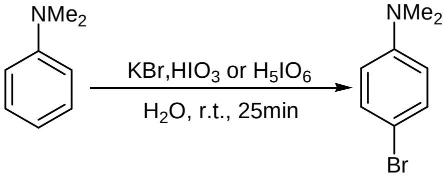
Organic halids are an important class of intermediates as they can be converted efficiently into other functionality by simple chemical transformations [1-3]. Due to the potential utility of aryl bromides in the synthesis of aryl esters, arylolefins and other useful compounds, bromination of aromatic compounds has been the subject of numerous studies. Recently, the oxidative halogenations of organic compounds by metal halides has emerged as an important alternative for the synthesis of such halo derivatives [4]. Despite the broad choice of options, however, many brominating methodologies are cumbersome, costly, and harsh; or involve use of toxic heavy metals or elemental bromine. The development of quick, inexpensive, widely applicable, and environmentally benign brominating agents is therefore still an active area of research. On the other hand, Replacement of expensive, toxic, flammable, not recyclable organic solvents with water is a challenge and in great demand from academia and chemical industries [5]. The use of water as the reaction medium has several benefits; water is a cheap and abundant, nontoxic, non-flammable and relatively green solvent. In this article a new environmentally friendly catalytic method is described for the efficient monobromination of arenes using iodic acid or periodic acid as the oxidant. The method is based on using potassium bromide and iodic acid as an effective catalyst in water at room temperature.



References:

[1] House, H. O. *In Modern Synthetic Reactions*; W. A. Benjamin Inc.: Menlo Park, CA, **1972**; 422.
[2] Liu, Y. H.; Zhou, S. L. *Org. Lett.* **2005**, *7*, 4609-4611.
[3] Johnsson, R.; Meijer, A.; Ellervik, U. iodination *Tetrahedron* **2005**, *61*, 11657-11663.
[4] Moriuchi, T.; Yamaguchi, M.; Kikushima, K.; Hirao, T. *Tetrahedron Lett.* **2007**, *48*, 2667-2670.
[5] Grieco, P. A. (Ed.), *Organic Synthesis in Water*, Blackie Academic and Professional, London, **1998.**

Ph_3P- and solvent-assisted thiocarbonylation of amines with CS_2 under mild aqueous conditions: synthesis of symmetric thioureas

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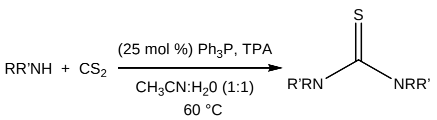
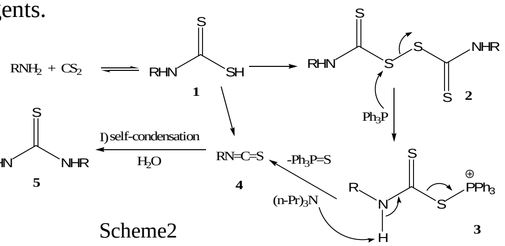
Thiourea moieties are important chemical building blocks that have numerous chemical and pharmaceutical applications [1]. Moreover, thiourea and its derivatives have attracted much attention owing to their application as useful intermediates in the synthesis of different chemicals compounds [2]. Conventional methods for the synthesis of 1,3-disubstituted thioureas are essentially based on the reaction of amines with isothiocynanates [3], thiocarbonaylating agents such as thiophosgene and dithiocarbamates [4], or carbon disulfide. In addition, symmetric 1,3-disubstituted thioureas are prepared by self-condensation of isothiocyanates under aqueous conditions in the presence of organic bases [5]. The most common method for synthesis of 1,3-disubstituted thioureas involves the reaction of primary amines with CS_2. This process is catalyzed by different reagents [6] such as ZnO/Al_2O_3 composites, alumina, MCM-TBD, mercury acetate and peptide coupling reagents. However, many methods suffer from limitations related to harsh reactions conditions such as high reaction temperature, use of a strong acid or base, and toxic reagents.



Scheme1



Scheme2

Here we report a simple one-pot procedure for the synthesis of symmetrical 1,3-disubstituted thioureas by reaction of amines with carbon disulfide in aqueous media in the presence of Ph_3P as a desulfurizing agent (Scheme 1).

In conclusion, an efficient, novel and simple method for one-pot synthesis of 1,3-disubstituted thioureas from primary amines and carbon disulfide under mild aqueous conditions was developed. The method avoids the use of toxic catalysts and reagents, such as thiophosgene and isothiocyanates, and hazardous conditions. It seems that formation of the isothiocyanates **4** may assisted by Ph_3P as a desulfurizing agent for S–S bond-containing intermediates **3**, and finely symmetric thioureas **5** are produced not only by self-condensation of isothiocyanate but also by attack of amines to isothiocyanate **4** which are assisted by water in the presence of tripropylamine (Scheme 2).

References:

[1] (a) Nowick, J. S.; Mahrus, S.; Smith, E. M.; Ziller, J. W. *J. Am. Chem. Soc.* **1996**, *118*, 1066; (b) Chalina, E. G.; Chakarova, L. *Eur. J. Med. Chem*. **1998**, *33*, 975.

[2] (a) Yadav, L. D. S.; Rai, V. K. *Tetrahedron* **2007**, *63*, 6924; (b) Kabalka, G. W.; Mereddy, A. R.; *Tetrahedron Lett.* **2006**, *47*, 5171.

[3] Rasmussen, C. R.; Villani, F. J. Jr.; et. al. *Synthesis* **1988**, 456.

[4] (a) Halimehjani, A. Z.; Pourshojaei, Y.; Saidi, M. R. *Tetrahedron Lett.* **2009**, *50*, 32.

[5] Blanco, J. L. J.; Barria, C. S.; Benito, J. M.; Fernandez, J. M. G. *Synthesis* **1999**, 1907.

[6] (a) Yamazaki, N.; Tomioka, T.; Higashi, F. *Synthesis* **1975**, 384; (b) Balleabeni, M.; Ballini, R.; Bigi, F.; Maggi, R.; Parrini, M.; Predieri, G.; Sartori, G. *J. Org. Chem*. **1999**, *64*, 1029.

Efficient synthesis of functionalized 2,5-dihydropyrrole derivatives by the reaction between aromatic amines, acetilenic esters and phenacyle bromide in the presence of triphenyl phosphine

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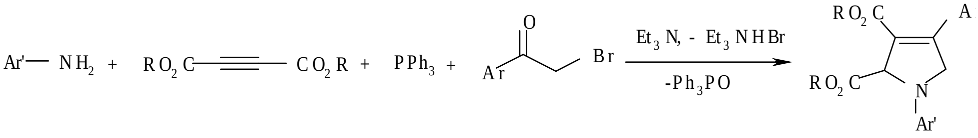
Development of simple synthetic routes for widely used organic compounds from readily available reagents is one of the major tasks in organic synthesis [1]. Dihydropyrroles are important compounds which exhibit wide range of biological activities and are useful intermediates in synthesizing of natural products. Some 2,4-bisaryl-2,5-dihydropyrrole derivatives have been recently studied as a novel patent, water solouble KSP inhibitors.

Addition reaction between phosphines and activated carbon-carbon triple bonds is well known to produce a reactive zwitterionic intermediate, which may be trapped by various electrophiles [2]. Reaction of triphenylphosphine with dimethyl acetylenedicarboxylate (DMAD) has been studied in the presence of a variety of organic acidic compounds, in order to trapp the zwitterionic intermediate. Trapping of PPh_3-DMAD zwitterion by an organic acidic compound containing a carbonyl group have been used as a one-pot and efficient route for the synthesis of a variety of heterocylclic and carbocyclic compounds [3].

Here we report an efficient, simple and one-pot synthetic method for some *N*-substituted 2,5-dihydropyrrole derivatives through the reaction between aromatic amines, acetilenic esters, phenacyle bromide in the presence of triphenyl phosphine.



References:

[1] Laszlo, P., *Organic Reactions: Simplicity and Logic*, Wiley, New York, **1995**.
[2] Yavari, I.; Adib, M.; Hojabri, L. *Tetrahedron*., **2002**, 58, 7213.
[3] Mosslemin, M. H.; Yavari, I.; Anary-Abbasinejad, M.; Nateghi, M. R. *Synthesis,* **2004**, 7, 1029.

Carboxymethylation of cellulose in nonaqueous ionic liquid media

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[b] *Member of young researcher club*

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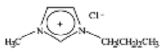
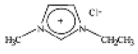
Cellulose is the most abundant polymer in nature and is composed of units of β-1,4-linked glucose. Cellulose fibers are present in all plant cell walls in combination with hemicelluloses, lignin, and extractives. The cellulose fiber is designed of nanosized fibers, often referred to as microfibrils, that have diameters in the range of 2-20 nm and lengths of up to several micrometers depending on their origin [1]. Cellulose nanofibers consist of cellulose crystallites, also known as cellulose nanowhiskers, that are linked to each other by amorphous cellulose domains [2-4]. Although the modulus of a cellulose crystal is about 138 GPa5 along the fiber axis, an assembly of crystallites connected by hydrogen bonds has a considerably lower elastic modulus have been known for almost one century. In 1914, Paul Walden described the synthesis and properties of the “first” ionic liquid, ethylammonium nitrate.

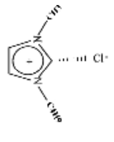
In this paper, we wish to report the application of the highly effective nonaqueous ionic liquids 1-ethyl-3-methyl imidazolium chloride as a reaction medium for the carboxymethylation of cellulose.



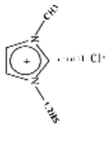
1-N-Butyl-3-methylimidazolium chloride (BMIMCl)



1-N-Ethyl-3-methylimidazolium chloride (EMIMCl)



(BMIMCl)



(EMIMCl)

References:

[1] Goto, T.; Harada, H.; Saiki, H. Fine structure of cellulose microfibrils in poplar gelatinous layer and valonia. *Wood Sci. Technol.* **1978**, *12* (3), 223.
[2] Fengel, D. Ultrastructural behavior of cell wall polysaccharides. *Tappi* **1970**, *53* (3), 497.
[3] Frey-Wyssling, A. Ultrastructure of wood. *Wood Sci. Technol.* **1968**, *2* (2), 73.
[4] Heyn, A. N. J. Ultrastructure of wood pulp with special reference to the elementary fibril of cellulose. *Tappi* **1977**, *60* (11), 159.

Synthesis of novel 2-azetidinones bearing biologically important amines

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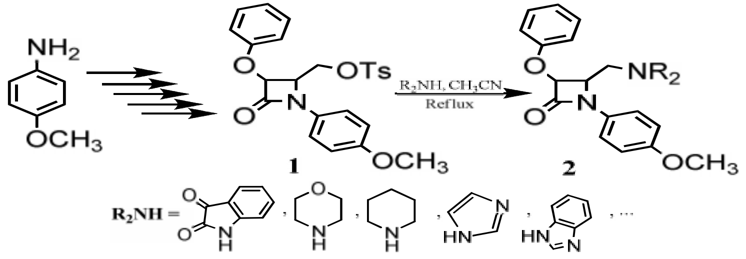
[*]Corresponding Author E-mail: Jarrah@susc.ac.ir

An interesting group of β-lactams are the monocyclic β-lactams such as nocardicins and monobactams[1-2]. In the late 1970s and early 1980s, the first classes of monocyclic β-lactam antibacterial agents were isolated from natural sources. It has been reported that monocyclic β-lactams have novel biological activities such as cytomegalovirus protease inhibitors, thrombin and tryptase inhibitors, cholesterol absorption inhibitors, human leukocyte elastease (HLE) inhibitors, porcine pancereatic elastease (PPE) inhibitors and anticancer activities[3]. The extensive use of common β-lactam[4] antibiotics in medicine has resulted in an increasing number of resistant strains of bacteria through mutation and β-lactamase gene transfer[5]. In order to oppose the destructive action of β-lactamases, one strategy consists of modifying the structure of the β-lactam antibiotic, aiming to render it insensitive to the β-lactamase attack. A second approach uses a reagent, typically a β-lactam derivative, which incapacitates the β-lactamase, in synergy with the β-lactam antibiotic.

It is evident from literature that bioamines such as isatin[6] and its derivatives are known to be associated with broad spectrum of biological activity like antibacterial, anti-inflammatory , analgesic , anti-viral , antifungal , anti-tubercular , anti-depressant[7].

Based on the mentioned facts, we decided to have both important molecules (β-lactam and bioamines) in the same molecule. To do this, tosylated β-lactam **1** was synthesized[8] in five steps and then it was refluxed in acetonitrile with bioamines to produce the monocyclic β-lactams **2**.



References:

[1] Alcaide, B.; Almendros, P.; Alonso, J. M.; Redondo, M. C. *J. Org. Chem.* **2003**, *68*, 1426
[2] Jarrahpour, A.; Zarei, M. *Molecules*. **2006**, *11*, 49
[3] Banik, B. K.; Becker, F. F.; Banik, I. *Bioorg. Med. Chem.* **2004**, *12*, 2523
[4] (a) Jarrahpour, A.; Shekarriz, M.; Taslimi, A. *Molecules.* **2004**, *9* ,29 (b) Niccolai, P.; Tarsi, L.; Thomas, R. *J. Chem. Commun.* **1997**, 2333
[5] Alcaide, B.; Almendros, P.; Rodrı´guez-Vicente, A.; Ruiz, M, Pilar. *Tetrahedron* **2005**, *61*, 2767
[6] (a) Jarrahpour, A.; Khalili, D. *Molecules*. **2006**, *11*, 59 (b) Jarrahpour, A.; Khalili, D. *Tetrahedron Lett*. **2007**, *48*, 7140 (c) Luntha, P.; Singh, G. S. *Eur. J. Med. Chem*. **2009**, *44*, 2265
[7] Patel, A ; Bari, S ; Talele, G ; Patel, J ; Sarangapani, M. 2006, *Iranian. J. Pharm. Res.* **2006**, *4*, 249
[8] Hakimelahi, G.H,; Li, P.; Moosavi-Movahedi, A. A.; Chamani, A.; Khodarahmi, G.A.; Ly, T.W,; Valiyev, F.; Leong, M.K.; Hakimelahi, S.; Shia, K.; Chao, I. *Org. Biomol. Chem*. **2003**,*1*, 2461.

Efficient and one pot synthesis and characterization of some novel bis(2-benzothiazole) derivatives

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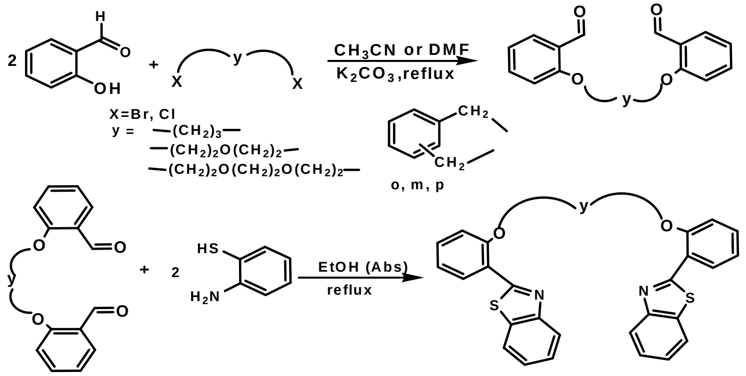
Benzothiazoles are a group of xenobiotic, heterocyclic chemicals which contain a benzene ring fused with a thiazole ring. Benzothiazoles rarely occur as natural products, but they form part of the molecular structure of a large number of natural products, biocides, drugs, food flavors, and industrial chemicals [1].

Benzothiazole derivatives have been well known for their biological and pharmaceutical activities, such as antitumor, antiviral, antimicrobial, activities and potent inhibitory activity [2]. 2-Arylbenzothiazoles have been known as important and useful compounds for pharmaceutical organic synthesis, as anticancer and Alzheimer's disease agents. There have been numerous reports for the synthetic routes of these compounds [3].

We have synthesized a series of new macroacyclic bis (2-benzothiazole) derivatives under free catalyst condition, condensation reaction of dialdehydes with 2-aminothiophenol in absolute ethanol in high yields and simple separation. Firstly the reaction of salicylaldehyde with some of aliphatic and benzilic dibromides and dichlorides, in the presence of K_2CO_3 as base in the appropriate solvent. In this new methodology, a number of dialdehydes were synthesized in excellent yields and short reaction times with advantages such as: simplicity work up, easily separation and simple purification.



References:

[1] Vincenzo, B.; Marco, N.; Roberto, F.; Domenico, R. *J. Agric. Food Chem.* **2000**, *48*, 1239.
[2] Lianqing, C.; Chuluo, Y.; Suyue, L.; Jingui, Q. *Spectrochimica Acta Part A*, **2007**, *68*, 317.
[3] Chin-Hsing, C.; Pin-Chih, Y.; Bo-Chi.; W. *Tett. Let.* **2008**, *49*, 4145.

Facile synthesis of novel dihydroimidazo[1,2-*a*]pyrimidines

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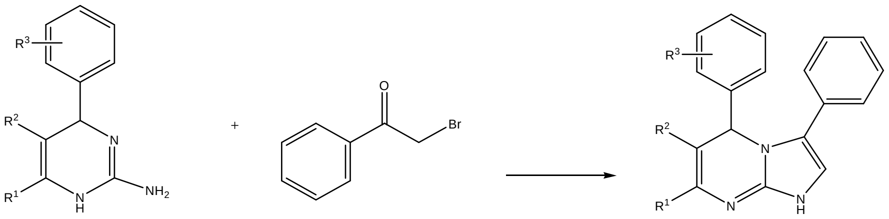
Imidazo[1,2-a]pyrimidines posses diverse biological activities and this structural motif is present in analgesics and inflammation inhibitors [1]. Also, Imidazo[1,2-*a*] pyrimidines represent a class of molecules capable of binding to multiple receptors with a high affinity giving useful biological activities such as antifungal, antibacterial, local anesthetic activity [2-3]. In recent years, several procedures for preparing of Imidazo[1,2-a]pyrimidines have been reported [4-5].

Herein, we would like to report, a facile synthesis of novel dihydroimidazo[1,2-*a*]pyrimidines by the reaction of 2-aminodihydropyrimidines generated from Biginelli and Biginelli-like reaction with *α*-bromoacetophenone in good yield and high purity. The structures of the products were confirmed through spectral analysis.



References:

[1] Freeman, C. G.; Turner, J. V.; Ward, A. D. *Aust. J. Chem.* **1987**, *31*, 179.
[2] Lyon, M.; Kercker, T. *Org.Lett.* **2004**, *26*, 4989.
[3] [Lober, S.; Hubner, H.; Gmeneir, P. *Bioorg. Med, Chem. Pharm. Bull.* **1992**, *40*, 1170.
[4] Nadipuram, A.; Kerwin, S. *Tetrahedron* **2006**, *62*, 3798.
[5] Lee, Y. S.; Lee, K. *J. Bull. Korean Chem. Soc.* **2002**, *23*, 1845.

A novel one-pot and efficient procedure for the synthesis of 3*H*-spiro[isobenzofuran-1,6'-pyrrolo[2,3-*d*]pyrimidine]-2',3,4',5'-tetraones

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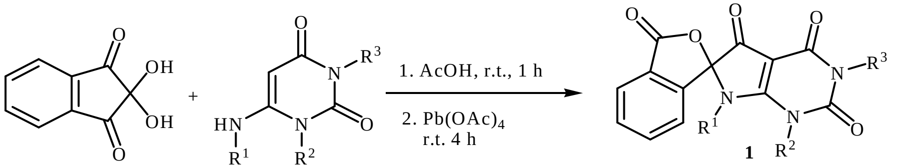
Oxygen and nitrogen containing heterocycles are getting immense importance in the area of pharmaceuticals and agrochemicals [1]. Substituted phthalides (isobenzofuran-1(3H)-ones) represent an important class of natural products that posses significant biological properties [1]. In particular, 3-substituted phthalides are vital heterocyclic motifs in many bioactive compounds such as isocoumarins, anthraquinones, anthracyclines, and several alkaloids [2].

Pyrrolo[2,3-d]pyrimidine derivatives are reported to possess various biological activities such as anti-HCV, anti-HIV type 1, anti-HSV, adenosine kinase inhibition, Aurora-A kinase inhibition and cAMP phosphodiesterase inhibition [3,4].

In continuation to our ongoing programs with the aim to develop more efficient synthetic processes for synthesis of biologically important oxygen and nitrogen containing heterocycles [5], we herein describe a novel and practical one-pot procedure for the preparation of some new derivatives of 3*H*-spiro[isobenzofuran-1,6'-pyrrolo[2,3-*d*]pyrimidine]-2',3,4',5'-tetraones **1**.



References:

[1] Lin, G.; Chan, S. S.-K.; Chung, H.-S.; Li, S.-L. Chemistry and Biological Action of Naturally Occurring Phthalides. In *Studies in Natural Products Chemistry*; Atta-ur-Rahman, Ed.; Elsevier: Amsterdam, 2005; Vol. 32, p 611.

[2] Mal, D.; Pahari, P.; De, S. R. *Tetrahedron* **2007**, *63*, 11781.

[3] (a) Ramesh, E.; Raghunathan, R. *Tetrahedron Lett.* **2008**, *49*, 2583; (b) Ramesh, E.; Raghunathan, R. *Tetrahedron Lett.* **2008**, *49*, 1812.

[4] Ramasamy, K.; Imamura, N.; Robins, R. K.; Revankar, G. R. *J. Heterocyc. Chem.* **2009**, *25*, 1893.

[5] (a) Mohammadizadeh, M. R.; Firoozi, N. *Tetrahedron Lett.* **2010**, *51*, 2467; (b) Mohammadizadeh, M. R.; Bahramzadeh, M.; Mohammadi, A. a.; Karimi, A. R. *Helv. Chim. Act.* **2010**, *93*, 153.

Silica sulfuric acid nanoparticles: An efficient and reusable catalyst for synthesis of naphthopyran, α-amino nitriles and chromene derivatives

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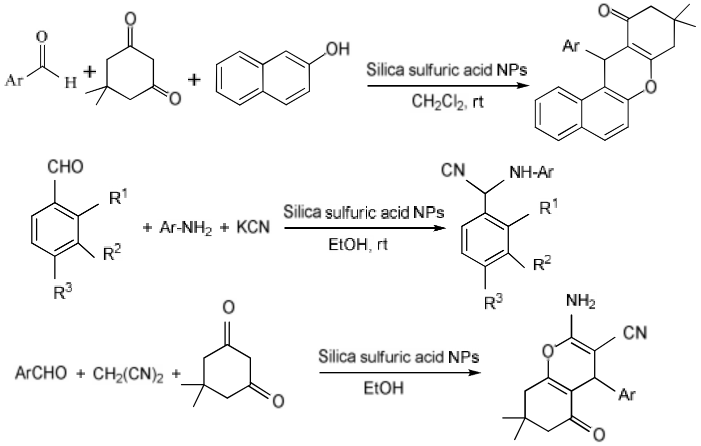
Naphthopyran derivatives are of special interest as photochromic compounds, which have a wide variety of applications such as ophthalmic glasses, electronic display systems, optical switches, and temporary or permanent memoriesl [1], α- amino nitriles are important and very useful class of intermediates for the synthesis of versatile α- amino acid [2] and 2-amino-2-chromenes are an important class of compounds found as the main components of many naturally occurring products employed as cosmetics and pigments and utilized as potential biodegradable agrochemicals [3].



Solid supported reagents have improved activity and selectivity than individual reagents. Because the surface area of the reagent is increased manifold [4]. In this work we report a mild procedure for the synthesis of different naphthopyrans, α- amino nitriles and chromenes by solid phase acidic catalyst with improved yields.

References:

[1] Coelho, P. J.; Carvalho, L. M.; Vermeersch, G.; Delbaere, S. *Tetrahedron*, **2009**, *65, 5369.*
[2] Horenstein, B. A.; Nakanishi, K. *J. Am. Chem. Soc.* **1989**, *111*, 6242.
[3] Hafez, E.A.; Elnagdi, M. H.; Elagamey, A. A.; El-Taweel, F. A. M. *Heterocycles*, **1987**, *26*, 903.
[4] Sadeghi, B.; Mirjalili, B. F.; Hashemi, M. M. *Tetrahedron Lett.* **2008**, *49*, 2575.

Citric acid as green and reusable catalyst for the synthesis of 2,3-dihydroquinazolin-4(*1H*)-ones in water

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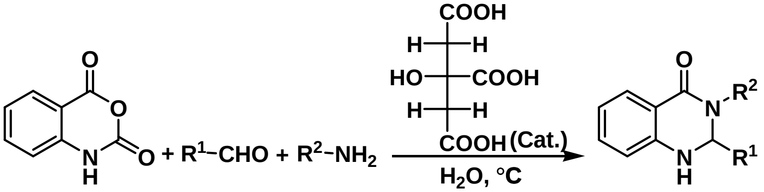
2,3-Dihydroquinazolinones are a class of heterocycles that attracted much attention because they have been reported to possess a wide range of pharmaceutical activities including antifertility, antibacterial, antitumor, antifungal, and mono amine oxidase inhibition [1]. Also these compounds can be readily oxidized to their quinazolin-4(3H)-one analogues that are important biologically active heterocyclic compounds [2]. Therefore, considerable efforts have been made to investigate efficient, simple, non-toxic and direct approaches toward the construction of 4(*3H*)-quinazolinone derivatives.

In continuing our studies about investigation of new catalysts or catalytic methods in organic reactions [3-4] we became interested to apply citric acid as an efficient catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones. Therefore isatoic anhydride, ammonium acetate (or primary amines) and a variety of aldehydes were condensed in the presence of catalytic amounts of citric acid in water at 80 ºC (Scheme 1).



Scheme 1

In summary, a new catalytic protocol to synthesize 2,3-dihydroquinazolin-4(*1H*)-one derivatives has been developed. The present protocol enjoys simple work-up, short reaction time, easy recovery and reuse of catalyst.

References:

[1] Hour, M.; Huang, L.; Kuo, S.; Xia, Y.; Bastow, K.; Nakanishi, Y.; Hamel, E.; Lee, K. *J. Med. Chem.* **2000**, *43*, 4479.
[2] Salehi, P.; Dabiri, M.; Zolfigol, M.A.; Baghbanzadeh, M. *Synlett* **2005**, 1155.
[3] Ghorbani-Choghamarani, A.; Goudarziafshar, H.; Nikoorazm, M.; Yousefi, S. *Can. J. Chem.* **2009**, *87*, 1144.
[4] Zolfigol, M.A.; Amani, K.; Ghorbani-Choghamarani, A.; Hajjami, M.; Ayazi-Nasrabadi, R.; Jafari, S. *Catal. Commun.* **2008**, *9*, 1739.

Studies on the synthesis and dynamic NMR properties of 1-ethyl 2,3 dialkyl 1-(acetylamino)-1-cyano-3-(1,1,1-triphenyl-λ^5-phosphanilidine)-1,2,3-propantricarboxylate

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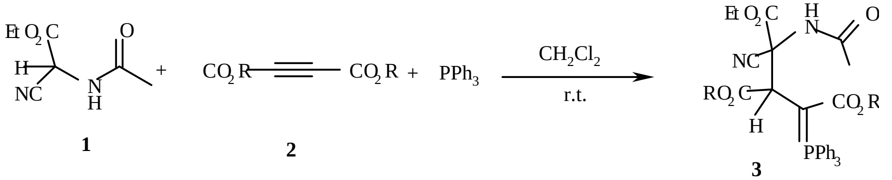
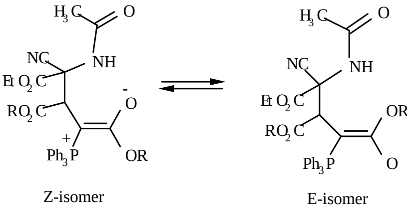
Stable crystalline phosphorus ylides **3a-b** were obtained in excellent from the 1:1:1 addition reaction between triphenylphosphine and dialkyl acetylenedicarboxylates **2** in the presence of ethyl acetamidocyanoacetate **1** as a CH-acid [1]. These stable ylides exist in solution as a mixture of two geometrical isomers(*E* and *Z*) as a result of restricted rotation around the carbon-carbon partial double bond resulting from conjugation of the ylide moiety with the adjacent carbonyl group on the NMR time scale at ambient temperature [2,3]. Assignment of the (*Z*)-configuration to the major geometric isomer is based on the ^{1}H chemical shift of the OR moiety, which is expected to be shielded as a result of the anisotropic effect of the phenyl groups [3]. The dynamic effects in the ylide moiety were investigated by ^{1}H NMR spectra. Rotational energy barrier ($\Delta G^{\#}$) for their interconversion process of rotational isomers of ethyl and methyl derivatives equal 17.263 and 16.180 KJ mol^{-1}, respectively.





Z-isomer E-isomer

2,3	R	Yield of 3 (%)
a	Me	80
b	Et	85

References:

[1] Asghari, S.; Taghipour, V. *Tetrahedron Lett.* **2008**, *49*, 1824.
[2] Yavari, I,; Zonouzi, A.; Hekmat-Shoar, R. *Tetrahedron Lett.* **1998**, *3*9, 3841.
[3] Habibi-Khorassani, S. M.; Maghsoodlou, M. T.; Ebrahimi, A.; Vasheghani-Farahani, F.; Mosaddeg, E.; Amini Kazemian, M. *Tetrahedron Lett.* **2009**, *50*, 3621.

Ab initio investigations of some of the molecular wires under the interaction of external electric field

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It has been demonstrated that both the geometric and electronic feature of the molecular wires are sensitive to the external field(EF)and may consequently result in a different transportation behavior[1,2].The effect of such a perturbation depends on the polarizability and electronic configuration of the molecule. In this report, we investigate transport properties of molecular wire based molecules sandwiched between metal cluster of AU.Linker such CN,SH,NS has been considered. The gold clusters and the terminated atoms were fixed at their optimal. As a representative example,the bond length variation under various EF for complexes 1 is shown in Fig.1.Also Table 1 gives a comparison of the energy levels of HOMO and LUMO levels as well as their gap (HLG) for the complexes.

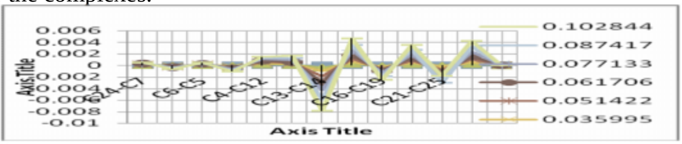


Fig. 1a.

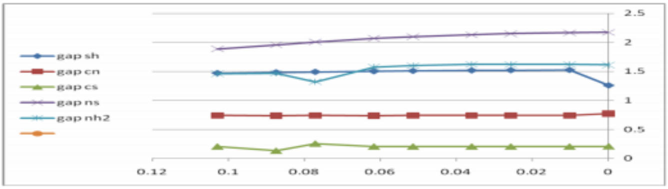
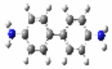


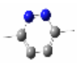
Table 1.

This is due to the localization of the LUMO energy level on the metal atoms.The addition of Au atoms stabilizes the HOMO energy levels of the molecule.On the other hand we investigated electron transport properties of NBN(NH2-Bridge-NH2) molecules sandwiched between two gold surfaces.Different bridges such NB1N,NB2N,NB3N,NB4N and NB0N(Fig.2)we conclude that with the increase of EF single bonds become shorter and double bonds become longer signifying an enhanced conjugation of molecular wire. Fig.2.

NBN



B1



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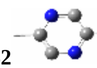

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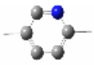

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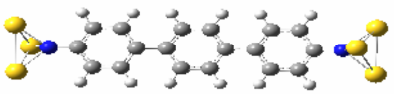

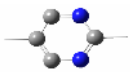

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References:

[1] Lu, S.Z.; Li, X.Y.; Liu, J.F.*Chem.Phys.* **2004**, *297*, 31.
[2] Seminario, J.M.; Zacarias, A.G.; Derosa, P.A. *J.Phys.Chem.A* **2001**, *105*, 792.

Synthesis of purine derivatives via amidine intermediate using diaminomaleonitrile

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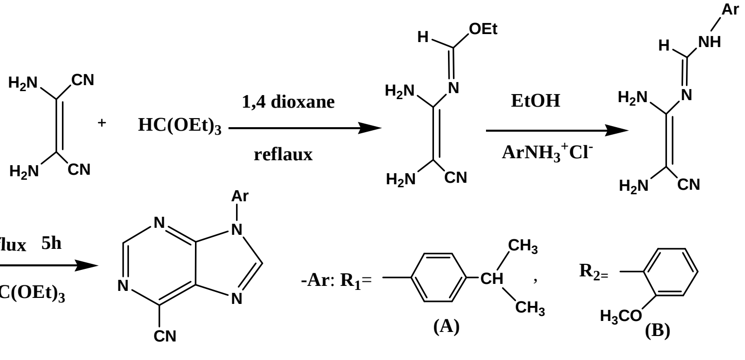
Purines are a class of heterocyclic compounds which play an important role in many biological processes. The most important natural occurrence of purines is in the nucleotides and nucleic acids; compounds which perform some of the most crucial functions in fundamental metabolism. The chemotherapeutic uses of purines and purine analogues have prompted tremendous efforts towards their synthesis, both in academia and in the pharmaceutical industry As the purine ring system is a fusion of two aromatic heterocyclces, pyrimidine and imidazole, a logical starting point for ring synthesis is an appropriately substituted pyrimidine or imidazole from which the second ring can be constructed by a cyclization process. In this paper we synthesized derivatives of ciyanopurine using diaminomaleonitrile from different aromatic amines. In first step we synthesized imidate and in second step synthesized different amidine using anilinum chloride catalyst.

In latest step cyanopurines synthesized in the presence of triethylortoformate under reflux conditions. In conclusion the yield of purine with (R_2) was higher than (R_1). These products identified by melting point, IR spectra, ^{1}HNMR.



Refrences:

[1] Booth B L, Dias A D and Proenca M F, *J. Chem. Soc. Perkin. Trans.* **1992**, *1*, 2119.
[2] Birkett P R and King H, *Tetrahedron*, 1993, *49*, 11029.
[3] Yahyazadeh A, Pourrostam B and Rabiee M, *Bull. Korean. Chem. Soc.* **2003**, *24*, 1723.

Synthesis of new 2,2-bis{[3,5-bis(1,1-dimethylethyl)-4-hydroxy]phenylmethyl}indan-1-ones and their alcohols as new GABA$_B$ potentiators

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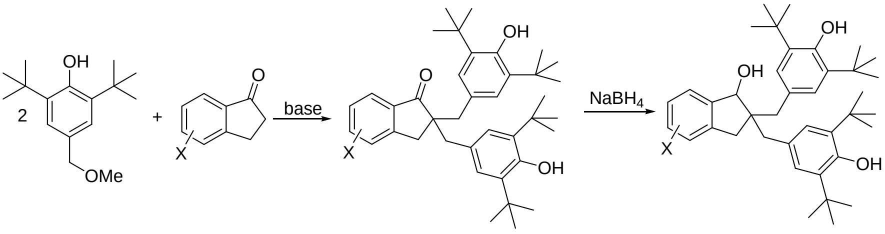
A series of compounds with general formula 3-(3,5-di-*tert*-alkyl-4-hydroxyphenyl)-2, 2-di-substituted propanals, are known to stabilize organic materials normally subjected to deterioration caused by heat, light and oxygen. In addition to being antioxidants, they are even more useful as intermediates for the preparation of high molecular weight antioxidants for polypropylene and other polymers [1].

We have previously reported the synthesis of 3-(2,6-di-tert-butyl-4-hydroxyphenyl)propan-1-ones and 3-(2,6-di-isopropyl-4-hydroxyphenyl)propan-1-ones [2,3]. Herein, we report the synthesis of new 2,2-Bis{[3,5-bis(1,1-dimethylethyl)-4-hydroxy]phenylmethyl}indan-1-one derivatives **1** which may have better antioxidant activity than the corresponding monosubstituted analogues. In order to produce a new series of potential GABA$_B$ receptor modulators. We have also reduced these carbonyl compounds to their corresponding alcohols **4**.



3 **2** **1** **4**

X= Cl, OMe

References:

[1] Biggo, G.; Concas, A.; Costa, E. E.; GABAergic Synaptic Transmission: *Molecular, pharmacological and clinical aspects* **1992.**

[2] Kerr, D. I. B.; Khalafy, J.; Ong, J.; Perkins, M. V.; Prager, R. H.; Puspawati, N. M.; Rimaz, M.; *Aust. J. Chem.* **2006**, *59*, 457.

[3] Kerr, D. I. B.; Khalafy, J.; Ong, J.; Prager, R. H.; Rimaz, M.; *J. Braz. Chem. Soc.* **2007**, *18*, 721.

Synthesis and characterization of new soluble thermally stable pyridine-based polyesters

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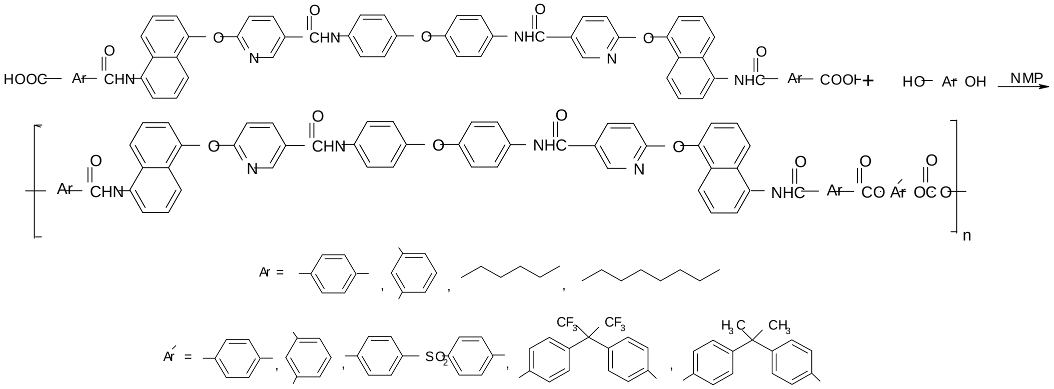
Polyesters are important class of high performance and engineering polymers, which find use in a number of diverse applications [1]. Development of polyesters for use at high temperature with improved solubility is an important goal [2,3].

Here we wish to express the synthesis of a novel diacids with preformed ether and amide groups and use it for the preparation of related polyesters. Thus, the solubility of the polyesters increased without extreme loss of their high thermal stability via introduction of polar and flexible groups in to the polymer backbone.



All monomers, model compound and polyesters are characterized. The physical properties of polymers including inherent viscosity, solubility behavior, thermal properties and thermal stabilities are studied.

References:

[1] Seymour, R. B.; Kirshenbaum, G. S. *High performance polymers, New York, Elsevier,* **1986**.
[2] Mehdipour-Ataei, S.; Maleki-moghaddam, R.; Nami, M. *Eur. Polym. J.* **2004**, *40*, 2523.
[3] Tamami, B.; Yeganeh, H.; Kohmareh, G. *Eur. Polym. J.* **2004**, *40*, 1651.

Synthesis of 1,5-benzothiazepines in the presence of ionic liquid

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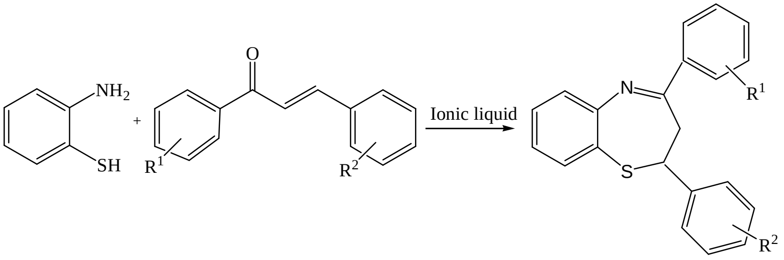
Chalcones, which are considered to be precursors of flavonoids and isoflavonoids, are abundant in dibble plants. Chemically they are open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β-unsaturated carbonyl system (1,3-diphenyl-2-propen-1-one). Chalcones exhibit many pharmacological activities, including anti-leishmanial [1], anti-inflammatory [2], antimitotic [3], anti-invasive and anti-tuberculosis [4].

1,5-Benzothiazepines play a unique role in drug discovery programs, as they display a wide spectrum of biological actives [5].

Herein, a simple and efficient method for the preparation of 1,5-Benzothiazepines from the reaction of Chalcones with 2-aminothiophenol using ionic liquid is reported. Simple procedure, high yields and easy work-up are merits of our method.



References:

[1] Nielsen, S. F.; Christensen, S. B.; Cruciani, G.; Kharazmi, A.; Liljefors, T. *J. Med. Chem.* **1998**, *41*, 4819.

[2] Matsuda, H.; Morikawa, T.; Ando, S.; Iwao, T.; Masayuki, Y. *Bioorg. Med. Chem.* **2003**, *11*, 1995.

[3] Ducki, S.; Forrest, R.; Hadfield, J. A.; Kendall, A.; Lawrence, N. J.; Mcgown, A. T.; Rennison, D. *Bioorg. Med. Chem.* Lett. **1998**, *8*, 1051.

[4] Lin, Y. M.; Zhou, Y.; Flavin, M. T.; Zhou, L. M.; Nie, W.; Chen, F. C. *Bioorg. Med. Chem.* **2002**, *10*, 2795.

[5] Wang, L.; Zhang, P.; Zhang, X.; Zhang, Y.; Li, Y.; Wang, L.; Wang, Y. *Eur. J. Med. Chem.* **2009**, *44*, 2815.

Solvent-free synthesis of amides, esters and thioesters using ($CaMg(CO_3)_2$) as a heterogeneous catalyst

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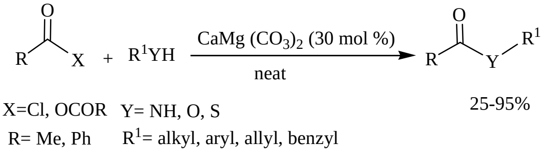
Heteroatom protection is conventionally carried out via the catalytic reaction of *SH*, *OH* and amino groups with anhydrides, acid chlorides or sulfonyl chlorides. Current contributions to this area have been highlighted by using heterogeneous catalysts [1].

Recently, minerals have been used as excellent heterogeneous catalysts in organic transformations with rewards of non-toxicity, reusability, eco-friendly and green nature of catalysts together with raising the activity of adsorbed materials and reaction rates [2]. In this pursuit we have acylation of alcohols [3] and our new approach is application of $CaMg(CO_3)_2$ as a new reusable heterogeneous mineral catalyst in the the solvent-free synthesis of amides, esters, thioesters, sulfonamides and sulfonate esters (Scheme1).



Scheme 1

Thus, we report here an efficient method for chemoselective acylation of of amines, alcohols and thiols under solvent-free conditions in the presence of catalytic amount of $CaMg(CO_3)_2$. Various aromatic, heteroaromatic, aryl and alkyl substrates were converted to the corresponding amide, ester and thioester derivatives in excellent yields. Selective acylation of amines in the presence of alcohols and secondary amines were also achieved by this method.

References:

[1] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104*, 199.

[2] (a) Sharghi, H.; Hosseini, M. *Synthesis* **2002**, 1057. (b) Hosseini-Sarvari, M.; Sharghi, H. *J. Org. Chem*. **2006**, *71*, 6652.

[3] (a) Tamaddon, F.; Amrollahi, M. A.; Sharafat, L. *Tetrahedron Lett.* **2005**, *46*, 7841. (b) Fitz, M.; Forró, E.; Vigóczki, E.; Lázár, L.; Fülöp, F. *Tetrahedron: Asym.* **2008**, *19*, 1114.

PEG - 400 as an Efficient Reaction Medium for the Synthesis of Hantzsch 1, 4 – dihydroprydines

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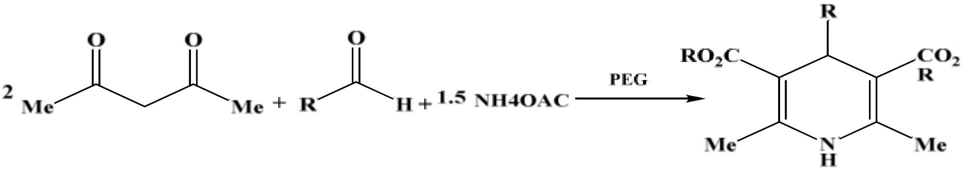
In recent years, an increasing interest has been focused on the synthesis of 1,4–dihydropyridines (1,4–DHPs) due to their significant biological activity. Reducing or eliminating the use of volatile organic solvents particularly chlorinated hydrocarbons can minimize the generation of waste, which is a requirement of one of the principles of green chemistry. Recently, PEG has attracted great attention as novel solvent for many organic reactions since it is relatively inexpensive, essentially nontoxic, readily available and biodegradable material. We have developed for the first time, an efficient protocol for synthesis of various substituted 1,4-dihydropyridines using one pot condensation of aldehydes with ethyl acetoacetate and ammonium acetate in PEG - 400 as reaction medium at 110^{o}C (Scheme).



(Scheme)

This procedure is operationally simple, environmentally benign and has high yield.

References:

[1] Ko, S; Yao, C-F; *J. Tetrahedron*. **2006**,62,7293.
[2] Lee, J. H*; J. Tetrahedron Letters*. **2005**,46,7329.

A conveniet one step synthesis of 3-methyl pyrazolo[5,4-d] benzopyranes

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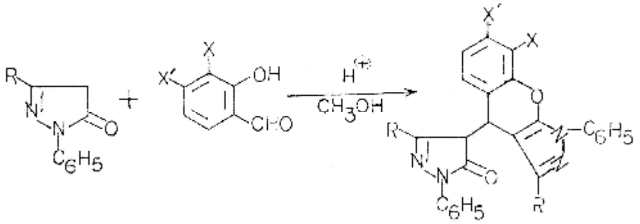
2-pyrazolin-5-ones individually or incombination are known to posses important various biological & pharmaceutical activities [1] ranging from antitumor [2] to anti-inflammatory [3], antipsychotic [4], antimicrobial [5], antiviral [6],and antifungal [7] activities . Synthesis of 3-methyl-1-phenyl-4-(3'-methyl-1'-phenyl-4'-5'-dihydro-5'-oxopyrazol-4'-y1)pyrazolo [5,4-d] -4H-1- benzopyran (1a): A solution of3-methyl-1-phenyl-2-pyrazolin-5-one2a (2g,0.011 mol) and 2-hydroxy-benzaldehyde 3a(0.70g,0.006mol) in, ethanol (50ml) in presence of hydrochloric acid (0.5ml) was refluxed on a steam bath for 36hrs.the solvent on distillation gave a solid which was recrystallised from chloroform-methanol(3:7) to give1a as pale brown shining crystals(1.61g), m.p.220°C. Pyrazolo[5,4-d]benzopyranes have been synthesized in one step in good yield by the reaction of3-methyl-1-phenyl- 2-pyrazolin-5-one with orthohydroxy benzaladehydes in presence if hydrocholoric acid.



(2a-2b) (3a-3b) [A]

References:

[1] Elguero, J.; In Comprehensive Heterocyclic Chemistry II Katritzky, A. R.; Rees, C. W.; Scriven, E. F. V., eds.;: NewYork, 1967; McDonald, E.; Jones, K.; Brough,P. A.; Drysdale, M. J.; Workman, P. ; Curr Top. Med. Chem. **2006**, *6*, 11936, 52.

[2] Lin, R.; Chiu, G.; Yu, Y.; Connolly, P. J.; Li, S.; Lu, Y.; Adams, M.; Fuentes-Pesquera, A. R.; Emanuel, S. L.; Greenberger, L. M.; Biooig. Med. Chem. Lett. **2007**, *17*, 4557.

[3] Gokhan-Kelekci, N.; Yabanoglu, S.; Kupeli, E.; Salgin, U.; Ozgen, 0.; Ucar, G.; Yesilada, E.; Kendi, E.; Yesilada, A.; Bilgin, A. A.; Bioorg. Med. Chem. **2007**, *15*, 5775;

[4] ‘Barceló , M.; Ravia, B.; Masaguer, C. F.; Dominuez, E.; Areias, F.M.; Brea, J.; Loza, M. I.; Bioorg. Med. Chem. Lett. **2007**, *17*, 4873.

[5] ‘Farag, A. M.; Mayhoub, A. S.; Barakat, S. E.; Bayomi, A. H.; Bioorg. Med. Chem. **2008**, *16*, 4569; Mahajan, R. N.; Havaldar, F. H.; Fernandes, P. S.; I Indian Chem. Soc. **1991**, *68*, 245.

[6] Larsen, J. S.; Zahran, M. A.; Pedersen, E. B.; Nielsen, C.; Monatsh. Chem. **1999,** *130*, 1167.

[7] Prakash, 0.; Kumar, R.; Parkash, V.; Eur I Med. C’hem. **2008,** *43*, 435.

Chemical composition of the essential oil of the aerial parts of *Adonis wolgensis* from north Iran

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The genus *Adonis* L. (Ranunculaceae) comprises about 30 species of herbaceous plants, which are mainly distributed in the temperate regions of Asia and Europe [1]. Nine taxa of this genus have been already reported from flora of Iran [2]. A literature survey showed that the *Adonis* species has been found to be rich in Flavonoids, Cardenolides and Phenolic glycosides [3-6]. There are no previous data available in the literature on the quantitative analysis of *A. wolgensis* essential oil's components, so the aim of the present research was to determine the chemical composition of *A. wolgensis* essential oil from north of Iran. The hydrodistillation of aerial parts of *A. wolgensis* gave oil in 0.2% (v/w) yield, based on the dry weight of the plant. The constituents of the volatile oil obtained were analyzed by gas chromatography–mass spectroscopy (GC–MS). The major constituents of the essential oil tested were palmitic acid (32.52%), methyl linolenate (12.07%) and phytol (10.32%).

The essential oil of *A. wolgensis* was also assayed for measurement of antimicrobial activity. But, the oil did not exhibit antimicrobial activity.

References:

[1] Wang, W. T. *Bull. Bot. Res*. **1994**, *14*, 1.
[2] Rechinger, K. H. *Flora Iranica*, Rechinger, K. H. ed., *Graz* (**1992**), no. *171*, 204.
[3] Komissarenko, N. F.; Korzennikova, E. P.; Yatsyuk, V. Ya. *Chem. Nat. Cmpd*. **1973**, *9*, 417.
[4] Komissarenko, N. F.; Korzennikova, E. P.; Yatsyuk, V. Ya. *Chem. Nat. Cmpd*. **1974**, *10*, 838.
[5] Pauli, G. F.; Junior, P. *Phytochemistry*, **1995**, *38*, 1245.
[6] Pauli, G. F.; Junior, P.; Berger, S.; Matthiesen, U. *J. Nat. Prod*. **1993,** *56*, 67.

A new efficient catalytic system for microwave promoted cyanation of aryl halides

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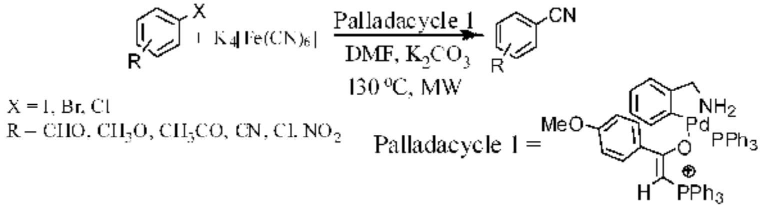
As aryl nitriles can be used in both laboratory and industrial scales [1] in the synthesis of a vast range of commercial compounds [2], development of new synthetic methods for cyanation of aryl halides and aryl triflates are attractive subject in organic synthesis. Also CN group is equal to functional groups such as carboxylic acids and their derivatives, aldehydes, amines, thiazoles, triazoles, oxadiazoles, etc., and can be applied for preparation of these functional groups [2].

Because almost all of the old methods for cyanation of aryl halides such as Sandmeyer reaction [3] and Rosenmund-von Braun reaction [4] have required harsh conditions, so, many researchers are trying to find new methods that can produce these compounds, efficiently. Microwave irradiation methodology is one of methods that have found a widespread advantage in organic and inorganic synthesis such as more energy efficient and higher reaction rates, and in many cases improves the yields in comparison to the conventional conditions [5]. Reaction rate improvement could be explained by considering the higher and more rapid temperature homogeneity that reached by employing microwave heating methods.

Herein, we wish to report the application of a new phosphine-based catalytic system for cyanation reaction of different aryl halides using $K_4[Fe(CN)_6]$ as a safe cyanating agent under microwave irradiation. The reactions were performed with reasonable reaction times and simple reaction conditions.



References

[1] Jiang, B.; Kan, Y.; Zhang, A. *Tetrahedron* **2001**, *57*, 158.
[2] Larock, R. C. *Comprehensive Organic Transformations* VCH: New York, **1989**.
[3] Sandmeyer, T. *Ber. Dtsch. Chem. Ges.* **1884**, *17*, 1633.
[4] Rosenmund, K. W.; Struck, E. *Ber. Dtsch. Chem. Ges.* **1919**, *2*, 1749.
[5] Cundy, C. S. *Collect. Czech. Chem. Commun.* 1998, *63*, 1699.

Ionic liquid, [bmim]Br, as an efficient promoting medium for synthesis of 2-amino-2-chromenes without the use of any catalyst

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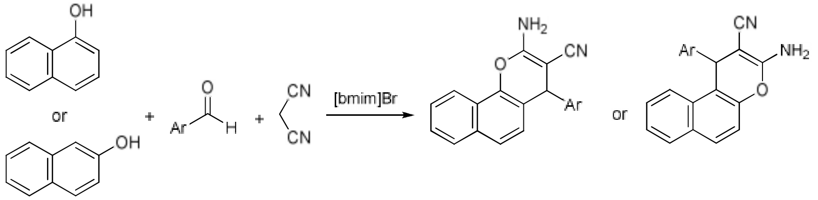
2-Amino-2-chromenes represent an important class of compounds being the main components of many naturally occurring products and are widely employed as food additives, cosmetic agents and utilized as potential biodegradable agrochemicals [1,2]. The most straightforward synthesis of this compounds involve the three-component condensation of an aldehyde, malononitrile, and α(or β)-naphthol in the presence of piperidine using acetonitrile or ethanol as a reaction solvent [3,4]. Recently, relatively benign catalysts such as cetyltrimethylammonium bromide (CTABr), I_2/K_2CO_3, and nano MgO in water have also been used in this reaction [5-7]. However, the application of some of these methods is limited due to the moderate yields of the products, longer reaction time and laborious work-up procedure.

Thus, in this work, we wish to report a simple and eco-friendly procedure for the synthesis of 2-amino-2-chromene derivatives via three-component condensation of an aldehyde, malononitrile, and α(or β)-naphthol using [bmim]Br, a neutral ionic liquid, as an efficient medium without any catalysts.



References:

[1] Hafez, E. A.; Elnagdi, M. H.; Elagamey, A. A.; El-Taweel, F. M. A. A. *Heterocycles*, **1987**, *26*, 903.
[2] Varma, R. S.; Dahiya, R. *J. Org. Chem.*, **1998**, *63*, 8038.
[3] Bloxham, J.; Dell, C. P.; Smith, C. W. *Heterocycles*, **1994**, *38*, 399.
[4] Elagamey, A. G. A.; El-Taweel, F. M. A. A. *Indian J. Chem.*, **1990**, *B29*, 885.
[5] Jin, T. S.; Xiao, J. C.; Wang, S. J.; Li, T. S. *Ultrason. Sonochem.*, **2004**, *11*, 393.
[6] Ren, Y. M.; Cai, C. *Catal. Commun.*, **2008**, *9*, 1017.
[7] Kumar, D.; Reddy, V. B.; Mishra, B. G.; Rana, R. K.; Nadagouda, M. N.; Varma, R. S.; *Tetrahedron*, **2007**, *63*, 3093.

Sulfamic acid as an cost-effective and green catalyst for efficient and simple synthesis of mono-and disubstituted 2,3-dihydroquinazolin-4(1H)-ones in water

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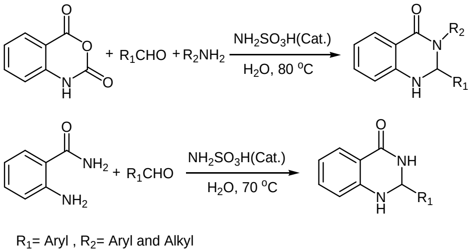
2,3-Dihydroquinazolinones are a class of heterocycles that attracted much attention because they have been reported to possess a wide range of pharmaceutical activities including antifertility, antibacterial, antitumor, antifungal, and mono amine oxidase inhibition [1]. The typical procedure for the synthesis of mon-substituted-2,3-dihydroquinazolin-4(1H)-ones involves the condensation reaction of anthranilamide with aldehyde in the presence of catalyst [2]. The disubstituted-2,3-dihydroquinazolin-4(1H)-ones are also synthesized through a multi-step reaction of isatoic anhydride and different types of amines and aldehydes using acid catalyst [3].

Sulfamic acid (SA, H_2NSO_3H) is a common inorganic acid with a mild acidity that is nonvolatile, noncorrosive, and utilized as a stable, low-cost, and commercially available reagent. More important, its water resistance makes it an outstanding alternative to metal catalysts, in different areas of organic synthesis, as an efficient and green heterogeneous catalyst [4].

In continuation of our efforts to develop more versatile methodologies in organic synthesis [5]. Herein, we report a simple and straightforward method for the preparation of mono-and disubstituted quinazolin-4(1H)-ones in the presence of catalytic amounts of SA as a green catalyst.



In summary, a very simple, efficient and eco-friendly synthesis of 2,3-dihydroquinazolin-4(1H)-ones has been devised. Work-up procedure was so simple and including filtration of mixture and washing the residue with ethanol followed by a recrystallisation step. We believe this method could be addressed for the combinatorial synthesis of 2,3-dihydroquinazolinones in drug discovery programs.

References:

[1] Hour, M.; Huang, L.; Kuo, S.; Xia. Y.; Bastow, K.; Nakanishi, Y.; Hamel, E.; Lee. K. *J. Med. Chem*. **2000**, *43*, 4479.
[2] Shaabani, A.; Maleki, A.; Mofakham, H.; *Synth. Commun.* **2008**, *38*, 3751.
[3] Dabiri, M.; Salehi, P.; Baghbanzadeh, M.; Zolfigol, M. A.; Agheb, M.; Haydari, S. *Catal.Commun*. **2008**, *9*, 785.
[4] Heravi, M. M.; Baghernejad, B.; Oskooie, H. A. *Cur. Org. Chem.* **2009**, *13*, 1002.
[5] Rostami, A.; Akradi, J. *Tetrahedron Lett.* **2010**, *51*, 3501.

DFT Studies and synthesis of mono and bis-4-methylpiperidineiummethyl-thiourea as corrosion inhibitors

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Corrosion protection is designed to prevent the corrosion of metal surfaces of equipment during transport and storage. The study of corrosion of mild steel and iron is a matter of tremendous theoretical and practical concern and as such has received a considerable amount of interest [1]. Acid solutions, widely used in industrial acid cleaning, acid descaling, acid pickling, and oil well acidizing, require the use of corrosion inhibitors in order to restrain their corrosion attack on metallic materials. The use of organic compounds containing oxygen, sulfur and especially nitrogen to reduce corrosion attack on steel has been studied in some detail [2]. The existing data show that most organic inhibitors adsorb on the metal surface by displacing water molecules on the surface and forming a compact barrier film [3].

Mono and bis- 4-methylpiperidineiummethyl-thiourea was developed as novel corrosion inhibitor. This compound has been synthesized and characterized by IR, Mass and NMR.

It is very stable compound and do not undergo any degradation under the stated conditions. An interesting feature of their moiety is the presence of heteroatoms (N–O) with lone pairs of electrons which invariably plays a dominant role in corrosion inhibition. As a part of our ongoing research program for synthesis and theoretical studies of corrosion inhibitors [4] in this work we report the synthesis of Mono and Bis-4-methylpiperidineiummethyl-thiourea as corrosion inhibitors.

Further work is underway in the laboratory involving the in-depth study of some of the most promising inhibitors from this study. Density functional (DFT) calculations have been carried out for the title compounds by performing HF and DFT levels of theory using the standard 6-31G* basis set. Predicted vibrational frequencies have compared with experimental IR spectra and they supported each other.

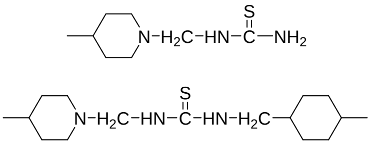

Fig. Molecular structures of Mono- 4-methylpiperidineiummethyl -thiourea and Bis-- 4-methylpiperidineiummethyl -thiourea .

References:

[1] Uhlig, H. H.; Revie, R. W, *Corrosion and Corrosion Control*, Wiley, New York, **1985**.
[2] Sykes, J. M. *Brit., Corros. J.* **1990**, *25*, 175.
[3] Muralidharan, S.; Phani, K. L. N.; Pitchumani, S.; Ravichandran, S. V. K.; Iyer, S., *J. Electrochem. Soc.* **1995**, *142*, 1478.
[4] Teimouri, A.; Najafi Chermahini, A. Frontiers of Chemical Engineering in China: In Press.

The synthesis of novel barbiturates a century after their clinical introduction

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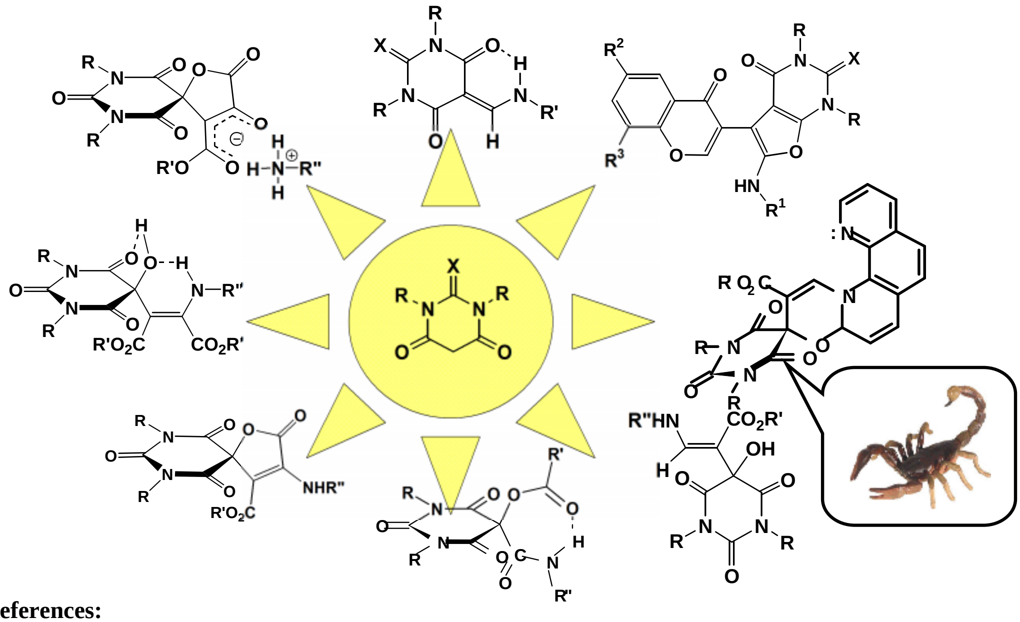
In the course of the 20th century, more than 2500 barbiturates were synthesized, 50 of which were eventually employed clinically. Their use was widespread and many still have some use today. One hundred years after the introduction in clinical pharmacology of the original compound, oxybarbiturates, in general, continue to be the selected drugs in the treatment of some serious forms of insomnia and in some types of epilepsy. Similarly, some thiobarbiturates and some ultrashort-acting barbiturates are still used today as inducers of general anesthesia [1].

In connection with our recent interest aimed at the development of efficient protocols for the preparation of biologically active heterocycles [2,3], herein some of our recent synthetic approaches to novel biologically interesting barbiturates are reported.



References:

[1] López-Munoz, F.; Ucha-Udabe, R.; Alamo, C. *Neuropsychiatric Disease and Treatment* **2005**, *1*, 329.
[2] Teimouri, M. B.; Abbasi, T.; Khavasi, H. R. *J. Chem. Res.* **2010**, 310.
[3] Teimouri, M. B.; Abbasi, T. *Tetrahedron* **2010**, *66*, 3795.

Synthesis and applications of poly (vinylpyrrolidone)-grafted silica as a polymeric cosolvent catalyst in reduction of carbonyl compounds

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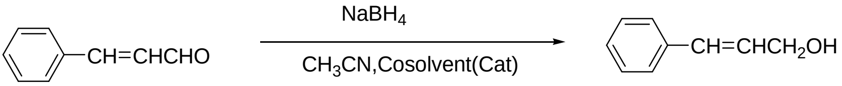
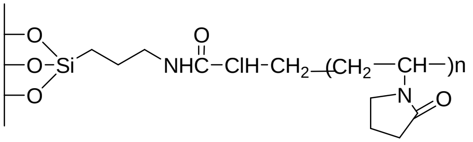
Polymeric phase transfer or cosolvent catalyst are the most attractive types of polymeric species for application in organic chemistry, because they provide great ease in separation and recycling of the catalyst and isolation of the product [1, 2]. Silica is chosen as a support because of its high mechanical resistance, its high thermal stability and its chemical reactivity through the silanol groups [3]. In here Poly (vinylpyrrolidone)-grafted silica is prepared and used as an effective heterogenouse polymeric cosolvent catalyst. As typical example aldehydes are reacted with $NaBH_4$ under this cosolvent system. A solution of a carbonyl compound and $NaBH_4$ in a wet THF is added to the poly (vinylpyrrolidone) grafted silica with stirring. The progress of the reaction will be followed by TLC and/or GC and the product is characterized by ^1H, ^{13}C-NMR and FT-IR spectroscopy technique.



Cosolvent :



References:

[1] Akelah, A. ; Moet, A. *Functionalized Polymers and Their Appiication* ; Chapman and Hall ; New York ; **1990**.
[2] *Synthesis and separations Using Functionalized Polymers*; Hodge, P.; Sherngton, D.C., Eds.; Wiley: New York, **1988** .
[3] A. Revillon, D. Leroux, *Reactive & Functional Polymers*, 1995, 26, 105.

The Synthesis of 3-(4-bromophenyl and 3-nitrophenyl)-5-bromomethyl isoxazole

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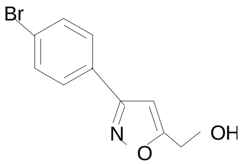
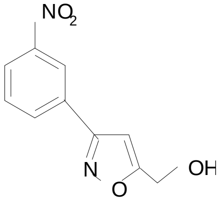
Isoxazoles and isoxazolines are very useful heterocycles[1] in organic medicinal chemistry.

[2a-e]isooazoline rings have been used by organic chemists for synthetic manipulation to aceess complex molecular architectures[1b].drugs such az lsocarboxazid, valdecoxib, oxacillin, leftunomide, and micafungin are the examples[2f] to substantiate the pharmaceutical acceptance of such heterocyclic systems. [1].

This research work describes the synthesis of new compound of isoxazole family. First, benzaldehyde (**1**) was transformed to benzaldoxime (**2**) by using NH_2OH in pyridine. The in situ generated nitriloxide from reaction between (**2**) and NaOCl, was reacted with propargylalcohol to produce 3-phenyl-5-hydroxymethyl isoxazole (**3**) in a cycloaddition procedure. Then, bromination of compound (**3**) with PBr_3 in CH_2Cl_2, to produce 3-phenyl-5-bromomethyl isoxazole (**4**). Bromination of compound **(4)** with Br_2 produced 3-(4-bromophenyl)-5-bromomethyl isoxazole **(5)** in high yield. Then, the nitration of compound (**3**) was occurred with HNO_3-H_2SO_4, and produced 3-(3-nitrophenyl)-5-hydroxymethyl isoxazole **(6)** as a new compound

The structure of all the synthesized compounds was characterized and confirmed by FT-IR and NMR spectroscopy techniques.





References:

1. Li G., Kakarla R., Gerritz S. W., *Tetrahedron Lett.* **2007,** *48,* 4595.

Three-component synthesis of functionalized 2,4-dioxothiazolidines

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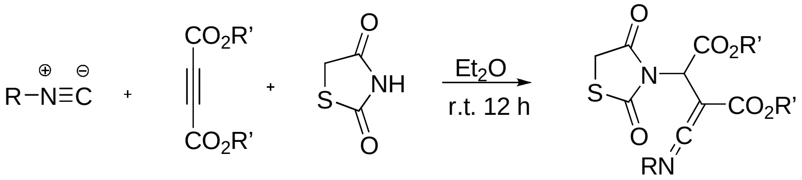
Multi-component reactions (MCRs), by virtue of the convergence, productivity, facile execution, and generally high yields of products, have attracted much attention from the point of combinatorial chemistry. Of pivotal importance in this area are the isocyanide based MCRs such as the versatile *Ugi* and *Passerini* reactions [1,2].

In recent years, the synthetic applications of multifunctional heteroallenes have been widely investigated [3]. In spite of extensive developments in the chemistry of modified ketenes and isocyanates, little attention has been paid to the synthesis of ketenimines [4].

We wish to report a simple one-pot synthesis of highly functionalized 2,4-dioxothiazolidines **4**. Thus, reaction of dialkyl acetylenedicarboxylates **2** with 2,4-thiazolidinedione **3a** in the presence of alkyl isocyanides leads to **4** in good yields. Also, the reaction of alkyl isocyanides with *DMAD* in the presence of 5-arylidene-2,4-thiazolidinediones **3b-g** led to corresponding 2,4-dioxothiazolidines in good yields.



1 **2** **3a** **4**

References

[1] Ugi, I. *Angew. Chem. Int. Ed. Eng.* **1982**, *21*, 810.
[2] Domling, A. and Ugi, I., *Angew. Chem. Int. Ed. Eng.* **2000**, *39*, 3169.
[3] Abbiati, G.; Cirrincione de Carvalho, A.; Rossi, E. *Tetrahedron.* **2003**, *59*, 7397.
[4] Yavari, I.; Zare, H.; Mohtat, B. *Mol Divers.* **2006**, *10*, 247.

Rapid *N*-alkylation of saccharin with trialkyl phosphites in the presence of dialkyl acetylenedicarboxylate

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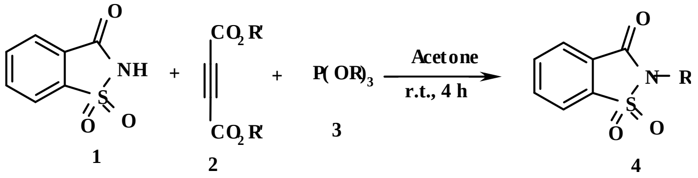
The *N*-alkylation of heterocyclic compounds bearing an acidic hydrogen atom attached to nitrogen is generally accomplished by treatment of these compounds with an appropriate base (sodium hydroxide or amide, metaloorganic compounds) followed by treatment of the resulting salts with an alkylating agent.[1] All these procedures require strictly anhydrous conditions and use of strongly ionizing solvents.[2] Herein we have described rapid N-alkylation of saccharin with trialkyl phosphites in the presence of dialkyl acetylenedicarboxylate in excellent yields.



4	R	R'	%Yield*
a	Me	CH_3	88
b	Et	C_2H_5	85
c	Bu	CH_3	91

* Isolated yields

The structures of **4a-c** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:

[1] Gilchrist, T. L. *Heterocyclic Chemistry*, 2nd ed.; Longman: London, 1992.
[2] Barco, A.; Benetti, S.; Pollini, G. P. *Synthesis*, **1976**, 124.

Synthesis of 9H-indeno[1, 2-b]pyrazine and 11H-indeno[1, 2-b]quinoxaline derivatives in one step reaction from 2-bromo-4-chloro-1-indanone

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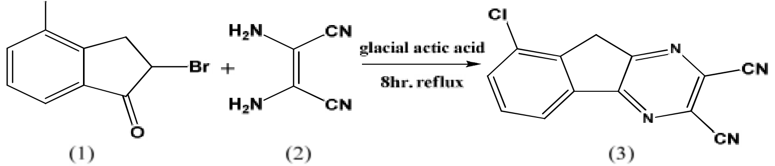
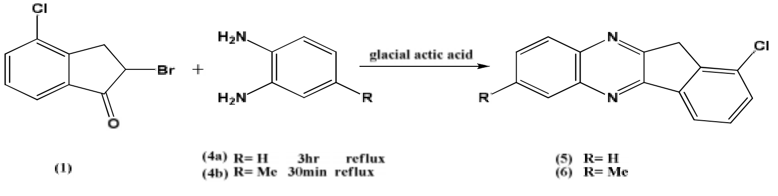
Quinoxaline derivatives are an important class of benzoheterocycles which has received much attention in recent years owing to their both biological properties and pharmaceutical applications [1, 2]. It was reported several methods to synthesize quinoxaline and pyrazine derivatives via α-hydroxy carbonyl [3], dicarbonyl compound [4]. The reaction of 2-bromo-4-chloro-1-indanone with 2,3-diaminomaleonitrile, benzene-1,2-diamine and 4-methylbenzene-1,2-diamine in glacial acetic acid gave 8-chloro-9H-indeno[1,2-b]pyrazine-2,3-dicarbonitrile, 1-chloro-11H-indeno[1,2-b]quinoxaline and 1-chloro-7-methyl-11H-indeno[1,2-b]quinoxaline in quantitative yield, respectively. When 2, 3-diaminopyridine and 3,4-diaminopyridine was treated with 2-bromo-4-chloro-1-indanone, 4-chloro-1-indanone as debrominated product was obtained.





References:

[1] S. Kotharkar, D. Shinde. *Bioorg. Med. Chem. Lett.,* **2006**, 16, 6181.
[2] O. Lenzi, V. Colotta , D. Catarzi and et al, *J. Med. Chem.,* **2006**, 49, 3916.
[3] J. Azizian, A. Karimi, Z. Kazemizadeh, A. Mohammadi and M.R. Mohammadizadeh, *Tetrahedron letters*, **2005**,46, 6155.
[4] M. Honari, M.M. Baradarani, *Arkivoc*, **2008**, xiv, 166.

Vitamin B_1 as a metal ion-free natural catalyst for sustainable quinoxaline ring condensation under sonochemical conditions

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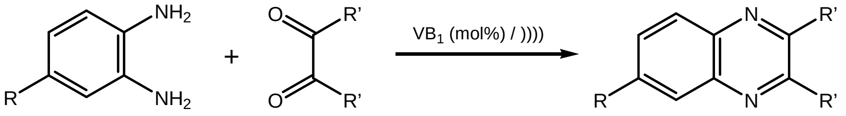
Quinoxalines are very important compounds due to their wide spectrum of biological activities behaving as anticancer, antibacterial, and activity as kinase inhibitors. Besides these, they are well known for their application in rigid subunits in macro cyclic receptors, electroluminescent materials, organic semiconductors and DNA cleaving agents. Considering the significant applications in the fields of medicinal, industrial and synthetic organic chemistry, there has been tremendous interest in developing efficient methods for the synthesis of quinoxalines [1–3].

In continuation of our work to develop new catalysts for the synthesis of quinoxaline derivatives [1–5], herein we wish to report a mild, efficient and environmentally benign method for the quinoxaline ring condensation in the presence of vitamin B_1 (VB_1) as catalyst under sonochemical conditions. The procedure can be performed for a broad scope of quinoxalines, however, the nature of the functional group on the aromatic ring of 1,2-diamine exerts a strong influence on the time and the reaction yield.



References:

[1] Darabi H. R, Mohandessi S, Aghapoor K, Mohsenzadeh F, *Catal Commun* **2007,** *8, 389.*

[2] Mohsenzadeh F, Aghapoor K, Darabi HR *J Braz Chem Soc* **2007,** *18, 297.*

[3] Darabi H. R, Tahoori F, Aghapoor K, Taala F, Mohsenzadeh F *J Braz Chem Soc* **2008,** *19, 1646*.

[4] Darabi H. R, Aghapoor K, Mohsenzadeh F, Taala F, Asadollahnejad N, Badiei A *Catal Lett* **2009**, *133*, 84.

[5] Aghapoor K, Darabi H. R, Mohsenzadeh F, Balavar Y, Daneshyar H *Transit Metal Chem* **2010**, *35*, 49.

Design, synthesis of 4-allyoxyaniline amides as potent inhibitors of lipoxygenase

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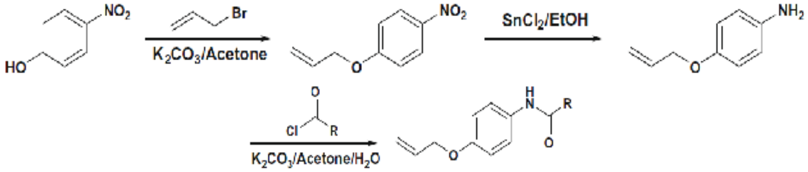
It is well documented that lipoxygenases (LOs) are non-heme iron-containing enzymes responsible for the oxidation of polyunsaturated fatty acids and esters to hydroperoxy derivatives. Among the mammalian lipoxygenases involved in the etiology of human disease, 5-lipoxygenase (5-LO) is now well established as a target for reducing the production of leukotrienes [1]. More recently, 15-lipoxygenase (15-LO) has emerged as an attractive target for therapeutic intervention.5 15-LO has been implicated in the progression of certain cancers [2] and chronic obstructive pulmonary disease (COPD) [3].

Herein we report a group of 4-allyloxyaniline amides as potential inhibitors of soybean 15-lipoxygenase (SLO). All compounds were docked in SLO active site and showed that allyloxy group of compounds is oriented towards the Fe^{3+}-OH moiety in the active site of enzyme and fixed by hydrogen bonding with two conserved His513 and Gln716. It is resulted that molecular volume of the amide moiety would be a major factor in inhibitory potency variation of the synthetic amides, where the hydrogen bonding of the amide group could also involve in the activity of the inhibitors.



References:

[1] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.
[2] Zhu, J.; Kilty, I.; Granger, H.; Gamble, E. *Am. J. Respir. Cell Mol. Biol.* **2002**, *27*, 666.
[3] Kelavkar, U. P.; Cohen, C.; Kamitani, H.; Eling, T. E.; Badr, K. F. *Carcinogenesis* **2000**, *21*, 1777.

Three-component reaction of alkyl isocyanides with acetylenic esters in the presence of pyridine-2-carboxaldoxime or α-furildioxime: Synthesis and dynamic NMR study of novel ketenimines and bis (ketenimines)

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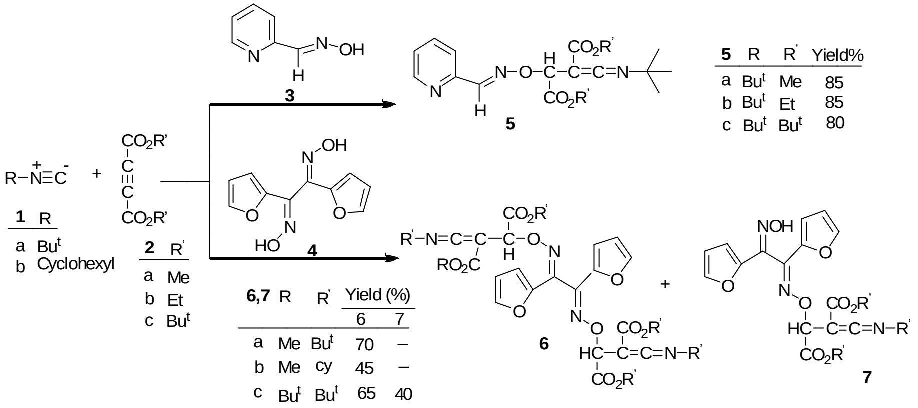
Ketenimines, a group of organic nitrogen heterocumulenes, are excellent building blocks for the synthesis of nitrogen heterocycles with different ring sized [1]. They commonly participate in pericyclic events such as electrocyclic ring closures [2], imino-ene type reaction [3] and [2+2] or [4+2] cycloaddition processes [4]. Our interest in the chemistry of ketenimines led us to the preparation and spectroscopic study of new examples of highly functionalized ketenimines and bis (ketenimines). We now report a facile one-pot synthesis of stable ketenimines and bis (ketenimines) using reaction of a mono oxime, pyridine-2-carboxaldoxime, and a dioxime, α-Furildioxime, as proton source/nucleophile with dialkyl acetylene dicarboxylates in the presence of alkyl isocyanides. This three-component condensation reaction leads to highly functionalized ketenimines **5a-5c** and bis (ketenimines) **6a-6c** in good yields. The structures of **(5a-5c)**, **(6a-6c)** and **(7a-7c)** were determined on the basis of their elemental analyses, mass spectra (MS) ^{1}H and ^{13}C NMR and IR spectroscopic data.



5	R	R'	Yield%
a	Bu^t	Me	85
b	Bu^t	Et	85
c	Bu^t	Bu^t	80

6,7	R	R'	Yield (%)	
			6	7
a	Me	Bu^t	70	–
b	Me	cy	45	–
c	Bu^t	Bu^t	65	40

References:

[1] Arrieta, A.; Cossio, FP.; Lecea, BJ. *Org Chem* **1999**, *64*, 1831.
[2] Molina, P.; Alajarin, M.; Vidal, A.; Fenau, DJ.; Declerq, JP. *J Org Chem* **1991**, *56*, 4008.
[3] Alajarin, M.; Vidal, A.; Tovar, F.; Sanchez, AP. *Tetrahedron Lett* **2002,** *43*, 6259.
[4] Alajarin, M.; Vidal A, Tovar, F.; Conesa, C. *Tetrahedron Lett* **1999**, *40*, 6127.

Characteristics and applications of nanocellulose as a high proficiency new raw material

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Cellulose has long been known as the most abundant natural biodegradable organic polymer, which is annually biosynthesized about 100 billion cubic meter in nature. Due to its sole properties such as rather low cost, renewability, reactivity and accessibility, etc., cellulose has found vast and extensive applications in various industries such as pulp and paper, food and pharmaceutics [1]. Nowadays, along with the development of nanotechnology, not only its applications have been extended, but also new capabilities such as the possibility of the production Microcrystalline Cellulose (M.C.C), Nano Fibrillated Cellulose (N.F.C) and Nano Whisker Cellulose (N.W.C) have been discovered. This paper is intended to represent the production methods, advantages and applications of these newly improved nanocellulose products. Cellulose is chemically a linear polymer consisted of β-D-glucopyranose units linked to each other through 1→4 glycosidic bonds. Cellubiose units (10.3 nm in length), are the basic structural elements of cellulose nanoscale materials and nanofibrill is formed through their connections [1]. The diameter and length of cellulose nanofibers are about 5-20 nm and 20000 nm, respectively, depending on cellulose source and preparation process. The tensile strength and modulus of cellulose nanofiber are 2-3 GPa and 150 GPa, respectively [2,3]. Because of the high aspect ratio of these nanoscale materials, they can be used as a superior reinforcement for the composites. Cellulose nanofibers are produced through chemical hydrolysis of the wood and other lignocellulosic materials combined with mechanical separation, but enzymatic treatment is also used. From economical aspect, the mechanical processes are better than chemical methods. Utilization of these materials in the textiles, advanced composite materials, aerospace and transportation, food, cosmetics, pharmaceuticals, drug delivery, coatings and paints, switchable optical devices, films for barrier and paper packaging industries is remarkable.

References:

[1] Klemm, D., Schumann, D., Kramer, F., Heϐler, N., Hornung, M., **2006**. Cellulose nanofibers as Innovative Polymers in Research and Application. Advance polymer science. 205: 49.
[2] Marielle Henriksson, Lars A. Berglund. Structure and Properties of Cellulose Nanocomposite Films Containing Melamine Formaldehyde. Journal of Applied Polymer Science, Vol. 106, 2817.
[3] Yano, H., Nakahara, S., Bio-composites produced from plant microfiber bundles with a nanometer unit web like network. Journal of materials science, **2004**. 39(5): 1635.

Synthesis and characterize of some new azo dyes based on hydroxy thioxanthone derivatives

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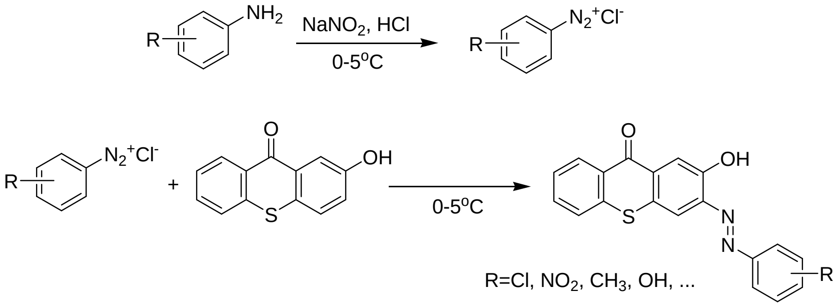
Azo dyes are the most important group of all synthetic dyes. These dyes possess a wide range of deep colors. In recent decades, organic color chemistry has been undergoing very exciting development as a result of the opportunities presented by dye applications in high technology fields: electronic devices, linear and non linear optics, reprography, sensors and biomedical uses. Many Azo compounds have been applied as chromogenic reagents for the determination of several metal ions [1].

The use of heterocyclic intermediates in the synthesis of Azo dyes is well established and the resultant dyes exhibit good tinctorial strength [2].

Thioxanthone and its derivatives are recognized as useful intermediates in the preparation of pharmaceuticals and are useful as photo-initiators [3,4].

Hydroxy thioxanthone derivatives can be useful as heterocyclic intermediates for synthesis new Azo dyes. Thioxanthone azo dyes were synthesized by the diazotization-coupling reaction shown in Scheme. Various aromatic amines were diazotized using sodium nitrite in the presence of hydrochloric acid at 0-5 ºC, followed by coupling with hydroxy thioxanthones to produce new azo dyes in good yield.



References:

[1] Noroozi-Pesyan, N.; Khalafy, J.; Malekpoor, Z. *JCCS*. **2009**, *56*, 1018.
[2] Karci, F.; Sener, N.; Yamac, M.; Sener, I.; Demircali, A. *Dyes and Pigments*. **2009**, *80*, 47.
[3] Vogel, H.; Minning, M. *ibid*., **1949**, *42*, 268.
[4] Blair, D. M.; Hawking, F.; Meeser, C. V.; Ross, W. F. *ibid*. **1949**, *4*, 68.

Synthesis of *E,E*-2-benzylidene-6-(nitrobenzylidene)cyclohexanones as potential cytotoxic agents

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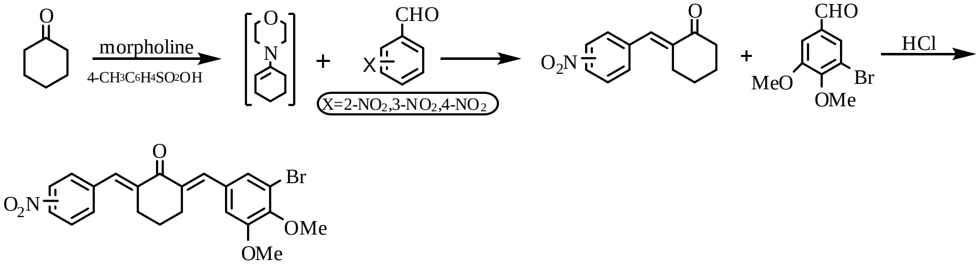
Benzylidene cyclohexanon, benzylidene cyclopentanon and benzylidene aceton derivatives show anti-bacterial, anti-oxidant, anti-inflammatory and cytotoxic activities that enable them to be used for drugs [1].

The objective of the present study is evaluation of the hypotheses that cytotoxic potencies were correlated with both the charge densities and the steric environment of the olefinic carbon atoms. So expansion of the cluster of compounds was indicated in order to draw meaningful conclusions pertaining to those structural features which contribute to cytotoxicity [2]. In this regard, we have synthesized a series of novel benzilidine cyclohexanon and evaluated their cytotoxic effect. The synthetic pathway is outlined as shown in the scheme.



Reference:

[1] Sardijman, Drs (ID) Reksohadiprodjo, Mochammad Samh (ID) Timmerman, Prof. Dr. Henk (NL). EP19980200519.

[2] U. Das, A. Doroudi, S. Das, B. Bandy, J. Balzarini, E. D.Clercq, J. R. Dimmock. Bio. Med. Chem. **2008**, *16*, 6261.

A novel and inexpensive method for the synthesis of benzothiazole derivatives using barium dichloride dihydrate as Lewis acid catalyst

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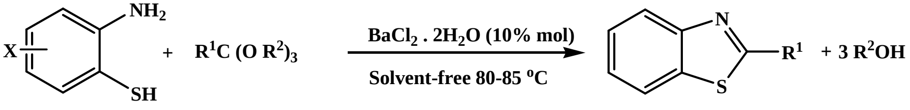
Aromatic heterocyclic compounds are valuable synthetic templates for the synthesis of new compounds with specific biological or material properties. Among Benz-fused heterocyclic compounds, benzothiazoles are an important class of aromatic heterocyclic compounds. They provide a common scaffold to various derivatives, which can be utilized as a wide variety of biologically active and medicinally significant compounds [1,2]. Numerous methods for the synthesis of benzothiazoles have been reported [3-5]. In general, these compounds could be achieved via the condensation of amino thiophenols with carboxylic acid derivatives such as ortho esters. Many of the reported methods suffer from one or more limitations such as long reaction times, harsh conditions, unsatisfactory product yields, use of expensive and toxic catalysts, critical product isolation procedures, use of volatile and carcinogenic organic solvents and co-occurrence of several side products.

In this research, we have presented a new application of barium dichloride dihydrate ($BaCl_2{\cdot}2H_2O$) as an effective Lewis acid catalyst for the synthesis of a variety of benzothiazole derivatives **3** based on the condensation of amino thiophenol derivatives **1** and ortho esters **2** under solvent-free conditions. Because of advantages such as clean reaction without using organic solvents as media and applying inexpensive catalyst, simple work-up procedure and the high yields of products, this method is important from an environmental point of view and economic considerations.



1 **2** **3**

R^1= H or Me R^2= Me or Et

X= H, Cl, Me

References:

[1] Sondhi, S. M.; Singh, N.; Kumar,A.; Lozach, O.; Meijer, L. *Bioorg. Med. Chem.* **2006**, *14*, 3758.
[2] Bonham, L.; Klein, P. *Bioorg. Med. Chem. Lett.* **2004**, *14*, 1455.
[3] Wipf, P.; Venkatraman, S. *Tetrahedron Lett.* **1996**, *37*, 4659.
[4] Phillips, A. J.; Uto, Y.; Wipf, P.; Reno, M. J.; Williams, D. R. *Org. Lett.* **2000**, *2*, 1165.
[5] Wuts, P. G. M.; Northuis, J. M.; Kwan, T. A. *J. Org. Chem.* **2000**, *65*, 9223.

Quantitative structural relationship and theoretical study of electrochemical properties of [Cp_2-Fe]@[SWCN(5,5)-Armchair-C_nH_{20}] complexes

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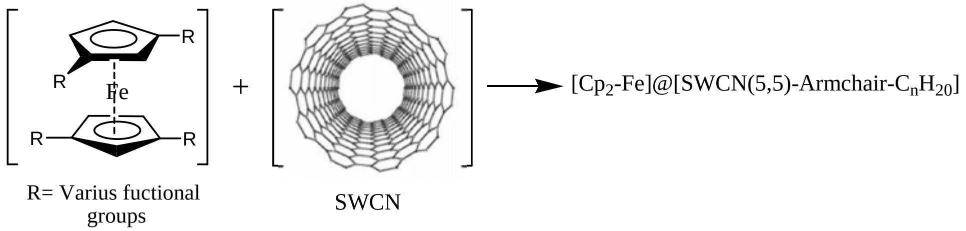
Nanoscale structures of carbon display an attractive variation of structural characteristics, and many useful forms have been synthesized and identified. One of these structures is the carbon nanotubes. Carbon nanotubes are either single-wall (SWCNT) or multi-wall; the former attract more attention due to their unique electronic, optical and spectroscopic properties. The electrochemical properties of the ferrocene (Cp_2-Fe) have been studied previously. The accommodation of (Cp_2-Fe) inside the SWCNT leads to significant periodic modifications of the electronic states of SWCNT. One of the main recognized structures of nanotubes is the (5, 5) single-wall tube (SWCN). A topological index is a mathematical invariant of a chemical graph, which shows a significant correlation with some chemical or physical property. They have been successfully used to construct effective and useful mathematical methods for finding good relationships between structural data and the properties of these materials. To establish a good structural relationship between the structure of molecules (Cp_2-Fe) and [SWCN(5,5)-Armchair-C_nH_{20}] (n = 20–190), the molecular degree of unsaturation (D_U) was used as one of the useful numerical and structural electrochemical properties of unsaturated compounds. In this study, the relationship between this index and electron affinity; the reduction potential (${}^{Red}E$) of [SWCN(5,5)-Armchair-C_nH_{20}] (n = 20–190); and the free energy of electron transfer (ΔG_{et}) as assessed using the Rehm–Weller equation between [SWCN(5,5)-Armchair-C_nH_{20}] (n = 20–190) and ferrocene (Cp_2-Fe) as [Cp_2-Fe]@[SWCN(5,5)-Armchair-C_nH_{20}] complexes.



References:

[1] A.A. Taherpour., *Chem. Phys. Lett.,* 469 (**2009**) 135.
[2] A.A. Taherpour., *Fulleren. Nanotube Carbon Nanostruct.* 16 (**2008**) 196.
[3] A.A. Taherpour., Aus. *J. Ed. Chem.* 65 (**2005**) 37.
[4] H. Shen., *Molecular Physics,* 105 (17-18) (**2007**) 2405.
[5] Pedro Molina, Aurelia Pastor, M. Jesu´ s Vilaplana., *Organometallics.,*16 (**1997**) 5836.

High thermal stability of novel organosolube polyamides based on quinoxalin bulky pendent group

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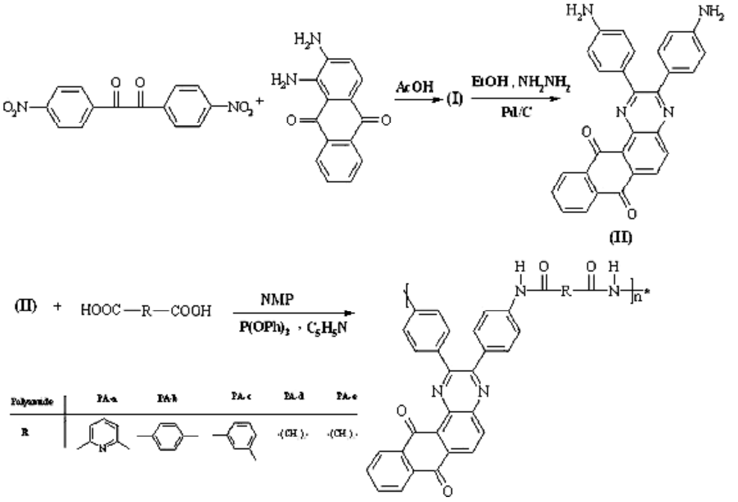
A new unsymmetrical diamine monomer containing quinoxalin-anthraquinone bulky pendent group was synthesized through the reaction of 4,4’ dinitro benzyl with 2,3 diamino anteraquinone gave 2,3-bis(4-nitrophenyl)naphtho[2,3]quinoxaline-7,12-dione(I). The nitro groups of this compound reduced in the presence of Pd/C in hydrazine and ethanol to afford 2,3-bis(4-aminophenyl)naphtho[2,3]quinoxaline-7,12-dione(II). A series of novel polyamides(PAs) containing quinoxalin-anthraquinone pendant group was prepared by direct polycondensation of the diamine monomer with various dicarboxylic acids. These PAs were suitable readily soluble in many organic solvents and their inherent viscosities were suitable and could be solution-cast into tough and flexible films. The PAs were characterized using FT-IR, ^{1}H NMR, UV–vis spectroscopy, fluorimetry and elemental analysis. Thermal properties of new PAs were evaluated by thermogravimetric analysis and differential scanning calorimetry [1-3].



References:

[1] Hsiao, S.H.; Liou, G.S.; Kung, Y.C.; Pan, H.Y; Kuo, C.H. *Eur. Polym. J.* **2009**; *45*, 2234.
[2] Ghaemy, M.; Alizadeh, R.; Behmadi, H. *Eur. Polym. J.* **2009**, *45*, 3108.
[3] Ghaemy, M.; Amini Nasab, S.M. *Reac. Funct.l Polym.***2010**, *70,* 306.

Theoretical study of the mechanism, regio- and stereoselectivity of the Diels–Alder reaction of para-substituted 1-phenyl-1,3-cyclopentadiene with cyclopent-2-enone

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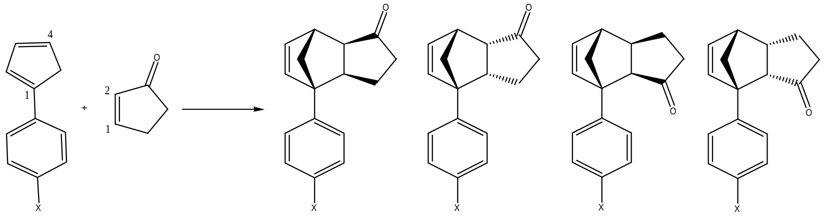
The stereo- and regioselectivity of the Diels-Alder reactions have been widely studied because of the synthetic value of these reactions [1]. A theoretical study of the mechanism, regio- and stereoselectivity of the Diels–Alder reactions of para-substituted 1-phenyl-1,3-cyclopentadiene where X= H, NO_2, CHO, CN, NH_2, OH and $NHCH_3$ with cyclopent-2-enone are carried out at the B3LYP/6-31G(d) using Gaussian 03. These cycloadditions can take place along four reactive channels corresponding to the endo and exo approaches and in each in two regioisomeric pathways with a concerted mechanism. Totally, four transition states and then four cycloadducts, namely, endo 1, exo 1, endo 2 and exo 2 have been located as following:



EXO1 ENDO1 EXO2 ENDO2

Calculated activation energies show that the endo 2 isomer is kinetically favored. Global and local reactivity descriptors [2] such as chemical potential (μ), chemical hardness (η), electrophilicity (ω), condensed form of Fukui functions (f), local softness differences (Δ), and the ratio of regioisomers (exo 1/exo 2) are calculated and presented in the following Table. According to the smaller values for $\Delta_{exo\ 2}$, interaction between dienes with dienophile would provide regioisomer 2 as a preferred regioisomer.

Global and local descriptors for para-substituted 1-phenyl-1,3-cyclopentadiene (diene) and cyclopent-2-enone (dienophile)

	X	f_k^-		f_k^+		f_k^+		f_k^-		μ(au.)	η(au.)	ω(au.)	$\Delta_{Exo\ 1}$	$\Delta_{Exo\ 2}$	Exo 1/ Exo 2
		C_1	C_4	C_1	C_2	C_1	C_4	C_1	C_2						
	H	0.115	0.166	-	-	-	-	-	-	-0.117	0.078	0.088	0.625	0.104	0.016
	NH_2	0.055	0.138	-	-	-	-	-	-	-0.100	0.074	0.068	0.955	0.111	0.003
	OH	0.080	0.151	-	-	-	-	-	-	-0.109	0.076	0.078	0.806	0.073	0.005
Diene	$NHCH_3$	0.035	0.126	-	-	-	-	-	-	-0.094	0.072	0.062	1.186	0.197	0.001
	NO_2			-	-	0.003	0.094	-	-	-0.155	0.064	0.186	0.816	0.009	0.019
	CN			-	-	0.035	0.110	-	-	-0.142	0.072	0.140	0.627	0.032	0.013
	CHO			-	-	0.019	0.102	-	-	-0.141	0.068	0.146	0.705	0.009	0.007
Dienophile	-	-	-							-0.140	0.096	0.103	-	-	-
				0.243	0.092										
								0.128	0.018						

References:

[1] Hirao, H.; Ohwada, T., *J. Phys. Chem. A.*, **2005**, *109*, 816.
[2] Domingo, L. R., *Tetrahedron*, **2002**, *58*, 3765.

A novel three-component reaction: Chemoselective synthesis of *new bisbenzofurans* in the presence of $H_3PW_{12}O_{40}.XH_2O$ as green and reusable catalysts

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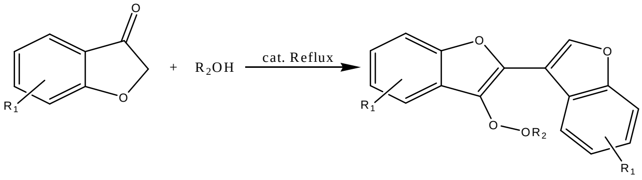
Benzofurans and their analogues constitute a major group of naturally-occurring compounds that are of particular interest because of their biological activity [1] such as cardiovascular [2], antitumor [3],….

Several methodologies are available for the synthesis of simple benzofurans but no methology for direct synthesis of benzofuran dimmers is explored to a great extent [4].Recently, a series of benzofuran dimmers were synthesized in the presence of Amberlyst 15 as a catalyst in toluene and showed good Protein phosphatase 1B(PTP-1B) inhibitory activity and in another report bis(benzofuranyl)methanes were obtained in the presence of $Bi(OTf)_3$ [5].

Due to the outstanding properties of benzofuran derivatives and ever-mounting environmental concern in the field of chemistry, here in we developed a novel route for the chemoselective synthesis of new 3-alkoxy-2,3'-bisbenzofuran derivatives via the new one-pot reaction of benzofuranones and alcohols in the presence of catalytic amounts of HPAs (Scheme 1).



1a-d 2a-d 3a-m

1a: R_1=H
1b: R_1=5-Cl
1c: R_1=5-Br
1d: R_1=6-OMe
1e: R_1=6-OEt
1f: R_1=6-Cl

2a: R_2=Et
2b: R_2=Me
2c: R_2=CH_2CH_2OH
2d: R_2=*n*-Bu

Scheme 1. Synthesis of 3-alkoxy-2-3'-bisbenzfuran

Refrences

[1] S. N. Aslam,P. C. Stevenson, S. J. Phythian, N. C. Veitch, D. R. Hall,Tetrahedron 62 (2006) 4214.
[2] G. bourgery, P. Dostert, A. Lacour, M. Langlois, B. Pourrias, J. Tisneversilles, J. Med. Chem. 24 (1981) 159.
[3] B. S. Yun, H. C. Kang, H. Koshino, S. H. Yu, I. D. Yoo. J. Nat. Prod. 64 (2001) 1230.
[4] (a) S. Mahboobi, A. U. S. Cenac, A. Sellmer, E. Eichhorn, S. Elz, F. D. Bohmer, C. Kazaz, Molecules, 10 (207) 2187; (b) D. S. Black, D. S. Craig, R. Rezaei. Chem. Commun. 8 (2002) 810.
[5] R. E. Chen, Y. L. Wang, Z. W. Chen, W. K. Su, Can. J. Chem. 86(2008) 885.

Synthesis of hybrid hetropolyoxometalate, (bmim)$_5$ [CoW$_{12}$O$_{40}$].xH$_2$O, and investigation of catalytic activity in synthesis of xanthenes

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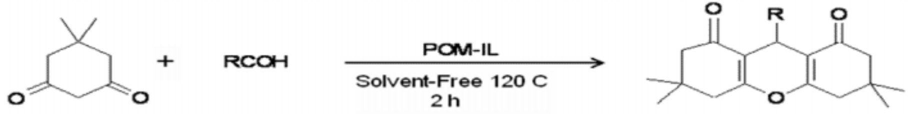
Polyoxometalates can be described as molecular blocks of metal oxide formed by MO6 octahedra sharing corners, edges and faces. There are two generic families, the isopolyoxometalates, which contain Mo, W or V in their highest oxidation states, and the heteropolyoxometalates, which contain at least one p- or d-block element as heteroatom, that represent a diverse range of molecular cluster with an almost unmatched range of physical properties and the ability to form dynamic structures and acting as a set of transferable building blocks that can be reliably utilized in the formation of new materials [1,2]. Xanthenes and benzoxanthenes have received much attention because of their wide range of therapeutic and biological properties, such as antibacterial, antiviral and anti-inflammatory activities. Furthermore, these compounds have emerged as sensitizers in photodynamic therapy [3,5]. In this paper, a novel organic – inorganic hybrid (bmIm)$_5$[W$_{12}$Co O$_{40}$].xH$_2$O (BmIm:1- buthyl, 3- methyl imidazolium) has been prepare[6,7], as a green, reusable, efficient and heterogeneous hybrid catalyst in synthesis of xanthenes derivatives under solvent-free conditions. The condensation reaction involving an aldehyde and diketone was efficiently promoted by hybrid catalyst.



Reference:

[1] Pope, M.T., *Heteropoly and Isopoly Oxometalates*: Springer, Berlin, **1983.**

[2] Borras-Almenar, J.J., Coronado, E., Muller, A., Pope, M., *Polyoxometalate Molecular Science*: Kluwer, Dordrecht, **2001.**

[3] J.P. Bacci, A.M. Kearney, D.L. Van Vranken, *J. Org. Chem*. **2005,** *70* , 9051.

[4] H. J. Schneider, D. Guttes, U. Schneider, *J. Am. Chem. Soc*. **1988,** *110*, 6449.

[5] A. Banerjee, A.K. Mukherjee, *Stain Technol*. **1981,** *56*, 83.

[6] L.C.W. Baker, T.P. McCutcheon, *J. Am. Chem. Soc.* **1956,** *78*, 4503; L.C.W. Baker, V.E. Simmons, *J. Am. Chem. Soc.* **1959,** *81*, 4744

[7] *Materials Chemistry and Physics*. **2008,** *112*, 853.

A new and convenient in-situ method for synthesis of new Categorie carbamates from cabamyl chloride using bis(trichloromethyl)carbonate

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Carbamate is a widespread functional group in organic synthesis. In general, carbamates are found as protecting groups for the amino function [1]. Carbamate derivatives are drawing increasing attention due to their desirable properties. They are extensively employed to synthesize biofunctional compounds, well exampled by as superior inhibitors of TryR or HIV. Recently, a number of cyclic urea derivatives have been synthesized and performed promising properties, especially some interesting pharmacological properties [2]. During the last decade, triphosgene [bis (trichloromethyl)carbonate] has become a versatile synthetic auxiliary for the synthesis of some important classes of organic compounds. This white crystalline compound has proven to be safe and advantageous over its gaseous congener, phosgene [3].

In this article, we have successfully employed this reagent for the direct conversion of amines to carbamates. Triphosgene is known to react with amines to produce carbamyl chlorides.N,N-Diphenyl carbamyl chloridereact with alcohols to produce carbamates.

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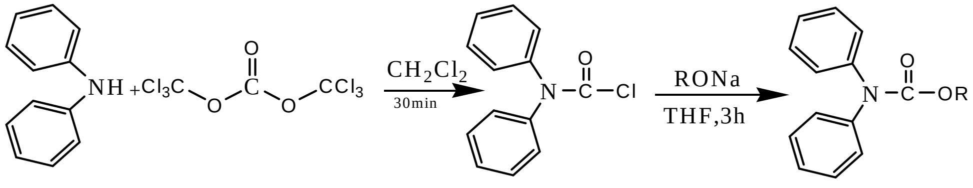

R : alkyl,aryl

References:

[1] Mormeneo, D.; Llebaria, A.; Delgado, A. *Science.* **2004**, 6831.
[2] Deng, J; Zhao, W.; Yang, W. *Science.* **2007**, 828.
[3] Krishna Swamg, D.; Bhawal, B, M.; Deshmukh, A, R, A, s .*Tetrahedron Lett*. **2000**, *41*, 417.

One-pot, three-component synthesis of dialkyl quinoline-2,3-dicarboxylates from triphenylphosphine, acetylenic esters, and amino derivatives of 2-aminobenzaldehyde in aqueousa acetone

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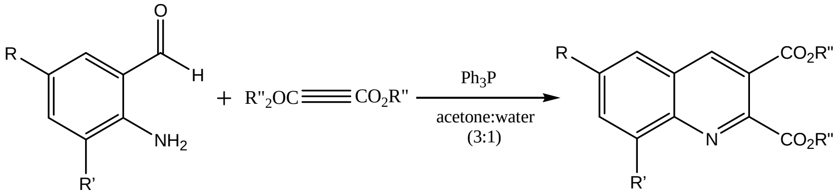
Quinolines [1] are interesting synthetic targets because they act as building blocks for a large number of natural products. In recent years there has been an increase in interest in the synthesis of quinoline compounds. This interest has resulted from the use of such compounds in variety of biological and synthetic applications [2]. While a number of synthetic methodologies for the quinoline ring system have been developed [3], the literature describing a novel one-pot cyclization method based on consecutive processes in rather scarce. In this article, we report on the one-pot synthesis of dialkyl quinoline-2,3-dicarboxylates (**4**) from the reaction of amino derivatives of 2-aminobenzaldehyde, dialkyl acetylenedicarboxylates , and triphenylphosphine in acetone-water (3:1).



4a R= Cl, R'= H, R"= Me
4b R= Br, R'= Br, R"= Me
4c R= Br, R'= Br, R"= Et

References:

[1] Hepworth, J. D. in *Comprehensive Heterocyclic Chemistry*, ed. Katritzky, A. R. and Rees, C. W. Pergamon Press, Oxford, **1984**, *2*, 165.
[2] Albrecht, R. *Progress in Drug Research*, ed. E. Jucker, Birkhauser Verlag, Basel, **1977**, *21*, 9.
[3] *The Chemistry of Heterocyclic Compounds*, ed. G. Jones, Wiley, New York, **1982**, *32*, 93; S. Radl and D. Bouzard, *Heterocycles*, **1992**, *34*, 2143.

Theoretical study of free energies of electron transfer quantitative structural relationship studies of C_n@X-[HbA] (HbA=hemoglobin A; X= α- and β-fumarate crosslinked hemoglobins (αXL & βXL)) and [R].C_n (R= Cytochrome-c peroxidase, cytochrome-c oxidase, tyrosinase and ascorbate oxidase) nanostructur complexes

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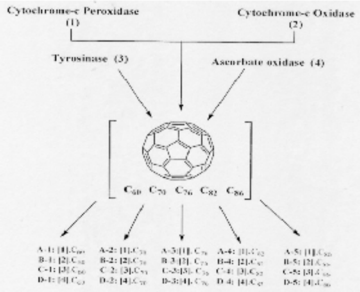
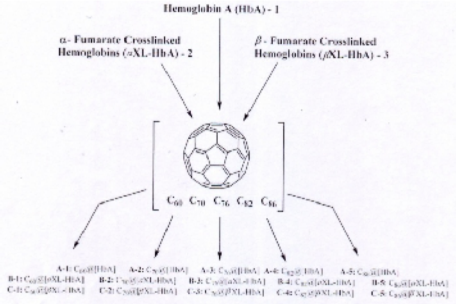
Various empty carbon fullerenes (C_n) with different carbon atoms have been obtained and investigated. The main component of the red blood cells, hemoglobin A (HbA) functions as an efficient oxygen carrier by reversibly binding oxygen at the ferrous ion of the heme groups [1]. Self-assembled monolayers of thiolated compounds are used as promoters for protein-electrode reactions [2].Topological indices are purported to correlate chemical structures with various chemical and physical properties. They have been successfully used to construct effective and useful mathematical methods to establish clear relationships between structural data and physical properties of these materials [3].In this study, the number of carbon atoms in the fullerenes was used as an index to establish a relationship between the structures of Hemoglobin A, α- and β-Fumarate Crosslinked Hemoglobins, HbA, αXL and βXL-[HbA], respectively, 1-3 as the most well-known blood molecular systems and fullerenes C_n (n=60, 70, 76, 82 and 86),and also the structures of Cytochrome-c peroxidase, Cytochrome-c oxidase, Tyrosinase and Ascorbate oxidase, 1-4 as the most well-known enzyme molecular systems and fullerenes C_n . The relationship between the number of carbon atoms and the free energies of electron transfer ($\Delta G_{et(}$) are assessed using the *Rehm-Weller* equation for supramolecular C_n@X-[HbA] and [R].$C_n$complexes.the result were used to calculate the free energies of electron transfer of the supramolecular complexes for fullerenes C_{60} to C_{300}.





References:

[1] Dragan, S. A.; Olsen, K. W.; Moore E. G.; Fitch, A.*Bioelectrochemistry*, **2008**, 73, 55.

[2] F. W. Scheller, et al., Reviews in Molecular Biotechnology, **2002**, 82, 411.

[3] Taherpour, A. A. *Fullerenes, Nanotubes and Carbon Nanostructures*, **2008**, 15, 279.

Generally applicable organocatalytic *N*-tert-Butoxycarbonylation of amines

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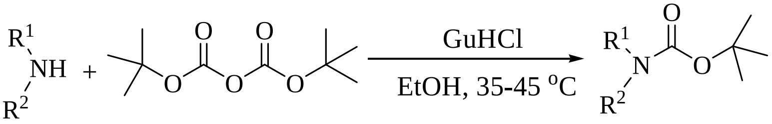
Synthetic organic chemistry depends on the concourse of reagents and catalysts to achieve the clean formation of new compounds, and suitable protecting groups are required to prevent the formation of undesired products. The development of mild and selective methods for the protection and deprotection of functional groups continues to be an important tool in the synthetic chemistry of polyfunctional molecules [1,2]. Protection of amino group is one of the most fundamental and useful transformation during the synthesis of peptides, amino acids and other natural products [3]. Due to the great stability toward catalytic hydrogenation and extreme resistance toward basic conditions and many other nucleophilic reagents [4], the *tert*-butoxycarbonyl (Boc) group has been widely employed to mask the amino function, finding widespread use in both organic and peptide [5] synthesis.

Herein we report an efficient method for chemoselective *N*-*tert*-butoxycarbonylation of amines, diamines, amino acids and peptides using guanidine hydrochloride as an organocatalyst in ethanol. The corresponding products were formed in excellent yields. Selective protections of alkylamines in the presence of aromatic or heteroaromatic amines were also achieved by this method.



R^1, R^2 = H, alkyl, aryl, amino acid, peptide

References:

[1] Greene, T. W.; Wuts, P. G. M. in *Protective Group in Organic Synthesis,* 3rd ed.; John Wiley and Sons, NewYork, **1999**.
[2] Kocienski, P. J. in *Protecting Groups*; George Thieme Verlag: Stuttgart-New York, **2004**.
[3] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104*, 199
[4] Xiuo, X. Y.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.
[5] Kaiser, E. S.; Picart, F.; Kubiak, T.; Tam, J. P.; Merrifield, R. B. *J. Org. Chem.* **1993**, *58*, 5167.

Reaction between benzoyl isothiocyanate and 2,6-dimethylphenyl isocyanide. synthesis of a sterically congested ten-membered ring sontaining S-S-S moiety

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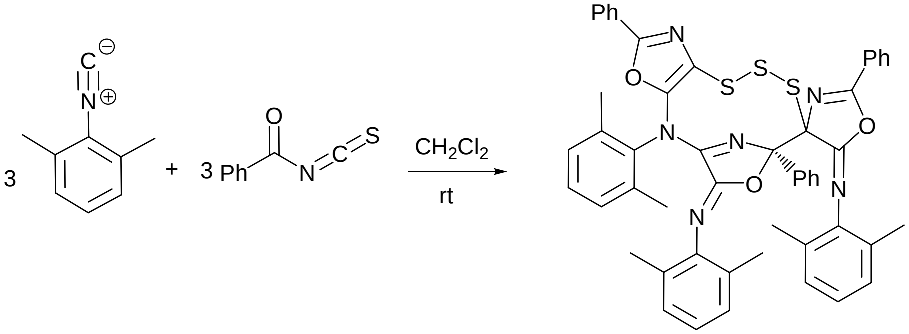
Multi-component reactions (MCRs) are useful organic reactions in which three or more starting materials react to give a product [1]. MCRs, by virtue of their convergence, productivity, facile execution, and generally high yields of products, have attracted much attention from the combinatorial chemistry. As part of our current studies on the development of new routes to heterocyclic systems [2], we now report the reaction between 2,6-dimethylphenyl isocyanide (**1**) and benzoyl isothiocyanate (**2**) in CH_2Cl_2, which leads to *N*-(2,6-dimethylphenyl)-4,16-bis[alkyimino]-2,11,18-triphenyl-3,12,17-trioxa-6,7,8-trithio-10,14,19-triazatricyclo-[10.2.1.0^{9,13}] pentadeca-1-azaspiro[4,10]pentadeca-1,11,15(19),13(9)-tetraene (**3**) in nearly quantitative yield[10] (Scheme 1). Dynamic effects are observed in the ^{1}H NMR spectrum of this compound for the restricted rotation around two of the Ar-N single bonds. Unambiguous evidence for the structure and stereochemistry of **3** was obtained from a single-crystal X-ray analysis [3].



References

[1] A. Doemling, *Chem. Rev.* **2006**, *106*, 17.
[2] Yavari, I.; Djahaniani, H. *Tetrahedron Lett*. **2006**, *47*, 2953.
[3] Crystallographic data CCDC-284910.

Synthesis and characterization of polyvinyl amine-Al_2O_3–SiO_2 as a novel heterogeneous basic catalyst and its application in Knoevenagel condensation

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The use of polymer-supported reagents provides an attractive and practical method for the clean and efficient preparation of novel chemical libraries with potential applications in the pharmaceutical or agrochemical industries [1]. Nevertheless, there are relatively a few examples of polymer applications in the field of heterogeneous organocatalysis. It may be originate from two drawbacks of most polymers: their low thermal stability, and/or their low mechanical stability [2]. One way to overcome these drawbacks is the use of organic–inorganic polymer composite instead of polymeric materials. Hybrid organic–inorganic polymers have been receiving an increasing interest from research groups, because of their unique properties. These materials combine some advantages of polymer compounds (easy processing with conventional techniques, elasticity and organic functionalities) with properties of inorganic oxides (hardness, thermal and chemical stability, transparency). Thus, the syntheses of organic–inorganic hybrid polymers with new framework structures are highly desirable [3]. In most cases, the incorporation of polymer species into the mesoporous silica and other inoganic materials are performed with the organosilica precursors. However, the organosilica precursors are either involve complicated synthesis and purification method or very expensive. Therefore, preparation of organic–inorganic hybrid polymers without using organosilica precursors is highly desirable [4].

In this work, a novel polymer–inorganic hybrid material (polyvinyl amine-Al_2O_3-SiO_2) is prepared by a very simple and inexpensive method without using any organosilane compound. This hybrid has a high density of nitrogen groups to act as the basic sites and, therefore, is expected to show high catalytic activity as a heterogeneous basic catalyst. The samples were characterized by XRD, XRF, FTIR, SEM, TG and BET. Catalytic activity of the composites were tested for the synthesis of α,β-unsaturated carbonyl compounds from condensation reaction between carbonyl compounds and diethylmalonate. Sample containing Al/Si molar ratio of 0.6 exhibited highest yield (98%) and selectivity (100%) at very short time (5 min) for the synthesis of α,β-unsaturated carbonyl compounds under solvent-free and room temperature conditions.

References:

[1] Ley, S. V.; Baxendale, I. R.; Bream, R. N.; Jackson, P. S.; Leach, A. G.; Longbottom, D. A.; Nesi, M.; Scott, J. S.; Storer, R. I.; Taylor, S.J. *J. Chem. Soc., Perkin Trans. 1*, **2000**, 3815.
[2] Goettmann, F.; Sanchez, C. *J. Mater. Chem.* **2007**, 24.
[3] MARK, J. E.; *Acc. Chem. Res.* **2006**, *39*, 881.
[4] Cheng, Q.; Pavlinek, V.; Li, C.; Lengalova, A.; He, Y.; Saha, P. *Mater. Chem. Phys.* **2006**, *98*, 504.

One-pot synthesis of 5,5-disubstituted hydantoins under ultrasonic and microwave irradiation.

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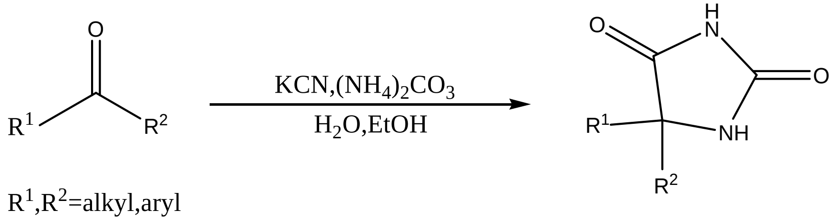
Hydantoins, 2,4-imidazolidine-diones,comprise a class of compounds that has been of considerable interest. hydantoin derivatives are synthetically valuable hydantoins substituted at C-5 are important medicinal compounds [1].

The Bucherer-Bergs reaction provides perhaps the best method for preparation of hydantoins [2]. Some 5,5-disubstituted α-hydantoins were synthesized from the corresponding ketones , aldehydes, diketones, and hydroxyl ketones with KCN and ammonium carbonate in good yield [3].

Herein, we report a rapid and highly efficient synthesis of hydantoin derivatives was achieved under ultrasonic irradiation and microwave irradiation in an additional reaction.



Refrences :

[1] Mahmoodi.N.; Khodaee.Z. *Arkivoc*, **2007**, 29.
[2] Gallienne.E.; Muccioli.G.;Lambert.D.;Shipman.M, *Tetrahedron lett*, **2008**, 6495.
[3] Faghihi.Kh.;Zamani.Kh.;Mobinikhaledi.A,*Turk. J. Chem*, **2004**, 345.

Synthesis and properties of new polyamide-imides based on 2,2'-sulfoxide-bis[4-methyl(2-trifluoromethyl)4-aminophenoxy) phenyl ether]

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Aromatic polyimides generally possess excellent thermal, mechanical, electrical, and chemical properties. Therefore, they are being used in many applications such as electrics, coatings, composite material, and membranes. However, the commercial use of these materials is often limited because of their poor solubility, and high softening or melting temperatures [1]. Recent studies demonstrated that polyimides with ether and trifluoromethyl groups exhibit some excellent physical properties, such as high solubility with low moisture uptake, low dielectric constant, and high optical transparency [2]. Also, major enhancement in processability can be achieved by modifying the substitution pattern of the aromatic units in the main chain, especially by inclusion of 1,2-linked units derived from ortho-catenated aromatic rings [3]. In addition, the presence of sulfoxide linkages can induce important new properties, such as improved solubility and miscibility with other polymers [4].

As part of our continuing efforts to develop easily processable high-performance polymers with good solubility and thermal stability [5], this work deals with the synthesis and characterization of novel series of fluorinated ortho-sulfoxide bridged poly(ether amide imide)s (PEAIs) based on novel aromatic diimide-diacid (DIDA). The polyamide-imides were obtained in high yields and possessed inherent viscosities in the range of 0.46–0.98 dL g^{-1}. All of the polymers were amorphous in nature and were readily soluble in various solvents. They showed good thermal stability with glass transition temperatures between 191-232 °C, 10% weight loss temperatures in excess of 490 °C, and char yields more than 50% at 700 °C in nitrogen atmosphere. Moreover, these PEAIs possessed low refractive indexes (n = 1.53-1.55) and low birefringence ($\Delta \approx 0.02$) due to the trifluoromethyl pendent groups and sulfoxide bridged ortho-catenated aromatic rings that interrupt chain packing and increase free volume.

References:

[1] Liaw, D. J.; Chen, W. H. *Eur. Polym. J.* **2006**, *91*, 1731.
[2] Hsiao, S. H.; Yang, C. P.; Huang, S. C. *Eur. Polym. J.* **2004**, *40*, 1063.
[3] Eastmond, G. C.; Paprotny, J. *Polymer*. **2004**, *45*, 1073.
[4] Oyama, T.; Naka, K.; Chujo, Y. *Macromolecules*. **1999**, *32*, 5240.
[5] Shockravi, A.; Abouzari-Lotf, E.; Javadi, A; Taheri, S. *Polym. J.* **2009**, *41*, 174.

Preparation of flavanones on the acidic SiO_2/H_2SO_4 surface

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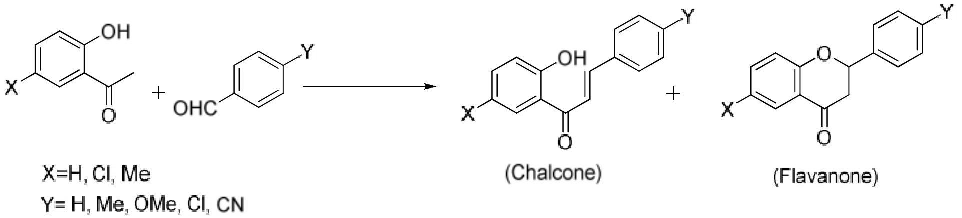
Flavanones are a subgroup of the Flavonoid family which are found in plants, fruits, vegetables & citrus [1]. Flavanones perform a variety of functions for example, antioxidant, antitumor, antibacterial & decreasing the blood pressure [2]. The most common method for the synthesis of flavanones includes the intra molecular conjugated addition of O-Hydroxy chalcone to the cyclic system of the corresponding Carbone (Michael addition) [3].

The purpose of this project was one-step synthesis of flavanones on the SiO_2/H_2SO_4acidic surface from benzaldehydes & 2´-hydroxyacetophenones which demonstrated better yields than pervious surfaces including (MgO, ZnO, BaO, K_2O, Na_2O) [4].

The synthesis of flavanones on the basic & neutral surfaces was also investigated in this project which result was not comparable with acidic ones [5].

The advantage of SiO_2/H_2SO_4surface include: biocompatibility, the variety of products with different starting materials, the easy preparation of the surface & its abundant, low-cost of the surface, none diminishing activity of the surface with time duration, also the easy extraction technique with filtration.

All of these advantages make $SiO_2/H_2SO_4$the best choice among all the pervious surfaces.



References:

[1] Flavonoids (isoflavonoids and neoflavonoids)., IUPAC Compendium of Chemical Terminology.
[2] Harborn, J.B.; Baxter, H. *The hand book of natural flavonoids*; John Wiely & Sons*:* Chichester, **1999**.
[3] Scoth. G.; *antioxidants: in Science, Technology, Medicine & Nutrition*; Albion publishing: Chichester, **1997**.
[4] Toda, F., et al., *J. Chem. Soc. Perkin Trans. I.*, **1990**, 3207.
[5] Palleros, D. R., *J. Chem. Educ.*, **2004**, *81*, 1345.

The study of solvation effects on an anticancer drug: Dacarbazine

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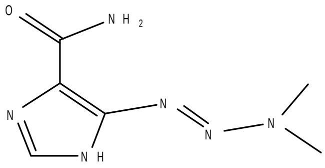
Dacarbazine, used as antineoplastic in the treatment of tumors. It belongs to the group of medicines called alkylating agents. It is used in the treatment of cancer of the lymph system and malignant melanoma a type of skin cancer. Dacarbazine, (DTIC-NSC-45388) is the single most active agent for the treatment of malignant melanoma. In addition to dacarbazine, other dimethyltriazenes have shown to demonstrate antitumor properties [1].

We have studied the solvent effects on values of Gibbs free energy, enthalpy, entropy and dipole moment in spread of solvents around dacarbazine [2]. The quantum mechanic calculations based on HF theory at the B3LYP/3-21G, 6-31G, 6-31G*, 6-31G** levels have been done, moreover. We have Compared resulted thermodynamic valuesin gas phase as well as various solvent when surround the dacarbazine molecule. We obtained the effects of differentdielectric constants on dacarbazine with the onsagar self-consistent model reaction field by applying hartree-fock theory and also we obtaind the effects of temperature on thermodynamic values of temozolomide in gas phase at 298k, and various solvent [3].



Reference

[1] Gunasekaran, S.; Kumaresan, S.; Arunbalaji, R.; Anand, and, Srinivasan, S. *Chem. Sci.* **2008**, *315*, 324.
[2] *Najafi, F.; Saedi, L.; Mollaamin, F.; Aghaie, H. V. J.of.Phy.and.Theor.Chem..* ***2010****,4 237.*
[3] Hooshyari. M.; Naderi, F.; Yari, M.; Khaleghian. M.; Monajjemi, M. *J. J.of.Phy.and.Theor.Chem.* **2009**, *173.*

One-pot synthesis of amidoalkyl naphthols by a three-component reaction under solvent-free conditions

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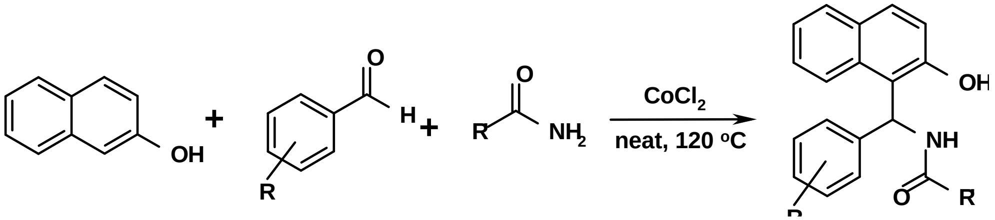
Multi-component reactions have proved to be remarkably successful in generating molecular complexity in a single synthetic operation. The preparation of 1-amidoalkyl-2-naphthols can be carried out by multi-component condensation of aryl aldehydes, 2-naphthol and acetonitrile or amide in the presence of Lewis or Brønsted acid catalysts [1-2]. However, some of these catalysts suffer from the drawback of green chemistry such as prolonged reaction times, low yields and toxicity of the catalyst. Therefore, introducing clean processes and utilizing eco-friendly and green catalysts which can be simply recycled at the end of reactions have been under permanent attention.

Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for several important organic transformations [3], we describe an efficient method for the synthesis of amidoalkyl naphthols by one-pot condensation reaction of 2-naphthol, aldehydes and amide using catalytic amounts of cobalt(II) chloride under solvent-free conditions at 1.5 to 2.5 h with 68% to 90% yields.



R= 4-nitro, 4-chloro, 4-bromo, 4-methyl,
4-flouro, 2,6-dichloro, 2,4-dichloro,
2-nitro, 2-chloro, 3-nitro, 2-chloro-6-flouro

R′= CH_3-, CH2=CH-

We b c, and a user-friendly process for the synthesis of 2,3-dihydroquinazolinones of biological and medicinal importance.

References:

[1] Shaterian, H. R.; Yarahmadi ,H. *Tetrahedron Lett.* **2008,** *49*, 1297.
[2] Nagarapu, L.; Baseeruddin, M.; Apuri, S.; Kantevari, S. *Catal. Commun.* **2007**, *8*, 1729.
[3] Karimi-Jaber, Z.; Keshavarzi, M. *Chin. Chem. Lett.* **2010**, *21*, 547.

Composition and antibacterial activity of the essential oils from flowers of *Astrodaucus orientalis* (L.) Drude.and leaves and flowers of *Prangos ferulacea(L.)*Lindle. growing wild in Iran

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The genus *Astrodaucus*is represented in the flora of Iran by two species [1]. Coumarins have been previously identified in a solvent extract of the aerial parts of *A.orientalis* [2]. Previously we reported the essential oils from aerial parts of. and *A.orientalis* collected from Fasham,Iran .In the oil,α-pinene (32.7%) and α-fenchyl acetate(14.5%), were predominated [3]. Fifteen species of the genus Prangos are found in Iran, among which five are endemic [1]. The water distilled oils obtained from the aerial parts of *P . latiloba* and *P . acaulis* have been the subject of our previous studies [4,5]. The aim of our study is to identify the constituents and antibacterial activity of the water distilled essential oil of flower of *A.orientalis* and leaves and flowers oils of *Prangos ferulacea*. The oils were analyzed by GC and GC/MS.Seventy-eight components in the flower oil of *A.orientalis*,which represented about 94.7% of the total oil, were identified.The oil of *A.orientalis* consisted of seventeen monoterpene hydrocarbons (62.1%),twenty-seven oxygenated monoterpenes(19.0%),fifteen sesquiterpene hydrocarbons (4.0%),ten oxygenated sesquiterpenes (6.3%) and nine non terpenoid compounds (3.3%).The major components of this oil were sabinene(16.5%)and α-pinene (11.0%).Other notable constituents were myrcene(7.0%),p-cymene(6.1%),α-thujene(6.1%)and β-pinene (5.2%).As can be seen from the above information,in the flower oil of *A.orientalis* monoterpenes (81.1%)predominated over sesquiterpenes(10.3%). Sixty-six components representing 96.5% and fifty-two constituents representing 90.4% were identified in the oils of leaves and flowers of *Prangos ferulacea*, respectively. The main components in the both oils were ß-pinene (29.6% and 20.6%), α-pinene (19.8 % and 7.8%), δ-3-carene (11.4% and 10.4% '') and ß-phellandrene (11.1% and 8.1%) respectively. According to these results, the composition of the leaves and flowers of *P.ferulacea* show significant similarity for the concentration of the main components. Both oils were rich in regard to monoterpenes (85.6% and 62.9%, respectively), the sesquiterpene fraction of the oils was relatively small, representing (10.5% and 27.4%), of the total oils, respectively. Antimicrobial activity was determined by measurement of growth inhibitory zone.All oils showed moderate activity against Gram-positive and Gram-negative bacteria.

Reference

[1] Mozaffarian, V., A Dictionary of Iranian Plant Names, Farhang Moaser, Publishers, Tehran, Iran, **1996,** 64,431.
[2] Muradyam , A . A. Tr. Bot. Inst. Akad. Nauk Amn. SSR. **1971**, 17, 136.
[3] Mazloomifar,H.;Bigdeli,M.;Saber-Tehrani,M.;Rustaiyan,A.;Masoudi,S.J.Essent. Oil Res. **2003**, 15,
[4] Masoudi,S.; Aghjani,Z.; Yari, M.; Rustaiyan, A.J. Essent. Oil Res., **1999**, 11, 767 .
[5] Rustaiyan, A.; Mazloomifar, H.; Masoudi, S.; Aghjani, Z.J. Essent.Oil Res.,**2006**,18,682.

A green method for the synthesis of 3-amido-2-aminothiophenes via Gewald reaction under aqueous conditions

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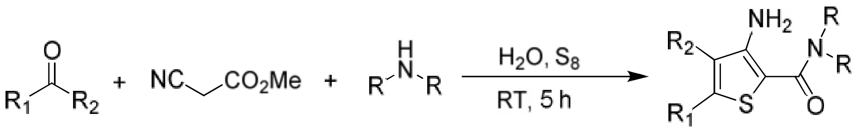
Aqueous conditions can significantly facilitate organic syntheses due to often increasing the rate and selectivity of the reactions and reducing the number of steps, if designed properly [1]. Consequently, conduction of organic transformations in water is very popular among synthetic chemists, nowadays.

Multicomponent reactions (MCRs) have increasingly gained popularity in synthetic organic chemistry in recent years because they offer one-pot combination of more than two reactants in one step allowing direct access to complex target molecules [2]. In this context, the one pot cyclocondensation of ketones (aldehydes) and 2-substituted acetonitrile derivatives with elemental sulfur, known as Gewald reaction [3], has been one of the most well studied MCRs in recent years. The reaction affords formation of 2-aminothiophenes with diverse pharmaceutical and biological properties [4]. To extend the scopes of the reaction, many alterations are made to the original Gewald's base catalyzed multi-component combination of α-mercapto ketones with cyanoacetate by variation of the components and the conditions [5].

In the present work, a green medium consisted of H_2O and Et_3N is employed for one pot combination of keones and aldehydes with appropriate active methylene compounds such as cyanoacetates and elemental sulfur to obtain their respective Gewald products in high yields and short reaction times at room temperature.



References:

[1] Filimonov, V. D.; Semenischeva, N. I.; Krasnokutskaya, E. A.; Tretyakov; A. N.; Hwang, H. Y. ; Chi, K.-W. *Synthesis* **2008**, 185.
[2] Kappe, C. O. *Acc. Chem. Res.* **2000**, *33*, 879.
[3] Gewald, K. *Chem. Heterocycl. Comp.* **1976**, *12*, 1077.
[4] Manhas, M. S.; Sharma, S. D.; Amin, S. G. *J. Med. Chem.* **1972**, *15*, 106.
[5] Hu, Y.; Wei, P.; Huang, H.; Han, S.-Q.; Quyang, P.-K. *Synth. Commun.* **2006**, *36*, 1543.

Synthesis of a new lariat diaza crown ether compounds

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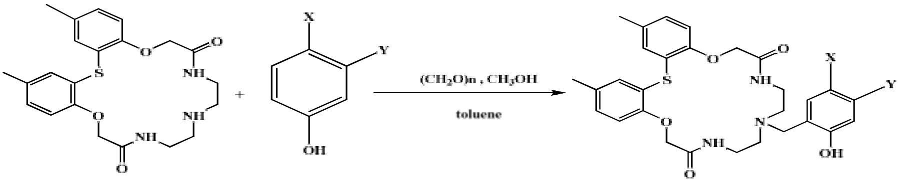
Macrocycles diamide derivatives are macrocyclic compounds, which possess similar properties to those of crown ethers. Macrocyclic diamides are valuable intermediates formed during the preparation of aza-crown compounds. They have high capability in selective and effective complexation with a variety of transition and heavy metals, molecular ions, and neutral molecules [1].

Macrocyclic polyethers with side groups containing donor atoms (lariat crown others) can form complexes with a three-dimensional coordination sphere, similar to that in cryptates, since the donor atoms of both the macroring and the side chains can be involved in the coordination. This gives rise to unusual complexing properties, which do not directly correlate with the extent of size matching between the cation and macroring cavity but strongly depend on the structure of side substituents [2].

The Mannich reaction is known to be a powerful method for the functionalization of azacrown ethers with additional ligating units [3].

Our purpose in this research work is preparation of lariat ether compound as cationic and molecular acceptor. Lariat ethers 1,2,3 were prepared by reaction of macrocyclic diamide and phenols in the presence of paraformaldehyde by refluxed in dry toluene.



1	X=CHO	Y=H
2	$X=NO_2$	Y=H
3	$X=CH_3$	$Y=CH_3$

References:

[1] Mashhadi Akbar Boojar, M.; Shockravi, A.; *Bioorganic & Medicinal Chemistry*. **2007**, *15*, 3437.

[2] V.Bordunov, A.; S.Bradshaw, J.; N.Zhang, X.; Kou, X.; Dally, N.K.; Yang, Z.; B.Savage, P.; M.Izatt, R.; *Tetrahedron*. **1997**, *53*, 17595.

[3] Su, N.; S.Bradshaw, J.; E.Krakowiak, K.; L.De Wall,S.; W.Gokel, G.; B.Savage, P.; M.Izatt, R.; *Tetrahedron*. **1999**, *55*, 9737.

Sulfamic acid (SA)/$NaNO_2$ as a novel heterogeneous system for the chemoselective *N*-nitrosation of secondary amines

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N-Nitroso amines are useful synthetic intermediates for the preparation of various *N*,*N*-bonded functionalities. Furthermore, owing to their easy lithiation, followed by reaction with electrophiles and subsequent denitrosation, they can be used for the electrophilic substitution of secondary amines at the α-carbon in a regio- and stereoselective manner [1].

The most general reagent for synthesis of nitrosoamines is nitrous acid, generated from sodium nitrite and acids [2]. However the used acid for generation of nitrous acid from sodium nitrite suffers from some disadvantages such as environmentally unfavorable, commercially unavailable and expensive, hence there is a need to develop new reagents which can overcome these drawbacks. Sulfamic acid is commercially available, environmentally compatible, cheap, easy to handle, and stable.

During the course of our studies on the development of new routes for the transformation of organic functional groups [3], herein we report an efficient and novel heterogeneous system of sulfamic acid/$NaNO_2$ for *N*-nitrosation of different type of secondary amines in dichloromethane at room temperature (Scheme 1).

$$R^1R^2NH \xrightarrow[CH_2Cl_2,\ r.t]{SA/NaNO_2,\ Wet\ SiO_2} R^1R^2N\text{-}N{=}O$$

Scheme 1

Summery, this procedure offers several major advantages:(1) the use of a eco-friendly, commercially available, cheap, and chemically stabile reagent; (2) efficient for the chemoselecti *N*-nitrosation of structurally diverse secondary amines in good to high yields at room temperature; (3) the method conforms to several of the guiding principles of green chemistry. We believe the present method to be an improvement with respect to other procedures

References:

[1] Olszewska, T.; Milewska, M. J.; Gdaniec, M.; Matuszynska, H.; Potonski, T. *J. Org. Chem.* **2001**, *66*, 501.
[2] Zolfigol, M. A.; Ghorbani-Choghamarani, A.; Hazarkhani, H. *Synlett* **2002**, 1002.
[3] Rostami, A.; Ahmad-Jangi, F.; Zarehbin, M. R.; Akradi, J. *Synth. Commun.* **2010**, *40*, 1500.

A novel approach to the synthesis of highly functionalized pyrroles

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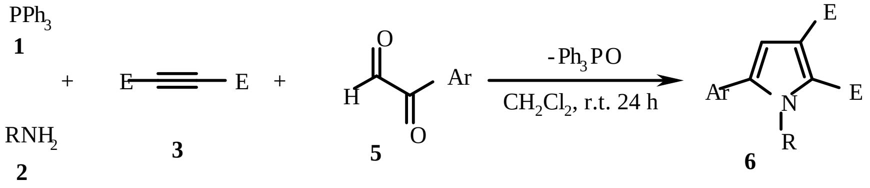
A new and efficient one-pot synthesis of polysubstituted pyrrole derivatives by three-component reaction between dialkyl acetylenedicarboxylates, aromatic amines, triphenylphosphine and arylglyoxals is described. The reactions were performed in dichloromethane at room temperature and neutral conditions and afforded high yields of products.

Being successful in this reaction, we decided to investigate the one-pot synthesis of dimethyl 5-(4-nitrophenyl)-1-phenylpyrrole-2,3-dicarboxylate 6a .Thus, equimolar amounts of triphenylphosphine, aniline and DMAD were mixed in dichloromethane as solvent. After stirring for one minute at room temperature, 4-nitrophenylglyoxal was added and the progress of the reaction was monitored by TLC. After 24 hours the TLC of the mixture of the reaction showed only the presence of pyrrole derivative 6a and triphenylphosphine oxide. Silica-gel chromatography afforded the product dimethyl 5-(4-nitrophenyl)-1-phenylpyrrole-2,3-dicarboxylate 6a in 85% yield [1-3].



References:

[1] Anary-Abbasinejad, M.; Anaraki-Ardakani, H.; Hosseini-Mehdiabad**,** H. *Phosphorus, Sulfur and Silicon***, 2008**, 183 (6), 1440.
[2] Yavari, I.; Adib, M.; Hojabri, L. *Tetrahedron*., **2002**, 58, 7213.
[3] Anary-Abbasinejad, M.; Mosslemin, M. H.; Hassanabadi, A.; Tabatabaee. M. *Synth. Commun*., **2008**, 38, 3700.

Melamine-$(H_2SO_4)_3$/$NaNO_2$: As an efficient system for the oxidation of urazoles

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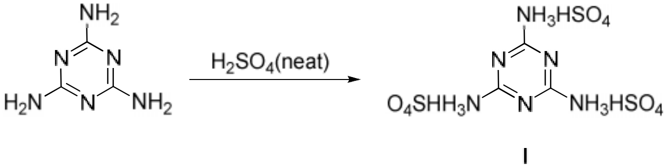
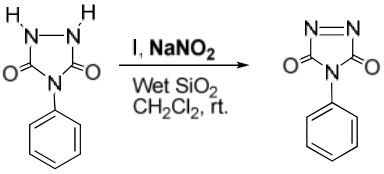
Solid acids have many advantages such as simplicity in handling, decreased reactor and plant corrosion problems, and more environmentally safe disposal. Also, wastes and by-products can be minimized or avoided by developing cleaner synthetic routes [1]. On the basis of our experiences in the application of solid acids [2], we found that melamine reacts with concentrated sulfuric acid to give Melamine-$(H_2SO_4)_3$. It is interesting to note that this exothermic reaction is easy and clean without any required work-up procedure (Scheme 1).



Scheme 1.

In continuation of our studies on the oxidation of urazoles [3], we were interested in using the Melamine-$(H_2SO_4)_3$ for the *in situ* generation of HNO_2 in combination with $NaNO_2$ and wet SiO_2 and eventually oxidation of urazoles and *bis*-urazols. Herein, we wish to report a simple, economical and effective method for oxidation of urazoles and *bis*-urazols under mild and heterogeneous conditions (Scheme 2).



Scheme 2.

References:

[1] Shirini, F.; Zolfigol, M. A.; Salehi, P.; Abedini, M. *Curr. Org. Chem.* **2008**, *12*, 183.
[2] Zolfigol, M. A.; Ghaemi, E.; Madrakian, E.; Ghorbani Choghamarani, A. *Mendeleev Commun.* **2006**, 41.
[3] Zolfigol, M. A., Bagherzadeh, M., Mallakpour, S., Chehardoli, G., Ghorbani-Choghamarani, A., Koukabi, N., Dehghanian, M., Doroudgar, M., *J. Mol. Catal. A: Chem.* **2007**, *270,* 219.

Synthesis and characterization of novel optically active aromatic–aliphatic poly(amide-imide)s comprising hydroxyphenyl benzamide linkages

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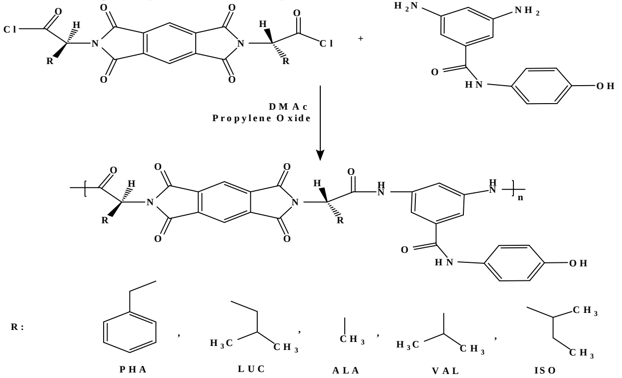
Wholly aromatic polyamides (aramide)s are a set of high temperature resistant polymers with good chemical resistance and thermal stability, low flammability and very good mechanical properties [1]. However, because of their limited solubility in organic solvents and high melting and glass transition temperatures they are difficult to process. Therefore, the interest have been focused on the preparation of polymers with improved processability while maintaining the thermal stability. Copolycondensation is one of the possible ways for modification of polymer properties. Thus, for the processing of polyamides many copolyamides, such as poly(sulfone-amide)s, poly(ether-amide)s, poly(amide-imide)s and other copolymers have been reported [2-4].

Here we wish to report the synthesis and characterization of novel optically active poly(amide-imide)s (PAIs) containing hydroxyphenyl groups in the side chain and chiral center in the main chain. The PAIs were synthesized by solution polycondensation reaction of different synthetic diacid chlorides containing chiral center with a diamine containing the hydroxyphenyl benzamide group at low temperature.



References:

[1] Mallakpour, S.; Rafiee, Z. *Polymer* **2008**, *49*, 3007.
[2] Ghaemy, M.; Barghamadi, M. *J. Appl. Polym. Sci*. **2009**,*111*, 1588.
[3] Pal, R R.; Patil, PS.; Salunkhe, MM.; Maldar, NN.; Wadgaonkar, PP. *Eur. Polym. J*. **2009**, *45*,953.
[4] Mallakpour, S.; Seyedjamali, H. *Colloid. Polym. Sci*. **2009**, *287*, 1111.

The multicomponent reaction of isocyanides, arylidenemalononitriles and acetylenedicarboxylate: a novel and simple synthesis of highly substituted cyclopentadienes

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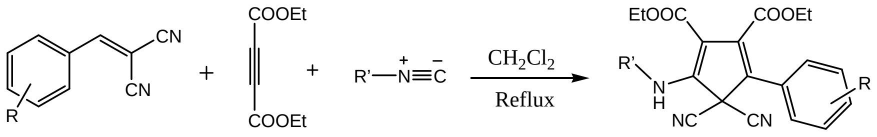
Cyclopentadienes (Cps) are highly useful synthetic intermediates. Considerable attention has been focused on the synthesis of substituted Cps as units for the construction of fused ring systems via inter- and intramolecular Diels–Alder reactions, as ligands in coordination chemistry and as homogeneous catalysis for olefin polymerization [1-3].

We report herein synthesis of polysubstituted Cps using simple starting materials. Thus, a mixture of arylidenemalononitriles **1**, acetylenedicarboxylate **2**, and isocyanides **3** underwent a smooth reaction in dry dichloromethane at reflux condition to afford diethyl 3-amino-4,4-dicyano-5-phenylcyclopenta-1,2-diene-1,2-dicarboxylates **4** in medium to good yields (Scheme 1).



1 **2** **3** **4**

Scheme 1

The structures of the isolated Cps **4** were confirmed by IR, ^{1}H, and ^{13}C NMR spectroscopy, two ethoxy groups resonated around 1.5 and 3.80 ppm and the amino proton appeared around 8.5 ppm as a singlet peak in the ^{1}H NMR spectrum. The ester carbonyl groups displayed ^{13}C resonance signals around 165 ppm and the signal around 110 ppm were attributed to the cyano groups.

References:

[1] Okuda, J. *Top. Curr. Chem.* **1991**, *160*, 97.
[2] Halterman, R. L. *Chem. Rev.* **1992**, *92*, 965.
[3] Fringuelli, F.; Taticchi, A. Dienes in the Diels–Alder Reaction; *John Wiley & Sons: New York*, **1990**.

Solvent-free *N*-alkyl and *N*-arylimides preparation from anhydrides catalyzed by starch

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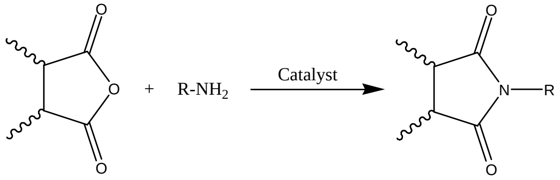
Imide derivatives are associated with various uses both in biology and synthetic chemistry [1]. Also these are good Michael acceptors and Diels-Alder dienophiles [2]. It is not surprising therefore, that preparation procedures for these compounds are in great demand.

The popular procedures include dehydrative condensation of an anhydride and amine at high temperature and cyclization of amic acid intermediates in presence of acidic reagents [3]. The direct N-alkylation of imides with alcohols under Mitsunobu reaction conditions is yet another popular method [4]. How ever many of these have short comings, such as poor yields, carcinogenic solvent media, and stoichiometric reagent require ment [5].

To address all these limitations we report here in, a solvent-free starch catalyzed imide synthesis under microwave irradiation. The results from experiments prove that starch acted as a very efficient catalyst. Also, the avoiding of carcinogenic solvents, high yields and shorter reaction times, undoubtedly offer many advantages over existing procedures.



R: alkyl, aryl
Catalyst: Starch

References:

[1] Da Settimo, A.; Primofiore, G.; Da Settimo, F.;Simorini,F.; La Motta, C.;Martinelli,A.; Boldrini, E.; *Eur.J. Med. Chem*, **1996**, 31, 49.
[2] Ohkubo, M.; Nishimura, T.; Jona, H.; Honma, T.; Morishima, H.; *Tetrahedron*, **1996**, 52, 8099.
[3] Braish, T.F.; Fox, D.E.; *Synlett*, **1992**,979.
[4] Walker, M.A.; *J. Org.Chem*, **1995**, 60, 5352.
[5] Reddy,P.Y.; Kondo, S.; Toru, T.; Ueno, Y.*; J.Org.Chem*, **1997**,62,2652.

Nanosized sulfated zirconia as solid acid catalyst for the synthesis of 2-substituted benzimidazoles

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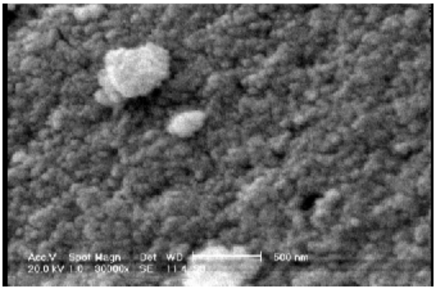
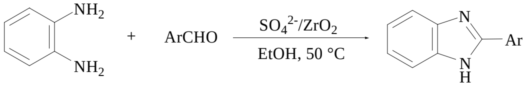
The use of solid acid catalyst has received considerable importance in organic synthesis because of their ease of handling, greater selectivity, simple workup and reusability. Among the various heterogeneous catalysts, zirconia has attracted considerable attention as both catalyst and catalyst support because of high thermal stability and amphoteric character of its surface hydroxyl groups [1]. Zirconia modified with sulfate anion act as strong solid acid catalyst in many organic transformation [2, 3]. In this research, we report an efficient method for the synthesis of 2-substituted benzimidazoles by the reaction of aldehydes and *o*-phenylenediamines in the presence of catalytic amount of nanosized sulfated zirconia under mild condition.





A variety of aldehydes were reacted with *o*-phenylenediamine in the presence of catalytic amount of SO_4^{2-}/ZrO_2 in EtOH at 50 °C and the corresponding 2-arylbenzimidazoles were obtained in high yields. The reusability experiments were also investigated and the results show that the catalyst is reusable with moderate change in its activity.

In conclusion, we introduced nanosized SO_4^{2-}/ZrO_2 as an efficient and eco-friendly catalyst for the synthesis of 2-arylbenzimidazoles. Simple workup, mild reaction conditions and reusability of the catalyst makes this procedure favorable and environmentally benign.

References:

[1] Devassy , B. M.; halligudi, S. B. *J. Mol. Catal. A: Chemical* **2006**, *8,* 253.
[2] Sainan, W.; Shuichi, M.; Kazunobu, T. *Tetrahedron Lett.* **2007**, *48,* 6449.
[3] Benjaram M. R.; Pavani, M. S.; Pandian, L. *J. Mol. Catal. A: Chemical* **2005**, *93,* 237.

"On water" organic synthesis: A clean and highly efficient synthesis of tetrahydrobenzodiazepines and dihydropyrazines via isocyanide-based multicomponent reactions of diamines

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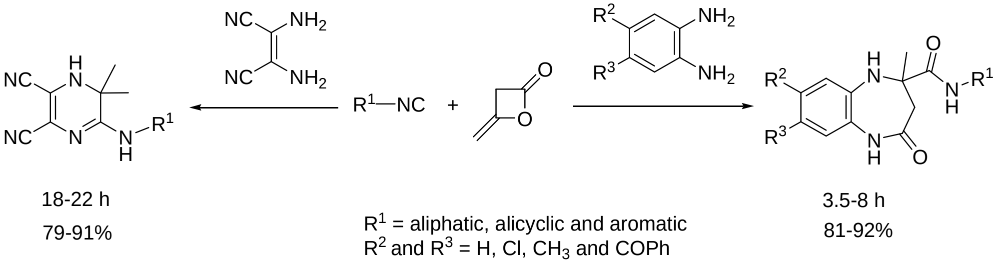
Benzodiazepines and pyrazines are important class of benzoheterocycles displaying a broad spectrum of biological activities which have made them privileged structures in medicinal chemistry [1,2]. Benzodiazepines as one of the most widely prescribed class of psychotropics, have remarkable central nervous system depressant activity, with various biological interest such as cancer, viral infection (HIV) [3-7].

Herein we report a highly efficient method for the synthesis of 2,3,4,5-tetrahydro-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide with regiochemical control and 1,6-dihydropyrazine-2,3-dicarbonitrile derivatives from condensation reaction of an isocyanide, diketene and 1,2-diamine compounds in water, at ambient temperature. This protocol has the advantages of high yields, less environmental impact and convenience of procedure.



References:

[1] Horton, D. A.; Bourne, G. T.; Smythe, M. L. *Chem. Rev.* **2003**, *103*, 893.
[2] Dembitsky, V. M.; Gloriozova, T. A.; Poroikov, V. V. *Mini-Rev. Med. Chem.* **2005**, *5*, 319.
[3] Michelini, S.; Cassano, G. B.; Frare, F.; Perugi, G. *Pharmacopsychiatry* **1996**, *29*, 127.
[4] Archer, G. A.; Sternbach, L. H. *Chem. Rev.* **1968**, *68*, 747.
[5] Knabe, J.; Buech, H. P.; Bender, S. *Arch. Pharm.* **1995**, *328*, 59.
[6] Atwal, K. S.; Bergey, J. L.; Hedberg, A.; Moreland, S. *J. Med. Chem.* **1987**, *30*, 635.
[7] Di Braccio, M.; Grossi, G.; Roma, G.; Vargiu, L.; Mura, M.; Marongiu, M. E. *Eur. J. Med. Chem.* **2001**, *36*, 935.

Chemoselective epoxidation of polybutadiene and hydroxyl-terminated polybutadiene using in situ generated dimethyl dioxirane (DMD) in the peresence of nanoclay

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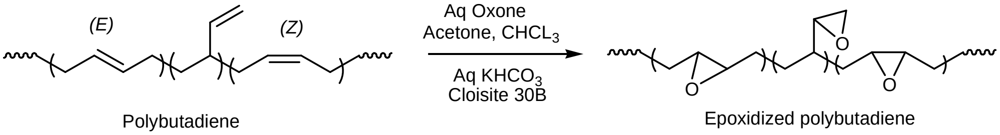
The introduction of one or more epoxy functional groups in non-polar polymer chains that contain non-conjugated carbon–carbon double bonds can increase the polarity of the final polymers and lead to the production of new special polymer products [1]. There are some experimental methods for the epoxidation of C=C bonds in the polymer structure such as, thermal oxidation [2], oxidation with Vo(acac)$_2$ complex [3] and epoxidation using peroxide [4] and peracids [5] but all of them have some advantages and disadvantages, for example the epoxidation process was accompanied by several side reactions and higher temperatures were needed in order to obtain higher conversion degrees. These drawbacks can be solved by using in situ-generated DMD in epoxidation of double bonds [6]. In situ generated DMDs are cyclic peroxides known as powerful, reactive and efficient oxidizing agents and DMD usually prepared from the reaction of acetone and aqueous "Oxone$^{®}$" ($2KHSO_5$, $KHSO_4$, K_2SO_4) in buffered conditions. In this report, the transformation of polybutadiene and hydroxyl terminated polybutadiene to the corresponding epoxidized one using in situ generated DMD accompanied by Cloisite30B as a phase-transfer catalyst was successfully done for the first time.



References:

[1] McGrath, M. P.; Sall, E. D.; Tremont S. *J. Chem. Rev.* **1995**, *95*, 381.
[2] Stenberg, B.; Ahlblad, G.; Reitberger, T.; Terselius, B. *Polymer. Degradation. Stab.* **1999**, *65*, 179.
[3] Gerbase, A. E.; Gregorio, J. R.; Martinelli, M.; von Holleben, M. L. A.; Jacobi, M. A. M.; Freitas, L.; Calcagno, C. I. W.; Mendes, A. N. F.; Pires, M. L. Catalysis. Today. **2000**, *57*, 241.
[4] Badran, B. M.; Abdel, E. M.; In Situ Epoxidation of Natural Rubber and Polybutadiene, *Chem Ind* (London), **1977**, 314.
[5] Saffer, A.; Johnson, B. L. *Ind Eng Chem,* **1948,** *40* (3), 538.
[6] Kachasakul, P.; Assabumrungrat, S.; Praserthdam, P.; Pancharoen, U. *Chem. Eng. J.* **2003**, *92*, 131.

A synthesis of diethyl alkylsulfanylmethylmalonates catalyzed by KOH in an ionic liquid

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[b]*Chemistry Department, Tarbiat Modares University, Tehran, Iran.*

Ionic liquids (ILs) have gained tremendous attention in the last 15 years [1–3]. They are, among other uses, solvents and are frequently fitted with attributes like ‘‘modern,’’ ‘‘green,’’ ‘‘designable,’’ ‘‘non-volatile,’’ ‘‘non-coordinating,’’ etc., although it is increasingly recognized that none of these labels should be used lightly. Nonetheless, many chemical reactions have been attempted and successfully performed in IL media, and oftentimes these systems show interesting and peculiar features.

As part of our current studies, on the development of in situ thia- Michael addition, we wish to report a one-pot synthesis of sulfanylmethylmalonates catalyzed by KOH. Thus, three-component reaction of aldehyde **1**, diethyl malonate **2**, and alkyl thiols **3** catalyzed by KOH proceeds smoothly in ionic liquid to produce diethyl alkylsulfanylmethylmalonates **4** in good yields (Scheme 1). The advantage of the present procedure is that the reaction is performed in green and environmentally benign media by simple mixing of the starting materials.

1 **2** **3** **4**

Scheme 1

References:

[1] Welton T. *Chem Rev* **1999,** *99*, 2071.
[2] Rogers R D, Seddon K R (eds) (**2002**) In: Ionic liquids: industrial applications to green chemistry. ACS, Symposium Series 818, American Chemical Society, Washington, DC.
[3] Wasserscheid P, Welton T (eds) (**2003**) Ionic liquids in synthesis. Wiley, Weinheim.

An efficient one-pot synthesis of 3-((1*H*-indol-3-yl)(p-tolyl)methyl)pentane-2,4-dione using indol, p-methylbenzaldehyde in the presence of CH-acids

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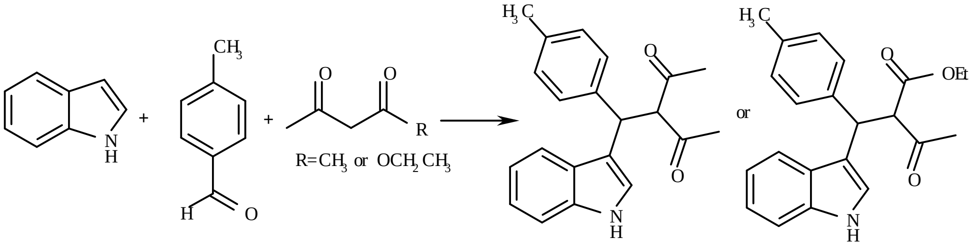
Multi-component reaction (MCRs), due to their productivity, simple procedures, convergence, and facile execution, are one of the best tools in combinationatorial chemistry [1,2]. As a result, the number of new MCRs has grown rapidly [3]. Nowadays, one-pot multicomponent reactions have emerged as valuable tools in organic synthesis for reducing operative steps and enhancing synthesis efficiency.

Here we report an efficient synthesis of 3-[(1*H*-indol-3-yl)(p-tolyl)methyl] pentane-2,4-dione and ethyl 2-((1H-indol-3-yl)(p-tolyl)methyl)-3-oxobutanoate analogues *via* one-pot reaction of commercial available indol, p-methylbenzaldehyde and CH-acids such as acetylacetone or ethyl acetoacetate in the presence of some of Lewis and Bronstead acid catalyst under argon atmosphere. The reaction provided the products in moderate to good yield.



The structures of these products were deduced from ^{1}H NMR, ^{13}C NMR and IR spectral data.

References:

[1] Terrett, N. K. *Combinatorial Chemistry*; Oxford University Press: New York, **1998.**

[2] Zhu, J. P.; Bienaymé, H. *Multicomponent Reactions*; Wiley-VCH: Weinheim, **2005**.

[3] (a)Orru, R. V. A,; Greef, M. Synthesis 2003, 1471; (b)Dömling, A.. *Curr. Opin Chem. Biol.* **2002**, 6, 306; (c) Dömling, A. *Chem. Rev*. **2006**, 106, 17-89.

A green Brønsted acid ionic liquid as an efficient catalyst for the one-pot, synthesis of α-aminonitriles , amidoalkyl naphthols and coumarins under solvent-free conditions

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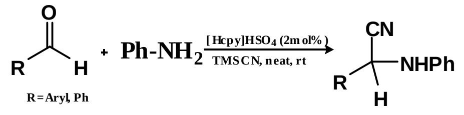
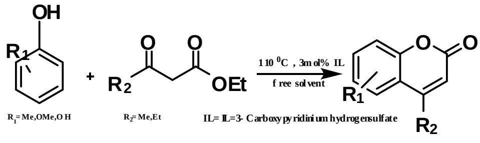
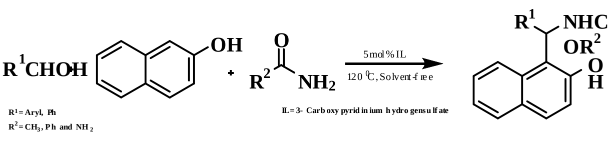
One of the fundamental aspects in Green Chemistry is linked to the number of steps in organic synthesis as well as atom economy. Multicomponent reactions (MCR) are thus becoming a more and more important class of the reactions, since they allow combining several starting materials in a single compound and in one-flask operation [1]. α-aminonitriles serve as efficient precursors for the synthesis of natural and unnatural α-amino acids [2], amidoalkyl-2-naphthols are ubiquitous to a variety of biologically important natural products and potent drugs including a number of nucleoside antibiotics and HIV protease inhibitors[3] and coumarins have varied bioactivities such as: antibacterial [4], anticancer [5]

We have found that acidic ionic liquids 3- Carboxypyridinium hydrogensulfate can be used as green, efficient and inexpensive catalysts for the synthesis of α-aminonitriles , amidoalkyl-2-naphthols and coumarins in good yields and short reaction times.

This compounds were prepared using this methodology as shown below. The structures of the products were determined from their spectral (^{1}H and ^{13}C NMR, IR) data.







References:

[1] Marek, I. *Tetrahedron.* 2005, *61*, 11309.
[2] Weinstock, L. M.; Davis, P.; Handelsman, B.; Tull, R. *J. Org. Chem.* 1967, *32*, 2823.
[3] Shen, A. Y.; Tsai, C. T.; Chen, C. L. *Eur. J. Med. Chem.* 1999, *34*, 877.
[4] Wang C. J.; Hsieh, Y, J.; Chu, C, Y.; Lin, Y, L.; Tseng , T. H.; *Cancer Lett.* 2002, *183*, 163.
[5] Kayser, O.; Kolodziej, H.; *Planta Med.* 1997, *63*, 508.

The study of volatile compounds, mineral content and antioxidant properties of *Carica papaya* L.

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Carica papaya L. is widely cultivated throughout the world and is used as a food and also as a traditional medicine, particularly as an antiseptic and contraceptive. The present study was investigated the composition of volatile compounds, mineral content and antioxidant properties of carica papaya collected from sarbaz area of sistan & baluchestan in Iran.

1) The volatile compounds were isolated from fresh papaya fruit by simultaneous steam distillation-solvent extraction according to Likens–Nickerson.Compounds were identified by capillary GC-MS [1].

2) The mineral composition (Na, Ca, Fe, Mn, Mg, K and Cu) of papaya fruit was determined by flame photometry method [2].

3) The antioxidant properties of dried papaya leaves were studied by DPPH and β-caroten linolic acid tests [3].

References:

[1] Pino, J. A.; Almora, K.; Marbot, R. *Flavour Fragr. J.* **2003**, *18*, 492.
[2] Wall, M. M. *J. Food Composition and Analysis,* **2006**, *19*, 434.
[3] Mehdipour, S.; Yasa, N.; Dehghan, G.; Khorasani, R.; Mohammadirad, A.; Rahimi, R.; Abdollahi, M. *Phytother. Res.* **2006**, *20*, 591.

Synthesis and characterization of nanocasted $AlPMo_{12}O_{40}$ and investigation of catalytic activity

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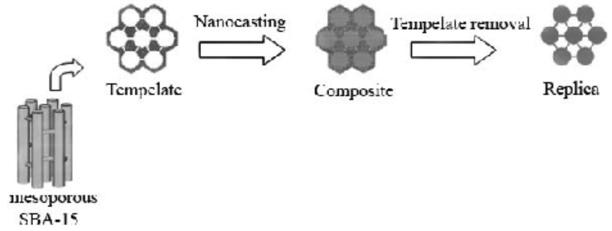
High-surface area inorganic materials have attracted widespread attention in diverse areas such as heterogeneous catalysis, adsorption, gas sensing, energy storage, drug delivery, biomedical applications, electrochemistry, etc. Because of this broad range of applications, a great effort has been made to review and update the methods of preparing such materials [1-3]. The application of the nanocasting technique to the fabrication of inorganic compounds implies that the fabrication of these products takes place in the nanospaces provided by the pores of a porous solid (hard template). After the synthesis of the material, the template framework is selectively removed and the inorganic product is obtained [4]. The catalytic performance of nanocasted $AlPMo_{12}O_{40}$ materials exceeded that of bulk $AlPMo_{12}O_{40}$, known as the most active among the acidic HPW salts. As part of our continued interest in developing "greener" methods for oxidation, we studied the UHP/ $AlPMo_{12}O_{40}$ (AlPMo) salt nanocrystal system for the aerobic oxidative of alcohols.



References:

[1] Raimondi, F.; Scherer, G. G.; Ko¨tz, R.; Wokaun, A. *Angew. Chem. Int. Ed.* **2005**, *44*, 2190.
[2] Medine, G. M.; Zaikovskii, V.; Klabunde, K. J. *J. Mater. Chem.* **2004**, *14*, 757.
[3] Carnes, C. L.; Stipp, J.; Klabunde, K. J. *Langmuir,* **2002**, *18*, 1352.
[4] Madhusudhan Rao, P.; Goldberg-Oppenheimer, P.; Kababya, S.; Vega, S.; Landau, M.V. *J. Mol. Catal. A: Chem.* **2007**, *275*, 214.

N-Bromo succinimid (NBS): A Novel and Efficient Catalyst for the Synthesis of 14-Aryl 14-*H*-dibenzo[*a,j*]xanthenes under Solvent-Free Conditions.

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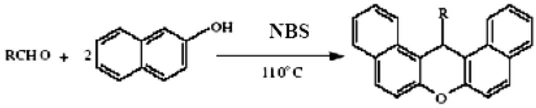
The synthesis of xanthenes, especially benzoxanthenes, has been of considerable interest to chemists because their oxygen heterocycles may contribute to potential antibacterial,[1] antiviral,[2] and anti-inflammatory activities.[3] For the synthesis of benzoxanthenes, various methods have been reported including the reaction of b-naphthol with formamide, 2-naphthol-1-methanol, and carbon monoxide. However, these methods have drawbacks such as poor yields, prolonged reaction time, using of toxic organic solvents, excess reagents/catalysts, and harsh reaction conditions. Due to these disadvantages, several reactions have been improved by the condensation of b-naphthol with aldehydes in the presence of a catalyst, such as p-TSA,[4] sulfamic acid, AcOH/H_2SO_4, iodine, $K_5CoW_{12}O_40$-$3H_2O$, cyanuric chloride, LiBr. However, searching another environmentally friendly catalyst and green solvents is still highly desirable.

In connection with our ongoing studies on *N*-Bromosuccinimide (NBS) as a versatile and convenient reagent used in various transformations, we describe an efficient method for the condensation of aromatic aldehydes with β-naphthol to the corresponding 14-aryl-14Hdibenzo[a,j]xanthanes using catalytic amounts of NBS under solvent-free conditions.(Scheme **1**).



Scheme **1**

The advantages or the characteristic aspects of the described method in this paper in comparison with other previously reported are the following: The yields of products are better than the pervious reported yields. In addition, the catalyst NBS is inexpensive, not moisture sensitive, sub-molar amounts of NBS are required. Longer reaction times are required when lesser amounts of NBS are employed. It is important to note that no furan derivatives were afforded when the reactions were carried out without using any NBS in the reaction.

References:

[1] Banerjee, A.; Mukherjee, A. K. *Stain Technol*. **1981**, *56*, 83.
[2] Sirkeeioglu, O.; Talinli, N.; Akar, A. *J. Chem. Res., Synop*. **1995**, 502.
[3] Knight, C. G.; Stephens, T. *Biochem. J.* **1989**, *258,* 683.
[4] Rajitha, B.; Kumar, B. S.; Reddy, Y. T.; *Tetrahedron Lett*. **2005**, *46,* 8691.

Facile synthesis and characterization of imines derived from indoline-2,3-dione

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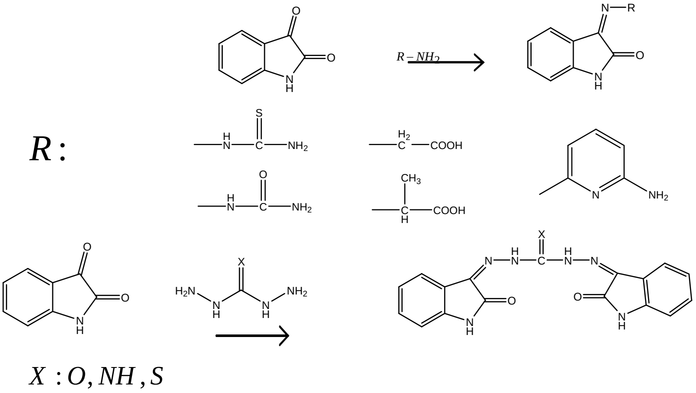
Imines have large numbers of applications in some fields such as, organic and inorganic chemistry, pharmacy, paint, plastic, liquid crystal, agronomy, biochemistry, physiology and so on [1] .

In this article the synthesis of imines derived from Indoline-2,3-dione is to be considered. These imines as long as we know are novel compounds. The mixture of Indoline-2,3-dione (0.01mol) and primary amine (0.01mol) in ethanol was stirred and heated at 70-75 ◦C and the progress of the reaction was monitored by TLC. The products were precipitated in high yield with no special procedure for purification is needed. The products were characterized by IR, ^{1}H NMR, ^{13}C NMR and elemental analysis.

One of the imines, Isatin- 3- thiosemicarbazone, was used in complex with Cu to get a (Isatin-3-thiosemicarbazone)Bis(triphenylphosphine)Copper(I)nitrate ($[Cu(PPh_3)_2(ITC)] NO_3$) as a yellow crystals in high yield.The preparation of other complexes using the synthesized imines is under investigations. Some imines derived from Indoline-2,3-dione are reported as anti HIV drugs [2]. The biological activity of the synthesized imines is under investigations by our research group.



References:

[1] R. Karvembu, C. Jayabalakrishnan, N. Dharmaraj, V. S.Renukdaevi, K. Natarajan, transiton Metal

[2] D. Sriram, T.Rattan and P.Yogeeswari, *Bioorganic & Medicinal chemistry*, **2004,** *12*, 5865.

Emulsion polymerization of styrene and optimized measurement of the conversion of the monomer to polymer

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In recent years the popularity of polystyrene has increased tremendously, particularly in view of more frequent use of this material in containers, in the automobile industry, in the toy industry, and in many other areas of commerce [1].

Emulsion polymerization is a unique chemical process widely used to produce waterborne resins with various colloidal and physiochemical properties [2].

Emulsion polymerization of styrene initiated by the radical initiator of potassium persulfate in the presence of sodium dodecyl sulfate (SDS) as an emulsifier was performed in which the conversion of styrene to polystyrene was improved and measured [3,4].

In this research work, different parameters such as temperature, the concentration of surfactant, the concentration of initiator, the proportion of monomer to water and the effect of agitation on the emulsion polymerization of styrene by conventional method was investigated. The results showed that the conversion of the monomer to polymer was 90% in fifty minutes.

References:

[1] James, M. Watson, Polymerization of styrene, Big Spring, Tex, June 22, **1993**, *636*,718.
[2] Chern, C.S.Emulsion polymerization mechanisms and kinetics 15 February **2006**, 443.
[3] Abedini, H. Shahrokhi, M. Inferential closed-loop control of particle size distribution of styrene emulsion polymerization, 24 January **2008**, 2378.
[4] Capek I, Lin S. Y., Hsu T. J., Chem C. S “Effect of Temperature on Styrene Emulsion Polymerization in the presence of Soduim Dodecyl Sulfate. II.”J Polym Sci: part A, Vol.*38*, **2000**, PP 1477.

Synthesis of bis-(1,4-dihydropyridines) via one pot multi component condensation in water using *nano* aluminum nitride as solid source of ammonia

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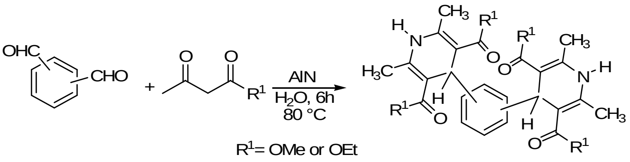
One of the most attractive synthetic strategies favored by organic chemists is the multi-component coupling reactions (MCRs), which allow the creation of several bonds in a single operation [1]. Numerous heterocyclic compounds have the ability to mimic structures of peptides and to bind reversibly to proteins [2]. An interesting example of useful scaffold is a 1,4-dihydropyridine (DHP) system, because of its ability to act as NAD(P)H analogue of 1,4-dihydronicotinamide [3]. They are the most important class of calcium-channel modulators [4] and have been introduced for the treatment of cardiovascular diseases such as nifedipine, nicradipine and amlodipine. In continuation of our investigation on the organic functional group transformation [4-5] we became interested to disclose a novel synthetic protocol for the preparation of bis-(1,4-dihydropyridine) derivatives by combination of *nano* aluminum nitride (**Figure 1**), dialdehyde and methyl acetoacetate or ethyl acetoacetate in water as solvent at 80 °C (Scheme 1).



Scheme 1

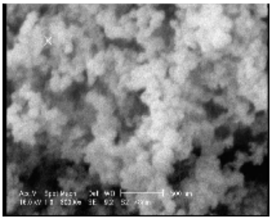


Figure 1 SEM image of nano aluminium nitride

Nano aluminium nitride has dual roles in this reaction. Aluminum nitride serves to generate a solution of ammonia via its reaction with water. On the other hand, $Al(OH)_3$ as other product of this reaction might be act as catalyst for the condensation of dialdehydes, β-dicarbonyl compounds and ammonia.

In summary, we have demonstrated that the combination of a dialdehydes, alkyl acetoacetate and *nano* aluminum nitride in water allows a practical preparation of bis-(1,4-dihydropyridines).

References:

[1] Kantam, M. L.; Ramani, T.; Chakrapani, L.; Choudary, B. M. *Catal. Commun.* **2009**, *10*, 370.
[2] Baskovc, J.; Bevk, D.; Stanovnik, B.; Svete, J. *J. Comb. Chem.* **2009**, *11*, 500.
[3] Zhu, X.-Q.; Liu, Y.; Zhao, B.-J.; Cheng, J.-P. *J. Org. Chem.* **2001**, *66*, 370.
[4] Ghorbani-Choghamarani, A.; Zolfigol, M.A.; Hajjami, M.; Darvishi, K.; Gholamnia, L. *Collect. Czech. Chem. Commun.* **2010**, *75*, 607.
[5] Ghorbani-Choghamarani, A.; Zolfigol, M.A.; Hajjami, M.; Jafai, S. *J. Chin. Chem. Soc.* **2008**, *55*, 1208.

Synthesis of sulfur-containing heterocyclic compounds from isothiocyanate derivatives as potential cytotoxic agents

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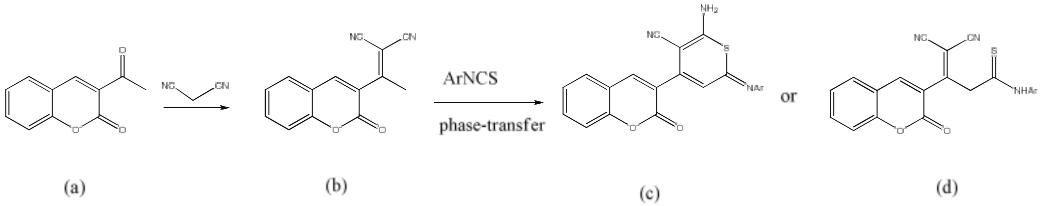
Coumarins have been found to exhibit a wide range of biological and controlled therapeutic activities in view of their extensive occurrence in nature and low toxicity [1].
The application of phase-transfer catalysis in carbanionic reactions provides one of the most important methods of organic synthesis because it simplifies procedures, eliminates expensive, inconvenient and dangerous reactions and solvents [2-4]. Compound (b) was allowed to react with isothiocyanate using soild-liquid phase-transfer catalysis techniques to give the compounds (c), (d) [5]. In this regard, we have synthesized a series of novel hetrocyclic compounds from isothiocyanate evaluate their cytotoxic effect .The synthetic pathway is outlined as shown in the scheme.



References:

[1] Imtyaz, A.; Khan, a Manohar, V.; Kulkarni, a, * M. Gopal, b M. S. Shaha3buddinb and Chung- Ming Sun. *Bioorganic & Medicinal Chemistry* Letters . **(2005)**, 15, *3584.*
[2] E. V. Dehmlow and S.S.Dehmlow, phase Transfer catalysis. 3 rded, VCH, Weinheim, **(1993)**.
[3] C. M.Starks, C. L. Liotta and M. Halpern, Phase Transfer Catalysis Fundamentals. Applications and Industrial perspectives, Chapman and Hall, New York, **(1994).**
[4] F. Montanari, S.Quici and S.Banfi, Comprehensive Supramolecular Chemistry, Pergamon, **(1996),** Vol.10; Reinhout, Ed., Ch.13.
[5] El-Sayed, A.M.; Abdel-Ghany, H.; *Heterocyclic chem*. **(2000)**, 37, *1233*.

Synthesis and application of itaconic acid containing copolymers as seed coating

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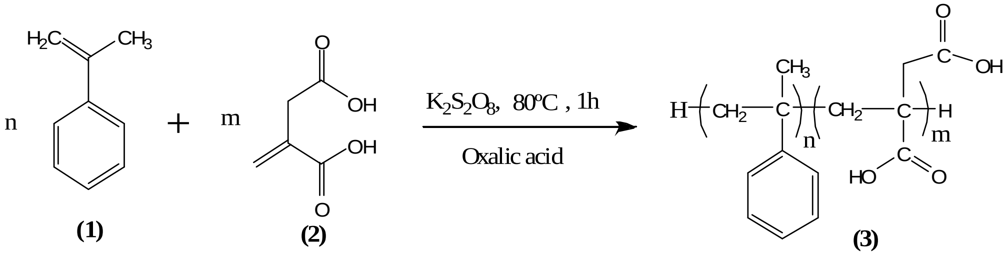
Seed treatment technology has application in control of growth regulators and fertilizers; and sizing and shaping of seeds to facilitate planting. These new uses often require improved application systems to better establish dosages and coverage of materials. Seed treatment technology also has application in control of insect vectors of plant pathogens, more efficient, and safer use of herbicides, application of growth regulators and fertilizers [1, 2].

In this study we try to report the chain copolymerization of itaconic acid as a main monomer and styrene, α-methylstyrene or methylmethacrylate as co-monomer in the presence of potassium persulfate, AIBN or fenton reagent as radical initiators. Also the effect of polymerization time and temperature was investigated. After that the application of co-polymer studied as seed coatings.

The results indicated that copolymerization of α- methylstyrene **(1)**, itaconic acid **(2)** and oxalic acid in the presence of $K_2S_2O_8$, at 80ºC and 1hr was the best procedure to produce sugar beet seed coating **(3)**.



(1) **(2)** **(3)**

References:

[1] Puoci, F. S; Lemma, F.; Spizzirri, U. G.; Cirillo, G.; Curcio, M.; Picci, N. *American Journal of Agricultural* and Biological Sciences, **2008**, 3(1), 299.

[2] Upadhyay, B. M.; Smith, E. G.; Clayton, G. W.; Harker, K. N.; O`Donovan, J. T.; Black shaw, R. E. *Agronomy Journal*. **2007**, 99, 489.

Molecular structures and nucleophilic mechanisms of acetylenic dicarboxylates: *ab initio* calculations

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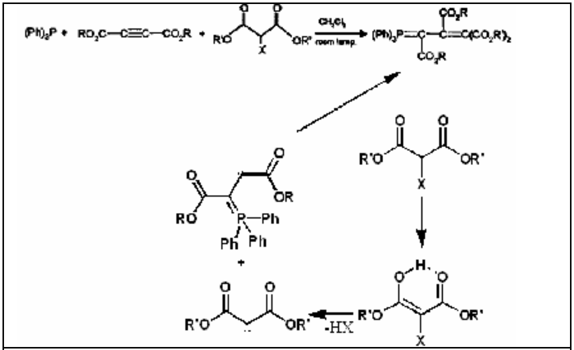
Despite of acetylenic dicarboxylates take part in nucleophilic addition. For example phosphorus ylides attacks acetylenic dicarboxylates (**1**) and in this way many interesting compounds were obtained [1]. In these work we propose a new mechanism for the reaction of acetylenic dicarboxylates with different compounds such as example shows in fig1. Base of this mechanism reaction proceeds from dicarbene intermediate. This intermediate is stabilized with PPh3. For investigation of this mechanism we calculated stability of different structure of acetylenic dicarboxylates : ROCOCCCOOR(R=Me, Et, *n*-Pr, *n*-Bu, *t*-Bu, Ph, *p*-CH_3-C_6H_4, *p*-NO_2-C_6H_4, *p*-OH-C_6H_4, *p*-NH_2-C_6H_4, *p*-OH-C_6H_4, *p*-CN-C_6H_4, *o*-CH_3-C_6H_4, *o*-NO_2-C_6H_4, *o*-OH-C_6H_4, *o*-NH_2-C_6H_4, *o*-OH-C_6H_4, *o*-CN-C_6H_4, *m*-CH_3-C_6H_4, *m*-NO_2-C_6H_4, *m*-OH-C_6H_4, *m*-NH_2-C_6H_4, *m*-OH-C_6H_4, *m*-CN-C_6H_4) with Hartree-Fock and B3LYP methods and 6-311++G** basis set. All computations carried out with Gaussian03 programm package [2].



Tetrahedron Letters 39 (1998) 1051–1054

References:

[1] *Journal of Organometallic Chemistry* **2005**, *690*, 2497.

[2] Frisch, M. J.; Trucks, G. W.; Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J. R.; J.A. Montgomery Jr. T. Vreven, K.N. Kudin, J.C.Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B.Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H.Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa,M.Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J.Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R.Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich,A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck,K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S.Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P.Piskorz, I. Komaromi, R. L. Martin, D.J. Fox, T. Keith, M.A. A1-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill,B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J.A. Pople,Gaussian, Inc. Wallingford CT, Gaussian 03, RevisionB.05, Gaussian, Inc. Pittsburgh, Pennsylvania, **2003**.

Effect of montmorillonite content on synthesis and swelling characterization of NOCC- poly(sodium acrylate) superabsorbent hydrogel composite

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Hydrogels are three-dimensional hydrophilic polymer networks capable of imbibing large amount of water [1]. For this reason they have been used widely in the field of drug delivery, immobilization of enzymes, dewatering of protein solutions, solute separation,baby diapers, soil for agriculture and horticulture, water-blocking tapes, absorbent pads, and numerous other applications [2].

Carboxymethyl chitosan (NOCC) is very important chitosan derivative showing very good water solubility and biocompatibility [3]. Recently, clay become the focus for the preparation of inorganic-organic superabsorbent composite to improve swelling properties, enhance hydrogel strength, and reduce production cost of corresponding superabsorbents [4].

Toxic heavy metals are released into environment from a number of industries such as mining, plating, dyeing, automobile manufacturing, metal processing [5]. The presence of these metals in the environment has become a serious threat for the human life as they enter into domestic water sources like rivers, lakes, ponds etc. These heavy metals are not biodegradable and their presence in water leads to bioaccumulation in living organism, causing health problems in animals, plants and human beings [6].

In the current research, a new superabsorbent hydrogel composites based on NOCC were prepared via graft polymerization of acrylic acid in the presence of nono-clay (MMT), crosslinker (MBA) and initiator (KPS). The effect of MMT content on the Swelling capacity of the hydrogel composite was studied. The chemical structure of the hydrogels was characterized by means of FT-IR spectroscopy. Morphology of samples was examined by scanning electron microscopy. Also, adsorption of toxic heavy metal cation (such as Cd^{2+}) was examined.

References:

[1] Pó R.; *Polymer Reviews*, **1994**, *34*, 607.
[2] Mahdavinia, G. R.; Mousavi , S. B.; Karimi, F.; Marandi, G. B.; Garabaghi, H.; Shahabvand, S.; *Express Polymer Letter*, **2009**, 3,5,279.
[3] Pang, H.T.; Cheng, X. G.; Park, H.J.; Cha, D.S.; & Kennedy, J. F.; *Carbohydrate Polymers*, **2007**, *69*, 419.
[4] Zang, J.; Wang, L,; Wang, A.; *Ind. Eng. Chem. Res*., **2007**, *46*, 2497.
[5] Rehman, H.; Shakirullah, M.; Ahmed I.; Shershah and hameedullah, *J. Chinese. Soc*, **2006**, *53*, 1045.
[6] Acemioglu, B.; Alma, M.H.; *J.Colloid Interf.Sci*, **2001**, *243*, 81.

Ultrasound-assisted synthesis of photochromic spirooxazine dyes

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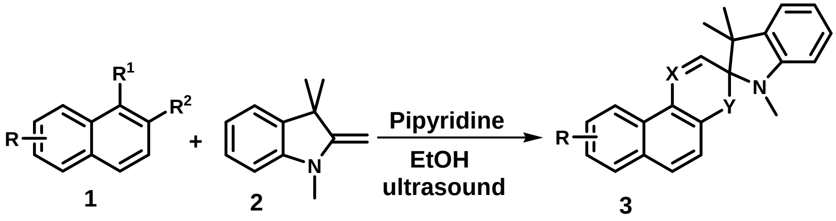
Among photochromic compounds, spirooxazine is one of the well-explored groups because of its excellent light fatigue resistance [1] and color change upon photo-irradiation. In fact, spirooxazine dye is much important for not only conventional dye-applications but also opto-electronics and bio-medicine [2]. Long reaction time and low yield in traditional methods made us explore a new approach for the synthesis of these intelligent materials.

Following our continued interests in the synthesis of heterocyclic compounds [3], we studied the synthesis of new derivatives of sprirooxazines (**3**) by the reaction of newly made nitrosonaphtols (**1**) and 1,3,3-trimethyl-2-methyleneindoline (**2**) using ultrasound irradiations (Scheme 1). The reaction gave the desired products in lower reaction time (2-15 min) and good yields. The reaction under classical condition furnished the products in much longer reaction time (5-47 h) and comparable yields. The structures of all products were identified by IR, ^{1}H NMR, ^{13}CNMR and Mass spectroscopy.



R^1 = OH, R^2 = NO; R^1 = NO, R^2 = OH.
R = 4-Cl, 6-Br, 7-OH, 1-(4-Nitrophenylazo).
X, Y = N, O.

Scheme 1

References:

[1] (a) Chu, N. Y. C. Proceedings of the 10th IUPAC symposium on photochemistry, Quantum yield for photo-degradation, Interlaken, Switzerland, **1998**. (b) Fu, Z.; Sun, B.; Chen, J.; Yuan, l. *Dyes Pigm*. **2008**, *76*, 515.

[2] (a) Zhang, P.; Meng, J. B.; Matsuura, T.; Wang, Y. M. *Chin. Chem. Lett*. **2002**, *13*, 299. (b) Berkovic, G.; Krongauz, V.; Weiss, V. *Chem. Rev*. **2000**, *133*, 1741.

[3] (a) Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301. (b) Mamaghani, M.; Dastmard, S. *Arkivoc* **2009,** *ii*, 168. (c) Samimi, H. A.; Mamaghani, M.; Tabatabaeian, T. *J. Heterocyclic Chem***.** **2008**, *45*, 1765. (d) Samimi, H. A.; Mamaghani, M.; Tabatabaeian, T. *Heterocycles* **2008**, *75 (11)*, 2825. (e) Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49 (9)*, 1450.

Preparation of a platinum complex and investigation of its catalytic activity in hydrosilylation reaction

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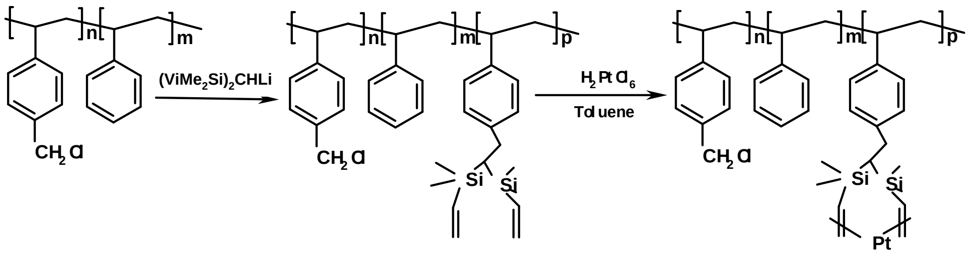
Hydrosilylation is the most important technique to form Si–C bonds and describes the addition of silicon hydrides to double or triple bonds [1]. Already Speier et al. [2] described these usually platinum catalyzed reactions to be highly exothermic and fast, making thermal management of the reaction crucial and thus, kinetic reaction analysis challenging. Hydrosilylation reactions may also be used for the synthesis of polymeric materials [3].

In this study, new catalytic systems based on bis(dimethylvinyl)methyl substituted polystyrene were prepared. Dendronized polystyrenes were obtained by modification of poly(styrene-co-chloromethylstyrene) precursors with $LiCH(SiMe_2CH=CH_2)_2$. Platinum was attached to the polymers via coordination to vinyl groups located on carbosilane moieties. Such the catalytic system makes an interesting alternative for heterogeneous platinum catalysts (Pt/charcoal, Pt/Cact and Pt/Al_2O_3) and also to Karstedt's catalyst, when used in hydrosilylation of vinylsilanes.



References:

[1] Fu, P.F.; Brard, L.; Li, Y.; Marks, T.J. *J. Am. Chem. Soc.* **1995**, 117, 7157.
[2] Speier, J.L.; Webster, J.A; Barnes, G.H. *J. Am. Chem. Soc.* **1957**, 79, 974.
[3] Brook, M.A. *Silicon in Organic, Organometallic, and Polymer Chemistry*. **2000**, John Wiley & Sons, New York

N,N′-Bis (benzoylacetone) ethylenediamine manganese(III) chloride: A reusable catalyst for an efficient, ecofriendly and clean synthesis of polyhydroquinolines and 4-H-Benzo[b]pyrans

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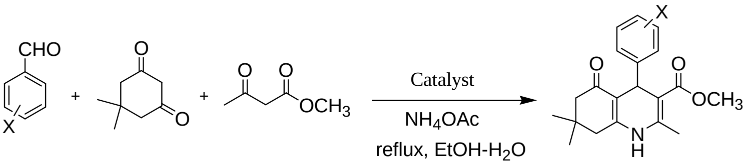
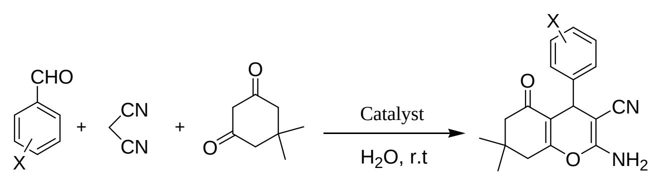
Heterocyclic compounds are of special interest because they show some biological and pharmacological activities [1]. Therefore, a number of methods have been reported for the synthesis of titled compounds. However, there are disadvantages to those methods such as low yield, prolonged reaction time and use of toxic organic solvents, harsh reaction conditions or tedious workup procedures.

Thus, a search for new reagents and the development of new methods are still of practical importance. We wish to report herein a simple and highly efficient procedure for preparation of polyhydroquinolines and 4-H-Benzo[b]pyran derivatives via multi-component condensation reaction using N,N′-bis (benzoylacetone) ethylenediamine manganese(III) chloride as a complex catalyst with high catalytic activity and reusability within short reaction times. All of compounds were obtained in high purity in excellent yields without any use of more purification and characterized by physical and spectroscopic data. This new methodology is of interest due to minimizing the cost operational hazards and environmental pollution, high yields, short reaction time, cost effective, simple work-up and reusability of catalyst.





References:

[1] Sayyafi, M.; Seyyedhamzeh, M.; Khavasi, H. R.; Bazgir, A. *Tetrahedron*. 2008, 64, 2375, and the references sited therein.

Study the anomeric effects (AE) on the stability of the cis- and trans-stereoisomers of 1,4,5,8-tetraoxadecalin, 1,4,5,8-tetrathiadecalin and 1,4,5,8-tetraselenadecalin

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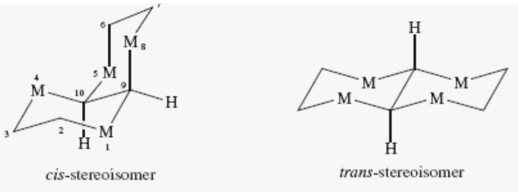
NBO analysis, hybrid-density functional theory (hybrid-DFT: B3LYP/6-311+G**//HF/6-311+G**) and ab initio molecular orbital (MO: MP2/6-311+G**//HF/6-311+G**) based methods were used to study the anomeric effects (AE) on the stability of the cis- and trans-stereoisomers of 1,4,5,8-tetraoxadecalin [1], 1,4,5,8-tetrathiadecalin [2] and 1,4,5,8-tetraselenadecalin [3]. The B3LYP/6-311+G**//HF/6-311+G** results revealed that the cis-stereoisomers of compounds 1–3 are more stable than their trans-stereoisomers by about 4.26, 1.03 and 0.70 kcal mol^{-1}, respectively. Also, the cis-stereoisomers of compounds 1–3 are more stable than their trans-stereoisomers by about 4.18, 2.11 and 01.18 kcal mol-1, respectively, as calculated at the MP2/6-311+G**//HF/6-311+G** level of theory. In addition, HF/6-311+G**//HF/6- 311+G** results revealed that the Gibbs free energy difference (Gcis _ Gtrans) values (e.g. GFEDcis–trans) between the cis- and trans-stereoisomers decrease from compound 1 to compound 3. On the other hand, the NBO analysis of donor–acceptor (bond-antibond) interactions revealed that the anomeric effects (AE) for compounds 1–3 are -22.08, -17.84 and -13.22 kcal mol^{-1}, respectively. The decrease of the AE could fairly explain the decrease of the GFEDcis–trans from compound 1 to compound 3. On the other hand, the decrease of the donor–acceptor interactions associated with LPaxM1→ σ*C9–O8 electronic delocalizations could fairly explain the increase of occupancies of LPaxM1 non-bonding orbitals and the decrease of occupancies of σ*C9–O8 anti-bonding orbitals from the cis-stereoisomers of compound 1 to compound 3.



cis-stereoisomer *trans*-stereoisomer

[Numbering used for compounds **1-3** (**1**: M=O; **2**: M=S; **3**: M=Se)]

References:

[1] F.H. Westheimer, in: M.S. Neman (Ed.), Steric Effects in Organic Chemistry, John Wiley & Sons, Inc., New York, **1956**.
[2] J.B. Hendrickson, *J. Am. Chem. Soc*. **1967,** *89*, 7036.
[3] F. Freeman, A. Phornvoranunt, W.J. Hehre, *J. Phys. Org. Chem.* **1998,** *11*, 831.

Synthesize of chelating nano polymer based on poly(styrene-alt-maleic anhydride) for removal of heavy metal ions from waste waters

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Environmental contamination with heavy metals gained lately more concern because of their high persistence, and the nervous system damage, and even cancer, caused by their accumulation at certain levels. A difficult problem encountered in the removal of the metal ions is that the target species are usually in low concentration and in complex mixtures .Numerous variables must be Considered in practice, such as : salinity, pH, temperature and the presence of organic substances [1].

Among various methods of heavy metal removal the last is generally preferred because of its high efficiency, ease of handling, and availability of different sorbents. Therefore, the most promising technique for removal of metal cations is their adsorption on organic sorbents containing chelating functional groups [2,3]. The development of high performance adsorbents (chelating polymers) in nano scale for removing heavy metal ions from wastewater is considered a research priority in the environmental field [4]. Traditionally, an advantage of nano polymeric materials is that they can be synthesized and processed on a large scale at relatively low cost.

A nano chelating resins, based on poly(styrene-alt-maleic anhydride) (PSMA), were synthesized by graft reaction of amino benzoic acid and diamino propane on PSMA backbone under ultrasonic irradiation and magnetic stirring bar. In the graft reaction various molar ration of amino benzoic acid to diamino propane was used. Also the different ratios of amine to PSMA were investigated. The prepared copolymers were examined for removal of Cu(II), Co(II), Cd(II) and ect. from aqueous solutions. The XRD analysis was done for obtained copolymers network and particle size of copolymers was calculated by sherer equation. The particle size of obtained copolymers was in nano scale in the range of 30–90 nm. The characteristic of copolymers was carried out by Fourier transform infrared spectroscopy (FT-IR) and differential scanning calorimetric (DSC) and Scanning electron micrographs (SEM).

References:

[1] R.L,Alberti.; M,Casciola.; U,Constantino. *Encyclopedia of Analytical Chemistry*. *Academic Press*, **1995**, *4*,2298
[2] B.L,Rivas.; B,Quilodran.; E,Quiroz. *J. Appl. Polym. Sci*. **2004**, *92*, 2908.
[3] A,Baraka.; P.J,Hall, M.J.Heslop. *React. Funct. Polym*.**2007**, *67*, 585.
[4] T,Kaliyappan.; P,Kannan . *ProgPolym Sci*.**2000**, *25*, 343.

Study of reaction between triphenylphosphine and dimethyl acetylene dicarboxylate in the presence of 3-choloroacetylacetone

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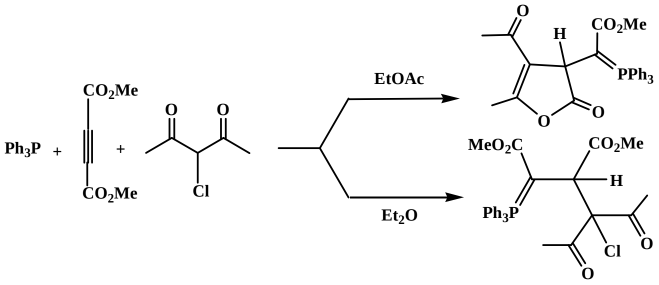
Phosphorus ylides are reactive intermediates, which take part in many valuable reactions in organic synthesis [1-5]. Several methods have been developed for the preparation of phosphorus ylides. These ylides are usually prepared by treatment of a phosphonium salt with a base, and phosphonium salts are usually prepared from the phosphine and an alkyl halide [1-5]. Phosphonium salts are also prepared by Michael addition of phosphorus nucleophiles to activated olefine and in other ways [1-5].

In the current work, Stable phosphorus ylides were obtained in good to excellent yields from the 1:1:1 addition reaction between triphenylphosphine, dimethyl acetylenedicarboxylate in the presence of CH-acids such as 3-choloroacetylacetone. Furthermore, useful information was obtained from studies of the solvent effect, on the product of reaction.

The ylide moiety of these compounds is strongly conjugated with the adjacent carbonyl group, and the rotation around the partial double bond in (E) and (Z) geometrical isomers is slow on the NMR time scale at an ambient temperature. In the present work, the two Z- and E- geometrical isomers were observed in the presence of different solvent.



References:

[1] Khorassani, S. M. H.; Maghsoodlou, M.T.; Ebrahimi, A.; Kazemian, M. A.; Zakarianejad, M *Phosphorus, Sulfur, and Silicon*. **2009**, *184, 11, 2959*.

[2] Maghsoodlou, M. T.; Hazeri, N.; Khorasani, S. M. H.; Moghaddam, H. M.; Nassiri, M.; Salehzadeh, J. *Phosphorus, Sulfur and Silicon* . **2009**, *184, 7, 1713*.

[3] Maghsoodlou, M. T.; Hazeri, N.; Afshari,G.; Niroumand, U. J. *Sulfur Chem*. **2006**, *181, 12, 2681*.

[4] Tian, H. Y.; Chen, Y. J.; Wang, D.; Bu,Y. P.; li, C.J. *Tetrahedron lett.* **2001**, *42, 1803*.

[5] Sikshin, S. A.; Hultin, P. G. *J. Org.C hem*. **2006**, *71, 5888*.

A green and efficient method for the synthesis of highly functionalized 4*H*-pyrano[3,2-*d*]isoxazoles via isocyanide-based reaction in ionic liquid media

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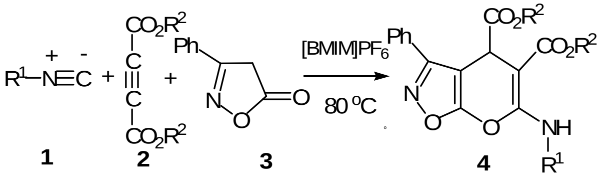
The design and development of convergent strategies to synthesize diverse arrays of drugs is an important objective in contemporary chemical biology and medical chemistry. Over the last years great interest has received to the chemistry of pyrano isoxazoles as important classes of biologically effective compounds. They are valuable to chemists because of their therapeutic applications [1]. One of the earliest approaches to synthesize of these compounds was done by Marcus and co-workers in 1967 [2]. Continuing the work of Marcus, Chantegrel and colleagues described the synthesis of the pyranoisoxazoles. Recent methods for the synthesis of pyrano isoxazoles include 1,3-dipolar cycloaddition of acetonitrile oxide to an α,β-unsaturated enone, intramolecular 1,3-dipolar nitro or nitrile oxide cycloaddition [3].

Ionic liquids, as environmentally benign solvents, offer an attractive alternative to conventional organic solvents because they are non-flammable, non-explosive and can be recycled. [4].

In continuation of our interest [5] in the development of methods for synthesis of heterocyclic compounds of biological importance, herein we describe a green method for the synthesis of highly substituted pyrano[3,2-d]isoxazoles **4** by the reaction of an isocyanide **1** with a dialkylacetylenedicarboxylate (DAAD) **2** and 3-phenylisoxazol-4-(5*H*)-one **3** via three-component reactions in ionic liquid media. The structures of the products were confirmed by their IR, mass, ^{1}H NMR and ^{13}C NMR spectra.



References:

[1] Parmer, V. S.; Sharma, N. K.; Husain, M.; Watterson, A. C.; et. al. *Bioorg. Med. Chem.* **2003**, *11*, 913.

[2] Marcus, E.; Chan, J. K.; Hughes, J. L. *J. Chem. Eng. Data* **1967**, *12*, 151.

[3] (a) Chantegrel, B.; Nadi, A. I.; Gelin, S. *J. Heterocyclic Chem.* **1985**, *22*, 1127. (b) Yamada, K.; Yamada, F.; Somei, M. *Heterocycles* **2003**, *2*, 685.

[4] Zhang, X. Y.; Li, Y. Z.; Fan, X. S.; Qu, G. R.; Hu, X. Y.; Wang, J. J. *Chinese Chem. Lett.* **2006**, *17*, 150.

[5] (a) Esmaeili, A. A.; Amini, S.; Bodaghi, A. *Synlett,* **2007**, 1452. (b) Esmaili, A. A.; Vesalipoor, H. *Synthesis,* **2009**, 1635.

New fluorinated poly(ether-imide)s based-on twisted binaphthyl rings: organosolubility, thin film optical behavior, and thermal properties

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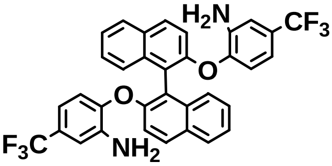
Aromatic polyimides are an important class of high performance materials due to their excellent thermo-oxidative stability, high radiation, solvent resistance, outstanding mechanical and electrical properties, therefore, all kinds of polyimides have been widely used in the fields of adhesives, composite matrices, fibers, films, foams, as well as microelectronic materials [1]. However, because of their chain rigidity and strong interchain interaction, most of the aromatic polyimides are insoluble in organic solvents and exhibit high softening temperatures, In addition, most polyimides have strong absorption in the visible region due to the existence of charge transfer complexes, so most polyimides show coloration from pale yellow to deep brown. Poor processability and deep coloration limit the applications of polyimides, especially in the fields that require good optical transparency.

In order to overcome these problems, several approaches such as introduction of flexibilizing groups , bulky groups, cardo groups, molecular asymmetry, pendent flexible groups, etc [2,3].

The objective of the present work is synthesis and characterization of a series of novel polyimides based on a new monomer namely 2,2′- bis (4-trifluoromethyl-2-aminophenoxy)-1,1′-binaphtyl **(I)**, by chemical polyimidization two-step method. Some properties of the polymers obtained including organosolubility, thermal stability, crystallinity, film quality, and solusion viscosity are also investigated.



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References:

[1] Hu, A. J.; He, T.; Yang S. Y. *Macromolecules.* **1999**, *32*, 8046.
[2] Shen, Z.; Guo, M.; Cheng, S. D.; Harris, F. W. *Macromolecules.* **2007**, *40*, 889.
[3] Hesegawa, M.; Horie, K. *Prog. Polym. Sci.* **2001**, *26*, 259.

Chemical composition of essential oil of *Teucrium polium* in Mazandaran

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The genus of *Teucrium* belongs to the *Labiatae* family. This genus includes 12 species in Iran [1]. Among the Species, *Teucrium polium* has been used in folk medicine to treat some diseases because it has useful effects such as anti-inflammatory, anti-bacterial, anti-nociceptive [2], anti-diabetic [3] and anti-oxidant [4].

Because of useful effects of this plant we decided to investigate chemical composition of essential oil of *Teucrium polium* in the heights of Mazandaran province and to find their difference.

Thus we collected the flowering aerial parts of this plant in 9 habitats in Mazandaran province and dried them. Then we subjected the dried flowering aerial parts to hydrodistillation using a clevenjer-type apparatus and obtained their oils. The oils were analyzed by GC and GC-MS methods and their components were identified in every height. The main components of *Teucrium polium and their percentag* were different in every habitat. Among the major compounds of oil of this plant we can indicate some of them. For example: Sabinene, Germacrene D, α-Pinene, β-Pinene.

References:

[1] Mozaffarian V. A Dictionary of Iranian Plant Names. Farhang Moaser: Tehran, Iran, **2007**; 542.

[2] Abdollahi. M, Karimpour, H,Monsef Esfehani, HR. Antinociceptive effects of *Teucrium polium* L. total extract and essential oil in mouse writhing test. Pharmacol. Res **2003**; 48, 31.

[3] Gharaibeh MN, Elayan HH, Salha AS. Hypoglycemic effects of *Teucrium polium,* J. Ethnopharmacol **1988**, 24, 93.

[4] Couladis M, Tzakou O, Verykokidou E, Harvala C. Screening of some Greek aromatic plants for antioxidant activity. *Phytother. Res.* **2003**, *17*, 194.

Novel approach for the stereoselective synthesis of Hesperadin analogoues

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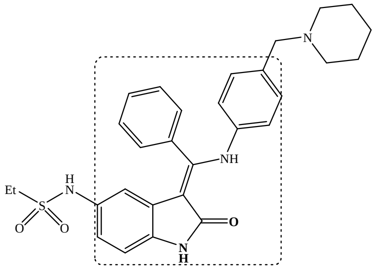
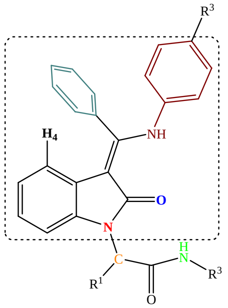
3-(aminomethylene)-2-oxindoles have recently captured attention due to a unique ability to inhibit protein kinase activities [1]. Hesperadin, a recently notified inhibitor, is one notable 3-(anilinoarylmethylene)-2-oxindoles [2]. This small molecule appears to inhibit Aurora B kinase. Aurora kinases are a family of mitotic serine/thereonine kinases. Hesperadin and other Aurora kinase inhibitors have received much attention especially in targeted cancer therapies [3].

In continuation of our research program [4], and in view of interesting biological activities, we introduced a highly efficient palladium catalyzed approach for the stereoselective synthesis of Hesperadin analogoues using the Ugi product.

In all cases, the sole product of this reaction is the *Z* isomer. The distinguished peak for all products is related to the NH peak which were observed at δ 11.86-12.13 ppm . This unusual chemical shift is related to internal hydrogen bonding between the amino group and the carbonyl group. In this Poster, we will present our results about this novel strategy and proposed mechanism.



Hesperadin



Synthesized Hesperadin Analogoues

References:

[1] Marti, C.; Carreira, E. M. *Eur. J. Org. Chem.* **2003**, 2209.
[2] S. Hauf, R. W. Cole, S. LaTerra, C. Zimmer, G. Schnapp, R. Walter, A. Heckel, J. van Meel, C. L. Rieder, J. M. Peters, *J. Cell. Biol.* **2003**, *161*, 281.
[3] Carvajal, R. O.; Tse, A.; Schwartz, G. K. *Clin. Cancer Res.* **2006**, *12*(23), 6869.
[4] M. Bararjanian, S. Balalaie, F. Rominger, B. Movassagh, H. R. Bijanzadeh, *J. Org. Chem*, **2010**, *75*, 2806.

Electrodeposition of zinc-nickel alloy coatings from an alkaline pyrophosphate bath

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Zinc alloy coatings containing one of the iron groups of metals (Ni, Co, Fe) have shown excellent corrosion resistance and paintability and therefore have already found numerous applications in various industrial sectors including the automotive industry [1]. Zn-Ni alloy coatings have attracted much attention because they possess higher corrosion resistance and other mechanical characteristics in comparison with zinc and other zinc alloy coatings [2-4]. It has been stated in several studies that corrosion resistance of electrodeposited Zn–Ni alloy coatings within a certain composition range (9–15 wt.%) can be significantly higher (5 to 6 times) than that for pure zinc. Acidic or alkaline plating baths can be used for Zn–Ni alloy deposition. However, an acidic bath usually produces a dual phase structure, which implies an unsatisfactory corrosion resistance of the coating. Meanwhile, the deposition in alkaline solutions, in contrast to the acidic ones, is less efficient but it produces more uniform plating and a single-phase alloy [5].

In the present work, Zn-Ni alloy coatings were electrodeposited from an alkaline pyrophosphate bath on low carbon steel substrate with direct current (DC). Pyrophosphate ion was used as a complexing agent. The effect of current density, Zn^{2+}/Ni^{2+} molar ratio and pyrophosphate ion concentration in bath on chemical composition, phase structure, surface morphology and corrosion resistance of coatings were investigated. The results showed that alloy with nickel content of 14%, single γ-phase structure (an intermediate phase with a composition Ni_5Zn_{21}) and higher corrosion resistance were obtained in current density of 15 A/dm^2, Zn^{2+}/Ni^{2+} of 6 and pyrophosphate ion concentration of 0.3 M.

References:

[1] C. N. Panagopoulos, K.G. Georgarakis, P.E. Agathocleous, Tribology International *36*, **2003**, 619.

[2] M. G. Hosseini, H. Ashassi-Sorkhabi, H.A.Y. Ghiasvand, Surface & Coatings Technology *202*, **2008**, 2897.

[3] H. Ashassi-Sorkhabi, A. Hagrah, N. Parvini-Ahmadi, J. Manzoori, Surface and Coatings Technology *140*, **2001**, 278.

[4] T. V. Byk , T. V. Gaevskaya, L. S. Tsybulskaya, Surface & Coatings Technology 202, **2008**, 5817.

[5] O. Girciene, L. Gudaviciute, R. Juskenas, R. Ramanauskas, *Surface & Coatings Technology 203*, **2009**, 3072.

Preparation of polyaniline/graphite nanosheet composite based on acrylic resin

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Conducting polymers exhibit a wide range of novel electrochemical and chemical properties that has led to their use in a diverse array of applications. Among the conductive polymers, polyaniline (PANi) is one of the most promising candidates for industrial application due to its good conductivity, special doping mechanism, and excellent chemical stability [1-3]. In order to develop a conducting network within polymer matrix with as small an amount of filler as possible one could consider using nanoscale fillers as conducting charges. When nanoscale conducting fillers is dispersed in polymer matrix, the particular morphology and structure developed provides the advantage information the conducting network. In this paper first expand graphite were prepared in the presence sulfuric acid and nitric acid by heated shock at high temprature for short time. The expand graphite was immersed in a aqueous alcohol solution and subjected in an ultrasonic bath to produced graphite nanosheet. The emulsion polymerization of butylacrylate with aniline in the presence graphite nanosheet were done by amonium persulfate in the presence of both anionic and cationic emulsifiers. Electrically conductive product composite was measured by four probe method. Study structure and surface morphology of nano graphite were investigated by scanning electron microscopy (SEM). The measurement of film was investigated by salt spray test. The corrosion resistant property of the coatings on steel was determined by electrochemical method. It was shown that coatings had provided good corrosion protection of steel in corrosive solution. Adhesion measurements on steel by cross-cut test demonstrate that of the blended coatings has significantly higher strength of adhesion compared to that observed for pure polyaniline. The excellent films can uses in several industry applications.

References:

[1] Plesu, N.; liescu, S.; Ilia, G.; Popa, A.; Muntean, C.; *Turk J Chem*, **2006**, 30, 155.
[2] Hosseini, S. H.; Dabiri, M., Ashrafi, M., *Polymer International*, **2006**, 55, 9, 1081.
[3] Hosseini, S. H.; Mohammadi, M., *Materials Science & Engineering C,* **2009**, 29, 1503.

A novel one pot synthesis of 1,4-aryl-14H-dibenzo[a,j]xanthenes catalysed by Melamine-formaldehyde resin under solvent-free condition.

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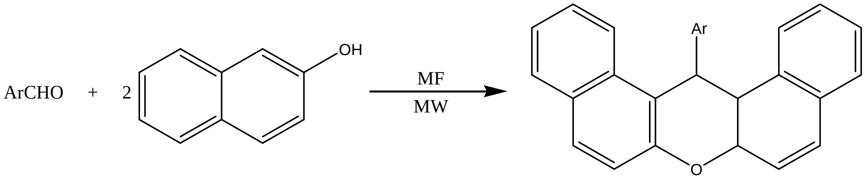
Research on xanthenes, especially benzoxanthenes, has emerged in organic synthesis due to their wide range of biological and therapeutic properties [1]. Xanthenes are also available from natural sources [2]. 14H-dibenzo[a,j]xanthenes and related products are prepared by reaction of

β-naphthol with formamide [3], 1-hydroxy-methyl-naphthalen-2-ol [4] and carbon monoxide [5].

While many procedures have been reported, disadvantages like low yield, prolonged reaction time, use of excess of reagents/catalysts and use of toxic organic solvents [6] prompted us to develop an alternate route for the synthesis of xanthene derivatives in improved yield, short reaction time and safe reaction conditions using Melamine-formaldehyde resin as catalyst.

At present study several aryl-14H-dibenzo[a,j]xanthenes were prepared by reaction of β-naphthol with aryl aldehydes in the presence of Melamine-formaldehyde resin as readily available catalyst and in the absence of catalyst.



MF: Melamine-formaldehyde resin
MW: Microwave

References:

[1] Ion, R.M.; Frackowiak, D.; Planner, A.; Wiktorowicz, K.; *Act Biochim, pol*. **1998**, *45*, 833.
[2] Kinjo, J.; Uemura, H.; Nohara, T.; Yamashita, M.; Marubayashi, N.; Yoshihira., K.;
[3] *Tetrahedron Lett*., **1995**, *36*, 5599.
[4] Papini, P.; Cimmarusti, R.; *Gazz.chim.Ital*. **1947**, *77*, 142.
[5] Sen, R. N.; Sarkar, N. N.; *J.Am.Chem.Soc*. **1925**, *47*, 1079.
[6] Ota, K.; Kito ,T.; *Bull.Chem.Soc.Jpn*. **1976**, *49*, 1176.
[7] Li, C.; *J.Chem.Res*, **2008**, 484.

New organotin(IV) complex of a new carbacylamidophosphate : Syntheses, spectroscopic study and crystal structure

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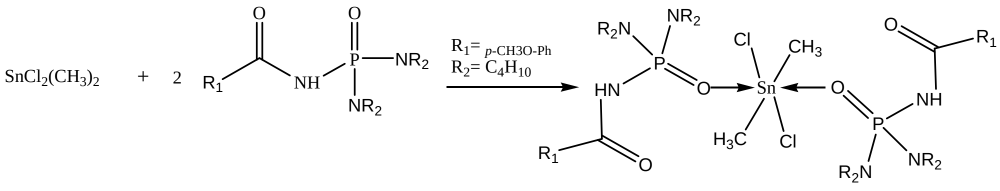
Organotin compounds are of great interest and they have been subject of diverse studies owing to their anticancer activity [1] as well as their applications as biocides [2]. Furthermore, the phosphorus compounds have wide agricultural applications because of their potent biocidal effect [3] and the presence of both organotin(IV) moieties and phosphorus moieties in a single molecular could produce a still more powerful and lasting effective complex.

In this work the new carbacylamidophosphate ligand with formula *p*-OCH_3-$C_6H_5C(O)NHP(O)(NC_4H_{10})_2$ (**1**) and its organotin(IV) complex with formula $SnCl_2(CH_3)_2(X)_2$, X = **1**, (**2**) were synthesized and characterized by ^{1}H, ^{13}C, ^{31}P NMR, IR spectroscopy and elemental analysis and were spectroscopically studied in comparison to each other. Structural properties of (**2**) was determined using single-crystal X-ray diffraction. The six coordinate organotin compound **2** with equal ligands in *trans* position was obtained according to the bottom Scheme 1. The crystallographic results showed that –Sn–Cl…H–N– major hydrogen bonds beside other electrostatic interactions produced a two dimensional polymeric chain in this complex' crystalline lattice.



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2

Scheme 1.

References:

[1] Gielen, M. *Appl. Organomet. Chem*. **2002**, *16*, 481.

[2] Sharma, V.; Sharma, R.K.; Bohra, R.;, Ratnani, R.; Jain, V.K.; Drake, J.E.; Hurshouse, M.B.; Light, M.E. *J. Organomet. Chem.* **2002**, *651*, 98.

[3] Singh, N.; Megharaj, M.; Gates, W. P.; Churchman, G. J.; Anderson, J.; Kookana, R. S.; Naidu, R.; Chen, Z.; Slade, P. G.; Sethunathan, N. *J. Agric. Food Chem.* **2003**, *51*, 2653. **2006**, *71*, 5888.

Synthesis and characterization of poly(4-vinylpyridinium hydrochloride)-CrO_3/SBA-15 as a selective heterogeneous oxidant for oxidation of alcohols

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The selective oxidation of alcohols to the corresponding aldehydes or ketones is a fundamental transformation in both laboratory synthesis and industrial production. Although many useful procedures for oxidation of different organic compounds (such as oxidantion with CrO_3, $KMnO_4$, MnO_2, etc.) have been reported [1], the main disadvantage of these reagents is the difficult working-up of the reaction mixture.

Hybrid organic–inorganic polymers had attracted considerable interest because of their unique properties. Thus, the syntheses of hybrid organic–inorganic polymers with new framework structures are highly desirable [2]. Functional polymers are specified as very efficient catalyst supports, since they provide the stabilizing steric bulk of their framework and several binding sites for simultaneous interactions with the particles and the substrates. Poly (4-vinylpyridine) (P4VP) is particularly attractive because of the strong affinity of the pyridyl group for metallic nanoparticles and because of its ability for interacting with polar species through hydrogen bonding. Moreover, P4VP could be quaternized and act as a catalyst with high catalytic activity in organic reactions [3].

In continuation of our study to develop new organic-inorganic hybrids, we found that the poly(4-vinylpyridinium hydrochloride)/SBA-15 is an excellent candidate for supported chromate in order to prepare a heterogeneous oxidant (P4VPHC-CrO_3/SBA-15). Our studies showed that the P4VPHC-CrO_3/SBA-15 serve as highly active heterogeneous oxidant catalyst for the selective oxidation of benzyl alcohol and its substituted homologues to their corresponding aldehydes. The existence of both organic and inorganic phase in this composite shows the critical effect on the catalytic activity. The merits of this methodology are its simplicity, fast, mild condition, and efficient selective oxidation of alcohols as well as catalyst reusability. Therefore it is believe that the synthetic method reported here would greatly contribute to the environmentally safer process.

References:

[1] Hudlicky, M. *Oxidations in organic chemistry,* American chemical society science, Washangton, DC, **1990**.
[2] Ostapenko, N.; Dovbeshko, G.; Kozlova, N.; Suto, S.; Watanabe, A. *Thin Solid Films* **2008**, *516*, 8944.
[3] Tamami, B.; Parvanak Borujeni, K. *Iran. Polym. J.* **2009**, *18*, 191.

Synthesis and characterization of $AlCl_3$ supported on heterogeneous catalyst based on aminated triazine rings on silica-gel for protection of alcohols and phenols

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A large number of heterogeneous polymer supported Lewis acids have been prepared by immobilization of the catalysts on polymers via coordination or covalent bonds [1]. Such catalysts are as active as their homogeneous counterparts while having the distinguishing characteristics of being easily separable from the reaction media, recyclability, greater selectivity, enhanced stability, non-toxicity, non-corrosiveness, and low cost [2]. Tetrahydropyranylation is one of the most frequently used processes to protect hydroxyl groups due to the remarkable stability of tetrahydropyranyl ethers under a variety of conditions such as, Grignard reagents, oxidative reagents and acylating reagents. Although different methods have been developed for protection of alcohols, many of these are associated with several drawbacks, which include long reaction times harsh and acidic conditions, poor selectivity, and formation polymeric by-products. In addition, some of these catalysts are not recyclable. Thus, there is still a need for mild and selective methods, especially using heterogeneous catalysts for this purpose [3, 4].

The goal of this work is to introduce $AlCl_3$ supported on new solid catalyst. Cyanuric chloride was chemically bound with surface hydroxyl groups of silica-gel followed by reaction with ethyelendiamine. $AlCl_3$ supported on aminated triazine (AT-$AlCl_3$) was prepared by addition of anhydrous aluminum chloride to aminated triazine (AT) in carbon tetrachloride under reflux condition. FT-IR and XRD were used to characterize AT-$AlCl_3$. Using this polymeric catalyst, different kinds of alcohols (primary, secondary, tertiary, benzylic and allylic) and phenols underwent tetrahydropyranylation in good to excellent yields. The mild reaction conditions, short reaction times, high to excellent yields, low cost and easy preparation and handling (as a bench top catalyst) of the polymeric catalyst as well as catalyst reusability are the obvious advantages of the present method.

References:

[1] Smith, K. Solid Supports and Catalysts in Organic Synthesis; Ellis Horwood: hichester, **1992**.
[2] Parvanak Borujeni, K.; Tamami, B. *Catal Commun*. **2007**, *66*, 1191..
[3] Hu,X.; Khuan Chuah,G.; Jaenicke,S. *Appl Catal A: Gen* **2001**, *217,* 1.
[4] Parvanak Borujeni, K.; Tamami, B. *Tetrahedron Lett*. **2004,** *45*, 715.

Synthesis of dimethyl 4, 5-diaryl 1H-pyrrole-2, 3-dicarboxlate derivatives

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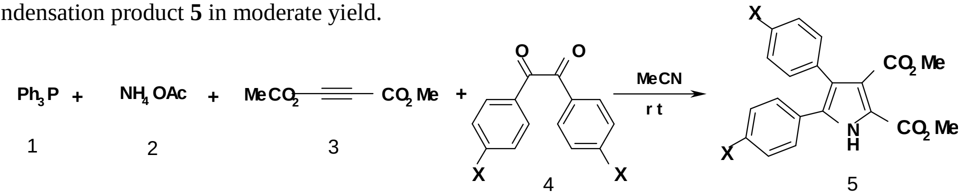
Pyrroles are important structural constituents of many bioactive natural products [1] therapeutic compounds [2] and new organic materials [3] and can serve as intermediates in organic synthesis [4]. Consequently, the efficient assembly of this class of molecule is a significant objective in synthetic chemistry.

In spite of a large number of methods reported for the synthesis of pyrroles, there is always considerable demand in exploring more milder, convenient, practical and benign reagents for their synthesis [5-6].

Herein, we report an efficient, inexpensive, convenient and mild synthetic route to highly substituted pyrroles in moderate yields without the use of catalyst. We carried out the reaction of triphenylphosphine **(1)**, ammonium acetate **(2)**, dimethyl acetylenedicarboxylate (DMAD) **(3)**, and substituted 1, 2-diaryl-1, 2 ethanedione **(4)** in dry acetonitrile at room temperature which gave the condensation product **5** in moderate yield.



X: H, Cl, Br, F, CH3, OCH3

The structure of compounds is supported with spectral data (^{1}HNMR, ^{13}CNMR, IR) and elemental analysis.

References:

[1] (a) Lindquist, N.; Fenical, W.; Van Duyne, G. D.; Clardy, J. *J. Org. Chem.* **1988**, *53*, 4570. (b) Boger, D. L.; Boyce, C. W.; Labroli, M. A.; Sehon, C. A.; Jin, Q. *J. Am. Chem. Soc.* **1999**, *121*, 54.

[2] (a) Colotta, V.; Cecchi, L.; Melani, F.; Filacchioni, G.; Martini, C.; Giannaccini, G.; Lucacchini, A. *J. Med. Chem.* **1990**, *33*, 2646-2651. (b) Cozzi, P.; Mongelli, N. *Curr. Pharm. Des.* **1998**, *4*, 181.

[3] Curran, D.; Grimshaw, J.; Perera, S. D. *Chem. Soc. Rev.* **1991**, *20*, 391.

[4] Boger, D.L.; Boyce, C.W.; Labrilli, M.A.; Sehon, C.A.; Jin, Q.; *J. Am. Chem. Soc*. **1999**, *121*, 54.

[5] Bharadwaj, A.R.; Scheidt, K.A.; *Org. Lett*. **2004**, *6*, 2465.

[6] Tejedor, D.; Gonzalez-Cruz, D.; Garcia-Tellado, F.; *J. Am. Chem. Soc*. **2004**, *126*, 8390.

Synthesis of 1,3-thiazines *via* multicomponent reaction of isothiocyanate, activated acetylene and isoquinoline in the presence of ZnO nanoparticles

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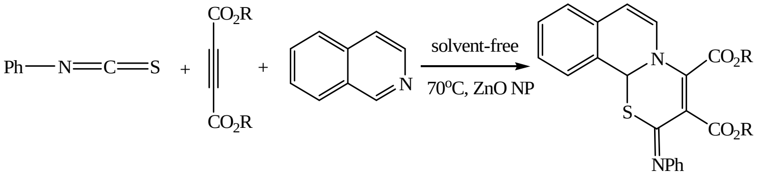
1,3-Thiazines and their derivatives possess remarkable biological activities such as antibacterial, antitumour, insecticidal and fungicidal [1-3]. These are also known as anti-radiation agents and used as radiation-sickness drugs [4]. Furthermore, the antibiotic activity of cephalosporins is due to the presence of 1,3-thiazine nucleus [5]. As regards chemical viewpoint, 1,3-thiazines are important synthetic intermediates in organic syntheses [6]. As part of our continuing interest in the development of new synthetic methods in heterocyclic chemistry and our interest in isoquinoline-based multi-component reactions, we describe an efficient synthesis of thiazine derivatives **4** *via* the reaction of isothiocyanate with activated acetylenes and isoquinoline under solvent-free conditions in the presence of ZnO nanoparticles at 70˚C.



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References:

[1] (a) Patel, H. S.; Patel, N. P. *Orient J Chem*, 1997, *13*, 69. (b) Madkour, H. M. F.; Salem, M. A. I.; Soliman, E. A.; Mahmoud, N. F. H. *Phosphorus Sulfur Silicon Relat Elem* **2001**, *170*, 15.
[2] Ingarsal, N.; Amutha, P.; Nagarajan, S. *J Sulfur Chem* **2006**, *27*, 455.
[3] (a) Bozsing, D.; Sohar, P.; Gigler, G.; Kovacs, G. *Eur J Med Chem,* **1996**, *31*, 663 (b) Tozkoparan, B.; Aktay, G.; Yeilada, E. *Il Farmaco* **2002**, *57*, 145.
[4] Campaigne, E.; Nargund, P. K. *J Org Chem* **1964**, *29*, 224.
[5] Barret, G. C.; Kane, V. V.; Lowe, G. *J Chem Soc* **1964**, 783.
[6] Schmidt, R. R. *Synthesis* **1972**, 333.

Synthesis and characterization of novel spiro heterocyclic systems (Uracil derivatives) from barbituric acids

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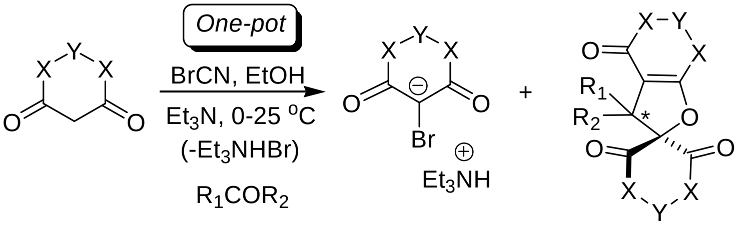
A large number of barbituric acid derivatives (Barbiturates) are widely used as medical agents for the treatment of neurological diseases, depressions, and memory impairment, as well as antitumor agents. 2-Thiobarbituric acid derivatives also are widely used as antibacterial agents, and they inhibit reverse transcriptase and show strong inhibitory activity agents, HIV-1 in vitro, antiphlogistic, antitumor, and hypocholesteremic agents [1].

They are also been used as dyes [2], PH-responding polymer[3] and preparation metal complexes[4]. Several spiro-barbituric acid derivatives in which the C-5 of barbituric acid is substituted by an unsubstituted cyclobutane or cyclohexane. Spiro compounds have been reported to possess biological activities that include narcotic hypotensive, skeletal muscle relaxant, analgesic anticonvulsant, CNS depressant anti-inflammatory activity [5]. Recently, we have reported the crystal structure of 1,1',3,3',5,5'-hexamethyl-1*H*,1'*H*-spiro[furo[2,3-d]pyrimidine-6,5'-pyrimidine]2,2',4,4',6'(3*H*,3'*H*,5*H*)-pentaone [6].

In the present work ,we report synthesis of heterocyclic stable spiro [furo[2,3-*d*]pyrimidine-6,5-pyrimidine]2,2',4,4',6'(3*H*,3'*H*,5H)-pentaones and triethylammonium-5-bromobabiturate salt from the condensation reaction and cyclization of barbituric acid with ethyl methyl ketone in the presence of cyanogen bromide and triethylamine in methanol.



X-Y-X = NH-CO-NH (**a**); CH_3N-CO-NCH_3 (**b**); NH-CS-NH (**c**)

References:

[1] Shul'ts, E. E.; Andreev, G. N.; Shakirov, M. M.; Komarova, N. I.; Bagryanskaya, I. Yu.; Gatilov, Yu. V.; Tolstikov, G. A; *Russian, Journal of Organic Chemistry*, **2009**, *45*, 87.

[2] Wang, S ; Kim, S. H; *Dyes and Pigment*s, **2009**, *80*, 314.

[3] Zhou, W. J ; Kurth, M. J; *Polymer*, **2001**, *42*, 345**.**

[4] Yilmaz, V. T; Aksoy, M. S; Sahin, O; *Inorg. Chim. Acta*. **2009**, *362*, 3703.

[5] Kesharwani, S; Sahu, N. K; Kohli1, D. V. *J; Pharm .chem*, **2009**, *43, 6*.

[6] Noroozi Pesyan, N.; Rastgar, S.; Hosseini, Y. *Acta Cryst. Section E* **2009**, *65*, 1444.

Application of double activating catalyst for the synthesis of pyran derivatives in green media

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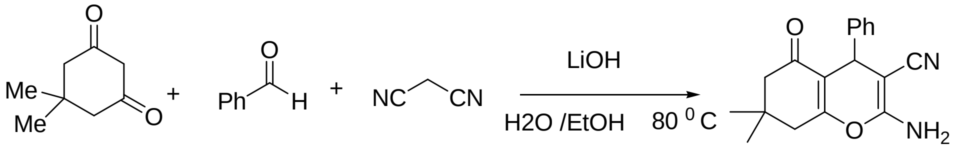
4H-benzopyran derivatives have attracted great attention recently in synthetic organic chemistry due to their wide range of biological activity and pharmacological property, such as anti-coagulant, anti-cancer, spasmolytic, diuretic, and anti-ancaphylactin [1]. These methods have some shortcomings in terms of poor yields, environmental pollution and expensive solvent, not easy work-up. Therefore, the improvements in such synthesis had been sought continuously [2]. It also has been reported that these compounds were synthesized by microwave irradiation [3] Although microwave irradiation in organic reactions is applicable in the laboratory, and it cannot be widely applied in industry. [4]

Herein we would like to report lithium hydroxide catalysed three-component cyclocondensation of aryl aldehydes, malonitriles and dimedone proceeds under reflux with H2O, EtOH as solvent conditions to give highly functionalised hydrobenzo[*b*]pyrans in excellent yields.



Reference:

[1] Wang, X . S.; Shi, D. Q.; Tu, S. J.; et al. *Synth Commun*, **2003**, *33, 119.*
[2] Fan, X. S.; Hu, X. Y.; Zhang, X .Y.; et al. *Aust. J. Chem*, **2004**, *57,* 1067.
[3] Jin, T. S.; Wang, A. Q.; Zhang, J. S.; et al. *(Chin. J. Org. Chem)*, **2004,** *24,* 1598.
[4] Shi, D. Q.; Mou, J.; Zhuang ,Q .Y.; et al. *Journal Chem. Res. (s)*, **2004**, *12,* 821.

Aza-Michael addition of aromatic amines to α,β-unsaturated compounds catalyzed by boric acid/glycerol in water

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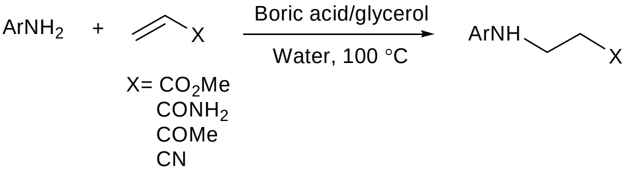
Owing to their wide range of biological activities and pharmacological properties, β-amino carbonyl compounds and derivatives are much sought after. Such compounds not only constitute components of biologically active natural products, they also serve as essential intermediates in the synthesis of β-amino acids and β-lactam antibiotics. Consequently, the development of novel synthetic methods for their synthesis has attracted sustained interest in organic synthesis [1, 3].

The selection of boric acid/glycerol as catalyst was because of some important reasons. Boric acid/glycerol is an environmentally, green, recyclable and cheap catalyst. The efficiency of boric acid improves with glycerol considerably [2].

Herein we want to report a convenient and versatile method for aza-micheal addition of aromatic amines. We implement boric acid/glycerol catalytic system to effort β-aza-substituent compounds from Michael acceptors.



References:

[1] Ying, A-G.; Liu, L.; Wua, G-F.; Chen, G.; Chen, X-Z.; Ye, W-D., *Tetrahedron Lett.* 2009, 50, 1653.
[2] Mukhopadhyay, C.; Datta, A.;. Butcher, R. J., *Tetrahedron Lett.* 2009, 50, 4246.
[3] Yang, L.; Xu, L-W.; Zhou, W.; Li, L.; Xia, C-G., *Tetrahedron Lett*. 2006, 47 , 7723.

Molecular imprinted polymer: Synthesis, characterization and applications as extractant for preconcentration and determination of Cefuroxime Sodium

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Recently molecularly imprinting polymer has been used for purification bioproduct. Molecular imprinted polymers (MIPs) were prepared from methacrylic acid and Allyl glycidil ether/ iminodiacetic acid as the functional monomer and N, N methylene diacrylamid as the cross-linker in methanol solution using cefuroxime sodium as the template molecule and 2,2-azobis-isobutyronitrile as the initiator. The .applied for drug determination from tablet matrixpolymer was by elemental analysis, IR and thermogravimetric analysis (TGA) and studied for preconcentration and determination of cefuroxime sodium using high performance liquid chromatography for drug monitoring. The effects of amount of the cross-linker, the ratio of template molecule and functional monomer, amount of solvent and amount of the radical initiator on the polymerization were examined. The polymerization also was performed in presence of Cu (II) which can coordinate the drug and retain it in polymer. Clearly, in the last polymerization manner, the polymer first was doped with Cu (II) then acted as a sorbent. The synthesized polymer was successfully applied for drug determination from tablet matrix.

References:

[1] Y. Pic´o, V. Andreu, Anal. Bioanal. Chem. 387 (**2007**) 1287.
[2] F.G. Tamayo, E. Turiel, A. Mart´ın-Esteban, J. Chromatogr. A 1152 (2007) 32.
[3] E. Turiel, G. Bordin, A.R. Rodr´ıguez, J. Sep. Sci. 28 (**2005**) 257.

An efficient one-pot three-component synthesis of new derivatives of indenoquinolines under ultrasound conditions

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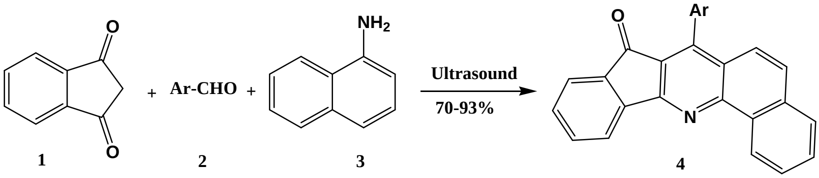
Quinolines have amazing intrinsic pharmacological and biological activities such as antimalaria, anti-asthmatic, antibacterial and antihypersensitive activities [1]. In addition, quinolines are valuable synthons used for the preparation of nanostructures and polymers that combine enhanced electronic, optoelectronic or non-linear optical properties with excellent mechanical properties [2]. In particular indenoquinoline derivatives showed a wide range of biological activities such as 5-HT-receptor binding activity, anti-inflammatory activity, and also act as antitumor agents, inhibitor for steroid reductase, acetylcholonesterase inhibitors, and antimalarial [3].

At present study in connection with our previous reports on the benign synthetic methods in organic chemistry [4], we wish to introduce an efficient protocol for the synthesis of new derivatives of indenoquinolines in one-pot three-component approach by the reaction of α-naphthylamine, arylaldehydes and indanedione under solvent-free conditions, using ultrasonic irradiations. This novel procedure furnished the desired indenoquinolines in reasonable reaction times and higher yields (70-93% yields). The structures of all products were confirmed by IR, ^{1}H NMR, and ^{13}C NMR spectroscopy.



References:

[1] Chen, Y. L.; Fang, K.; Sheu, J. Y.; Hsu, S. L.; Tzeng, C. C. *J. Med. Chem.* **2001**, *44*, 2374.

[2] Jegou, G.; Janekhe, S. A. *Macromolecule* **2001**, *34*, 7926.

[3] Jiang, B.; Si, Y. G. *J. Org. Chem.* **2002**, *67*, 9449.

[4] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K. *Molecules* **2009**, *14*, 1468; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *Heterocycles* **2008**, *75*, 2825; Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N. O.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49*, 1450.

Synthesis, characterization and catalytic activity of nanospinels $Cu_{1-x}Co_xFe_2O_4$ in t-butylation of p-cresol

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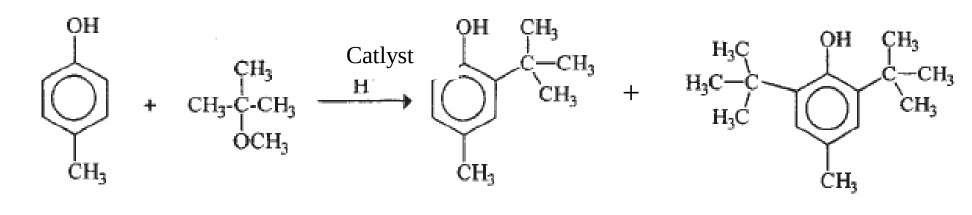
The synthesis of nano crystalline spinel has been investigated intensively in the recent year due to their unique potential application in high density magnetic recording, microwave devices, magnetic fluids and also as an absorbent material to remove sufur-containing materials from hot-coat gas [1]. Herein we try to synthesis nanospinels with general formula using hydrothermal method for the production of alkylated phenol:
$Cu_{1-x}Co_xFe_2O_4$ (x=0, 0.25, 0.5, 0.75, 1)

The x-ray diffraction (XRD) and scaning electron microscopy (SEM) confirmed the formation of nanosized.

The alkylated phenol products are used as raw materials for the manufacture of a variety of resins, durable surface coatings, varnishes, antioxidants, and etce [2]. Use of antioxidants in composite propellant formulation is unavoidable. These materials are added to the propellants to import stability to the formulation during storage time. One of these antioxidants is A.O.2246 that used in HTPB as stabilizer [3]. A.O.2246 is synthesised from 2-t-butyl–para cresol which is an intermediate in this process. The adventages of these nanospinels is more active surface that make this catalyst more effective in compare with microcatalysts and also results in better selectivity of product. Reaction scheme is shown below: Catalyst



References:

[1] Bid, S.; Pradan, S. K. *Materials Chemistry and Physics*. **2003**, *82*, 27.
[2] Hao-Yu, Shen.; Zaher, M. A.; Judeh and Chi Bun ching. *Tetrahedron Letters*. **2003**, *44*, 981.
[3] Gurvich, Y. A.; Grinberg, A. A. U.S. Patent, 4,087469, **1978**.

Application of ionic liquids immobilized on silica in drug delivery system

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A drug delivery system is capable of carrying agents and releasing them at a specific location and rate. The main objective of such systems is to control the dosage and duration of the drug effect without harm to the patient while improving the patient's health[1]. Due to the emergence of new drugs of larger sizes, higher dose sensitivity, and poor stability in biological systems, a more efficient and controlled release system was developed[2]. Ionic liquids (ILs) are salts in liquid form and already have a wide range of applications, from use in drug delivery to fuel cells and batteries.

In this work Silica nanoparticles linked through ionic liquid are synthesized. The first approach utilized a 1-methyl-3-(3-trimethoxysilylpropyl)imidazolium chloride to link the silica nanoparticles. Then, the hollow microspheres were produced by removing the silica cores through chemical etching with hydrofluoric acid[3].The composition of the composites hybrid materials was determined by scanning electron microscopy (SEM) and FT-IR.

Equilibrium swelling studies were carried out in enzyme-free simulated gastric and intestinal fluids (SGF and SIF, respectively). Insulin was entrapped in these hybrids and the in vitro release profiles were established separately in both (SGF, pH 1) and (SIF, pH 7.4)[4].

References:

[1] Wang, S. Micropor. Mesopor. Mater. **2009**, 117, 1.
[2] Vallet-Regi, M.; Balas, F.; Arcos, D. Agnew. Chem. Int. Ed. **2007**, 46, 7548.
[3] Sikshi, S. A.; Hultin, P. G. J. Org. Chem. **2006**, 71, 5888.
[4] M. Galehassadi, M. Mahkam, F. Hosseinzadeh. e-Polymers **2007**, no. 028

Synthesis of spiro[indole-3,8'-phenaleno[1,2-b]pyran]-9'-carbonitriles and by a one-pot, four-component Reactions

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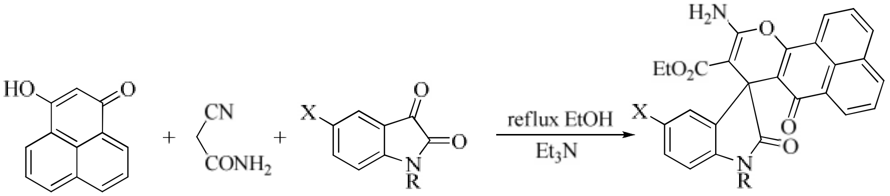
Modern synthetic design demands high efficiency in terms of minimization of synthetic steps together with maximization of complexity [1]. One of the best methods to fulfill these goals is the development and use of multicomponent reactions (MCRs) which consist of several simultaneous bond-forming reactions and allow the high efficient synthesis of complex molecules starting from simple substrates in a one-pot manner [2]. MCRs are economically and environmentally very advantageous because multi-step syntheses produce considerable amounts of waste mainly due to complex isolation procedures often involving expensive, toxic and hazardous solvents after each step.

Indole and indoline fragments are important moieties of a large number of a variety of natural products and medicinal agents [3], and some of indolines, spiro-annulated with heterocycles in the 3-position, have shown high biological activity [4]. The spirooxindole system is the core structure of many pharmacological agents and natural alkaloids [5].

In the current work, we have reported a new four-component method for the synthesis of spiro[indole-3,8'-phenaleno[1,2-*b*]pyran]-9'-carbonitriles by a reaction of isatins, 2-cyanoacetamide, alcohols and 1*H*-phenalene-1,3(2*H*)-dione.



References:

[1] Trost, B. M. *Science* **1991**, *254*, 1471.
[2] Orru, R. V. A.; de Greef, M. *Synthesis* **2003**, 1471
[3] Sundberg, R. J. *The Chemistry of Indoles*; Academic: New York, NY, **1996**.
[4] (a) Joshi, K. C.; Chand, P. *Pharmazie* **1982**, 37; (b) Da-Silva, J. F. M.; Garden, S. J.; Pinto, A. C. *J. Braz. Chem. Soc*. **2001**, *12*, 273.
[5] Ma, J.; Hecht, S. M. *Chem. Commun.* **2004**, 1190.

Synthesis of star polymethylmethacrylate by ATRP

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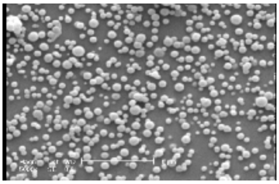
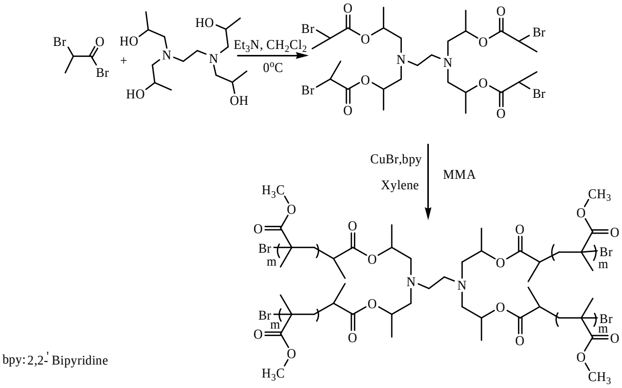
Tetra-functionalized bromide initiator have been synthesized by esterification reaction of the Ethylenediamine-*N,N,N',N'*-tetra-2-propanol to produce star polymer by core-first method [1-3]. The multifunctional initiator (core) have been used with methyl methacrylate (MMA) as a monomer, CuBr as the catalyst and 2,2'-bipyridine ligands in the synthesis of methyl methacrylic star polymers by atom transfer radical polymerization (ATRP) [4]. Under these conditions, tetra-arm star polymers were synthesized with high conversion, low polydispersity and nearly monomodal molecular weight distributions. These polymers were recognized by different instrumental methods such as FT-IR, ^{1}H NMR and also scanning and tunneling electron microscopes. Formation of star polymers were confirmed by spherical ingredients in their pictures. GPC of the hydrolyzed star polymers are monomodal, which is the characteristics of living systems. The molecular weights of the linear polymers are near to ¼ molecular weights of star polymers.





References:

[1] Matyjaszewski, K.; Gao, H. *Macromolecules.* **2008**, *41*, 1118.
[2] Hussain, H.; Tan, B. H.; Gudipati, C. S.; Xaio, Y HE. J. *Polym. Sci. PartA: Polym. Chem.* **2008**, *46*, 7287.
[3] Kimani, S.M.; Moratti, S. C. *Macromol. Rapid Common.* **2006,** *27*, 1887.
[4] Huaming, SUN. ; Ziwei GAO. ; Lin YANG.; Lingxiang GAO. *Front. Chem. China.* **2009**, *4(1),* 89.

Synthesis and photochromic properties of (3,3 dipheniyl -3H-benzo (f) chromene-1-yl) methanol

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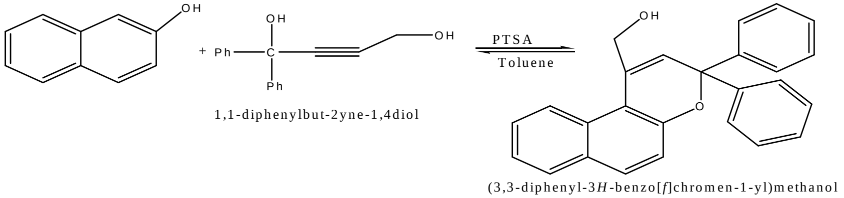
(3,3 diphenyl -3H- benzo (f) chomene-1-yl) methanol were synthesized from reaction between 1,1-diphenylbut-2yne-1,4diol and β-Naphtol in toluene solvent and P-toluensulphonic acid (PTSA) as a catalyst (scheme 1).

Synthesis of naphtopyrans (benzo chromenes) from propargyl alcohol with hydrogen groups at the 1-position is difficult, because for closing pyran ring in this compounds ,non-hydrogen groups at the 1-position is required [1]. Naphtopyrans containing aryl groups at the 3-position have improved fatigue resistance compared with compounds substituted at the 3-position with groups containing hydrogens. Also aryl groups at the 3-position in naphtopyrans cause to increase of photochromic properties, because aryl groups in open-ring isomer of naphtopyrans lead to increase of resonance and creating a bathochromic shift [2,3].

As a result for synthesis of (3,3 dipheniyl -3H-benzo (f) chomene-1-yl) methanol optimization and increase of photochromic properties, primarily ,the 1-positon of propargyl alcohol were substituted by aryl groups and then synthesized compounds were investigated by UV, IR, NMR spectrums.



Scheme 1

References

[1] J. Cottam and R. Livingston, 6,6- Diphenylnaphtho(1',2' : 2,3)pyran and 1,3-diphenyl-3-(1-hydroxy-2-naphthyl)propan-1 -one, *J. Chem. Soc.*, **1964**, 5528.

[2] J. Cottam and R. Livingston, 6,6-Diphenyl-6H -naphtho(2'3' : 2,3)pyran and 4,6-diphenyl-4H -naphtho(2',3' : 2,3)pyran, *J. Chem. Soc.*, **1965**, 6646.

[3] J. Kolc and R. S. Becker, Spectroscopy and photochemistry of naturally occurring and synthetic chromenes, Photochem. Photobiol., **1970**, *12*, 383.

Synthesis of elastomeric hydrogels

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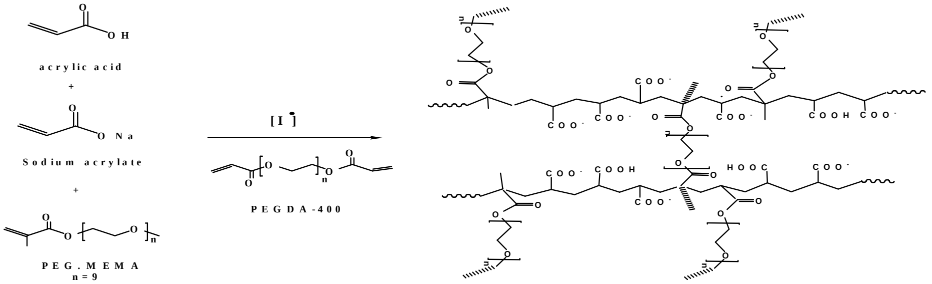
Hydrogels are three dimensional polymeric networks which can absorb and retain water [1,2]. The majority of hydrogels have glass transition temperature (Tg) above room temperature. An elastomeric hydrogel was prepared in this research based on poly(ethylene glycol) methyl ether methacrylate (PEGMEMA) and acrylic acid (AA) through solution polymerization [2]. Ammonium persulphate (APS)/tetramethyl ethylenediamine (TMEDA) was used as an initiating system for the free radical polymerization and polyethyleneglycol diacrylate (PEGDA 400) was used as a cross-linker (Scheme 1).

Hydrogels were characterized by FT-IR, swelling behavior and gel content. Thermal behavior was determined by thermogravimetric analysis (TGA) and dynamic mechanical thermal analysis (DMTA). Swelling was increased from 4.5 to 38.6 g/g with the AA enhancement from 0 to 81%. The gels with high PEGMEMA content had low Tg (Tg of homopoly(PEGMEMA) was -50 °C). It was increased with AA content enhancement. The samples with high AA content did not possess elastomeric behavior at room temperature. Gels having elastomeic behavior can be used as sealants.



Scheme 1. Synthetic scheme for preparation of elastomeric hydrogel.

References:

[1] Buchholz, F. L.; Graham, T. Modern. *Superabsorbent Polymer Technology*; *Wiley-VCH: New York.* **1998**, 252.
[2] Zohuriaan-Mehr M. J.; Kabiri, K**.** *Iran. Polym. J.* **2008**, *17*, 451.

Ring opening of epoxides with nitrogen heterocycles catalyzed by MCM-41 under solvent-free conditions

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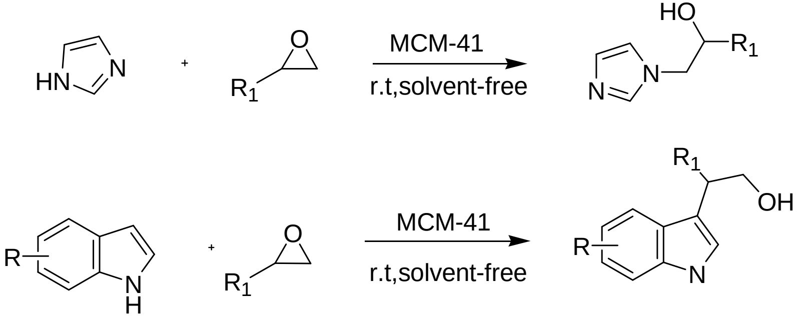
Indole and imidazole derivatives are important heterocyclic compounds and have wide application in medicinal chemistry [1].

In particular, 3-alkylindole derivatives have significant biological and pharmacological importance. Due to the nucleophilic nature of indolyl and imidazole compounds, various methods have been developed for the alkylation of indoles and imidazoles [2].

Ring opening of aliphatic and aromatic epoxides with nitrogen heterocycles such as indoles and imidazoles under solvent-free conditions at room temperature is reported. The reaction takes place with a S_N2 pathway affording alkylated derivatives with high regioselectivity. Treatment of indole with styrene oxide resulted in the formation of 2-(3'-indolyl)-2-phenylethanol in 85% yield using 0.05 g MCM-41.



References:

[1] Li, J. T.; Dai, H. G.; Lin, Z. P. *Prog. Chem.* **2007**, *19*, 751.
[2] Bandini, M.; Melloni, A.; Tommasi, S.; Umani-Ronchi, A. *Synlett* **2005**, 1199.

5,6,7,8-Tetrahydro-ß-Naphthyl Chlorothionoformate As A Powerful Dealkylating Agent of Tertiary Amines

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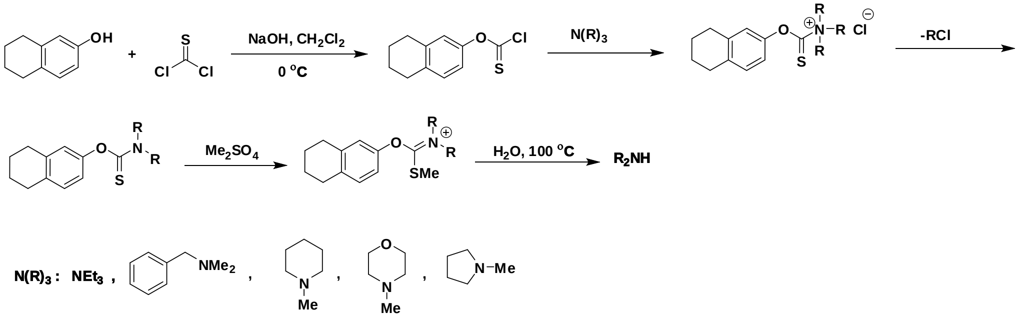
N-Dealkylation and more specifically debenzylations are important in organic synthesis and structural determination. Many carbon chloridates (chloroformates) [1] have been used as reagents for acylative dealkylation and so far as many different methods and reagents are used for dealkylation of tertiary amines. Reagent such as: Dithiols [1], Niobium pentachloride [2], propargly oxyloxycarbonyl [3]' boron triboromide [4]. We have previously reported the dealkylation of tertiary amines with thiophosgene [5],1-chloroethylchlorothionoformate [6], p-chloro and 2,4,6- tribromophenyl chlorothionoformate [7] and more recently ortho-nitrophenyl chlorothionoformate **[**8]. The reactivity of these reagents was found to be comparable to that of a number of previously used method.

In this research we have made a new reagent that the rate of a reactions and alkyl group cleavage selectivity in certain amines with this reagent are comparable to another dealkylating agent. To the solution of 5,6-7,8-Ttrahydro-*β*-Naphthol in aqueous sodium hydroxide at 0 °C was added thiophosgene in dichloromethane to give 5,6-7,8-Ttrahydro-ß-Naphthyl chloroformate as pure yellow oil in 90% yield, the structure of this reagent was identified by NMR and IR spectra.

The reaction of this reagent with different tertiary amines caused deethylation of triethylamine, debenzylation of *N,N*-dimethylbenzylamine, demethylation of 1-methylpiperidine and *N*-methylmorpholine, and with pyrrolidine let to ring opening products very rapidly at room temperature in very good yields. The sequence steps of dealkylation reaction shown below:



References:

[1] Bethaby A. Buck-Koehntop et.al., *j. Org. Chem* **2006**,*691*,1748.
[2] Yukinori Sudo,et al.*Eur. j. Org. Chem* **2006**, 752.
[3] Ramakrishna G. Bhat,et al. *Tetrahedron Lett.* **2004**, *45,* 7983.
[4] Timothy S. Keizer, et al. *Jorganchem*.**2003**, *666*, 103.
[5] Baradarani, M. M.; Prager, R. H. *Tetrahedron Lett.* **1999**, *40*, 7403.
[6] Baradarani, M. M., Prager, R. H. *J. Sci. I.R.Iran.* **2001**,*12*,27,(Chem**.**Abstr.2002,136,262753).
[7] Heidari, M.; Baradarani, M.M. *Arkivoc*, **2006**,167.
[8] Aghazadeh, M.; Bradarani, M. M. *African Journal of pure and applied chemistry* **2008**, *2(7)*, 64.

A facile synthesis of novel spiroindane-1,3-diones via one-pot three-component [3+2] azomethine ylide cycloaddition

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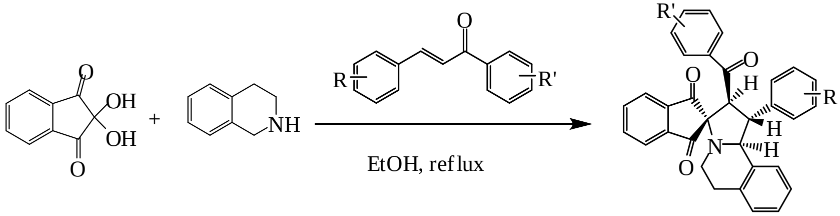
1,3-Dipolar cycloaddition reactions provide an efficient approach for the synthesis of five-membered ring heterocycles [1]. High stereospecificity and stereoselectivity associated with these reactions make them synthetically important [2]. Azomethine ylides are reactive and versatile 1,3-dipoles which readily react with various dipolarophiles to afford pyrrolidines and pyrrolizidines. These compounds are central skeleton for numerous alkaloids and constitute classes of compounds with significant biological activity [3].

Spiro compounds in particular spiropyrrolidines have gained much attention as a result of their interesting biological activities such as antimicrobial, antitumor and antibiotic properties [4]. The synthesis and antimicobacterial activity of spiro and dispiroindanediones have reported recently [5].

Herein, we report the facile synthesis of novel spiroindane-1,3-diones via the one-pot three-component condensation of azomethine ylide generated in situ from ninhydrin and 1, 2, 3, 4- tetrahydroisoquinoline with chalcone derivatives. The structure and regiochemistry of the cycloadducts were characterized with spectroscopic data and X-Ray crystal structure analysis.



References:

[1] Padwa, A.; *In Synthetic Applications of 1,3-Dipolar Cycloaddition Chemistry Toward Heterocycles and Natural Products*; John Wiley & Sons, 2002.

[2] Pandey, G.; Sahoo, A. K.; Gadre, S. R.; Bagul, T. D.; Phalgune, U. D. *J. Org. Chem.* **1999**, *64*, 4990.

[3] (a) Padwa, A. *In Comprehensive Organic Synthesis*; Trost B. M. and Flemming I., Eds.;, Pergamon: Oxford, 1991, vol. 4, pp 1085; (b) Fejes, I.; Nyerges, M.; Szollosy, A.; Blasko, G.; Toke, L. *Tetrahedron* **2001**, *57*, 1129.

[4] Kozikowski, A. P. *Acc. Chem. Res*. **1984**, *17*, 410.

[5] (a) Suresh Babu, A. R.; Raghunathan, R.; Satiskumar, B. K. *Tetrahedron Lett.* **2009**, *50*, 2818; (b) Lakshmi, N. V.; Thirumurugan, P.; Perumal, P. T. *Tetrahedron Lett*. **2010**, *51*, 1064.

Multi-walled carbon nanotubes/linear dendritic copolymers supramoleculesand their application as anticancer drug delivery systems

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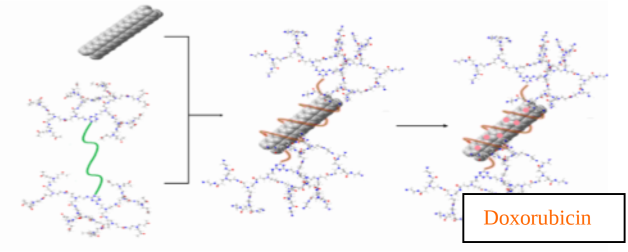
Carbon nanotubes have attracted considerable attention because of their unique atomic structure, high surface area-volume ratio and excellent electronic, mechanical and thermal properties .They have a wide range of potential applications including nanoelectronic, sensors, fillers in composites materials and others [2,4,5].Carbon nanotubes are also promising materials for nanomedicine .They have potential applications as carriers for delivery of drugs, RNA, DNA, peptides and other biological activemolecules into cells because of the ability to cross cell membranes [1].

In this work a versatile method for the preparation of dispersed nanotubes using Linear-dendritic co-polymers in water and their application in cancer therapy is presented . Oxidized Multi-walled carbon nanotubes (MWNTs) were easily solubilized in water by non-covalentfunctionalization with Linear-dendritic copolymers. In order to investigate their potential application in nanomedicine and to understand their limitation and capability as nanoexcipients in biological systems short term in vitro cytotoxicity tests were connected on cancer cell lines and it was proved thatsolubilized systems are able to form supramolecular complexes with anticancer drugs such as doxorubicinvia p–p stacking interactions and enhance theirtoxicity activity [3].The chemical structure, morphology, thermal properties,molar mass and size of nanomaterials were determined using IR, ^{13}C NMR, ^{1}H NMR, Raman spectroscopy, TEM,TGA, DSC, GPC and DLS.



References:

[1] Adeli M, Mirab N. *Polymer* **2009**; *50*: 3528.
[2] Yu H, Jin Y. *J. Phys Chem . C* **2008.**
[3] Ali-Boucetta H; Al-Jamal Kh; Kostarelos K *Chem .Commun.*, **2008**; 459.
[4] Qin Sh .Qin D. *Chem. Mater* **2005**; 17: 2131.
[5] Wang Zh, Liu Q, Chen Y. *Carbon* **2007**; 45: 285.

$KAl(SO_4)_2.12H_2O$ as a recyclable Lewis acid catalyst for synthesis spirooxindoles in aqueous media

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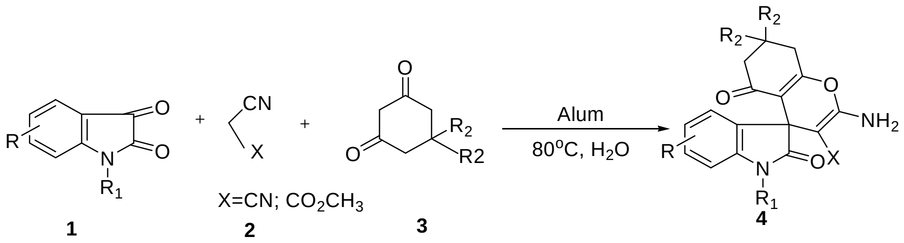
Multicomponent reactions (MCRs), an important subclass of tandem reaction, are one-pot processes in which three or four easily accessible component react to form a single product, which incorporates essentially all the carbon atoms of the starting materials [1].

Recently, a great attention has been focused on the use of water as green solvent in organic transformations. Water is a desirable solvent for chemical reactions because it is safe, non-toxic, environmentally friendly, readily available, and inexpensive compared to organic solvents [2].

The spirooxindole system is the core structure of some pharmacological agents and natural alkaloids [3].

We report an efficient method for synthesis spirooxindoles in aqueous media. A mixture of isatin (1mmol), malononitrile or methylcyanoacetate (1mmol), 5,5-dimethyl-1,3-cyclohexanedione (1 mmol) in the presence of $KAl(SO_4)_2.12H_2O$ in water were mixed at 80^oC for the appropriate time.

In conclusion, we demonstrated a simple procedure for synthesis of spirooxindoles in water using $KAl(SO_4)_2.12H_2O$ as inexpensive and efficient catalyst. High yields and simple workup procedure are some advantage of this protocol.



References:

[1] Zhu, J. *Eur. J. Org. Chem*. **2003**, 1133.
[2] Li, C. J. *Chem. Rev*. **2005**, *105*, 3095.
[3] Sebahar, P.R.; Williams, R. M. *J. Am. Chem. Soc*. **2000**, *122*, 5666.

A new method for the synthesis of 1,3,4-thiadiazole derivatives under solvent-free conditions with using $H_4SiW_{12}O_{40}$ and $H_3PW_{12}O_{40}$

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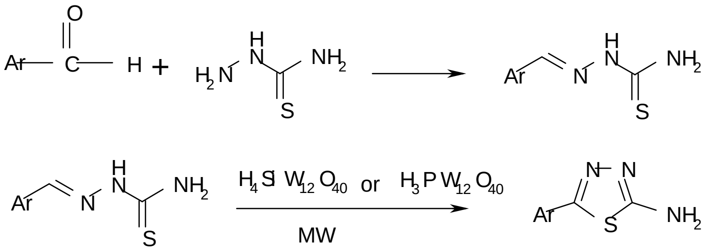
1,3,4-Thiadiazole derivatives have been of great interest as antitumour compounds for several scores of years. At first the attention was focused on 2-aminothiadiazole and its simple derivatives[1-2]. 2-Aminothiadiazole was introduced into phase II clinical trials in patients with different tumours: renal, colon, ovarian and others [3].

In recent years, the use of solid acids as heterogeneous catalysts has received considerable attention in different areas of organic synthesis. Amongst the various heterogeneous catalysts, heteropoly acids (HPAs) are the most attractive, because of their flexibility in modifying the acid strength, environmental compatibility, no toxicity and experimental simplicity. The use of HPA as a catalyst makes the process convenient and environmentally benign [4].

Herein we report an efficient, novel, fast and modified method for synthesis of 1,3,4-thiadiazole derivatives under microwave irradiation in the presence of catalytic amount of $H_4SiW_{12}O_{40}$ and $H_3PW_{12}O_{40}$ under solvent-free condition.



References:

[1] Donald, H.L. *Cancer Chemother. Pharmacol.* **1980**, *4*, 215
[2] Nelson, J.A.; Rose, L.M.; Bennet, L. *Cancer Res.* **1977**, *37*, 182.
[3] Asbury, R.F.; Blessing, J.A.; Moore, D. *Am. J. Cli. Oncol.* **1996**, *19*, 400.
[4] Heravi, M.M.; Rajabzadeh, G.; Bamoharram, F. Seifi, N. J. *Mol Catal A: Chem.* **2006**, *256*, 238.

Convenient one-pot synthesis of 4-thiazolidinones and derivatives under room temperature and solvent- free condition

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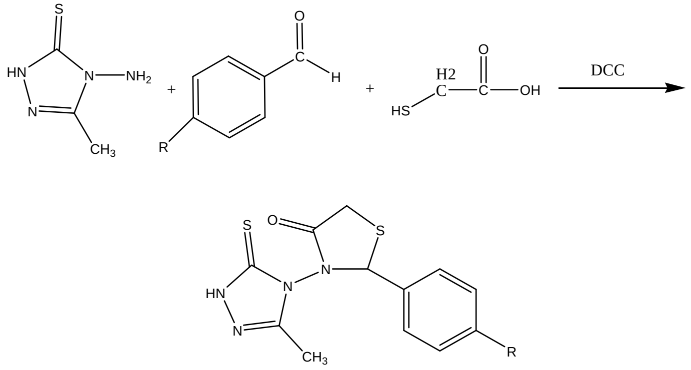
Thiazolidinone was prepared by cyclization of Schiff base with thioglycolic acid. Reaction is proceeding by nucleophilic attack of anion of mercapto acetic acid upon the carbon atom of Schiff base, followed by the capture of proton by nitrogen , and subsequent cyclization with removal of water molecule. N-hetrocyclic compounds such as 1,2,4-triazoles and 4-thiazolidinones may display some significant biological activities like anti-HIV , anticonvulsant, anti-inflammatory , antimicrobial ,antitubercular, anticancer, antitumor, antibacterial, antifungal, antiviral, anesthetic, diuretics, nematicidal and antihistaminic activity [1-3].

In a one-pot method, 5-amino triazole , benzaldehyde derivatives and mercapto acetic acid were converted into new 4-thiazolidinone compounds.The reactions procced with good yield and all products were characterized well with ^{1}HNMR, ^{13}CNMR and MASS analaysis.

We report an efficient, convenient and mild procedure in the presence of catalytic amount of DCC. The reaction also is easily carried under solvent- free conditions.



References:

[1] Srivastava, T.; Haq, W.; Katti, S. B. *Med. Chem. Divi.* ***2002****, 58, 7619.*
[2] Bahghat, M. M.; Maghraby, A. S.; Heiba, M.E.; Ruppel, *Arch. Pham. Res.* ***2005****, 28, 1002.*
[3] Dandia, A.; Singh, R.; KHaturia, S.; Morgant, G.; Loupy, A. *Bio. Med. Chem.* ***2006****, 14, 2409.*

Regioselective ring opening of epoxides in 5-isopropyl-2,3-*cis*-epoxy cyclohexanole by azide

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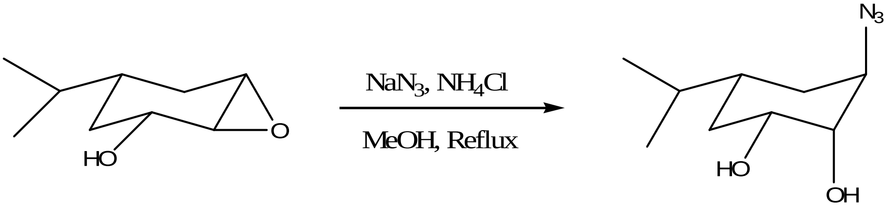
The ring opening of epoxides is one of the most important ways to synthesis different α-substituted alcohols. One of the most important problems in these types of epoxide ring opening is regioselectivity [1].

By attacking an azide ion to epoxide an α azido alcohole produced which could be easily converted to corresponding α amino alcohol. The ring opening of epoxides by azide anion takes place in presence of weak acids such as ammonium chloride. At first glance it appears that the azide anion could attack on either carbon of epoxide group.

In this work we investigated regioselective ring opening of 5-isopropyl-2,3-*cis*-epoxy cyclohexanole (**1**) by azide to provide corresponding 5-isopropyl-3-azido-1,2-cyclohexanediole (**2**).



1 2

However, azide attack at C-2, leads to a twist chair-like transition state (*cis*-diequatorial ring opening) which energetically is disfavored. On the other hand, azide attack at C-3, provides a chair-like transition state (*trans*-diaxial ring opening) which is lower in energy and thus favored. Thus, the ring opening of epoxides is generally under kinetic control and gives *trans*-diaxial products (**2**).

Our calculations for transition states of both attack on C-2 and C-3 positions justified our work. The calculations are done by Gaussian 98 program in AM1 method [2].

References:

[1] J. Lewiński, P. Horeglad, E. Tratkiewicz, I. Justyniak, Z. Ochal; *J. Org. Met. Chem. 690,* **2005**, 3697.

[2] Frisch, M. J. *et al.*GAUSSIAN98, Revision A.7, Gaussian, Inc., Pittsburgh, PA, **1998**.

Novel one-pot, three-component condensation reaction: an efficient approach for the synthesis of γ-Iminolactone derivatives in the presence of water

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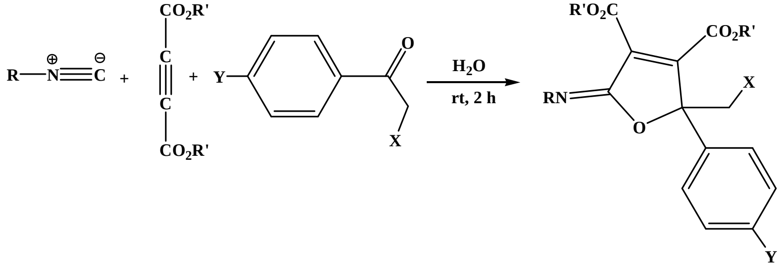
Recently, a great attention has been focused on the use of water as green solvent in various organic transformations. In addition to its abundance and for economical and safety reasons, water has naturally become as a substitute and an alternative environmentally benign solvent in organic synthesis [1]. Due to atom economy, simplicity, and amenability to automated synthesis, multicomponent condensation reactions (MCRs) have an advantageous position among other reactions. The ability of on isonitrile to undergo easy R-addition with a nuclophile and on electrophile under mild conditions has made them popular reactants for the development of novel MCRs [2]. Recently, iminolactones have been the subject of great consideration because of their effects as antibacterialagents, aldosterone inhibitors, and proper precursors for the preparation of a wide spectrum of natural compounds [3]. As part of our ongoing program to develop efficient and robust methods for the preparation of organic compounds [4], we describe a clean and efficient process for three-component reaction between alkyl isocyanides, dialkyl acetylenedicarboxylates and phenacyl halides in water at room temperature, leading to yield γ-iminolactone derivatives. The structures of the products were deduced from their IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. In summary, we have fund water as novel reaction medium for the synthesis of highly functionalized γ-iminolactones derivatives. This procedure offers significant advantages such as operational simplicity, mild reaction conditions, enhanced rates, ease of isolation of products, cleaner reaction profiles and eco-friendly nature of the solvent, which makes it useful and attractive strategy for the synthesis of γ-iminolactones derivatives.



Reference

[1] Grieco, P. A. *Organic Synthesis in Water*; Blackie Academic and Professional: London, **1998**.
[2] Domling, A. *Chem. Rev*. **2006**, *106*, 17.
[3] Ambrosi, Oliaruso, M. A.; Wolf, J. F. In Synthesis of Lactones and Lactams. Wiley, New York. **1993**
[4] Ramazani, A.; Rezaei, A. *Org Lett*. **2010**, *12*, 2852.

The synthesis and characterization of 4-(5-((cyclohexylamino)isoazol-3-yl)-2-methoxyphenol

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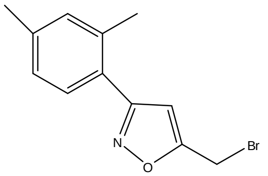
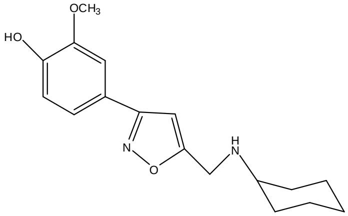
Isoxazole derivatives have been used a key intermediates in synthesis and have been investigated intensively for the last several years because of their biological activities [1]. In spite of this wide spectrum of properties, the number of isoxazoles trisubstituted by different functional groups, useful as scaffolds in the synthesis of many differently trisubstituted isoxazole, is scarce [2].

In this research work, 4-hydroxy-3-methoxybenzaldehyde (**1**) was transformed to 4-hydroxy-3-methoxybenzaldehyde oxime (**2**) by using NH_2OH in pyridine. The in situ generated nitriloxide from reaction between (**2)** and NaOCl, was reacted with propargylalcohol to produce 4-(5-(hydroxymethyl) isoxazol-3-yl)-2-methoxyphenol (**3**) in a cycloaddition procedure. Then compound **(3)** reacted with amins such as cyclohexylamin and produced 4-(5-((cyclohexylamino)isoazol-3-yl)-2-methoxyphenol (**4**). Also, 2,4-dimethylbenzaldehyde (**5**) was transformed to 2,4-dimethylbenzaldoxime (6) by using NH_2OH in pyridine. The in situ generated nitriloxide from reaction between (**6)** and NaOCl, was reacted with propargylalcohol to produce 3-(2, 4-dimethylphenyl)-5-hydroxymethyl isoxazole (**7**) in a cycloaddition procedure. Then, bromination of compound (**7**) with PBr_3 in CH_2Cl_2, to produce 3-(2, 4-methylphenyl)-5-bromomethyl isoxazole (**8**).

The structure of all the synthesized compounds was characterized and confirmed by FT-IR and NMR spectroscopy techniques.





References:
[1] Lee, Y., Kim, B. H., *Med. Chem. Lett.* **12** (2002) 1395.
[2] Ruano, J., Fajardo, C., Martin, M. R., *Tetrahedron* **61** (2005) 4363.

A DFT study on physical organic aspects of the Fischer carbene intermediate

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One of the most important synthetic applications for Fischer carbenes is the benzannulation reaction involving the coupling of α,ß-unsaturated carbene complexes and alkynes. This reaction results in the formation of phenols or naphthoquinones and proceeds with considerable regioselectivity when the substituents on the alkyne are distinctly different in size. This formal [3+2+1] cycloaddition proceeds by sequential coupling of the alkyne, carbene and one carbonyl ligand at a $Cr(CO)_3$ template. The proposed mechanisms of this reaction have been made based on experimental and theoretical studies.

Fischer carbenes are important starting materials for C-C bond formation via coupling reactions between carbene and wide variety of substituted alkenes or alkynes. This DFT study shed light on unique fundamental organic/organometallic aspects for the C(OMe)Me carbene in the free form and in case of bonding with $M(CO)_4$ (M= Cr, Mo, W). The data illustrate that the structures of the title intermediates include a unique structure stabilizing intramolecular M…C-H interaction.

This conclusion was made based on calculated NMR data (for carbon and hydrogen), structural parameters, energy calculations of conformers (C-C conformation), selected IR stretching frequencies (C-O, C-C, and C-H), and atomic charges. The agostic interaction is most efficient in case of chromium and in general is described as an overlap between the σ-bond electron pair of C-H with an empty d-orbital of the metal. These characterized examples are new addition to the orbital interaction theory.

Analysis of the data revealed that bonding the carbene C(OMe)Me to $M(CO)_4$ (M= Cr, Mo, W) causes dramatic changes in many of the theoretical organic aspects; the structure, relative stability of conformers, atomic charges, infrared frequencies, and ^{1}H- and ^{13}C-NMR chemical shifts. The results from these aspects illustrate a unique case of [M]…C2-H1 interaction. Although this interaction weakens the C_2-H_1 bond but it causes an overall stability for the electronic structure of the molecule. In general, the greater effect from chromium is attributed to the shorter Cr-C_1 distance. This is a new addition to the “Orbital Interaction Theory” [1] and to the literature information about the organic/organometallic reactive intermediates. This type of stabilizing interaction is known in the chemical literature and is called “agostic interaction” [2].

References:

[1] Rauk A, Second Edition, New York: Wiley, **2001**.
[2] Clot E and Eisenstein O, *Structure and Bonding*, **2004**, *113*, 1.

Comparing the effect of Tin(IV) Porphyrin complexes with a commercial catalyst, DBTDL, on preparation of new polyurethanes based on cyclopeptide moiety

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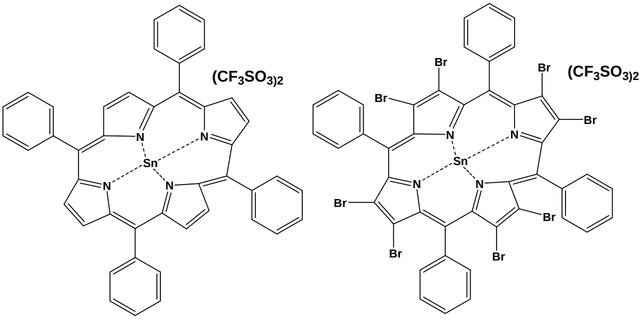
Electron deficient metalloporphyrins such as Fe(tpp)OTf, has been used as mild Lewis acid catalysts in organic synthesis. Some Metalloporphyrins were also designed to mimic the function of cytochrome P-450, Leading to finding a number of catalysts such for the selective oxidation of hydrocarbons [1]. Tin(IV) porphyrins have been investigated for applications such as catalysis, biomedicine, and synthesis of nano materials [2].

New electron deficient tin (IV) porphyrins were used as efficient catalysts for the reaction of 4,4'-methylene-bis-(4-phenylisocyanate) (MDI), *L*-leucine anhydride cyclodipeptide (LAC) and polyethyleneglycols-400 (PEG-400). Similar experiments conducted with a commercial catalyst, dibutyltin dilaurate (DBTDL). Molar ratio of catalysts, polymerization reaction time, viscosity and yield of the resulting poly (ether-urethane-urea)s (PEUU) under different catalytic conditions were compared. We found tin (IV) porphyrins catalysts afford higher reaction rate, viscosity and yield.



tin (IV) porphyrins catalysis

References

[1] Moghadam M, Tangestaninejad S, Mirkhani V, Mohammadpoor-Baltork I, Taghavi S A. *Catal Comm*, **2007**, 8, 2087.
[2] Moghadam M, Tangestaninejad S, Mirkhani V, Mohammadpoor- Baltork I, Shaibani R. *J Mol Catal: A: Chem* **2004**, 219,73.
[3] Moghadam M, Tangestaninejad S, Mirkhani V, Mohammadpoor-Baltork I, Taghavi S A. *J Mol Catal: A: Chem*, 2007, 274, 217.

Eco-friendly synthesis of poly(ether-urethane)s based on PTMG in phosphonium ionic liquids

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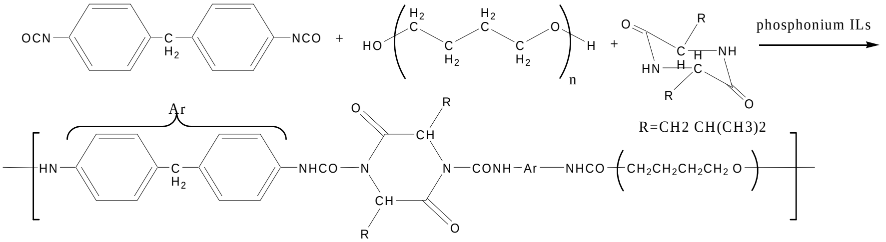
In response to public concern about the effects of plastics in the environment it has become a widely accepted opinion that degradable polymers have a well-grounded job in solving waste problem. Some important classes of degradable polymers are polymers based on α-amino acids and their different derivatives. Amino acid anhydrides as important precursors prepared from amino acids are known as good candidates for preparation of degradable polymers [1]. On the other hands, ionic liquids (IL)s are advanced, technological solvents that can be designed to fit a particular application. ILs offer new and interesting chemical and physical properties, but it is the negligible vapor pressure exhibited by ILs that has primarily attracted the attention of many researchers [2]. ILs have been referred to as "designer solvents" and millions of different ILs could potentially be synthesized and optimized for specific applications [3].

In this work for the first time a new series of poly (ether-urethane)s (PEU)s containing L-leucine anhydride was prepared by the reaction of L-leucine anhydride, 4,4′-methylene bis(phenyl isocyanate) and polytetramethylene-etherglycol (PTMG) in different phosphonium type ILs under microwave irradiation. After establishing the best conditions, we compared our results with conventional methodologies described in literature and reported in our laboratories [4]. The results showed that when ILs were used as reaction media, the reaction time was drastically decreased and viscosity, yield and polymer thermal properties were improved comparing with conventional solvents and conventional heating methods. The resulting polymers had inherent viscosities in the range of 0.4-0.62 dL/g and showed their 5% of weight loss at about 320 °C by TGA.



References:

[1] Nakano, K.; Sumitomo, Y.; Kondo, K. *Macromolecules* .**1997**, *30,* 852.
[2] Lozinskaya, E.I.; Shaplov, A.S.; Vygodskii, Ya.S. *Eur Polym J* .**2004**, *40*, 2065.
[3] Hussey, C. *Pure Appl. Chem.* **1988**, *60*.1763.
[4] Rafiemanzelat, F.; Abdollahi, E. *J Appl Polym Sci.* **2010**, submitted for publication.

A green method for the synthesis of tri substituted imidazole derivatives in the presence of In (OTf)$_3$, $CrCl_3{\cdot}6H_2O$ and $SbCl_3$ As en efficient and reusable catalysts under solvent-free condition

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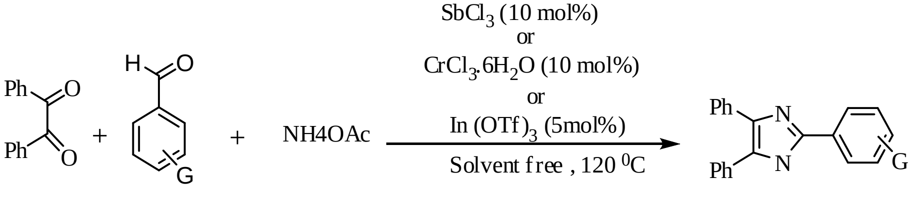
In recent years, with an increase in emphasis on environmentally-friendly chemistry, green methods are more preferable [1]. Tri substituted imidazole derivatives are of considerable interest as they possess a wide rang of biological properties and have been used extensively as pharmaceutical agents for the treatment of different diseases. A large number of drugs containing this functionality are in clinical use, including anti bacterial, diuretics, anticonvulsants, hypoglycemic, and HIV protease inhibitors [2]. tri substituted imidazole derivatives are preferred due to the ease of administration, wide spectrum of antimicrobial activity, no interference with the host defense mechanism, and relative freedom from problems of super infection [3]. In this article, an easy effective, cheap and environmentally adapted methods for synthesis tri substituted imidazole derivatives by condensation benzil and ammonium acetate with different substituted aromatic aldehydes in the presence of a catalytic amount of In (OTf) $_3$, $CrCl_3.6H_2O$ and $SbCl_3$ are explained as an effective and reusable catalysts under solvent-free condition in 120 °C (scheme).



G= H, CH_3, NO_2,Cl, Br, OCH_3

Scheme

References:

[1] G. Nagalkshmi. *E. J. Chem.*, **2008**, *5*, 447.
[2] D. Wahyuningrum.; S. Achmad. ; Y. M. Syah.; B. Bundjali.; B. Ariwahjoedi. ; *Int. J. Electrochem. Sci.*, **2008,** *3*, 154.
[3] D. Sharma.; B. Narasimhan.; P. Kumar. V. Judge.; R. Narang.; E. D. Clercq.; J. Balzarini.; *Eur. J. Med Chem*. **2009**, *44,* 2347.

The synthesis and characterization and optical properties of novel compound on based of pyridine rings

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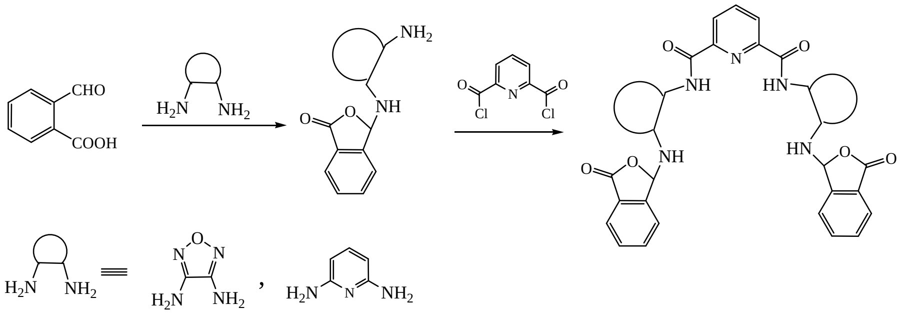
The ligands involving pyridine rings have received considerable attention in the literature because of their very important role in biological systems, they may also be used as anti-inflammatory agents [1] and can display widely varying coordination behavior, functioning as a bidentate, tridentate, meridian or bridging ligand [2, 3].in other hand, Compounds based on the furazan ring (1, 2, 5-oxadiazole) have appealing molecular properties that enhance their potential usefulness as energetic materials. Modification of polymeric materials1, 2, 5-oxadiazole derivative biological properties: antimicrobial antituberculous, spasmolytic, and muscle relaxant activity.(1, 2, 5-oxadiazole) derivatives are used as pharmaceuticals, analytical reagents, propellants and explosives, and starting materials in organic synthesis [4]. Thus, much attention has been focused on 2, 6-diaminopyridine and 2, 6-pyridinedicarboxylic acid chloride to synthesis of novel pyridine rings and furazan compounds to obtain new materials for pharmaceuticals and analytical reagents .the products were characterized by means IR, ^{1}H, ^{13}C NMR.



References:

[1] E. Opozda , W.Łasocha , *Journal of Molecular Structure,* **2003 ,***657* , 199.
[2] C. Yenikaya, M.Poyraz, *Polyhedron* **2009,** *28,* 3526.
[3] S. Khan, S. Nami , K.S. Siddiqi , *Spectrochimica Acta Part A* , **2009 ,***72* , 421.
[4] B. P. Xiang Chea, K.J. Du *Propellants. Explosives, Pyrotechnics* **2000,** *25*, 241.

N-Bromosuccinimide or 1,3-di(chloro or bromo)-5,5-dimethylhydantoin: as a mild and efficient catalyst for the synthesis of 2-arylbenzothiazoles and 2,4,5-triaryl-1*H*-imidazoles from aromatic aldehydes

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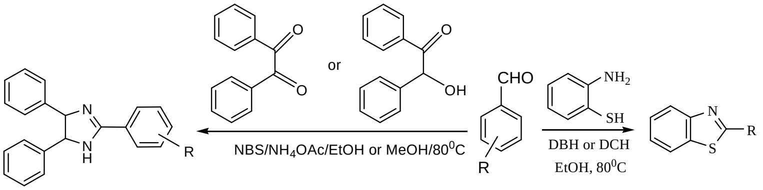
Over the century, imidazoles have received significant attention due to their reactions and biochemical properties. Even today, research in imidazole chemistry continues. Compounds with an imidazole moiety have biological and pharmaceutical importance [1]. Several substituted imidazoles are known as inhibitors of P 38 kinase [2]. 2-Arylbenzothiazoles have been investigated entensively by organic chemists due to their medicinal properties such as antitumour drugs and antiviral. Also, some benzotiazoles have been found in some organism [3-4]. Therefore, it has attracted continuous interested to develop methods for the synthesis of 2-arylbenzothiazoles and 2,4,5-triaryl-1H-imidazoles.

In continuation of our ongoing research for the development of simple and efficient methods for the synthesis of various heterocyclic compounds [5], herein we wish to report a simple, economic, and efficient one-pot method for the synthesis of 2,4,5-triaryl-1H-imidazoles from benzoin or benzil, ammonium acetate, and aromatic aldehydes using *N*-bromosuccinimide (NBS) as the catalyst and also by condensation of 2-aminithiophenol with aldehydes under thermal conditions in EtOH catalyzed by 1,3-Di(chloro or bromo)-5,5-dimethylhydantoin. The present protocols offers significant improvements for the synthesis of 2,4,5-triaryl-1H-imidazoles and 2-arylbenzothiazoles with regard to yield of products, simplicity in operation, and cheap catalyst.



3a-m **1a-m** **2a-m**

References:

[1] Zhang, C.; Sarshar, S.; Morgan, E. J.; Krane, S.; Rodarte, J.C.; Benbatoul, K. D.; Dixon, R.; Mjalli, A. M. M. *Bioorg. Med. Chem.* **2000**, *10*, 2603.

[2] Lee, J. C.; Laydon, J. T.; McDonnell, P. C.; Gallagher, T.F.; Kumar, S.; Green, D.; McNully, D.; Blumenthal, M.; Heys**,** J.R.; Landvatter, S.W.; Strickler, J. E.; McLauhlin, M.M.; Siemens, I. R.; Fisher, S. M.; Livi, J. P.; White, J. R.; Adams, J. L.; Young, P. R. *Nature* **1994**, *372*, 739.

[3] Wattenberg, L. W.; Page, M. A.; Leong, J. L. *Cancer. Res.* **1968**, *28*, 2539.

[4] Paget, C. J.; Kisner, K.; Stone, R. L.; Denlog, D. C. *J. Med. Chem.* **1969**, *12*, 1016.

[5] Zolfigol, M. A.; Azarifar, D.; Mallakpour, S.; Mohammadpoor-Baltork, I.; Forghaniha, A.; Maleki, B.; Abdollahi-Alibeik, *Tetrahedron lett.* **2006**, *47*, 833.

Synthesis of Baylis-Hillman adducts by reaction of 4-pyrone-2-carboxaldehydes with various conjugated ketones and esters

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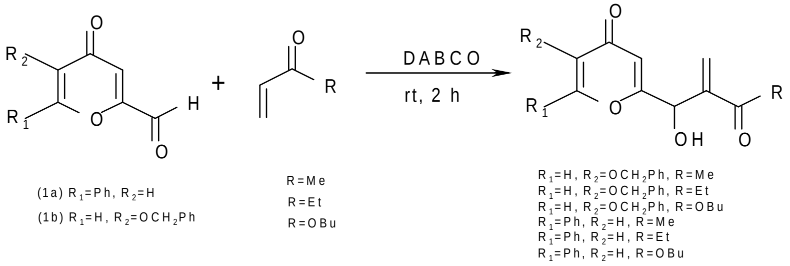
The Baylis-Hillman reaction provides a simple and atom economic synthesis of *β*-hydroxy-α-methylene esters, nitrils, ketones, etc [1]. This reaction which mainly entails a tertiary amine-catalyzed coupling of an α,*β*-unsaturated carbonyl compound with an aldehyde is a superior carbon-carbon bond-forming reaction, since it gives synthetically useful chiral building blocks that are allylic alcohols [2,3,4].

Herein we report synthesis of some Baylis-Hillman adducts by reaction of alkyl vinyl ketones and acrylates with 4-pyrone-2-carboxaldehydes. In this direction 4-oxo-6-phenyl-4*H*-pyran-2-carboxaldehyde(1a) and 5-benzyloxy-2-carboxaldehyde-4*H*-pyran-4-one(1b) (1 mmol) were treated with alkyl vinyl ketones and buthylacrylate (2 mmol) in the presence of DABCO(1,4-diazabicyclo[2,2,2]octane) (1 mmol) for 2 hours.The best solvent in the reaction of alkyl vinyl ketones was THF while in the case of buthylacrylate we used H_2O:Dioxane(1:1) as solvent. All reaction products were purified by PLC on silicagel and were characterized by IR, ^1H NMR, ^{13}C NMR spectral data and CHNS analysis. Finally we intended to synthesize heterocyclic compounds by using Baylis-Hillman adducts.



References:

[1] Sohtome, Y.; Tanatani, A.; Hashimoto, Y. *Tetrahedron letters*. **2004**, *45*, 5589.
[2] Shahrisa, A.; Ghasemi, Z. *Chemistry of Heterocyclic compounds*. **2010**, *1*, 37.
[3] Singh, V.; Batra, S. *Tetrahedron*. **2008**, *64*, 4511.
[4] Song, Y.; Ke, H.; Wang, N.; Wang, L. *Tetrahedron*. **2009**, *65*, 9086.

Synthesis and characterization of UV-curable hybrid urethane methacrylate silica nanocomposites for clear coatings

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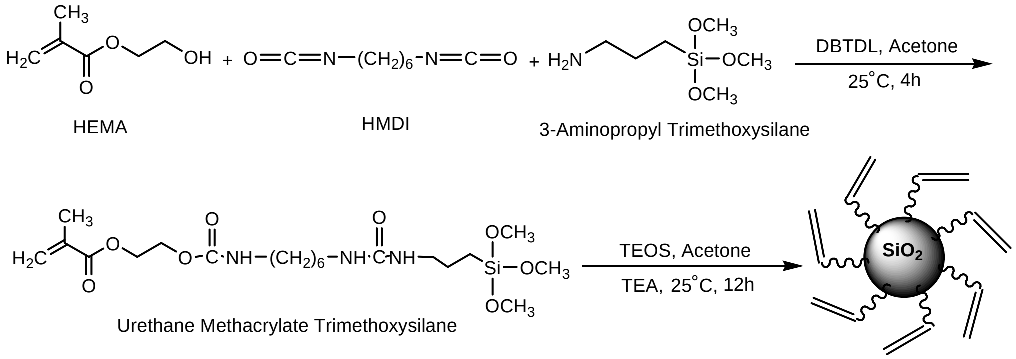
The UV-curable hybrid urethane methacrylate silica nanocomposites were synthesized in two steps. First, urethane methacrylate trimethoxysilane was synthesized by hexamethylene diisocyanate (HMDI), 3-aminopropyl trimethoxysilane and hydroxyethyl methacrylate (HEMA) in presence of acetone as solvent and dibutyldtin dilaurate (DBTDL) as catalyst. Next, UV-curable hybrid urethane methacrylate nano-silica composites were prepared by urethane methacrylate trimethoxysilane and tetraethyl orthosilicate (TEOS) in presence of triethyl amine (TEA) as catalyst. The UV-curable hybrid urethane methacrylate silica nanocomposites used as automobile clear coatings. These have been characterized with ^{1}H-NMR, FT-IR and SEM.



References:

[1] Xu J.; Pang W.; Shi W. *Thin Solid Films.* **2006**, *514*, 69.
[2] Uhl F.; Webster D.; Davuluri S.; Wong S. *European Polymer Journal*, **2006,** *42*, 2596.
[3] Mishra R.; Mishra A.; Raju K. *European Polymer Journal,***2009**, *45*, 960.

Fe_3O_4 nanoparticles as an efficient and reusable catalyst for the synthesis of calix [4] resorcinarenes

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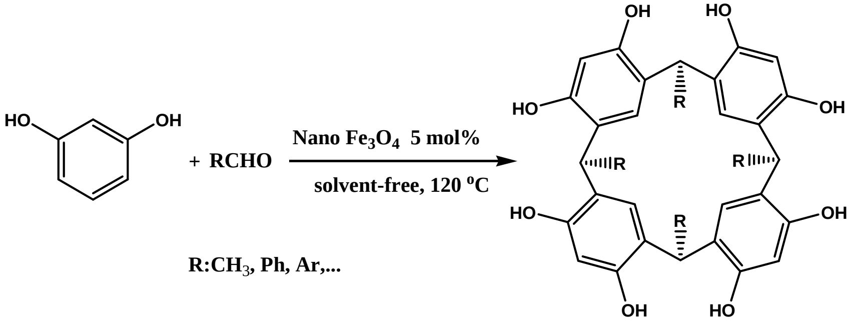
The use of the solid state in synthetic organic chemistry conveys enormous advantages in terms of separation and purification of materials. In this research, Calix [4] resorcinarenes are synthesized from the condensation of resorcinol with aldehydes by use of Fe_3O_4 nanoparticles as catalyst under solvent-free conditions.

Calix [4] resorcinarenes**,** a subclass of calixarenes, are cyclic tetramers which have found application as supramolecular tectons [1] and host molecules [2] as components in liquid crystals, HPLC stationary phases [3] and surface reforming agents.

Easy synthesis and stability of catalyst, simple work-up procedure and the high yields, short reaction times , mild reaction conditions , recyclability , inexpensive and eco-friendly nature of the catalyst make the method attractive for the synthesis of various Calix[4]resorcinarenes(Scheme).



References:

[1] MacGillivray, L. R..; Atwood, J. L. *J. Solid State Chem.* **2000**, *152*, 199; MacGillivray, L. R.; Diamente, P. R.; Reid, J. L.; Ripmeester, J. A. *Chem. Commun.* **2000**, 359; Harrison, R. G.; Dalley N. K.; Nazarenko, A. Y. *Chem. Commun.*, **2000**, 1387.

[2] Martinez, G. M.; Teran, C. R.; Tlapanco, O. A.; Toscano A.; Cruz-Almanza, R. *Fullerene Sci. Technol.* **2000**, *8*, 475; Tucci, F. C.; Renslo, A. R.; Rudkevich D. M.; Rebek, J. *Angew. Chem., Int. Ed.* **2000**, *39*, 1076.

[3] Pietraszkiewicz, O.; Pietraszkiewicz, M.;*J. Inclusion Phenom. Macrocycl. Chem.* **1999**, *35*, 261.

Synthesis of 2-(4-Halosubstituted phenyl)-4,5-diphenyl-1*H*-imidazoles using silica supported $CuSO_4$ as an effective and reusable catalyst at solvent free condition

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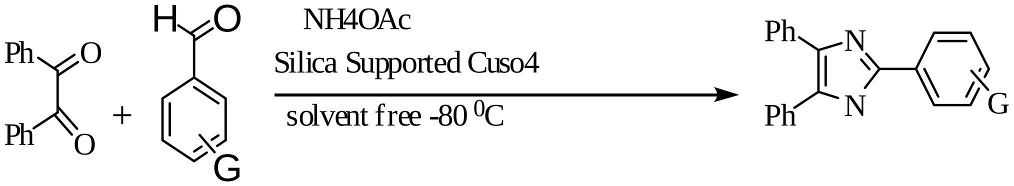
A simple and efficient method for the imidazol derivatives synthesis from the condensation benzil and ammonium acetate with different4-halosubstituted aromatic aldehydes in the presence of a catalytic amount of Silica Supported $CuSO_4$ is described The reason proposed for higher catalytic activity of Silica Supported $CuSO_4$ is a combination effect of the small particle size and high-density surface defects [1-3]. The practical and simple method led to excellent yields of the 2-(4-halosubstituted phenyl)-4,5-diphenyl-1Himidazoles under mild conditions and within short times [4].



References:

[1] Sushma Drabu, Nitin Kumar and Siddeswaran Munirjan, Indian J. Heterocycl. Chem.2005, 15, 195.
[2] Renukadevi P, Biradar J S, Hiremath S P and Manjunath S Y, Indian J. Heterocycl. Chem. 1997, 6, 277.
[3] Cozzi P, Carganico G, Fusar D, Grossoni M, Menichincheri M, Pinciroli V, Tonani R, Vaghi F and Salvati P, J. Med. Chem. 1993, 36, 2964.
[4] Jag Mohan and Ashok Kumar, Indian J. Heterocycl. Chem. 2002, 12, 41.

Influence of nanoclay on biodegradability of polyurethane bio-nanocomposite based on chitin

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Biodegradable polyurethane has received considerable attention over the past two decades because it has excellent physical properties, and good biocompatibility and biodegradability [1]. This kind of polymers is generally synthesized by incorporating soft segments susceptible to hydrolysis, such as poly (ε-caprolactone), poly (glycolide), poly (lactide) into polyurethane. Poly (ε-caprolactone) is a biodegradable, biocompatible, and semi-crystalline aliphatic polyester [2]. It is degradable hydrolytically; however, it has not been utilized as frequently as other degradable aliphatic polyesters due to its low degradation rate [3].

The introduction of a polysaccharide chain extender such as chitin can accelerate the degradation rate. Chitin is crystalline polysaccharide and degradable enzymatically by microorganisms [4]. In nanocomposites with an exfoliated morphology due to high miscibility between the polymer matrix and the organic modifier, spherulite nucleation is low. The bulk crystallization rate is slower, and the extent of crystallinity is much lower than that of neat polymer [5].

In this study we synthesized novel polyurethane bio-nanocomposite based on chitin with different proportion of modified nanoclay, by in-situ polymerization. The state of dispersion of nanoclay particles and its effects on crystallization of synthesized samples was analyzed by WAXD. The results showed that the nanoclay was exfoliated in bio-nanocomposites, and reduce the crystallinity. To study the biodegradability of synthesized samples, we used hydrolytic degradation test. Since water molecules can easily diffuse into the amorphous region of the polymer, the hydrolytic degradation occurs preferentially in the amorphous region rather than the crystalline region, and then exfoliated nanoclay could develop the rate of hydrolytic degradation due to the effect of nanoclay on crystalline reduction of the nanocomposites. Also, X-ray and TEM studies showed that most of the nanoclays are exfoliated in the polymer matrix.

References:

[1] Lamba, N.;Cooper, SL.; Polyurethane in biomedical application, New York : CRC Press ; **1998**.
[2] Wang, W.; Ping, P.;Chen, X., *Eur. Polym. J.*, **2006**, 42, 1240.
[3] Pena, J.;Corrales, T.; Doadrio, A. L., *Polym. Degrad. Stab.*, **2006**, 91, 1424.
[4] Zia, K. M.;Barikani, M.; Bhatti, I. A.; Zuber, M.; Bhatti, H. N., *J. Appl. Polmy. Sci.*,**2008** , 110, 769.
[5] Krikorian,V.;Pochan, D. J., *Macromolecules*, **2004**, 37, 6480.

A novel three-components reaction of a secondary amine and 2-hydroxybenzaldehyde derivative with an isocyanide in the presence of water: an efficient one-pot synthesis of benzo[b]furan derivatives and theoretical studies

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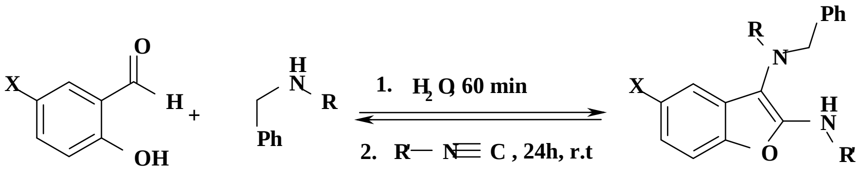
Three-components reactions of an amine derivative and an aldehyde derivative with an isocyanide derivative have been extensively investigated [1-6], In this work, reaction of an isocyanide with an iminium ion intermediate, formed by reaction between 2-hydroxybenzaldehyde derivative and secondary amine in the presence of water proceeds smoothly at room temperature to afford benzo[*b*]furan derivatives in high yield. The structures of these compounds were confirmed by IR, ^{1}H NMR and ^{13}C NMR spectroscopy.

DFT calculations were also carried out on benzo[*b*]furan and its derivatives containing heavy atoms, using B3LYP/6-31G* level of theory by the GAUSSIAN 98 program. The geometrical parameters, HOMO and LUMO energies, dipole moments and charges on atoms of benzo[*b*]furan derivatives were calculated. The detailed results and their discussions would be presented.



References:

[1] Ugi, I.; Lohberger, S.; Karl, R.. In Comprehensive Organic Synthesis; Trost, B. M., Fleming, I., Eds.; Pergamon Press: Oxford, **1991**; Vol. 2, pp 1083–1106.
[2] Dömling, A.; Ugi, I. *Angew. Chem., Int. Ed.* **2000**, *39*, 3169.
[3] Ugi, I. *Angew. Chem., Int. Ed. Engl*. **1982**, *21*, 810.
[4] Nair, V.; Rajesh, C.; Vinod, A. U.; Bindu, S.; Sreekanth, A. R.; Mathess, J. S.; Balagopal, L. *Acc. Chem. Res*. **2003**, *36*, 899.
[5] Yoshida Z, Shibata M, Sugimoto T, *Tetrahedron Letters*, **1984**, *25*, 4223.
[6] Ueno M, Murata I, Kitahara Y, *Tetrahedron Letters*, **1965**, *6*, 2967.

Synthesis of trisubstituted amidines in the presence of solid acid catalysts under solvent –free conditions

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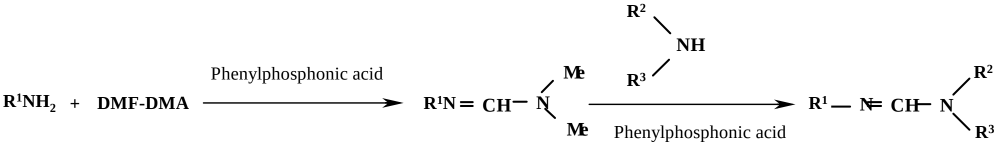
Amidines are an important class of biologically active molecules[1]. Aamidines have been used as pharmacological agents, primarily as pesticides like amitraz and histamine receptor antagonists. Their application as building blocks in polymers, bleaching agents for paper, and ligands in transition metal complexes has also been reported [2-3].

We were particularly interested in developing a facile and straightforward synthetic procedure for preparation of trisubstituted amidines. Furthermore, transformations that increase molecular diversity through a few synthetic steps are well suited for automated parallel solvent-free phase synthesis, as well as being of substantial interest [4].

In this study, we have developed a new and highly efficient method for synthesis of asymmetry amidines using phenyl phosphonjc acid as a catalyst under solvent-free condition. When an amine is treated with *N*,*N*-dimethylformamide dimethyl acetal (DMF-DMA) in the presence of phenylphosphonjc acid after 10-20 min. a quantitative yield of the compound١ is formed. Treatment of compound ***1*** with secondry amines undr solvent-free condition, afforded the amjdines ***2*** in good to excellent yield.



R^1,R^2,R^3= aryl, alkyl

1 ***2***

References:

[1] Flinn, C.; Poirier , R. A. *J. Phys. Chem. A.***2003,** *107,* 11174.
[2] Leung, V. K. S.; Chan, T. Y. K.; Yeung, V. T. F.*J. Toxicol.ÐClinical Toxicol.* **1999**, *37*, 513.
[3] Baxter, G. D.; Barker, S. C. *Insect Biochem. Mol. Biol.* **1999,** 29, 461.
[4] Porcheddu, A.; Giacomelli, G.; Piredda, I. *J. Comb. Chem.* **2009,** *11,* 126.

A facial synthesis for xanthene derivatives by silica supported $CuSO_4$ as an effective and reusable catalyst in water

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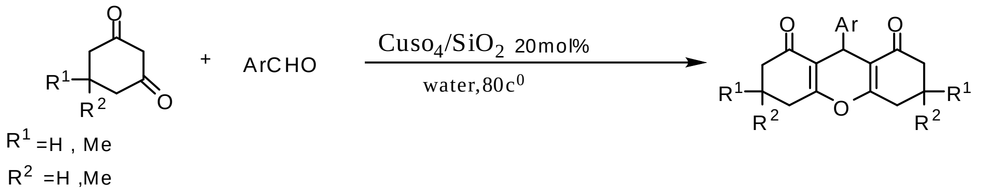
In this article, an easy effective, cheap and environmentally adapted method for synthesis xanthene derivatives by condencation reaction between dimedon with aromatic aldehyds in water as solvent in the presence of silica supported $CuSO_4$ as an effective and reusable catalyst. In recent times, the use of Silica Supported $CuSO_4$ and' green' solvents in organic synthetic processes has gained considerable importance. This method provides several advantages such as simple work-up, environmental friendliness and shorter reaction time along with high yields [1-2].



References

[1] S. Kantevari, R. Bantu, L. Nagarapu, J. Mol. Catal. A: Chem. 2007, 269, 53.

[2] Z. Zhang, Y. Lui, Catal. Commun. 2008, 9, 1715.

[3] K. Venkatesan, S. S. Pujari, R. J. Lahoti, K. V. Srinivasan, Ultrason. Sonochem. 2008, 15, 4548.

[4] H. N. Karade, M. Sathe, M. P. Kaushik, Arkivoc. 2007, 13, 252-258.

Synthesis of 3,4-dihydropyrimidin-2(1*H*)-one azo dyes in the presence of $SbCl_5.SiO_2$ at room temperature

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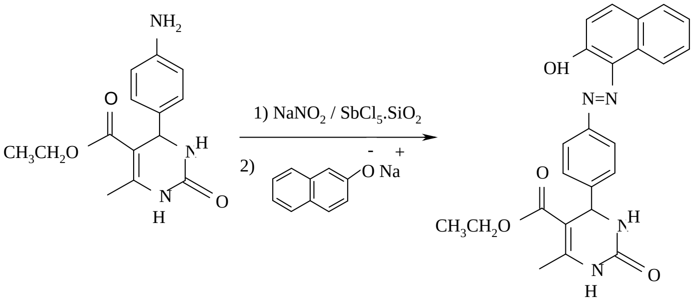
Azo compounds are the most widely class of industrial synthesized organic dyes due to their versatile application in various fields, such as dyeing textile fiber, biological–pharmacological activities and advanced application in organic synthesis [1]. Dihydropyrimidines (thiones) are important compounds exhibiting broad spectra of pharmacological activities [2]. Azo dyes have been synthesized *via* coupling of diazotized aromatic amines with activated aromatic compound. According to literature, aromatic amines have been converted to diazonium salts in the presence of $NaNO_2$ and mineral acid at 0-5 °C. In this report, we have synthesized the 3,4-dihydropyrimidin-2(1*H*)-one azo dyes from biginelli products in the presence of $NaNO_2$ and $SbCl_5$ /SiO_2 at room temperature (Scheme 1).



In conclusion, we have developed an efficient and environmentally benign methodologies for the synthesis of azo dyes in room temperature. The advantages of these methods are reduced reaction times, higher yields, mild reaction condition, easy purification and economic viability of the catalyst.

References:

[1] Karci, F.; Demircali, A.; Sener, I.; *Dyes Pigm*. **2006**, *71*, 90.
[2] Kappe, C. O. *Tetrahedron* **1993**, *49*, 6937.

One pot synthesis of 2-aryl-benzimidazoles and benzothiazoles catalyzed by trans-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane/HCl system

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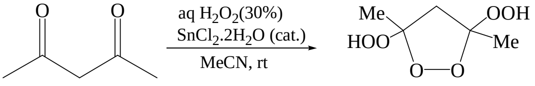
As a part of our ongoing research in the synthesis of *gem*-dihydroperoxides [1-3], and their applications in various organic transformations [4], *trans*-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane has been efficiently prepared in high yield from $SnCl_2.2H_2O$-catalized reaction of acetylacetone with aqueous H_2O_2 (30%) in acetonitrile at room temperature (Scheme **1**) [4].



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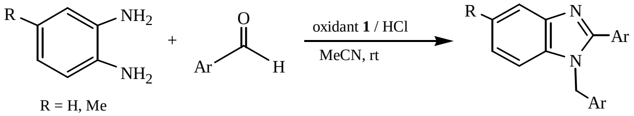
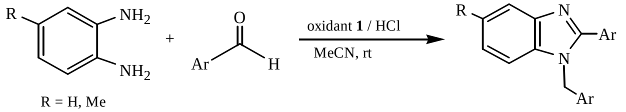
Scheme 1

Trans-3,5-dihydroperoxy-3,5-dimethyl-1,2-dioxolane in the presence of HCl was successfully used for the first time as the oxygen source for the efficient condensation of 1,2-phenylenediamines and 2-aminothiophenoles with various aldehydes into their corresponding 1-benzyl-2-arylbenzimidazoles and 2-arylbenzothiazoles respectively under mild condition (Schemes **2** and **3**). All the reactions proceed smoothly in MeCN at room temperature to provide the products in excellent yields.



Scheme 2.



Scheme 2.

References:

[1] Zmitek, K.; Zupan, M.; Iskra, J. Synthetic strategies for a biologically important class of *gem*-dihydroperoxide and perketal derivatives. *Org. Biomol. Chem.* **2007**, *5*, 3895. (a review).
[2] Azarifar, D.; Khosravi, K.; Soleimani, F. *Synthesis* 2009, 2553.
[3] Azarifar, D.; Khosravi, K.; Soleimani, F. *Molecules*, **2010**, *15*, 1433.
[4] Azarifar, D.; Khosravi, K. *Eur. J. Chem.* **2010**, *1*, 15.

Synthesis of tetrahydrobenzo[b]chromene and 3,4-dihydropyrano[3,2-C]chromene derivatives

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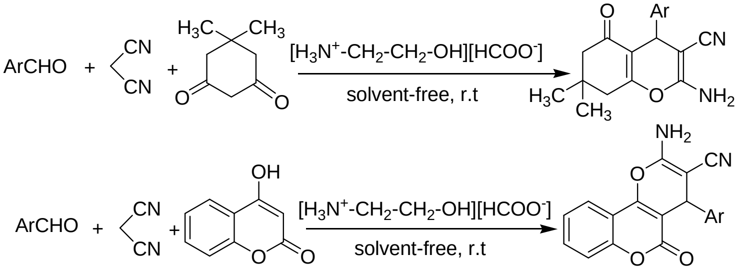
There has been an increasing interest in exploiting the potential of ionic liquids as a reaction media to develop green methodologies; allowing reuse of the catalysts or reagents [1]. This properties and applications prompted us to initiate a systematic exploration on preparation of organic compounds with the help of ionic liquids [2].

In this work, three-component synthesis of tetrahydrobenzo[b]chromene derivatives [3,4] and 3,4-dihydropyrano[3,2-c]chromene derivatives [5,6] by condensing aldehydes, malonitrile, and dimedone or 4-hydroxycoumarin using a catalytic amount of 2-hydroxyethylammonium formate under solvent-free conditions at room temperature is reported (Scheme).



Scheme

A series of differently substituted tetrahydrobenzo[b]pyrans and 3,4-dihydropyrano[3,2-c]chromene derivatives were prepared successfully under solvent-free conditions. The mechanism proposed for the reaction using ionic liquid as catalyst is also described *via* Knoevenagel condensation, Micheal addition and followed cyclization. We also investigated the recycling of the catalyst under solvent-free conditions. The recovered catalyst was reused five runs without any loss of its activities.

References:

[1] M. Khurana, J.; Magoo, D. *Tetrahedron lett*. **2009**, *50,* 7300.
[2] Rebeiro, G.L.; Khadilkar, B.M. *Synthesis*. **2001**, *2001*, 0370.
[3] Wang, L.M.; Shao, J.H.; Tian, H.; Wang, Y.H.; Liu, B. *J. Fluorine. chem*. **2006**, *127*, 97.
[4] Seifi, M.; Sheibani, H. *Catal. Lett*. 2008, *126*, 275.Heravi, M. M.; Alimadadi jani, B.; Derikvand, F.; Bamoharram,F. F.; Oskooei, H. A. *Catal Commun*. **2008**, *10*, 272.
[5] Khurana, J. M.; Kumar, S. *Tetrahedrone Lett*. **2009**, *50,* 4125.

Synthesis of dithiocarbamate by markovnikov addition reaction in aqueous medium

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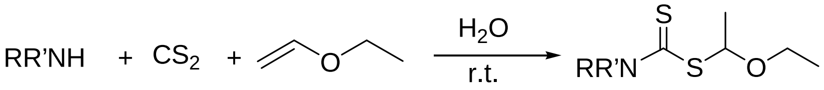
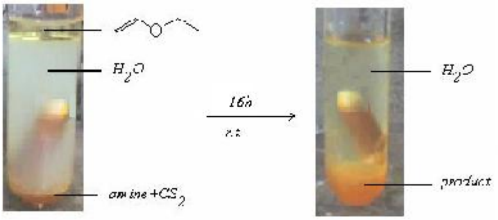
Dithiocarbamates are valuable compounds due to their interesting chemistry and wide utility. These compounds have shown wide applications as pesticides, fungicides in agriculture, sulfur vulcanization in rubber manufacturing [1-3] and radical chain transfer agents in the reversible addition fragmentation chain transfer (RAFT) polymerizations [4].

Here we report an efficient, novel, and invironmentally benign procedure for the Markovnikov addition reaction of dithiocarbamates to alkyl vinyl ethers in aqueous medium without using catalyst at room temperature. The results of the present work show the desired products in excellent yields.





References:

[1] Marinovich, M. ; Viviani, B. ; Capra, V. ; Corsini, E. ; Anselmi, L. ; D'Agostino, G. ; D. Nucci, A. ; Binaglia, M. ; Tonini, M. ; Galli, C. L. Chem. Res. Toxicol. 2002, 15, 26.
[2] Len, C. ; Boulogne-Merlot, A. S. ; Postel, D. ; Ronco, G. ; Villa, P. ; Goubert, C. ; Jeufrault, E. ; Mathon, B. ; Simon, H. ; Agric. *J. Food Chem.* **1996**, *44*, 2856.
[3] Bergendorff, O. ; Hansson, C. ; Agric. *J. Food Chem.* **2002**, *50*, 1092.
[4] Bathfield, M. ; D'Agosto, F. ; Spitz, R. ; Charreyre, M. T. ; Delair, T. *J. Am. Chem. Soc.* **2006**, *128*, 2546.

Chlorodiphenylphosphine/2,3-Dichloro-5,6-dicyanobenzoquinone as a new, selective and neutral system for the mild conversion of aldehydes to *gem*-dichlorides

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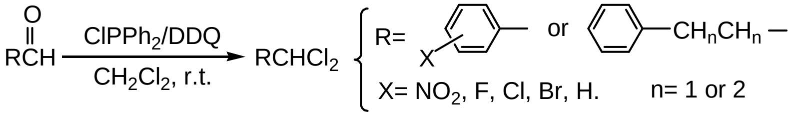
The conversion of aldehydes and ketones to the corresponding *gem*-dichlorides is a very important transformation in organic synthesis because these compounds can serve as precursors to transition metal alkylidenes for carbonyl olefination [1] and also the product dichloroarylmethanes are of value in the pharmaceutical and agricultural industries [2]. Some methods generating geminal dichlorides include for example the use of acid halides in the presence of acid catalysts [3] and $(PhO)_3P/Cl_2$ [4] etc. However, some reported methods in this area contain some disadvantages such as use of toxic reagents, operation at high temperature or in acidic conditions, long reaction times, low selectivity, unsuitability for carbonyl compounds containing enolizable hydrogens, formation of undesired products and low yields. Consequently, there is a need for the development of new methods within neutral media that are more convenient for this important synthetic transformation. In continuation of our works on the new applications of trivalent phosphorus in organic synthesis [5], we now report a mild conversion of aldehydes to their corresponding *gem*-dichlorides using a mixture of chlorodiphenylphosphine and 2,3-dichloro-5,6-dicyanobenzoquinone ($ClPPh_2$/DDQ; 2.5:2.5) under neutral conditions (Scheme). Aldehydes can be efficiently converted to their corresponding *gem*-dichlorides in the presence of ketones, epoxides, amides, carboxylic esters, and phenols with excellent chemoselectivity *via* this method.



In conclusion, the present investigation has demonstrated that the use of $ClPPh_2$/DDQ offers a simple, mild and convenient method avoiding the use of molecular halogen with its harsh handling for the conversion of aldehydes to their corresponding *gem*-dichlorides. Availability and ease of handling of the reagent, high yields, excellent selectivity, easy work up, operation at room temperature in neutral media, and applicability for carbonyl compounds containing enolizable hydrogens can be considered as other advantages of this method. Further studies toward the other applications of this reagent in organic synthesis are in progress in our laboratory.

References:

[1] Takeda, T.; Sasaki, R.; Fujiwara, T. *J. Org. Chem.* **1998**, *63*, 7286.
[2] Olivan, M.; Caulton, K. G. *Inorg. Chem.* **1999**, *38*, 566.
[3] Wolfson, A.; Shokin, O.; Tavor, D. *J. Mol. Catal. A: Chemical* **2005**, *226*, 69.
[4] Spaggiari, A.; Vaccari, D.; Davoli, P.; Torre, G.; Prati, F. *J. Org. Chem.* **2007**, *72*, 2216.
[5] Aghapour, G.; Afzali, A. *Synth. Commun.* **2008**, *38*, 4023.

The structure of 3-(1-Methylpyrrolidin-2-ylidene)-3H-indole sesquihydrate and 1-[(*E*)-4-(5-Bromo-1*H*-indol-3-yl)-1-methyl-2, 5, 6, 7-tetrahydro-1*H*-azepin-2-ylidene] propan-2-one crystals

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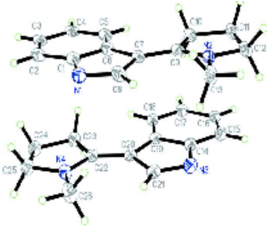
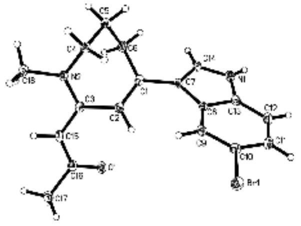
Vilsmeier reaction of indole using a tertiary amide in combination with phosphorous oxychloride give rise to 3-acylindoles corresponding to the acyl residue of the amide. However, when 1-methylpyrrolidin-2-one is used as the amide component, 3-(1-Methylpyrrolidin-2-ylidene)-3H-indole **(1)** is the product. In order to understand the chemical reactivity of **(1)**, we felt it was important to crystallographically establish the planar structure, predicted by resonance contributor, and also to verify the geometry of the exocyclic double bond. The asymmetric unit of **(1)** contains two similar molecules of **(1)**, together with three water molecules. The two molecules are essentially planar. In the crystal, the two crystallography different molecules are linked by O-H…N hydrogen bonds to a network of hydrogen-bonded water molecules. O-H…O interactions are also present.



$C_{13}H_{14}N_2.1.5H_2O$ **(1)**



$C_{18}H_{19}BrN_2O$ **(2)**

5-Bromo-3-(1-methylpyrrolidin-2-ylidene)-3*H*-indole was shown to be a remarkably strong base. The reaction of 5-Bromo-3-(1-methylpyrrolidin-2-ylidene)-3*H*-indole with pentane-2,4-dione give 1-[(*E*)-4-(5-Bromo-1*H*-indol-3-yl)-1-methyl-2,5,6,7-tetrahydro-1*H*-azepin-2-ylidene]propan-2-one **(2)** as yellow needle crystals (after crystallization in n-hexane/acetone).

The seven membered azepine ring adopts a twist-boat conformation. The planar 5-bromoindole bicycle is not coplanar with the enone in the seven-membered azepine ring. The N-H…O hydrogen bond between the indole ring and carbonyl group is present.

References:

[1] Al-khawaja, I. K.; Beddoes, R. L.; Joule, J. A.; Mills, O, S. *J. Chem. Res (s).* **1984**, 2738.
[2] Bishop, D. I.; Al-khawaja, I. K.; Joule, J. A. *J. Chem. Res (s).* **1981**, 4279.
[3] Helliwell, M. ; Aghazadeh, M. ; Baradarani, M. M. ; Joule, J. A. *Acta Cryst*. E*65*, **2009**, 03114.
[4] Helliwell, M. ; Aghazadeh, M. ; Baradarani, M. M. ; Joule, J. A. *Acta Cryst*. E*66*, **2010**, 01532.

Synthesis of a novel class of aza crown macrocycles and lariat crown ethers containing two 1,2,4-triazole rings and naphthalene as subunits

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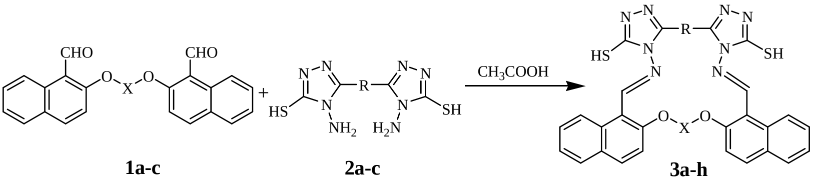
Since Pedersen's discovery of crown ethers and their abilities to bind strongly with metal ions in 1967 [1], the study of crown ethers has grown at an incredible rate. The incorporation of oxygen, nitrogen and sulfur donor atoms in the macrocycles will also markedly affect their complexing properties because of the hard (O, N) and soft (S) character of the donor atoms and the exodentate tendency of the sulfide linkages [2]. Other changes involve the insertion of aromatic and/or heterocyclic ring systems into the macrocycles [3]; heterocyclic groups provide rigidity and are able, in some cases, to form complexes through their soft donor atoms [4]. The wide interest in the construction of synthetic macrocyclic compounds containing five- and six-membered heterocyclic rings as subunits has led to the preparation of a range of such compounds which have been shown to possess very interesting properties in a variety of fields [5].

In continuation of our effort to develop the synthesis of new azathiacrown macrocycles and lariat ether [6,7], we report here the synthesis of a series of 18–21 membered aza crown macrocycles fused with two 1,2,4-triazole rings containing N, O inside the macrocyclic ring as donor atoms and possess pendant thiol groups as precursor for the synthesis of lariat ether macrocycles.



1a-c **2a-c** **3a-h**

References:

[1] Gatto, V. J.; Gokel, G. W. *J. Am. Chem. S*oc. **1984,** *106*, 8240.
[2] Richard, E. D.; Milton, D. G. *J. Am. Chem. Soc.* **1976**, *98,* 762.
[3] Newkome, G. R.; Sauer, J. D.; Rober, J. M.; Hager, D. C. *Chem. Rev.* **1977**, *77*, 513.
[4] Bradshaw, J. S. *In Comprehensive Supramolecular Chemistry*; Gokel, G. W. (Ed.); Pergamon: New York, **1996**, PP. *1*, 35.
[5] Weber, E.; Kohler, H. J.; Reuter, H. J. *J. Org. Chem.* **1991**, *56*, 1236.
[6] Foroughifar, N.; Mobinikhaledi, A.; Ebrahimi, S.; Moghanian, H.; Bodaghi Fard, M. A.; Kalhor, M.; *Tetrahedron Lett.* **2009,** *50,* 836.
[7] Foroughifar, N.; Mobinikhaledi, A.; Ebrahimi, S.; *Synthesis* **2009**, *15,* 2557.

A novel and efficient one-pot method for synthesis of 2-imino-4-oxo-6-aryl-1,2,3,4-tetrahydropyrimidine-5-carbonitrile under mild reaction

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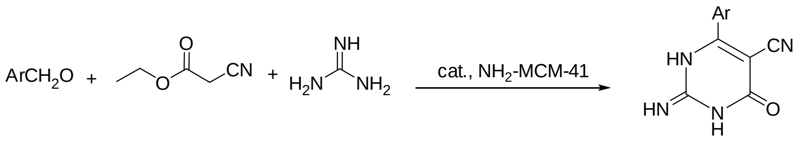
Heterocycles are ubiquitous to among pharmaceutical compounds [1]. Pyrimidine moiety is an important class of *N*-containing heterocycles widely used as key building blocks for pharmaceutical agents. It exhibits a wide spectrum of pharmacophore as it acts as bactericidal, fungicidal [2], analgesic [3], antihypertensive [4] and anti-tumor agents [5]. Alternative strategies for synthesis of the pyrimidine derivatives involving different catalysts and conditions have been developed.

In continuation of our investigations on the synthesis of dihydropyrimidines (DHPMs) [6], herein we describe a novel and efficient one-pot method for the preparation of 2-imino-4-oxo-6-aryl-1,2,3,4-tetrahydropyrimidine-5-carbonitrile derivatives from cyclocondensation of aldehydes, ethyl cyanoacetate and guanidine using a catalytic amount of functionalized MCM-41 under mild conditions reaction. This new method has the advantage to give high yields, to be completed in short reaction times, without using any strong mineral alkaline and simple product isolation procedure.



References:

- [1] Eicher, T.; Hauptmann, S. The Chemistry of Heterocycles, second ed. Wiley-VCH, Weinheim, **2003**.
- [2] Pershin, N.G.; Sherbakova, L. I.; Zykova, T. N.; Sakolova, V. N. *World Rev. Pest. Contr.* **1972**, *35*, 466.
- [3] Regnier, G.; Canevar, L.; Le, R. J.; Douarec, J. C.; Halstop, S.; Daussy, J. *J. Med. Chem.* **1972**, *15*, 295.
- [4] Winter, C. A.; Fisley, E. A. R.; Nuss, G. W. *Proc. Soc. Exp. Biol. Med.* **1962**, *111*, 544.
- [5] Suguira, K.; Schmid, A. F.; Schmid, M. M.; Brown, F. G. *Cancer Chemother. Rep.*, Part 2, 3 (1) 1973, 231.
- [6] (a) Mirza-Aghayan, M; Bolourtchian, M.; Hoseini, M. *Synth. Commun.*, **2004**, 34, 3335; (b) Mirza-Aghayan, M., Moradi, A.; Bolourtchian, M.; Boukherroub, R. *Synth. Commun.* **2010**, *40*, 8; (c) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. *J. Iran. Chem. Soc.* **2010**, *7*, 269.

Study of the wittig reaction of 1,3,4-thiadiazol-2-yl-amines with dialkyl acetylendicarboxylates in the presence of triphenylphosphine

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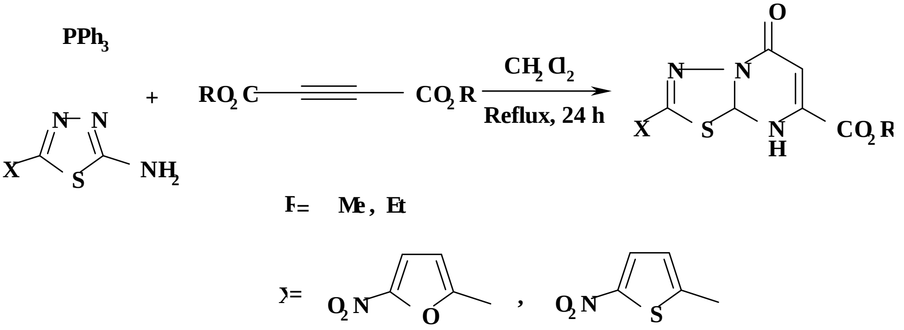
During recent years there has been intense investigation of different classes of thiadiazole compounds, many of which are known to possess interesting biological properties.They are also known to possess antiviral activity and especially effective againts HIV [1].

It is known that many 1,3,4-thiadiazole and 1,2,4-triazole derivatives have biological activity, with their antibacterial, antimycobacterial, antimycotic, antifungal, antidepressive and cardiotonic, action being notable [2].

The wittig reaction has evolved to include many variations that constitute some of the most powerful processes for the construcation of carbon-carbon bonds.The importance of intramolecular wittig reactions in the synsthesis of cycloalkenes and unsaturated heterocyclic compounds can hardly be overestimated [3].

Herein we report the reaction of 1,3,4-thiadiazol-2-yl-amines with dialkyl acetylenedicarboxylats in the presence of triphenylphosphine.



References:

[1] Mayekar, S. A.; Mulwad, V. V.; *Indian J. Chem.* **2008**, *47B,* 1438.
[2] Ashutosh, B.; Ankur, J.; kumar, N. R.; Sonia, G.; Niharika, S.; Vivek, D.; Pramod, S.; *J Pharmaceutical Sciences and Drug Researc,* **2009**, *1(3)* ,207.
[3] Yavari, I.; Adib, M.; Sayahi, M. H.; *Tetrahadran Lett.* **2002**, *43,* 2972.

Novel soluble, heat-resistant, optically active polyesters

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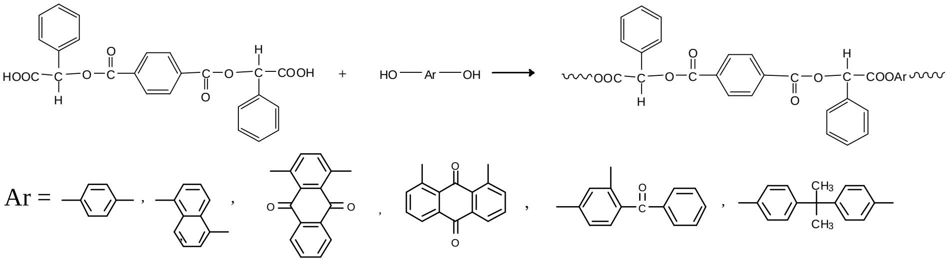
Aromatic polyesters (polyarylates) are one of the most important classes of high temperature polymers that have good heat-resistance. But their industrial uses are limited by their difficult processability due to their high melting point, high glass transition temperature and limited solubility in most organic solvents [1,2]. On the other hand, some certain properties could be introduced to the polymers by structural modification. One example in this field is preparation of optically active polymers which may take part an important position in the molecular arrangement and assembly that is critical for optoelectronics supramolecular structure [3]. Therefore, much attention has been paid to different synthetic methods in this area for improving their solubility and processability (including introduction of flexible groups, bulky groups and disruption of symmetry and regularity of main chain) through the design and synthesis of new and specific monomer to obtain polymers with improved solubility while maintaining thermal stability. In this research, a new optically active diacid was prepared and named terephthalic acid bis-(carboxyphenylmethyl) ester (TBE), was used as monomer for the preparation of related optically active polyesters. Polycondensation reaction of this monomer with different aromatic diols in the presence of benzene sulfonyl chloride led to preparation of different polyesters.



HQ (1) DHN (2) 1,4-DHAQ (3) 1,8-DHAQ (4) DHBP (5) BPA (6)

The prepared monomer and all the polymers were characterized by conventional methods. Thermal and physical properties of the polyesters including thermal stability, thermal behavior, solution viscosity, and solubility behavior in addition to optical activity were studied and they showed nice balance of mentioned properties including enhanced solubility, heat-resistant, and optical activity.

References:

[1] Cassidy, P. E. Thermally stable polymers. Dekker: New York, **1980**.
[2] Mehdipour-Ataei, S.; Zigheimat, F. *Des. Mono. Polym.* **2007**, *10*, 145.
[3] Peng, G.; Li, Q.; Yang, Y.; Wang, H.; Li, W. *Polym. Adv. Technol.* **2008**, *19*, 1629.

Synthesis of some structurally rigid glycoluril-derived molecular clips

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In recent years a series of synthetic receptors derived from the concave molecule glycoluril have been developed by Nolte's group [1-3]. These U-shaped receptors, which are known molecular clips, bind dihydroxybenzenes by hydrogen bonding interactions between the hydroxyl groups of the guest and the urea carbonyl groups of the host and by π-π stacking interactions between the guest and the host side-walls. Also, molecular clips with large variety of side walls have been synthesized and the supramolecular chemistry of these clips has been extensively studied [4,5].

We report herein the synthesis of a series of new structurally rigid glycoluril clips with different amounts of steric hindrance around their cavities. The geometry of the clips would be the result of a balance of the two factors: 1) The length of the used alkyl chain for applying of the more rigidity to the glycoluril scaffold of the clips, and 2) the extent of the steric interactions around the cavity because of the methyl substituents.

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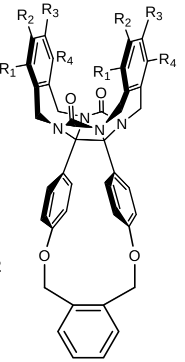
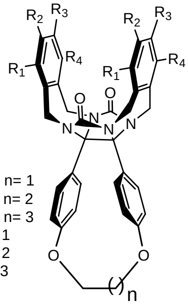
2a R_1 , R_2 , R_3 , R_4 = H
2b R_1 , R_4 = H; R_2 , R_3 = Me
2c R_1 , R_2 , R_3 , R_4 = Me



2

1a R_1 , R_2 , R_3 , R_4 = H; n= 1
1b R_1 , R_2 , R_3 , R_4 = H; n= 2
1c R_1 , R_2 , R_3 , R_4 = H; n= 3
1d R_1 , R_4 = H; R_2 , R_3 = Me; n= 1
1e R_1 , R_4 = H; R_2 , R_3 = Me; n= 2
1f R_1 , R_4 = H; R_2 , R_3 = Me; n= 3
1g R_1 , R_2 , R_3 , R_4 = Me; n= 1
1h R_1 , R_2 , R_3 , R_4 = Me; n= 2
1i R_1 , R_2 , R_3 , R_4 = Me; n= 3



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References:

[1] Sijbesma, R. P.; Nolte, R. J. M. *Top. Curr. Chem.* **1995**, 179, 25.
[2] Rowan, A. E.; Elemans, J. A. A. W.; Nolte, R. J. M. *Acc. Chem. Res.* **1999**, 32, 995.
[3] Elemans, J. A. A. W.; Rowan, A. E.; Nolte, R. J. M. *Ind. Eng. Chem. Res.* **2000**, 39, 3419.
[4] Reek, J. N. H.; Elemans, J. A. A. W.; Nolte, R. J. M. *J. Org. Chem.* **1997**, 62, 2234.
[5] Reek, J. N. H.; Priem, A. H.; Engelkamp, H.; Rowan, A. E.; Elemans, J. A. A. W.; Nolte, R. J. M. *J. Am. Chem. Soc.* **1997**, 119, 9956.

Synthesis of meso-substituted porphyrin immobilised on SBA-15 surface

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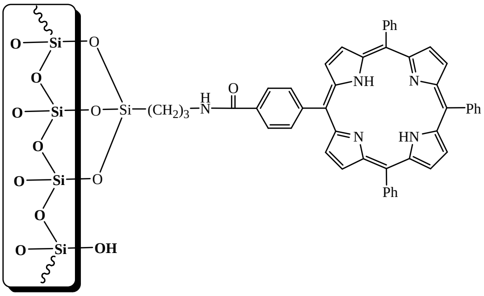
Inorganic–organic hybrids are now attracting much attention in terms of new functional materials. Recently, many researchers have studied the incorporation of dyes into micro or mesoporous materials such as zeolite, mesoporous silica SBA-15 and clay minerals [1–3]. The resulting materials may exhibit unique physicochemical properties and are expected to be used as adsorbents, catalysts and catalyst supports and in optical and electrical applications. In these cases, silica gel (SiO_2) has been widely used as the carrier, because of its wide surface area and ability to be immobilized [4–6]. The objective of this work is the development of new catalytic systems based on the amine-functionalized nanosilica that are capable of immobilization of heavy metal cations, water treatment and industrial effluent treatment plants.

Preparation of 4-(methoxycarbonyl)phenyltriphenylporphyrin was performed using the Lindsey method [7]. The synthesized porphyrin was hydrolyzed in basic media .SBA-15 was synthesized and characterized using X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Thermogravimetric Analysis (TGA) and Fourier Transfer Infrared spectroscopy (FT-IR). Then it was modified using 3-aminopropyltriethoxysilane and grafted to the surface of the functionalized porphyrin. The grafted material was characterized with FT-IR spectroscopy.



References:

[1] Ogawa, M.; Nakamura, T.; Mori, J.; Kuroda, K. *Micropor. Mesopor.Mater.* **2001**, *48*, 159.
[2] Xi, H.; Zhang, Y.; Li, Z., Qian, X.; Yin, J.; Zhu, Z. *J. Mater. Sci. Lett.* **2002**, *21*, 1817.
[3] Takagi, S.; Tryk, D. A.; Inoue, H. *J. Phys. Chem.* **2002,** *106*, 5455.
[4] Rodrigues, M. A.; Tada, D. B.; Poloto, M. J.; Baptista, M. S. J. *Non-Cryst. Solids* **2002,** *304*, 116.
[5] Zhang, X. ; Jin, Z.; Li, Y.; Li, S.; Lu, G. *J. Power Sources*, **2007,** 166, 74.
[6] Latour, V.; Pigot, T.; Mocho, P.; Blanc, S.; Lacombe, S. *Catal. Today* **2005,** *101*, 359.
[7] Lindsey, J. S.; Wagner, R. W.; *J. Org. Chem.* **1989,** *54*, 828.

Puckering energy of 4-X-3-hydro,1-oxa-3-aza cyclopent-4-en-2-ylidene and their rings for M = C, Si, Ge, Sn and Pb (where X = H, F, Cl, Br and I)

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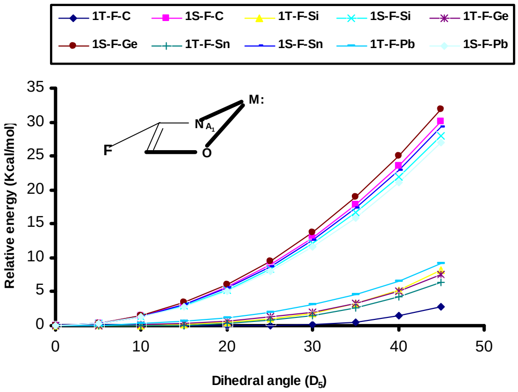
Divalent carbenes and their heavier analogues are intensely reactive, and the studies of their properties are often made through matrix isolation techniques [1]. Among the relatively more stable carbenes, the cyclic species, and their halogenated derivatives, have held a special place in the chemistry of divalent carbon intermediates.

In order to confirm global minima, for carbenes and their heavier analogues, energy surface studies are necessary [2], since puckering of cyclopent-4-en-2-ylidene rings and their heavier analogues may alter positions of the global minima. Puckering energy are presented for carbenes (which include 4-X-M-cyclopent-4-en-2-ylidene rings) as a function of dihedral angle N-M-O-C (for M = C, Si, Ge, Sn and Pb). The puckering energy appears higher for singlet states than their corresponding triplet states.



References:

[1] P.P. Gaspar, R. West, in: Z. Rappoport, Y. Apeloig (Eds.), Chemistry of Organic Silicon Compounds, vol. 2, Wiley, Chichester, 1997, p. 2436.

[2] M.Z. Kassaee , S. Arshadi, M. Acedy, E. Vessally Journal of Organometallic Chemistry 690 (2005) 3427–3439.

A simple, efficient and green procedure for synthesis of 2-amino-4-substituted hexahydroquinoline derivatives in/on water

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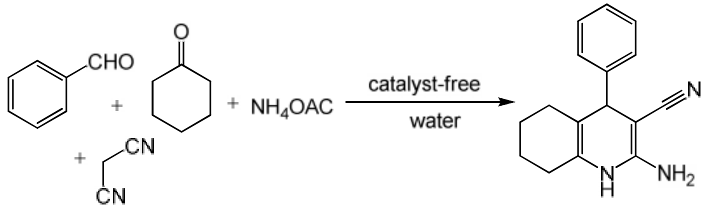
Green chemistry emphasizes the development of environmentally benign chemical processes and technologies [1]. Designing organic reactions in aqueous media is attractive area in green chemistry [2]. Water is an abundant and environmentally benign solvent. Developing a simple, ecofriendly reaction protocol for the synthsis of compound libraries of medicinal scaffolds is an attractive area of research in both academic and pharmaceutical R&D [3].

Quinoline derivatives are important biologically active compound showing anticancers, antimalarialas and antibacterials activity [4].

In the light of these facts, and as a continuation of our work, the present work reports the synthesis of some novel 2-amino-4-substituted hexahydroquinoline derivatives by a four-component catalyst-free reaction in aqueous media. Green aspects of this reaction include: (i) being a multi-component reaction is step economic, (ii) water is being used as the reaction medium therefore use of conventional volatile organic solvents is avoided, (iii) avoidance of catalyst.



References:

[1] P. T. Anastas, J. C. Warner, *Green Chemistry: Theory and Practic,* Oxford University Press, Oxford, UK, 1998; P. T. Anastas, T. Williamson, *Green Chemistry, Frontiers in Benign Chemical Synthesis and Process,* Oxford University Press, Oxford, UK, **1998**

[2] C. I. Herrerias, X. Yao, Z. Li, C. Li, *Chem. Rev.*, **2007**, *107*, 2546; C. J. Li, T. H. Chan, *Comprehensive Organic Reactions in Aqueous Media*, Eds. John Wiley & Sons, **2007**; P. A. Grieco, *Organic Reactions in Water*, Thomson Science, Glasgow, Scotland, **1998**.

[3] A. Dömling, *Chem. Rev.*, **2006**, *106*, 17; I. Kanizsai, S. Gyónfalvi, Z. Szadonyi, R. Sillanpä and F. Fülöp, *Green Chem.*, **2007**, *9*, 357.

[4] M. M. Ghorab, F. A. Ragab, M. M. Hamed, *Eur, J. Med. Chem.* **2009**, *44*, 4211-4217.

Study of the essential oils composition of leaves and flowers of Calendula tripterocarpa and Centaurea rhizantha from Iran

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The genus *Calendula* and *Centaurea* (compositae) comprises species, which are found wild in Iran [1,2]. The oils of *Calendula* species have been the subject of only a few investigations. Chemical compositions of some *Calendula* species have shown flavonoids, iridoids, phenyl-ethanoid glycosides, diterpene glycosyl esters and nortriterpenes [3]. These latter investigations refer to *C. zuvandica* from Turkey [4], *C. pseudoscabiosa subsp. pseudoscabiosa* and *C. hadimensis* from Turkey [5]. In our research on the essential oil of the plants of Iran, we have investigated on the composition of the essential oils of leaves and flowers of *Calendula tripterocarpa* and *Centaurea rhizantha.*

The oil was separately isolated from the leaves and flowers of *Calendula tripterocarpa* and *Centaurea rhizantha* for 3 h with a Clevenger-type apparatus and an average of 150gr was used for each experiment.

The composition of essential oil samples obtained by hydrodistillation of the leaves and flowers of *Calendula tripterocarpa* and *Centaurea rhizantha*, were investigated by GC and GC–MS. Fifteen components in the leaves oil of *Calendula tripterocarpa* 93.6% of the total oil, and 17 components in the flower oil of *Calendula tripterocarpa*, representing 96% of the total oil, were identified. Thirty components were identified in the leaves oil of *Centaurea rhizantha* with caryophyllene oxide (18.5%), spathulenol (15.9 %) and 2-methoxy-4-vinil phenol (9.3 %) as main constituents. Twenty-three compounds were characterized in the flower oil of *Centaurea rhizantha* with 1, 8-cineole (61.7 %), trans-pinocarveol (7.7 %) and p-cymene (4.1 %) as main components.

References:

[1] Newall, C. A.; *A Guide for Health care Professionals*. Pharmaceutical Press: London, **1996**, 231.
[2] Rechinger, K. H.; *Flora Iranica*. Graz, Austria, **1982**, 158.
[3] Bal, Y.; Kaban, S.; Kirimer, N.; *J. Essent. Oil Res.* **1989**, 55, 105.
[4] Dural, H.; *Journal of Sys. & ecology*, **2003**, 31,1417.
[5] Flamini, G.; Ertugrul, K.; cioni, P. L.; *Journal of Biochem. Syst. Ecol***. 2002**, 30, 953.

Electronic effects at α and β-position for the energy surface of divalent five-membered ring XC_4H_3M (X= H, F, Cl and Br; M=C, Si and Ge)

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Carbenes have been extensively studied both experimentally and theoretically [1]. Moreover, there has been significant synthetic interest in the production of the silylene and germylene analogues of the carbene [2,3]. The five-membered cyclic conjugated carbene, cyclopentadienylidene, has been observed in the interstellar space [4]. In this work, thermal energy gaps, ΔE_{s-t}; enthalpy gaps, ΔH_{s-t}; Gibbs free energy gaps, ΔG_{s-t}, between singlet (s) and triplet (t) states of XC_4H_3M were calculated using the GAUSSIAN 98 program DFT calculations indicated that increase electronegativity of substituents at α positon cause to intensify ΔG_{s-t} and decrease electronegativity of substituents lead to reduce the ΔG_{s-t} of XC_4H_3M. (X= -F > -Cl > -Br > -H). Also, for example when X = F the order of values ΔG_{s-t} is: (FC_4H_3C < FC_4H_3Si < FC_4H_3Ge). Studying the relationship between all parameters (different energy types, electron energies of the frontier molecular orbitals (HOMO and LUMO), chemical hardness (η), chemical potential (μ), Dipole Moment (D), electrophilicity (ω), geometry parameters (Non-dihedral) and total charge on atom) are studied.Also DFT calculations indicated that Gibbs free energy gaps, ΔG_{s-t} were changed at β position in the following order when M = C; Cl(-9.92 kcal/mol) > Br (-9.69 kcal/mol)> CH_3 (-9.67 kcal/mol)> H (-9.59 kcal/mol) > CF_3(-9.42 kcal/mol) > F (-9.31 kcal/mol)> NO_2 (-8.60 kcal/mol) > OH(-8.57 kcal/mol) > NH_2(-6.33 kcal/mol). ΔG_{s-t} was changed in the following order when M = Si; NH_2 (23.27 kcal/mol)> OH (20.17 kcal/mol)> F (19.56 kcal/mol)> Cl (18.57 kcal/mol)> Br (18.36 kcal/mol)> CH_3 (17.06 kcal/mol)> H (15.26 kcal/mol)> CF_3 (14.44 kcal/mol)> NO_2 (13.11 kcal/mol). Morever, in the following order when M = Ge; NH_2 (30.82 kcal/mol) > OH (27.92 kcal/mol)> F (27.36 kcal/mol) > Cl (25.97 kcal/mol)> Br (25.66 kcal/mol)> CH_3 (24.03 kcal/mol)> H (22.79 kcal/mol)> CF_3 (22.59 kcal/mol)> NO_2 (21.72 kcal/mol). The details would be presented and discussed.

References:

[1] Parham, W.E., Loew, F.C., Schweizer, E.E, *Journal of Organic Chemistry 24*,**1959**, 1900.
[2] Atwell, W.H., Weyenberg, D.R., *J. Am. Chem. Soc. 90*, **1968**, 3438.
[3] Sefcik, M.D., Ring, M.A., *Journal of Organometallic Chemistry* 59, **1973**, 167.
[4] Collins, C.L., Davy, R.D., Schaefer III, H.F. *Chemical Physics Letters* 171, **1990**, 259.

The synthesis and characterization of 5-(4-methylphenyl)-2-alkyl-2H-tetrazole

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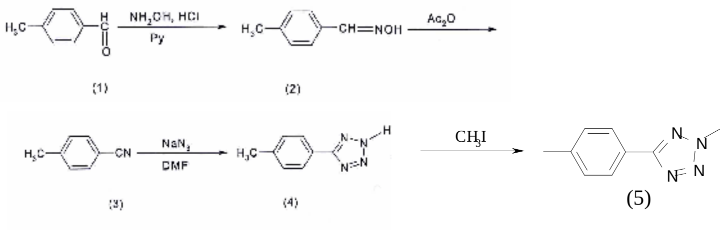
The chemistry of tetrazoles has gained increasing attention since the early 1980s, mainly due to their role in variety of synthetic and industrial processes [1]. Alkylation of tetrazoles in basic medium leads to formation of 1- and 2-alkyl tetrazole isomers. Generally, it appears that electron-donating substitutions at the 5-position of tetrazoles tend slightly to favor alkylation at position 1 of tetrazole anions, while electron-withdrawing substitutents tend to favor alkylation at position 2 [2]. In this research work, we described the synthesis of new compounds of these families. Therefore 4-methyl benzaldehyde (1) was converted to 4-methyl benzaldoxime (2) , by using NH2OH, dehydration of compound 2 with acetic Anhydride obtained 4-methyl benzonitrile (3) , The 5-(4-methyl phenyl)- 2H- tetrazole (4) was synthesized by [3+2] cycloaddition reaction between compound 3 and NaN3 . Then, compound 4 reacted with CH3I and produced 2-methyl-5-phenyl-2H-tetrazole(5). The structures of all the synthesized compounds were confirmed by FT-IR, 1HNMR and 13 CNMR spectroscopies.



References:

[1] Butler, R.N. *The Comprehensive Heterocyclic Chemistry II*, **1996**, *4*, 621.

[2] Dabbagh, H.A.; Mansoori, Y.; Jafary, M.; Rostami, M. *Journal Chemistry Research,* **2000**, *5*, 442.

Conformational effects of the IsoLeusyn side chain on the stability of structure for HOC-GLY-L-ILE-GLY-NH_2 tripeptide motif Ab initio study

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During the past 50 years, protein chemists have simplified their approach to study of protein folding by separating the problem of backbone conformation from side-chain conformation, as well as from the problems of nearest neighbors and long-rang interactions [1].
Tripeptide models are increasingly in peptide folding studies. In a tripeptide, three amino acid residues are bound together at their amid groups, forming a short oligopeptid chain, although the amino acids and peptides present in living systems exclusively were L isomers, the D isomers are often found in the cell walls of bacteria and in antibiotics that attack them [2].
In this study, we want to find most stable structure, conformations of the HCO-GLY-L-ILEU-GLY-NH_2 were optimized by using Ab initio calculations at the HF/6-31G(d) level of theory. our tripeptide divided into three separate segments which defined by their torsional angles, φ, ψ, ω as presented (Fig. 1).

side chain has two dihedral angels : χ_1,χ_2 that we have rotation around them in two stages, first: different conformers that obtained from the rotation of Isoleusyn side chain around $<N_4C_6C_8C_{12}$ dihedral angle (χ_1) at 30^0 intervals from 0^0 to 360^0, second: χ_1 was kept in three minima and then rotation around $<C_6C_8C_{12}C_{13}$ dihedral angle (χ_2) similar to previous stage.

Our results indicate that:

1- Three minima for χ_1 are in gauche(-), gauche(+), anti states with: -593322.65, -593322.35, -593321.79 Kcal/Mol energies, respectively.

2-Three minima for χ_2 are in:180, 210, 240 angels when the χ_1 was kept in gauche(-) state.

3-The gauche(-) – gauche(-) is the most stable conformer with: -593322.70 Kcal/Mol energy.

4-The angels of optimized backbone structure are close to 180.

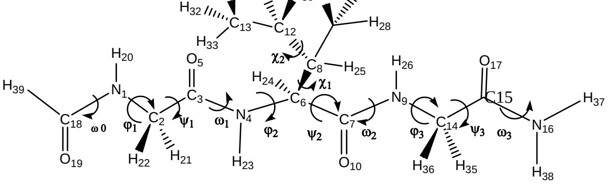

Fig. 1. Schematic diagram with torsional angle definitions for HCO-GLY-ISLEU-GLY-NH_2

References:

[1] Chou P.Y.; Fasman G., *Biochemistry*. **1974**, *13*, 211.
[2] Perczel, A.; McAllister, M.A.; Csa´sza´r, P.; Csizmadia I.G., *Am J.Chem. Soc*. **1993**, *288*, 115.

Regioselective synthesis of spiro bridgehead bicyclic *N*-heterocycles via 1, 3 - dipolar cycloaddition reaction of azomethin ylides

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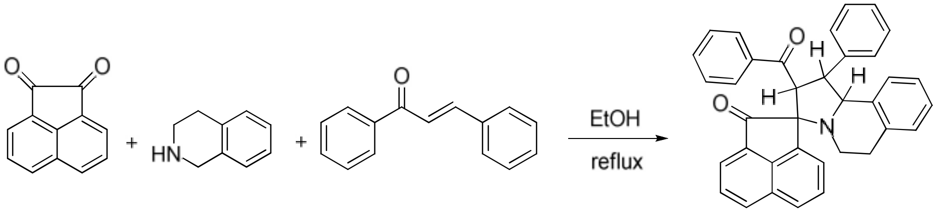
Multicomponent 1,3-dipolar cycloaddition reactions are considered to be one of the most useful processes for the construction of five membered heterocyclic ring systems[1]. In particular, the chemistry of the azomethine ylide has gained significance in recent years for the construction of nitrogen-containing five-membered heterocycles, which are often the central ring systems of numerous natural products [2]. Among the various nitrogen-containing heterocycles, functionalized pyrrolidine alkaloids constitute classes of compounds with significant biological activity [3].

In this letter, we have chosen 1,2,3,4- tetrahydroisoquinoline, acenaphthaquinone and various chalcones for our studies. The reaction of acenaphthaquinone with 1,2,3,4-tetrahydroisoquinoline in boiling ethanol grives rise to the intermediate azomethine ylide which has been trapped by variety derivatives of chalcon to produce bridgehead bicyclic cycloadducts, as evidenced by thin layer chromatography and mass, ^{1}H and ^{13}C NMR spectral.



References:

[1] Harwood, L. M.; Vickers, R. J. In *The Chemistry of Heterocyclic Compounds: Synthetic Applications of 1,3-Dipolar Cycloaddition Chemistry Toward Heterocycles and Natural Products*; Padwa, A., Pearson, W. H., Eds.; Wiley and Sons: New York, NY, **2002**;.

[2] Poornachandran, M.; Raghunathan, R.; *Synthetic Communications*. **2007**, 37, 2507.

[3] (a) Suresh Babu, A. R.; Raghunathan, R.; Tetrahedron Lett. **2007**, *48*, 6809; (b)Molineux, R. J. *In Alkaloids: Chemical and Biological Perpsective*; S. W. Pelletier (Ed.); Wiley: New York, **1987**; Chapter 1.

A new chalcon derivative isolated from Viburnum lantana L.

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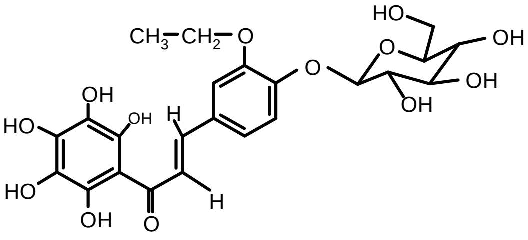
Chalcon derivatives one of important secondary metabolism products, occur in the plants and classified in flavonoids group. These compounds have some very important medicine and biological especially antiradical, antioxidant and prevent cancer effects [1]. *Viburnum* is one of the genuses in Caprifoliaceae family and *V. lantana* is permanent shrub, and one of the species in *Viburnum* [2, 3]. Leaves and fruits of *V. lantana* have been reported to be used to astringent, anti-inflammatory and therapeutic in folk medicine.

In this study, the leaves of plants was collected from Khalkhal area and dried in shade and then subjected to methanol extraction. A new glycosyl flavonoid (chalcon derivative) Trans–3–Ethoxy–4–O-(glucopyranoside) – 2', 3', 4', 5', 6' –pentahydroxy chalcone (compound **1**) has been isolated from the leaves of *Viburnum lantana* L. and purified by column chromatography, TLC and preparative TLC techniques. The structure was elucidated by using ^{1}H-NMR, ^{13}C-NMR and Mass spectroscopy methods and 2D- NMR such as HMQC, HMBC and HOMODEC. experiments.



(1)

References:

[1] Picard, D.; The biochemistry of green tea polyphenols and their potential application in human skin cancer; Alt Med. Rev., **1996,** 1, 31 and 103- 111.
[2] Mozaffarian, V.; *A Dictionary of Iranian Plants Names,* Farhang Moaser, Tehran, **2007**.
[3] Ghahreman, A. *Iranian colour flora*, Research Institute of Forests and Rangelands with Tehran University; (**2003**), Vol. 20, No 2499.

Synthesis of photoactive and thermal polyimides from diamine containing triaryl imidazole pendent group

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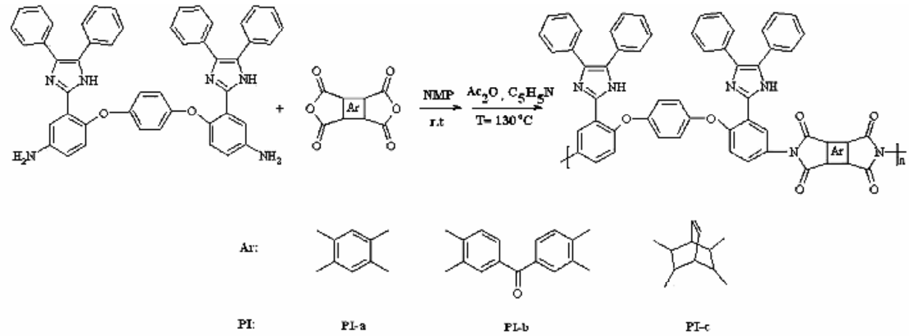
Novel fluorescent polyimides (PIs) were prepared from a new diamine, of 4-(4-(4-amino-2-(4,5-diphenyl-1H-imidazol-2-yl)phenoxy)phenoxy)-3-(4,5-diphenyl-1H-imidazol-2-yl)benzenamine, and three tetracarbonylic dianhydrides. The new symmetrical diamine was successfully synthesized by the nucleophilic substitution reaction of hydroquinone with 2-(2-chloro-5-nitrophenyl)-4, 5-diphenyl-1H-imidazole (**I**). The PIs are amorphous and soluble in polar aprotic solvents and demonstrate a film-forming capability; their inherent viscosities ranged from 0.43 to 0.82 dL/g. They had useful levels of thermal stability associated with relatively high T_gs (245-274 °C), 10% weight loss temperatures in excess of 500 °C, and char yields at 600 °C in air up to 62%. The PIs show emission in dilute (0.2 g/dL) DMAc solution with photoluminescence (PL) quantum yields in the range of 0.11-0.25 The chemiluminescence activity of PIs in the presence of peroxyoxalate was also investigated.



References:

[1] Ghaemy, M.; Alizadeh, R. *Eur. Polym. J.* **2009**, *45*, 1681.
[2] Ghaemy, M.; Alizadeh, R.; Behmadi, H. *Eur. Polym. J.* 2009, *45*, 3108.
[3] Ghaemy, M.; Barghamadi, M. *J. Appl .Polym.Sci.* **2009**, *112,* 815.

Conventional and microwave-assisted facile one-pot synthesis of *N*-substituted pyrrole-2,3,4,5-tetracarboxylates under neat conditions

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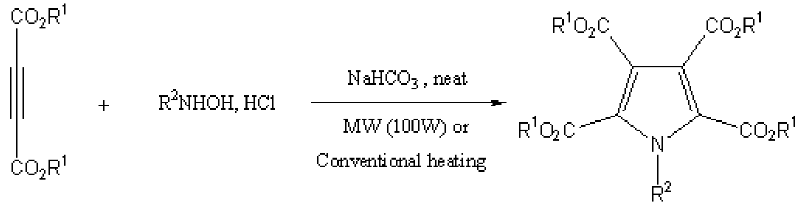
Synthesis of pyrrole containing compounds is very important for the synthetic organic community since this ring system is often embedded in important natural products and medicinally active compounds [1]. Many synthetic methods have been developed for the preparation of these compounds [2]. The most widely used method is the Paal–Knorr synthesis, which involves the reaction of 1,4-dicarbonyl compounds and their masked equivalents, such as 2,5-dimethoxytetrahydrofuran, with primary amines.

Many of the methods including 1,3-dipolar cycloaddition reactions, aza-Wittig reactions, reductive coupling and Hantzsch syntheses, were reported for the synthesis of pyrroles [3].

In this work, we report the results of our studies involving the reactions of (dimethyl- and diethyl-)acethylenedicarboxylates with N-monosubstituted hydroxylamines in the presence of $NaHCO_3$, which lead to a synthesis of highly substituted pyrroles.

Tetramethyl l-methylpyrrole-2,3,4,5-tetracarboxylate was obtained as a major product in good yield. We have developed a convenient and efficient synthetic approach to synthesize penta-substituted pyrroles using conventional heating and MW irradiation under neat conditions



References:

[1] Eicher, T.; Hauptmann, S.; Speicher, A. The Chemistry of heterocycles; 2nd ed., *Wiley-VCH: Weinheim, Germany*, **2003**, 97.
[2] Gilchrist, T. L. *J. Chem. Soc. Perkin Trans* **1998**, 1, 615.
[3] Polackova, V.; Veverkova, E.; Toma, S.; Bogdal, D. *Synth. Commun*. **2009**, 39, 1871.

Molecular capsule in water

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We have described a calix[4]arene derivatives which forms highly stable molecular capsules with complementary cationic half-spheres in polar solvents[1].

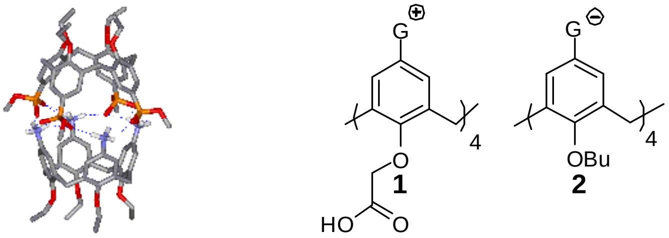

Figure 1) Left: The optimized structures of molecular capsule of calix[4]arene Right: structure of calix[4]arene halfspheres **1** and **2**

Because most biological processes take place in an aqueous environment, the synthesis of supramolecular containers for molecular recognition in water is a challenge [2].

Herein we report the formation and characterization of a novel type of capsules resulting from the self-association between oppositely charged complementary building blocks in water. After synthesis of new water soluble calix [4]arene half-spheres with four negatively charged groups at the upper rim, and the complementary halfsphere with four positively charged groups, we have also measured the binding constant between the halfspheres and this water-soluble capsule (**1**,**2**) opens new ways for the use of supramolecular structures as molecular receptors or drug delivery systems in physiological media.

References:

[1] Zadmard, R.; Schrader,T.; Grawe, T.; Kraft, A.; *Org. Lett*. **2002**, *4*, 1687.
[2] Corbellini, F.; Costanzo, L.; Crego-Calama, M.; Geremia, S.; Reinhoudt, N.; *J. Am. Chem. Soc.* **2003**, *125*, 9946.

Synthesis and characterization of an in-substituted ketenimine

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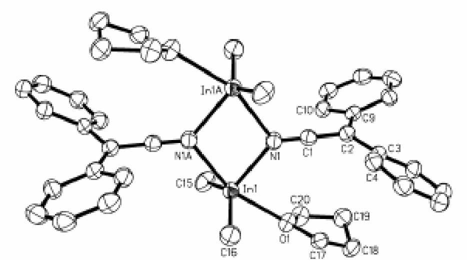
The metalane $TlMe_3$ acts as a simple Lewis acid during the reaction with acetonitrile, initiating the well-known nitrile trimerization to a 1,3,5-triazine [1]. The reaction of $InMe_3$ with acetonitrile gives the product of a trimerization but a metalla-substituted heterocycle [2]. Herein we report the reaction of $InMe_3$ with a phenyl-substituted acetonitrile Ph_2CHCN. This reaction in boiling toloul gives not the product of a trimerization but a metalla-substituted ketenimine which crystallize after addition of THF as the dimer $[Ph_2C{=}C{=}NInMe_2(THF)]_2$ (**1**). The reaction was monitored by ^1H-NMR spectroscopy, exhibiting an equilibrium with a 0.5 product to nitrile ratio of 82:18 mol%. CsF accelerates this reaction as well. Quite similarly, the reaction between $GaMe_3$ and Ph_2CHCN proceeds to give $[Ph_2C{=}C{=}NGaMe_2]_2$ (**2**) (no crystal structure), but the position of the equilibrium is more unfavorable (34:66 mol%). A complete transfer to (**1**) or (**2**) was observed when $[Ph_2C{=}C{=}NLi(OEt_2)_2]_2$ (**3**) was added to Me_2InCl or Me_2GaCl.



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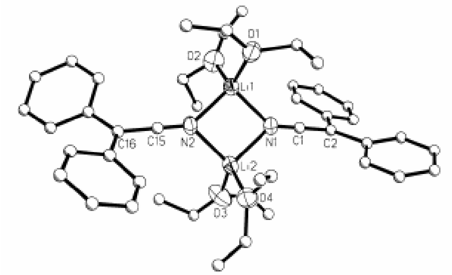

(3)

References:

[1] March, J. *Advanced Organic Chemistry, 3rd ed.* ; Wiley : New York, **1985**.
[2] Kopp, M. R, ; Neumueller, B. *Z. Anorg. Allg. Chem.* **1999**, *625*, 1246.

Pseudo five-component reaction between 3-formylchromones, Meldrum's acid, isocyanides and amines or alcohols: diversity-oriented synthesis of novel chromones

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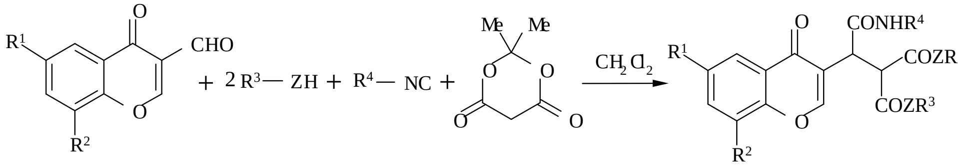
Diversity-oriented synthesis (DOS) is an emerging field involving the synthesis of combinatorial libraries of diverse small molecules for biological screening [1,2].

Chromone (4*H*-chromen-4-one, 4*H*-1-benzopyran-4-one) is a parent compound for an important class of oxygen-containing heterocyclic compounds with a benzoannelated γ-pyrone ring. This heterocyclic system is frequently encountered in the vegetable world, most often as flavone (2-phenylchromone), flavonol (3-hydroxy-2-phenylchromone) and isoflavone (3-phenylchromone) derivatives, which form the group of flavonoids flower and fruit pigments [3]. These compounds exhibit various types of biological activities [4] and find use as substrates in the preparation of many pharmaceuticals including some antitumour drugs [5]. Alkylchromones are less naturally abundant; nevertheless, some of them are also known to be biologically active. For example, of therapeutic interest are 3-methyl- and 2, 5, 8-tri-methylchromones [4,6].

In continuation of our studies on the chemistry of isocyanides [7,8], we wish to report a pseudo five-component reaction approach to the efficient synthesis of novel chromone derivatives using amines or alcohols, 3-formylchromones and isocyanides in the presence of Meldrum's acid in dry CH_2Cl_2 at room temperature.



References:

[1] Schreiber, S. L. *Science* **2000**, 287, 1964.
[2] Tan, D. S. *Nat. Chem. Biol.* **2005**, *1*, 74.
[3] Barton, D.; Ollis, W. D. (Eds), in "Comprehensive Organic Chemistry", Vol. 4, Oxford: Pergamon Press, **1979**.
[4] Ellis, G.P.in "The Chemistry of Heterocyclic Compounds", Vol. 31, New York: Wiley, **1977**,p. 749.
[5] McGarry, L. W.; Detty, M. R. *J. Org. Chem.* **1990**, *55*, 4349.
[6] Sosnovskikh, V. Y. *Russ. Chem. Rev.* **2003**, *72*, 489.
[7] Teimouri, M. B.; Mansouri, F, *J. Comb. Chem.* **2008**, *10*, 507;
[8] Teimouri, M. B. ; Mansouri, F. ; Bazhrang, R. *Tetrahedron* **2010**, *66*, 259.

Vinyl ester type naproxen polymeric prodrugs: synthesis, characterization and in vitro hydrolysis

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In recent years, polymeric prodrugs have gained prominence in pharmaceutical field, since they can effectively control the rate of drug release, administrate at low dosage, improve site-specificity and increase therapeutic benefit [1-3]. Naproxen or 2-(6-methoxy-2-naphtyl) propionic acid, is an important class of non-steroidal anti-inflammatory drugs (NSAIDs), which widely used for alleviation of pain and inflammation associated with tissue injury. The use of NSAIDs is also limited by their irritant side effects on the gastro-enteric mucous and by their frequent poor water solubility. These problems can be solved by the preparation of polymeric prodrug backbones *via* hydrolyzable bonds [4].

In the present work, naproxen vinyl ester (NVE), as a polymerizable monomer was synthesized by refluxing a solution of naproxen and mercuric acetate (as a catalyst) in vinyl acetate containing concentrated sulfuric acid. Sodium acetate was then added to quench the catalyst and filtered. The solution concentrated and purified by silica gel column chromatography to obtain NVE.

The resulting NVE monomer was copolymerized with 2-hydroxyethyl methacrylate and methyl methacrylate monomers (in 1:3 mole ratios) by free radical polymerization method. The structure of the obtained polymers was characterized by FT-IR, ^{1}H-NMR, elemental analysis and GPC. Study of naproxen release from the synthesized polymers was performed into dialysis bags by hydrolysis in different buffered solutions (pH 1, 7.4 and 10) at physiological conditions. Detection of hydrolysis solutions by UV spectroscopy at selected intervals showed that the naproxen can be released by hydrolysis of the ester bond at the side of drug moiety. The release profiles indicated that the hydrolytic behavior of polymeric prodrugs is strongly based on the polymer hydrophilicity and the pH value of the hydrolysis solution.

References:

[1] Babazadeh, M.; Mosanejhad, T. *Iran. Polym. J.* **2009**, *18*, 179.
[2] Babazadeh, M. *Int. J. Pharm.* **2008**, *356*, 167.
[3] Babazadeh, M. *J. Appl. Polym. Sci.* **2007**, *104*, 2403.
[4] Babazadeh, M.; Edjlali, L.; Rashidian, L. *J. Polym. Res.* **2007**, *14*, 207.

Intercalated conducting polyaniline–clay nanocomposites and their electrical characteristics

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A nanocomposite material, which consists of polyaniline (PANI) and inorganic Na+-montmorillonite (MMT), was synthesized via a microemulsion polymerization method, in which the Na+-MMT was forced to be swollen, following insertion of a mixture of aniline monomer, sodium lauryl sulfate and pentanol under sonication into its gallery [1]. The d-spacing of the PANI/Na+-MMT nanocomposite was found to become wider about 2.3A ˚ than that of the pure Na+-MMT particles, due to the successful intercalation of PANI into Na+-MMT layers [2,3]. The electrorheological (ER) fluid based on the fabricated PANI/Na+-MMT nanocomposite was prepared by dispersing the particles in insulating silicone oil [4]. Dynamic mechanical properties of the ER fluid were investigated via an oscillatory test using a vertical oscillation rheometer.

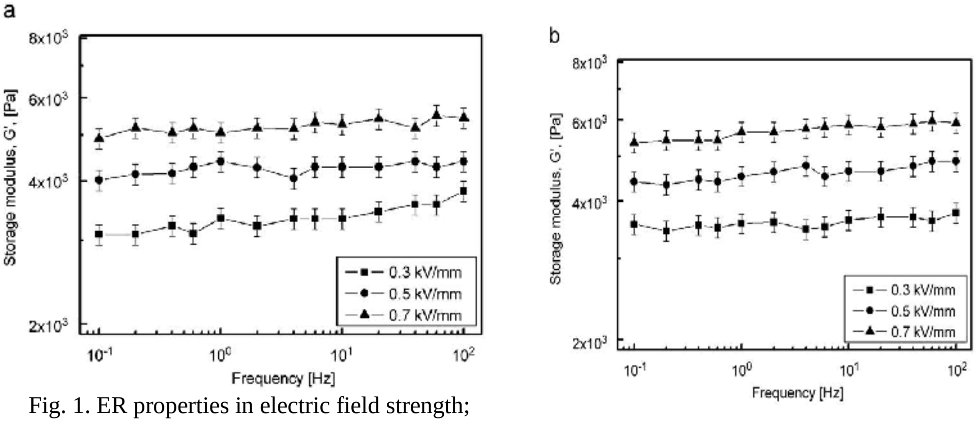

Fig. 1. ER properties in electric field strength;
frequency sweep test of: (a) Na+-MMT and (b) PANI/Na+-MMT composite.

References:

[1] O. Quadrat, J. Stejskal, *J. Ind. Eng. Chem*. **2006,** 12, 352–361.
[2] H. Van Hoang, R. Holze, *Chem. Mater.* **2006,** 18, 1976–1980.
[3] H.M. Lee, H.J. Choi, *Mol. Cryst. Liq. Cryst.* **2007,** 463, 221–225.
[4] W. Kim, M.S. Cho, H.J. Choi, S.G. Kim, C.A. Kim, M.S. Jhon, *Polym. Test*. **2001,** 20, 913–918.

p -Toluene sulfonyl chloride: A recyclable catalyst for the synthesis of trisubstituted and 1,2,4,5-tetrasubstituted imidazoles under solvent-free conditions

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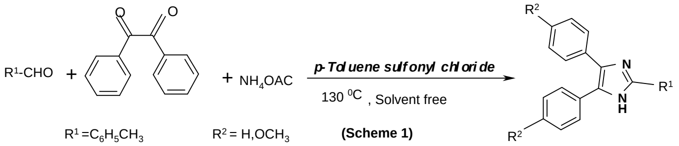
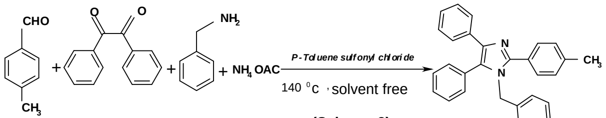
Imidazole and their derivatives, which usually possess diverse biological activities, play important roles as versatile building blocks for the synthesis of natural products and as therapeutic agents. In particular, 2,4,5-trisubstituted imidazoles are biologically active and occur in structures of a number of herbicides [1], fungicides or as inhibitors of IL-1 or P38 MAP kinase. Therefore, the synthesis of these imidazole derivatives has attracted much attention in organic synthesis. The classical route to 2,4,5-trisubstituted imidazoles involves the multi-component reaction of aldehydes, benzil and ammonium acetate under Solvent-free Conditions[2].

Multi-component reactions (MCRs) have proved to be remarkably successful in generating products in a single synthetic operation [3]. One of such reaction is synthetic route to imidazole ring. The tetrasubstituted imidazole is a core section in many biological systems such as Losartan and Olmesartan [4]. Herein, we introduced *p* -Toluene sulfonyl chloride as an efficient and reusable catalyst for the synthesis of 1,2,4,5-tetrasubstituted imidazoles. These reactions were accomplished via four components benzil, aromatic aldehydes, amines and ammonium acetate under solvent-free conditions.



(Scheme 1)



(Scheme 2)

References:

[1] Golan, D.E.; Armstrong, A.W.; Principles of Pharmacology: The Pathophysiologic Basis of Drug Therapy, Wolters Kluwer Health, **2007.**

[2] Liebl, R.; Handte, R.; Mildenberger, H.; Bauer, K.; Bieringer, H.; Ger. Offen De 3,604,042, **1987**; *Chem. Abstr*. **1987**, *108*,6018.

[3] Eilbracht, P.; Schimdt, A. *Chem. Rev*.**1999**,*99*, 3329.

[4] Koike, H.; Konse, T.; Sada, T.; Ikeda, T.; Hyogo, A.; Hinman, D.; Saito, Yanagisawa, H.; *Ann. Rep. Sankyo Res. Lab*. **2005**,*1*,55.

Synthesis of 2-Imino-hexahydroquinazolin-5(6*H*)-one derivatives under mild conditions

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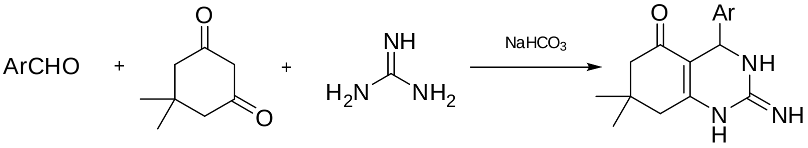
Recently, the Biginelli reaction has found great interest because of their therapeutic and pharmacological activities as calcium channel blockers, α-1a-adrenergic receptor antagonists, antihypertensive agents, neuropeptide Y (NPY) antagonists, antiviral, antitumour, antibacterial agents and anti-inflamatory activities [1]. Consequently syntheses of these compounds have gained importance and plethora of improved synthetic methodologies has recently been reported [2].

In continuation of our investigations in the Biginelli reaction [3], herein we describe a simple and efficient one-pot method for the 2-imino-hexahydroquinazolin-5(6*H*)-one derivatives. In this work we introduce a new three-component reaction of aldehydes **1a-i**, dimedone **2** and guanidine chloride **3** in presence of $NaHCO_3$ as base that provides an easy access to 2-imino-hexahydroquinazolin-5(6*H*)-one derivatives **4a-i** with high yields, short reaction times and simplicity of operation.



1a-i **2** **3** **4a-i**

References:

[1] (a) Kappe, C. O. *Eur, J. Med. Chem*. **2000**, 35, 1043; (b) Ma, Y.; Qian, C.; Wang, L.; Yang, M. *J. Org. Chem*., **2000**, 65, 3864.
[2] (a) Li, W.; Lam, Y. *J. Comb. Chem*., **2005**, *7*, 721; (b) Huang, Y.; Yang, F.; Zhu, C. *J. Am. Chem. Soc.*, **2005**, *127*, 16386.
[3] (a) Mirza-Aghayan, M.; Bolourtchian, M.; Hoseini, M. Synth. Commun., **2004**, *34*, 3335; (b) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M.; Boukherrob, R. Synth. Commun., **2010**, *40*, 8; (c) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. J. Iran. Chem. Soc. **2010**, *7*, 269; (d) Mirza-Aghayan, M.; Baie Lashaki, T.; Rahimifard, M.; Boukherroub, R.; Tarlani, A. A. *submitted for publication*.

Sodium dihydrogen phosphate (NaH_2PO_4) catalyzed three-component reaction of aldehydes, amines and cyanides: a high yielding synthesis of α-aminonitriles under solvent-free conditions

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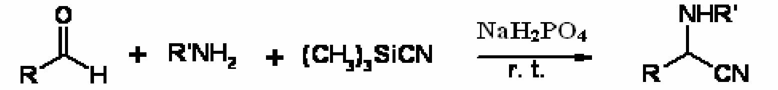
α-Aminonitriles are not only versatile intermediates for the synthesis of α-amino acids and various nitrogen containing heterocycles such as imidazoles and thiadiazoles but also exhibit a valuable dual reactivity, which has been utilized in a broad range of synthetic applications [1].

The Strecker reaction provides one of the most important methods for the synthesis of α-aminonitriles. Numerous modifications have been made to the original Strecker reaction, using a variety of cyanating agents such as hydrogen cyanide, sodium or potassium cyanide, Bu_3SnCN, bis (dialkylamino) cyanoboranes, diethylphosphorocyanidate, and trimethylsilyle cyanide (TMSCN). TMSCN is a safer, more effective, and more easily handled anion source compared to others. The efficiency of the reaction has been increased by the use of catalysts [2-3].

Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for one-pot multi-component reactions [4], we would like to introduce the first procedure for Sodium dihydrogen phosphate (NaH_2PO_4) promoted combination of aldehydes, amines, and TMSCN leading to the synthesis of a-aminonitriles under solvent-free conditions at room temperature.



This method offers some advantages in terms of simplicity of performance, low reaction times, solvent-free condition, low cost, and it follows along the line of green chemistry. The catalyst is readily available and inexpensive and can conveniently be handled and removed from the reaction mixture.

References:

[1] Gonzalez-Vera, J.A.; Garcia-Lopez, M.T.; Herranz, R. *J. Org. Chem*. **2005**, *70*, 3660.
[2] Mojtahedi, M.M.; Abaee, M.S.; Abbasi, H. *J. Iran. Chem. Soc.,* **2006**, *3*, 93.
[3] Reddy, B.M.; Thirupathi, B.; Patil, M.K. *J. Mol. Catal. A: Chem*. **2009**, *307*, 154.
[4] Karimi-Jaberi, Z. Amiri, M. *Heteroatom Chem.* **2010**, *21*, 96.

Palladium-mediated synthesis of 1,2-disubstituted-1*H*-benzo[f]indole-4,9-diones by sequential coupling/ring closure

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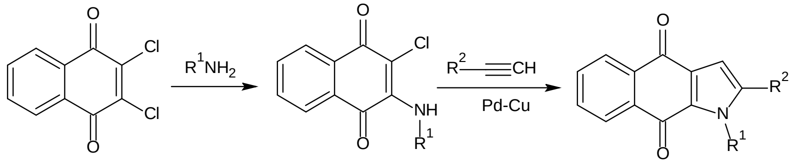
Heterocyclic quinone scaffolds often represent an important class of biologically active molecules. There have been a few reports on substituted-1*H*-benzo[f]indole-4,9-diones, exhibiting cytotoxic activities against cancer cell lines [1].

We have recently reported the synthesis of pyrrolo[2,3-b]quinoxalines via palladium catalyzed hydroamination [2]. In this work, we wish to report an eficeient way for the synthesis of 1,2-disubstituted-1*H*-benzo[f]indole-4,9-diones **3** from 2,3-dichloro-1,4-naphthoquinone **1** and primary amines with terminal alkynes in the presence of the palladium-copper catalyst. The structures of the products were deduced from their elemental analyses and spectroscopic data.



1 2 3

R^1: alkyl, aryl
R^2: phenyl

References:

[1] Seo, J.-M.; Kim, T.-J.; Jin, Y.-R.; Han, H.-J.; Ryu, C.-K.; Sheen, Y. Y.; Kim, D.-W.;Yun, Y.-P. Eur. *J. Pharmacol.* **2008**, *586*, 74.
[2] Keivanloo, A.; Bakherad, M.; Rahimi, a.; Taheri, S. A. N. *Tetrahedron Lett*. **2010**, *51*, 2409.

Synthesis of PVA/TiO_2 nanocomposite: Using γ- aminopropyltriethoxysilane as a coupling agent

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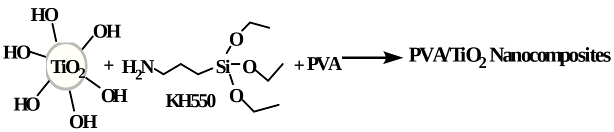
In recent decades, the synthesis of inorganic-polymer nanocomposite materials has been intensely studied due to their improved properties and widespread potential applications. The composites can combine the properties of inorganic particles such as mechanical strength and thermal stability with the processability and flexibility of organic polymers. Titanium dioxide (TiO_2) nanoparticles have attracted considerable interests because of their chemical, electrical and optical properties, high photoelectric conversion efficiency and high photocatalytic activity [1]. Polyvinyl alcohol (PVA) is a biodegradable and biocompatible polymer with excellent mechanical strength and thermal stability. PVA has multiple applications such as textile industry, paper coating, medical and cosmetic [2]. TiO_2/polymer nanocomposites show a special property such as capability of intensely absorbing Uv radiation as well as excellent transparency for the visible light [3].

In this study, γ-aminopropyltriethoxysilane was used to functionalize TiO_2 nanoparticles which make it organophilic. This surface modification of TiO_2 will increase dispersity of modified nanoparticles in the polymer matrix (Scheme 1). PVA/TiO_2 nanocomposites were prepared using ultrasound irradiation. The obtained nanocomposites were characterized by fourier transform infrared (FT–IR), ultraviolet-visible (UV–vis) diffuse reflectance spectroscopy, X-ray diffraction (XRD), thermalgravimetric analysis (TGA) as well as scanning and transmission electron microscopy (SEM, TEM). TEM image of nanocomposite (Fig. 1) show that the particle sizes are between 30-50 nm.



Scheme 1

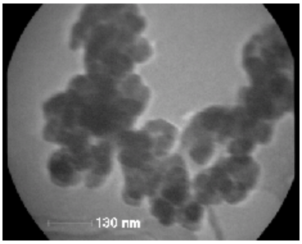


Fig. 1

References:

[1] Xiaochuan, C. *J, mater, sci, lett*. **2002**, *21*, 1637.
[2] Finch, C. *Poly (vinyl alcohol); Properties and Applications*. John Wiley and Sons: Vannessa, G.; Jacobs, D. **2005**.
[3] Malladi, S.; Mallikarjunagouda, B.; Ravindra, S.; Tejraj, M. *J, Membrane Sci*. **2006**, 281 95.

Study of the Wittig reaction of [5-(5-nitrothiophen-2-yl)-1,3,4-thiadiazol-2-amine] with acetylen dicarboxylate esters in the presence triphenyl phospithe

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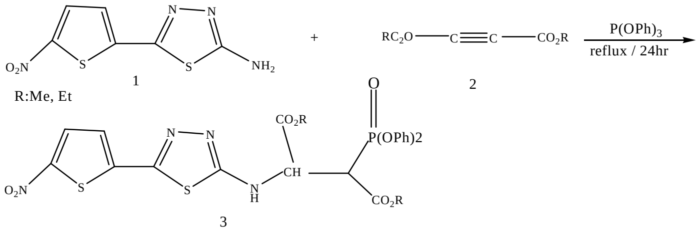
Nitrogen-containing heterocyclic compounds occupy an place important in modern chemistry. They are widely used in industry, medicine, veterinary, and agriculture[1]. The resistance towards available drugs is rapidly becoming a major worldwide problem. The need to design new compounds to deal with this resistance has become one of the most important areas of research today. Thiadiazole is a versatile moiety that exhibits a wide variety of biological activities[2].

Multicomponent reactions (MCR) have emerged as a powerful tool for delivering the molecular diversity needed in the combinatorial approaches for the preparation of bioactive compounds·[3]. Organophosphorus compounds have found a wide range of applications in the areas of industrial, agricultural, and medicinal chemistry owing to their biological and physical properties as well as their utility as synthetic intermediates[4].

Herein we report synthesis new ylides from reaction of [5-(5-nitrothiophen-2-yl)-1,3,4-thiadiazol-2-amine] with triphenyl phosphite and acetylen dicarboxylate esters under counditions reflex and solvent toluene lead to 3.



References:

[1] Strunskaya, E. I.; Yanilkin, V. V.; Bredikhina, Z. A.; Nastapova, N. V.; Morozov, V. I.; Maksimyuk, N. I.; Sharafutdinova, D. R.;Bredikhin, A.A. *Russian Journal of General Chemistry, 73,* **2003**, 806.

[2] Siddiquia, N.; Ahujaa, P.; Ahsana, W.; Pandeyab, S. N.; Alama, M. S. *Journal of Chemical and Pharmaceutical Research*, **2009**, *1*(*1*), 19.

[3] Ding, Q. ; Wang, B.; Wu, J. *Tetrahedron*, *63*, **2007**, 12166.

[4] rezaei, Z.; Firouzabadi, H.; Iranpoor, N.; Ghaderi, A.; Jafari, M. R. *European Journal of Medicinal Chemistry*, *44*, **2009**, 4266.

Preparation and characterization of conducting polyaniline/silica composite by silica-supported camphor sulfonic acid and perchloric acid

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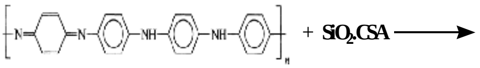
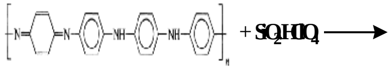
Polyaniline (PANI) has attracted considerable attention since MacDiarmid and coworkers reinvestigated this material as a conducting polymer due to its simple synthesis, good environmental stability, and adequate level of electrical conductivity [1]. Polyaniline is unique among conducting polymers in that its electrical properties can be reversibly controlled both by charge-transfer doping and by protonation.

In recent years, composites of PANI and inorganic compounds have been synthesized in order to get new materials with modified properties. Among those inorganic materials, silica (SiO_2) has received great attention because of its unique properties and wide applications. Nano- and mesoporous silica particles have been included in the composites through many ways; including surface polymerization of aniline adsorbed on silica surfaces, in situ hydrolysis and condensation of tetraethyl orthosilicate (TEOS) in PANI solutions or on solid PANI surfaces, etc. Although silica is insulating, some of the composites were at the same conductivity level as that of PANI, and some even displayed enhanced conductivity which may be due to the change in morphology of the conductive PANI in the hybrids, providing potential applications of the composites in electrochemistry and related fields [2].

Based on solid-states reactions [3], in present study, polyaniline (emeraldine base) which synthesized by IUPAC method [4] doped with addition of silica-supported camphor sulfonic acid (SiO_2.CSA) or silica-supported perchloric acid ($SiO_2.HClO_4$) as a chiral solid dopant acid. We used two acids to show the effect of doping process on the cinductivity. The achieved polyaniline composite showed the properties of semi conductive polymers, therefore, we were successful in doping process. The whole of processes have done in room temperature. Doped composite was characterized by using FT-IR, UV-VIS and four-probe conductivity measurement.



Polyaniline (emeraldine base)



Polyaniline (emeraldine base)

References:

[1] MacDiarmid, A.G.; Chiang, J.C.; Halpern, M.; Huang, W.S.; Mu, S.L.; etal. *Mol. Cryst. Liq. Cryst.* **1985**, *121*, 173.
[2] *Liu, X.X.; etal. Electrochimica Acta* **2008**, *53*, 4693.
[3] Modarresi-Alam, A.R.; Solaimani, M.; Pakseresht, M.; Farzaneh Jobaneh, E. *The First Throughout Seminar of Basic Science in Nanotechnology, Imam Hussein University, 9-10 December 2009, 523.*
[4] Stejskal, J.; Gilbert, R.G. *Pure Appl. Chem.* **2002**, *74*, 857.

Cyanoric chloride: A novel promoter for oxidation of sulfides to sulfones

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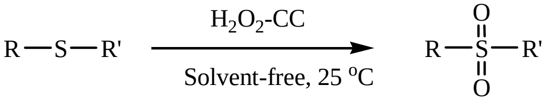
During the last few decades, a central objective in synthetic organic chemistry has been to develop greener and more economically competitive processes for the efficient synthesis of biologically active compounds with potential application in the pharmaceutical or agrochemical industries. Organic reactions under solvent-free conditions have gained in popularity in recent years [1]. The solvent-free approach is simple with amazing versatility. It reduces the use of organic solvents and minimizes the formation of other waste. The reactions occur under mild conditions and usually require easier workup procedures and simpler equipment. Moreover, solvent-free processes often exhibit significant rate enhancements due to increased reactant concentrations [2].

Sulfones are useful reagents in organic synthesis and they are also valuable synthetic intermediates for the construction of chemically and biologically important molecules [3]. The increasing interest and applications of sulfones have stimulated investigations on new methodologies for the preparation of these compounds.

Herein, we wish to report an efficient protocol in which H_2O_2 has been used as the oxidizing agent in the presence of CC for the chemoselective oxidation of sulfides to their sulfones in excellent yields and short reaction times (Scheme 1).



$$R{-}S{-}R' \xrightarrow[\text{Solvent-free, 25 }^{o}\text{C}]{H_2O_2\text{-CC}} R{-}\overset{\overset{\large O}{\|}}{\underset{\underset{\large O}{\|}}{S}}{-}R'$$

Scheme 1.

References:

[1] Tanaka, K. *Solvent-Free Organic Synthesis;* Wiley-VCH: Weinheim, Germany, 2003.
[2] (a) Fringuelli, F.; Girotti, R.; Pizzo, F.; Vaccaro, L. *Org. Lett.* **2006**, *8*, 2487. (b) Tucker, J. L. *Org. Process Res. Dev.* **2006**, *10*, 315. (c) Yusubov, M. S.; Wirth, T. *Org. Lett.* **2005**, *7*, 519. (d) Tanaka, K.; Toda, F. *Chem. Rev.* **2000**, *100*, 1025. (e) Shibahara, F.; Nozaki, K.; Hiyama, T. *J. Am. Chem. Soc.* **2003**, *125*, 8555.
[3] (a) Patai, S.; Rappoport, Z. *Synthesis of Sulfones Sulfoxides and Cyclic Sulfides*, John Wiley, Chichester, 1994. (b) Mikolajczyk, M. *Tetrahedron* **1986**, *42*, 5459. (c) Simpkins, N. S. *Sulphones in Organic Synthesis*, Pergamon Press, Oxford, 1993. (d) Prilezhaeva, E. N. *Russian Chem. Rev*. **2000**, *69*, 367.

A novel catalysis for synthesis of (4, 10-dinitro-2, 6, 8, 12-tetraoxa-4, 10-diazaisowurtzitane (TEX)

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The energetic materials play an important role in aeronautics, the weapons industry and other high-tech fields at present [1]. Cage crystal molecules containing the nitro group are important and widely used as energetic materials [2] due to high energetic density and high tension, such as 4, 10-dinitro-2, 6, 8, 12-tetraoxa-4, 10-diazaisowurtzitane (TEX) [3]. The synthesis and development of the most prominent and relatively new powerful explosive with wurtzitane ring system containing nitramine (R_2NNO_2) functionalities have attracted much interest [4]. TEX and Hexanitrohexzaazaisowurtzitane (HNIW or CL-20) are the most prominent molecules in this class. Ever since the report of the synthesis of 4, 10-dinitro-2, 6, 8, 12-tetraoxa-4, 10-diazaisowurtzitane (TEX) was first synthesized in 1990 by Ramakrishna et. al. TEX usually prepared via nitration of precursors with concentrated nitric acid and sulfuric acid [5]. But there are lots of difficulties with these old methods like strong acidic and thermal condition that decomposed the product and cause low yields, hazardous waste and difficulties with product separation. We report herein for the first time the use of many efficient catalysts and mild reaction condition for synthesis of TEX. By the use of this nitrating agent, the reaction eliminated the use of concentrated sulfuric acid and was environmental friendly. The structure of the compound was characterized by elemental analysis, IR, 1H NMR and MS. Meanwhile, the effects of reaction temperature, time and other factors on yield were analyzed.

References:

[1] D.H. Andrews, Phys. Rev. **1990**, *36*, 544.
[2] R. M. Richard and D. W. Ball, J. Hazard Mater. **2009**, *164*, 1595.
[3] P.F. Pagoria, G.S. Lee, A.R. Mitchell, R.D. Schmidt, Thermochimica Acta. **2002**, *384*, 187.
[4] P. E. Eaton, T.W. Cole, J. Am. Chem. Soc. **1964**, *86*, 3157.
[5] V. R. Ramakrishnan, M. Vedachalam, and J. H. Boyer, Heterocycles, **1990,** *31*, 479.

Preparation and characterization of conducting nano composites based on poly (aniline-co-3aminobenzoic acid) and poly (aniline-co-ethyl 3 amino benzoate) copolymers

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Polyaniline (PANI) is one of the most investigated intrinsically conducting polymers [1]. Copolymerization of aniline with aniline derivatives is caused the promising ways of improving the properties of PANI. In this work, firstly ethyl 3-aminobenzoate was synthesized from 3-aminobenzoic acid by direct esterification [2]. Then the copolymerization ethyl 3-aminobenzoate with aniline was carried out by sonochemical polymerization in aqueous hydrochloric acid using ammonium persulfate (APS) as an initiator lead to produced poly(aniline-co-ethyl 3 amino benzoate) (PAE3ABO) nano particles[3]. Finally the nanocomposites poly (aniline-co-ethyl 3 aminobenzoate)/poly (styrene-alternative-maleic acid) (PSMA)/poly styrene (PS) were prepared.

Biodegradable conductive composite poly (aniline-co-3aminobenzoic acid)-Starch was also prepared by template polymerization of aniline and 3aminobenzoic acid with native starch activated in acid medium by magnetic stirring. The influence of various organic and inorganic acids as dopant on the electrical conductivity of the starch-poly (aniline-co-3aminobenzoic acid) composites was investigated [4]. The electrical conductivity of composites was increased by increasing the amount of poly (aniline-co-3aminobenzoic acid) and poly (aniline-co-ethyl 3 amino benzoate). The conductive composites were characterized by FT-IR, and DSC analysis. The scanning electronic microcopy SEM images were prepared from composites. The conductivity of obtained composites measured with four point method.

References:

[1] Seong Cho, M.; Young Park, S.; Yeon Hwang, J. Materials Science and Engineering. 2004, 24, 15.
[2] Horacio, J.; Salavagione Diego, F.; Maria, C. Journal of Polymer Science: Part A. 2004, 42, 5587.
[3] Najafi Moghadama, P.; Khalafy, J.; Taheri T. Polym. Adv. Technol. 2010, 21, 235.
[4] Gemeay, A.; Mansour, I. A.; El-Sharkawy, R. G.; Zaki, A. European Polymer Journal. 2005, 41, 2578.

Novel poly(*O*-toluidine)/silica composite; Polymerization of *O*-toluidine with $FeCl_3.6H_2O$ as the oxidant and dopant in the presence of silica

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Polyaniline (PAn) has potential commercial applications in electronic, optical, and anticorrosion industries. However, the PAn still needs to be improved in mechanical properties for use in harsh environments. Moreover, the PAn may be necessarily to adhere tightly to inorganic substrates such as ceramics, metals, and glass during the applications. The incompatibility between organic PAn and inorganic substrates would lead to a poor stability and durability for the applications. An organic/inorganic hybrid as PAn/SiO_2 can solve these difficulties. Generally, the organic/inorganic hybrids possess the processibility property of organic materials as well as excellent hardness and good adhesion of inorganic materials [1-2].

Solid–state reactions (solvent-free) devoid of a number of above serious disadvantages are more appropriate, especially for high-disperse silica. From the standpoint of “green chemistry”, significant efforts have been made to find an alternative to organic solvents [3].

In this paper, the in situ composites were synthesized by solid-state polymerization of *O*-toluidine with iron (III) chloride hexahydrate as the oxidant and dopant in the presence of silica particles. The composite was characterized by Fourier transform infrared (FT-IR) spectra, ultraviolet visible (UV-Vis) spectrometry and conductivity measurements. Scanning electron microscopy (SEM) was done to study the morphology of composite.

References:

[1] Wei, Y.; Yeh, J.M.; Jin, D.; Jia, X.; Wang, J.; Jang, G.W.; Chen, C.; Gumbs, R.W. *Chem. Mater*, **1995**, *7*, 969.
[2] Wang, Y.; Wang, X; Li, J.; Mo, Z.; Zhao, X.; Jing, X.; Wang, F. *Adv. Mater.*, **2001**, *13*, 1582.
[3] Modarresi-Alam, A.R.; Khamooshi, F., et al. *Tetrahedron*, **2007**, *63*, 8723.

3-Aminopropylated silica gel as an efficient and recyclable catalyst for the synthesis of *β*-phosphonomalonates

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Owing to the synthetic and biological values of phosphonates, their chemistry has stimulated an increasing interest and the development of new methodologies for their preparation is an important goal in organic synthesis [1-3]. Direct phosphorus-carbon bond formation represents one of the most versatile and powerful tools for the synthesis of phosphonates. Amongst these methods, phospha-Michael addition, that is, the addition of a phosphorous nucleophile to an electron-deficient alkene has evoked remarkable attention by organic chemists.

Use of heterogeneous solid base catalysts is of current interest in chemistry and industry because solid bases offer many advantageous such as simplicity in handling, more environmentally safe disposal and less plant corrosion problems [4,5]. Amine functionalized silica gel such as 3-aminopropylated silica gel (AP-SiO_2) is one of the organic-inorganic hybrid materials that have been applied as effective solid base catalyst in organic transformations. In these types of solid base catalysts, the reactive centres are highly mobile similar to that of homogeneous catalysts and at the same time these species have the advantage of being recyclable in the same fashion as heterogeneous catalysts.

Here, we report an efficient method for the synthesis of a variety of β-phosphonomalonates by 3-aminopropylated silica gel as a catalyst. Good to high yields, short reaction times, simple work-up, ease of catalyst recovery, no by-product formation and re-usability of the catalyst without appreciable loss of activity make this method attractive and a useful contribution to the present methodologies.

References:

[1] Engel, R. *Chem. Rev*. **1977**, *77*, 349.
[2] Smith, J. D.; Ed.: Hilderbrand, R. L. *CRC: Boca Raton, FL*, **1983**, 31.
[3] Conrad,K. A.; Lee,S. M. *Clin. Pharmacol. Ther*. **1981,** *30*, 114.
[4] Ballini, R.; Bosica, G.; Livi, D.; Palmieri, A.; Maggi, R.; Sartori, G. *Tetrahedron Lett*. **2003**, *44*, 2271.
[5] Macquarrie, D. J.; Maggi, R.; Mazzacani, A.; Sartori, G.; Sartorio, R. *Appl. Catal. A: Gen*. **2003**, *246*, 183.

One-pot synthesis of 1,2,4,5-tetrasubstituted and 2,4,5-trisubstituted imidazoles by Na_3PO_4 as efficient and reusable catalyst

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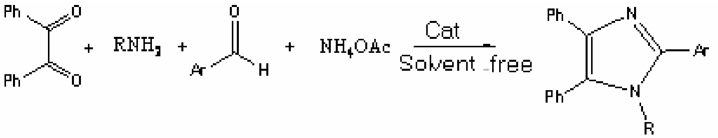
Tree-Sodium phosphate (Na_3PO_4) efficiently catalyzes the condensation reaction of benzil, aldehydes, amines and ammonium acetate in a four-component reaction under solvent-free conditions. The reaction proceeds rapidly and affords the corresponding tetra-substituted imidazoles in high yields. Also an efficient route was developed for the synthesis of tri-substituted imidazoles from condensation of benzil, aldehydes and ammonium acetate using Na_3PO_4.

Multicomponent reaction (MCR) condensations involve three or more compounds reacting in a single event, but consecutively to form new products, which contains the essential parts of all the starting materials [1].

The developing of new MCRs, and improving known multi-component reactions are an area of considerable current interest [2]. One such reaction is the synthesis of imidazoles. The prevalence of imidazoles in natural products and pharmacologically active compounds has instituted a diverse array of synthetic approaches to these heterocycles [3].

There are several methods for the synthesis of highly substituted imidazoles [4]. Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for several important organic transformations in this paper we report a simple and environmentally benign methodology for the synthesis of tetrasubstituted imidazoles via direct four-component condensation reaction between aldehydes, 1,2-diketones, amines, and ammonium acetate using catalytic amounts of Na_3PO_4 under solvent-free conditions.



References:

[1] Domling, A.; Ugi, I. *Angew Chem Int Ed* **2000**, *39*, 3168.
[2] Eilbracht, P.; Barfacker, L.; Buss, C.; Hollmann, C.; Kitsos-Rzychon, B. E.; Kranemann, C. L.; Rische, T.; Roggenbuck, R.; Schimdt, A. *Chem Rev* **1999**, *99*, 3329.
[3] Sisko, J. *J Org Chem* **1998**, *63*, 4529.
[4] Katritzky, A.R.; Boulton, A.J. (Eds.), *Advances in Heterocyclic Chemistry; Academic: New York,* **1980**; Vol. 27.

One-pot, three-component reaction of *tert*-butyl isocyanide, alkyl propiolates and 2-thioxo-4-thiazolidinone

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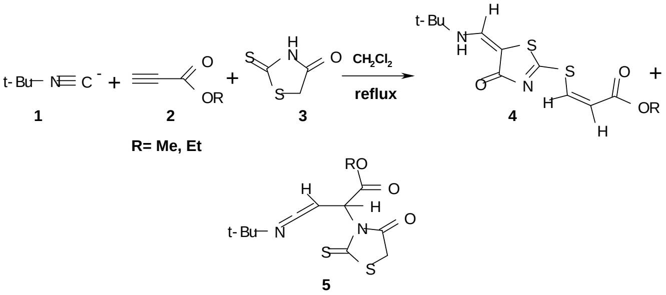
Rhodanine derivatives are attractive compounds due to their biological activities. They are anticonvulsant, antibacterial, antiviral and antidiabetic in nature [1]. A long-term study on the clinical effects of the rhodanine-based Epalrestat for antidiabetic demonstrated that it is well tolerated [2]. Due to various possibilities of chemical derivatization of the rhodanine ring, rhodanine-based compounds will probably remain a privileged scaffold in drug discovery. Therefore, the synthesis of these compounds is of considerable interest.

On the other hand, the isocyanide based multicomponent reactions (I-MCRs) are extremely useful tools for synthesis of combinatorial libraries of compounds and structurally complex molecules [3].

This prompted us to examine the isocyanide based multicomponent reaction of Rhodanie (**2**) with alkyl propiolates (**3**). The reactions proceeded in refluxing dichloromethane and afforded alkyl (Z)-3-({5-[(E)-1-(*tert*-butylamino)methylidene]-4-oxo-4,5-dihydro-1,3-thiazol-2-yl} sulfanyl)-2-propenoates (4) and alkyl 3-[(*tert*-butylimino)methylene]-3-(4-oxo-2-thioxo-1,3-thiazolan-3-yl)propanoates (5) in moderate yields. The structure of products was deduced from their X-ray crystallography, ^{1}H NMR, ^{13}C NMR, Mass and IR spectral data.



References:

[1] Momose, Y.; Meguro, K.; Ikeda, H.; Hatanaka, C.; Oi, S.; Sohda, T. *Chem. Pharm. Bull.* **1991**, *39 (6)*, 1440.
[2] Hotta, N. *Diabetes Care* **2006**, *29*, 1538.
[3] Domling, A. *Chem. Rev.* **2006**, *106*, 17.

Synthesis of fluorinated silyl ethers

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Most of the currently used inhalation anesthetics are halogen-containing volatile anesthetics that were developed in the 1960s and 1970s [1]. Among these are isoflurane, sevoflurane, and desflurane (Fig 1). Many of the inhalation anesthetics developed during this period are still in use today and a novel compound, as an inhalation anesthetic has not been introduced yet [2,3]. Synthesis of new inhalation anesthetics such as Sevoflurane, 1,1,1,3,3,3-hexafluoro-2-(fluoromethoxy)- propane, one of the most widely used inhalation anesthetics and Desflurane, 2,2,2-trifluoro-1-fluoroethyl-difluoromethyl ether) has recently been performed in our research group.

It seems to us that, fluorinated silyl ethers, 1 and 2, could potentially be applied for the synthesis of target molecules. Such Si analogues of currently used inhalation anesthetics can be suitable candidates for this purpose. In this study, the reaction of two fluorinated alcohols, 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP) and 2,2,2-trifluoroethanol, with dimethyldichlorosilane followed by a fluorination reaction is investigated (Scheme 1). As shown in scheme 1, in the first step, two products, 1 and 2, were obtained, as intermediates, which then were reacted with fluorinating agents such as KF, $Me_4N^+F^-$and BF_3 in order to produce the desired fluorinated silyl ethers (Target molecules)

The intermediates, 1 and 2, were analyzed by ^1H, ^{13}C and ^{19}FNMR.

Scheme 1

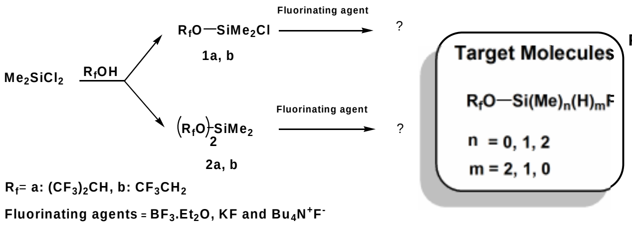
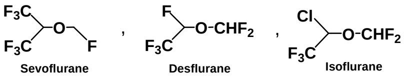


Fig 1



References:

[1] Bovill, J. G., Inhalation Anaesthesia: From Diethyl Ether to Xenon, Handbook of Experimental Pharmacology, Modern Anesthetics, **2008,** 182**.**

[2] Ramakrishna, Kornpati ; Behme, Chris ; Schure, Ralph, M.; and Bieniarz, Christopher, *Org. Proc. Res. Dev.* **2000,** *4 (6),* 581.

[3] Lee, Bora; Kim, Jin Hyung; Lee, Hyungjoo; Ahn, Byoung Sung; *J. Fluor. Chem.* **2007**, *128*, 110.

Synthesis of ethyl 2-(benzo[d]oxazol-2-ylamino)-1H-indole-3-carboxylates

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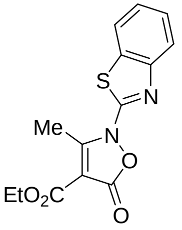
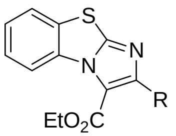
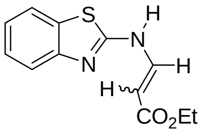
The synthesis of isoxazol-5(2H)-one with benzothiazole substituted on nitrogen **1** have been reported by prager and co-workers [1]. It has been reported [2] that the 2-benzothiazol-2-yl isoxazolones **1** and **2** gave the corresponding imidazobenzothiazoles **3** and **4** on photolysis in ethyl acetate/trifluoroacetic acid, and the acrylate **5** was obtained from the photolysis of **1** in methanol.



1 R = H
2 R = Me

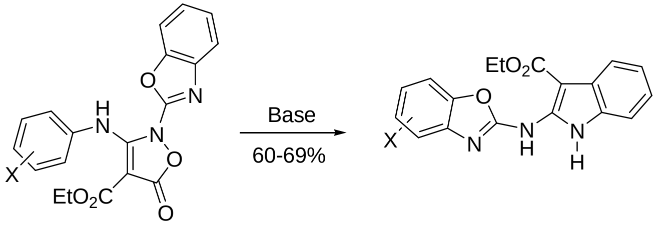


3 R=H
4 R=Me



5

In this work a number of 3-arylaminoisoxazolones **6** substituted with nitrogen heterocycles on *N*-2 with a benzoxazole ring have been synthesized. Annelated aminoindole **7** are obtained in excellent yields on their treatment with base in ethanol, which are presumed to arise by intramolecular cyclization of an imino carbene intermediate.



6 **7**

X = 2-Br , 3-Br , 2-Me , 3-Me , 3-OMe , 4-NO_2

References:

[1] Hung, T. V.; Janowski, W. K.; Prager, R. H. *Aust. J. Chem*. **1985**, *38*, 931.
[2] Prager, R. H.; Singh, Y.; Weber, B. *Aust. J. Chem*. **1994**, *47*, 1249.

Essential oil composition and antibacterial activity of *Chaerophyllum macropodum*

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Essential oil from aerial part of *chaerophyllum macropodum*, were collected from Ramsar Area in May 2010 [1] was obtained by hydrodistillation and analyzed by GC and GC-MS. The 95.9% containing forty-two compounds were identified. The main identified compounds were linalool (49.8%), limonene (7.8%), bicyclogermacrene (4.9%) and *α-santalol* (4.6%). The oxygenated monoterpens was main compounds of the oil. The against four gram-positive (*staphylococcus aureus, bacillus cereus and bacillus subtilis*) and two gram-negative (*Escherichia coli, canadida albicans*) bacteria with the 1-4 mg.mL^{-1} and 1-0.5 mg.mL^{-1} MIC, respectively.

References:

[1] A. Zargar/Medicinal plants / Tehran University press (**1992**).

Synthesis of monocyclic *B*-Lactam-bound polyacrylate nanoparticles by emulsion polymerization

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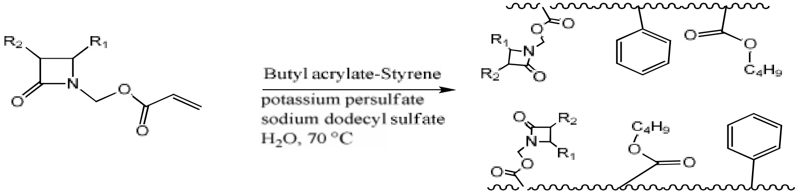
Several natural and synthetic compounds, containing the β-Lactam nucleus, are of clinical importance due to their high antibiotic activity [1]. Large efforts have been made on the synthesis and structural modification of the β-Lactam nucleus to increase antimicrobial activity [2]. However, the rapid emergence of bacterial strains resistant to most generally used members of this class of compounds requires a continuous effort for the design and synthesis of novel derivatives that are stable to β-lactamases and possess high potency and broad spectrum activity both in vitro and in vivo [3-4].

Nanotechnology is a rare phenomenon in recent history that has galvanized practically every sector of the research, engineering and business community. The ability to characterize, manipulate and organize matter systematically at the nanometer scale is spurring a revolution in science, technology and inevitably drug delivery and therapeutics. Nanosized systems are predisposed to being transformed into a more sophisticated system associated with its physical dimension of less than 100 nm. Nanotechnology promises to generate a library of sophisticated drug delivery systems that integrate molecular recognition, diagnostic and feedback. In short, these systems are functionally behaving like specialized living cells [5].

In this article we describe the preparation of emulsified polyacrylate nanoparticles in which a monocyclic β-Lactam is covalently conjugated onto the polymeric framework. These nanoparticles will be prepared in water by emulsion polymerization of an acrylated monocyclic β-Lactam pre-dissolved in a mixture of butyl acrylate and styrene in the presence of sodium dodecyl sulfate (surfactant) and potassium persulfate (radical initiator) [6-7].



References:

[1] Jarrahpour, A.; Zarei, M. *Tetradehron lett*. **2007**, *48*, 8712.
[2] Singh, G. S. *Mini-Rev. Med. Chem*. **2004**, *4*, 69.
[3] Shah, A. A.; Hasan, F.; Ahmed, S.; Hameed, A. *Res. Microbiol.* **2004**, *155*, 409.
[4] Jarrahpour, A.; Zarei, M. *Tetradehron.* **2009**, *65*, 2927.
[5] Lee.V. H. L. *Adv. Drug. Deliv. Rev.*. **2004**, *56*, 1527.
[6] Turos, E.; Reddy, G. S. K.; Greenhalgh, K.; Ramaraju,P.; Abeylath, S. C.; Jang, S.; Dickeyc, S.; Limc, D. V. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 3468.
[7] Turos, E.; Shim, J. Y.; Wang, Y.; Greenhalgh, K.; Reddy, G. S. K.; Dickey, S.; Lim, D. V. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 53.

New and efficient catalytic preparation of nicotinamides as diet supplement via hydration of cyanopyridines

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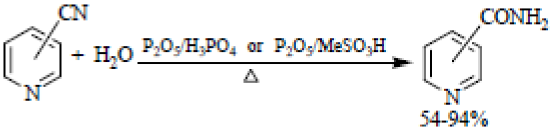
Nicotinamides constitute the major backbone of important biological active compounds with special roles as human and animal diet supplement. One of the most promising nicotinamides is 3-nicotinamide which has protective ability against disease arising from Vitamin B deficiency [1-2]. Nicotinamides are generally produced via the acid or base catalyzed hydration of cyanopyridines [3]. The major problem in the hydration of cyanopyridines to nicotinamides is formation of nicotinic acids as competitive products. It is obvious that, in catalytic hydration of cyano compounds, the nature and strength of the catalyst affect on the percentage formation of amide and acid [3].

Although, the details of catalysts and reaction conditions have been protected by patents, the development of more effective hydration protocols for cyanopyridines is already of interest. Therefore, as a continuation of our recent research devoted to amide synthesis [4] we report herein, two different catalytic systems for preparation of nicotinamides via cyanopyridines hydration (Scheme 1).



Scheme 1

References:

[1] (a) Gale, E. A. M. *Horm. Metab. Res.* **1996**, *28*, 361. (b) Burkart, V.; Blaeser, K.; Kolb, H. *Horm. Metab. Res.* **1999**, *31*, 641.
[2] Meneely, K. M.; Lamb, A. L. *Biochem.* **2007**, *46*, 1193.
[3] Bazi, F.; Badaoui, H. E.; Tamani, S.; Sokori, S.; Solhy, A.; Macquarrie, D. J.; Sebti, S. *Appl. Catal. A.: Gen.* **2006**, *301*, 211.
[4] Tamaddon, F.; Khoobi, M.; Keshavarz, E. *Tetrahedron Lett.* **2007**, *48*, 3643.

Essential oil composition of *Ranunculus Kochii*

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The genus *Ranunculus* belongs to the family Ranunculaceae, which comprises 50 genera and 2000 species, distributed throughout the northern hemisphere. It is also found in southern temperate regions in the tropics where they are usually confined to higher altitudes. Previous phytochemical studies of the genus *Ranunculus* revealed the presence of flavonoids, alkaloids, triterpene saponins, and lactones such as ranunculin and protoanemonin [1-4]. There is a report on the essential oils analysis of *R. Constantinopolitanus* and *R. Arvensis* in the literature [5]. However, no previous work has been reported on the essential oil analysis of *R. Kochii*. Thus, the systematic research was carried out by the extraction of the essential oil constituents of the aerial part of plant by hydrodistillation in Clevenger-type apparatus. The obtained essential oils were then investigated by GC-MS technique. The main components of essential oil were Pentacosane (15.08%), Tricosane (12.50%), Eicosane (12.22%) and Methyl linolenate (7.42%).

References:

[1] Gluchoff-Fiasson, K.; Fiasson, J. L.; Waton, H. *Phytochemistry*, **1997**, 45, 1063.

[2] Bonora, A.; Tosi, B.; Dallmolio, G.; Bruni, A. *Phytochemistry*, **1990**, 29, 2389.

[3] Marston, A.; Cabo, M.; Lubrano, C.; Robin, J. R.; Fromageot, C.; Hostettmann, K. *Nat. Prod. Commun.* **2006**, 1, 27.

[4] Saber, A.; Mahran, G. H.; El-Alfy, T. *Planta Med*. **1968**, 16, 231.

[5] Terzioglu, S.; Yasar, A.; Yayli, N.; Yilmaz, N.; Karaoglu, S.; Yayli, N. *Asian J. Chem*. **2008**, 20, 3277.

Homocoupling of aryl halides under microwave irradiation using a new palladium complex

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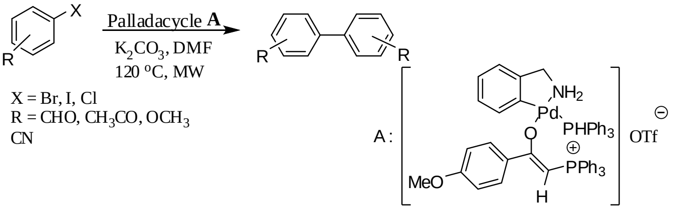
The development of organometallic catalysts has had a dramatic influence in organic chemistry in the past several decades. During this time, there have been significant advances in metal catalyzed cross-coupling reactions for the formation of carbon-carbon and carbon-heteroatom bonds [1,2]. One of the most significant advancements in this field, was the development of palladium(0)-catalyzed cross-coupling reactions [1,2].

In the past few years, heating and driving chemical reactions using microwave (MW) irradiation has been must popular area in the organic synthesis. The main advantages of employing Microwave heating adjusted with transition metals, are the significant rate enhancements, the higher product yields and dropping the level of byproducts from (thermal) side-reactions [3].

Herein, we wish to report the application of orthopalladate complex $[Pd\{C_6H_2(CH_2CH_2NH_2)\text{-}(OMe)_2,3,4\}\ (\mu\text{-}Br)]_2$ (**A**) in homocoupling reaction of various aryl halides under microwave irradiations. After the optimization of reaction conditions, homocoupling reactions were carried out using a very small amount of catalyst. The resulted yields were very excellent and required time for completion the reaction in comparison to traditional conditions was decreased from hours to minutes by application of MWI.



References:

[1] Antilla, J. C.; Klapars, A.; Buchwald, S. L. *J. Am. Chem. Soc.* **2002**, *124*, 11684.
[2] Baranano, D.; Mann, G.; Hartwig, J. F. *Curr. Org. Chem.* **1997**, *1*, 287.
[3] Leadbeater, N. E. *Chem. Commun*. **2005,** 2881.

Catalytic selective oxidation of methane: The forefront in the challenge for more useful chemicals

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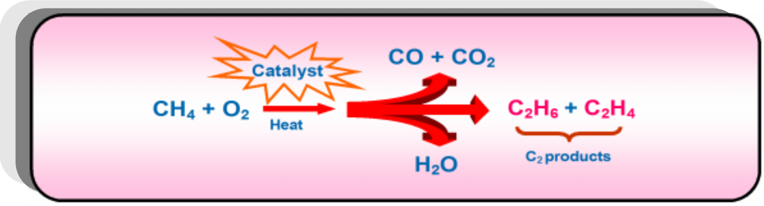
Selective oxidation catalysis has been and will be playing a leading role in the ambitious project of amore sustainable industrial chemistry [1]. In fact, selective oxidation is one of the reactions with the greatest potential for improvement, and in recent years this has led to the development of a series of better processes, as has been widely documented in various papers.

Recently, extensive research efforts have been focused on the utilization of methane chemistry as a future source for fuels and chemicals [2,3]. Among the various schemes for converting methane into more valuable petrochemical feedstocks, oxidative coupling of methane (OCM) using metal oxides as catalysts, has become a promising alternative approach for the economical utilization of natural gas [4]. Indeed, OCM is direct selective oxidation of methane by oxygen to ethylene or ethane (C_2-products) in the presence of catalyst at high temperature [5].

Iran holds the world’s second largest natural gas reserves, 974 trillion cubic feet, representing 16 percent, of the total world reserves [6]. Iran’s gas endowment is far from fully developed. Therefore, a serious multilateral attention to the development of new efficient methods for natural gas upgrading processes into value-added products, such as ethylene (a feedstock for petrochemicals), is strongly desirable.

In the present work, the effectiveness of alkaline metals doped titania-supported ceria catalyst systems on the OCM reaction is examined and the systems are found to be excellent novel candidates for the C_2 formations. In this work, we are able to achieve a good C_2 selectivity (~50%) at an acceptable CH_4 conversion (~50%) as a good result reported worldwide.



References:

[1] Centi, G.; Perathoner, S.; Abate, S. in: Mizuno, N. (Ed.), “Modern Heterogeneous Oxidation Catalysis. Design, Reactions and Characterization”, Wiley-VCH, Weinheim, **2009**.
[2] Burch, R.; Tsang, S. C. *Current Opinion in Solid State & Materials Science* **1997**, *2*, 90.
[3] Roberts, C. B.; Elbashir, N. O. *Fuel Process. Technol.* **2003**, *83*, 1.
[4] Zaman, J. *Fuel Process. Technol.* **1999**, *58*, 61.
[5] Bhasin, M. M.; Slocum, D. W., (Eds.), “Methane and Alkane Conversion Chemistry”, NY, **1995**.
[6] “Worldwide Look at Reserves and Production,” *Oil & Gas Journal* **2006**, *104*, 22.

Selective bromination of 4-chloro-1-indanone under various conditions

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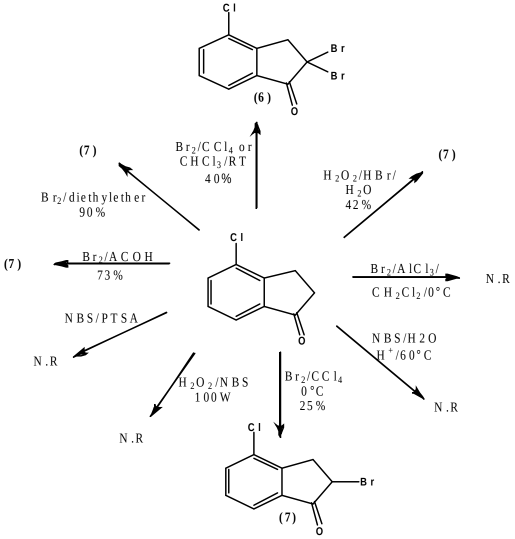
Bromoaromatic compounds are widely used as intermediates in the manufacture of pharmaceuticals, organochemical and especially chemical products [1]. Some famous chemical reactions such as Suzuki, Negashi, and Sonogashiro started with bromoarens or acetylenic condensation via metal catalyzed cross coupling reaction [2]. In this work we study preparation of 4-chloroindan-1-one and the investigated bromination of this compound in various conditions such as different solvents, different temperatures, various area of pH and corresponding product of indanone characterized by H^1-NMR, C^{13}-NMR and FT-IR spectral data (Scheme 1).



References:
[1] Choi, T.; Ma, E. *Molecules*, **2007**, 12, 74.
[2] Jung, W.; Ma, E. *Yakhak Hoeji*, **2003**, 47, 1.

Pyridine 2,6-dicarboxylic acid as a bifunctional organocatalyst for hydrophosphonylation of aldehydes and ketones in water

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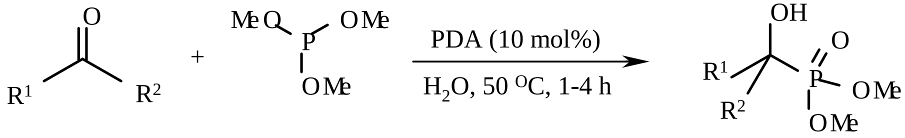
α-hydroxy phosphonates and the corresponding phosphonic acids display a wide spectrum of biological activity [1]. α-hydroxy phosphonic acid derivatives have been shown to be very important enzyme inhibitors. For example, they are inhibitors of such important medicinal enzymes as rennin [2] or human immunodeficiency protease and polymerase [3]. Many of these compounds have attracted attention because of their antibacterial, antivirus, antibiotic and pesticidal activities [4].

Upon the recent strong attention to environmentally benign protocols, the search of new and efficient catalysts, able to promote organic reactions under green conditions, is an area of continuous interest for production of α-hydroxy phosphonates. In this regard and in connection of our previous work [5], we report here the synthesis of α-hydroxy phosphonate derivatives in the presence of a catalytic amount of pyridine 2,6-dicarboxylic acid (PDA) in aqueous media. The catalyst can either be recovered or after separation of the product remaining aqueous layer can be used directly in the subsequent reactions.



References:

[1] Patel, D. V.; Rielly-Gauvin, K.; Ryono, D. E. *Tetrahedron Lett*. **1990**, *31*, 5591.
[2] Patel, D. V.; Rielly-Gauvin, K.; Ryono, D. E. *Tetrahedron Lett*. **1990**, *31*, 5587.
[3] Szymanska, A.; Szymczak, M.; Boryski, J.; Stawinski, J.; Kraszewski, A.; Collu, G.; Sanna, G.; Giliberti, G.; Loddo, R.; La Colla, P. *Bioorg. Med. Chem*. **2006**, *14,* 1924.
[4] Hammerschmidt, F. *Angew. Chem., Int. Ed. Engl.* **1994**, *33*, 341.
[5] Tajbakhsh, M.; Heydari, A.; Khalilzadeh, M. A.; Lakouraj, M. M.; Zamenian, B.; Khaksar, S. *Synlett* **2007**, 2347.

Novel synthesis of 4H-quinolizine deravatives using dialkyl carbodiimides via MCRs

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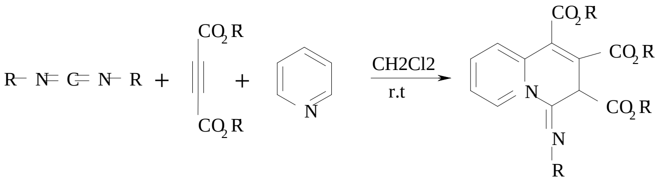
Multi-component reactions (MCRs) are useful organic reactions in which three or more starting materials react to give a product [1]. MCRs, by virtue of their convergence, productivity, facile execution, and generally high yields of products, have attracted much attention from the combinatorial chemistry. Quinolizines are of considerable interest due to their widespread occurrence in natural products, particularly in the field of alkaloids [2]. Although many routes to the basic ring systems are known [3] new general synthetic approaches are still highly desirable.As part of our current studies on the development of new routes to heterocyclic systems [4], we now report the reaction between dialkyl acetylendicarboxylates (**1**) and dialkyl carbodiimid (**2**) in the presence of pyridine (**3**) in CH_2Cl_2, which leads to 4*H*-quinolizine derivatives (**4**) with double insertion of the dialkyl acetylendicarboxylates in good yield (Scheme 1).



1	R
a	^{i}Pr
b	cyclohexyl

2	R'
a	Me
b	Et

4	R	R'
a	^{i}Pr	Me
b	^{i}Pr	Et
c	cyclohexyl	Me
d	cyclohexyl	Et

References:
[1] A. Doemling, *Chem. Rev.* **2006**, *106*, 17.
[2] W.Eberbach, W.Maier, *Tetrahedron Lett*., **1989**, 30, 5591-5594.
[3] F. J. Swinbourne, J. H. Hunt, G. Klinkert, *Adv. Heterocycl.Chem*. **1978**, 23, 103.
[4] Yavari, I.; Djahaniani, H. *Tetrahedron Lett*. **2006**, *47*, 2953.

Synthesis and characterization of new thermally stable polyesters containing pendent naphthalene groups

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Polyesters (PE)s are one of the most versatile polymers. They contain widely different materials with large applications, which are produced by a variety of manufacturing techniques. They have in common the ester group in the main chain, which is a polar group and brings about inter and intramolecular chain interactions that may reflect in some properties such as low solubility, mobility of the chain and melting characterizations. In addition, PEs often have limited heat and flame resistance, so these materials are inappropriate for many important applications. Several approaches have been proposed to develop structurally modified polymers having increased solubility, in order to improve their processability while maintaining a good thermal stability, based on the incorporation of flexible segments bearing ester, sulfone, amide, ether and sulfide moieties in the polymer backbone, without sacrificing heat resistance [1,2]. Also, major enhancement in processability can be achieved by modifying the substitution pattern of the aromatic units in the main chain, especially by inclusion of 1,2-linked units derived from *ortho*-catenated aromatic rings. In addition, the presence of thioether linkages can induce important new properties, such as less water absorption, better fire-retardant properties, and higher refractive indices for the resulting polymers [3].

As part of our continuing efforts to develop easily processable high-performance polymers with good solubility and thermal stability [4], this work deals with the synthesis and characterization of novel series of *ortho*-sulfide bridged poly(sulfide ester)s (PSE)s by the polycondensation reactions of a sulfide containing diol (1,1'-thiobis(2-naphthol)) (TBN) with various aromatic diacids. The resulting new polyesters were obtained in good yields and possessed inherent viscosities in the range of 0.68–1.03 dL g^{-1}. All of the polymers were amorphous in nature, showed excellent solubility and could be easily dissolved in amide-type polar aprotic solvents and even dissolved in less polar solvents. They showed good thermal stability with the glass transition temperatures between 223-285 °C, the 10% weight loss of 451–507 °C in nitrogen and 443–501 °C in air, and the residue at 700 °C of 44–59% in nitrogen.

References:

[1] Liaw, D. J.; Hsu, J. J.; Liaw, B. Y. J. *Polym. Sci., Part A: Polym. Chem*. **2001**, *39*, 2951.
[2] Shockravi, A.; Mehdipour-Ataei, Sh.; Abouzari-Lotf, E.; Zakeri, M. Eur. *Polym. J*. **2007**, *43*, 620.
[3] Berti, C.; Celli, A.; Marianucci, E.; Vannini, M. *Eur. Polym. J*. **2007**, *43*, 2453.
[4] Shockravi, A.; Abouzari-Lotf, E.; Javadi, A.; Atabaki, F. *Eur. Polym. J*. **2009**, *45*, 1599.

Multicomponent, one pot, and green method for the synthesis of β-aryl-β-mercapto ketones using Et_2NH and H_2O as a solvent

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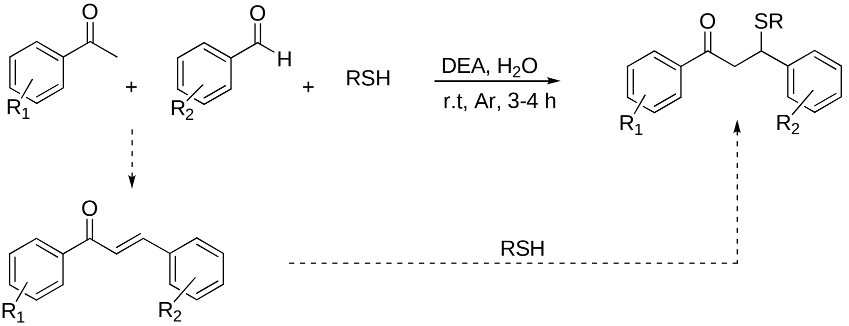
Multi-component reactions (MCRs) are among very useful methods in synthetic organic chemistry. The major advantages of MCRs are conduction of the whole process in one step, often higher yields, use of relatively small and simple reactants to construct complex molecules, and no need to isolate and purify the intermediates [1]. As a consequence of these advantages, investigations to develop new and efficient multi-component reactions are currently very popular in organic chemistry and are also favorable from "green chemistry" point of view.

β-Aryl-β-mercapto carbonyls with their various biological properties are valuable synthetic scaffolds in synthetic and medicinal chemistry [2]. Traditionally, their synthesis is performed via multi-step synthesis, where the chalcones are first synthesized from the condensation of acetophenone with aldehydes and then react with thiols to get the final products. Based on our experience on the use of aqueous conditioned organic transformations [3], we conducted the one-pot synthesis of various β-keto sulfides from their respective acetophenone, aldehydes, and thiol derivatives.



References:

[1] Kappe, C. O. *Acc. Chem. Res.* **2000**, *33*, 879.
[2] Kaye, P. T.; Nocanda, X. W. *Synthesis* **2001**, 2389.
[3] Abaee, M. S.; Mojtahedi, M. M. Forghani, S.; Ghandchi, N. M.; Forouzani, M. Sharifi, R. Chaharnazm. B. *J. Braz. Chem. Soc.* **2009**, *20*, 1895.

$PVP-(H_2SO_4)_n/NaNO_2$: As an efficient system for the nitrosation of secondary amines under mild and heterogeneous conditions

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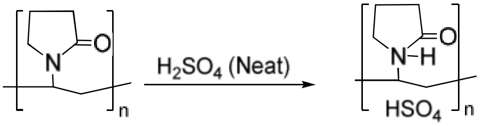
Solid acids have many advantages such as simplicity in handling, decreased reactor and plant corrosion problems, and more environmentally safe disposal. Also, wastes and by-products can be minimized or avoided by developing cleaner synthetic routes [1]. On the basis of our experiences in the application of solid acids [2], we found that poly vinyl pyrrolidone (PVP) reacts with concentrated sulfuric acid to give $PVP-(H_2SO_4)_n$. It is interesting to note that this exothermic reaction is easy and clean without any required work-up procedure (Scheme 1).



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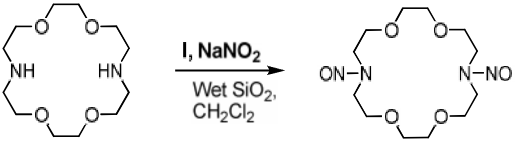
Scheme 1.

In continuation of our studies on the nitrosation of secondary amines [3], we were interested in using the **TTSA** for the *in situ* generation of HNO_2 in combination with $NaNO_2$ and wet SiO_2 and eventually nitrosation of secondary amines. Herein, we wish to report a simple, economical and effective method for nitrosation of secondary amines under mild and heterogeneous conditions (Scheme 2).



Scheme 2.

References:

[1] Shirini, F.; Zolfigol, M. A.; Salehi, P.; Abedini, M. *Curr. Org. Chem.* **2008**, *12*, 183.
[2] Zolfigol, M. A.; Ghaemi, E.; Madrakian, E.; Ghorbani Choghamarani, A. *Mendeleev Commun.* **2006**, 41.

Inherent viscosity approximation of bioactive polymers using QSPR technique

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Aromatic polyamides are considered to be high-performance materials due to their superior thermal and mechanical properties, which make them precious for advanced technologies [1,2]. The ability to predict the physical-chemical properties of polymeric materials from the molecular structure of their repeating units prior to their synthesis is of great value in designing polymers. So the expansion of a substitute method such as quantitative structure-property relationship (QSPR) would be useful for the theoretical calculation of physical-chemical values.

Inherent viscosity of polymer in a solvent is of significant chemical and thermo-dynamical interest as well as of great practical significance [3].

In this work QSPR studies were carried out to discover the correlation between structural features of novel optically active polymers with their physicochemical properties for the first time.

Number	Amino acid containing polymers	η_{inh} (EXP)	η_{inh} (PLS)	η_{inh} (ANN)
1	Alanine	0.21	0.26	0.20
2	Isoleucine	0.48	0.40	0.46
3	Leucine	0.23	0.29	0.25
4	Phenylalanine	0.30	0.36	0.32
5	Valine	0.18	0.23	0.19

References:

[1] Mallakpour, S.; Moghaddam, E. *Iran. Polym. J.* **2006**, *15*,547.
[2] Chen, J.; Nan, Q.; Guo, L.; Zhou, Y. *J. Appl. Polym. Sci.* **2010**, *115*, 2190.
[3] Golmohammadi, H.; Fatemi, MH. *Electrophoresis* **2005**, *26*, 3438.

N-chloroquinuclidinium chloride: a novel and reusable oxidizing agent for conversion of alcohols, THP and silyl ethers into their carbonyl compounds in water

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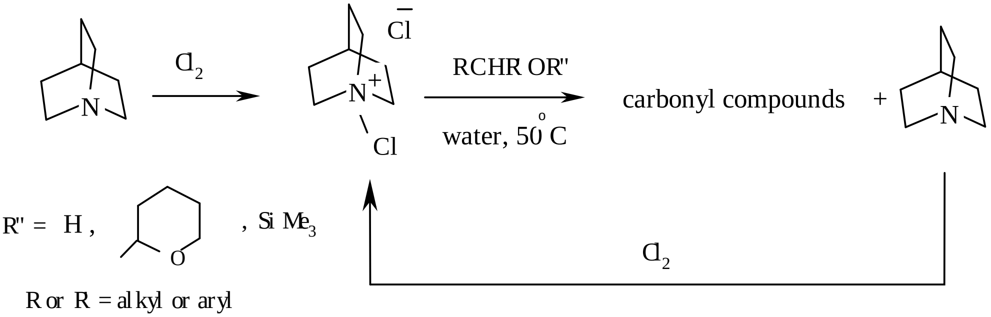
The oxidation of alcohols plays an important role in organic synthesis while the development of new oxidative processes continues to draw attention in spite of the availability of numerous oxidizing reagents [1]. Silyl and THP (tetrahydropyranyl) ethers are extensively used as protective groups for alcohols in synthetic chemistry because of their low cost, efficiency of preparation, stability under the intended reaction conditions, easy and selective removal, but the direct synthesis of carbonyl compounds from THP or silyl ethers is not widespread in the literature.[2] In our ongoing programmed to find new oxidants for organic materials [3], we now report the preparation of N-chloroquinuclidinium chlorideas a new efficient and reusable reagent for the oxidation of alcohols, THP and silyl ethers in water as a solvent [4]. In the oxidation reactions it is almost quantitatively converted quinuclidine which can be chlorinated and reused several times.



References:
[1] Zhou, L.; Yu, X.; Lin Pu *Tetrahedron Letters*, **2010,** *51, 475.*
[2] Krishmaveni, N.S.; Surendra, K.; Reddy, M.A. *J. Org. Chem.* **2003,** 68, 2018.
[3] Tajbakhsh,M.; Habibzadeh, S. *J. Chem. Research (S),* **2007,** 259; Tajbakhsh, M.; Heravi, M. M.; Habibazadeh, S. *Synthetic Communications,* **2007**, 37: 1–7.
[4] Narender, M.; S. Reddy, M.; Kumar, P.; Nageswar, Y. V. D.; Rao, K. R. *Tetrahedron Lett.* **2005,** 46, 1971.

Direct oxidative conversion of alcohols and aldehydes into nitriles

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Nitriles are useful functional groups in synthetic organic chemistry. They are also valuable intermediates that can be transformed to a variety of biologically important substances such as oxazoles, thiazoles, triazoles, oxadiazoles, and tetrazoles [1]. Nitriles are potentially valuable precursors for the synthesis of well-known drugs such as verapamil, indoprofen, cicloprofen, and naproxen. The most common and well-known procedure for the preparation of nitriles is the nucleophilic displacement of substrates with suitable leaving groups such as halogen compounds, aryl sulfonates, alcohols, esters, ethers, nitro or amino compounds and diazonium salts with inorganic cyanide ions [2]. These antiquated procedures have serious disadvantages such as use of toxic inorganic cyanides, production of wasteful inorganic salts, and harsh reaction conditions.

Therefore to improve above-mentioned disadvantages and introducing new methodologies [3-5] we report here an efficient method for the oxidative conversion of aldehydes and primary alcohols into nitriles using periodic acid and catalytic amounts of potassium iodide in the presence of aqueous ammonia (Scheme 1).

$$\mathrm{RCH_2OH \text{ or } RCHO} \xrightarrow[\mathrm{NH_3(aq)}]{\mathrm{H_5IO_6/KI}} \mathrm{RCN}$$

Scheme 1

Described method here offers the advantage of shorter reaction times, mild reaction conditions, non-toxicity, cost effective reagent and easy workup of products.

References:

[1] Rajagopal, G.; Kim, S.S. *Tetrahedron* **2009**, *65*, 4351.
[2] Soltani-Rad, M.N.; Khalafi-Nezhad, A.; Behrouzb, S.; Faghihi, M.A. Tetrahedron Lett. **2007**, *48*, 6779.
[3] Ghorbani-Choghamarani, A.; Amani, K.; Zolfigol, M.A.; Hajjami, M.; Ayazi-Nasrabadi R. *J. Chin. Chem. Soc.* **2009**, *56*, 255.
[4] Ghorbani-Choghamarani, A.; Rezaei, S. *J. Chin. Chem. Soc.* **2009**, *56*, 251.
[5] Ghorbani-Choghamarani A., Goudarziafshar H., Nikoorazm M., Yousefi S.: *Lett. Org. Chem.* **2009**, *6*, 535.

Optimized synthesis and characterization of NOCC-g- Poly(acrylic acid-co- 2-acrylamido- 2-methylpropane sulfonic acid) superabsorbent hydrogel

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Hydrogels are water-swollen, crosslinked polymeric structures produced by the simple reaction of one or more monomers, which find an extremely wide range of applications in the fields of medicine, pharmacy, biotechnology, agriculture, and controlled release of drugs [1]. Chitosan and its derivates have also been investigated as polymeric drug carriers for the optimization of drug delivery in the pharmaceutical field because of their biocompatibility and biodegradability. However, the application of chitosan was limited for using as a drug carrier owing to its insolubility at neutral or high pH region. To improve the solubility of chitosan, a series of hydrophilic groups have been introduced into its skeleton [2].

In recent years, water-soluble derivatives of chitosan (carboxymethyl chitosan, N,O-carboxymethyl chitosan and carboxyl chitosan, etc.) were used to blend with alginate to prepare Ca^{2+}- crosslinked hydrogel beads which generally exhibited pH-sensitive and ionic-sensitive swelling and drug release properties [3–5].

In this work we attempt to synthesize novel hydrogel with desirable capacity of swelling, fast kinetic and good mechanical strength in presence of N, O-Carboxymethyl Chitosan modified polysaccharide, AA/ AMPS as monomers, MBA as a crosslinker, APS as a initiator. The reaction variables that affect in the synthesis and swelling behavior oh hydrogels were optimized. Also, the effect of swelling media (salt solutions and various pH Values) was investigated. Morphology of optimized hydrogel was examined by scanning electron microscopy.The chemical structure of samples was characterized by FTIR spectroscopy.

References:

[1] El-Sherif, H.; El-Masry, M. Polym. Adv. *Technol*., **2008**, *19*, 342.
[2] Kato, Y.; Onishi, H.; Machida, Y. *Biomaterials*, **2004**, *25*, 907.
[3] Chen, LY.; Tian, ZG.; Du, YM. *Biomaterials* , **2004**, *25*, 3725.
[4] Liu, ZH.; Jiao, YP.; Zhang, ZY. *J Appl Polymer Sci*, **2007**, *103*, 3164.
[5] Yan, LF.; Qian, F.; Zhu, QS. *Polym Int* , **2001**, *50*, 1370.

Kinetic investigation of the platinum-catalyzed hydrosilylation based on tris(dimethylvinylsilyl)methyl substituted polystyrene

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Sterically overloaded tris(trimethylsilyl)methane (‘‘trisyl”) and its derivatives, due to the exceptional steric hindrance and structural versatility, have been studied extensively in organometallic chemistry [1]. More recently, these moieties have found their place in the field of polymer chemistry, and have been applied for preparation of novel polymeric materials [2,3] and catalytic systems [4]. Trisyl-type moieties were also recently applied for the synthesis of carbosilane scaffolds for new platinum catalysts [5].

Herein, a new polymeric support based on multifunctional, exceptionally sterically hindered carbosilane moieties, grafted onto crosslinked poly(styrene-*co*-chloromethylstyrene), was prepared. It offers well accessible, coordination-active sites (–$CH=CH_2$ moieties) that can be used for preparation of novel catalysts. Tris(dimethylvinylsilyl) methyl groups exert quasi-dendritic effect to polystyrene. Platinum was attached to the synthesized poly(styrene)-*co*-[1,1,1-tris(dimethylvinyl)ethylstyrenes] via coordination to vinyl groups. A kinetic investigation of the platinum-catalyzed hydrosilylation of triethylsilane with trimethylvinylsilane was performed by using gas chromatography (GC). This new heterogenized platinum hydrosilylation catalyst can be recovered and reused several times without significant loss of its activity.

References:

[1] Eaborn, C.; Smith, J.D. J. *Chem. Soc., Dalton Trans.* **2001**, (10), 1541.
[2] Kowalewska, A.; Stanczyk, W.A.; Boileau, S.; Lestel, L.; Smith, J.D. *Polymer* **1999**, 40, 813.
[3] Safa, K.D.; Babazadeh, M.; Namazi, H.; Mahkam, M.; Asadi, M.G. *Eur. Polym. J.* **2004**, 40, 459.
[4] Kowalewska, A.; Stanczyk, W.A.; Eckberg, R.P., *Appl. Catal. A – Gen.* **2005**, 287, 54.
[5] Kowalewska, A.; Stanczyk, W.A., *ARKIVOC* **2006**, 110.

Synthesis of tetrahydrobenzo[a]xanthene-11-one dyes in the presence of $Bi(NO_3)_3.5H_2O/SiO_2$

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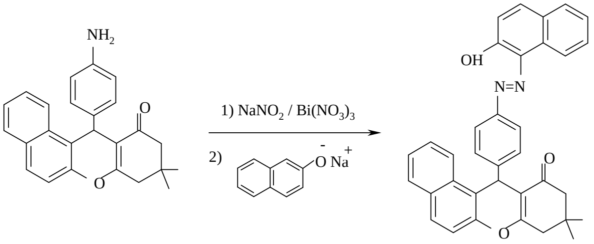
Azo compounds are the most widely class of industrial synthesized organic dyes due to their versatile application in various fields, such as dyeing textile fiber, biological–pharmacological activities and advanced application in organic synthesis [1]. On the other hand, benzoxanthenes are important biologically active heterocyclic compounds, which possess antiviral [2], anti-inflammatory [3], and antibacterial activities [4]. Azo dyes have been synthesized *via* coupling of diazotized aromatic amines with activated aromatic compound. Aromatic amines have been converted to diazonium salts in the presence of $NaNO_2$ and mineral acid at 0-5 °C. In this report, we have synthesized the azo dyes from aromatic amines in the presence of $NaNO_2$ and 50%$Bi(NO_3)_3.5H_2O/SiO_2$ in room temperature (Scheme 1).



In conclusion, we have developed three efficient and environmentally benign methodologies for the synthesis of 12-aryl/ alkyl-8,9,10,12-tetrahydrobenzo[a]xanthene-11-ones and 12-aryl-8,12-dihydro-7-oxa-8,10-diazabenzo[a]anthracene-9,11-diones by a one-pot, multi-component reaction. The advantages of these methods are reduced reaction times, higher yields, mild reaction condition, easy purification and economic viability of the catalyst.

References:

[1] Karci, F.; Demircali, A.; Sener, I.; *Dyes Pigm*. **2006**, *71*, 90.
[2] Lambert, R. W.; Martin, J. A.; Merrett, J. H.; parkes, K. E.B.; Thomas, G. J. PCT Int. Appl. WO9706178, **1997**.
[3] Poupelin, J. P.; Saint-Ruf, G.; Foussard-Blanpin, O.; Marcisse, G.; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem*. **1978**, *13*, 67.
[4] Hideo, T.; Teruomi, J. (Sankyo Co.) Jpn. Patent 56005480, 1981.

Preparation of cross-linked aniline and formaldehyde resin grafted onto chitosan

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In recent years, considerable effort has been devoted to developing new methods to synthesize polyaniline (PANi) to achieve better mechanical properties while maintaining high conductivity. The most common strategy that has been implemented is to change the oxidizing agent employed in the chemical polymerization reaction [1]. A new strategy has been employed to control the cross-linking of polyaniline that allows the synthesis of high molecular weight, conducting copolymers [2]. The new method utilizes anilineformaldehyde condensates (AFC) to establish the upper limit of possible cross-link sites in an AFC polyaniline copolymer. In the last work, we have synthesized PANi grafted onto polyvinylpropionate and its sensing behavior studied for pesticide poisons. Then prepared chemical and electrochemical of cross-linked aniline sulfide resin [3,4]. In this word, we have synthesized novel conducting polymer by employ cross-linked aniline and formaldehyde resin grafted onto chitosan. First, we prepared different molecular weights grafted copolymer of aniline onto chitosan by using ammonium persulfate as initiator. Chitosan and aniline are oxidized to form through a cation radical mechanism.

Then, grafted copolymer can be polycondensed by introduce formaldehyde to solution resin in the acidic media. The final copolymer was identified by FTIR, UV-visible and ^{1}H, ^{13}C-NMR spectroscopies. The thermal properties of polymer were studied by thermogravimetric (TGA) and differential scanning calorimetry (DSC). Electrical conductivity of copolymer has been studied by four-point probe method and produced 4.9×10^{-4} S/cm conductivity for it.

References:

[1] Y. Cao; A. Andretta; A. J. Heeger; P. Smith; *Polymer* **1989**, *30*, 2305.
[2] Liu, G.; Freund, M. S.; *Macromolecules* **1997**, *30*, 5660.
[3] Hosseini, S. H.; Ghavami A., *Iranian Polym. J.*, **2005**, 14, 7, 617.
[4] Hosseini, S.H.; Malekdar, M.; Naghdi, N.; *Polymer Journal*, **2010** (In press, *PJ2010097R*).

Synthesis and spectroscopic study of some new N-carbonyl phosphoramidates

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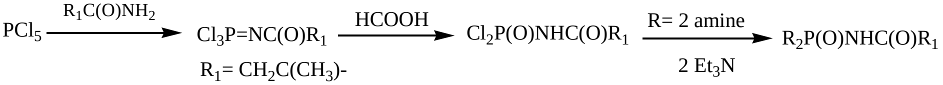
The extensive application of N-carbonyl phosphoramidate compounds with general formula $R_1C(O)NHP(O)R_2$ in medicine fields, plant growth regulators, extraction of lanthanide metals and preparation of O,O′-donor ligands include an important part of phosphorous chemistry [1-4]. In this work four novel phosphoric triamide compounds with formula $CH_2ClCHCH_3C(O)NHP(O)R_2$, R= isopropylamine (**1**); isobutylamine (**2**); tert-butylamine (**3**) and allylamine (**4**) were synthesized according to the Scheme 1 and characterized by ^1H, ^{13}C, ^{31}P NMR, IR spectroscopy and CHN elemental analysis. Results showed that in all of compounds two protons of CH_2Cl- moiety were diastrotopic and indicated two separate signals for the two non-equivalent protons in the range of 3.35 - 3.77 ppm and coupled with neigboring protons in pattern of dd. Also, the protons of CH_3 groups of two NH-CH$(CH_3)_2$ moieties in(**1**) are diastrotopic and indicate two separate singlet signals for the two non-equivalent CH_3 in 1 ppm and 1.05 ppm, but the protons of CH_3 groups of two NH-CH_2-CH$(CH_3)_2$ moieties in(**2**) are equivalent and appear in 0.8 ppm. ^{13}C NMR spectra of (**1**) indicate two non-equivalent cabons of NH-CH $(CH_3)_2$ moieties too. It is interesting that aminic protons in these compounds indicate two separate triplet signals in the range of 3.23 - 4.56 ppm.



$$PCl_5 \xrightarrow{R_1C(O)NH_2} \underset{R_1= CH_2C(CH_3)-}{Cl_3P{=}NC(O)R_1} \xrightarrow{HCOOH} Cl_2P(O)NHC(O)R_1 \xrightarrow[2\ Et_3N]{R= 2\ amine} R_2P(O)NHC(O)R_1$$

Scheme 1

References:

[1] Yule, S. M.; Boddy, A. V.; Cole, M.; Price, L.; Wyllie, R.; Tasso, M. J.; Perasson, A. D.J.; Idle, J; *Br. J. Clin. Pharmacol.* **1996**, *41*, 13.
[2] Wathsworth, W. S.; Emmons, W. D.; *J. Org. Chem.* **1964**, *29*, 2816.
[3] Rahimii R.; Abdoli M.; *Pest. Biochem. Physiol.* **2007**, *88*, 115.
[4] Singh, N.; Megharaj, M.; Gates, W. P.; Churchman, G. J.; Anderson, J.; Kookana, R. S.; Naidu, R.; Chen, Z.; Slade, P. G.; Sethunathan, N.; *J. Agric. Food Chem.* **2003**, *51*, 2653.

Synthesis of 1,2-dihydroisoquinolines *via* multicomponent reactions of NH-acides in water

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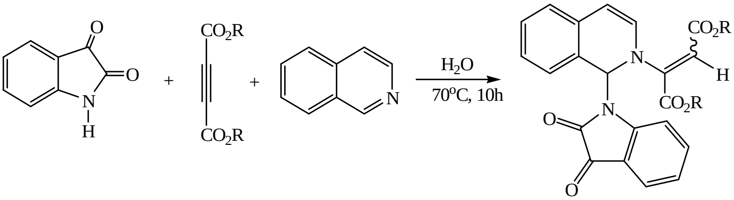
Multicomponent reactions (MCRs) are fast and appropriate solutions for the synthesis of different classes of compounds and are important in synthetic organic chemistry [1-2]. 1,2-Dihydroisoquinolines, as basic scaffolds in many natural products and pharmaceuticals that show significant biological activities [3-5], have promoted considerable efforts toward their synthesis. Thus, it is desired to increase novel methods to build up the new 1,2-dihydroisoquinoline-based structures.

As part of our continuing interest in the development of new synthetic methods in heterocyclic chemistry and our interest in isoquinoline-based multi-component reactions, we describe an efficient synthesis of 1,2-dihydroisoquinolines **4** *via* the reaction of isatin with activated acetylenes and isoquinoline in water at 70˚C.



1 **2** **3** **4**

References:

[1] Szymanski, W.; Zwolinska, M.; Ostaszewski. R. *Tetrahedron* **2007**, *63*, 7647.
[2] Nair, V.; Rajesh, C.; Vinod, A.U.; Bindu, S.; Sreekanth, A.R.; Mathen, J.S.; Balagopal. L. *Acc. Chem. Res* . **2003**, *36*, 899-907.
[3] Kaneda, T.; Takeuchi, Y.; Matsui, H.; Shimizu, K.; Urakawa, N.; Nakajyo, S. *J. Pharm. Sci.* **2005**, *98*, 275-282.
[4] Marchand, C.; Antony, S.; Kohn, K.W.; Cushman, M.; Ioanoviciu, A.; Staker, B.L.; Burgin, A.B.; Stewart, L.; Pommier,Y. *Mol Cancer Ther* **2006**, *5*, 287-295.
[5] Bentley, K.W.; The Isoquinoline Alkaloids*; Pergamon Press: London,* **1965**.

Synthesis and characterization of a cyclic 5,6-dihydro-1,3-dimethyl-5,6-bis-[1',3'-dimethyl-2',4',6'-trioxo-pyrimid(5',5')yl]furo[2,3-d]uracil (Uracil derivatives)

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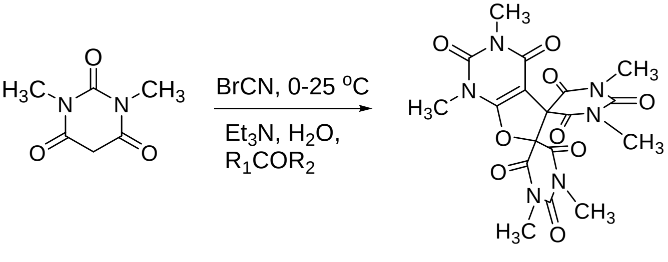
Barbiturates (barbituric acid derivatives) are a class of drugs that act as central nervous system depressants and by virtue of this; they produce a wide spectrum of effects, from mild sedation to anaesthesia and are also effective as anxiolytics and as anticonvulsants. They have additional pharmacological potentialas analeptics, immunomodulating and anti-AIDS agents and, also as anticancer remedies [1].

Spiro barbiturates are a class of compounds with interesting pharmacological and physiological activity [2]. Thus, the discovery of new synthetic possessing biological activity, whether isolated from natural sources or rationally designed pharmaceutical agents, has inspired chemists to find novel and diverse approaches to their synthesis [3].

Now, we report a new synthesis of cyclic stable heterocyclic trimeric form from the self-condensation reaction 1,3-dimethyl barbituric acid and cyclization with triethylammonium-5-bromobabiturate salt.



References:

[1] (a) Maquoi, E.; Sounni, N. E.; Devy, L.; Oliver, F.; Frankenne, F.; Krell, H. W.; Grams, F.; Foidart, J. M.; Noel, A. *Clin. Cancer Res.* **2004**, *10* , 4038; (b) Uhlmann, C.; Froscher, W. *CNS Neurosci. Ther*. **2009**, *15*, 24; (c) Grams, F.; Brandstetter, H.; D'Alo, S.; Gepperd, D.; Krel, H.W.; Leinert, H.; Livi, V.; Menta, E.; Oliva, A.; Zimmermann, G. *Biol. Chem*. **2001**, *382* , 1277.

[2] Michail, N. E. ; Anatolii, N. V. ; Nikita, O. S. ; Tatiana, A . Z; Valentina, M. M.; Gennady, I. N. *Tetrahedron Lett* . **2010** , *51*, 428.

[3] Parajapati, D.; Thakur, A. *J. Tetrahedron Lett*. **2005**, *46*, 1433.

Synthesis of bisphenolic compounds over heterogeneous zirconium lewis acids

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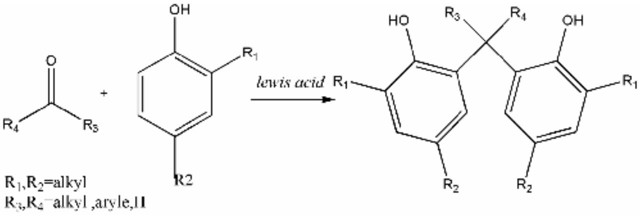
Bisphenols are important chemical intermediates for the preparation of industrially important epoxy resins and polycarbonates that are used in molting, casting, sealing, coating, encapsulating, adhesives and etc [1]. Bisphenols are classified as a group of phenolic antioxidants and therefore can be used as a part of composite solid propellants.

The most common method for synthesis of bisphenols is condensation of a ketone or aldehyde with a phenolic compound in the presence of an acidic condensing agent. However the use of homogeneous acid catalysts poses several problems such as difficulty in separation and recovery of disposal of catalyst and toxicity. In order to overcome these drawbacks, many solid acid catalysts were attempted in bisphenols synthesis. Although these solid catalysts such as zeolites, heteropoly acids, heteropolyacids supported on K_{10} clay and other, were reported to be active for bisphenol synthesis, but these catalysts also have disadvantages of low conversion, higher reaction temperature or prolonged reaction time [2,3].

Herein we try to use nano sized zirconium Lewis acids as heterogeneous condensation catalyst to reach this purpose and compare these acid's activity with micro samples.



References:

[1] Udayakumar, Seshachalam.; Ajaikumar, Samikannu.; Pandurangan, Arumugam.; *Catalysis Communications.* **2007**, *366*, 374.
[2] Lijie Hou; Qinghai, Cai. *Catal.Lett. 111,* **2006**.
[3] Wasilewska, M.*; Spectrochemica Acta,* part B, **1997**, *52*, 1321.

Convenient preparation of a highly substituted Imidazoles catalyzed by MCM-41 under solvent-free conditions

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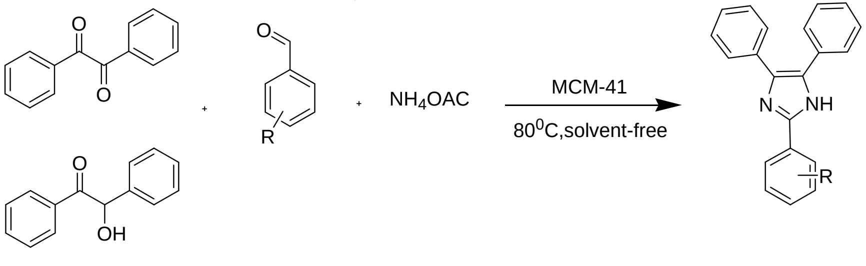
Recently, multi-component reactions (MCRs) have attracted considerable attention since they are performed without the need to isolate any intermediate and save both energy and raw materials and also reduce time. The synthesis, reactions and biological properties of substituted imidazole constitute a significant part of modern heterocyclic chemistry. Multi-substituted imidazoles, an important class of pharmaceutical compounds, exhibit a wide spectrum of biological activity [1]. Highly substituted imidazoles like lepidilines A and B exhibit micromolar cytotoxicity against several human cancer cell lines. Trifenagrel is a potent 2,4,5-triarylimidazole that reduces platelet aggregation in several animal species and humans. In recent years, substituted imidazoles are substantially used in ionic liquids that have been given a new approach to ‘Green Chemistry’. The imidazole compounds are also used in photography as photosensitive compound [2].

In this Letter, we have presented a novel, mild, and efficient method for the synthesis of tri and tetrasubstituted imidazoles. We herein report the use of recyclable, MCM-41 catalyst for an improved and rapid one- pot synthesis of 2, 4, 5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles in excellent yields.



References:

[1] Lombardino, J. G.; Wiseman, E.H. *J. Med. Chem.* **1974,** *17*, 1182–1188.

[2] Satoru I (**1989**) Japn Kokkai Tokyo Koho *117*: 867. Nagawade, R. R.; Shinde, D. B. *Acta Chim. Slov.* **2007**, *54*, 642

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An expedient approach for the synthesis of spiropyrrolidine oxindoles through 1,3-dipolar cycloaddition reactions

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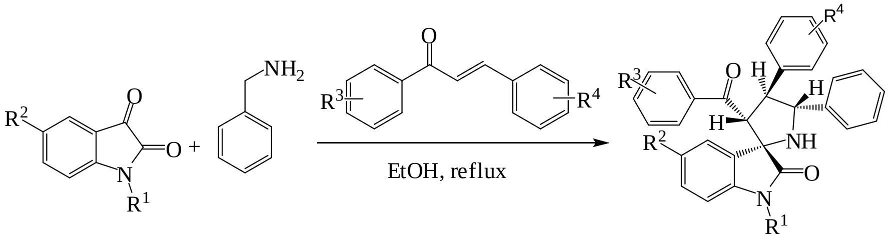
Multicomponent 1,3-dipolar cycloaddition reactions are considered to be one of the most useful processes for the construction of five-membered heterocyclic ring systems because of their high regioselectivity and stereoselectivity [1].The chemistry of azomethine ylides has gained significance in recent years as it serves as an expedient route for the construction of pyrrolidines and pyrrolizidines, which constitute the central skeleton of numerous natural products [2].

Spiro compounds are also known for their antimycobacterial properties [3]. Spirooxindole ring systems are the central skeleton for numerous alkaloids and pharmacologically important compounds [4].

In this work, we present the facile synthesis of novel spiropyrrolidine oxindoles through regio and stereoselective [3+2] cycloaddition reaction of azomethine ylides prepared *in situ* from isatin derivatives and benzylamine with the conjugated double bond of chalcone derivatives.



References:

[1] Tsuge, O.; Kanemasa, S. *In Advances in Heterocyclic Chemistry*; Katritzky, A. R., Ed.; Academic: San Diego, CA, 1989; Vol. 45, p 231
[2] Fejes, I.; Nyerges, M.; Szollosy, A.; Blasko, G.; Toke, L. *Tetrahedron* **2001**, *57*, 1129.
[3] Howe, R. K.; Shelton, B. R. *J. Org. Chem.***1990**, *55*, 4603
[4] Kang, T.-H.; Matsumoto, K.; Murakami, Y.; Takayama, H.; Kitajima, M.; Aimi, N.; Watanabe, H. Eur. *J. Pharmacol*. **2002**, *444*, 39.

PET aminoalcoholysis reaction optimization

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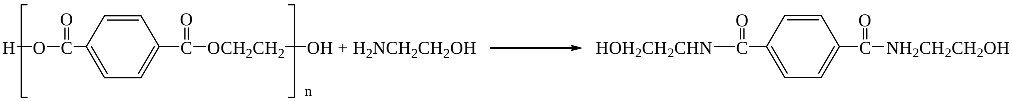
Heretofore many different ways have been used for polyester poly ethylene terephthalate (PET) chemical recycling. In this project, PET aminoalcoholysis reaction was investigated in order to provide a suitable way for PET waste omitting and also preparing polyol products for preparation of other compounds such as resins [2].

In researches done by Shukla and colleagues, different catalysts effects and their value on BHETA yield was investigated [1].

In this study, effect of 2 agents such as time and molar ratio of reacting parts was studied for reaction progress to attaining the monomerical units. Poly ethylene terephthalate with Aminoalcohols (PET:Aminoalcohol) was reacted with 2 molar ratios 1:3 and 1:6 in presence of sodium acetate as catalyst. Each reaction was performed separately once in 5 and once in 8 hours in 160-190 °C.

Finally, reactions progress was investigated by laboratory tests such as hydroxyl value determination and total nitrogen measurement based on ASTM standards.



BHETA

PET

Reference

[1] Ellison, M. S. ; Fisher, L. D.; Alger, K. W. ; Zeronian, S. H.; *J. Appl. Polym. Sci*. **1982,** 27:247.
[2] Shukla, S.R. ; Harad, A.M. ; *Polymer Degradation and Stability* **2006** 91, 1850.

Anchoring of a Cu(II) on to modified triazine ring supported on silica-gel and its application for oxidation of benzylic alcohols

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The oxidation of alcohols to aldehydes and ketones is a widely used chemical transformation in organic synthesis. The products are important precursors and intermediates in the synthesis of many drugs [1-2]. The traditional inorganic oxidant, such as permanganate and dichromate, however, are toxic and produce a large amount of waste. The separation and disposal of this waste increases steps in chemical processes.

Also, extensive research was devoted to immobilize transition metal complexes on solid supports, because such heterogenization of homogeneous catalyst may combine ease of product separation with the selectivity of the complexes [3].

In this work, a new catalyst for oxidation of benzylic alcohol was prepared by functionalization of silica-gel. Amino functionalized triazine supported on silica-gel was prepared by reaction of cyanuric chloride with silica-gel followed by diethylenetriamine treatment. It was characterized by FT-IR spectroscopy and XRD, and then was applied as a coordination agent for Cu(II) ion. The content of copper in this catalyst was determined by atomic adsorption spectrometry. This novel transition metal supported on heterogeneous surface was effectively used as a catalyst for selective oxidation of various benzylic alcohols in present of H_2O_2 in hexane as a solvent to their corresponding aldehydes in high yield and short reaction time. The reusability of this heterogeneous catalyst was also investigated. The main advantages of this catalyst for oxidation reaction are simple workup of reaction, catalyst preparation is easy and relatively not expensive, and finally this catalyst can be reused without modification or signification loss in it is activity.

References:

[1] Trakarnpruk, W.;Hoonsart, P. *Chin. J. Catal.* **2007**, *28(4)*, 290.
[2] Miller, M. M.; Scherrington, D. C. *J. Catal.* **1995**, *152*, 368.
[3] Salavati, N. M.; Amiri, A.; *Applied Catalysis A: General.* **2005,** *290*, 46.

Removal of heavy metal ions from industrial wastewater by chelating polymers based melamine modified poly(styrene-alt-maleic anhydride) in nano sacle

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Environmental contamination by heavy metal ions is a serious problem owing to their tendency to accumulate in living organisms and toxicities in relatively low concentration [1-2]. The aim of present work was to investigate the preparation of new chelating copolymers and to evaluate their performance in metal ions adsorptions from aqueous solution [3]. Chelating copolymers were synthesized by graft reaction of melamine into poly(styrene-alt-maleic anhydride). The prepared copolymer was further reacted by 1,3-diaminopropane as crosslinking agent in presence of ultrasonic irradiations for preparation of polymeric network in nano scale. The characterization of prepared copolymers was done by FT-IR analysis, SEM and XRD. The obtained copolymers were used for removal of heavy metal ions such as Cu(II), Ni(II), Cr(III), and Co(II) from aqueous solutions. The obtained copolymers in nano scale with long surface area provide a maximum interaction of metal ions and the chelating functional groups on the surface. The amount of metal uptake by the chelating polymer was determined by spectrometric analysis

References:

[1] Shukla, S.R.; Pai, R. S.; Shendarkar, A.D. Absorbtion of Ni(II), Zn(II) and Fe(II) on modified coir fibres. *Sep Purif Technol.* **2006**, 47, 141.

[2] Denizli, A.; Ozkan,G.;Arica,M.Y. Preparation and characterization of magnetic polymethyl methacrylate microbeads carrying ethylene diamine for removal of Cu(II), Cd(II), Pb(II) and Hg(II) frome aqueous solution . *J Apple Polym Sci* .**2000**, 78, 81.

[3] Iemma, F.; Cirillo, G.; Spizzirri, U.G.; Puoci, F.; Parisi, O. I.; Picci,N. Removal of metal ions from aqueous solution by chelating polymeric microspheres bearing phytic acid derivative. *European PolymerJournal* .**2008,** 44, 1183**.**

p-Toluene sulfonic acid-catalyzed microwave synthesis of symmetrical bisamides by reaction between aromatic aldehydes and amides

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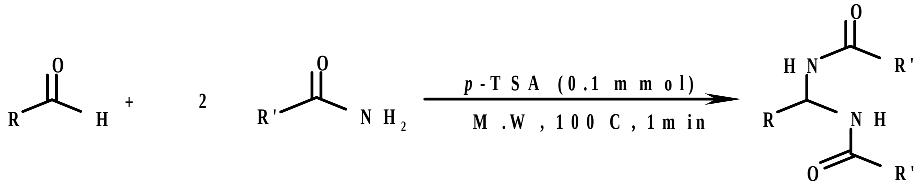
Bisamides are useful synthetic intermediates. Pyrolysis of benzylidenebisbenzamides afforded *N*-benzoylbenzaldimine derivatives, which has been used for the synthesis of *N*-(α-alkoxybenzy1)benzamides [1]. Bisamides are also important fragments for the introduction of *gem*-diaminoalkyl residues in retro-in verso pseudopeptide derivatives [2] by treating the corresponding amide with iodobenzene bistrifluoroacetate [3,4]. Herein we have developed a highly efficient synthesis of symetrical bisamide derivatives from aldehydes and amides under microwave conditions. The advantages of the reported method are inexpensive and easily available starting materials, simple reaction conditions, high yields, single-product reaction and simple workup procedure.



References:

[1] Breuer, S. W.; Bernarth, T.; Ben-Ishai, D. *Tetrahedron*, **1967**, 23, 2869.
[2] Nunami, K. I.; Yamazaki, T.; Goodman, M. *Biopolymers*, **1991**, 31, 1503.
[3] Rodriguez, M.; Dubreuil, P.; Bali, J. P.; Martinez, J. *J. Med. Chem.*, **1987**, 30, 758.
[4] Pernak, J.; Mrowczynski, B.; Weglewski, J. *Synthesis*, **1994**, 1415.

Synthesis of monocyclic *β*-lactam-conjugated polyacrylate nanoparticles

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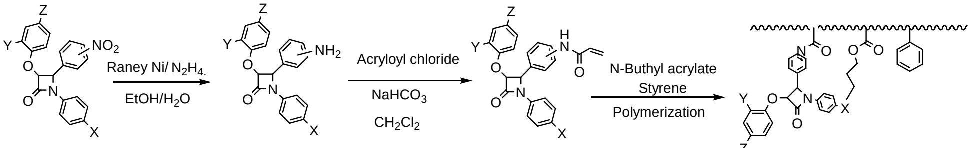
Azetidinones which are part of antibiotics structure are known to exhibit interesting biological activity [1]. However, microorganisms have built up resistance against the most traditional β-lactam antibiotics due to the wide-spread overuse of antibiotics. Therefore, the phenomenon of bacterial resistance forces the continuous modification of structure of known active compounds and the development of new ones [2]. Recently drug delivery vehicles have been developed to improve bioavailability, efficacy, and specificity of pharmaceutical compounds, particularly for anticancer agents, but nanoparticles have received surprisingly little attention in the antibiotic and infectious disease area [3].

So we became interested in the synthesis of 2-azetidinones as nanoparticles. For this, the nitrophenyl β-lactams **1** were reduced to aminophenyl β-lactams **2** by Raney Ni and hydrazine hydrate in EtOH/H_2O (9:1). β-Lactam monomers **3** were then obtained by reaction of free amines with acryloyl chloride at room temperature. Acrylated β-lactams **3** (5% w/w) was dissolved in a 7:3 (w/ w) ratio of butyl acrylate and styrene at 70°C, ultrapurified water, SDS (1% w/w) and initiator ($K_2S_2O_8$) (0.5% w/w) was then added to the solution and stirred at 70°C for 6 to 8 hours under a nitrogen atmosphere.



1 2 3

X= OMe, OEt, Cl
Y= H, Cl
Z= H, Cl

References:

[1] Jubie, S.; Gowramma, B.; Muthal, N. K.; Kalirajan, R.; Gomathi S.; Elango, K. *Int. J. Chemtech Res.***2009,** 1, 153.
[2] Vatmurge, N. S.; Hazra, B. G.; Pore, V.S.; Shirazi, F.; Chavan, P.S.; Deshpande, M.V. *Bioorg. Med. Chem. Lett.***2008,** 18, 2043.
[3] Turos, E.; Shim, J. Y.; Wang, Y.; Greenhalgh, K.; G. Reddy, G. S. K.; Dickey, S.; Lim, D. V. *Bioorg. Med. Chem. Lett.***2007**, 17, 53.

Synthesis and characterization of (*E*)-3-(methylthiobenzylidene)-2,3-dihydro-7-methoxychromen-4-one derivatives as potential anticancers

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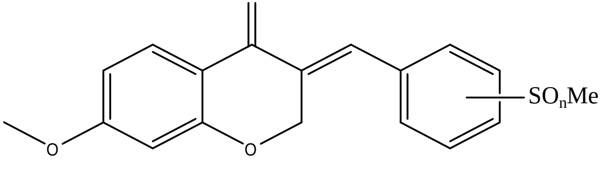
Flavonoids, occurring widely throughout the plant kingdom, are one of the most representative families of plant secondary metabolites and display a remarkable spectrum of biological activities [1]. It should be especially noted that developing flavonoids as anticancer agents has interested medicinal chemists for many years [2]. Some kinds of molecular mechanisms of flavonoids were identified as carcinogen inactivation, antiproliferation, cell cycle arrest, induction of apoptosis and differentiation, inhibition of angiogenesis, antioxidation and reversal of multidrug resistance [3].

On the basis of the above observations, we reasoned that (*E*)-3-(methylthiobenzylidene)-2,3-dihydro-7-methoxychromen-4-one derivatives might display anticancer activity with different feature from that of flavanoids.

They were synthesized by one-pot reactions of methylthiobenzaldehyde and 2,3-dihydro-7-methoxychromen-4-one.The purity of the synthesized compound was confirmed by chromatography. The structure of compound was characterized using IR, ^{1}HNMR spectra.



References:

[1] (a) Lazaro, M. L. Curr. *Med. Chem.* **2002**, *2,* 691; (b) Beulter, J. A.; Hamel, E.; Vlietinck, A. J.; Haemers, A.; Rajan, P.; Roitman, J. N.; Cardellina, J. H.; Boyd, M. R. *J. Med. Chem.* **1998***, 41,* 2333; (b) Whitting, D. A. *Nat. Prod. Rep.* **2001***, 18,* 583.
[2] a) Di Carlo, G.; Mascolo, N.; Izzo, A. A.; Capasso, F. *Life Sci.* **1999***, 65,* 337; (b) Samuelsen, A. B. J. *Ethnopharmacol.* **2000***, 71,* 1.
[3] Ren, W.; Qiao, Z.; Wang, H.; Zhang, L. *Med. Res. Rev.* **2003***, 23,* 519.

Synthesis of 4-amino-2-oxo-1,2-dihydro-1,8-naphthyridine-3-carbonitrile derivatives

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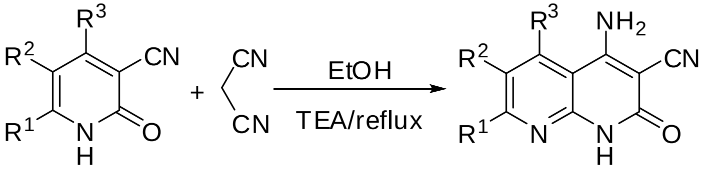
Cyanopyridones and aminopyridines separately show wide range of biological and pharmaceutical activities. For example cyanopyridones act as anti-inflammatory, analgestic, anti-pyretic, β-adrenolytic, antimicrobial, and antihypertensive [1] and aminopyridine compounds, were identified as a primary hit of IKK-β inhibitors [2]. They also show analgesic, antipyretic, β-adrenolytic and antihypertensive properties [3]. These applications led us to develop a new synthetic method for synthesis of new series of highly substituted 4-amino-2-oxo-1,2-dihydro-1,8-naphthyridine-3-carbonitriles that formed from both cyanopyridones and aminopyridines skeleton as a new attractive biological active molecules.

We wish to report here, synthesis of the target molecules from the reaction of 3-cyano-2-pyridone derivatives and malononitrile in the presence of triethanolamine at reflux condition.



R^1, R^2, R^3 = alkyl and aryl

References:

[1] Dejohn, D.; Domogala, J. M.; Kaltenbronn, J. S.; Krolls, U. *J. Heterocyclic Chem.* **1983**, *20*, 1295.
[2] Murata, T.; Shimada, M.; Sakakibara, S.;Yoshino, T.; Kadono, H.; Masuda, T.; Shimazaki, M.; Shintani, T.; Fuchikami, K.; Sakai, K.; Inbe, H.; Takeshita, K.; Niki, T.; Umeda, M.; Bacon, K. B.; Ziegelbauer, K. B.; Lowinger, T. B. *Bioorg. Med. Chem. Lett.* **2003**, *13*, 913.
[3] Manna, F.; Chimenti, F.; Bolasco, A.; Filippeli, A.; Palla, A.; Filippeli, W.; Lampa, E.; Mercantini, R. *Eur. J. Med. Chem.* **1992**, *27*, 627.

7-Deazaadenines: Synthesis of new pyrrolo[2,3-d]pyrimidin-4-amine derivatives

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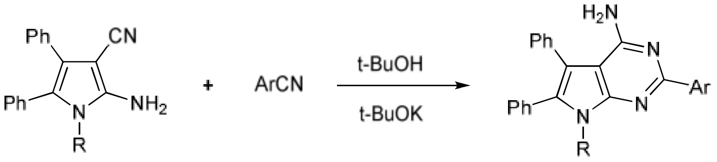
Pyrrolo[2,3-d]pyrimidin-4-amine may be regarded as an analogue of adenine in which its N-7 has been replaced by a CH group and therefore can be named as 7-deazaadenine. Literature reports had already established pyrrolo[2,3-d]pyrimidins as antitumor [1], antimicrobial [2], antiangiogenic [3] agents with potential application as enzyme inhibitors [4]. Moreover, these compounds have been shown to induce neurogenesis in murine embryonic stem cells [5]. To the best of our knowledge, heterocyclisation of 2-amino-4,5-diphenyl-1H-pyrrole-3-carbonitrile **1** with aryl nitriles **2** has not been reported in the literature.

Thus, cyclocondensation of 2-amino-4,5-diphenyl-1H-pyrrole-3-carbonitriles **1** with aryl nitriles **2** in the presence of potassium t-butoxide in t-butanol under reflux gave products identified as 5,6-diphenyl-7H-pyrrolo[2,3-d]pyrimidine-4-amines **3** in good yields.



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References:

[1] Acs, G.; Reich, E.; Mori, M. *Proc. Nat. Sci.*, **1964**, *52*, 493.
[2] Mohamed, M. S.; Rashad, A. E.; Zaki, M. E. A.; Fatahala, S. S. *Acta Pharm.*, **2005**, *55*, 237.
[3] Gangjee, A.; Namjoshi, O. A.; Yu, J.; Ihnat, M. A.; Thorpe, J. E.; Warnke, L. A. *Bioorg. Med. Chem.*, **2008**, *16*, 5514.
[4] Gibson, C. L.; Rosa, S. L.; Ohta, K.; Boyle, P. H.; Leurquin, F.; Lemacon, A.; Suckling, C. J.; *Tetrahedron*, **2004**, *60*, 943.
[5] Ding, S.; Wu, T. Y. H.; Brinker, A.; Peters, E. C.; Hur, W.; Gray, N. S.; Schultz, P. G. *Proc. Natl. Acad. Sci.*, **2003**, *100*, 7632.

First report on solvent-free synthesis of monobenzylidine derivatives of thiopyranone under catalysis of $MgBr_2.OEt_2$

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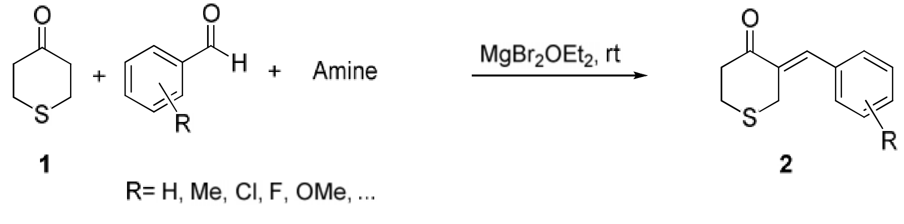
Although the aldol condensation as an important carbon-carbon bond forming reaction has witnessed much recent progress, there are still demands for the development of new efficient procedures for this reaction involving inexpensive and recyclable catalytic systems, preferably under solvent-free conditions. The broad utility of α,β-unsaturated carbonyl compounds in organic chemistry has continued to attract considerable interest to develop new methods for their synthesis [1].

In the framework of our investigations on aldol condensation of various cyclic ketones [2], we would like to herein report a new synthetic method for monobenzylidenes of thiopyran-4-one system. Consequently, a solvent free preparation of monobenzylidines of thiopyran **1** is performed at room temperature under trace quantities of magnesium bromide diethyl etherate catalyst to obtain products of type **2**.



The reaction is also applied to other cyclic ketones like cyclohexanone as giving high yields of the respective products in short times.

References:

[1] Hallgas, B.; Dobos, Z.; Agocs, A.; Idei, M.; Keri, G.; Lorand, T.; Meszaros, G. *J. Chromatogr. B* **2007**, *856*, 148.
[2] Abaee, M. S.; Mojtahedi, M. M.; Hamidi, V.; Mesbah, A. W.; Massa, W. *Synthesis* **2008**, 2122; Abaee, M. S.; Mojtahedi, M. M.; Zahedi, M. M.; Sharifi, R.; Khavasi, H. *Synthesis* **2007**, 3339.

A novel approach to the synthesis of iminophosphoranes

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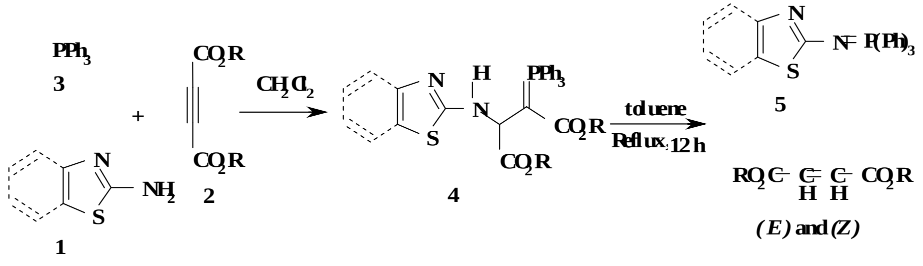
It is known that iminophosphoranes are important reagents and intermediates, their use for the introduction of imine units organic synthesis [1,2]. In the realm of ylide compounds and their value for a variety of industrial, biological and chemical synthetic uses, phosphorus ylides are playing increasingly pivotal roles.[3-5] The stabilized phosphoranes(4) obtained from the three-component reaction between dialkyl acetylenedicarboxylates (2) and 2-aminothiazole or 2-aminobenzothiazole(1) in the presence of triphenylphosphine(3), undergo a smooth reaction in boiling toluene to produce iminophosphoranes(5) in good yields.



References:

[1] Molina, P.; Vilaplana, M.J. *Synthesis*, **1994**, 1197.
[2] Palacios, F.; Ochoa de Retana, A.M.; Martinez de Marigorta, E.; . Rodriguez M.; Pagalday, J. *Tetrahedron,* **2003**, *59*, 2617.
[3] Islami, M. R.; Amrollahi, M. A.; Iranmanesh M., *Arkivoc,* **2009**, 35.
[4] Yavari,I.; Islami, M. R.; Bijanzadeh, H. R., *Tetrahedron*, **1999,** *55*, 5547.
[5] Shen, Y. *Acc. Chem. Res.*, **1998**, *31*, 584.

Fischer indole synthesis by melamine-formaldeyde resin supported acids under solvent-free condition

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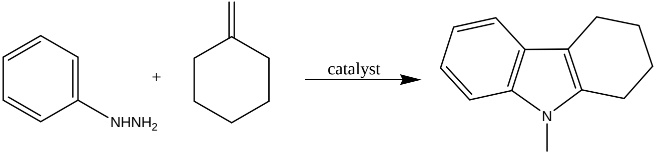
The indole ring system is probably the most ubiquitous heterocycle that represents an important stuctural component in many pharmacologically active compounds [1]. Since its discovery in the 1880s by Emil Fischer,various catalysts have been used to effect the cyclization of arylhydrazones derived from ketones.Alternative catalysts, including Bronsted acids,Lewis acids and solid acids have been reported for the synthesis of the indole nucleus, but the search for new catalysts is still being actively pursued because the reported Bronsted and Lewis acids are environmentally unfriendly, hazardous, or difficult to reuse, and they are usually required in large amounts.In addition, traditional organic solvents are still used which can have a considerable environmental impact[2].

With the approach to minimize the use of hazardous materials or volatile solvents in reaction, solvent-free condition has attracted much attention because of their advantageous properties, which include reagents immobilized on the porous solid supports, good dispersion of active reagent sites, associated selectivity and easier work- up[3].

On the basis of the above facts, herein we wish to report a new method for the one-pot synthesis of the Fischer indole scaffold with the use of ecofriendly solvent-free Melamine-formaldehyde resin supported acids which act as catalysts as well. The products are obtained in high yield,good purity, and without further purification. In unsymmetrical cases, regiospecific formation of a single product with more substitutes in the indole ring is obtained, which indicates that the Melamine-formaldehyde resin supported acid provides a good catalyst for synthesis of indoles and has a high selectivity.



Catalyst : Melamin-formaldehyde resin supported acid

References:

[1] Humphrey, G.R.; Kuethe, J.T.; *Chem Rev*, **2006,** 106, 2875.
[2] An, J.; Bagnell, L.; Cablewski, T.; Strauss, C.R.; Trainor, R.W.; *J.Org.Chem*, **1997,** 62, 2505.
[3] Tanaka, K.; Toda, F.; *Chem Rev*, **2000,** 100, 1025.

H_2O_2/CC As an efficient reagent system for the conversion of thiols to sulfonyl chlorides

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With new pharmacological targets continuously being discovered, novel biologically active leads are urgently needed, and this has stimulated a search for techniques capable of providing large numbers of pharmaceutically interesting compounds.

Oxidation is an important chemical process, prevalent throughout chemistry. It leads to significant changes in the properties of organic and biological compounds [1-2].

Sulfonyl chlorides are precursors with extensive uses in organic synthesis. The most typical method for the preparation of sulfonyl chlorides is the oxidative chlorination of sulfur compounds; thiols, sulfides, thioacetates and thiocarbamates, with aqueous chlorine [3].

A variety of methods are reported in the literature for the synthesis of sulfonyl chlorides [4]. However, various drawbacks such as low yields, long reaction times, harsh reaction conditions, tedious work up, use of expensive reagents, use of toxic agents and special efforts required to prepare the reagent associated with many of these methods.

As part of our continuing studies on the use of hydrogen peroxide in organic synthesis [5] herein, we introduce for the first time H_2O_2/CC as valuable reagent system for the direct oxidative chlorination of thiol derivatives to the corresponding sulfonyl chlorides (Scheme 1).

$$\mathrm{R{-}SH} \xrightarrow[\mathrm{CH_3CN,\ rt}]{\mathrm{H_2O_2\text{-}CC}} \mathrm{R{-}SO_2Cl}$$

R = Alkyl, Aryl

CC = Cyanuric chloride

Scheme 1.

References:

[1] Suto, Y.; Yamagiwa, N.; Torisawa, Y. *Tetrahedron Lett*. **2008**, *49*, 5732.
[2] Polshettiwar, V.; Varma, R. S. *Tetrahedron Lett*. **2008**, *49*, 2661.
[3] Olah, C. A.; Arvanaghi, M.; Ohannesian, L.; Surya, P. G. K. *Synthesis* **1984**, 785.
[4] (a) Bahrami, K. *Tetrahedron Lett.* **2006**, *47*, 2009. (b) Bahrami, K.; Khodaei, M. M.; Kavianinia, I. *Synthesis* **2007**, 547. (c) Bahrami, K.; Khodaei, M. M.; Naali, F. *J. Org. Chem.* **2008**, *73*, 6835; (d) Bahrami, K.; Khodaei, M. M.; Tirandaz, Y. *Synthesis* **2009**, 369.

Synthesis and characterization Schiff base ligands and their complexes with U(VI) and Pb(II)

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Schiff bases are a versatile class of ligands having great physiological and biological activities, and have found use as insecticides, anticoagulants, antitumour agents, antioxidants and plant growth regulators [1]. Their metal complexes have found applications in various chemical processes like nonlinear optics, sensors, medicine, etc. [2]. Furthermore, schiff bases incorporating heterocyclic moieties are well known for their metal binding ability and exhibit interesting coordinating behavior with transition metal ions [3], which makes them interesting from the structural point of view also. Schiff bases ligands can act as bidentate, tridentate or tetradentate ligands depending on the nature of heterocyclic ring substituents attached to the hydrazone unit. These ligands due to their facile keto–enol tautomerization and the availability of several potential donor sites can coordinate with metals. Schiff bases have interesting ligation properties due to presence of several coordination sites[1,4]. The ligands L_1H, L_2H, L_3H and L_4H were prepared by the condensation of 2-hydroxy-1-naphthaldehyde with 3-hydroxy-2-naphthoichydrazide, nicotinicacid hydrazide, 4-nitro-1,3-phenylendiamine and 2-amino-3-hydroxypyridine respectively in methanol and the ligands L1, L2 and L3 were prepared by the condensation of 1-Naphtylamine with 2-hydroxybenzaldehyde, 5-bromo-2-hydroxybenzaldehyde and 2-hydroxy-1-naphthaldehyde respectively in methanol medium. On refluxing the methanolic solution for 72 h yellow colouration were observed. The precipitates were collected by filtration and washed with methanol. All synthesized compounds were identified and confirmed by elemental analyses, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy. U(VI) and lead(II) complexes with the new schiff bases ligands (L_1H, L_2H, L_3H, L_4H, L1,L2 and L3) have been synthesized and characterized by CHN elemental analysis,IR, ^{1}H NMR, ^{13}C NMR spectroscopy.

References:

[1] Y.P. Kitaev, B.I. Buzykin, T.V. Troepolskaya, Russ. Chem. Rev. **1970**, 6, 441.
[2] M. Bakir, I. Hassan, T. Johnson, O. Brown, O. Green, C. Gyles, M.D. Coley, J. Mol. Struct., **2004**, 68, 213.
[3] A.E. Dissouky, O.A. Fulij, S.S. Kandil, J. Coord. Chem. **2004**, 7, 57.
[4] Z.Y. Yang, R. D. Yang, F.S. Li, K.B. Yu, *Polyhedron*, **2000**, 19, 2599.

Solvent effect on the H-bond strength of tri fluoro acetyl acetone

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Trifluoroacetyl acetone at ambient temperature is about 97% in the cis-enol form [1]. The molecules of this compound, depend on the position of the carbonyl group, could be in one of two possible tautomer forms, carbonyl be near the methyl group, 4TFAA or near the trifluorimethyl group, 2TFAA [2]. NMR Studies on TFAA also show that the chemical shift of the proton engaged in the intramolecular H-bond, unlike its parent acetylacetone, is very sensitive to the choice of solvent [2]. In this work, the effect of solvent on the position of equilibrium between these two tautomers and on the H-bond strength in both of tautomers will be studied.

Calculations:

All calculations have been done using Gaussian 03. Optimizations and frequency calculations have been done at the B3LYP level using 6-31G** and 6-311++G** basis sets. The NMR shielding constants were calculated, at the B3LYP/6-311++G** level, using the standard GIAO (Gauge-Independent Atomic Orbital) approach [3].

The results of calculations indicate that the H-bond in 2TFAA is considerably stronger than that in 4TFAA. However, in spite of this fact, 4TFAA is more stable than 2TFAA. These phenomena could be interpreted by considering the steric effect.

The optimized structures in the solvents, using Onsager and PCM methods, indicate that the H-bond of 2TFAA in polar solvents is considerably stronger than in non-polar solvents. It is interesting that this is not the case for 4TFAA, which is weaker in more polar solvents. These results have been discussed and interpreted on the basis of charge distribution in both molecules.

References:

[1] M. Zahedi-Tabrizi, F. Tayyari, A. Jalali, S.F. Tayyari, *Spectrochim. Acta*, 63A (**2006**) 387.
[2] R. L. Lintvadt, H.F. Holtzclaw, *J. Am. Chem. Soc.* 88 (**1966**) 2713.
[3] B. Osmialowski, R. Gawinecki, *Magn. Reson. Chem.* 39 (**2001**) 334 and references cited therein.

Preparation of thermally stable optically active aromatic polyamide-imides under green conditions

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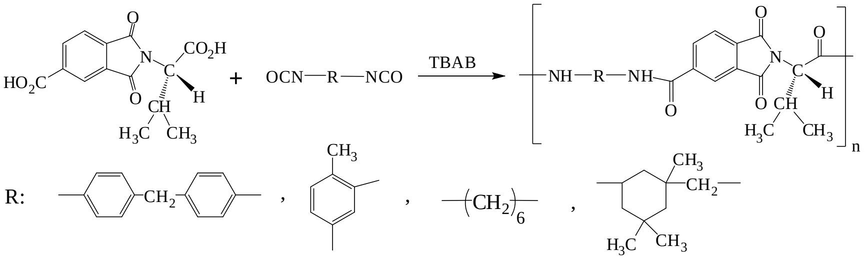
Ionic liquids (ILs) are viewed as a novel class of green benign solvents, which promise to have widespread application in industry, possibly replacing currently used organic solvents, due to unique properties such as negligible vapor pressures, high thermal and chemical stability, broad liquid temperature ranges and high specific solvent abilities [1]. Aromatic polyimides are thermally stable polymers, which demonstrate excellent mechanical and electrical properties [2]. However, these polymers are difficult to process due to their high softening temperatures and poor solubility in organic solvents [3]. Poly(amide-imide)s (**PAI**)s are one of the classes of copolyimides, which combine the advantages of high-thermal stability and processability [4].

In the work presented here, we wish to report a green and safe method for the preparation of thermally stable and optically active aromatic **PAI**s bearing amide-imidic linkage in the polymer backbone with the aim of removing the use of volatile organic compound. These **PAI**s were synthesized via direct polycondensation of different aliphatic and aromatic diisocyanates with a chiral diacid monomer under conventional heating technique in tetrabuthyl ammonium bromide (TBAB) as a molten IL. This method was compared with a classical method in a medium consisting of *N*-methyl-2-pyrrolidinone and *N*,*N*-dimethylacetamide as a solvent and the results are comparable. These polymers are thermally stable and soluble in amide-type solvents. Some structural characterization and physical properties of these new optically active polymers are reported.



References:

[1] Mallakpour, S.; Dinari, M. *Polym. Bull.* **2009**, *63*,623.
[2] Yang, C. P.; Chen, R. S.; Hung, K. S. *Polymer.* **2001**, *42*, 4569.
[3] Kim, Y. J.; Chung, I. S.; In, I.; Kim, S. Y. *Polymer.* **2005**, *46*, 3992.
[4] Liaw, D. J.; Chen, W. H. *Polym. Degrad. Stab.* **2006**, *91*, 1731.

Three-component Hantzsch reaction for the synthesis of 1,4-dihydropyridines using TiO_2 nanoparticle

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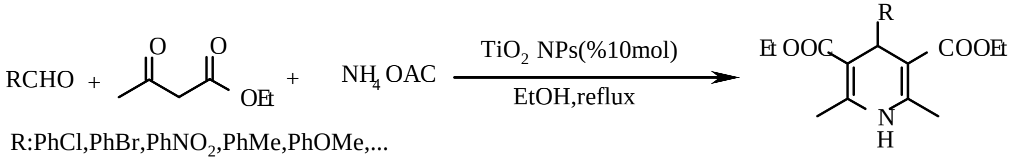
Nanotechnology is of growing importance in many branches of research because of the opportunity for miniaturization and the interesting properties associated with small particle size [1]. In recent decades, nanostructured materials have attracted much attention for their novel electronic, magnetic, optical, chemical, and mechanical properties due to their unique characteristics which are different from bulk materials [2].

Specifically, nanoparticles have great potential for use as a catalyst for a variety of organic and inorganic reactions due to their high surface-to-volume ratio [3]. On the other hand, 1,4-dihydropyridines (1,4-DHPs), as important ‘‘privileged scaffolds,’’ are very attractive targets for medicinal synthesis. A recent literature survey revealed that 1,4-DHPs have several biological applications.

In this study, an efficient one-step synthesis of 1,4-dihydropyridines in good to excellent yields via the TiO_2 nanoparticle- catalyzed Hantzsch three-component reaction of an aldehyde, ethyl acetoacetate and ammonium acetate is described. The present methodology offers several advantages such as simple procedure, excellent yields, and short reaction time.



References:

[1] Rautio, J.; Pera¨ma¨ki, P.; Honkamo ,J.; Jantunen, H. *Microchem. J.* **2009**, *91*, 272.
[2] Xia, YN.; Yang, PD.; Sun, YG.; Wu, YY.; Mayers, B.; Gates, B.; Yin, YD.; Kin, F.; Yan, HQ. *Adv. Mater*. **2003**, *15*, 353.
[3] Narayanan, R.; El-Sayed, MA. *J. Phys. Chem. B.* **2005**, *109,* 12663

Tautomerism and vibrational assignment of cyclohexane-1,2-dione

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It has been shown that cyclohexane-1,2-dione (CHDO) is completely in the enol form in sample [1]. This compound, at least theoretically, is capable to exist as different tautomers and conformers. The aim of this project is study of the structure, tautomerisation, and vibrational assignment of CHDO.

The calculations of geometrical parameters were performed using the Gaussian 03 program package and B3LYP approach in conjunction with the 6-31G(d,p) and 6-311G(d,p) basis sets without any symmetry restrictions. The harmonic vibrational frequencies and IR and Raman intensities have been obtained at the B3LYP/6-311G(d,p) level of theory.

After fully optimization, the relative energies (calculated at the 6-311G(d,p)) of the possible tautomers and conformers of CHDO have been calculated. According to our calculation, the cis-enol form is the most stable tautomer and is considerably more stable than diketo form and the trans-enol form. Therefore, existing of any other tautomer in the sample is unlikely. Our calculations indicate that the content of the keto form in the sample, at least at the ambient temperature, is less than 1%.

Coparison of the relative energies of the cis-enol form and the trans-enol form indicates the hydrogen bond strength (the energy difference between cis- and trans-enol forms) is about 7 kcal/mol.

In this work we also discuss the vibrational spectra of this compound and compare those frequencies which directly relate to the H-bond strength with the several β-diketones [2, 3] and relate the H-bond strength to the O-H···O bond angle.

References:

[1] Samanta, A. K.; Pandey, P.; Bandyopadhyay, B.; Chakrabort, T., *J. Mol. Struct.* **2010,** *963* , 234.
[2] Zahedi-Tabrizi, M.; Tayyari, F.; Moosavi-Tekyeh, Z.; Jalali, A.; Tayyari, S.F., *Spectrochim. Acta.* **2006,** *A65* , 387.
[3] Tayyari, S.F.; Emampour, J.S.; Vakili, M.; Nekoei, A.R.; Eshghi, H.; Salemi, S.; Hassanpour, M., *J. Mol. Struct.* **2006,** *794*, 204.

One-pot reaction of alkyl isocyanides with α-chloro ketone derivatives in the presence of acetylenic esters

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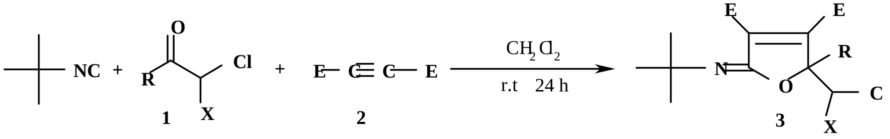
Isocyanides are compounds with an extraordinary functional group; its unusual valence structure and reactivity have been discussed for over one and a half centuries [1]. One of the classic reactivities in the chemistry of isocyanide is heterocyclic synthesis [2,3]. Here we describe a three- component condensation in which *tert*-butyl isocyanide react with α-chloro ketone derivatives **1** in the presence of acetylenic esters **2** in one-pot to afford γ-iminolactone derivative **3** in good yields. The structures of **4a-f** were deduced from their IR, ^{1}H and ^{13}C NMR Spectra.



1,2	*E*	*R*	*X*	*Yield of **3** (%)*
a	CO_2Me	CH_3	*H*	*95*
b	CO_2Et	CH_3	*H*	*90*
c	CO_2Me	CH_2Cl	*H*	*95*
d	CO_2Et	CH_2Cl	*H*	*90*
e	CO_2Me	*Ph*	*Cl*	*95*
f	CO_2Et	*Ph*	*Cl*	*90*
g	CO_2Me	CH_3	*Cl*	*90*
h	CO_2Et	CH_3	*Cl*	*85*

References:

[1] Weber, L. *Curr. Med. Chem.* **2002**, *9*, 2085.
[2] (a) Ugi, I. ; Lohberger, s. ; Karl, R. In Comprehensive Organic Synthesis; Trost, b. M., Fleming, I., Eds.; Pergamon Press: Oxford, 1991, vol.2, pp 1083-1106. (b) Domling, A.; Ugi, I. *Angew. Chem. Int. Ed.* **2000**, *39,* 3169.
[3] Nair, V.; Kajesh, C.; Vinod, A. U.; Binda, S.; Sreekanth, A. R.; Mathess, J. S.; Balagopal, L. *Acc. Chem. Res.* **2003**, *36,* 899.

Brønsted-acidic ionic liquids as efficient and reusable catalysts for the facile dehydration of aldoximes into nitriles

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The cyano moiety is a highly important one not only due to its synthetic value as precursor to other functionalities [1-2] but also due to its presence in a variety of natural products, pharmaceuticals, and bioactive molecules [3, 4]. Thus, methods for preparing organic nitriles are highly desirable. The most efficient route reported for preparing nitriles and one that has received much recent attention involves the dehydration of aldoximes that is one of the cleanest routes avoiding inorganic cyanides. A number of dehydration agents have been employed for this transformation including N-chlorosuccinimide/pyridine in CH_3CN [5], thionyl chloride [6], triphenylphosphine/I_2 [7], etc. Although these methods may be effective at dehydrating aldoxidmes, most of them encounter some limitations such as long reaction times, unsatisfactory yields, harsh reaction conditions, expensive or not readily available reagents, hazardous organic solvents and tedious work-up procedure.

Prompted by these findings herein we wish to report a green and efficient methodology for the dehydration of aldoximes to nitriles using two halogen-free Brønsted-acidic ILs, 3-methyl-1-(4-sulfonic acid)butylimidazolium hydrogen sulfate $[(CH_2)_4SO_3HMIM][HSO_4]$ and N-(4-sulfonic acid)butylpyridinium hydrogen sulfate $[(CH_2)_4SO_3HPY][HSO_4]$.

$$\mathrm{Ar{-}CH{=}NOH} \xrightarrow{\text{Brønsted-acidic ILs}} \mathrm{Ar{-}C{\equiv}N}$$

References:

[1] Tennant, G. In *Comprehensive Organic Chemistry*, Barton, D.; Ollis, D. W.; Sutherland, I. O. Ed.; Pergamon: Oxford, **1979**, Vol. *1*, p. 528.
[2] Srinivas, K. V. N. S.; Reddy, E. B.; Biswanath, D. *Synlett.*, **2002**, *4*, 625.
[3] Miller, J. S.; Manson, J. L. *Acc. Chem. Res.*, **2001**, *34*, 563.
[4] Romero, M.; Renard, P.; Caignard, D. H.; Atassi, G.; Solans, X.; Constans, P.; Bailly, C.; Pujol, M. D. *J. Med. Chem.*, **2007**, *50*, 294.
[5] Gucma, M.; Golebiewski, W. M. *Synthesis*, **2008**, *13*, 1997.
[6] Telvekar, V. N.; Akamanchi, K. G. *Synth. Commun.*, **2004**, *34*, 2331.
[7] Narsaiah, A. V.; Sreenu, D.; Nagaiah, K. *Synth. Commun.*, **2006**, *36*, 137.

An efficient one pot synthesis of highly functionalised 3,3-dispiropyrrolidine bisoxindoles via [3+2] cycloaddition

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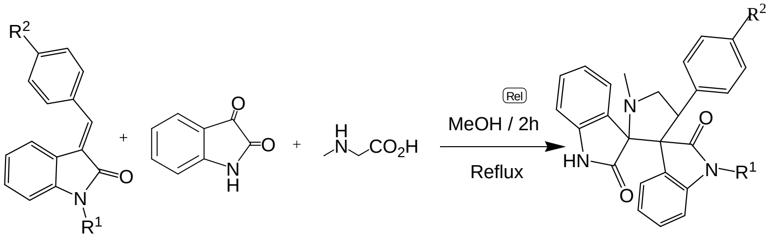
3-Spiro and dispirooxindoles and their derivatives have become important synthetic targets as these structural frameworks form the core units of many naturally occurring molecules that possess significant biological activities. These derivatives have served as potential synthetic intermediates for the total synthesis of alkaloids, drug intermediates and clinical pharmaceuticals.

1,3-Dipolar cycloaddition reactions constitute one of the most fundamental reactions for the stereoselective construction of five-membered heterocyclic compounds. Azomethine ylides are a class of powerful reagents used in [**1,3**]-dipolar cycloaddition reactions which in general afford a range of pharmacologically important heterocyclic compounds.

In this report we used (*E*)- Arylideneindolinone derivations as unusual dipolarophiles for the synthesis dispirooxindoleswith potential biological significance. We observed that when the dipolarophiles **1**a–g, were subjected to **1,3**-dipolar cycloaddition with the azomethine ylide generated in situ by decarboxylation condensation of isatin **2** and sarcosin **3** in methanol, a mixture of cycloadducts **4**a–g was obtained.



1a-g **2** **3** **4a-g**

R^1:Me, Et, Ph
R^2: Me,OH,OMe,Br

References:

[1] Naerts, A. J.; DeGroote, M. A.; Orme, I. M. *Trends Microbiol.* **2008**, *16*, 48.

[2] Mioka, H. Curr. *Pharm. Des.* **2006**, *12*, 4047.

[3] Illiams, K. J.; Duncan, K. *Curr. Mol. Med.* **2007**, *7*, 297.

Meta phosphoric acid $(HPO3)_n$ as an efficient catalyst for the synthesis of some oxygenated heterocyclic compounds such as octahydro xanthene derivatives

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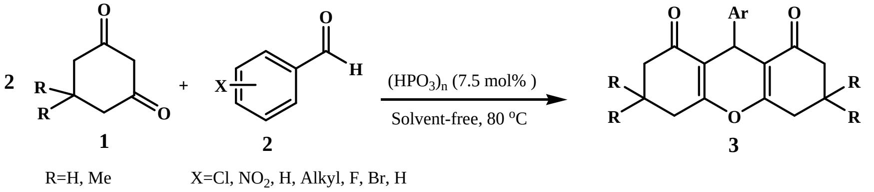
Organic chemistry researchers from both academia and industry have started giving serious thought to the detrimental effect of non-green processes and chemicals on the environment. They have successfully developed several environmentally benign procedures to avoid, or at least minimise, these effects.

Among oxygenated heterocyclic compounds, xanthene derivatives are particularly important for different reasons such as biologic and treatment properties such as anti virus, anti phlogosis and anti bacteria [1-3].

Herein, A simple, efficient and cost-effective method for the synthesis of 1,8-dioxo-octahydroxanthene **3** derivatives via cyclocondensation of dimedone or 1,3 cyclohexadion **1** with aldehydes **2** in the presence of meta phosphoric acid $(HPO3)_n$ as a highly efficient catalyst under solvent-free conditions at 80 °C was described.

This method is important from an environmental point of view and economic considerations, because it produces little waste, Simple preparation and stability of catalyst, simple work-up procedure and the high yields of products, short reaction times and avoiding from use of toxic organic solvents as media. Scheme of the general reaction is presented below.



References:

[1] Lambert, R. W.; Martin, J. A.; Merrett, J. H.; Parkes, K. E. B.; Thomas, G. J. *Chem. Abstr*. **1997**, *126*, 2123.

[2] Hideo, T.; Koho, J. T. *Chem. Abstr*. **1981**, 95.

[3] Poupelin, J. P.; Saint- Rut, G. ; Foussard-Blanpin, O.; Narcisse, G. ; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.* **1978**, *13*, 67.

Chemical modification of glycidyl methacrylate polymers with 9- anthracenecarboxylic acid groups

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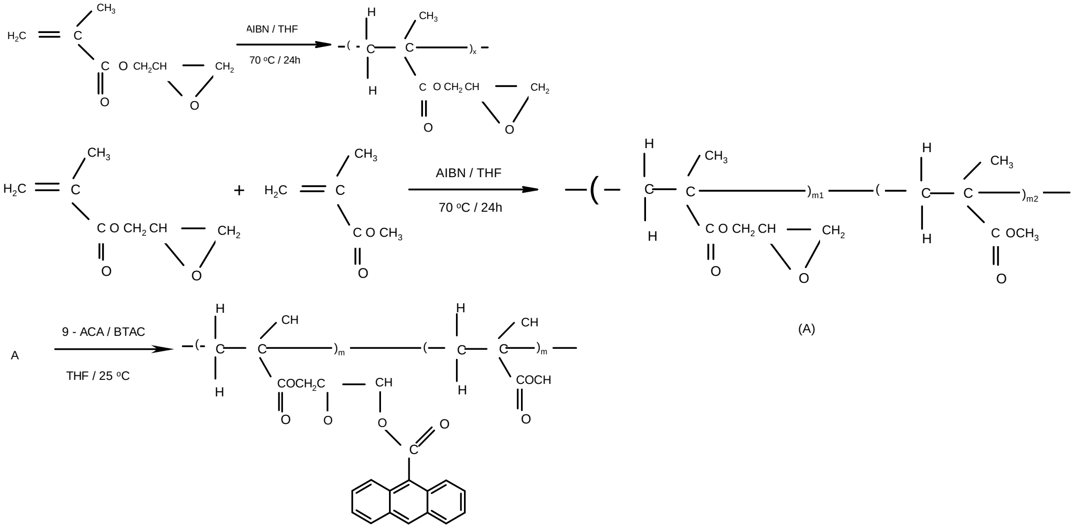
Glycidyl methacrylate (GMA) has been homopolymerized and copolymerized practically like any other acrylic monomer by means of free radical initiators known to selectively attack the methacrylic double bonds [1]. In this work the homopolymer of glycidyl methacrylate (GMA) and its rondom copolymer with methyl methacrylate (MMA) were synthesized by free radical polymerization method in tetrahydrofuran (THF) solution at 70 ± 1°C using azobis (isobutyronitrile) (AIBN) as initiator to give the copolymer in good yields [2]. Then copolymers of glycidyl methacrylate have been modified by incorporation of 9-anthracenecarboxylate groups through the ring opening reaction of the epoxy group. The structure of all the resulted polymers was characterized and confirmed by FT-IR and ^{1}H-NMR spectroscopic techniques. It was found that these polymers with 9-anthracenecarboxylic acid (9-ACA) moieties have high thermal stability. The presence of bulk 9- anthracenecarboxylate graups in polymer side chains leads to a different applications in polymer industry, and a series of novel modified polymers are obtained [3,4].



Reference:

[1] Iwakura, Y., Toda, F., Ito. T. Aoshima, K., *Polym. Let*. **1987**, 5, 29.
[2] Okamoto, y., urakawa, K., Yuki, H., *Polym. J.*, **1978**, 10(4), 473.
[3] Safa, K. D., Nasirtabrizi, M. H., *Eur. Polym. J.*, **2005**, 41, 2310.
[4] Safa, K. D., Nasirtabrizi, M. H., Tofangdarzadeh. Sh. *Iran Polym. J.* **2008**, 14(1), 39.

Synthesis of poly(methyl methacrylate) with terpyridine via Reversible addition fragmentation chain transfer (RAFT) polymerization

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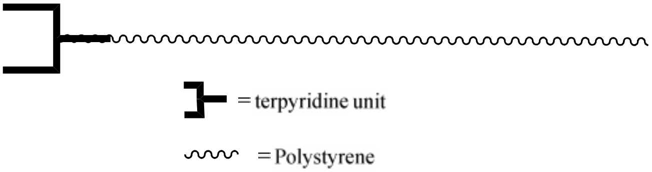
Reversible Addition–Fragmentation chain Transfer (RAFT) polymerization has developed into one of the leading controlled/living radical polymerization techniques since its invention by the CSIRO group in 1998 [1]. It enables the formation of polymeric materials with controlled molecular weights, low polydispersities, and complex macromolecular architectures, such as block, comb, star, and hyperbranched copolymers [2].

The mediating compounds employed in most RAFT polymerizations are dithioesters, Z-C(=S)S-R, which have been developed in great structural variety with respect to their leaving R-groups and to their stabilizing Z-moieties [3]. The terpyridine as an Z-group increase heat stability of the polymer. The hydroxyl group in the terpyridine was converted into thiocarbonyl-thio compound (xantate) as chain transfer agent, and was further used to mediate the RAFT polymerization of methyl methacrylate.

All of the materials were characterized by FT-IR, H-NMR spectroscopy and thermal analysis. The number-average molecular weight and polydispersity index (PDI) of the poly(methyl methacrylate) were determined by gel permeation chromatography (GPC).



References:

[1] Chiefari, J.; Chong, Y. K.; Thang, S. H. *Macromolecules* **1998**, *31*, 5559.
[2] Barner, L.; Barner-Kowollik, C.; Davis, T. P.; Stenzel, M. H. *Macromolecules* **2007**, *28*, 539.
[3] Chong, Y. K.; Krstina, J.; Le, T. P. T.; Moad, G.; Postma, A.; Rizzardo, E.; Thang, S. H. *Macromolecules* **2003**, *36*, 2256.

Synthesis of an optical brightening agent, 4,4'-bis(4-methoxystyryl)-biphenyl

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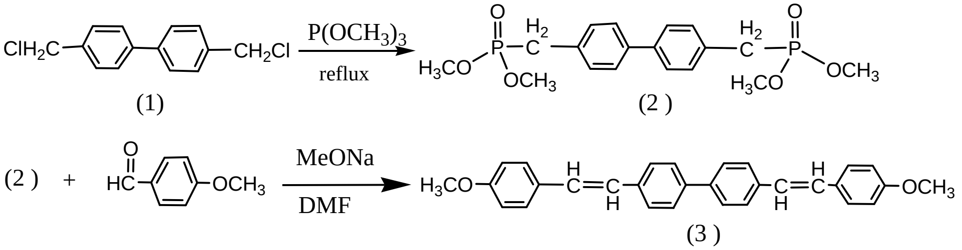
Optical brightening or withening agents, due to attraction of ultraviolet waves and reflection in green to ultraviolet area can be used in plastic, textile, fabric, paper and detergent industries [1-4]. 4,4'-bis(4-methoxy styryl)-biphenyl, an optical brightener, has been synthesized and characterized in this work.

The agent was synthesized through a two step reaction. Refluxing 4,4'- bis(cholromethyl)–biphenyl(1) with trimethyl phosphite resulted in preparation of a phosphonate intermediate, 4,4'- bis- (dimethoxyphosphonomethyl)-biphenyl (2). The phosphonate intermediate was then reacted with para-methoxybenzaldehyde in presence of sodium methoxide in DMF as salvent resulting in production of 4,4'-bis(4-methoxy styryl)-biphenyl (3), a new optically active agent.

The product was characterized by ^{13}CNMR , ^{1}HNMR and UV spectra .



References:

[1] Christian Luethi; Kurt Weber; US patent No,4602087, **1986.**
[2] Kurt Weber; Peter Liecheti; US patent No,3984399, **1976.**
[3] Kentarro Okuma ; Yuji Tachibana ; *Bull. Chem. Soc. Jpn.* **1988,** *61*,4323.
[4] Christian Luethi; US patent No, 3907904, **1974.**

Chemical composition and antibacterial activity of the essential oil from leaves of *Ferula ovina* (Boiss.) Boiss.growing wild in Iran

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The genus *Ferula* comprises perennial herds distributed from the Mediterranian region to central Asia.Thirty species of genus *Ferula* are found in Iran,among which 15 are endemic [1]. Several species of the genus *Ferula* are used in traditional medicine,e.g. the roots of *F.persica* have been used in folk medicine to treat diabetes [2].There have been several studies of the genus *Ferula*.The reported compounds were mainly coumarins and sesquiterpene esters .

Conversely,only afew studies have reported the chemical composition of *Ferula* essential oils.Perviously,we reported the essential oil composition of *F.stenocarpa*. *F.microcolea*, *F.hirtella*, *F.macrocolea* and *F.galbaniflua* [3-6].

The present work presents the chemical composition and antibacterial activity of the essential oil of leaf of *F.ovina* growing wild in Haraz road in July 2009. The colorless oil were obtained by hydrodistillation , using a Clevenger-type apparatus for 4h and analyzed by GC and GC/MS.

Sixty-nine components in the leaf oil of *F.ovina* , which represented about 93.8% of the total oil , were identified . The leaf oil of *F.ovina* consisted of sixteen monoterpene hydrocarbons (53.6%) , thirty-two oxygenated monoterpenes (34.1%), eleven sesquiterpene hydrocarbons(2.6%), seven oxygenated sesquiterpenes(3.1%),and three non terpenoid compounds(0.4%). The major components of this oil were α- pinene(22.5%), bornyl acetate (14.1%) and camphene (11.0%). Other notable constituents were borneol(6.5%) and limonene (6.4%). As can be seen from the above information, in the leaf oil of the plant monoterpenes(87.7%), perdominated over sesquiterpenes(5.7%). Antibacterial activity was measured using the growth inhibitory zones. The oil of the plant showed significant antibacterial activity against Gram-positive bacteria.

Reference:

[1] Mozaffarian,V.A Dictionary of Plant Names, Farhang Moaser Publishers,Tehran, Iran, **1996.**
[2] Diab,Y**;**Doimazon,R.;Bessiere,J.M.Flav. Frag. J. **2001**, 16, 120.
[3] Rustaiyan,A.;Assadi,F.;Monfared,A;Masoudi,S.;Yari,M.J.Essent.Oil Res. **2001**, 13, 181.
[4] Akhgar,M.R.;Rustaiyan,A.;Masoudi,S.;Bigdeli,M.J.Essent.Oil Res.**2005**,17,237.
[5] Rustaiyan,A.;Nadimi,M;Mazloomifar,H.;Masoudi,S.J.Essent.Oil Res.**2005**,17,55.
[6] Rustaiyan,A.;Monfared,A.;Masoudi,S.;Ameri,N.J.Essent.Oil Res.**2002**,14,286.

DFT study of electronic properties of some β -alkyle thiophene oligomers

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The electro synthesis of electrically conducting organic polymers, first described with poly pyrrole, and then continued with other different monomers [1]. Poly thiophene is one of conductive polymers has been studied in many research places in the world. In our previous work, we studied some of characteristics of monomers of alkyle thiophene [2]. But in the present work, we consider the electro synthesis of 3-alkyle thiophenes by calculation of electronic properties of their oligomers (including dimer to hexamer). We applied G03 program package and our calculations were done of two level of theory, HF/6-31G** and B3LYP/6-31G**. Behavior of HLGs (HOMO-LUMO Gaps) in all oligomers has shown that HLG decrease with increasing length of oligomer for each monomer and also decrease with increasing length of substituent. The results show that long oligomers with long substituent have the lower HLG. Also, optimized structural properties demonstrate that radical cation oligomers have more planar structure compared corresponding neutral oligomers. This behavior observed to aromaticity of this compound. Finally the calculations show that oligomers of 3-propyle thiophene have the best conditions to candidate as conductive polymers among 3-alkyle thiophenes and conductivity of larger oligomers is more.

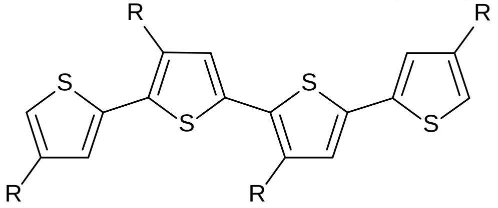

Fig 1. Structure isomer of the 3-alkyle thiophene tetramer,R= CH_3, C_2H_5, C_3H_7.

References:

[1] T. A. Skothiem, R. Elsenbaumer, J. Reynolds, *Handbook of Conducting Polymers*, Marcel Dekker, New York, **1998**

[2] H. Nikoofard, Z. Kalantar, M. Khorrami, *13th Iranian Physical Chemistry seminar*, Shiraz University and Shiraz University of Technology, Iran.

Acidic alumina as heterogeneous catalyst for the preparation of 2*H*-indazolo[2,1-b]phthalazine-trione derivatives under solvent-free conditions

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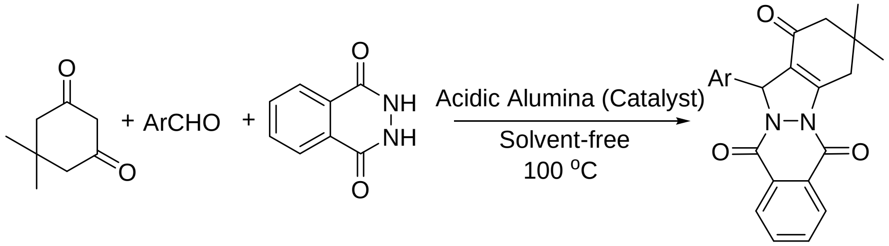
Heterocyclic compounds occur very widely in nature and are essential to life. Among a large variety of heterocyclic compounds, heterocycles containing phthalazine moiety are of interest because they show some pharmacological and biological activities [1]. An efficient protocol for the one-pot preparation of 2*H*-indazolo[2,1-b]phthalazine-trione derivatives [2] *via* a three-component condensation reaction of phthalhydrazide, dimedone, and aromatic aldehydes under solvent-free conditions in high to excellent yields and short reaction times using acidic alumina as catalyst is described (Scheme). This methodology offers significant improvements with regard to the scope of this transformation, simplicity in operation, and green aspects by avoiding expensive or corrosive catalysts.



Scheme

References:

[1] (a) Al´-Assar, F.; Zelenin, K. N.; Lesiovskaya, E. E.; Bezhan, I. P.; Chakchir, B. A. *Pharm. Chem. J.* **2002**, *36*, 598.; (b) Jain, R. P.; Vederas, J. C. *Bioorg. Med. Chem. Lett.* **2004**, *14*, 3655.; (c) Carling, R. W.; Moore, K. W.; Street, L. J.; Wild, D.; Isted, C.; Leeson, P. D.; Thomas, S.; O'Conner, D.; McKernan, R. M.; Quirk, K.; Cook, S. M.; Atack, J. R.; Waftord, K. A.; Thompson, S. A.; Dawson, G. R.; Ferris, P.; Castro, J. L. *J. Med. Chem.* **2004**, *47*, 1807.
[2] Sayyafi, M.; Seyyedhamzeh, M.; Khavasi, H. R.; Bazgir, A. *Tetrahedron* **2008**, *64*, 2375.

A novel approach to the synthesis of highly functionalized pyridines

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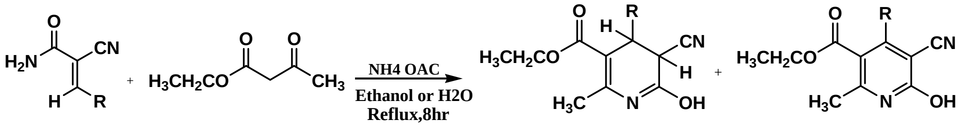
Pyridines are of interest because of the occurrence of their saturated and partially saturated derivatives in biologically active compounds and natural products such as NAD nucleotides, pyridoxol (vitamin B_6), and pyridine alkaloids [1]. Due to their π-stacking ability, some pyridines are used in supramolecular chemistry [2]. Some examples are used as pharmaceuticals (as antimalarial, vasodilator, anesthetic, anticonvulsant, and antiepileptic), dyes, additives (as antioxidant), agrochemicals (as fungicidal, pesticidal, and herbicidal), veterinary (as anthelmintic, antibacterial, and antiparasitic), and also in qualitative and quantitative analysis [3].

Herein we report A new and efficient one-pot synthesis of polysubstituted pyridine derivatives by four-component reaction between cyanoacetamide, aryl aldehydes and ethyl acetoacetate with ammonium acetate. The reactions were performed in water and ethanol under reflux conditions and afforded high yields of products.



(A) (B)

References:

[1] Yates, F. S. *In Comprehensive heterocyclic chemistry, Boulton, A. J. and McKillop, A. Eds.* (Pergamon, Oxford, **1984**), Vol. 2, p. 511.
[2] Jones, R. A. In Pyrroles, *Part II: The synthesis, reactivity, and physical properties of substituted pyrroles* (Wiley, New York, **1992**).
[3] Gilchrist, T. L. *J. Chem. Soc., Perkin Trans. 1*, **2001**, 2491.

Efficient one-pot synthesis of 3,4-dihydro pyrano[*c*]chromens in aqueous media

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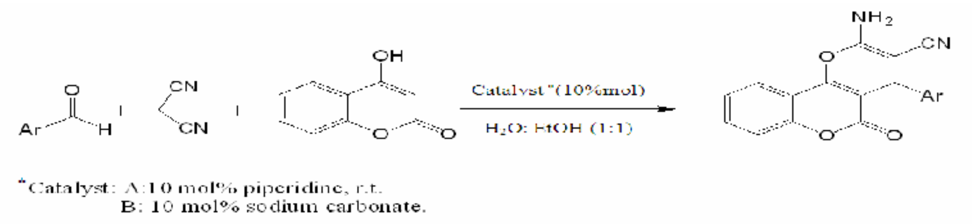
Dihydro pyrano[*c*]chromens and their derivatives have a wide range of biological activities [1-2]. There are different methods for the synthesis of this skeleton, but some of them have some drawbacks. Finding a suitable method for the synthesis of this scaffold is an interesting subject in organic synthesis.

As a part of our studies aimed to develop simple and efficient synthesis of heterocyclic skeletons [3], herein, we described a green protocol for the synthesis of 3,4-dihydro pyrano[*c*]coumarines via three-component reaction of 4-hydroxy coumarin, malononitril and benzaldehydes in the presence of catalytic amount of piperidine or sodium carbonate (10%) in mixture of 1:1 H_2O:EtOH.

The amount of catalyst was optimized and the product had good diversity. The structures of the products were deduced according to spectroscopic data.

The details of the proposed mechanism will be discussed in the conference.



References:

[1] Jitender M. Khurana , Sanjay Kumar *Tetrahedron Lett.* **2009**, *50,* 4125.
[2] El-saghier, A.M.A. ; Naili, M.B.; Rommash, B.K.; Saleh, N.A.; Kreddan,K.M. *Arkivoc* **2007**(Xvi) 83.
[3] Abdolmohammadi, S; Balalaie, S; *Tetrahedron Lett.* **2007**, *48,* 3299

A fast, simple and convenient procedure for the synthesis of 1-amidoalkyl 2-naphthols by using [Hmim][HSO_4] as an efficient and reusable catalyst under solvent-free conditions

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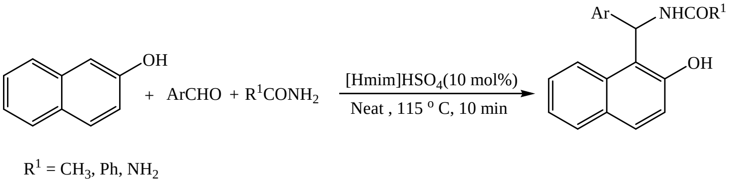
It was found that compounds containing 1,3-amino-oxygenated functional groups were frequently used as biologically active natural products and potent drugs such as nucleoside antibiotics and HIV protease inhibitors. It is noteworthy that 1-amidoalkyl 2-naphthols can be converted to useful and important biological building blocks. For example, 1-amidoalkyl 2-naphthols can be hydrolyzed to 1-aminoalkyl 2-naphthol derivations that these compounds show hypotensive and bradycardiac effects [1]. 1-Amidoalkyl 2-naphthols can be prepared by multicomponent condensation of aldehydes, 2-naphthols and acetonitrile or various amides in the presence of Lewis or Brønsted acids [2, 3]. Because of the great potential of room temperature ionic liquids as environmentally benign media for the catalytic processes, chemists have currently focused on organic reactions catalyzed by ionic liquids. Brönsted acidic ionic liquids combining the advantageous characteristics of solid acids and mineral acids are designed to replace traditional mineral liquid acids, such as sulfuric acid and hydrochloric acid, in chemical processes. Ionic liquids with Brönsted acidic counter ions have been used as acid catalysts and provide a useful medium under solvent-free conditions because of their polar nature. Several organic reactions catalyzed by ionic liquids have been reported with high performance. Herein we report an efficient, fast, and convenient procedure for the one-pot three-component synthesis of amidoalkyl naphthol derivatives from a variety of aryl aldehydes, 2-naphthol and different kind of amides (acetamide, benzamide and urea) in the presence of [Hmim][HSO_4] as a Brönsted acidic ionic liquid under solvent-free conditions.



Reference:

[1] Shen, A. Y.; Tsai, C. T.; Chen, C. L. *Eur. J. Med. Chem.* **1999**, *34*, 877.
[2] Khodaei, M. M.; Khosropour, A. R.; Moghanian, H. *Synlett* **2006**, 916.
[3] Shaterian, H. R.; Yarahmadi, H.; Ghashang, M. *Tetrahedron* **2008**, *64*, 1263.

A novel catalyst-free route to the synthesis of 1,3,4-oxadiazole-2-thione derivatives

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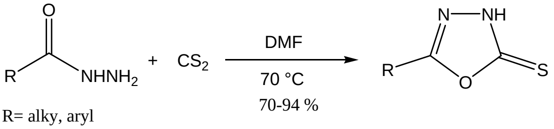
1,3,4-oxadiazole-2-thione derivatives are an important class of five-member heterocyclic compounds which have attracted much attention due to their applications as key intermediates in organic synthesis, studies of biological activity and theoretical calculations and investigation chemistry.[1] In addition, their derivatives represent an important type of heterocyclic compound in the field of coordination chemistry because of their potential multifunctional donor sites, via either exocyclic sulfur or endo cyclic nitrogen.[2] Although many studies have been reported concerning the biological activities and structural investigations of 1,3,4-oxadiazole-2-thione derivatives, we have found only a few procedures describing the synthesis of these compounds in the literature. By far the most common strategy for the synthesis of 1,3,4-oxadiazole-2-thiones involve the interaction of acid hydrazides with carbon disulfide in the presence of alcoholic potassium hydroxide.[3]

These issues have prompted us to investigate the synthesis of 1,3,4-oxadiazole-2-thiones in catalyst-free and mild solution conditions. Various aliphatic, aromatic or heteroaromatic hydrazide were tested, which all gave the target products in good to excellent yields . In fact, from these reactions, we have isolated 1,3,4-oxadiazole-2-thiones with no evidence for the formation of any by-products such as 1,5-dibenzoylthiocarbazide or 1,3,5-thiadiazole derivatives .



In conclusion, we have developed a novel and efficient catalyst-free and solvent assisted protocol for the synthesis of 5-substituted 1,3,4-oxadiazole-2-thiones with potential synthetic and pharmacological interest. Catalyst-free conditions, excellent yields, a simplified purification process, short reaction times, ease and safe handling are the main advantages of this method.

References:

[1] (a) Jain, N.; Pathak, D. P.; Mishra, P.; Jain, S. *J. Iran. Chem. Soc.* **2009**, *6*, 77; (b) Hoggsrth, E. *J. Chem. Soc*. **1952**, 4811; (c) Vijayaraghavan, S.; Somani, R. R.; Shirodkar, P. Y.; Kadam, V. J. *International J. Pharm. Tech. Res*. **2009**, *1*, 811.

[2] (a) **Singh**, N. K.; Kushawaha, S. K.; Bharty, M. K.; Dulare, R.; Butcher, R. J. *J. Molecular Structure* **2009**, *936*, 257; (b) Singh, M.; Butcher, R. J.; Singh, N. K. *Polyhedron* **2009**, *28*, 95.

[3] (a) Khali, M. A.; El-Khawass, S. M.; Kassem, M. G. *Sci. Pharm*. **1980**, *48*, 344; (b) Belkadi, M.; Othman, A. A. *Arkivoc* **2006**, *11*, 183; (c) Charistos, D. A.; Vagenas, G. V.; Tzavellas, L. C. *J. Heterocyclic Chem.* **1994**, *31*, 1593; (d) Sandstrom, J.; Wennerbeck, I. *Acta. Chem. Scand*. **1966**, *20*, 57.

Synthesis and characterization of mono- and bicycle heterocyclic derivatives containing 1,3,4-thiadiazole and thiadiazine rings

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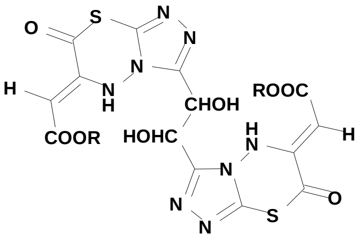
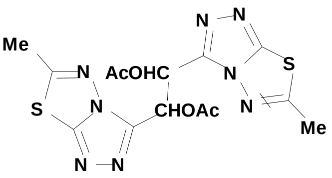
During recent years there have been investigation of different classes of 1,3,4-thiadiazoles and thiadiazines derivatives, many of which have demonstrated a broad spectrum of biological activity in both agrochemical and pharmaceutical fields showing antibacterial, antimicrobial, insecticidal, herbicidal/fungicidal and antitumor activity [1-2].

In addition, compounds incorporating both 1,2,4-triazole and 1,3,4-thiadiazole rings have been attracting widespread attention due to their diverse pharmacological properties such as antimicrobial, anti-inflammatory, analgesic, and antitumor activities [3-4]. Consequently, in view of the above facts and as a part of an ongoing investigation into biologically more active and less toxic substances, our current interest is focused on the synthesis of a series of new 1,3,4-thiadiazole and condensed 1,2,4-triazolothiadiazine derivatives.





References:

[1] Ates, O.; Kocabalkanli, A.; Sanis, G.; Ekinci, A.; Vidin. A.; *Drug Res.*,**1997**, *47*, 1134.
[2] Li, X.; Wang, Y.; Chen, W.; Huang, Q.; Liu, C.; Song, G.; *J. Flurine Chem.*, **2003**, *123*, 163.
[3] Amir, M.; Shikha, K. *Eur. J. Med. Chem*., **2004**, *39*, 535.
[4] Palaska, E.; Sahin, G.; Kelicen, P.; Durlu, N.T.; Altinok, G. *Farmaco*, **2002**, *57*, 101.

Iodine: A versatile catalyst in the synthesis of resorcinarenes

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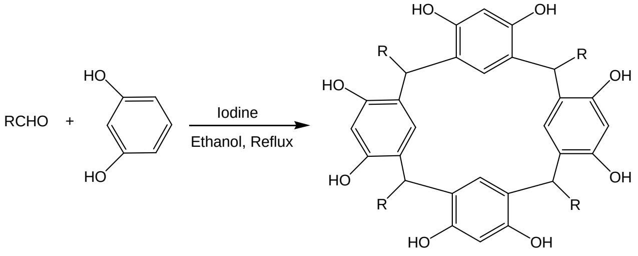
Interest in the chemistry of resorcinarene has increased in recent years. They serve as starting materials for variety of cavitands or compounds that contain a cavity that can accommodate other ions or molecules [1]. Resorcinarene derivatives can exhibit liquid crystalline behavior [2]. They have also found application as HPLC stationary phases [3].

Resorcinarenes can be prepared by acid-catalyzed condensation of an aldehyde with resorcinol [4].

A number of methods have been developed for the synthesis of resorcinarene involving various catalyst such as $Yb(OTf)_3$ [5], $Bi(OTf)_3$ [6]. A solvent free synthesis of resorcinarenes using *p*-TsOH as the catalyst has also been reported. These procedures suffer from either the use of large quantities of concentrated HCl, use toxic catalysts or require long reaction times.

In this work catalytic amount of iodine (I_2) was found to be an effective catalyst for the condensation reaction of aldehydes with resorcinol in the ethanol and reflux condition. This method is metal-free, and generates good yields of products. Using catalytic amount of molecular iodine devoid the use of expensive, corrosive reagents, toxic solvents and provides the operational simplicity.



References:

[1] Niederhoffer, E. C; Timmons, J. H; Martell, *A .E .Chem. Rev.* **1984**, *84*, 137.
[2] Erdtman, H.; Hogberg, S; Abrahamsson, S.; Nilsson, B. *Tetrahedron Letters* **1986**, *9*, 1679.
[3] Hogberg, A. G. S. *J. Am. Chem. Soc.* **1980**,*102*,6046
[4] Baeyer, A, *BerDtschchemGes* **1872**, *5*, 25.
[5] Morikawa, O.; Yanagimoto, M.; Sakakibara, H.; Kobayashi, K.; Konishi, H.; *Tetraherdron Letters* **2004**, *45*, 5731.
[6] Peterson, K. E.; Smith, R. C; Mohan, R. S. *Tetraherdron Letters* **2003**, *44*, 7723.

Ring opening of epoxides with various thiols for the synthesis of β-hydroxy sulfides under ultrasonic conditions

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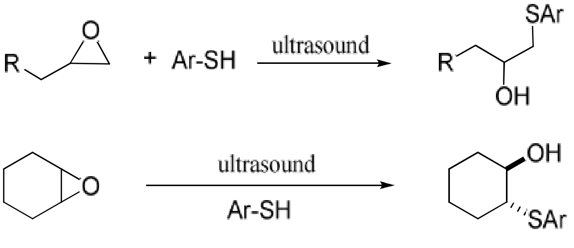
Ring opening of epoxides with thiols is an important method in organic synthesis and has found much uses in pharmaceutical and natural product chemistry, particularly for the synthesis of leukotrienes [1]. Recent approaches for the synthesis of β-hydroxy sulfides have been involving nucleophilic ring opening of epoxides with thiols under various sets of conditions [2] In many of these cases, the ring opening of epoxides is carried out in a solvent and in the presence of equimolar quantities of a Lewis acid or other additives.

The use of ultrasound irradiation in the synthesis of many organic chemicals at ambient temperature is now well documented [3]. Consequently, many protocols have been developed to carry out organic transformations in shorter reaction times and under milder and more environmentally friendly conditions. In continuation of our studies to develop environmentally friendly processes and in the framework of our investigations on ring opening of epoxides [4], we would like to herein report an efficient protocol for ultrasound promoted thiolysis of epoxides in pure water free from any additive or pH adjustment.



References

[1] Hammarstrom, S.; Samuelsson, B.; Clark, D. A.; Goto, G.; Marfat, A.; Mioskowski, C.; Corey, E. *J. Biochem. Biophys. Res. Commum.* **1980**, *92*, 946.
[2] Maiti, A. K.; Bhattacharyya, P. *Tetrahedron* **1994**, *50*, 10483.
[3] Mason, T. J. *Chem. Soc. Rev.* **1997**, *26*, 443.
[4] Mojtahedi, M. M.; Abaee, M. S.; Heravi, M. M.; Behbahani, F. K. *Monatsh. Chem.* **2007**, *138*, 95.

5, 5′-Dimethyl-3,3′-azoisoxazole as a new heterogeneous azo reagent for esterification of phenols and selective esterification of benzylic alcohols under Mitsunobu condition

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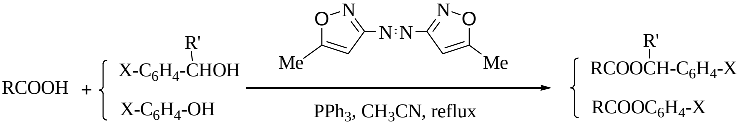
There are a number of chemical transformations that are highly profitable from a synthetic point of view, but are often plagued by purification difficulties. Infamous in this respect and often exploited approach is Mitsunobu reaction. In this reaction, a unique dehydration occurs between alcohols and various Brønsted-Lowry acids utilizing a combination of diethyl azodicarboxylate (DEAD) - triphenylphosphine (TPP).[1] This reaction historically faced purification challenges and often haunts the chemist in the isolation of the desired product from phosphine oxide and hydrazinodicarboxylate as by-products.[2] The mentioned laborious purification encountered with this reaction and motivation for extension of this important reaction in our research group[3] prompted us to design new heterogeneous azo reagent 5,5′-Dimethyl-3,3′-azoisoxazole that suggest an attractive approach to solve the separation problem in Mitsunobu reaction. After the successful synthesis of this heterogeneous azo reagent, we used 5,5′-Dimethyl-3,3′-azoisoxazole in conjunction with PPh_3 for esterification of phenols and highly selective esterification of benzylic alcohols (Scheme 1).



R = Alkyl, Aryl, Vinyl
R' = H, Me
X = H, Me, iso-Pr, t-Bu, OMe, Cl, Br, NO_2

The easy synthesis of this reagent in one step, facility in product isolation, separation of the hydrazine by-products that encountered with the Mitsunobu reaction and its recyclability are the most important advantages of this new azo reagent.

References:

[1] Mitsunobu, O. *Synthesis* **1981**, 1. b) Kumara Swamy, K. C.; Bhuvan Kumar, N. N.; Balaraman, E.; Pavan Kumar, K. V. P. *Chem. Rev.* **2009**, *109*, 2551.
[2] Dandapani, S.; Curran, D. P. *Chem. Eur. J.* **2004**, *10*, 3130.
[3] a) Iranpoor, N.; Firouzabadi, H.; Khalili, D.; Motevalli, S. *J. Org. Chem.* **2008**, *73*, 4882. b) N. Iranpoor, N.; Firouzabadi, H.; Nowrouzi, N.; Khalili, D. *Tetrahedron* **2009**, *65*, 3893.

Synthesis and characterization of some pyrazoles under sand-bath condition using silica phosphoric acid.

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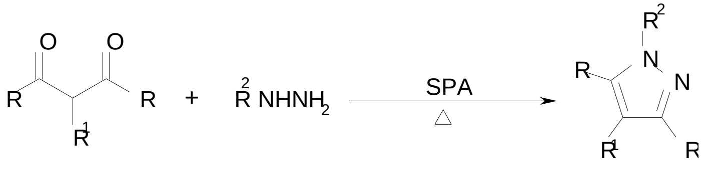
The toxicity and volatile nature of many organic solvents, particularly chlorinated hydrocarbons that are widely used in huge amounts for organic reactions have posed a serious threat to the environment [1]. Thus, design of solvent -free catalytic reaction has received tremendous attention in recent times in the area of green synthesis [2]. One important aspect of clean technology will be the use of environmentally friendly catalysis typically involving the use of solid acid catalyst that can be easily recovered when the reaction is complete. Employing such an approach results in minimal pollution and waste material production. The application of such catalysts to fine chemical manufacturing is likely to be increasingly important in the future. Pyrazoles are valuable bioactive heterocyclic, which are shown to possess important biological and pharmaceutical activities such as antimicrobial, antiviral, anti tumor, anti-inflamatory, antifungal. antidepressant and anticonvulsant activities. [3]

We report here the synthesis and characterization of some pyrazoles we prepared by condensation reaction of β-diketone and hydrazine derivatives using silica phosphoric acid (SPA). ***The*** structure of products have been characterized by several spectroscopic techniques such as IR,UV, ^{1}H-NMR and ^{13}C-NMR.



R: alkyl,aryl, R^1: H,Cl R^2: H, aryl

References

[1] W.M. Nelson, in: P.T. Anastas, T.C. Williamson (Eds.), "Green Chemistry", Oxford University Press, Oxford, **1998**,

[2] (a) K. Tanaka, F. Toda, *Chem. Rev.* , **2000**, 100,1025; (b) G.W.V. Cave, C.L. Raston, J.L. Scott, *Chem. Commun.,* **2001**, 2159-2160; (c) J.O. Metzger, *Angew. Chem., Int. Ed*., **1998,** 37,2975.

[3] Hatheway, G. J.; Hansch, C.; Kim, K. H.; Milstein, S. R.;Schimhdt, C. L.;Smith, R. N.; Quin, F. R. *J, Med. Chem*.**,1978**, 21 , 563-574.

Efficient synthesis of thioesteres from α-halo carbonyl compounds

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Thioesters represent organic derivatives of wide interest due to their wide range of biological activity and considerable applications in drug development [1] and industry [2]. Thioesters are important synthetic intermediates in organic synthesis and are used for peptide coupling, acyl transfer, protecting groups for thiols and also as coupling partners in organometallic [3] Also, thioesters show distinctive chemical properties compared to oxoesters and their enhanced reactivity has successfully been employed in a wide range of synthetic organic transformations. The most well known approach to the synthesis of thioesrers is the direct reaction of the corresponding thiols with a suitable acid chloride or acid anhydride. Thioesters have also been prepared by the reaction of esters or N-acylbenzotriazoles with thiols [4]. However, this method employs thiol and long reaction times, and the overall yields are not satisfactory (16-31%). Although most of these approaches provide efficient access to thioesters, they suffer from the use of corrosive reagents, harsh reaction conditions, expensive catalysts or reagents, and unfriendly organic solvents. Nevertheless, the greatest disadvantage of the previously mentioned methods is the application environmentally benign reaction courses is a major goal for organic synthesis. Therefore, we were eager to develop a single-step and quite eco-friendly method for the synthesis of diverse thioesters. Herein, we report the first development, to our knowledge, of a straightforward and versatile method to obtain thioesters using the reaction of tertiary thioamides and α-halo carbonyl compounds in aqueous media and the presence of catalytic amounts of NaI, and hexadecyltrimethylammonioum bromide (HTAB).

References:

[1] Olsen, J.; Björnsdottir, I.; Tjörnelund, J.; Hansen, S. H. *J. Pharm. Biomed. Anal.*, **2002**, *29*, 7.
[2] Matsumoto, K.; Costner, E. A.; Nishimura, I.; Ueda, M.; Willson, C.G. *Macromolecules*, **2008**, *41*,5674.
[3] Purushothaman, G.; Ravindran, S.V.; Srinivasan, C. *J. Org. Chem*., **2009**, *74*, 6291.
[4] Zali Boeini, H.; Eshghi Kashan, M. *Green Chem*., **2009**, *11*, 1987.

Construction of a new polymeric coating and its use as a replacement for the bumper cars in auto industry

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In this project ,that is according to the standards of common polymer and compatible with environment and according to the resistance and safety standards , we provide the basic application of this project in the automobile industry and in car sprhay[1].

Today , this compound can be used as substituente for hard and fragile shields[2] .

Herein we report an efficient method for making of this polymeric coverage: this polymer was designed very soft and elastike and impact of approach shot back to the primary mode, and it is acceptable to avoid risks and economic side . the polymeric coating is used from compounds such as fillers , resins,special solvent i.e. kardora and polyethylene foam(PE) for felexibility and plasticity.

Including benefits of this polymeric coverage is: 1)High chemical resistance, 2)Resistance to moisture, 3)Resistance to acidic rains, 4)Resistance radiation of X and UV and so on.

Another benefit of this coverage is that within the composite material in the cold season and hot season are not colded and melted.

References:

[1] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Biosensors and Bioelectronics.* **2010**, *25*, 2149.
[2] Wang, Y.; Dave, R.; Pfeffer, R. *The Journal of Supercritical Fluids*. **2004**, *28*, 85.

NMR study and AIM analysis for the ylide rotamers from the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates in the presence of 1-amino-anthraquinone

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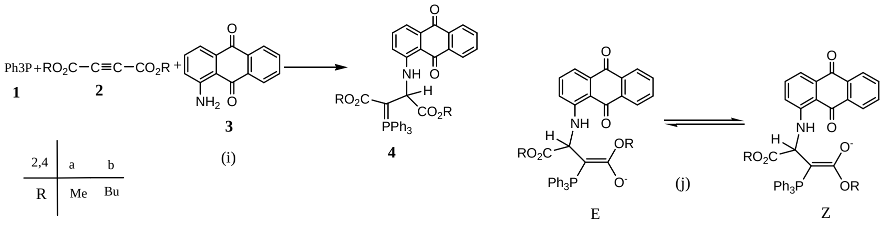
Stable crystalline phosphorus ylide **4** have been synthesized in excellent yield from the 1:1:1 addition reaction between triphenylphosphine **1** and dialkyl acetylenedicarboxylates **2** in the presence of 1-amino-anthraquinone **3** compound. These stable ylides exist in solution as a mixture of the two geometrical isomers as a result of restricted rotation around the carbon-carbon partial double bond resulting from conjugation of the ylide moiety with the adjacent carbonyl group [1-4]. In the recent work, an NMR study and the stability of the Z- and E-isomers were undertaken for the two rotamers of phosphorus ylides involving 1-amino-anthraquinone 4 by natural population analysis (NPA) and atoms in molecules (AIM) method. The individual chemical shifts have been characterized by NMR calculation at HF/6-31G (d,p) level of theory for the two E-4 and Z-4 (major and minor) geometrical isomers. The total spin-spin coupling constant is the sum of four components: the paramagnetics spin-orbit, Fermi contact and spin-dipole terms, the value of chemical shifts (δ) and coupling constants (y_{x-y}) were theoretically calculated. There was a good agreement between both the experimental and theoretical chemical shifts (δ) and coupling constants (y_{x-y}).



References:

[1] S. M. Habibi-Khorassani, A. Ebrahimi, M. T. Maghsoodlou, H. Saravani, M. Zakarianezhad, M. Ghahramaninejat, M. A. Kazemian, M. Nassiri, Z. Khajehali, *Progress in Reaction Kinetics and Mechanism*, **2009**, *34*, 301.

[2] S. M. Habibi-Khorassani, A. Ebrahimi, M. T. Maghsoodlou, Z. Ghahghayi, H. Ghasempour, M.A.Kazemian, *Journal of Sulfur Chemistry*, **2010**, *31*, 153.

[3] S. M. Habibi-Khorassani, M. T. Maghsoodlou, M.Zakarianezhad, M.Nassiri, M.A.Kazemian, P.Karimi, *Heteroatom Chemistry*, **2008**, *8*, 723.

[4] S. M. Habibi-Khorassani, M. T. Maghsoodlou, A. Ebrahimi, H.Roohi, M.Zakarianezhad, H.R.Dasmeh, M.Moradian, *Phosphorus, Sulphur and sillicon*, **2006**, *181*, 1103.

Synthesis of novel chromeno[4,3-b]pyridine

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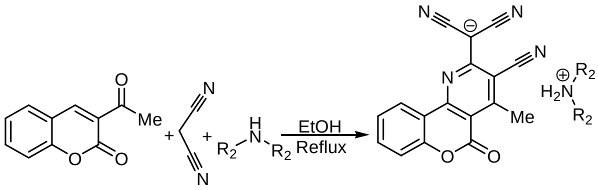
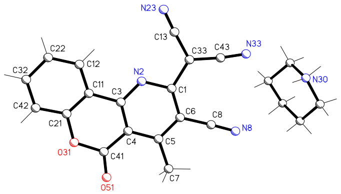
Fused 3,4-heterocyclic coumarin derivatives exhibit a wide range of biological activities. Specifically, those bearing a benzopyranone–pyridine or piperidine skeleton were found to interact with DNA, to transfer energy in photophysical processes, to be potential platelet activating factor antagonists, depressant or hypotensive activators and potent antipsychotic agents, whereas others exhibited antibacterial, antitumor, anticholinergic, and antimicrobial activities [1]. Also, some naturally occurring fused heterocyclic chromone alkaloids, such as shumanniophytine and isoshumanniophytine, were found to possess antiviral activity [2].

In view of these properties and in continuation of our research program on the synthesis of heterocyclic compounds, we report herein the synthesis of new chromeno[4,3-b]pyridine organic salt. The structure of product was determined by X-ray crystallography.





References:

[1] D. R. Gautam, J. Protopappas, K. C. Fylaktakidou, K. E. Litinas , D. N. Nicolaides, C. A. Tsoleridis, *Tetrahedron Lett.* **2009**, *50*, 448.

[2] (a) Houghton, P. J.; Woldemariam, T. Z.; Mahmood, N. *J. Pharm. Pharmacol*. **1994**, *46*, 1061; (b) Houghton, P. J.; Woldemariam, T. Z.; Khan, A. I.; Burke, A.; Mahmood, N. *Antivir. Res.* **1994**, *25*, 235.

Starch as a new catalyst for mild and efficient aminolysis of epoxides under solvent-free condition

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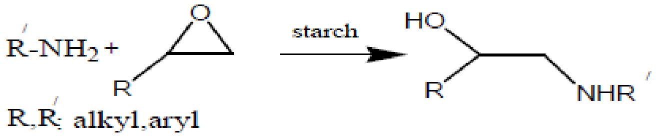
The synthesis of β-amino alcohol is an important theme in both organic chemistry and medicinal science [1]. The ring–opening addition reactions of 1,2-epoxides with ammonia or amines, and their synthetic equivalents, is one of the most widely used methods for β-amino alcohol synthesis [2]. Several useful modifications of the classical procedures have been demonstrated recently, however, there are still intrinsic limitations on the general utility of epoxide aminolysis [3].

Solvent-free reaction are of great importance in organic synthesis as it reduces the environmental pollution and bring down the handling costs due to simplification of work up technique[4].

We have found that the use of starch allows the ring opening of epoxides by various aromatic and aliphatic amines. Meanwhile, the impact of some important factors such as reaction time, structurally different and kind of epoxides and amines on the efficiency of this method was studied.



References:

[1] Ager, D. J.; Prakash, I.; Schaad, D.R.; *Chem .Rev.* **1996**, 96, 835.
[2] Williams, D.B.G.; Lawton, M.; *Tetrahedron lett.* **2006**, 47, 6557.
[3] Azizi, N.; Saidi, M.R.; *Tetrahedron*. **2007**, 63, 888.
[4] Smith, K.; *Solid Supports and Catalyst in Organic Synthesis*, Ellis Horwood, Chichester, **1992**.

A green synthesis of novel poly(amide-imide)s modified with siloxane linkage under microwave in conjunction with imidazolium based ionic liquids

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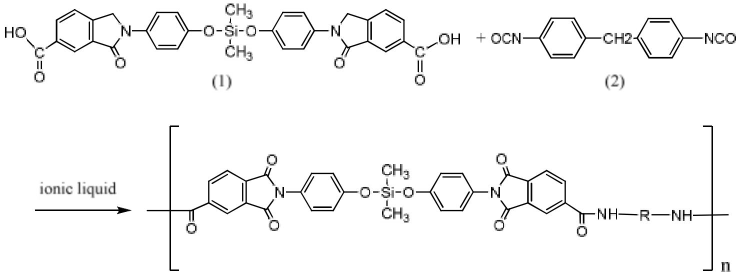
Ionic liquids (ILs), which have been widely promoted as “green solvents”, are attracting much attention for applications in many fields of chemistry and industry due to their chemical stability, thermal stability, low vapor pressure and high ionic conductivity properties. Over the last few years, ILs have been popularly used as solvents for organic synthesis, catalysis, and also been used as media for extraction processes [1–2].

Microwave radiation as a non-conventional energy source has become a very useful and popular technology in organic chemistry, polymerization for optimizing and accelerating of chemical reactions. These reactions are very fast and completed within a short period of time. Microwave enhanced synthesis actually generates higher yield and purer products than traditional heating. Recently microwave radiation has been used for the synthesis of novel polymers [3,4].

In this paper, we wish to report a convenient, cost effective and environmentally benign green chemical method for the synthesis of poly(amide-imide)s with siloxane linkage by using imidazolium-based Ionic liquids, under microwave irradiation condition. The step-growth polymerization reactions of 4,4’-dimethylsiloxane-bis(4-phenyl-N-trimellitylimide) (1) with 4,4’-methylene-bis(4-phenylisocyanate) (2) was performed through isocyanate route for direct amidation reaction. The resulting polymers have moderate viscosities and good yield and thermal stability. They were characterized with FT-IR, H^1-NMR and thermogravimetric analysis techniques.



References:

[1] Lu et al. *J. Prog Polym Sci.* **2009**, *34*, 431.
[2] Van Rantwijk, F.; Sheldon, R. A. *Chem Rev*. **2007**, *107*, 2757.
[3] Sinnwell, S.; Ritter, H. *J. Macromol Rapid Commun*. **2005**, *26*, 160.
[4] Mallakpour, S.; Rafiemanzelat, F.; *J. Appl. Polym. Sci*. **2004**, 93, 1647.

Synthesis of 2,6-di(1-benzofuran-2-yl)-4-aryl pyridines

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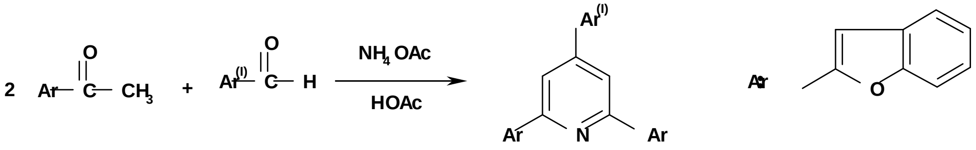
The pyridine ring systems are of interest because of the occurrence of their saturated and partially saturated derivatives in biologically active compounds and natural products such as NAD nucleotides, pyridoxol (vitamin B6), and pyridine alkaloids [1]. Due to their π-stacking ability, some pyridines are used in supramolecular chemistry [2].

Owing to their wide range of pharmacological activity and industrial and synthesis applications, a number of methods have been reported for the synthesis of Kröhnke-type pyridines [3]. Previously, 2,4,6-triarylpyridines have been prepared by the condensation of 1,5-diketones with formamide-formic acid [4] and by other synthetic procedures including the Chichibabin method [5–7].

Knowing the chemical and pharmacological importance of the Kröhnke pyridines, we have recently focused on introducing a facile and efficient synthesis of these pyridines. Thus, a range of 2,6-di(1-benzofuran-2-yl)-4-aryl pyridines were synthesized by heating a mixture of 2-acetylbenzofuran, aromatic aldehydes and NH_4OAc in the presence of acetic acid as solvent. The products recrystallized and showed a single spot on TLC and were pure enough for all practical purposes.



References:

[1] Balasubramanian, M.; Keay, J. G. *In Comprehensive Heterocyclic Chemistry II*; Katritzky, A. R., Rees, C. W., Scriven, E. V. F., Eds.; Pergamon Press: London, **1996**; Vol. 5, Chapter 6, pp 245–300.
[2] Constable, E. C.; Housecroft, C. E.; Neuburger, M.; Phillips, D.; Raithby, P. R.; Schofield, E.; Sparr, E.; Tocher, D. A.; Zehnder, M.; Zimmermann, Y. *J. Chem. Soc. Dalton Trans*. **2000**, 2219; Cave, G. W. V.; Hardie, M. J.; Roberts, B. A.; Raston, C. L. Eur. *J. Org. Chem*. **2001**, 3227; Jetti, R. K. R.; Nagia, A.; Xue, F.; Mak, T. C. W. *Chem. Commun*. **2001**, 919; Watson, Z. C.; Bampos, N.; Sanders, J. K. M. *New J. Chem*. **1998**, 1135.
[3] Chubb, F.; Hay, A.S.; Sandin, R.B. *J. A. Chem. Soc*. **1953,** *75*, 6042.
[4] W. Dilthey, J. Prakt. *Chem*. 102 (**1921**) 209.
[5] Lombard, R.; Stephen, J.P. *Bull. Soc. Chim. Fr*. **1958,** 1458.
[6] Zecher, W.; Krohnke, F. *Chem. Ber*. **1961,** *94,* 690.
[7] Frank, R.L.; Seven, R.P. *J. A. Chem. Soc*. **1949,** *71,* 2629.

Synthesis of tetrahydrobenzo[a]xanthene-11-one derivatives catalyzed by $RuCl_3.nH_2O$

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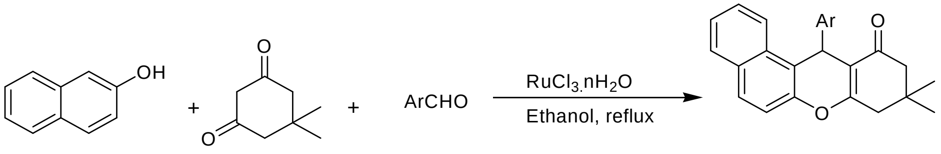
Xanthenes are important biologically active heterocycles. They possess antibacterial and antiviral activities [1]. Furthermore, these heterocycles display useful spectroscopic properties and are used as dyes [2], in laser technologies [3] and as fluorescent materials for the visualization of biomolecules. Thus, the development of new and simple synthetic methods for the efficient preparation of new xanthenes is an interesting challenge.

It is evident from the recent literature that Ru^{III} salts have invoked enormous interest as potential Lewis acid catalyst in various organic transformations such as oxidation reactions of alkanes [4], oxidative cyanation of amines [5] and many others. These salts have received considerable attention due to their low redox potential, high electron transfer ability, high coordination ability to heteroatoms, unique reactivity of metallic species and intermediates such as oxo-metals, metallacycles and metal carbene complexes.

Herein, we are reporting the reaction of aromatic aldehydes, 2-naphthol and dimedone for the formation of tetrahydrobenzo[a]xanthene-11-one in presence of catalytic amount of $RuCl_3.nH_2O$ under reflux conditions in ethanol as solvent. All the products are known compounds and were characterized by melting point and IR spectroscopic data. The advantages of this method are reduced reaction times, higher yields, mild reaction condition, and easy purification.



References:

[1] Ko, S.; Yao, C.F. *Tetrahedron Lett.* **2006**, *47*, 8827
[2] Banerjee, A.; Mukherjee, A. K. *Stain Technol*. **1981**, *56*, 83.
[3] Ahmad, M.; King, T. A. *J. Phys. D: Appl. Phys*. **2002**, *35*, 1473.
[4] Komiya, N.; Noji, S.; Murahashi, S. *Chem. Commun*. **2001**, 65.
[5] Murahashi, S.; Komiya, N.; Terai, H.; Nakae, T. *J. Am. Chem. Soc*. **2003**, *125*, 15312.

Effect of ZnO nanotubes in ring opening of epoxides with aniline in poly ethylene glycol as a solvent

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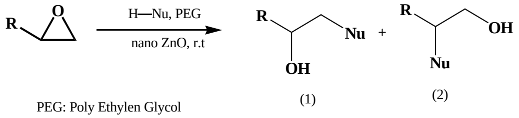
Epoxides have been recognized as important and versatile synthetic intermediates in organic synthesis [1]. They can be easily prepared and the strain of their three-membered ring together with the polarization of the c-o bonds make them susceptible to reaction with a large variety of reagents such as electrophiles, nucleophiles, acids, bases, reducing agents and same oxidizing agents [2]. The ring opening epoxides by amines is an important route for the preparation of *β*-amino alcohols [3]. Ring opening of epoxides with diverse nucleophiles is an important transformation in organic synthesis that generates a variety of useful building blocks with hydroxyl functionalities [4].Catalytic technologies are critical to present and future energy, chemical process, and environmental industries.The “nano” in nanocatalysts refers to very small particles [5].

Different methods have been reported for ring opening of epoxides in scientific resources.Epoxide rings in the present of different nucleophiles will be opened and causes 1 and 2 synthesis.

Herein we prepare ZnO nanotube (fig 1) as a nano catalyst in the ring opening of epoxides in the presence of PEG as a solvent and amine nucleophile in room temperature. At the end of reactions, *β*- amino alcohols were obtained with very good yields at the short time. So ZnO nano catalyst is effective in the ring opening of epoxides.



PEG: Poly Ethylen Glycol

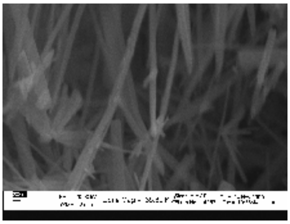


Fig 1: SEM image of ZnO nanotubes

References:

[1] Rao, A. S.; Paknikar, S. K.; Kirtane, J. G. *Tetrahedron* **1983**, *39*, 2323.

[2] Moller, F. In Methoden der organischem Chemie (Houben-Weyl); Muller, E., Ed., 4th ed.; Thieme Verlag: Stuttgart, **1957** ; *11/1*, PP. 311.

[3] D. M. Hodgson, A. R. Gibbs, G. P. Lee, *Tetrahedron* **1996**, 52, 14361.

[4] Jacobson, E. N. Acc. *Chem. Res.* **2000**, *33*, 421.

[5] Avgouropoulos, G., Loannides, T., Papadopoulou, C., Batista, J., & Matralis, H. K. *Catal. Today*, **2002** , *75*, 157.

Gas-phase thermochemistry of deprotonated & protonated Cytosine nucleosides: comprehensive DFT study of energetic & conformational properties

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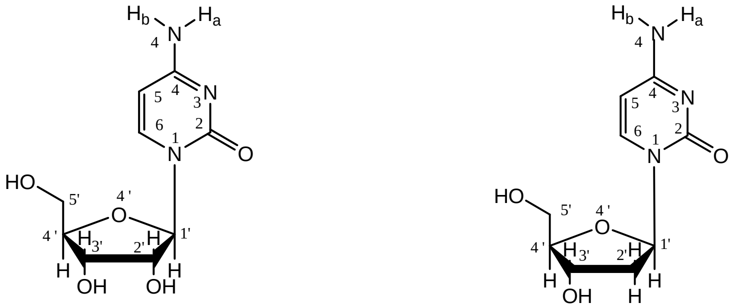
Nucleosides are the structural units of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA), containing the genetic code of each organism and play important roles in different biochemical processes [1]. Gas-phase acidities and basicity of nucleosides (as nucleic acids constituents) combined with the knowledge of deprotonation or deprotonation sites, could improve our understanding of chemical reactions basic to biological systems [2, 3]. In an effort to understand the intrinsic properties of cytosine nucleosides, we examined their gas phase proton dissociation energies ($\Delta H_{\text{acidity}}$), proton affinities, bond dissociation energy (BDE), electron affinities values of these molecules by using quantum mechanical calculations with B3LYP method in conjunction with the 6-311++G (d,p) basis set. In this work, we establish that the $N4H_a$ is the most acidic sites of cytidine and deoxycytidine molecules have a gas phase acidities of 338.5 and 341.6 kcal/mol respectively. Furthermore, the energy and geometry of different conformers of these molecules during deprotonation and protonation have been analyzed by considering sugar puckering, stability of N-glycosidic bond and anti or syn orientations of cytosine nucleobase with respect to the sugar.



Cytidine

Deoxycytidine

Scheme . Chemical structures of Cytidine & Deoxycytidine explored in this study

References:

[1] Osti, F. Corradini, F. G, Hanau, S. Matteuzzi, M., Gambari, R. *Haematologica,* **1997**, *82*, 395.
[2] Ponnuswamy, P.; Gromiha, M. *J. Theor. Biol.* **1994**, *169*, 419.
[3] Kong ,W, Engel. K, Wang. J, *Curr. Drug Metab.* **2004**, *5*, 63.

Clean synthesis of 1,8-dioxo-octahydroxanthene derivatives catalyzed by P_2O_5/Al_2O_3 and Silphos under solvent-free conditions

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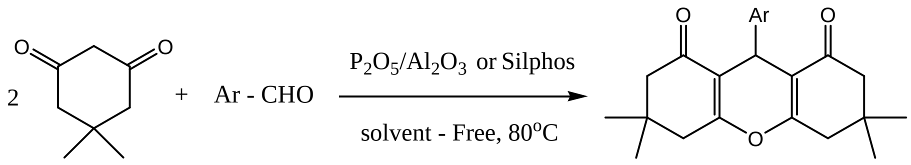
Heterogeneous catalysts have gained interesting attraction in recent years due to economic and environmental considerations. Phosphorus pentoxide/Alumina is an inexpensive, green, commercially available and heterogeneous catalytic system which has been used in several organic transformations [1]. Silphos (Silicaphosphine) is a cheap and stable reagent which can be used as a new source of filterable phosphine. Xanthenes are important classes of compounds that find use as dyes, fluorescent materials for visualization of bio-molecules and laser technologies due to their useful spectroscopic properties [2].

Even though there are many methods reported in the literature for the synthesis of xanthenes [3,4], we thought that there is scope for further innovation towards milder reaction conditions, short reaction time and better yields.

In the present work, we achieved that P_2O_5/Al_2O_3 is a highly efficient catalyst for the synthesis of *1,8*-dioxo-octahydroxanthenes from dimedone and aryl aldehydes solvent-free conditions.

In continuation of our investigations with Silphos as a heterogeneous phosphine reagen for the synthesis of *1,8*-dioxo-octahydroxanthenes: (Scheme1).



Scheme 1

References:

[1] Naeimi, H.; Salimi, F.; Rabiei, Kh. *J. Mol. Catal. A: Chem.* **2006**, *260*, 100.

[2] (a) Menchen, S.M.; Benson, S.C.; Lam, J.Y.L; Zhen, W.; Sun, D.; Rosenblum, B.B.; Khan, S.H.; Taing, M.; *US Patent*, **2003**, 6, 583, 168; (b) Banerjee, A.; Mukherjee, A.K.; *Stain Technol*.
1981, *56*, 83.

[3] Das, B.; Thirupathi, P.; Reddy, K.R.; Ravikanth, B.; Nagarapu, L. *Catal Commun*. **2007**, *8*, 535.

[4] Das, B.; Thirupathi, P.; Mahender, I.; Reddy, V.S.; Koteswara Rao, Y.; *J. Mol. Catal. A: Chem.* **2006**, *247*, 233.

A facile synthesis of novel optically active R,R-2-(4-[2-[4-(5-Chloro-3-halo-pyridin-2-yloxy)-phenoxy]-propionyloxy]-phenoxy)-propionic acid esters using cyanuric chloride as potential herbicide

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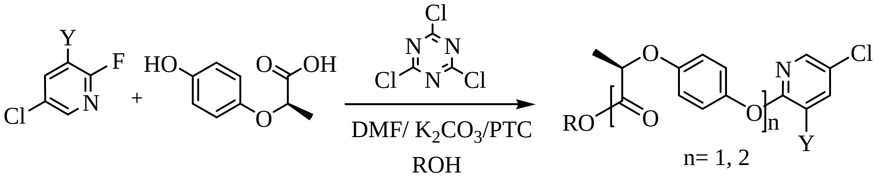
Aryloxyphenoxypropionate herbicides (APPH) are an interesting and highly effective class of herbicides in the international market over the past decade. Up to now, more than 20 kinds of APPH, such as clodinafop propargyl, were commercialized all over the world [1].

Traditionally APPH were prepared by coupling of alcohols with acid chloride generated from the parent carboxylic acid. The typical reagents employed to prepare an acid chloride from a carboxylic acid are corrosive $SOCl_2$, PCl_3 or toxic phosgene [2]. This method suffers from several disadvantages and can be cumbersome in a pilot plant. Due to the vigorous conditions and formation of strong acid during the process, sensitivity of optically active carboxylic acids and the disadvantages associated with the use of acid chlorides, esterification of carboxylic acids is an active area of research. Carboxylic acids activated by cyanuric chloride CC has been used in many chemical transformations [3] and can be a valid alternative route to the classical preparation method of APPH.

In this article, we have developed a facile process suitable for large-scale production of APPH using carboxylic acids, CC as a mild and inexpensive reagent and phase transfer catalyst (PTC) benzyltriphenylphosphonium bromide.



R = $-CH_3$, $-CH_2CH_3$, $-CH_2CH_2CH_3$,$-CH(CH_3)_2$ $-CH_2CH_2CH_2CH_3$, $-CH_2\text{-}C \equiv CH$
Y= Cl, F

References:

[1] Li, H. P. Pestic. Sci. Adm. **2004**, *25*, 28.
[2] Schurter, R. Rempfler, H. US pat. 4,713,109, **1987**.
[3] Blotny, G. *Tetrahedron* **2006**, *62*, 9507.

Comparative study of extraction yields and free-radical scavenging activity for *Allium cepa* extracts prepared by microwave-assisted and Soxhlet method

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Methods for extraction of bioactive materials are recently attended. *Allium* is one of the most famous geniuses of medicinal plants in east and west [1, 2]. Onion (*Allium cepa)* is one of oldest cultivated plants and is used both for food and medicinal applications [3, 4]. In this study, effect of microwave irradiations on extraction yields and antioxidant activity of extracts was investigated; we also compared heating and irradiating methods. The results show that although microwaves increase yields but probably damage the molecular structure of bioactive compounds or is not enabled to extract these compounds as much as Soxhlet method**.**

References:

[1] Zill-e-Huma, Maryline Abert Vian, Jean Francois Maingonnat and Farid Chemat, *Chromatography***. 2009**, *1216,* 7700.

[2] Bektas Tepe, Munevver Sokmen, H. Askin Akpulat and Atalay Sokmen. *Food chemistry*, **2004**. *92*, 89.

[3] J. Santas, R. Carbó, M.H. Gordon and M.P. Almajano, *Food Chem.* **2008**, *107*, 1210.

[4] Apak , R, Guclu, K., Demirata,B ., Ozyurek, M, Celik , S. E ., Bektasolu, B., Berker K. I., and Ozyurt, D., *Molecules***. 2007***, 12, 1496*.

Synthesis of *N*-substituted pyrroles in water in the presence of organocatalyst

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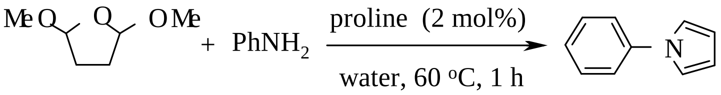
Pyrrole derivatives are key intermediates not only in the synthesis of drugs, pigments, and pharmaceuticals, but also for the development of organic functional materials .Substituted pyrroles are an important class of compounds displaying remarkable pharmacological properties such as antibacterial, antiviral, anti-inflammatory, antitumoral, and antioxidant activities. Furthermore, they are useful intermediates in the synthesis of natural products and heterocycles4 and are also widely used in the materials area.

Consequently, a wide range of procedures has been developed for the construction of pyrroles. Herein we evaluated the synthesis of several N-substituted pyrroles which are readily prepared from the reaction of 2, 5-dimethoxytetrahydrofuran and aryl/alkyl, sulfonyl and acyl amines in presence of organocatalyst in water as solvent offers short reaction times, mild and green reaction conditions and easy work-up.



References:

[1] N. Azizi, A. Khajeh-Amiri, *Synlett*, **2009**, *14*, 2245.
[2] A. R. Ekkati, D. K. Bates, *Synthesis*, **2003**, 1959.

Synthesis of new graphene-aryl isothiocyanate derivatives

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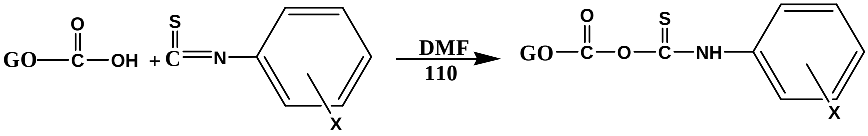
The recent explosion of scientific activity around the newly discovered two-dimensional material graphene is unprecedented since the discovery of the high temperature superconductors in the late 1980s.[1] Graphene sheets have been investigated due to its excellent electrical, thermal and optical properties, high-specific surface area, and ease of chemical functionalization which actually helps in tuning its properties.[2] Also Functionalized graphene sheet (FGS) was recently introduced as a new nano-sized conductive filler[3] for various composite applications. Very recently, synthesis of some functionalized graphite oxides were reported by treatment of graphite oxide (GO) with organic isocyanates. These isocyanate-treated GOs (iGOs) can then be exfoliated into functionalized graphene oxide nanoplates that can form a stable dispersion in polar aprotic solvents.[4]

In this report we wish to introduce some novel graphene-arylisothiocyanate derivatives by the reaction of graphene oxide with substituted arylisothiocyanates in refluxing DMF followed by reduction of the obtained compounds. Characterization of the obtained materials was carried out by XRD, UV, conductivity, IR and NMR methods.



References:

[1] M. Klintenberg, S. Lebegue, C. Ortiz1, B. Sanyal, J. Fransson, O. Eriksson, *J. Phys. Condens. Matter.* **2009,** *21*, 335502.

[2] C. Srinivasan, R. Saraswathi, Curr. Sci. 25 **2009**, *97*, 1115.

[3] D. A. Nguyen, Y. R. Lee, A. V. Raghu, H. Jeong, C. Shinb, B. K. Kimc, *Polym. Int.* **2009**, *58*, 412.

[4] S. Stankovich, R. D. Piner, S. T. Nguyen, R. S. Ruoff, *Carbon*, **2006**, *44*, 3342.

Synthesis and characterization of 2- pyridine carbaldehyde Schiff base complex supported on poly vinyl amine/SBA-15 hybrid and it's application for oxidation of alcohols

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Oxidation catalysis constitutes an important research area because it represents the core of a variety of chemical processes for producing bulk and fine chemicals. Therefore, the design of active, selective, and recyclable heterogeneous catalysts is a challenging goal in the field of oxidation catalysis [1]. Organic–inorganic hybridizing materials, especially the composites consisting of nano-inorganic particles and polymer resin, have received considerable attention recently due to the resultant materials are supposed to have better mechanical and/or thermal properties [2].

Mesoporous silica materials have been widely used as useful and versatile solid supports to construct various hybrid materials in catalysis, enzyme immobilization and drug delivery due to their large tunable pore dimensions, high surface areas and great diversity in surface functionalization. Therefore covalent anchoring of the Schiff base complexes onto a functionalized siliceous mesoporous material with large pore diameters seems to be promising [3,4]. The mesoporous SBA-15 materials are more versatile than other mesoporous supports because of their large pore diameter permitting easy diffusion of bulky reactants and products during the reactions [5].

Poly vinyl amine/mesoporous SBA-15 (PVAm/SBA-15) composites were prepared by in situ polymerization. Schiff base functionalized SBA–15 mesoporous materials were synthesized by post-grafting of 2-pyridine carbaldehyde on to PVAm/SBA-15 and followed by the introduction of Co(II) ions via a ligand exchenge reaction. The composite materials were characterized by XRD, FT-IR, BET and SEM techniques. This composite catalyst was subsequently utilized as an efficient and selective catalyst in oxidation of benzylalcohol to benzaldehyde using tert-butylhydro peroxide as an oxidant. The chemical and instrumental parameters have been optimized and the effect of the interferences has been determined.

References:

[1] Ettedgui, J.; Neumann, R. *J. Am. Chem. Soc.* **2009,** *131*, 4.
[2] Run, M. T.; Wu, S. Z.; Zhang, D. Y.; Wu, G. *Mater. Chem. Phys.* **2007**, *105*, 341.
[3] Yang, Y.; Guan, J.; Qiu, P.; Kan, Q. *Appl. Surf. Sci.* **2010**, *256*, 3346.
[4] Hu, J.; Li, K.; Li, W.; Ma, F.; Guo, Y. *Appl.Catal. A:* Gen. **2009**, *364*, 211.
[5] Yang, Y.; Zhang, Y.; Hao, S.; Guan, J.; Ding, H.; Shang, F.; Qiu, P.; Kan, Q. *Appl. Catal. A:Gen.* **2010**, *in press*.

Synthesis of 8H- (1, 2, 4) triazolo (4,3, -a) pyrimidine derivatives using heteropolyacid

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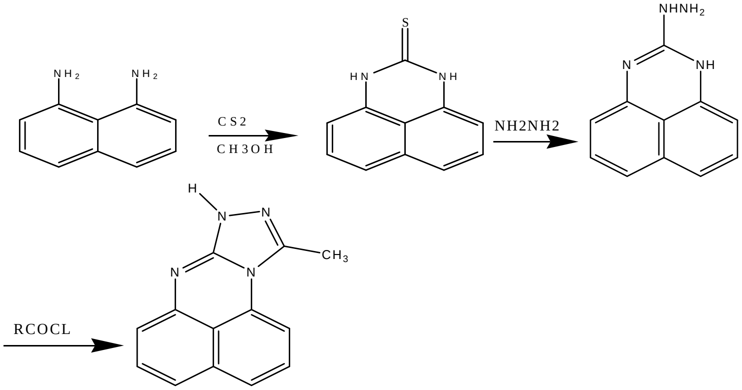
The pyrimidine and the derivatives are not natural compounds. For the first time in 1909 this compound was made by Sakhes from reaction of 1, 8-Diaminonaphtalene with formic acid [1].Some pyrimidine derivatives have biological activities such as medication for blood hypertension [2]. In common methods for the synthesis of heterocyclic compounds, acidic catalysts like sulfuric acid, nitric acid [3], perchloric acid and silica sulfuric acid are used [4]. Some of these catalysts are toxic and corrosive, and separation of them creates a lot of problems. Therefore, extensive researches have been done for replacement of them. Solid acids, especially heteropolyacids, have good advantages which have attracted chemists. These include easy preparing, low cost, ecofriendly, and high thermal stability. Furthermore, they are strong Brønsted acids [5, 6]. Application of Heteropolyacids as catalyst is under growing. These compounds have special properties such as certain structure, ability to change acidic properties or oxidation –reduction with change in structure of them, ability to absorb and release electrons, high active protons and they have more efficiency than common acidic catalysts, such as ionic exchange resines and zeoliets.These acids are used in industry and many organic reactions such as water elimination of alcohols, alkylation and esterification.



References:

[1] J. M. Herbert, P.D. Woodgate, W.A. Denny, *J. Med. Chem*. **1987,** *30*, 2081.
[2] U. Burkhardt, S.John, *Ger (East)*, 232, 919 (Cl.Co7D 513/09).
[3] T. Jin. S. Zhang, T.Li, *Synth commun*. **2002,** *32* , 1874.
[4] P. Salehi, M. Dabiri, M. A. Zolfigol, *Tetrahedron Lett,* **2003,** *44* , 2889.
[5] O. Okuhara. N. Mizuno, M. Misono, *Adv. Catal*, **1996,** *41*, 113.
[6] M. Misono, *Catal Lett*, **1992,** *12*, 963.

Metal oxide nanoparticles as a recyclable heterogeneous catalyst for synthesis of 5-subsitituted 1H-tetrazoles via the [3+2] cycloaddition of benzonitrile and trimethylsilyl azide

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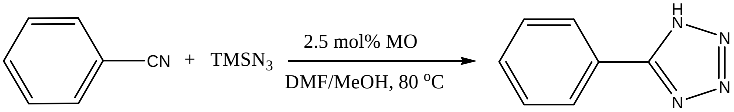
Tetrazoles have been reported applications in pharmaceuticals as lipophilic spacers and carboxylic acid surrogates, in material sciences as specialty explosives and information recording systems, and in coordination chemistry as ligands [1]. The synthesis of 5-substituted 1H-tetrazoles from nitriles has received much attention recently, and new preparative methods have appeared [2].

Recently, heterogeneous catalysts have become attractive from both economic and industrial points of view as compared to homogeneous catalysts. Nanoparticles metal oxides have excellent applications as heterogeneous catalysts. In general, nanoscale heterogeneous catalysts offer higher surface area and lower coordinating sites, which are responsible for the higher catalytic activity [3]. Copper zinc and nickel oxide nanoparticles are useful examples of reusable heterogeneous catalysts, which have been studied in few recent years [4-5]. As per our ongoing research program aimed at the development of environmentally benign synthetic methodologies for widely used heterocyclic compounds inspired us to report a novel and rapid synthesis of 5-subsitituted 1H-tetrazoles using some metal oxide nanoparticles such as MgO, NiO, CuO, MnO and ZnO as the efficient and commercially available catalysts. We successfully synthesized these nanoparticles in average size between 10-50 nm. The characterizations of nanoparticles were carried out by X-Ray diffraction (XRD), scanning electron microscopy (SEM), IR spectroscopy, thermal gravimetry analysis and differential thermal analysis (TGA/DTA)



References:

[1] Hert, R. J. *Bioorg. Med. Chem.* **2002**, *10*, 3379.
[2] Curran, D. P.; Hadida, S.; Kim, S.-Y. *Tetrahedron*, **1999**, *55*, 8997.
[3] Pacchioni, G. *Surf. Rev. Lett*. **2000**, *7*, 277.
[4] Hu, J.Q.; Bando, Y.; Zhan, J.H.; Li, Y.B.; Sekiguchi, T. *Appl. Phys. Lett*. **2003**, *83*, 4414.
[5] Kantam, M.L.; Ramani, T.; Chakrapani, L.; Choudary, B.M. *Catal. Commun*. **2009**, *10*, 370.

An efficient conversion of oximes into carbonyl compounds catalyzed by sodium molybdate

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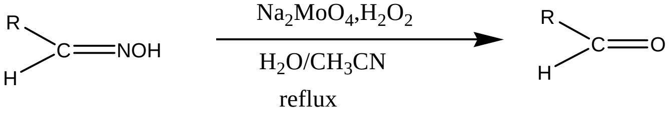
Oximes are extensively used for purification and characterization of carbonyl compounds and in the preparation of amides via the Beckmann rearrangement.On the other hand, Oximes could be prepared from non-carbonyl compounds and the regeneration of carbonyl compounds from Oximes represents a potential rout for syntheses of ketones and aldehydes.

Fortunately we have developed a new procedure for deoximation of various aldehyde oximes to their corresponding carbonyl compounds using H_2O_2 as a green oxidant catalyzed by sodium molybdate in the mixture of water and acetonitril (2:1 V/V) at reflux temperature (Scheme).



(Scheme)

The reaction was clean and no side product was detected in the reaction mixture.

References:

[1] A. I. Bosch, P. Cruz, E.Diez-Barra, A. Loupy, F. Langa, *Synlett*, **1995**, 1259.
[2] G. W. Kabalka, P. P. Wadgaonkar, R. D. Pace, *Synth. Commun*. **1990**, 20, 2453.

New methods to the synthesis of pyrazolo[3,4-d]pyrimidin-4-one derivatives

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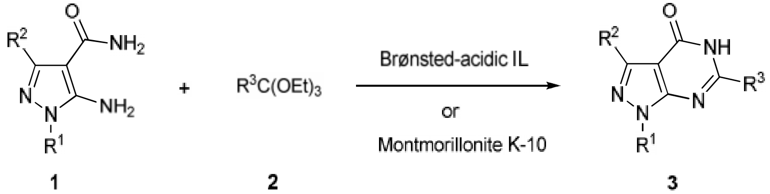
Pyrazolo[3,4-d]pyrimidines are a large group of heterocycles with diverse and interesting biological activities [1, 2]. Also, a number of these compounds have been considered as inhibitors of the Plasmodium falciparum PfPK7 protein kinase [3], cyclin-dependent kinases [4] and GSK-3 [5]. Various methods have already been proposed for the synthesis of these compounds and the most general ones involve heterocyclization of suitably functionalized pyrimidines or pyrazoles with different electrophiles and nucleophiles [6-8]. However, many of these methods are associated with some limitations such as long reaction times, unsatisfactory yields, harsh reaction conditions, hazardous organic solvents and tedious work-up procedure.

Thus, herein we wish to report two simple, efficient, high-yielding, and environmentally friendly methods for the synthesis of pyrazolo[3,4-d]pyrimidin-4-ones through cyclocondensation of 5-aminopyrazole-4-carboxamides with orthoesters using a Brønsted-acidic ionic liquid, 3-methyl-1-(4-sulfonic acid)butylimidazolium hydrogen sulfate [$(CH_2)_4SO_3HMIM$][HSO_4] and Montmorillonite K-10 clay as efficient, reusable, and eco-friendly catalysts under solvent-free conditions. The catalysts can be reused after a simple work-up, with a slight decline of their activities being observed. Other advantages of these protocols are high yields, very short reaction times, easy work-up, and omitting any volatile and hazardous organic solvents.



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References:

[1] Khobragade, C. N.; Bodade, R. G.; Konda, S. G.; et al. *Eur. J. Med. Chem.*, **2010**, 45, 1635.
[2] Wang, H. Q.; Zhou, W. P.; Wang, Y. Y.; et al. *J. Agric. Food. Chem.*, **2008**, *56*, 7321.
[3] Klein, M.; Diner, P.; Dorin-Semblat, D.; et al. *Org. Biomol. Chem.*, **2009**, *7*, 3421.
[4] Markwalder, J. A.; Arnone, M. R.; Benfield, P. A.; et al. *J. Med. Chem.*, **2004**, *47*, 5894.
[5] Peat, A. J.; Boucheron, J. A.; Dickerson, S. H.; et al. *Bioorg. Med. Chem. Lett.*, **2004**, *14*, 2121.
[6] El-Dean, A. M. K.; Geies, A. A. *J. Chem. Res. (s).*, **1997**, *10*, 352.
[7] Chen, W. Q.; Jin, G. Y. Phosphorus, Sulfur Silicon Relat. Elem., **2002**, 177, 1193.
[8] Bhuyan, P. J.; Borah, H. N.; Sandhu, J. S.; *Tetrahedron Lett.*, **2002**, *43*, 895.

Isocyanide based multi- component synthesis of pyrrolidine derivatives catalyzed by TiO_2

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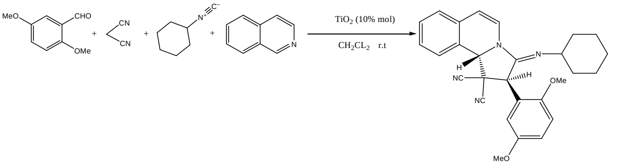
Many substituted quinoline and isoquinoline are subject of extensive researches due to biological, medical, photografic and other useful applications. Thus, the chemistry, synthesis and properties of this fused system analogues have been frequently reviewed .Using new method of four-component reaction between (isoquinoline or quinoline), isocyanide, benzaldehyde derivatives and malonitrile in presence of catalized by amount TiO_2 leading to new pyrrolidine derivatives. At first TiO_2 as a catalyst facilitate knoevenagel condensation of benzaldehydes and malonitrile to give related alkene and then whit quinoline or isoqinoline and isocyanide, give new pyrrolidine derivatives (major proudacts A and B). The products were identified by ^{1}HNMR, ^{13}CNMR, MASS and IR spectra datas.



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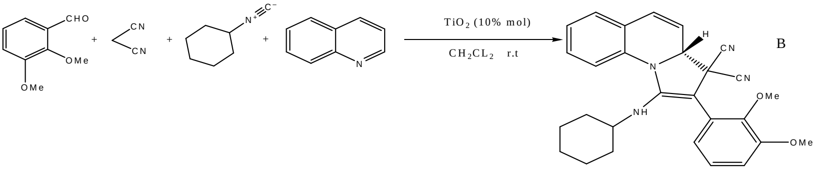

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References:
[1] Chai, W.; breitenbucher, *J. G.bioorg. Med. Cem.* **2003**, 5, 43.
[2] Goff, D, A, *Tetrahedron letter*. **1999**, 40, 5409.
[3] M. Mironov, V. Mokrushin, S. Maltsev. *Synlett*. **2003**, 02, 06.

Practical and mild synthesis of [3,2, A] carbazole, pyrrole and β-aminoketone under mild reaction conditions

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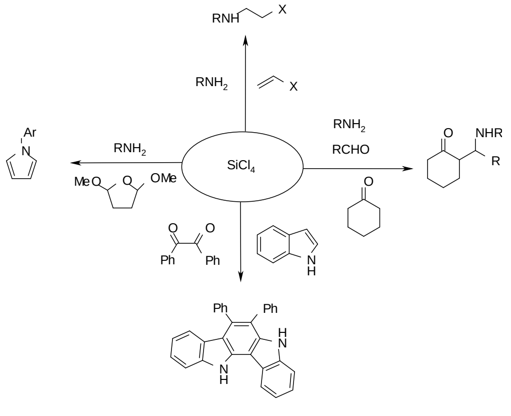
Simple silicone compounds, which are highly reactive species, have attracted much attention from the standpoint of not only fundamental chemistry but also applied chemistry such as material chemistry and organic synthesis. Simple silicone have been used as catalyst for the synthesis of a variety of carbon compounds.

In continuation of our research interest for developing a green organic chemistry by performing organic transformations under solvent-free conditions, herein we report operationally simple, atom economical, and scalable synthesis of [3,2, A] carbazole, pyrrole and β-aminoketone from simple starting material is shown to proceed readily with high yield in the presence of silicone tetrachloride. The scope of the reaction is quite broad; a variety of aromatic and aliphatic, activated and unactivated aldehydes as well as amines and indoles have all been shown to be viable substrates for this reaction.



References:

[1] Vijay Nair, Viday Nandialath, Keecherikunnel G, Abhilash and Eringathodi Suresh; *Org. Biomol. Chem*,. 2008, 6, 1738.
[2] Larisa N. Yudina, Jan Bergman; *Tetrahedron, Volume 59, Issue 8, 17 February 2003, Pages 1265.*

Melamine sulfonic acid as an efficient catalyst for the one-pot synthesis of *β*-acetamido ketones

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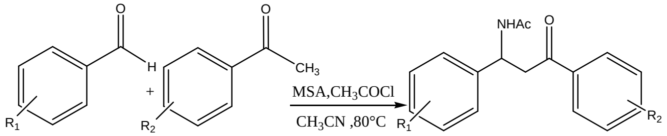
One-pot multi component reactions (MCR$_S$) are of increasing importance in organic and medicinal chemistry [1]. In the past decade, there has been tremendous development in three- and four-component reactions. These processes are performed without isolation of any intermediates, thus reducing time and saving both energy and raw materials.

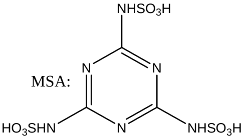
Dakin-West reaction is the best known route for the synthesis of *β*-acetamido ketones. This involves the condensation of an α-amino acid with acetic anhydride in the presence of a base. *β*-acetamido ketones are important for their biological and pharmaceutical properties ,and in the preparation of antibiotic drugs such as nikkomycine or neopolyoxines.

Recently several modified procedures for the Dakin-West condensation reaction were reported [2]. In continuation of our interest on the catalytic activities of solid acids,Now we want to report that Melamine Sulfonic Acid can be efficiently catalyzed condensation reaction of aryl aldehyde, aryl ketone and acetyl chloride in acetonitrile (Scheme 1). The β-acetamido ketones were produced in short reaction time with high yields.



R_1=H,NO_2,OMe,Cl R_2=H,NO_2,Cl

scheme1



References:

[1] Kappe, C. O, *Acc. Chem. Res.* **2000**, 33, 879.

[2] Khodaei, M. M, Khosropour, A. R, *Tetrahedron Lett*. **2005**, 46, 2105.

$\{[K.18\text{-}Crown\text{-}6]Br_3\}_n$: A unique tribromide-type catalyst for the selective protection of aliphatic and aromatic amines

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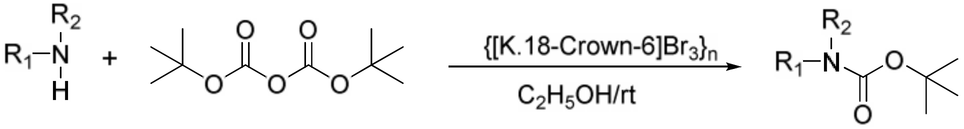
Organic tribromide reagents (OTBs) are preferable as oxidants to molecular bromine, owing to the hazards associated with elemental bromine. Several tribromides have been reported [1]. Very recently, we reported $\{[K.18\text{-crown-}6]Br_3\}_n$, a unique tribromide with a columnar nanotube-like structure. It would be extremely useful to develop further synthetic protocols for the synthesis of OTBs [2].

The presence of the amine functionality in a wide range of biologically active compounds makes protection of amines an important and interesting exercise in synthetic organic and medicinal chemistry [1]. Many mild and selective methods for the protection of amine groups have been developed for many different organic transformations. Among them the commercially available di-*tert* butyl dicarbonate [*(Boc)$_2$O*] has become an efficient reagent for the clean and rapid introduction of the *tert*-butoxy carbonyl (Boc) protecting group at the amine functionality. Due to the stability of *N-tert*-butylcarbamates towards many reagents, this protection of amines is used frequently [3].

In continuation of our studies on the protection of organic functional groups [4], we were interested in using the di-*tert*-butyl dicarbonate (*diboc*) for the simple and effective protection of amines in the presence of a catalytic amount of $\{[K.18\text{-crown-}6]Br_3\}_n$.



References:

[1] Zolfigol, M. A.; Chehardoli, G.; Ghaemi, E.; Madrakian, E.; Zare, R.; Azadbakht, T.; Niknam, K.; Mallakpour, S *Monatsh. Chem.* **2008**, *139*, 261.
[2] Zolfigol, M. A.; Chehardoli, G.; Salehzadeh, S.; Adams, H.; Ward, M. D. *Tetrahedron Lett*. **2007**, *48*, 7969.
[3] Sikshi, S. A.; Hultin, P. G. *J. Org. Chem*. **2006**, *71*, 5888.
[4] Shirini, F., Zolfigol, M. A., Abri, A. R., *Monatsh. Chem.* **2008**, *139*, 17.

The optimization of reaction condition in one-pot synthesis of benzimidazoles

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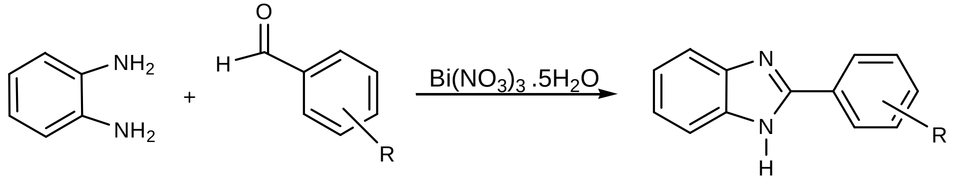
Benzimidazole nucleus is an important heterocyclic ringر because of its synthetic utility and broad range of pharmacological activities [1]. These heterocycles show various pharmaceutical properties such ac antiviral, antibacterial, antibiotic, antifungal, anticancer, antitumor and anti-inflammatory activities [2].

A variety of Methods are available for synthesis of benzimidazoles include the condensation of *o*-aryldiamines and aldehydes in refluxing nitrobenzene, the condensation of *o*-aryldiamines with carboxylic acids or their derivatives in the presence of strong acids such as polyphosphoric acid or mineral acids [3].

In previous work, we investigated the catalytic effect of $Bi(NO_3)_3 .5H_2O$ in one-pot synthesis of benzimidazoles from condensation of *o*-phenylenediamines with aldehydes [4].



Here, we report the modification of procedure to improve the reaction yields and rates. The solvent, temperature, reaction time and the amount of catalyst were main parameter whose effect was examined on the reaction yields and rates. The best results were achieved in dioxane at 75˚C using 1mmol catalyst.

References:

[1] Smith, A. A.; Ibrahim, K. S.; Parimalakrishnan, S.; Muthu, A. K. *J. Applied chemistry*. **2008**, 1,4.
[2] Mohammadpoor-Baltork, I.; Moghadam, M.; Tangestaninejad, S.; Mirkhani, V. *J. Iran Chem*. **2008**, 5, S65-S70.
[3] Nagawade, R. R. ; Shinde, D. B. *J. Chinese Chemical Letters* . **2006**, 17, 453.
[4] Mosavi, M.; Dorostkar, Z. The National Chemistry Conference, May **2010**, Islamic Azad University, Shahreza Branch, 229.

Sorption of Cd(II), Pb(II), Ni(II) and Zn(II) to bone char from aqueous solution and real samples using bone char

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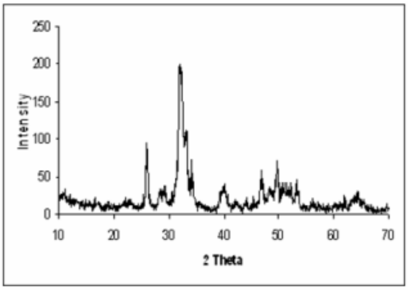
Human poisoning from toxic metals have occurred as a result of drinking water contaminated with toxic metals such as Pb and Cd. Various technologies such as ion exchange, adsorption and coagulation have been employed for metals removal from water. In recent years, many low-cost sorbents including agricultural waste and byproducts have also been tested in batch and fixed bed sorption systems by a number of authors [1-3].

In this research, Bone char has been investigated as biosorbent for Cd(II), Pb(II), Ni(II) and Zn(II) from aqueous solution and real samples. It is derived from the carbonization of the crushed animal bones by heating them to 700 °C for 6 h. The crushed bone, after the heating process was powdered and sieved through a 400 mesh sieve. It was characterized with FT-IR, XRD (fig), BET and SEM. The sorption of toxic metals such as Pb, Cd, Ni and Zn onto bone char in an agitated batch sorber has been studied. The adsorption isotherm studies for metal ions clearly indicated that the adsorptive behavior of them on bone char was fitted to Freundlich isotherm that is generally used to describe the adsorption processes. In the case of the real samples, was not showed any effect on tissue and the efficiency of sorption was as well as aqueous solution. The speed of heavy metal adsorption depends on several parameters, including particle size and porosity of the adsorbent as well as molecular structure of the adsorbed compound. In this work, the adsorption of mentioned metals by bone char little influenced by contact time that means the remaining concentration of metal ions in solution were not appreciably changed from 1 to 24 h and revealed that a contact time of 2 h was sufficient for equilibrium to be established.

We concluded that Bone char was a suitable adsorbent for the removal of mentioned metals from aqueous solution and chosen real samples.



References

[1] Field, R.A. *Meat Science.* **2000**, *55*, 255.
[2] Wu, Y., Zhang, Sh., Guo, X., Huang , H., *Bioresource Technology*. **2008**, *99*, 7709.
[3] Pan, X., Wang, J., Zhang, D. *Desalination*. **2009**, *249*, 609.

Dependence of the ${}^{n}J_{P\text{-}X}$ (n = 2, 3 and X = H, C) on the hybridization and ring size in novle heterocycles of *N*-phosphinyl urea

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1, 3-Disubstituted ureas were reported as new, potent and stable inhibitors of sEH (Epoxide hydrolases), HIV-1 protease inhibitors, plant growth regulators and anticonvulsant medicinal preparations [1]. Also, compounds with phosphorus-containing structures are an important part of chemistry because of their applications in medicine, fertilizers, pesticides and plant growth regulators [2].

One class of these compounds are *N*-phosphinylureas (containing -NHC(O)NHP(O)- backbone), which are important because of their various biological activities, as extractants, analytical reagent and structural fragments for construction of metal-containing macrocycles, ureas inhibitors and anticancer drugs [3, 4]. On the other hand, stereochemistry, P – C and P - H coupling constants in some five and six – membered rings containing phosphorus were studied [5].

To further investigate this area, we report synthesis of heterocycles of *N*-phosphinylurea (**1** – **4**) with formula $\rho\text{-}CH_3C_6H_4NHC(O)NHP(O)NH(CH_2)_nNH$ (n = 2 (**1**), 3 (**2**)), $\rho\text{-}CH_3C_6H_4NHC(O)NHP(O)NHC_6H_4NH$(**3**) and $\rho\text{-}CH_3C_6H_4NHC(O)NHP(O)NHC_{10}H_6NH$(**4**) by reaction of dichlorophosphinylureas and the desired amines (ethylendiamine, 1, 3-diaminopropane, 1, 2-phenylendiamine and 1, 8-naphtalendiamine) in the presence of an HCl scavenger (an excess amount of the corresponding amine or triethylamine) in acetonitril as solvent. Precipitates were characterized to find effective parameters for ${}^{n}J_{(P,\,X)}$ coupling constants (X = H, C).

Refrenses:

[1] Struga, M.; Kossakowski, J.; Kedzierska, E.; Fidecka, S.; Stefańska, J.; *Chem. Pharm. Bull.* **2007**, *55*, 796.
[2] Baldwin, A.; Huang, Z.; Jounaidi, Y.; Waxman, D. J.; Arch. *Biochem. Biophys*. **2003**, *409*, 197.
[3] Shaidarova, L. G.; Gedmina, A. V.; Brusko, V. V.; Zabirov, N. G.; Ulakhovich, N. A.; Budnikov, H. K.; *Anal. Sci.* **2001**, *17*, 957.
[4] Zon, G., *Prog. Med. Chem*., **1982**, *19*, 205.
[5] Wrackmeyer, B. Kupce, E. Schmidpeter, A. *Magn. Reson. Chem*. **1991**, *29*, 1045.

Melamine-formaldehyde resin supported lewis acids catalysed Fridel-Crafts addition of indoles to epoxides: a facile route to produce indolyl derivatives

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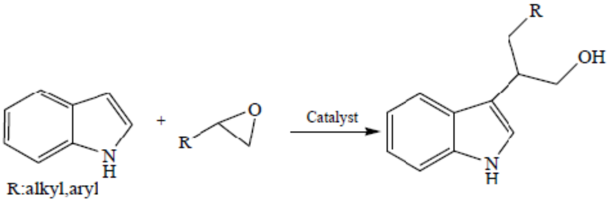
Epoxides are versatile intermediates in organic synthesis. Not only these compounds are easily prepared from a variety of starting materials, but inherent polarity and strain of their three membered rings make them susceptible to reaction with a large number of reagents, electrophiles, nucleophiles, aids, bases, and some reducing and oxidizing agent [1]. Indol is a key motif in many pharmacologically and biologically active compounds as well as in many natural products it belongs to the class of the alkaloids and a direct synthesis of indolyl derivatives is desired [2].

Organic synthesis in the absence of solvent is a powerful tool for the generation of structurally diverse molecules, due to their special selectivity, the ease of set-up and work-up arousing great interest. Moreover, solvent-free reactions sometimes are faster, taking just afew minutes rather than hours to complete. This aspect, coupled with the lower overall costs of running a reaction without solvent and no specially needed equipment, could become a decisive factor [3].

Herein, we have reported a new direct protocol for the preparation of indolyl derivatives via a Friedel-Crafts catalyzed ring opening of epoxides. The use of Lewis acids as catalyst besides to guarantee a general tolerance toward the presence of different functional group on the indole motif, allows the isolation of the indolyl alcohols in good chemical yields.



R:alkyl,aryl
Catalyst:lewis acid on Melamine-formaldehyde resin

References:

[1] Meskens, F. A. J. *Synthesis*, **1981**, 501.
[2] Walsh,T.; Toupence, R. B.; Ujjainwalla, F.; Young, J. R.; Goulet, M. T. *Tetrahedron*, **2001**, 57, 5233.
[3] Tanaka, K.; Toda, F. *Chem Rev*, **2000**, 100, 1025.

Synthesis of new isoxazolines with 1,3-dipolar cycloaddition of nitrile oxides and alkenes

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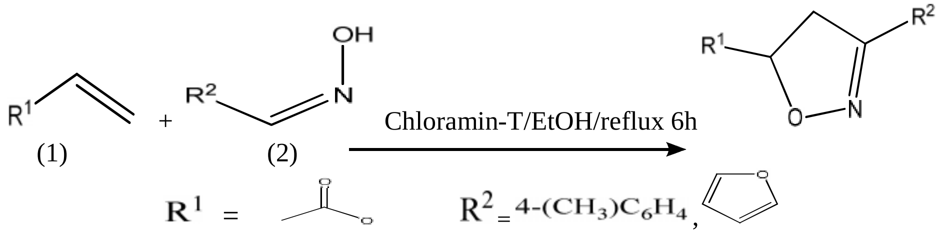
The addition of a 1,3-dipole to an alkene for the synthesis of five-membered rings is a classic reaction in organic chemistry.The 1,3-dipolar cycloaddition (1,3-DC) reactions are used for the preparation of molecules of fundamental importance for both academia and industry[1]. isoxazole is one of the most useful compounds, which was found as an important unit in many biologically and pharmaceutical active compounds[2].

The1,3-DC reaction of nitrile oxides with alkenes provides a straightforward access to 2-isoxazolines[3]. Reaction of aldoximes with chloramin-T leads to formation of nitrile oxides which can react in situ intra or intermolecularly with olefinic compounds to produce isoxazolines in good yield [4].

Herein we report the use of N-chloro-N-sodio-4-methylbenzene-sulfonamide known as chloramines-T as an efficient method to affored new of 2-isoxazolines during (1,3-DC) reaction.

The cycloaddition is carried out by heating an equimolecular mixture of an alken 1, aldoxime 2, and chloramin-T trihydrate in ethanol under reflux for 6h.



The role of chloramin-T in these transformation may be chloration of aldoxime [5].

References:

[1] Kurt V.Gothelf and Karl Anker Jorgenson,*Chem..Rev*. **1998**, 98, 863.
[2] Weissberger, A.*chem.Herterocycle.Compd*.**1962**.
[3] Kanemasa , s; Tsuge, O, *Heterocycles* **1990**, 30, 719.
[4] Alfred Hassner,K.M.Lokanatha Rai, *Synthesis* **1989,** 57.
[5] Corey, E.J., Estreicher,H. *Tetrahedron lett,* **1980**.21, 1117.

DFT exploratory study on the conformational features of the HCO-Gly-$_L$-Val-NH_2 dipeptide

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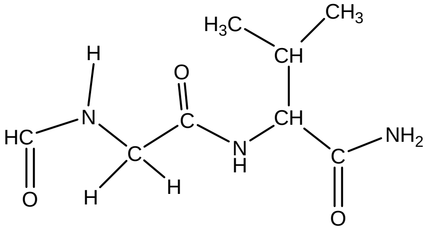
Conformation of an important system, the HCO-Gly-$_L$-Val-$NH_{2,}$ protected dipeptide , of been calculated by using B3LYP/6-31G* level of theory in the gas phase. At first the side chain's angel of valine (χ) changed at 30.0 intervals from 0.0 to 360.0 and their geometries optimized. Three minima Gauche+ (χ = 60), Gauche-(χ = -60) and Anti (χ = 180) were obtained that the gauche- conformer has the lowest energy.

And then for gauche - by using frequency calculation at B3LYP/6-31G* level with varying dihedral angles Ψ1 and φ1 for GLY, Ψ2 and φ2 for VAL, thermodynamic properties were determined. We optimized and performed the calculations of frequency for every dihedral's angel seperately instead of different amount at 30.0 intervals between 0.0 to 360.0. For each one we found the angel that it had the most stable in energy and thermo dynamics functions.

RESULTS: Calculations show that for most stable conformer Ψ1, φ1, Ψ2, φ2 are 180,180,150,240 respectively. Thermodynamic properties G , H, E and S are for the angles Ψ1 ,φ1,Ψ2,φ2are(441547.5849,441547.5849,441546.7585,441552.3853),(441507.9552,441507.9552,441509.0263,441512.8384),(441518.5588,441518.5588,441519.1957,441523.5569)and (132.919,132.919,126.553,132.64) respectively. G, H and E are according to kcal/mol and S is cal/mol k.



References:

[1] Cindy P. chun , Ashton A. Conner , Gregory A. Chass .THEOCHEM 2004.
[2] M. A. McAllister, A. Perczel, J. Mol. Struct. (THEOCHEM) 1993.
[3] A. Perczel, M. McAllister, P. Csazar 1998.

Silica-bonded *N,N,N-* tri sufamic acid (propyl diethylen tri amine) as an efficient and recyclable solid acid catalyst for the synthesis of 4,40-(arylmethylene)bis(1H-pyrazol-5-ols)

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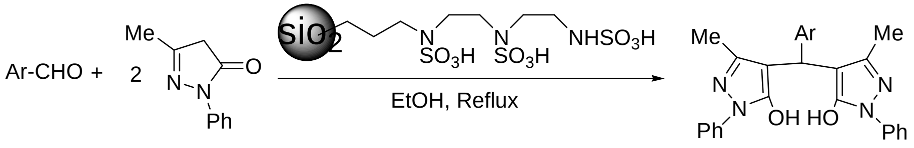
Pyrazoles are an important class of bio-active drug targets in the pharmaceutical industry, as they are the core structure of numerous biologically active compounds [1]. For example, they exhibit antianxiety, antipyretic, analgesic, and anti-inflammatory properties. 2,4-Dihydro-3H-pyrazol-3-one derivatives including 4,40-(arylmethylene) bis(3-methyl-phenyl-1H-pyrazol-5-ols) have a broad spectrum of approved biological activity, being used as anti-inflammatory, antipyretic[2].

In this article we introduced a new catalyst for the prepatation of 4,40(arylmethylene) bis (1H-pyrazol-5-ols) by condensation reaction of aromatic aldehydes with 3-methyl-l-phenyl-5-pyrazolone in the presence of silica-bonded N,N,N- tri sufamic acid (propyl diethylen tri amine) as catalyst. This condensation reaction was performed in ethanol under refluxing conditions giving 4, 40-alkylmethylene-bis(3-methyl-5-pyrazolones) in 75–90% yields.



References:

[1] McDonald, E.; Jones, K.; Brough, P. A.; Drysdale, M. J.; Workman, P. Curr. *Top. Med. Chem.* **2006**, *6*, 1193.

[2] Sugiura, S.; Ohno, S.; Ohtani, O.; Izumi, K.; Kitamikado, T.; Asai, H.; Kato, K. *J. Med. Chem.* **1977**, *20*, 80.

Polyacylation of unactivated aromatic compounds

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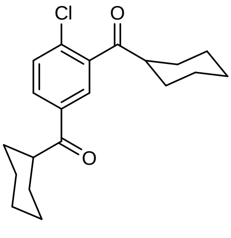
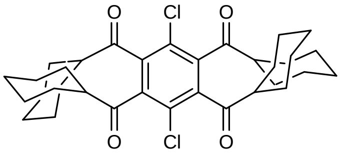
Many synthesis methods have been developed for the preparation of aromatic ketones which are important intermediates for the preparation of fine chemicals in pharmaceuticals. One of the most common is friedel-crafts acylation that is generally carried out by using aluminum trichloride as a lewis acid. The reaction of benzonitryl derivatives with grinyard reagents have also been used for this purpose. chlorophenyl cyclopentyl ketone, as a fundamental precursor of ketamine, have been synthesized using magnesium bromide and chlorobenzonitryl [1]. Ketamine is an old anaesthetic. It has been safely used for induction and maintenance of general anaesthesia since the second part of the 20th century and also plays a well-established role in analgesia [2]. It has been recommended for use in a variety of areas including controlling pain, therapy of asthma, intracranial procedures, hemorrhagic or septic shocks [3].

In this project, acylation of unactivated derivatives of benzene such as chlorobenzene, 1,4-dichlorobenzene and 4-chlorobenzoic acid have been carried out using an easy and known strategy at 80^0C in the presence of aluminum chloride as a reagent to give aromatic ketones. The products were characterized by IR, ^{1}HNMR, ^{13}CNMR and MS spectroscopy. Of interest to this project is the preparation of halophenyl ketones involving 2 or 4 acyl groups, as shown. Such key materials are going to be used in the preparation of new α-phenyl cycloheptanones.





References:

[1] Swain, C. G. J. Amer. Chem. Soc. **1947**, *69*, 2306.
[2] Marije aan het Rot, K. A.; Collins, J. W.; Murrough, A. M. Biological Psychiatry. **2010**, *67*, 139.
[3] Erk, G.; Örnek, D.; Dönmez, N.F. International Journal of Pediatric Otorhinolaryngology. **2007**, *71*, 937.

Theoretical studies on tautomerism of isoxazole derivatives in the gas phase

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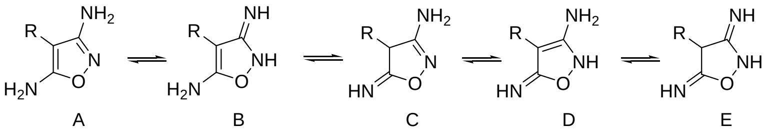
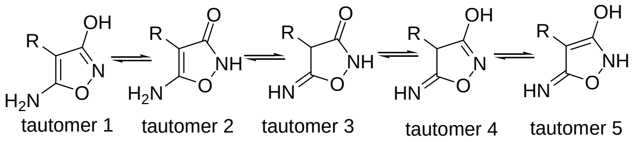
Isoxazoles play interesting roles in medicinal and agricultural chemistry and serve as important synthetic building blocks. Synthesis of substituted isoxazole derivatives is particularly important because a lot of compounds containing the isoxazole ring system are known to have variety of biological activities in pharmaceutical and agriculturalareas. Their range of uses includes medicinal,herbicidal, fungicidal, pesticidal applications, dyes,insulating oils, and lubricant [1].

Ab initio and DFT molecular orbital calculations have been performed on the intramolecular tautomerism of all five isomers of isoxazole in the gas phase. All stationary points' transition structures were optimized at the HF/6-311++G(d,p) and B3LYP/6-311++G(d,p) levels of theory and confirmed by frequency calculations. The intrinsic reaction coordinates (IRC) for the tautomeric processes were traced to connect the transition structures and the corresponding substituted tautomeric pairs. The energy barriers calculated at various levels of theory are reported for each tautomeric interconversion.



R=H, CH_3, F, CL, NO, NO_2, CN, C≡CH



R= OH, NO_2, Cl, Me, NH_2, CN

The results of HF and DFT calculations show that compound **2** and **A** is the most stable tautomer in the gas phase in order of **2> 1> 5> 4> 3 , A>C>D>B>E**

Reference

[1] (a) Kim, H. J.; Hwang, K. J.; Lee, J. H. *Biosci Biotech Biochem* **1994**, *58*, 1191; (b) Hwang, K. J.; Kim, H. J.; Lee, J. H. *Korean J Med Chem* **1994**, *4*, 2.

One-pot synthesis of 2,4,5-trisubstituted imidazole derivatives with DAHP and 2-morpholinoethanesulfonic acid as catalysts

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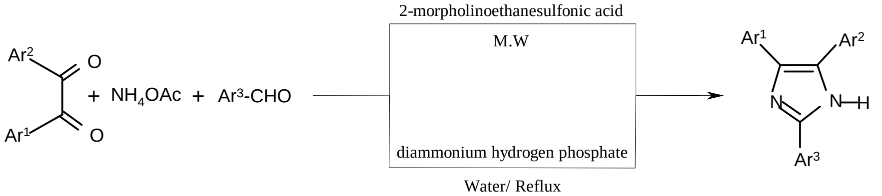
Nowadays, several of biologically active compounds are efficiently synthesized by highly elegant multi-component reactions [1]. Multi-component reactions are the processes that trigger the conversion of three or more starting materials in one-pot to a highly functionalized product displaying maximum molecular diversity, complexity, and impressive selectivity. Therefore, these reactions are highly atom economic, eco-friendly, and synthetically efficient in terms of decreasing the time, the number of reaction steps, and the consumption of chemicals and solvents used [2]. Multi-substituted imidazoles, an important class of pharmaceutical compounds, exhibit a wide spectrum of biological activity [3-5]. In this study diammonium hydrogen phosphate $(NH_4)_2HPO_4$ (DAHP) and 2-morpholinoethanesulfonic acid has been used as efficient catalysts for an improved and rapid synthesis of 2,4,5-trisubstituted imidazoles by a three-component, one-pot condensation of 1,2-diketones and aryl aldehydes with ammonium acetate in excellent yields under mild conditions. The effects of two catalysts in yields of reaction and times were investigated. The results shown that 2-morpholinoethanesulfonic acid was effective than DAHP in times and yields of reaction. The present methodology offers several advantages such as excellent yields and the use of non-toxic and inexpensive catalyst.



References:

[1] Ugi, I.; Domling, A.; Gruber, B.; Almstetter, M. *Croat. Chem. Acta.* **1997**, *70*, 631.
[2] Wasilke, J.C.; Obrey, S.J.; Baker, R.T.; Bazan, G.C. *Chem. Rev.* **2005**, *105*, 1001.
[3] Lombardino, J. G.; Wiseman, E. H. *J. Med. Chem.* **1974**, *17*, 1182.
[4] Laufer, S. A.; Zimmermann, W.; Ruff, K. J. *J. Med. Chem.* **2004**, *47*, 6311.
[5] Wolkenberg, S. E.; Wisnoski, D. D.; Leister, W. H.; Wang, Y.; Zhao, Z.; Lindsley, C. W. *Org. Lett.* **2004**, *6*, 1453.

One-pot synthesis of 3-cyano-2-pyridones by reaction between aromatic aldehydes, 2-cyanoacetamide and ethyl acetoacetate

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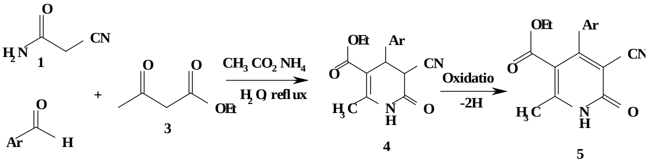
Substituted 3-cyano-2-pyridones derivatives are important intermediates in the pharmaceutical, dye, and photo industries. Synthesis of these compounds have been widely studied using conventional heating in the presence of various catalysts and usually in polar solvents.[1] The 2-pyridones are a class of important heteroaromatic compounds. 3-cyano-2-pyridones have been prepared by the cyclization of cyanoacetamide condensated with 2-aryl-3-dimethylamino-2-propenals.[2,3] Here we report a simple one-pot method for preparation of 3-cyanoacetamide, aromatic aldehydes, ethyl acetoacetate and amonium-acetate in boiling water after 12h afforded 3-cyano-2-pyridone derivaties in good yeilds.



5	Ar	% yield
a	C_6H_5	90
b	4-Cl C_6H_4	87
c	4- $NO_2C_6H_4$	92
d	2- $NO_2C_6H_4$	90
e	4-Me C_6H_4	87

References:

[1] Paulvannan, K.; Chen, T. *J. Org. Chem.* **2000**, *65*, 6160.
[2] Gomez-Parra, V.; Gomez, M. C.; Sanchez F.; Stefani, V. *Arch. Pharm. (Weinheim)* **1992**, *325*, 483.
[3] Julia, M.; Pinhas H.; Igolen, J. *Bull. Soc. Chim.* **1966**, 2387.

Three-component reaction between triphenylphosphine, dialkyl acetylenedicarboxylate and 2-aminothiazole or 2-aminobenzothiazole in the presence of arylglyoxals : An efficient one-pot synthesis of highly functionalized pyrroles

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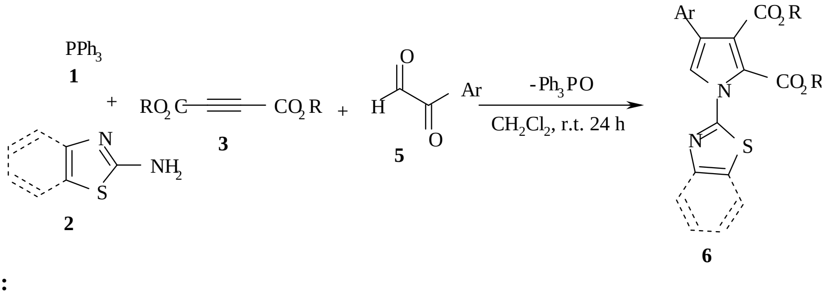
Pyrroles are heterocycles of great importance because of their presence in numerous natural products like heme, vitamin B_{12}, and various cytochrome enzymes. Some of the recently isolated pyrrole containing marine natural products have been found to exhibit considerable cytotoxicity and function as multidrug resistant (MDR) reversal agents. Many of these biologically active compounds have emerged as chemotherapeutic agents [1].Addition reaction between phosphines and activated carbon-carbon triple bonds is well known to produce a reactive zwitterionic intermediate, which may be trapped by various electrophiles[2]. Reaction of triphenylphosphine with dimethyl acetylenedicarboxylate (DMAD) has been studied in the presence of a variety of organic acidic compounds, in order to trapp the zwitterionic intermediate. Trapping of PPh_3-DMAD zwitterion by an organic acidic compound containing a carbonyl group have been used as a one-pot and efficient route for the synthesis of a variety of heterocylclic and carbocyclic compounds [3].

Here we report an extention of this route for the synthesis of polysubstituted pyrrole derivatives by three-component reaction between dialkyl acetylenedicarboxylates, triphenylphosphine, 2-aminothiazole or 2-aminobenzothiazole in the presence of arylglyoxals.



References:

[1] Sundberg, R. J. *In Comprehensive Heterocyclic Chemistry*; Katritzky, A., Rees, C. W., Scriven, E. F. V., Eds.; Pergamon: Oxford, 1996; Vol. 2, p 119.
[2] Anary-Abbasinejad, M.; Anaraki-Ardakani, H.; Hosseini-Mehdiabad**,** H. *Phosphorus, Sulfur and Silicon and the Related Elements***, 2008**, 183 (6), 1440.
[3] Mosslemin, M. H.; Yavari, I.; Anary-abbasinejad, M.; Nateghi, M. R. *Synthesis*, **2004**, 7, 1029.

Synthesis and characterization of three linear asymmetric N_2S diamines compounds

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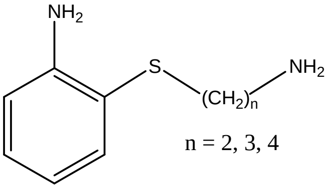
Interest in asymmetric compounds is growing on account of their unique structural properties. The preparation of asymmetric amines, however, is usually more elaborate than the synthesis of symmetric amines. The development of simple methods for the preparation of asymmetric amines is important. The non-symmetric structure of these compounds allows for selective functionalization at non-equivalent amino group(s) [1-3]. An asymmetric tridentate ligand permitted more detailed comparisons of the coordination chemistry of divalent group 12 metal ions to be made than related symmetric ligands [4].

Three asymmetric linear diamine, 2-(2-aminoethylthio)benzenamine, 2-(3-aminopropylthio)benzenamine and 2-(4-aminobutylthio)benzenamine were synthesized by reaction of 2-aminobenzenethiol with N-(2-bromoethyl)phthalimide or N-(3-bromopropyl) phthalimide or N-(4-bromobutyl)phthalimide respectively, so that leading to asymmetrical linear diamine that contain one primary aromatic amine group and one primary aliphatic amine groups. All the asymmetric diamines have been characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and EI mass.



References:

[1] M. Bandini, Pier G. Cozzi, and A. Umani-Ronchi. *Pure Appl. Chem.* **2001**.*73*, 325.
[2] L. Dai, X. Hou, W. Deng, S. You and Y. Zhou. *Pure Appl. Chem*. **1999**. *71*, 140.
[3] H. Keypour, S. salehzadeh, R.G. Pritchard and R.V. Parish, *Inorg. Chem.* **2000**, *39*, 5787.
[4] D.C. Bebout, W. Lai, S.M. Stamps, S. M. Berry, R.J. Butcher, *Polyhedron*, **2008**, *27*, 1591.

Theoretical studies on tautomerism of new azo dyes synthesized from 4-amino phenyl tetrazole

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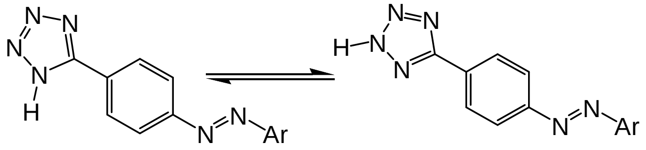
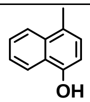
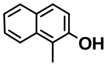
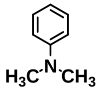
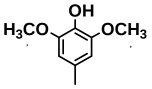
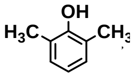
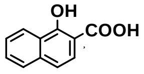
Azo dyes constitute the largest group of commonly availabledyes and pigments .Due to their colour, azo dyesare used as pigments, indicators of solvent polarity, of molecular environments and of chemical environments; they are also widely used as histological stains andin the colorimetric analysis of pharmaceuticals [1]. Tetrazole derivatives find a wide range of pharmaceutical applications, where they act as stimulants or sedatives on the centralnervous system. These compounds have antimicrobial, antiinflammatory, antilipemic, and antiallergic activities cis-peptide bondmimics. Recently some publications describing the tautomerism of 5-substituted tetrazoles by ab initio method became available. for all the substituents at the position 5 of the ring the 2H-tautomeres was found are the most stable in the gas phase and the difference in energy between 1H- and 2H-tautomers depends only slightly on the nature of substituent R [2].



Ar						
E_{2H}-E_{1H}	**-1.90**	**-2.19**	**-1.74**	**-1.89**	**-1.80**	**-1.87**

In this research some novel azo dyes synthesized from tetrazole in our laboratory have been studied using HF method by 6-31G(d) basis function investigated. Based on these calculations the 2*H* tetrazoles was found to be more stable than 1*H* ones.

References:

[1] . Nathan SS, Murthy SK. *Organic chemistry made simple*. London: W.H. Allen; **1968**.
[2] .A Najafi Chermahini, A Ghaedi, A Teimouri, *J. Mol. Struct. Theochem* **867** (2008) 78.

Density functional theory study of intermolecular interactions of cyclic pyrazol dimmers

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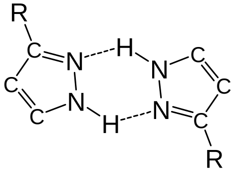
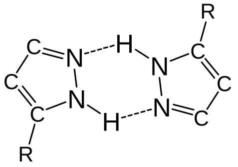
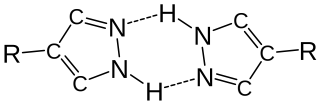
Substituted pyrazoles are an important class of heterocyclic compounds used in the pharmaceutical industry, since they form the core structures of many commercial drugs such as Zometapine [1]. They are also known to show a wide range of biological properties such as selective Human C1s inhibition [2]. Hydrogen bond is an important type of nancovalent intractions that is present in the many chemical and biologiacal sysrems [3,4]. In the present study we have investigate interaction energies in dimers of substituted pyrazoles, which show different patterns of hydrogen bonding.



A



B



C

Density Functional Theory at B3LYP/6-31++G(d,p) level is employed to study of the hydrogen bonding between pyrazol dimers in the gas phase. The following substituents have been taken into consideration: H, F, Cl, CH_3, NH_2, NO and NO_2. It was found that the strongest hydrogen bonding obtained by NO_2, NH_2 and H as the substituent in the **A**, **B** and **C** dimers respectively.

References:

[1] De Wald, H. A.; Lobbestael, S.; Poschel, B. P. H. *J. Med. Chem.* **1981**, *24*, 982.
[2] Pitt, G. R.; Batt, A. R.; Haigh, R. M.; Penson, A. M.; Robson, P. A.; Rooker, D. P.; Tartar, A. L.; Trim, J. E.; Yea, C. R.; Roe, M. B. Bioorg. *Med. Chem. Lett.* **2004**, *14*, 3043.
[3] J. Zabrocki, G.D. Smith, J.B Jr Dunbar, H. Iijima, G.R. Marshall, *J. Am. Chem. Soc.* **1988,** *110*, 5875.
[4] S.Schelyer, Hydrogen bonding; Oxford Univecity Press: New York, **1997**.

Facile one-Pot multicomponent synthesis of b-acetamido ketones with a catalytic amount of 22% Co/CeO2 - ZrO2 nano catalyst as heterogeneous catalyst

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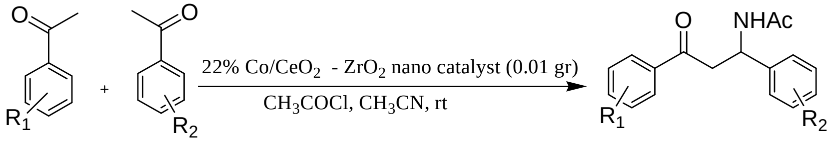
The MCRs for the synthesis of β-acetamido carbonyl compounds has been gained considerable attention in organic synthesis. The products, containing of β-acetamido carbonyl skeletons, are found in a number of biologically or pharmalogically important compounds such as nikkomycine or neopolyoxines [1-3]. The best known rout for the synthesis of these compounds is the Dakin-West reaction [4],Some of catalysts have been reported for the synthesis of β-acetamido carbonyl compounds. In this work, we wish to report a mild, efficient and novel prtocol multi-component condensation reaction utilizing a catalytic amount of 22% Co/CeO_2- ZrO_2 Nano Catalyst as a green, reusable, recycle and none toxic catalyst for the synthesis of β-acetamido ketones in the present of aromatic aldehydes derivatives, acetophenone derivatives, acetyl chloride and acetonitril at room temperature under mild conditions(Scheme 1). The use of this Catalyst makes this process convenient, and environment-friendly.



Scheme 1

References:

[1] Daehn, U.; Hagenmaier, H.; Hoehn, H.; Koening, W. A.; Wolf, G.; Zaehner, H.; *Arch. Microbiol 107*: 143; Kobinata, K.; Uramato, M.; Nishii, M.; Kusakabe, H.; Nakamura, G.; Isono, K.. *Agric. Biol.* **1980**, *44*, 1709.
[2] Casimir, J. R.; Turetta, C.; Ettouati, L.; Paris, J. *Tetrahedron Lett.* **1995**, *36*, 4797.
[3] Godfrey, A. G.; Brooks, D. A.; Hay, L. A.; Peters, M.; McCarthy, J. R.; Mitchell, D. *J. Org. Chem.* **2003**, *68*, 2623.
[4] Dakin, H. D.; West, R. *J. Biol. Chem.* **1928**, *78*, 745.

Cyanorosulfuric acid catalyzed synthesis of dibenzoxanthenes under solvent-free condition

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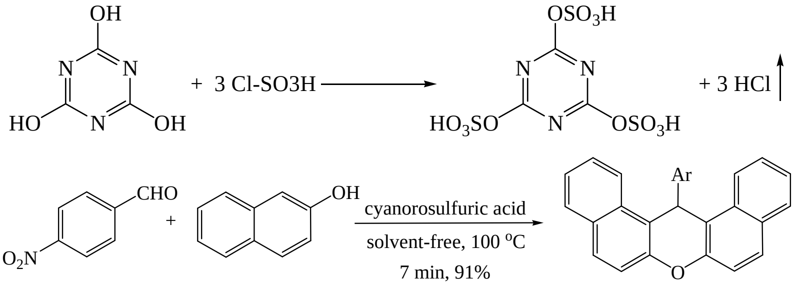
dibenzoxanthenes are important intermediates as they display biological and therapeutic properties such as anti-bacterial, anti-viral activities and anti-inflammatory [1]. A wide variety of reagents have been used for the preparation of dibenzoxanthenes, by the reaction of β-naphthol with aromatic aldehydes, including sulfamic acid, Yb(OTf)3, *p* -TSA, silica sulfuric acid [4].

Herein, we report an efficient method for the synthesis of dibenzoxanthenes by the condensation of aldehydes with *β* -naphthol under solvent-free conditions in good to excellent yields in the presence of catalytic amount of cyanorosulfuric acid. The novel catalyst was synthesized through the reaction of cyanoric acid and chlorosulfonic acid was added dropwise over a period of 1 h at room temperature. HCl evolved immediately. After completion of the addition, the mixture was shaken for 1 h, while the residual HCl was eliminated by suction. Then the mixture was washed with diethyl ether to remove the unreacted chlorosulfonic acid. Finally, a grayish solid material was obtained.



Reference:

[1] Vennerstrom, J. L.; Makler, M. T. *Antimicrob. Agents Chemother.* **1995**, *39*, 2671-2677.
[2] Furumiya, K.; Mizutani, T. *J. Toxicol. Environ. Health A*, **2008,** *71*, 1307-1313.
[3] Setnescu, R.; Jipa, S. *J. Optoelectron. Adv. Mater.***2006**, *8*, 682-686.
[4] a) Rajitha, B.; Kumar, B. S.; Reddy, Y. T.; Reddy, P. N.; Sreenivasulu, N. *Tetrahedron Lett*. **2005**, *46*, 8691; b) Wang, L. M.; Sui, Y. Y.; Zhang, L. *Chin. J. Chem*, **2008**, *26*, 1105. c) Khosropour, AR.; Khodaei, MM.; Moghannian, H. *Synlett* **2005**, *955*, 8. d) Shaterian, HR.; Ghashang, M.; Hassankhani, A. Dyes and Pigments. **2008,** *76*, 564.

Synthesis of 2-(3-oxocycloalk-1-enylamino)nicotinonitrile derivatives

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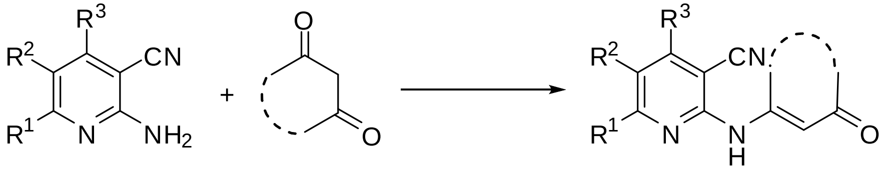
The enaminone derivatives are very important synthons for the synthesis of various heterocyclic and biologically active analogues including anti-imflammatory, antitumor, antibacterial agents [1] and intermediates for the synthesis of several amino acids, peptides and alkaloids [2], also 2-amino-3-cyanopyridines show analgesic, antipyretic, β-adrenolytic and antihypertensive properties [3].

Due to the wide range of utility in pharmaceutical industry, several methods have been developed for the synthesis of these compounds. Various activators such as zinc perchlorate, cerium chloride alumina, silica [4] and … have been reported for this transformation. However, many of these methods have some drawbacks, which include expensive and stoichiometric amounts of reagents and also require extended reaction times. Therefore, the development of a simple, more convenient and eco-friendly approaches is desirable. Also, the objective of this work was to design enaminone of cyanopyridines that would possess potential medicinal properties. The reaction between 1,3-diketones and 2-amino-3-cyanopyridines yielded secondary enaminone of cyanopyridines, in ethanol at reflux conditions respectively.



R^1, R^2, R^3 = alkyl and aryl

References:

[1] Spivey, A. C.; Srikaran, R.; Diaper, C. M. *Org. Biomol. Chem.* **2003**, *1*, 1638.

[2] Palmieri, G.; Cimmerelli, C. *J. Org. Chem.* **1997**, *62*, 1033.

[3] Manna, F.; Chimenti, F.; Bolasco, A.; Filippeli, A.; Palla, A.; Filippeli, W.; Lampa, E.; Mercantini, R. *Eur. J. Med. Chem.* **1992**, *27*, 627.

[4] a) Lin, J.; Zhang, L. F. *Monatsh. Chem.* **2007**, *138*, 77. b) Zhang, Z. H.; Yin, L.; Wand, Y. M. *Adv. Synth. Catal.* **2006**, *384*, 184.

Reaction of 2,3-dibromo-1,4-naphtaquinone with two equivalents of benzotriazole

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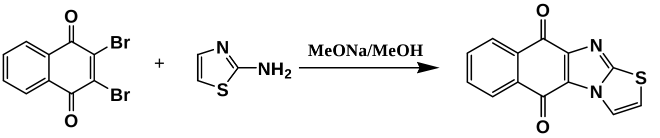
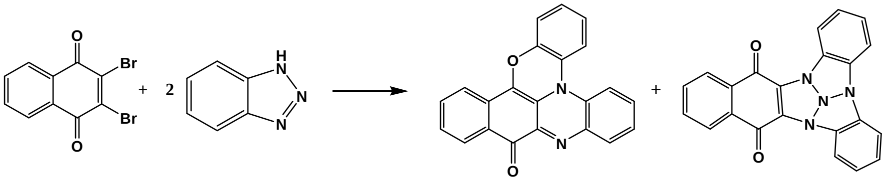
We have reported the reaction of 2,3-dibromo-1,4-naphtaquinone with 2-amino thiazole in MeONa/MeOH (2eq) at 60 ºC to give naphtho[2,3-d]thiazolo[3,2-a]imidazole-5,10-dione as shown in Scheme 1 [1].



Scheme 1

Heating two equivalents of benzotriazole (**1**) with 2,3-dibromo naphthaquinone at 130-140 ºC gave a mixture of product that separated by T.L.C. with chloroform as eluent. Two fractions were detected as (**1**) and (**2**) compounds (Scheme 2). These compounds were produced by loss of N_2 [2-5]. The structure of (**1**) and (**2**) were confirmed by ^{1}H-NMR, ^{13}C-NMR, FT-IR and mass spectral data.



1 **2**

Scheme 2

References:

[1] Khalafy, J.; Ghezelbash, Z. D.; Mahmoody, M. *Chemistry of Heterocyclic Compounds*. **2010**. inpress.
[2] Molla Ebrahimlo, A. R.; Khalafy, J. *Arkivoc.* **2008**, *xiii*, 65.
[3] Molla Ebrahimlo, A. R.; Khalafy, J.; Prager, R. H. *Aust. J. Chem.* **2009**, *62*, 126.
[4] Khalafy, J.; Prager, R. H.; Smith, J. A. *J. Chem. Res (M).* **1999**, 518.
[5] Molla Ebrahimlo, A. R.; Khalafy, J.; Poursattar Marjani, A.; Prager, R. H. *Arkivoc* **2009**, *xii*, 17.

Modification and characterization of nanoclay with cationic surfactant

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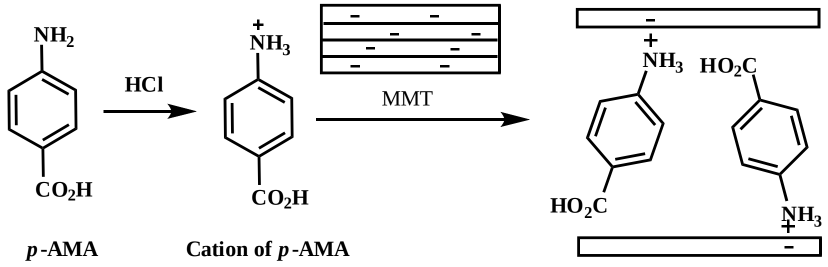
Montmorillonites (MMT) have attracted significant attention because of their high cation exchange and swelling capacity, high surface areas and consequential strong adsorption capacities [1]. Nature MMT consisted of layered silicates carrying negative charges that formed ionic bonds with metal cations in the intergallery of the layered silicates. These silicates also contained dangling hydroxyl end groups on their surfaces [2]. The existence of ionic bonds and the ability of forming hydrogen-bonding with water made MMT highly hydrophilic, and thus pure MMT is difficult to be mixed with hydrophobic polymeric materials. To improve the affinity of MMT toward organic materials, it is necessary to modify MMT by replacing the metal cations in the intergallery of silicates with various organic cation molecules. The most popular surface treatment agent or intercalant for MMT is quaternary ammonium salts, which have a cation-exchange capacity with the inorganic cations on the silicate surface [3]. In this work, MMT was modified with the ammonium salt of *p*-amino benzoic acid. The amine end group of swelling agent was changed into cations to interact chemically with the negatively charged silicate layers upon heating. The nanostructure of the OMMT was analyzed by X-ray diffraction, fourier transform infrared, dispersibility measurement and transmission electron microscopy. The thermal properties were characterized by thermogravimetric analysis. The results show that the surfactants have been intercalated into the MMT layers successfully.



***p*-AMA**   **Cation of *p*-AMA**   ***p*-ABA - MMT**

References:

[1] de Paiva, L.B.; Morales, A. r.; Diaz, F. R. *Appl. Clay Sci*. **2008**, 42, 8.
[2] Tyan, H. L.; Leu, C. M.; Wei, K. H. *Mater. Sci.* **2001**, *13*, 222.
[3] Zhou, L.; Chen, H.; Jiang, X.; Lu, Fang.; Zhou, Y.; Yin, W.; Ji, X. *J. Colloid Interface Sci.* **2009**, *332*, 16.

Synthesis of primary *O*-thiocarbamates by silica sulfuric acid as effective catalyst in various solvents

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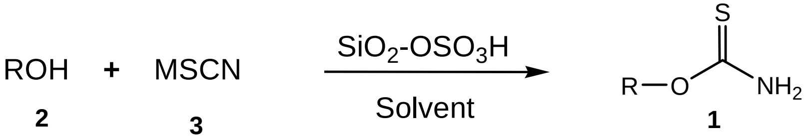
Thiocarbamates have received much attention due to their interesting technological, biological and synthetic applications. Their formation employs harsh reaction conditions such as the use of strong bases, high temperatures, and long reaction times. In addition, modifications have been reported to use thiophosgene, chlorothioformates, and isothiocyanates, which are costly and toxic reagents [1]. Thus, we were prompted to embark on improved procedures. Recently, we reported a highly efficient SSA promoted solid state synthesis of alkyl and aryl carbamates and thiocarbamates, which utilizes non-toxic reagents under mild conditions[2].

Now, in this work, a simple and efficient methodology approach to prepare primary *O*-thiocarbamates **1** has been introduced from compounds **2**, and salts of thiocyanate **3** in the presence of silica sulfuric acid in solvents of chloroform, dichloromethane and 1,2-dichloroethylene, Scheme 1. However, to the best of our knowledge there has been no report in literature on synthesis of primary thiocarbamates using solid acids (such as SSA) under solution condition.



References:

[1] Walter, W.; Bode, K.-D. *Angew. Chem. Int. Ed. Eng*. **1967**, *6* , 281-293.
[2] a) Modarresi-Alam, A. R.; Najafi, P.; Rostamizadeh, M.; Keykha, H.; Bijanzadeh, H.-R.; Kleinpeter, E. *J. Org. Chem.* **2007**, *72*, 2208-2211. b) Modarresi-Alam, A. R.: Dindarloo Inaloo, I., *International Symposium on Catalysis and Find Chemicals (C&FC 2009)*, December 13-17, **2009**, Korea University.

Preparation, characterization and thermal behavior of polymers containing *α,β*-epoxysilanes

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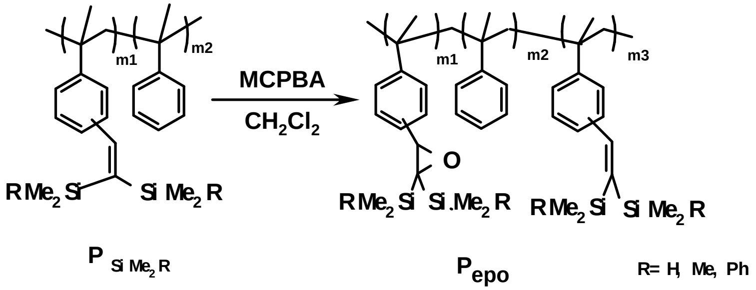
For simplicity, versatility, controlled architecture, and even distribution and ready accessibility of functional groups, functional polymers are generally better prepared by modification of preexisting polymers, rather than by copolymerization with specialty monomers. We have been studying the synthesis of organosilicon containing polymers, which have new structures [1,2].

Epoxidation of vinylsilanes furnish α,β-epoxysilanes, a class of compounds of considerable interest to the organic chemists [3]. The presence of trialkyl group provides regioselective control in the opening of epoxide by variety of nucleophiles. The polymers **P$_{SiMe2R}$** which were obtained via Peterson olefination reaction of $(RMe_2Si)_3CLi$ (R = H, Me and Ph) and formylated poly(α-methylstyrene) were reacted with MCPBA in CH_2Cl_2 at room temperature for 28 h and gave the polymers bearing epoxybis(silanes) groups. In order to examine the thermal behaviors of the polymers, thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) were used.



References:

[1] Safa, K.D.; Hassanpour, A.; Tofangdarzadeh, S. *J. Organomet. Chem.* **2008**, *693*, 3622.
[2] Safa, K.D.; Hassanpour, A.; Tofangdarzadeh, S. *Synth. commun.* **2009**, *39*, 1.
[3] Srikanth, A.; Nagendrappa, G.; Chandrasekaran, S. *Tetrahedron.* **2003**, *59*, 7761.

Solvent free ortho-formylation of some phenol derivatives under microwave irradiation

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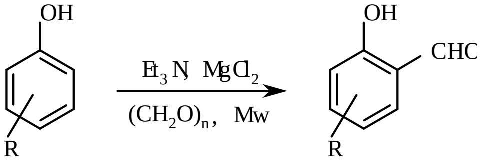
One of the potentially most useful and versatile functional groups to be introduced is the formyl group. Formyl compounds owe their usefulness as synthetic intermediates to the presence of the polarizable carbon-oxygen double bond that governs their chemical reactivity. The polarizability of the formyl carbonyl group is reflected in hard donor oxygen (hard base) and a fairly hard acceptor carbon (hard acid) [1].

However, Formate and the formyl groups have significant importance in tissue metabolism. Formylation of aromatic compounds is an important reaction in synthetic organic chemistry and numerous methods are available [2]. Recently, there have been a number of reviews discussing reactions of dialdehydes in organic synthesis [3], carbonylation using carbon monoxide, and synthesis of carbonyl compounds using a variety of coupling reaction [4, 5].

In this research, phenols are mono-formylated using a mixture of paraformaldehyde, $MgCl_2$ and Et_3N under microwave irradiation. This method gives improved yield and fewer by-products and renders the use of solvent superfluous. The structure of products have confirmed with spectroscopic data such as; IR, ^{1}H NMR and Ms spectra.



R=H, Me, t-Bu, OMe

References:

[1] Olah, G. A.; Ohannasian, L.; Arvanaghi, M. *Chem. Rev*. **1987**, *87*, 671.
[2] Akselsen, Ø. W.; Skattebøl, L.; Hansen, T. V. *Tetrahedron Lett*. **2009**, *50*, 6339.
[3] Botteahi, C.; Soccolini, F. *Synthesis* **1985**, 592.
[4] Narayana, C.; Periasamy, M. *Synthesis* **1985**, 253.
[5] Martin, S. F. *Synthesis* **1979**, 633.

Synthesis of copolymers of maleic anhydride and their reaction with 9-antracene methanol.

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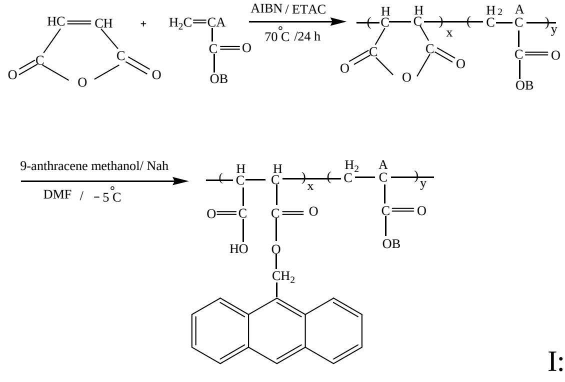
In recent years many researchers have been interested in synthesis and characterization of copolymerizations of maleic anhydride (MAN) [1].

MAN is an exellent monomer which can provide reactive anhydrid or carboxylic groups with nucleophilic molecules [2].

Because of the extremely low tendency of MAN to homopolymerize four copolymers of MAN with methyl methacrylate (MMA), ethyl methacrylate (EMA), methyl acrylate (MA) and ethyl acrylate (EA) in 1:1 ratios were synthesized by free radical polymerization method in ethyl acetate (ETAC) solution at $70\underline{+}1^{\circ}$C using azobis (izobutyronitrile) (AIBN) as initator to give the polymer in good yields [3,4]. Then, copolymers of MAN have been modified by incorporation of highly sterically hindered demanding 9-antracene methanol throught the MAN motieties. The structure of all the resulted polymers was characterized and confirmed by FT-IR, ^{1}HNMR spectroscopic techniques. It was found that these polymers with 9-antracene methanol groups in polymer side chains leads to a different in the rigidity and glass transition temprature of polymer as shown by dynamic mechanical thermal analysis (DMTA). The results show that, with the incorporation of 9-antracene methanol group in the polymers side chains a series of novel modified polymers can be obtained.



I: A=H, CH_3
II: B= CH_3, C_2H_5

References:

[1] Wang, K.; Huang, W.; Xia, P.; Gao,Ch.; Yan, D. *Reactive & Func*
[2] Zhou, J.; Wang, C.; Chen, T.; Yu, H.; Yung, Q. *Polymer*, **2005**, 46, 11157.
[3] Nieuwhof, R. P.; Marcelis, A.T.M.; Sudholter, E.J.R. *Macromolecules*, **1999**, 32, 1398.
[4] Boztug, A.;Basan, S. *Journal of Molecular structure*, **2007**, 830, 1.

Synthesis and NMR study of some pyrimidine-pyrrolidone couples

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Pyrrole and pyrimidine rings are among the most prevalent heterocyclic nucleuses, which are present as the basic cores in many natural products, potent pharmaceutical compounds, and various kinds of functional materials [1-3]. Despite numerous diverse approaches so far developed towards the synthesis of pyrroles and pyrimidines, it is still challenging to prepare polysubstituted pyrroles and pyrimidines from readily available building blocks [4]. This communication explains a two step approach that was adopted for efficient synthesis of some novel Dialkyl 1-(4,6-dimethoxypyrimidine-2-yl)-2,5-dihydro-3-alkoxyprrole-4,5-dicarbixylates. To the best of our knowledge these products represent an unprecedented class of pyrimidine-pyrrole coupling compounds. The structures of these products were precisely elucidated by their NMR as well as Mass spectral data. The ^{1}H NMR spectra of some products have shown a restricted rotation about the C-N bond between the two nucleuses. A discussion about the possible origins of the restricted rotation in these molecules with respect to their associate barrier energy will be presented in our communication. Several derivatives of the title compounds were synthesized by using different derivatives of the starting materials to show the scope of the present route. Because of the unique structural framework of the herein reported products we anticipate that they will receive more attention from biologists and medicinal chemists for bioactivity screenings.

References:

[1] G. Aridoss, S. Balasubramanian, P. Parthiban, S. Kabilan, *Eur. J. Med. Chem.* 42 (**2007**) 851.
[2] H. Hoffmann, T. Lindel, *Synthesis* (**2003**) 1753.
[3] W. Zhao, E. M. Carreira, *Chem. Eur. J.* 12 (**2006**) 7254.
[4] I. Yavari, A. R. Alborzi, B. Mohtat, *Dyes and Pigments* 68 (**2006**) 85.

Hydrazino acetamides: An Ab initio and NBO study

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The hydrogen bond was discovered almost 100 years ago, but still is a topic of vital scientific research [1]. The reason for this long-lasting interest lies in the eminent importance of hydrogen bonds for the structure, function, and dynamics of a vast number of chemical systems, which range from inorganic to biological chemistry [2].

Replacing the C^{β} atoms in the β-amino acid constituents of β-peptides by nitrogen atoms leads to hydrazino peptides [3]. First attempts of peptide modification by α-hydrazino acids providing bioactive peptides have been done in the early 1970s [4]. Now, peptide with single α-hydrazino amino acids are accessible and even a solid phase synthesis for hydrazino peptides by N-electrophilic amination has been elaborated [5].

Thus, a systematic examination of the possibilities of secondary structure formation in hydrazine peptides and its peculiarities could be useful. For this purpose, are employed quantum chemical and molecular mechanics methods which have provided an overview on the conformational aspects in the parent β-peptides [6].

The goal of the present study is to investigate the NBO analysis of hydrogen bonded systems, the charge transfer between the lone pairs of proton acceptor and anti bonds of proton donor and better understanding of the H-bond interaction in a more general context.

References:

[1] Pimentel, G. C.; McClellan, A. L. *the Hydrogen Bond*, Freeman, San Francisco, **1960**.
[2] Richardson, J. S. *Adv. Protein Chem.* **1981**, *34*, 167.
[3] Creighton, T. E. *Proteins: Structures and Molecular Principles*, 2nd ed.; Freeman: New York, **1993**.
[4] Ashkenasy, N.; Horne, W. S.; Ghadiri, M. R. *Small* **2006**, *1*, 99.
[5] Frackenpohl, J.; Arvidsson, P. I.; Schreiber, J. V.; Seebach, D. *Chem. Bio. Chem.* **2001**, *2*, 445.
[6] Ball, P. *Designing the Molecular World*; Princeton University Press: Princeton, **1994**.

Catalyst-free synthesis of 4,4-(arylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ols) unther ultrasonic irradiation

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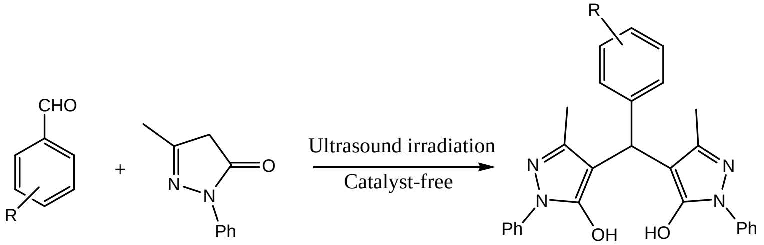
‘‘Sonochemistry”, is a new trend in organic chemistry, offering a versatile and facile pathway for a large variety of syntheses [1]. The temperature of hot spots caused by the collapse of acoustic caves is generally as high as more than several hundred degrees, this energy can be transferred to the organic molecules and absorbed by them to dramatically raise their intrinsic energy [2]. Due to the thermal effect of ultrasound wave, therefore, much larger amount of molecules can meet the demand for the active energy in a given reaction, leading to the apparent improvement of the reaction efficiency with increased rates and reduced reaction time [2].

Pyrazoles are an important class of bio-active drug targets in the pharmaceutical industry, as thy are core structure of numerous biologically active compounds [3,4]. Numerous methods for the preparation of 4,4′-(arylmethylene) bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols) from aromatic aldehydes and 5-methel-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one have been reported, however, the majority suffer from at least one of the the following disadvantages: use of expensive reagents, tedious work up procedure, longer reaction time, harsh reactions conditions .

In this work we introduced a new method for the preparation of 4,4′-(arylmethylene) bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols), by the reaction of aldehyde and 5-methel-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one unther ultrasound irradiation catalyst-free conditions.



References:

[1] Mason, T.J.;*Ultrason.sonochem*. **2007**, *14*, 476-483

[2] Zang, H.; Zhang, Y.; Zang, y.; Cheng, B.-W. *Ultraso. Sonochem*. **2010** .*17*, 495-499

[3] Mcdonald, E.; Jone, K.; Brough, P. A.; Drysdale, M.; Wrkman, P. *Curr. Top. Med. Chem*. **2006**, *6*, 116.

[4] Elguero, J.;Goya, P.; Jagerovic, N.; Silva, A. *Targets Heterocycl.Syst*. **2002**, *6*, 62.

Silica bonded acidic ionic liquid: A recyclable catalyst for the synthesis of trisubstituted and 1,2,4,5-tetrasubstituted imidazoles under solvent-free conditions

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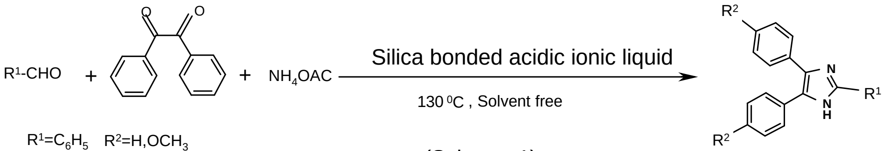
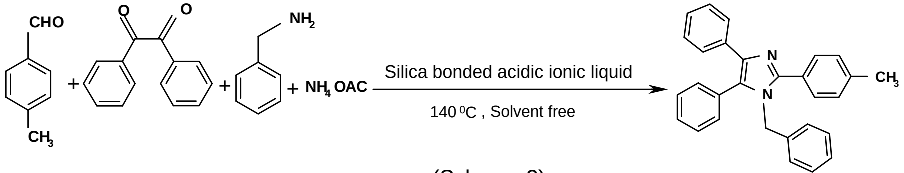
Multi-component reactions (MCRs) have proved to be remarkably successful in generating products in a single synthetic operation [1]. One of such reaction is synthetic route to imidazole ring. The tetrasubstituted imidazole is a core section in many biological systems such as Losartan and Olmesartan [2].

Silica bonded acidic ionic liquid is an efficient and reusable catalyst for the synthesis of 2,4,5-trisubstituted imidazoles via the reaction of benzil, an aromatic aldehyde and ammonium acetate under solvent-free conditions (scheme 1).also silica bonded acidic ionic liquid as an efficient and reusable catalyst for the synthesis of 1,2,4,5-tetrasubstituted imidazoles. These reactions were accomplished via four components benzil, aromatic aldehydes, amines and ammonium acetate under solvent-free conditions (scheme 2).



(Scheme 1)



(Scheme 2)

References

[1] Eilbracht, P.; Schimdt, A. *Chem. Rev*.**1999**, *99*, 3329.
[2] Koike, H.; Konse, T.; Sada, T.; Ikeda, T.; Hyogo, A.; Hinman, D.; Saito, Yanagisawa, H.; *Ann. Rep. Sankyo Res. Lab.* **2005**, *1*, 55.

Synthesis and characterization of aziridine derivatives in the presence of phase transfer catalyst (PTC)

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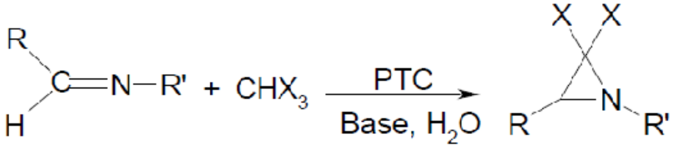
Three-membered nitrogen heterocycles are highly reactive molecules, in part due to ring strain. As a consequence of their high reactivity, these small heterocycles play an important role in organic chemistry and as intermediates in synthesis of both organicpharmaceutical and natural product intermediates [1]. Among three-membered heterocycles, aziridines constitute a particularly versatile class of molecule, and as discussed in recent book [2,3], both physical properties and chemical reactions of aziridines have been the subject of numerous theoretical and experimental investigations which have proved invaluable in understanding the mechanism of drug action of pharmaceuticals containing aziridine warheads for instance, the antitumor drug Aziridines, are constituents of several molecules presenting biological activity, for example, azinomycins and mytomycins [4,5].

It is therefore of great importance to develop and use synthetic methodologies for preparation of these compounds. Here we decide to report the synthesis of various aziridine derivatives through the reaction of imines compounds and chloroform in the presence a base in the presence of phase transfer catalyst (PTC).



References:

[1] Sweeney, J. B. *Chem. Soc. Rev*. **2002**, *31*, 247.
[2] Dahanukar, V. H.; Zavialov, L. A. *Curr. Opin. Drug Discov. Dev*. **2002**, *5*, 918.
[3] Yudin (Ed.), A.K. Wiley-VCH, Weinheim, **2006** p. 494.
[4] Sapse, A. M.; Rothchild, R.; Jain, D. C.; Hernandez, G. A. *J. Mol. Model*. **2007**, *13*, 1169.
[5] Khlebnikov, A. F.; Novikov, M. S.; Kostikov, R. R. *Russ. Chem. Rev*. **2005**, *74*, 171.

Preparation of photodecolorization of Dye pollutant Acid Red 52 in water by using Fenton reagent+Zno/Bentonite+UV processes

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In this paper Mineralization and decolourization of colored textile wastewater was investigated by using Fenton Reagent +Zno/Bentonite+UVprocesses. Acid red 52 (AR52) was used as an dye model. The effect of decolourization parameters such as iron (III) concentration, Zno/Bentonite concentration, temperature of reaction, initial concentration of the dye and H_2O_2 and initial pH of the dye solution on the degradation efficiency of the process were investigated [1]. The maximum iron (III) concentration was set to maximum allowable discharge level to environment [2-3]. The results indicated that by using 38ppm of H_2O_2 and 100ppm of the catalyst at pH 5, about 97% total Acid red 52 could be removed after 100 min in a batch photo-reactor. The rate of decolourization reaction decreased by increasing dye concentration and in the presence of the hydrogen peroxide. Therfor by a comparative study, decolourization of AR52 was also performed by photocatalysis that is comprised with the hydrogen peroxide and combined Photo-Fenton – photocatalysis processes [4-5]. Moreover, the decolorization of Acid red 52 was observed to be more difficult under the same operating conditions. The structure, surface and morphology properties of the structure Zno on Bentonite have been investigated by XRD, SEM techniques.From kinetic view the reaction was first order and study of reaction rate was carried out with the use of first order kinetic equation. Acceptable results were gained in this examination [6]. The results showed that the Photo-Fenton process had the decolourization capability of colored wastewater at different dye concentrations and in the presence of the hydrogen peroxide.

References:

[1] Meric¸ S.; Kaptan, D.; Olmez, T. *Chemosphere* **2004**, 54, 435.
[2] Kang ,S. F.; Liao, C. H.;Chen, M. C. *Chemosphere* **2002**, 46, 923.
[3] Arslan, I.; Balcioglu, IA.; Bahnemann, DW. *Dyes and Pigments* **2000**, 47, 207.
[4] Feng, J.; Hu, X.; Yue, P. L.; Zhu, H. Y.; Lu, GQ. *Water Research* **2003**, 37, 3776.
[5] Neamtu, M.; Yediler, A.; Siminiceanu, I.; Kettrup, A. *Journal of Photochemistry and Photobiology:A Chemistry* **2001**, 141, 247.
[6] Park, H.; Choi, W. *Journal of Photochemistry and Photobiology A: Chemistry***, 2003,** 159, 24.

Stereoselective synthesis of novel spiropyrrolidineoxindoles through [3+2] cycloaddition reaction of azomethine ylides

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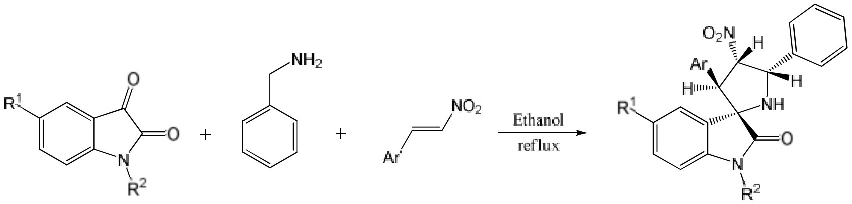
The [3+2] cycloaddition of azomethine ylide with electron-deficient conjugated double bonds is one of the important methods for the construction of heterocyclic five-membered rings, for example, pyrrolidines, which are used as important building blocks in the synthesis of natural products as well as pharmaceuticals [1].

Functionalised pyrrolidine, pyrrolizidines and oxindole alkaloids constitute classes of compounds with significant biological activity and the spiro oxindole ring system is a structural feature found in a variety of oxindole alkaloids [2]. Of particular interest, spiropyrrolidinyloxindole ring systems are also found in a number of alkaloids like horsfiline, spirotryprostatine A and B, elacomine, etc [3].

We wish to report the facile synthesis of novel spiropyrrolidineoxindoles through regio and stereoselective [3+2] cycloaddition reaction of azomethine ylides prepared from isatin derivatives and benzylamine with derivatives of β- nitrostyrene as dipolarophiles.



References:

[1] Hazra, A.; Paira, P.; Sahu, K. B.; Naskar, S.; Saha, P.; Paira, R.; Mondal, S.; Maity, A.; Luger, P.;
Weber, M.; Mondal, N. B.; Banerjee, S. *Tetrahedron Lett.* **2010**, *51,* 1585.
[2] Jayashankaran, J.; Manian, R. D. R. S.; Raghunathan, R. *Tetrahedron Lett*. **2004**, *45,* 7303.
[3] Subramaiyan, G.; Raghunathan, R.; Nethaji, M. *Tetrahedron*. **2002,** *58*, 9075.

Efficient synthesis of 1,3,5-triaryl-2-pyrazolines by Melamine-formaldehyde resin supported acids under solvent-free condition

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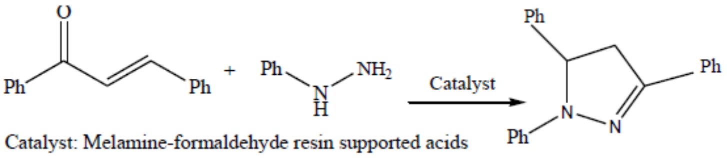
Pyrazoline derivatives have been found to possess a broad spectrum of biological activities [1]. Among various pyrazoline derivatives, 1,3,5-triaryl-2-pyrazolines seem to be the most frequently studied pyrazoline type compound. A variety of methods have been reported for the preparation of this class of compound [2]. However, in spite af their potential utility, some of reported methods suffer from drawbacks such as long reaction times, cumbersome product isolation procedures and environmental concerns.

The use of solid supports as reaction media in organic synthesis is increasingly widespread due to improved efficiency of many surface bound reagents. Further, with the advent of microwave dielectric heating, the rate of several reactions can be promoted to afford faster and cleaner conversion [3].

One of the most commonly used methods for preparation of 1,3,5-triaryl-2-pyrazolines is the cyclization of chalcones with phenylhydrazine.

The purpose of this work was to examine the optimal condition for reaction of phenylhydrazine with different chalcones using Melamine-formaldehyde resin supported acid as a catalyst under solvent –free condition. The stability and cheapness, low toxicity, heterogeneous nature of the reactions, high yields of the products and short reaction time are notable advantages of this method.



References:

[1] Turan-Zitouni, G.; Chevallet, P.; Kilic, F. S; Erol, K. *Eur. j. Med. Chem*, **2000**, *35*, 635.
[2] Kidwai, M.; Kukreja, S,; Thakura, R. *Lett. Org. Chem*. **2006**, *3*, 135.
[3] Tanaka, K.; Toda, F. *Chem Rev*, **2000**, *100*, 1025.

One-pot synthesis of pyrazoles through a tandem coupling-cyclization sequence

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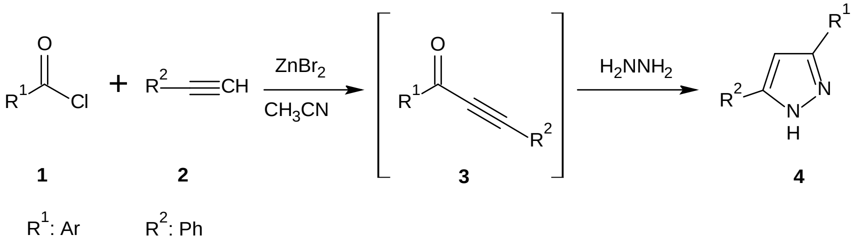
Pyrazoles and their derivatives, which are a large class of N-containing heterocycles, possess important biological and pharmaceutical activities, and are also useful synthetic building blocks and metal ligands in organic chemistry [1].

In continuation of our studies on the development of novel routes for synthesis of heterocycles via palladium-catalyzed heteroannulation [2], we report an efficient one-pot procedure for the synthesis of pyrazoles from acid chlorides, phenylacetylen and hydrazine. Ynones **3** were synthesized in situ from acid chlorides **1** and phenylacetylen **2** in the presence of $ZnBr_2$, and were then converted to pyrazoles **4** by reaction with hydrazine. The structures of the products were deduced from their elemental analyses and spectroscopic data.



References:

[1] Singh, P.; Paul, K.; Holzer, W. *Bioorg. Med. Chem.* **2006**, *14*, 5061.

[2] Heravi, M. M.; Kivanlooa, A.; Rahimizadeh, A.; Bakavoli, M.; Ghassemzadeh. M. *J. Heterocyclic Chem.* **2007,** *44*, 1.

Synthesis of quinolines derivatives *via* Friedlander annulation

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As a privileged fragment, quinoline is a ubiquitous subunit in many quinoline-containing natural products with remarkable biological activities [1]. Members of this family have wide applications in medicinal chemistry, being used as antimalarial, antiinflammatory, antiasthmatic, antibacterial, antihypertensive, and tyrosine kinase inhibiting agents. In addition, quinolines are valuable synthons, used for the preparation of nano- and mesostructures with enhanced electronic and photonic properties [2]. Though some methods such as the Skraup, Doebner–von Miller, and Combes reactions are available, the protocol reported by Friedlander is one of the most simple and straightforward methods for the synthesis of polysubstituted uinolines. The Friedlander annulation, that is, a condensation followed by a cyclodehydration between 2-aminoaryl ketones and amethylene ketones, is catalyzed by both acids and bases. Brounsted acids like sulfamic acid, hydrochloric acid, sulfuric acid, *p*-toluene sulfonic acid and phosphoric acid were widely used as catalysts. Recently, Lewis acids such as $FeCl_3$, $Mg(ClO_4)_2$, $ZnCl_2$, $SnCl_2$, $Bi(OTf)_3$, $Sc(OTf)_3$, silver phosphotungstate, sodium fluoride, and $NaAuCl_4,2H_2O$ have been reported to be effective for the synthesis of quinolines. However, many of these procedures also suffered from harsh reaction conditions, low yields, difficulties in work-up and relatively expensive reagents. Therefore the development of a simple, eco-benign, low cost protocol is still desirable. In recent years the optimal use of material and energy are important factors for environmental protection, so more attention has been paid to the application of inorganic acidic salts in organic synthesis. This techniques has reduced pollution, low cost, process simplicity and easier workup.Herein, Boron sulfonic acid used, as a catalyst for Friedlander quinoline synthesist (Fig 1).

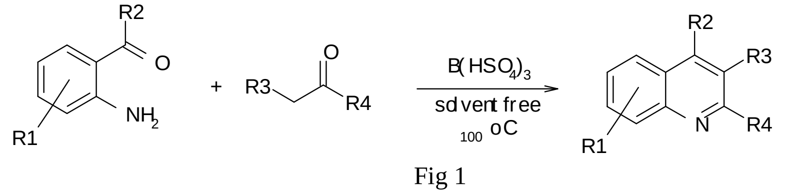

Fig 1

$B(HSO_4)_3$ was easily prepared according to a procedure reported elsewhere [3], by addition of chlorosulfonic acid to boric acid under N_2 atmosphere at room temperature.

References:

[1] (*a*) Y. L. Chen, K. C. Fang, J. Y. Sheu, S. L. Hsu and C. C. Tzeng, *J. Med. Chem.*, **2001**, *44*, 2374; (*b*) G. Roma, M. D. Braccio, G. Grossi and M. Chia, *Eur. J. Med. Chem.*, **2000**, *35*, 1021

[2] (*a*) A.K. Aggarwal and S. A. Jenekhe, *Macromolecules*, **1991**, *24*, 6806; (*b*) S. A. Jenekhe, L. Lu and M. M. Alam, *Macromolecules*, **2001**, *34*, 7315.

[3] A. R. Kiasat and M. F. Mehrjardi, *J. Braz. Chem. Soc.*, **2008**, *19*, 1595.

Poly (ethylene) glycol as a green and reusable solvent in the synthesis of some Indazoles as opaque drugs

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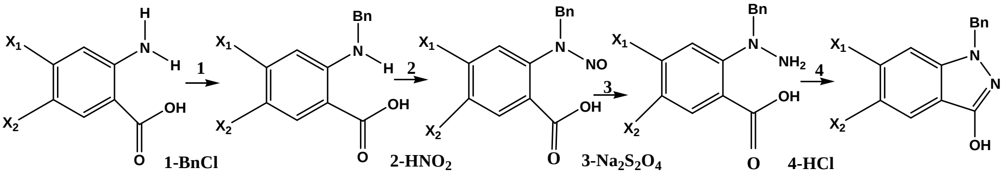
In pharmaceutical approach, Opaque drugs are used to absorb X-ray to help medicines to see internal organs. The most popular opaque drug is barium sulfate but its problem is its very high osmolality. The second and new vast family of opaque compounds is halide derivatives of amino benzoic acids like amidotrizoic acid and Iobenzamic acid. Polar functional group (-COOH) makes molecule polar and increases its solubility in water. Indeed, it modified its lipophilicity and decreases its half-life and makes it easy to defecate. On contrast, heavy halogen (usually iodine) increases its lipophilicity by increasing its half-life [1].

As we reported earlier, this duality (hydrophile-lipophile) might theoretically be explained by dipole moment term. By using semi-empirical AM1 method [2], we had calculated the dipole moment of Amidotrizoic acid and Iobenzamic acid and concluded that to have a good effect, our opaque reagents must have the same interval amounts. Later we have theoretically studied some Anthranilic acid derivatives and calculated their dipole moments and introduced them as new alternative candidate as opaque compounds. There, we declared that the facile methods for their preparation and the simple possibility of changing the number of iodine atoms were the advantages of our compounds [3]. In recent work we would like to extend our procedure by using PEG as solvent which provides green conditions with better total yield.



References:

[1] Catzung, Pharmakology, Translated by N. Ghotbi and E. Esfandiary ; Arjomand Pob., **1374**.
[2] A. D. Daniels, J. M. Millam, and G. E. Scueria; *J. Chem. Phys.*, **1997**, *107*, 425.
[3] A. Amoozadeh, *et al.* 6th Iranian Biophysical Chemistry Conference, 7-9 September **2004**, Damghan University of Basic Sciences P. 53.

Brønsted acidic ionic liquid [BMIM]HSO$_4$: a green catalyst and recyclable medium for the synthesis of quinolones

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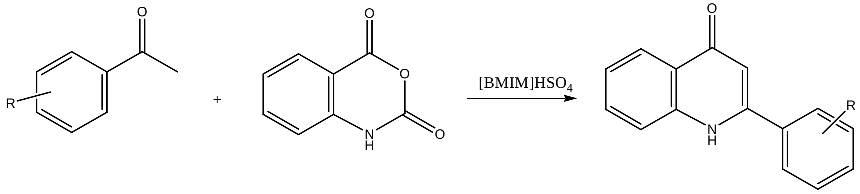
Quinolone derivatives were initially discovered as bacterial DNA gyrase inhibitors, and thus, developed as antibacterial agents [1]. Recently, DNA topoisomerase II has emerged as the pharmacological target for this class of quinolone compounds [2]. Also, 2-phenyl-4-quinolones were identified as novel antimitotic agents [3]. Previously reported quinolone synthesis typically employed forcing conditions of elevated temperature and/or strong bases and explicitly employed carbonyl condensation to yield the heterocycle [4-5].

Herein, for the first time, we wish to report an efficient, facile and solvent free procedure for the synthesis of quinolones by the reaction of isatoicanhydride and acetophenon derivatives using 1-buthyl-3-methlylimidazolium hydrogen sulfate ([BMIM]HSO$_4$) as ionic liquid. An advantage of this ionic liquid is that it is recyclable as reaction medium. Simple work up, solvent free, completely compatible with environment and descend reaction time for a few minute with improved yield as compared to reported method are other advantages of this procedure.



References:

[1] Goss, W. A.; Cook, T. M.; Corcoran, J. W., Hahn, F. E. *Antibiotics*; Springer: New York, **1975**; Vol. *3*, p 174.

[2] Tomita, K.; Tsuzuki, Y.; Shibamori, K.; Tashima, M.; Kajikawa, F.; Sato, Y.; Kashimoto, S.; Hino, K. *J. Med. Chem.* **2002**, *45*, 5564.

[3] Li, L.; Wang, H. K.; Kuo, S. C.; Wu, T. S.; Mauger, A.; Lin, C. M.; Hamel, E.; Lee, K. H. *J. Med. Chem.* **1994**, *37*, 3400.

[4] Li, L.; Wang, H. K.; Kuo, S. C.; Wu, T. S.; Lednicer, D.; Lin, C. M.; Hamel, E.; Lee, K. H. *J. Med. Chem.* **1994**, *37*, 1126.

[5] Kuo, S. C.; Lee, H. Z.; Juang, J. P.; Lin, Y. T.; Wu, T. S.; Chang, J. J.; Lendicer, D.; Paull, K. D.; Lin, C. M.; Hamel, E.; Lee, K. H. *J. Med. Chem.* **1993**, *36*, 1149.

Oxidation of benzoins to benzils using manganez(Π) schiff base complexes and H_2O_2

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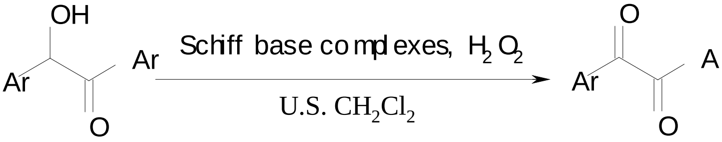
Benzils have received a great deal of attention because of their practical applications, i.e. as photosensitive agents and synthetic agents in organic and pharmaceutical chemistry [1]. Oxidation of benzoin derivatives with an oxidizing agent is a common method for the preparation of benzils. There are many reagents for this oxidation such as nitric acid [2], fehling's solution [2], thallium nitrate [3], clayfen [4], ammonium nitrate-copper acetate [5], iron (Ш) chloride [6], bismuth (Ш) nitrate-copper (Π) acetate [7], ferric nitrate [8], silica-supported manganese dioxide [9], alumina or silica gel [10], commercial alumina [11].

Oxidation of benzoins derivatives with an oxidizing agent is a common method for the preparation of benzils. Although a large number of reagent are known in the literature for such transformation the development of newer reagent oxidation method to permit better selectivity and with easy wok-up procedure continues to receive attention.

We report herein a simple and convenint procedure for the synthesis of a variety of benzils from the corresponding benzoins with manganez (Π) Schiff base complexes and H_2O_2 under ultrasound irradiation.



Referencecs:

[1] Matsushita Electric Industrial Co.Ltd., *Jpn.Kokai Tokkyo Koho,* 8198203, **1981**(Chem. ABSTRC.,**1981**,95,1881163 v).
[2]. J. S. Buck and S. S. Jenkins, *J. Am. Chem. Soc.,*1929, **51**, 2163 and references therein.
[3]. (a) A. Mckillop, B. P.Swann and E. C. Taylor, *Tetrahedron Lett.,* 1970, 5281; (b) A. Mckillop, B. P. Swann and M. E. Ford, *J. Am. Chem. Soc.,* 1973, **95**, 3641.
[4]. M. Bessermann, A. Cornelis and P. Laszlo, *C. R. Acad. Sci. Ser. C,* 1984, **299**, 427.
[5]. M. Weiss and M. Appel, *J. Am. Chem. Soc.,* 1948, **70**, 3666.
[6]. Y. M. Zhou, X. R. Ye and X. Q. Xin, *Synth. Commun.,* 1999, **29**, 2229.
[7]. S. A. Tymonko, B. A. Nattier and R. S. Mohan, *Tetrahedron Lett.,* 1999, **40**, 7657.
[8]. A. M. Paul, A. C. Khandekar, M. A. Shenoy, *Synth. Commun.,* 2003, **33**, 2581.
[9]. Khandekar, A. M. Paul, B. M. Khadilkar, *Synth. Commun.,* 2002, **32,** 2931.
[10]. N. Noroozi-pesyan, A. H. Dabbagh, *Molecules*, 2005, **10**, 1364.
[11]. K. Skobridis, V. Theodorou, E. Weber, *www. arkat-usa. Org.,* 2006, **13**, 102.

Synthesis and characterization of new polyamides from 5-(2-(6-methyl pyridine-2-yl)-1,3-dioxoisoidoline-6-carboxamido) isophthalic acid as a novel monomer

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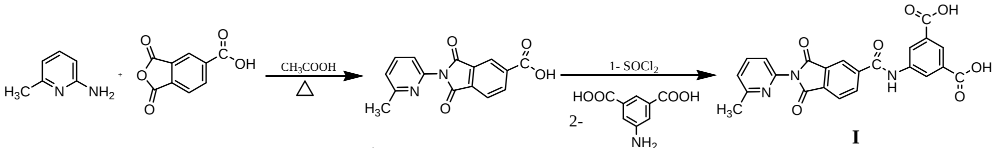
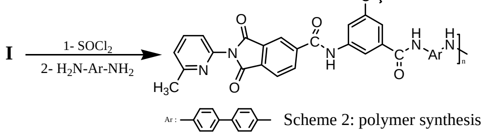
Wholly aromatic polyamides exhibit a number of useful properties such as high thermal stability, chemical resistance, and low flammability, and they have excellent mechanical properties as fibers [1,2]. One of problem with high temperature polymers especially rigid polyamides is their poor processability caused by low solubility in organic solvents and high melting of softening temperatures. One approach to improve the processability without changing their outstanding properties is to introduce a long and polar group pendent at the polymer backbone [3,4]. Recently, polyamides containing pyridine ring, have been synthesized. It has been shown that the interaction of pyridine rings in the polymers usually enhances their thermal stability, solubility, and adhesion to metal [5,6].

In this research a novel diacid monomer which includes pyridine ring as a pendent group has been synthesized (scheme 1), and then the monomer has been chlorinated and polymerized by different diamines (scheme 2), with excellent yields (80%). Eight Polyamides, which have been synthesized, were characterized by ^{1}HNMR, FT-IR spectroscopy and CHN analysis. The FT-IR spectra of the following polyamide showed characteristic bands of amide group at 3421 cm^{-1} (N-H stretching), and two bands at 1780 and 1725 cm^{-1} corresponding to the cyclic imide groups; a broad band at 1658 cm^{-1} corresponding to amide carbonyl groups; a band at 2924 cm^{-1} corresponding to C-H aliphatic units. The ^{1}HNMR spectra showed two peaks, at 10.70 and 10.74 which confirm presence of amide protons. Inherent viscosity of polyamides is in the range of 0.18 to 0.2 dl/g that show the molecular weighs of them are moderate. Solubility of these polymers are appropriate and good in polar aprotic solvents. The thermal stabilities of these polymers are excellent.



Scheme 1: monomer synthesis



Scheme 2: polymer synthesis

References:

[1] Morgan, P. W. *Chemtech*. **1979**, *9*, 316.
[2] Cassidy P. E. *Thermally stable polymers*. **1980**.
[3] Ferrero, E.; Espeso, F.; Campa, G.; Abajo, J.; Lozano, A.E.; *J. Polym. Sci. part A*, **2002**, *40*, 3711.
[4] Diakoumakos, C.D.; Mikroyannidis, J. *A. Eur.Polym. J*. **1995**, *31*, 761.
[5] Banihashemi, A.; Vakili, M. R. *e-polymer*. **2007**, *008*, 1.
[6] Kuoxi, X.; Peizhi, H.; Lihua, C.*J. Natural Sci*. **2006**, *11*, 602.

Oxidation of some aryl alcohols by a Manganese (III) schiff base complex

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The oxidative conversion of alcohols to the corresponding aldehydes and ketones is one of the important transformations in organic reaction. The obtained carbonyl compounds are applied as basic substances preparation of many organic compounds. Many attempts have led to presentation of various oxidation systems for the oxidation of alcohols. But designing of new catalytic or non-catalytic systems that can develop both environmentally and availability of the oxidant point of view is in demand yet. Among the various oxidants, metallooxoanions such as chromium oxoanions based reagents are widely used in for the oxidation of the variety of compounds including alcohols under aqueous or non- aqueous conditions. Recently Inorganic Schiff base complexes have been used for the catalytic running of various oxidations. Manganese (III) Schiff base complexes also provide a rich series of structural types that can be used as models for the magnetic and structural properties of manganoenzymes [1-7]. In this research a four dentate N_2O_2 Schiff base ligand entitled as bis (2-hydroxyacetophenone)-1,2-propanediimine was synthesized and and then metallated by manganese(II) chloride. The compounds were identified by IR, ^{1}HNMR, and UV-Vis spectra. Then the catalytic activity of this complex was investigated. The results showed good catalytic activity in the oxidation of a variety of alcohols to corresponding carbonyl derivatives in the presence of periodate as mild oxidant. Optimization of some effective parameters such as solvent, axial ligand, amount of oxidant and catalyst and reaction times were performed.

References:

[1] Sakuratani, K.; Togo, H. *Synthesis* **2003**, 21.
[2] Tashiro, A.; Mitsuishi, A.; Irie, R.; Katsuki, T. *Synlett* **, 2003**, 1868.
[3] Zolfigol, M. A.; Shirini, F.; Mohammadpoor-Baltork, I.; Ghorbani-Choghamarani, A.; Hajami, M.; Sedaghat, A. M. *Mendeleev Communications* **2005**, *15*, 113.
[4] Larson, E.; Lah, M.S.; Li, X.; Bonadies, J.A.; Pecoraro, V.L. *Inorg. Chem*. **1992**, *31*, 373.
[5] Dutta, R.L.; Ray, R.K. *J. Indian Chem. Soc*. **1977**, LIV, 1096.
[6] Barker, J. E.; Ren, T. *Tetrahedron Lett*. **2004**, *45*, 4681.
[7] Mirkhani, V.; Tangestaninejad, S.; Moghadam, M.; Mohammadpoor-Baltork, I.; Kargar, H. *J. Mol.Catal . A: Chem*. **2005**, *242*, 251.

Theoretical evaluation of acidity constants of some 1-hydroxy-9,10-anthraquinone derivatives using QSAR/QSPR methods considering the solvent effects

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A clear connection between the macroscopic and microscopic properties of matter can be provided using the fact that, there exist a close relationship between bulk properties of compounds and the molecular structure [1]. One of the main approaches for computing physical and chemical properties is the quantitative structure relationship (QSAR) [2]. This method is mathematical equations relating chemical structure to a wide variety of physical properties. Acid base properties of organic molecules affect their toxicity, chromatographic retention behavior and pharmaceutical properties [3]. Among the organic molecules 9,10-Anthraquinones, as the largest group of naturally occurring quinines, are of importance both in industry and medicine.

In a QSAR study which was done in order to evaluate the acidity constants of some recently synthesized 9,10-anthraquinones in mixture of water/methanol solvent quantum chemical descriptors were calculated in gas phase using ab initio calculations [4]. Then a genetic algorithm based neural network model (GA-NN) was applied for the prediction of the acidity constants. The nonlinear complex relationships between the acidity constants of antheraquinones and their quantum chemical descriptors was found and used to reproduce the acidity constants within relative errors of lower than 2%. Although the method shows a promise for prediction of acidity constant of antheraquinones, the complex relation found between acidity constants and quantum descriptors makes it difficult to have a clear verification on the effects of quantum descriptors on the PH of the system. This might be ascribed to the fact that the quantum descriptors were calculated in gas phase and the effect of solvent on electronic correlation of antheraquinones was ignored.

Herein, we have considered the solvent (water/methanol) effects in *ab initio* calculation of quantum chemical descriptors. The Onsager method was used to solve the wave equation in HF/6-311G* level of theory in solvent, using quassian 98 program. The quantum descriptors, dipole moment, hardness, highest positive local charge and root mean square of the charges are found to be in direct response with acidity constants of antheraquinones. Multiple linear regressions (MLR) principle was used to construct the linear relationship between the aforementioned quantum descriptors obtained in solvent, and the acidity constants. The mathematical relation was used to reproduce the acidity constants within relative errors of less than 4%. The value of the regression coefficient square (R^2) found to be higher than 0.932.

References:

[1] H. Eslami, *Aiche J.* **2001,** 47, 2585.
[2] M. Ravi, A. J. Hopfinger, R. E. Hormann, L. Dinan, *J. chem. Inf. Comput. Sci*. **2001**, 41, 1587.
[3] P. Alines, *J. Planar Chromatogr. Mod. TLC* **1996,** 9, 52.
[4] B. Hemmateenejad, A. M. Safarpour, F. Taghavi, *Journal of molecular Structure* **2003**, 635, 183.

Synthesis of diethyl ether from sub- and supercritical ethanol using homogeneous catalysts

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Supercritical fluids are good alternative for environmentally unsafe organic solvents, because of their tunable physicochemical properties with temperature and pressure. Also they possess a wide range of gas-like to liquid-like properties and can be employed as unique media to overcome poor solubility strength of gases and hindered mass transport in conventional liquids.

Among supercritical fluids, ethanol, offer novel media for both chemical reactions and separations, because it has an accessible critical properties (T c = 241 ◦C, Pc = 6.14MPa) and it is less corrosive and more reactive. Several industrially important reactions such as catalytic etherification have been successfully done in hot alcohols [1-3].

Diethyl ether because of its high volatility and low autoignition temperature is a valuable, chemical and an attractive alternate fuel for motor vehicles. Diethyl ether has been synthesized in sub- and supercritical ethanol in the presence of homogeneous catalysts namely sulfuric acid and p-toluene sulfonic acid in good yields. In the temperature range of (100-300) ^{o}C and pressure of 8 MPa and a reactor volume of 22 mL a 50% yield and 80% selectivity was achieved. The separation of product is easily performed by evaporation at the reactor exit.

The analysis of products was done by GC-FID after extracting the catalyst with the aqueous sodium hydrogen carbonate solution. Some gaseous compounds was produced as a by-product during the reaction that is under investigation.

References

[1] Gray, W.; Smail, F.; Hitzler, M.; Ross, S.; Poliakoff, M. *Am. Chem. Soc*. **1999,** *121*, 10711.
[2] Habenicht, C.; Kam, L.; Wilschut, M.; Antal, M. *Ind. Eng. Chem. Res*, **1995**, *34,* 3784.
[3] Usui, Y.; Wakai, C.; Matubayasi, N.; Nakahara, M. *Chemistry Letters*, **2004**, *33,* 394.

Synthesis of new nanomonocyclic β-lactams

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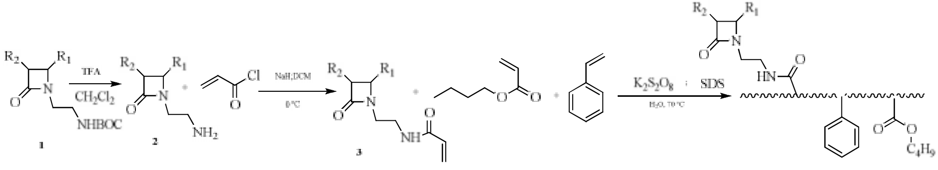
The development of antibiotics for control of pathogenic bacteria has been of pressing need in this era of drug resistant infections [1]. The application of lipophilic agents to combat such infections likewise has limited effectiveness due to uptake and delivery issues resulting from low water solubility and biodistribution[2]. The ability to deliver antibacterial drugs to infections in fatty tissue or on the surface of implanted medical devices, for example, where microbial biofilms often develop, ultimately determines if the infection can be cleared without surgical intervention [3]. New drug delivery vehicles such as liposomes and nanoparticles offer a promising way to improve bioavailability, efficacy, and specificity of pharmaceutical compounds in general. Polyacrylate nanoparticle antibiotics, or nanobiotics, appear to be an effective enhancer of activity for water-insoluble antibiotics. Turos et al reported an easy, one-step preparation of antibiotic-conjugated polyacrylate frameworks in aqueous media and have the ability to incorporate water-insoluble drugs directly onto the polymer framework without the need for post-synthetic modification of the nanoparticles [4-5]. In this paper nanoparticles were prepared in water by emulsion polymerization of an acrylated β-lactam (monomer **3**) analogue pre-dissolved in a 7:3 (w:w) mixture of butyl acrylate and styrene in the presence of sodium dodecyl sulfate (surfactant) and potassium persulfate (radical initiator). To prepare monomer **3**, β-lactam **1** was synthesized from a [2+2] cycloaddition reaction of an imine with a ketene. Then the BOC protecting group was removed by using TFA to obtain β-lactam **2**. Treatment of **2** with acryloyl chloride in the presence of NaH afforded monomer **3**.



References:

1. Zafeiris, S. *Nature* **2004**, 431, 892.
2. Patel, V. R.; Amiji, M. M. *Pharm. Res.* **1996**, 13, 588.
3. Costerton, J. W.; Stewart, P. S.; Greenberg, E. P. *Science* **1999**, 284, 1318.
4.Turos, E.; Reddy, G. S. K.; Greenhalgh, K.; Ramaraju,P.; Abeylath, S. C.; Jang, S.; Dickeyc, S.; Limc, D. V. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 3468
5. Turos, E.; Shim, J. Y.; Wang, Y.; Greenhalgh, K.; Reddy, G. S. K.; Dickey, S.; Lim, D. V. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 5.

Molecular iodine catalyzed efficient and highly rapid synthesis of 3-aminoimidazo [1,2-a] pyridines under solvent free conditions

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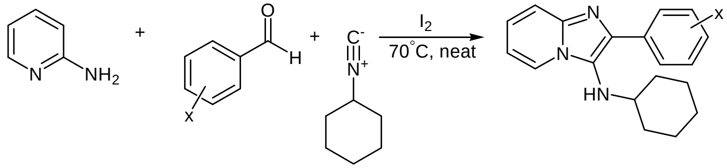
The imidazo[1,2-a] annulated nitrogen heterocycles bearing pyridine, pyrazine and pyrimidine moieties constitute a class of biologically active compounds that are potent antiinflamatory agents, as well as antibacterial agents, inhibitors of gastric acids secretion, and calcium channel blockers [1]. Hence, development of a green, simple, efficient, and general method for the synthesis of these widely used organic compounds, from readily available reagents, remains one of the major challenges in organic synthesis. In recent years, the use of molecular iodine [2] has received considerable attention as a mild, inexpensive, nontoxic, readily available Lewis acid catalyst for various organic transformations.

Herein, in connection with our previous work using molecular iodine [3] we designed a facile three-component, one-pot synthesis of 3-amino- imidazo[1,2-a]pyridines in the presence of molecular iodine as catalyst to provide a new methodology with short reaction times. (Scheme 1)



Scheme 1

References:

[1] Odell, L. R.; Nilsson, M. T.; Gising, J.; Lagerlund, O.; Muthas, D.; Nordqvist, A.; Karlén, A.; Larhed, M. *Bioorganic & Medicinal Chemistry Letters* **2009**, *19*, 4790.
[2] Gao, S.; Tzeng, T.; Sastry, M. N. V.; Chu, C.; Liu, J.; Lin, C.; Yao, C. *Tetrahedron Lett*. **2006**, *47*, 1889.
[3] Rostamizadeh, S.; Amani, A. M.; Aryan, R.; Ghaieni, H. R.; Shadjou, N. *Synth. Commun*. **2008**, *38*, 3567.

Ammonium chloride an efficient catalyst for synthesis of 1,4-dihydropyridine derivatives

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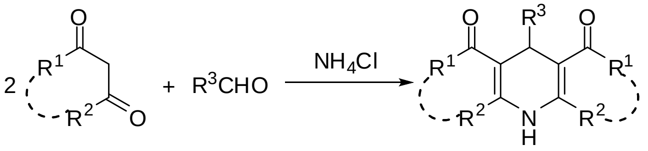
Recent studies have revealed that 1,4-dihydropyridines exhibit several medicinal and biological applications which include calcium channel blockers, platelet anti-aggregation and anti-diabetic agents [1].

Even though a number of modified methods under improved conditions have been reported, many of them suffer from drawbacks such as unsatisfactory yields, high temperatures and long reaction times [2]. Thus, the development of an efficient and versatile method for the preparation of 1,4-dihydropyridines is an active ongoing research area and there is scope for further improvement toward milder reaction conditions and improved yields. The versatility of ammonium chloride as a useful reagent in organic synthesis is well established [3]. As a continuation of our studies of ammonium chloride [4], we report a novel, efficient and improved synthesis for 1,4-dihydropyridines by using readily available and inexpensive ammonium chloride in refluxing ethanol.



R^1, R^2 = Alkyl

R^3 = Alkyl, Aryl

References:

[1] Sabitha, G.; Reddy, G. S. K. K.; Reddy, Ch. S.; Yadav, J. S. *Tetrahedron. Lett.* **2003**, *44*, 4129.
[2] Ohberg, L.; Westman, J. *Synlett* **2001**, 1296.
[3] Naya, S. I.; Iida, Y.; Nitta, M. *Tetrahedron* **2004**, *60*, 459.
[4] Azizian, J.; Teimouri, F.; Mohammadizadeh, M. R. *Catal. Commun.* **2007**, *8*, 1117.

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University of Mazandaran,
Babolsar,Iran 13-15 October 2010

۲۱ تا ۲۳ مهرماه ۱۳۸۹
بابلسر- دانشگاه مازندران
دانشکده شیمی

Synthesis, purification and characterization of O,O-dimethylchlorophosphorothioate from $PSCl_3$ and CH_3OH

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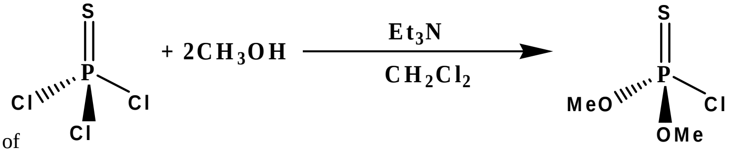
O,O-dimethylchlorophosphorothioate (DMPCT) is intermediate for preparation of phosphoroamidothioate insecticides. In particular, it has been used for producing *O,S*-dimethylphosphoroamidothioate and applied in the flotation agents, plasticizers, lubricating oil additives, rubber vulcanization accelerators, and many other useful chemicals [1]. In this paper,thiophosphoryl chloride ($PSCl_3$) reacts with methanol at low temperature to give DMPCT [2]. The synthesis method of DMPCT has been shown in following scheme:



Reaction scheme of synthesis for (DMPCT) of thiophosphoryl chloride in presence of triethylamine.

Here in we report synthesis DMPCT from inexpensive starting materials, thiophosphoryl chloride, methanol and triethylamin in dichloromethane as solvent [3]. In this research the One-Pot synthesis of DMPCT and increasing the yield of reaction product has been done by changing in different parameters, such as the mole ratio of reactants, solvent and catalyst. Purification has been done by washing with 75ml (3× 25 ml) water (precooled to less than 5°C) and the structure of DMPCT has been characterized by ^{31}P, $^{31}P\{H\}$, ^{1}H, ^{13}C-NMR and IR spectroscopy and GC-Mass [4]. The biological activity potential of the DMPCT was calculated using PASS software (1.193 version) programmed from which the probability of hundreds of biological activities can be predicted simultaneously.The probability of acetylcholinesteras inhibition in human and contribution of atoms in reduction or rising of acetylcholinesteras inhibition was also investigated.

References:

[1] John, P.; Chupp, C.; Kirk, W.; Peter, E. *U.S. Pat.* **1963,** 3, 089, 890.
[2] Zayed, S. M.A.D.; Mahdy, F. *Chemosphere, 70,* **2008**, 1653.
[3] Steven, E.E.; Gladstone, Mo. *U.S. Pat.* 4, 401, 605, **1983**.
[4] Peng, P.Y.; Jiang, C.Y.; Wang, Y.P. *J. Appl. Chem. 18,* **2001**, 257.

One-pot synthesis of highly functionalized stable ketenimines by three component reaction between of cyclohexyl isocyanide, Dialkyl acetylenedicarboxylate and methyl 2-acetyl-3-oxobutanoate (or 4,4,4-Trifluoro 3-oxothio-butyrate).

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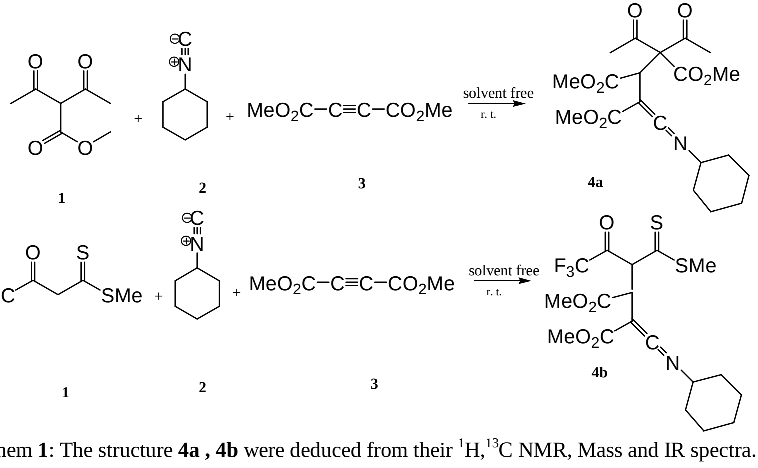
In recent years, ketenimines have attracted as dehydrating agents for peptide synthesis, as complexing agent for transition metal ions, and as coreagents for DMSO oxidation [1, 2]. The addition of nucleophilic carbens such as isocyanides to dialkyl acetylenedicarboxilates has been investigated in detail by a number of research groups.

Here we wish to report the results of our studies on the reaction between cyclohexylisocyanide **2** and dialkyl acetylendicarboxylate **3** in the presence of methyl 2-acetyl-3-oxobutanoate (or 4,4,4-Trifluoro 3-oxothio-butyrate) **1** that undergoes a smooth **1:1:1** addition reaction under solvent-free conditions at room temperature (schem **1**). This three component condensation reaction produces functionalized ketenimines **4a ,(4b)** in fairly good yield.



Schem **1**: The structure **4a , 4b** were deduced from their ^{1}H,^{13}C NMR, Mass and IR spectra.

References:

[1] Ugi, I., *Angew. Chem. Int. Ed. Eng.*, **1982**, *21*, 810.
[2] Tidwell, T. T. *Acc. Chem. Res.*, **1990**, *23*, 273.
[3] Krow, G. R. *Angew. Chem. Int. Ed. Engl.* **1971**, *10*, 435.

Synthesis of one interest polypiridylamide organic compound for preprating a new Zinc(II) coordination polymer as organometalic structure

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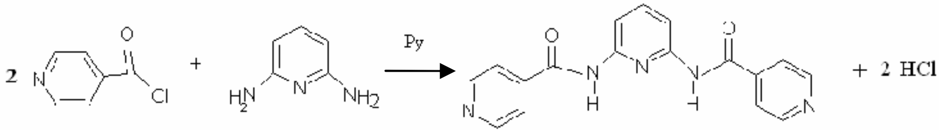
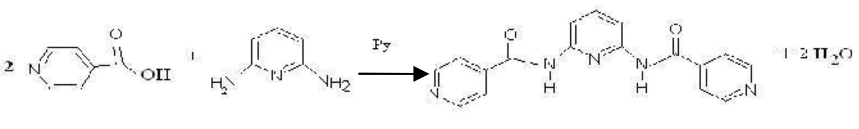
In recent years, some important potential applications, such as catalysis, magnetism, gas storage and molecular recognition of the functional coordination complexes have been drawn considerable attention to these compounds [1]. The amidic groups as coordinated ligand have many application such as catalysis, biologically and so on [2]. Hydrogen bonding is one important role in synthesis of coordination polymer [3]. This sort of bonding shapes between C=O groups and every hydrogen donating atom , also between NH groups and any hydrogen accepting groups, so growth of these structures are facilated. Using from “organic–inorganic hybrid material” term instead of coordination polymer compound is completely correct [4]. pyridylamide ligands to that these polymers are.

Herein we report the vagg method for synthesis of N,N´-Bis(4-pyridylcarbonyl)-2,6-diaminopyridine as organic compound and utilize it for preparing one new zinc(II) coordination polymer $\{Zn(L)_2(DMF)_4\}.ClO_4$ (**1**). We use from slow evaporation to prepare this coordination polymer. Organic ligand and compound **1** has been characterized by IR, ^{1}HNMR and ^{13}CNMR spectroscopy, also we used single X-ray crystallography to characterize compound **1.**

The organic structure, N,N´-Bis(4-pyridylcarbonyl)-2,6-diaminopyridine, also has obtained from the other reagent but this method [5] is more expensive than vagg. We show two methods in this scheme.



Vagg Method:



References:

[1] Wang, C. X.; Du, Ch. X.; Li. Y. H.; Wu, Y. J. *Inorganic Chemistry Communications* **2005**, *8,* 379.
[2] Bondy,Ch. R.; Loeb, S. J. *Coordination Chemistry Reviews* **2003,** *240,* 77.
[3] Amirnasr, M.; Schenk, K. J.; Meghdadi, S. *Inorganica Chimica Acta* **2002**, *338, 19*.
[4] Robin, A.Y.; Fromm, K. M. *Coordination Chemistry Reviews*. **2006**, *250,* 2127.
[5] Shin, Y. W.; Kim, T. H.; Lee, K. Y.; Park, K. M.; Han, S. W.; Lee, Sh. S.; Kim, J. S.; Kim, J. *Bull.Korean Chem. Soc.* **2005**, *26,* 473.

Novel methods to synthesis of sulfonamide compounds *via* isocyanide-based multicomponent reactions

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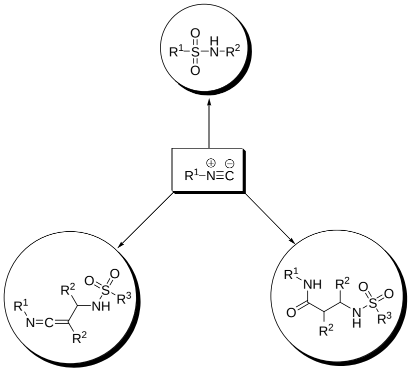
The amide and sulfonamide bonds are the most important linkages in organic chemistry and constitute the key functional group in peptides, polymers, many natural products and pharmaceuticals. [1,2].

In view of our current studies on IMCRs involving zwitterionic species [3] and our interest in chemistry of sulfonamides and amides [4], herein we describe an environmentally benign approach to the synthesis of ketenimine sulfonamide derivatives and bifunctional sulfonamide-amide compounds.



References:

[1] (a) Cupido, T.; Tulla-Puche, J.; Spengler, J.; Alberico, F. *Curr. Opin. Drug Discovery Dev.* **2007**, *10*, 768–783; (b) Bode, J. W. *Curr. Opin. Drug Discovery Dev.* **2006**, *9*, 765.

[2] Smil, D.; Leit, S.; Ajamian, A.; Allan, M.; Chantigny, Y. A.; Déziel, R.; Therrien, E.; Wahhab, A.; Manku, S. International Patent WO 07/143822, **2007**.

[3] (a) Shaabani, A.; Soleimani, E.; Sarvary, A.; Rezayan, A. H. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 3968; (b) Shaabani, A.; Sarvary, A.; Rezayan, A. H.; Keshipour. S. *Tetrahedron* **2009**, *65*, 3492; (c) Shaabani, A.; Ghadari, R.; Sarvary, A.; Rezayan, A. H. *J. Org. Chem.* **2009**, *74*, 4372; (d) Shaabani, A.; Rezayan, A. H.; Rahmati, A.; Sarvary, A. *Synlett* **2007**, 1458; (e) Shaabani, A.; Soleimani, E.; Rezayan, A. H.; Sarvary, A.; Khavasi, H. R. *Org. Lett.* **2008**, *10*, 2581; (f) Shaabani, A.; Rezayan, A. H.; Keshipour, S.; Sarvary, A.; Ng, S. W. *Org. Lett.* **2009**, *11*, 3342.

[4] Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.* **2007**, *48*, 2185-2188; (b) Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.* **2007**, *48*, 6137.

Metaborosulfric acid: A novel catalyst to for the friedlander quinoline synthesis and *α,β*-unsaturated aldol products

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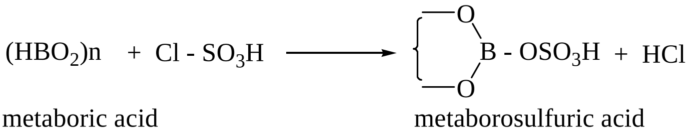
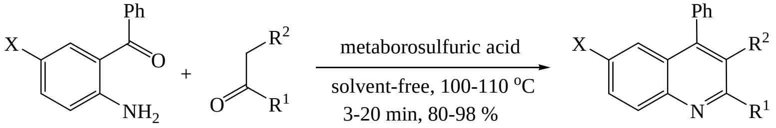
Quinolines are important heterocyclic systems, constituting the structure of many naturally occurring products with interesting pharmacological properties [1]. Among the various synthetic methods in quinoline synthesis, Friedlander condensation is an extremely useful and versatile method for the direct construction of a quinoline ring [2]. Cross-aldol condensation of aromatic aldehydes with ketones is an important synthetic reaction for the preparation of α,α'-bis(arylmethylidene)ketones and 1,5-Diarylpentadien -3-ones. These benzylidene derivatives are intermediates of various pharmaceuticals, agrochemicals and perfumes [3].

Herein, we report the first application of metaborosulfuric acid as an efficient catalyst for the preparation of quinolines from *o*-aminoarylketones and different ketones under solvent-free conditions in high yields at 110 °C. Furthermore, we report the preparation of α,β-unsaturated aldol products from aromatic aldehydes and ketones in the presence of metaborosulfuric acid in dichloroethane in excellent yields.





X = H, Cl R^1, R^2 = alkyl, aryl

Reference:

[1] (a) Chen, YL.; Fang, KC.; Shen, JY.; Hsu, SL.; Tzeng, CC. *J. Med. Chem.* **2001**, 44, 2374; (b) Roma, G.; Braccio, MD.; Grossi, G.; Mattioli, F.; Ghia, M. *J. Med. Chem.* **2000**, 35, 1021.

[2] Li, J. J.; Corey, E. J., Eds, *Name Reactions in Heterocyclic Chemistry*, Wiley & Sons: Hoboken, NJ, 2005, p 411.

[3] Artico, M.; Santo, R.D.; Costi, R.; Novellino, E.; Greco, G.; Massa, S.; Tramontano, E.; Marongiu, M.E.; Montis, A.D.; Colla, P.L. *J. Med. Chem.* **1998**, *41*, 3948.

Syntheses of two new symmetric 1,2,3,4-substituted pyrroles; A new synthetic route and mechanism

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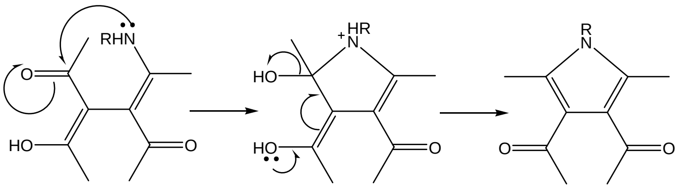
Pyrrole derivatives represent a class of heterocycles of great importance because of displaying biological activity and also being versatile building blocks in organic synthesis [1]. Although many efficient syntheses of pyrroles have been reported, developing new synthetic methods remains an attractive goal [2-6].

In this work we report a new method for synthesis of two new symmetric 1,2,3,4-substituted pyrroles and present a plausible mechanism for this reaction as shown below. In this reaction tetraacetylethane and ammonium acetate or methyl amine solution were used as starting materials in solvent of benzene. The yields of the reaction are good to moderate. The structures of the compounds were characterized by elemental analysis and ^{1}HNMR, ^{13}CNMR and IR spectroscopies.



R= H, Me

References:

[1] Arcadi, A.; Di Giuseppe, S.; Marinelli, F.; Rossi, E. *Tetrahedron: Asymmetry* **2001**, *12,* 2715.
[2] Dieter, R. K.; Yu, H. *Org. Lett*. **2001**, 2283.
[3] Farcas, S.; Namy, J.-L. *Tetrahedron* **2001**, 57, 4881.
[4] Ranu, B. C.; Hajra, A. *Tetrahedron* **2001**, 57, 4767.
[5] Attanasi, O. A.; Filippone, P.; Perrulli, F. R.; Santeusanio, S. *Tetrahedron* **2001**, 57, 1387.
[6] Aeltterman, W.; De Kimpe, N.; Tyvorskii, V.; Kulinkovich, O. *J. Org. Chem.* **2001**, 66, 53.

Phosphonato ester synthesis from reaction between tri phenyl phosphite, dialkyl acetylenedicarboxylate and nitrogen compound

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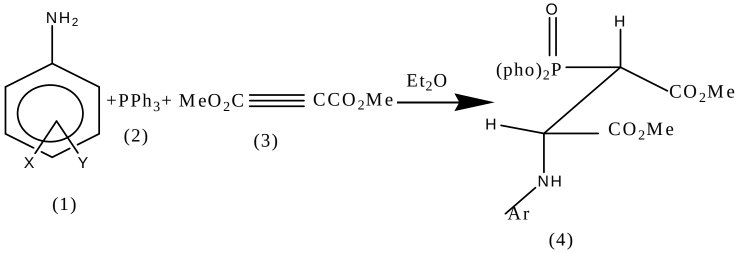
Development of simple synthetic routes for widely-used organic compounds from readily available reagents is one of the major tasks in organic chemistry .Phosphorus compounds are of great interesting compounds because pharmaceutical and biological activities that include anti-inflammatory, cardiotonic, inotropic, antihypertensive, antimicrobial propreties [1-3].We wish to describe have on efficient synthetic route to anilin containing stable phosphonato ester. Thus reaction of tri phenylphosphite (2) with dialkyl acetylenedicarboxylate (3) in the presence of N-H aromatic compounds (1) at diethyl ether, leads to the corresponding phosphonato ester (4) in excellent yield .The ^{1}H, ^{13}C ,^{31}P NMR spectra of ylide (4) is consistent.



X	Y
2-Cl	4-Cl
3-NO_2	4-Cl
2-CH_3	4-NO_2
4-CL	2-NO_2
3-CL	4-Cl

References:

[1] Maghsoodlou,M.T;HabibiKhorassani,S.M;Rofouei,M.K;Adhamdoust,S.R;Nassiri,M.Arkivoc, **2006**,xii,145.

[2] Sheldrick, G.M.Acta Cryst A **2008**, 64,112.

[3] Li,Y.X.;Wang,S.H.;Li,Z.M.;Su,N.;Zhao,W.G.Carbohyd Res **2006**,341,2867.

Synthesis of a new heterocyclic system Fluoreno[1,2-*d*]imidazol-10-one

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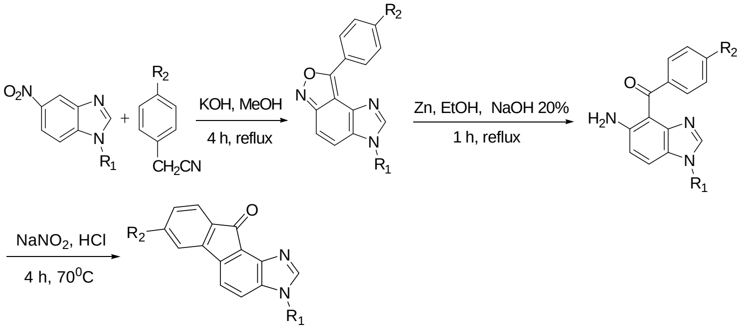
Fluorenones (fluorine-9-ones) are among the oldest classes of bioactive compounds, which are widely used as antiviral [1] and anticancer agents and act as the key synthetic intermediates in many reactions. Also, fluorenones with a suitable functionality can be used as a fluorescent electrophilic reagent [2]. Recently, they have mainly been considered as an important unit in polymer chemistry. The fluorenone structural unit provides both rigidly planarized biphenyl units within the polymer backbone and the possibility of remote functionalization at C-9, the latter offer the prospect of improving both polymer processibility and mediating potential interchain interactions in films [3].

Owing to our growing interest in the synthesis of bioactive heterocycles [4], we became interested in examining the cyclization of diazotized compounds to new fluoreno [1,2-*d*]imidazol-10-ones. This research has demonstrated that the cyclization of diazotized *o*-amino-ketones is a reliable work, which can be extended to the synthesis of other new heterocyclic compounds.



References:

[1] Alcaro, S. Arena, A. Di Bella, R. Neri, S. Ottanà, R. Ortuso, F. Pavone, B. rincone, A. Vigorita, M.G. *Bioorg. Med. Chem.*, **2005**, *13*, 3371.

[2] Garascia, R. J. Fries, E. F. Ching, C. *J. Org. Chem.*, **1951**, *17*, 226.

[3] Fuson, R. C. Bollero, A. G. Heins, C. F. *J. Org. Chem.*, **1961**, *27*, 2644.

[4] Mechoulam, R. Sondheimer, F. *J. Am. Chem. Soc.*, 1958, **80**, 4386.

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۲۱ تا ۲۳ مهرماه ۱۳۸۹
بابلسر ـ دانشگاه مازندران
دانشکده شیمی

Regioselective ring opening of epoxides with amines using SBSSA under solvent-free conditions

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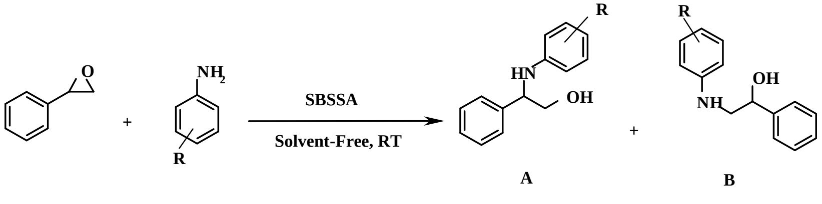
Due to their ease of formation and high reactivity, epoxides are important and useful synthetic intermediates in organic synthesis. The strain of their three-membered ring together with the polarization of the C–O bonds makes epoxides susceptible to reaction with a large variety of reagents such as nucleophiles, electrophiles, acids, bases, reducing agents and some of the oxidizing reagents [1]. Epoxides are efficiently converted into functionalized alcohols, as a handle for further manipulations, by employing various nucleophilic ring-opening reactions. This method provides a suitable route for the formation of C–C, C–N, C–O, C–P, C–S, C–N_3, C–X (X = halogen) δ-bonds [2]. This reaction, which is usually carried out with a large excess of nucleophiles at elevated temperature with long reaction times and drastic conditions, often fails when the nucleophile or the epoxides is sterically too bulky or the nucleophile having poor nucleophilicity or low boiling point is used [3].

Herein we carried out the reaction between styrene oxide and aniline derivatives in the peresence of SBSSA (Silica-bonded S-sulfonic acid), the corresponding amino alcohols (Scheme 1) were obtained in high yield at room temperature under solvent-free conditions. The regioselectivity in the reaction of these unsymmetrical epoxides is governed by both steric and electronic effects.



R	Yield (%)	A:B
H	98	95:5
CH3	95	90:10

Scheme 1

References:

[1] Nielsen, L.P.C. Jacobsen, E.N. In ***Aziridines and Epoxides*** in. ***Organic Synthesis*** (***Ed***.: ***A. K. Yudin***) ***Wiley-VCH***, ***Weinheim***, ***2006***.

[2] Pastor, I.M. Yus, M. *Curr.Org. Chem*. **2005**, *9*, 1.

[3] Bandini, M. Melloni, A. Tommasi, S. Umani-Ronchi, A. *Synlett*. **2005**, 1199.

Convenient one-pot synthesis of 3-(5-Aryl-1,3,4-oxadiazol-2-yl)-3-hydroxy-2-butanone derivatives via multicomponent reaction of (*N*-isocyanimino)triphenylphosphorane

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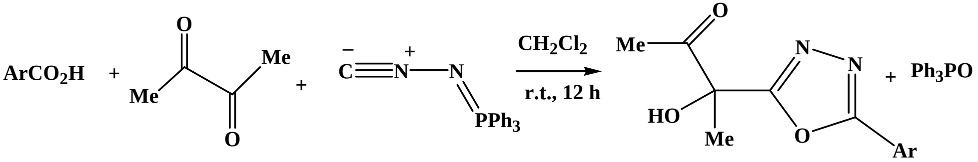
Due to the atom economy, convergent character and simplicity of one-pot procedures, multi-component condensation reactions (MCRs) have an advantageous position among other reactions. The development of novel MCRs is receiving growing interest from industrial chemistry research groups and represents a challenge for organic chemists [1]. 1,3,4-Oxadiazoles have attracted interest in medicinal chemistry as surrogates of carboxylic acids, esters, and carboxamides. They are an important class of heterocyclic compounds that have a wide range of pharmaceutical and biological activities including antimicrobial, anti-fungal, anti-inflammatory, and antihypertensive [2]. As part of our ongoing program to develop efficient and robust methods for the preparation of heterocyclic compounds [3], we report a hitherto unknown, one-pot three-component reaction, which, starting from readily available biacetyl, carboxylic acid derivative and (*N*-isocyanimino)triphenylphosphorane affords 3-(5-aryl-1,3,4-oxadiazol-2-yl)-3-hydroxy-2-butanones. The structures of the products were deduced from their IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. In summary, we have found a new and efficient method for the synthesis of sterically congested 2,5-disubstituted 1,3,4-oxadiazoles derivatives. Its ease of work-up, high yields and fairly mild reaction conditions make it a useful addition to modern synthetic methodologies.



Reference:

[1] Ramazani, A.; Rezaei, A. *Org Lett*. **2010**, *12*, 2852.
[2] Ambrosi, G.; Formica, M.; Fusi, V.; Giorgi, L.; Macedi, E.; Micheloni, M.; Piersanti, G.; Pontellini, R. *Org. Biomol. Chem.* **2010**, *8*, 1471.
[3] Ramazani, A.; Mahyari, T. M.; Rouhani, M.; Rezaei, A. *Tetrahedron Lett.* **2009**, *50*, 5625.

Encapsulation of methane molecules into the C_{60} fullerene: DFT simulation

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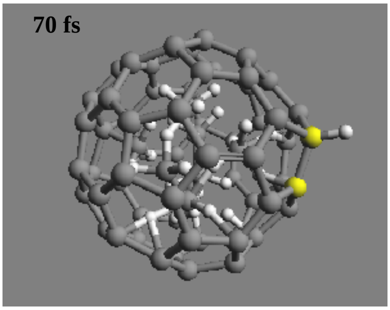
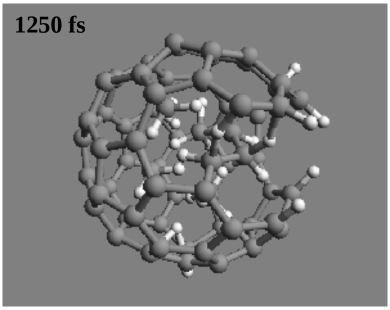
Natural gas adsorbed on porous materials have been attracting an increasing interest since they are a promising alternative to compressed natural gas as a suitable nonpollution vehicular fuel and for bulk transportation [1]. Methane is one of the major components of natural gas therefore its adsorption behavior in confined pores is of practical and theoretical interest [2]. Discovery of novel materials, such as fullerene nanocages has drawn much attention in recent years, because of their unique properties. There have been several works devoted to the investigation of the possibility of formation of endohedral complexes between diatomic molecule and fullerene nanocages [3, 4].

Here we present the results of our theoretical investigation by using the DFT method on methane deposition into the C_{60} fullerene, and its potential applications as a suitable material for energy storage. Endohedrally methane doped C_{60} systems, $n\mathrm{CH_4@C_{60}}$ (n: 1–7) have been examined and their formation energy and the CH_4–CH_4 and CH_4–wall repulsive energies are calculated as functions of the number of encapsulated methane molecules, N_{CH4}. The presently results revealed that C_{60} cage may accommodate quite a number of methane molecule. Although structures with a large amount of encapsulated methane are highly endothermic, they have metastable structures. The maximum number of methane molecules inside C_{60}, which can form a metastable structure is determined to be $N_{\mathrm{CH4}} = 6$. It was also found that for $N_{\mathrm{CH4}} = 7$ the capsule side wall eventually breaks and the mechanism of its breaking is studied by DFT-molecular dynamics (DFT-MD) simulations.





References:

[1] Kroto, H. W. *Int. J. Mass Spectrometry & Ion Processes* **1994**, *138*, 1.
[2] Aradi, B.; Hourahine, B.; and Frauenheim, Th. *J. Phys. Chem.* A **2007**, *111*, 5678.
[3] Ganji, M. D., *Nanotechnology* **2008**, *19*, 025709.
[4] Ganji, M. D., *Phys. E* **2009**, *41*, 1406.

A novel one-pot four-component synthesis of pyrimido [6,1-*a*]isoquinolines

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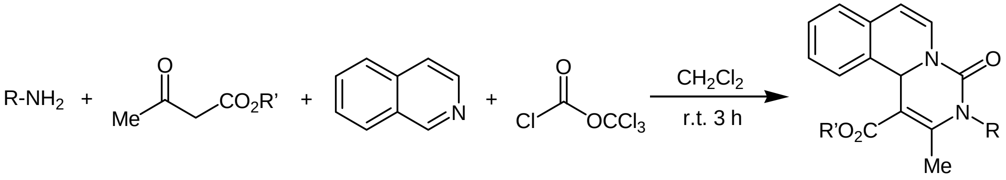
Bridgehead nitrogen heterocycles are of interest because they constitute an important class of natural and unnatural products, many of which exhibit useful biological activity and are used in pharmaceutical preparations [1]. A broad range of biological activities has been reported for compounds containing the pyrimido[6,1-*a*]isoquinoline ring system, amongst the reported ones are antihypertensive, bronchodilator, blood pressure lowering, anti inflammatory and anti-allergic activities [2]. This makes the pyrimido[6,1-*a*]isoquinoline skeleton an important synthetic target and a lot of research has been directed towards it.

An interesting and versatile pyrimido[6,1-*a*]isoquinoline synthesis involves enamines [3]. Enamines are versatile building blocks for the synthesis of various bicyclic and tricyclic structures bearing a bridgehead nitrogen atom. In the course of our research programon the design of new routes for the synthesis of a variety of active biologically nitrogen heterocycles in our laboratory via one-pot synthesis and reactions of enaminones [4], herein, we describe a simple, one-pot, four-component synthesis of pyrimido[6,1-*a*]isoquinoline-4-one derivatives. Thus, reaction between an enaminone, derived from the addition of various primary amines to alkyl acetoacetates, with trichloromethylchloroformate (diphosgene) in the presence of isoquinoline in dry dichloromethane at ambient temperature to produce pyrimido[6,1-*a*]isoquinoline derivatives.



References:

[1] Hermecz, I.; Vasvari-Debreczy, L.; Matyus, P. In *Comprehensive Heterocyclic Chemistry*; Katritzky, A. R., Rees, C. W.,Scriven, E. V. F., Eds.; Pergamon: London, **1996**; Chapter 8.23, pp 563.

[2] (a) Griffin, R. J.; Fontana, G.; Golding, B. T.; Guiard, S.; Hardcastle, I. R.; Leahy, J. J. J.; Martin, N.; Richardson, C.; Rigoreau, L.; Stockley, M.; Smith, G. C. M. *J. Med. Chem.* **2005**, *48*, 569; (b) Swinbourne, J. F.; Hunt, H. J.; Klinkert, G. *Adv. Heterocycl. Chem.* **1987**, *23*, 103.

[3] Tu, S.; Li, C.;G, Li.; Cao, L.; Shao, Q.; Zhou, D.; Jiang, B.; Zhou, J.; Xia, M. *J. Comb. Chem.* **2007**, *9*, 1144.

[4] (a) Alizadeh, A.; Rezvanian, A.; Zhu, L. G. *Tetrahedron* **2008**, *64*, 351; (b) Alizadeh, A.; Rezvanian, A. *Synthesis* **2008**, *11*, 1747; (c) Alizadeh, A.; Rezvanian, A.; Bijanzadeh, H. R. *Synthesis* **2008**, *5*, 725.

A remarkably simple formylation reaction catalyzed by amine functionalized ordered nanoporous silica

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Formylation reaction is a useful reaction in synthetic organic chemistry. The products of formylation are valuable intermediates in the construction of various pharmaceutically important compounds. They are also useful reagents in Vilsmeier formylation reactions. Moreover, they are Lewis bases and can catalyze several organic transformations. The formyl group is also an important protecting group in peptide synthesis [1].

A number of formylation methods have been reported in recent years. Acetic formic anhydridecontinues to be the most widely used formylating reagent, but it is sensitive to atmospheric moisture and cannot be stored due to decomposition to acetic acid and carbon monoxide. Many other useful formylation reagents have been reported such as chloral, activated formic acid using DCC or EDCI, activated formic acid esters, KF-Al_2O_3, ammonium formates, CDMT, solidsupported reagents, and other reagents [2].

Herein, we report a practical formylation procedure using formic acid in the presence of amine functionalized ordered nanoporous silica under solvent-free conditions brings about highly and efficient formylation to give the corresponding products in good to high yields.

References:

[1] Das, B.; Krishnaiah, M.; Balasubramanyam,P.; Veeranjaneyulu,B.; Kumar,N. *Tetrahedron Lett.* **2008**, *49*, 2225.
[2] Hosseini-Sarvari, M.; Sharghi,H. *J.Org.Chem.* **2006**, *71*, 6652.

Synthesis of new heterocyclic system: [1,2,4]triazolo[3',4':6,1]pyridazino [4,3-*e*][1,3,4] thiadiazine

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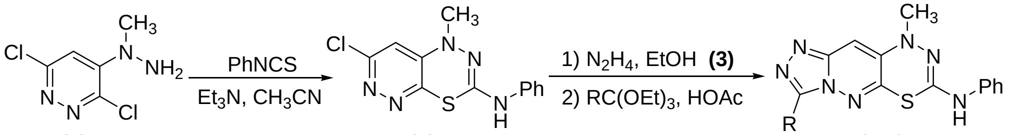
Triazoles, in particular fused 1,2,4-triazoles, are an important class of heterocyclic compounds which express antifungal [1] and bactericidal [2] activities. On the other hand, pyridazinothiadiazines are also important heterocycles which are of interest as potential inhibitors of cyclic nucleotide phosphodiesterase [3] and dyestuff [4]. Therefore, the synthesis of triazolopyridazinothiadiazines should be interesting from pharmacological and synthetic point of views.

We here now describe a method for the synthesis of novel heterocyclic ring system of 1,2,4-teriazoles fused to pyridazino[4,3-e][1,3,4]thiadiazine. Initially, the treatment of compound **(1)** with phenylisothiocyanate afforded the 2-anilino-7-chloro-1-methyl-1H-pyridazino[4,3-*e*][1,3,4]thiadiazine **(2)**. The reaction of precursor **(2)** with hydrazine hydrate in ethanol led to the substitution of chlorine atom with hydrazine and gave the corresponding 2-anilino-7-hydrazinyl-1-methyl-1H-pyridazino[4,3-*e*][1,3,4]thiadiazine **(3)**. The latter product subsequently underwent cyclocondensation with different triethylorthoesters in acetic acid to give the desired tricyclic heterocyclic compounds [1,2,4]triazolo[3',4':6,1]pyridazino[4,3-*e*][1,3,4] thiadiazine **(4a-c)** in good to excellent yields.



(1) **(2)** **4(a-c)**

References:

[1] El-Hawash, S. A.; Habib, N. S.; Fanaki, N. H. *Pharmazie* **1999**, *54,* 808.
[2] Brown, D. J.; Iwai, Y. *Aust. J. Chem.* **1979**, *32,* 2727.
[3] Naka, T.; Furukawa, Y. *Chem. Pharm. Bull.* **1979**, *27,* 1965.
[4] Elliot, A. J. *US Patent* 4, 025*, 510,* **1977** [*Chem. Abstr.* 87: 153420h].

Synthesis of the new chiral palladate salt from chiral ionic liquid

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The development of chiral transition metal complexes to catalyze asymmetric organic reactions represents one of the most important achievements of modern organometallic chemistry, and high selective catalysts are now available to catalyze an impressive range of reactions [1]. Polar aprotic solvents such as DMF and CH_3CN are the most commonly used solvents in these reactions. Replacement of these traditional but toxic organic solvents by ionic liquids (ILs) has been the object of numerous studies. ILs are of special interest due to their specific properties: they present good chemical and thermal stability, low vapour pressure, wide liquid range, good solubility for a wide range of organic and inorganic reagents and they allow the facile separation of the products and recycling of the ILs containing the catalysts [2]. In addition to this, the use of ILs in the C-C coupling reactions has opened new insights and perspectives: (i) ILs containing imidazolium cations stabilize ligand-free precursors of catalysts, consequently catalysts like palladium acetate proved to be efficient even at low concentrations and have been widely used; (ii) When performed in ILs, the reaction rate was significantly increased [3].

Herein we report an efficient method for synthesis of the new chiral palladate salt from chiral ionic liquid. Palladium-containing chiral IL catalysts (Figure 1) were generated from palladium chloride ($PdCl_2$) and the appropriate chiral IL. This catalyst could use in the asymmetric Pd-catalyzed reactions such as asymmetric heck reaction.

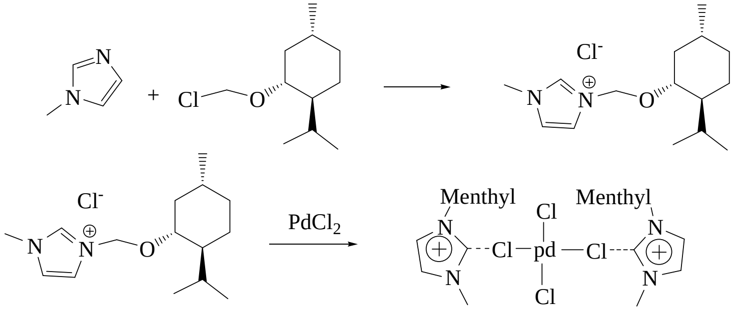

Figure 1

References:

[1] Minato, M.; Kaneko, T.; Masauji, S.; Ito, T. *Journal of Organometallic Chemistry*. **2006**, *691*, 2483.

[2] Hajipour, A. R.; Rafiee, F. *J. Iran. Chem. Soc.* **2009**, 6, 647.

[3] Gayet, F.; Marty, J.; Viguerie, N. *J. Phys. Chem*. **2008**, *61*.

Synthesis of monomer bearing imide ring and vinylic functions and its uses in the styrene emulsion copolymerization

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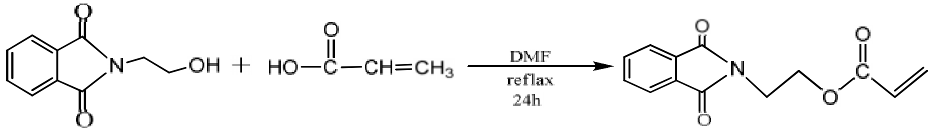
N-maleimide monomers are of particular interest because of their relatively high heat-resistance, flame retardancy and reactivity of their double bond. They could, therefore, be copolymerized with monomers such as ethylene or propylene system or vinylic monomers in the cause of having double bond or blended with functional materials for the purpose of modification [1-4].

In this study a new imide ring containing vinylic monomer, Acryloxyethylphthalimide (AEPI), was synthesized in two steps. First, phthalic anhydride and ethanolamine was reacted in the presence of methanol at 115-125°C to obtained N-(2-hydroxyethyl) phthalimide. Then the product was reacted with acrylic acid in the presence of dimetyl formamide and tetra isopropyltitanate as solvent and catalyst, respectively. In the second part of this work, a series of imide ring containing styrene – acrylate latexes have been successfully prepared by the emulsion polymerization. The polymerization was performed with methacrylic acid (MAA) and auxiliary agents at 80 ◦C in the presence of ammonium peroxodisulfate (APS) as the initiator. Alkyl phenol ether sulfate and Arkupal N-300 were used as anionic and nonionic emulsifiers, respectively. The resulting monomers and copolymers were characterized by using Fourier transform infrared spectroscopy (FTIR) as well as 1H and 13C nuclear magnetic resonance spectroscopy. Thermal properties of the copolymers were studied by using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The morphology of copolymers was also investigated by scanning electron microscopy (SEM). The obtained copolymers have high solid content (53%) with high thermal stability and can be used in emulsion paints as a binder.



References:

[1] Wang, H.; Wei,J.; Jiang, X.; Yin, J. *Polymer Intentional*. **2006**, *55*, 930.
[2] Gaina, C.; Gaina, V. *Designed Monomer and Polymers*. **2004**, *7*, 235.
[3] Bezdushna, E.; Ritter, H. *Macromol.Rapid Comm*. **2005**, *26*, 1087.
[4] Ahn, K. D.; Chung, C. M.; Koo, D. I. *Chem. Mater*. **1994**, *6*, 1452.

Synthesis of cysteine *β*-amyloid segment (25-35) peptide

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The Alzheimer's disease (AD) is a neurodegenerative illness, which effects millions of people worldwide. The Aß-amyloid peptides are the major constituents of senile plaques in Alzheimer's disease (AD) [1–3]. Formation of Aβ involves sequential cleavage of the β-amyloid precursor protein (APP) by two proteases, β-secretase and γ-secretase. Cleavage of APP by β -secretase, leads to the generation and extracellular release of APPs- β, and intracellular C-terminal fragments (CTFs) bearing the complete A β domain. A key event in the pathogenesis is the conversion of A β peptides from soluble oligomers to aggregated, fibrillary forms and eventually amyloid deposits called neuritic plaques. A great deal of evidence indicates that the Aß-amyloid peptides, in the form of soluble ß-sheet oligomers, are highly toxic and directly involved in the pathogenesis of AD [4].

β-Amyloid peptide fragment 25-35 potentiated induced opening of mitochondrial channels and caused swelling of mitochondria. These changes were accompanied by accumulation of lipid peroxidation products in mitochondria. Aβ (25-35) fragment is highly toxic segments of β -amyloid peptides that promote inflammatory processes in astrocytes and fibrillary aggregation of A β.

In continuation of our research work, the Cys-beta amyloid (25-35) was synthesized using solid phase peptide synthesis strategy. Coupling of amino acids and synthesis of *C*-terminal peptide was done on the surface of 2-chloro-trityl chloride resin. The progress of coupling was monitored using Kaiser test.The product was purified using HPLC, and finally the structure of the peptide was deduced using HR-ESI. The investigation of biological activity of the peptide is under progress.

H-Cys-Gly-Ser-Asn-Lys-Gly-Ala-Ile-Ile-Gly-Leu-Met-OH
β- amyloid Segment (25-35) sequence

References:

[1] Cohen, A.; Calkins. E. *Nature*. **1959**, *183*, 1202.
[2] Glenner, G.; Wong, CW. *Biochem. Biophys. Res. Commun.* **1984**, *120*, 885.
[3] Miller, D.; Papayannopoulos, I.; Styles, J.; Bobin, S.; Lin, Y.; Biemann, K.; Iqbal, K. *Arch. Biochem. Biophys.* **1993**, *301*, 41.
[4] Ikonomovic, M.; Uryu, K.; Abrahamson, E.; Ciallella, J.; Trojanowski, J.; Lee, V.; Clark, R.; Marion, D.; Wisniewsk, S.; DeKosky, S. *Exp. Neurol.* **2004**, *190*, 192.

Synthesis of 1,4 diazepines derivatives that used of 6-benzylpyrimidine2,4(1H,3H)-dione with benzaldehydes

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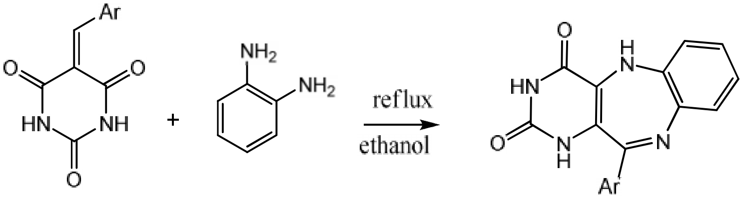
To modify heterocyclic systems chemically has always been a problem for the medicinal chemists in search of compounds with bio-pharmacological activity [1].

Lately the syntheses of analoges possessing heterocycles or even more fused systems such as a pyrimidine ring attracted attention since they showed to be promising pharmacophores [2], from which we can focus on diazepines.

Diazepines derivatives are very important and well-known in medicinal chemistry. among the active derivatives of these compounds, are 1,3 and 1,4 diazepines which have been taken in to consideration in medicinal pharmacy because of their active sites positioning [1]. Also they show a wide range of pharmacologic activities [3].

In this mong 1,4 diazepine system is considered today a relevant pharmacophre in wide range of biological activities , with special examples in the well- known benzodiazepines extensively studied synthetically and pharmacologically [4].In this work we have diescribed the synthesis of 1, 4 diazepines derivatives that used of 6- benzylpyrimidine-2, 4(1H,3H)-dione with benzaldehydes. All of the products were identified by ^{1}HNMR, ^{13}CNMR, FT-IR spectroscopy and element analysis.



Ar = benzaldehyde, 4-chloro benzaldehye, 4- methoxy benzaldehyde, furan-2-carbaldyde, thiophene-2-carbaldyde, 4-(dimehylamino) benzaldehyde, 4-nitr benzaldehyde, 3-nitrobenzaldehyde, 4-methylbenzaldehyde.

References:

[1] Incerti , M ; Acquotti , D ; Sandor , P ; Vicini , P . *Tetrahedron* **2oo9**, *65*, 7487.

[2] Insusasty , B ;Orozco ,F ; Lizarazo , C ;Quiroga , J ; Abonia , R ; Hursthouse , M ;N ogueras , M ; Cabo , *J. Bio&Med chem*. **2008**, *16* , 8492.

[3] Insuasty , B ; García , A ; Quiroga ,J; Abonia, R ; Nogueras , A ; Cobo , J. *Eur. J. Med. Chem,* **2010**, 1.

[4] Schutz, h. Benzodiazepines; *Springer: Heidelberg* , **1982**.

Efficient synthesis of Biginelli compounds using cobalt hydrogen sulfate

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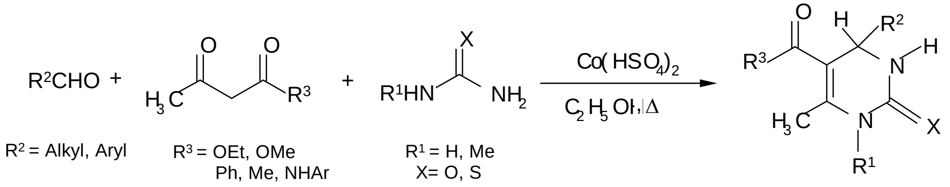
2-Oxo-1,2,3,4-tetrahydropyrimidines (THPMs) and their derivatives have shown a wide range of important pharmacological and biological properties including antimicrobial [1], anticancer [2] and antihypertensive [3] activities.

Because of the importance of THPMs, several new and improved procedures in the presence of various catalysts such as Lewis acids, Lewis bases, BrØnsted acids, heteropoly acids, ionic liquids, etc. have been reported [4].

Nowadays, much effort has been done to the use of inorganic reagents in organic reactions because of their advantages such as milder reaction conditions and easier work up. Due to stability, cheapness and milder reaction conditions, many works devoted to the usage of metal hydrogen sulfates (MHSs) for this purpose [5].

We wish to introduce cobalt hydrogen sulfate as an efficient catalyst for the synthesis of various 5-acyl, 5-carboalkoxy and 5-carboxamide-2-oxo(thioxo)-1,2,3,4-tetrahydropyrimidines. The results will be presented.



References:

[1] Virsodia, V.; Pissurlenkar, R.R.S.; Manvar, D.; Dholakia, C.; Adlakha, P.; Shah, A.; Coutinho, E.C. *Eur. J. Med. Chem.* **2008**, *43,* 2103.
[2] Ibrahim, D.A.; El-Metwally, A.M. *Eur. J. Med. Chem.* **2010**, *45,* 1158.
[3] Singh, K.; Arora, D.; Falkowski, D.; Liu, Q.; Moreland, R.S. *Eur. J. Org. Chem*. **2009**, 3258.
[4] Kolosov, M.A.; Orlov, V.D.; Beloborodov, D.A.; Dotsenko, V.V. *Mol. Diversity* **2009**, *13,* 5.
[5] Momeni, A.R.; Sadeghi, M. *Appl. Catal., A* **2009**, *357,* 100.

New macrocycles from cyanuric chloride

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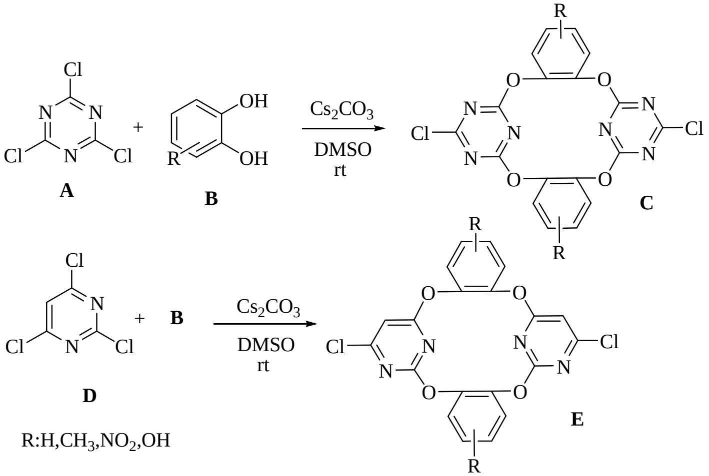
The perfection of the outline and synthesis of new and functional macrocyclic system has always been one reason to upgrade the significant progress in supramolecular chemistry. One of the recent instances is the eruptive studies of calixarene chemistry [1]. Because of the easy availability, unrivaled conformational and cavity structures,And recognition properties, calixarenes have been developed into an necessary section of supramolecular chemistry. Calix[n]arenas received much regard for decades in supramolecular chemistry due to their special molecular structure [2]. significant endeavors are now assigned in derivatizing the basic calixarene skeletons, and the more new expansions are the preparation of analogys by superseded the methylenic bridges by heteroatoms in order to improve their properties [3].

As per our ongoing research program aimed at the synthesized of fluorinated macrocyclic compounds [4], herein we would like to report synthesis of some macrocycle with common formula **C** and **E** from the reaction of various compounds containing bis-hydroxy groups with compound **A** and **D** respectively.



References:

[1] Kim, J. S.; Quang, D. T. *Chem. Rev*. **2007**, *107*, 3780.
[2] Baldini, L.; Casnati, A.; Sansone, F.; Ungaro, R. *Chem. Soc. Rev*. **2007**, *36*, 254.
[3] Katz, J. L.; Feldman, M. B.; Conry, R. R. *Org. Lett*. **2005**, *7*, 91
[4] Ranjbar-Karimi, R.; Sandford, G.; Yufit, D. S.; Howard, J. A. K. *J. Fluorine Chem*. **2008**, *129*, 307.

Synthesis and characterization of azo-calixarene amino pyridine derivatives as chromogenic selective sensor

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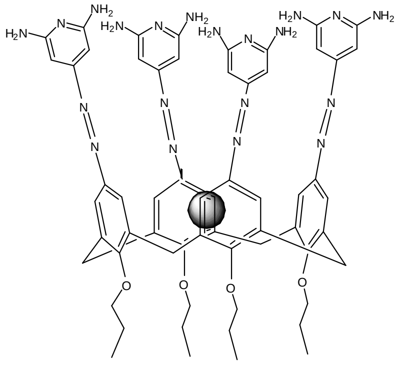
The macrocyclic ring in calixarenes acts as a molecular backbone to which ligating functional groups are attached [1]. Introduction of azo groups into the calix[n]arene framework confers chromogenicity to their molecular architecture, which can be utilize for development of specific molecular diagnostics and sensor material [2]. Azo phenol groups are one of the most frequently employed functions as a signaling device for the design of chromogenic ionophores, and many derivatives based on the calixarenes exhibit a pronounced chromogenic behavior towards a variety of cations [3].

In this paper synthesis of azocalixarenes derivatives based on 2,6-diamino pyridine as chromogenic compounds have been presented. The structure of azo calix was characterized with ^{1}H-NMR, ^{13}C-NMR, IR, UV-Vis and elemental analysis. The obtained azo derivatives with a large size cavity and a couple of azo functions can be acted as a chromogenic sensor toward transition metal cations. The host-guest behavior of this receptor has been investigated in presence of transition metal cations such as Pb^{2+}, Cd^{2+}.



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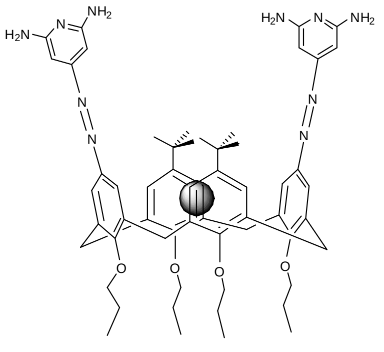

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References:

[1] Ludwig, R; Khm Dzung, T.K; Sensor.**2002**, 2, 397.
[2] Chawla, H.M; Pratap singh, S; Narugan sahu,S. Tetrahedron. **2006**, 62, 7854.
[3] Hyun Kim, T; Ho Kim, S; Vantan, L; Jinseo, Y; Young Park, S. Talanta. **2007**, 71, 1294.

Synthesis of alkyl 2-(-9-Arylidene-5-aryl-3, 5, 6, 7, 8, 9-hexahydro-2H-thiazolo [2,3-b] quinazolin-2-ylidene) acetate derivatives

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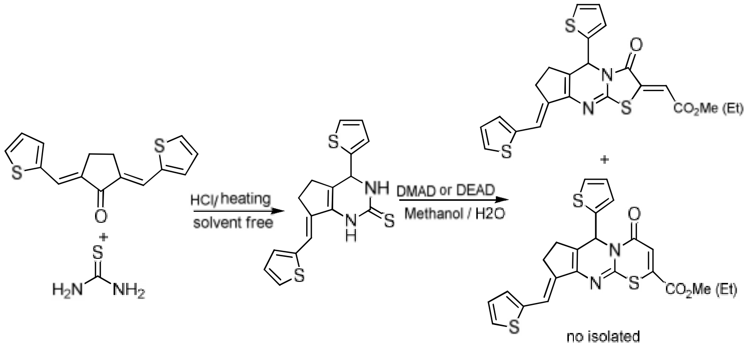
Many pyrimidine derivatives have been reported to possess useful medicinal and biological activities [1]. In the last few years, various pyrimidinone and pyrimidindione derivatives substituted either at C-5 or C-6 positions have emerged in the field of chemotherapy [2]. Recently, the pyrimidinone derivatives 2-methylthio-6-[(2-alkylamino) ethyl]-4(3H)-pyrimidinones have been shown to posses activity against positive strand (vesicular stomatitis virus) RNA virus [3].

Recently, interest in the synthesis of 1,2,4-triazoles (Biginelli compounds) and their derivatives has increased tremendously because of their diverse therapeutic and pharmacological properties such as anti-inflammatory, antibacterial, anticonvulsant, dephlogisticate, antidepressant, and antifungal agents. Recently we have reported synthesis a series of thiazoline compounds from reaction of thiosemicarbazone derivatives of aldehydes and ketoses with alkyl acetylenic esters [4]. Interest in this case synthesis of thiazoline rings and properties their due to we synthesis new dihydropyrimidino thiazine and dihydro-2H-thiazolo pyrimidine derivatives with use of 3,4-dihydropyrimidin 2(1H) ones derivatives and dimethyl acethlenedicarboxylate (DMAD), diethyl acetylene dicarboxiylate(DEAD). The results of ^{1}H NMR, ^{13}C NMR, FT-IR and UV spectra confirmed the formation of these products.



References:

[1] Barton, D. H. R.; Ollis, W. D., *Comprehensive organic synthesis; Pergamon: Oxford.* **1974,** 493.
Parlato, M. C.; Mugnaini C.; Renzulli M. L.; Corelli, F.; Botta M. *ARKIVOC.* **2004** (v), 349.

[2] Botta, M.; Occhionero, F.; Nicoletti, R.; Mastromarino, P.; Conti, C.; Margini, M.; S Aladino; *J. Bioorg. Med. Chem.* **1999,** *9*, 1925.

[3] Darekordi, A.; Saidi, K.; Islami, M. R. *Arkivoc.*2**007**, 180.

Synthesis of some new azacrown ethers as new receptors

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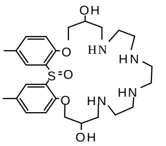
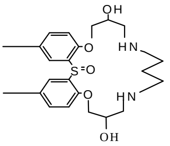
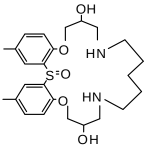
There has been a continued interest in the synthesis and chemistry of macrocyclic ligands because of their ability to form various complexes with organic, inorganic, cations, anions and biological molecules such as antibodies and enzymes for widespread applications. Crown ethers are artificial macrocycles that show wide applications in industry, medical, chemistry, and nuclear energy, phase transfer catalysis in organic synthesis and nano technology and materials [1]. These ligands can link to solid phases such as silica gel, for using in different fields. How ever, they are very expensive owing to their difficult synthesis, tedious purifications and, in most cases, very low yield [2].

In this research work, we hope to prepare some new ligands as azacrown ethers, by reaction of prepared bis epoxide compound with suitable aliphatic diamines, which have been functionalized with OH group in their rings.

For this purpose, the bis cresyl sulfoxid reacted with epichlorohydrine to give bis epoxide compound. The new ligands were synthesized by reaction of bis epoxide with proper diamines. The structures of all prepared compounds have proved by spectral date including IR, ^{1}H NMR and ^{13}C NMR.







References

[1] Krakowiak. K. E., Bradshaw. J. S., Kent Dalley. N., Zhu. C., Yi. G., Curtis. J. C., Li. D., Izatt. R. M., **1992**, 57, 3166.
[2] Bradshaw. J. S., Krakowiak. K. E., Izatt. R. M., Tetrahedron. **2000**, 48, 4475.

An efficient one-pot three component synthesis of pyranoquinoline derivatives

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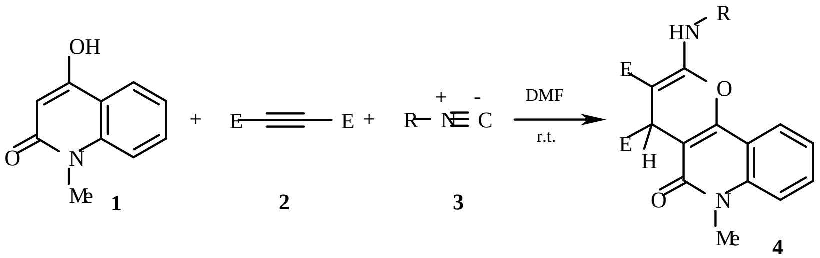
In recent years, pyranoquinoline derivatives have gained significant importance because of the wide range of their biological and pharmacological activities [1]. In view of the highly pronounced properties of pyranoquinolines several methods have been reported for the synthesis of these tricyclic compounds [2].

Herein, as part of our current studies on the synthesis of heterocyclic systems [3,4], we describe an efficient approach for the synthesis of pyranoquinoline derivatives *via* a one-pot three component reaction of 4-hydroxy-1-methyl-2(1*H*)-quinolinone **1** and dialkyl acetylenedicarboxylate **2** in the presence of alkylisocyanide **3** that leads to pyranoquinoline derivatives **4**.



	R	E	Yield (%)
4a	^{t}Bu	CO_2Me	80
4b	^{t}Bu	CO_2Et	85
4c	^{t}Bu	$CO_2{}^tBu$	76
4d	cyclohexyl	CO_2Me	88
4e	cyclohexyl	CO_2Et	85

The Structure of **4** was deduced from its ^1H, ^{13}C NMR, IR and mass spectra data.

References:

[1] Anniyappan, M.; Muralidharan, D.;Perumal, P. T. *Tetrahedron Lett.* **2003**, *18*, 3653.
[2] McLaughlin, M. J.; Hsung, R. P. *J. Org. Chem.* **2001**, *66*, 1049.
[3] Asghari, S; Salimi, A.; Qandalee, M. *Monatsh. Chem.* **2008**, 139, 1217.
[4] Asghari, S.; Tajbakhsh, M.; Taghipour, V. *Tetrahedron lett.* **2008**, *49*, 1824.

Synthesis of conducting and magnetic nanocomposite of $BaFe_{12}O_{19}/Fe_3O_4$/PEG multi-core/shell structure based polypyrrole

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The ferrite compounds and Fe_3O_4 have exhibited unique electric and magnetic properties based on the transfer of electrons between Fe^{2+} and Fe^{3+} in the octahedral sites. As an important magnetic material, Fe_3O_4 nanoparticles have been widely used in mineral separation, heat transfer applications, protein separation, efficient hyperthermia for cancer therapy, biosensors, MR contrast agents, dynamic sealing, recovery of metal irons, microwave adsorbing materials and so on [1-4].

In this paper, first, $BaFe_{12}O_{19}/Fe_3O_4$ nanocomposites with core-shell structure were successfully synthesized with two-step coprecipitation method. Then, we have prepared multi core-shell structure by adding PEG (polyethylene glycol) via one step masking shell method. Final shell was synthesized by in situ polymerization of pyrrole in the presence of $BaFe_{12}O_{19}/Fe_3O_4$/PEG nanoparticles to synthesize $BaFe_{12}O_{19}/Fe_3O_4$/PEG/PPy nanocomposite. The samples were studied by FTIR, X-ray diffraction (XRD), transmission electron microscope (TEM), atomic force microscopy (AFM), scanning electron microscopy (SEM) and vibrating sample magnetometer (VSM). XRD and TEM results indicated that the obtained nanoparticles have core-shell morphology. And FTIR spectra confirm, PEG masking and PPy final shell in the multi core-shell structure of the nanocomposites. Comparison of VSM measurements showed that core material, the coercivity and saturation magnetization of multi core-shell nanocomposites decrease obviously.

References:

[1] Bao,J., Chen,W., Liu, T.T., Zhu, Y.L., Jin, P.Y., Wang, L.Y., Liu, J.F, Wei, Li, Y.D. *Nano*, **2007**, 1, 4, 293.
[2] Dubus, S., Gravel, J.F., Drogoff, B.L., Nobert, P., Veres, T., Boudreau, D., *Anal. Chem.* **2006**, 78, 12, 4457.
[3] Brahler, M., Georgieva, R., Buske, N., Muller, A., Muller, S., Pinkernelle, J., Teichgraber, U., Voigt, A., Baumler,H., *Nano Lett.*, **2006**, 6, 11, 2505.
[4] Donia, A.M., Atia, A.A., Elwakeel, K.Z., *Hydrometallurgy*, **2007**, 87, 197.

The regioselective one pot synthesis of 2-alkyl-4*H*-benzo[1,4]thiazine-3-ones in ionic liquid

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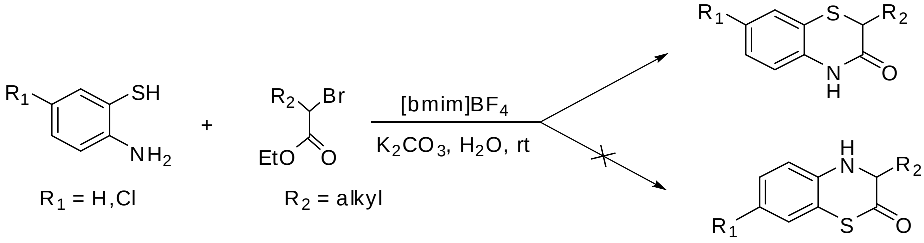
1,4-Benzothiazine is a molecule of interest to chemists and biologists due to being a subunit of various tissues such as feathers [1] and as a precursor for the synthesis of many biologically active heterocyclic molecules [2]. 1,4-Benzothiazine derivatives are found to possess a wide spectrum of biological activities such as antimicrobial, antifungal, anthelmintic activity [3] and aldose reductase inhibition property [4].

A series of 2-alkyl-4*H*-benzo[1,4]thiazine-3-ones were synthesized in high yields and in [bmim][BF_4] ionic liquid as the reaction medium via the cyclization of commercially available 2-amino thiophenols and ethyl-2-bromo-alkyl acetates in the presence of K_2CO_3 and water. Surprisingly, 3-alkyl-3,4-dihydrobenzo-[1,4]thiazine-2-ones did not form, as evidenced by the ^1H NMR spectra of the products.

As a result, a new efficient and one-pot regioselective synthesis of 2-alkyl-4*H*-benzo[1,4]thiazine-3-ones in [bmim][BF_4] is developed at room temperature. The ease of separation of benzothiazine products from the reaction medium is the foremost advantage of this process.



References:

[1] R. R. Gupta, Phenothiazines and 1,4 Benzothiazines: *Chemical and Biomedical Aspects*, Elsevier, Amsterdam, **1988**.
[2] J. Krapcho, A. Szabo, and J. William, *J. Med. Chem*,.**1963**, *6,* 214.
[3] C. V. R. Sastry, K. S. Rao, V. S. H. Krishnan, and K. Rastogi, *Indian J. Chem*., **1990**, *29B*, 297.
[4] T. Aotsuka, H. Hosono, T. Kurihara, Y. Nukihara, T. Matusi, and F. Kobayashi, *Chem. Pharm. Bull*., **1994**, *42*, 1264.

Synthesis and characterization of 1-amino -1-thioethyl-1, 1-diphosphonic acid and study of its effect on cancer cells and activated proteins

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The aminoethane-1, 1-diphosphonic acids constitute an important and interesting class of bisphosphonates analogues of the inorganic pyrophosphate with non-hydrolysable P-C-P structure, commonly known as bisphosphonates, strongly inhibit bone resorption. For more than 20 years, they have been used successfully for the treatment of bone disorders such as Paget's disease, cancer related hypercalcemia and post menopausal osteoporosis. Hypoxia is a unique physiological characteristic of solid tumors and is, therefore, an important therapeutic target [1]. The oxygen deficiency of solid tumors often leads to resistance to ionizing radiation and to many chemotherapeutic drugs. On the other hand, it also provides an opportunity for selective anticancer chemotherapy. Hypoxic tumor cells are known to have a greater capacity for reductive reactions as compared to well-oxygenated normal cells. Presently comprising nearly 1billion US$ of the global pharmaceutical market [2-4]. They are believed to act as complexing agents of bone calcium ions or affect enzyme essential metal ions. Their interaction with farnesyl Pyrophosphate synthase, glutamine synthase suggested as molecular targets, have shown that their action most strongly depends on the complexation on the metal ion present in the active centre of the enzyme [5]. On the other hand, the binding of bisphosphonates to calcified tissues is the basis for the use of these compounds as skeletal markers in nuclear medicine [6]. In other to prepare a synthetically useful bisphosphonic acid derivative with higher coordination ability and reactive moiety in the chelating system we choose Ethyl thiocyanate as initial material. Ethyl thiocyanate treated with a phosphorus tribromide, stirred 20 hrs at room temp. The mixture was decomposed with ice water, purified and recrystalized. The structure of 1-amino-1-thioethyl-1, 1-diphosphonic acid was characterized and confirmed by spectroscopic methods (IR, ^{13}C NMR, ^{1}H NMR).

References:

[1] Brown, J. M. *Methods Enzymol,* **2007**, 435, 297.
[2] R. Rawls, *Chem. Eng. News*, **1998**, 94, 38.
[3] R.E. Coleman, *Ann. Oncol,* **2000**, 11, 179.
[4] F.H. Ebetino, M. D. Francis, M. J. Rogers, R. G. G. Russell, Rev. *Contemp. Pharmacother,* **1998**, 9, 233.
[5] De Klark, J, J.M.H; Van Dijk , A.; Van Rijk, P. P.; et-al, *J. Nucl. Med*. **1991**, 32, 1082
[6] Pauwels, E. K.; Blom, J., et –al, *Eur. J. Nucl. Med*. **1983**, 8, 118

Fischer indole synthesis by using the $H_3PW_{12}O_{40}$ heteropolyacid as a green and reusable heterogeneous catalyst

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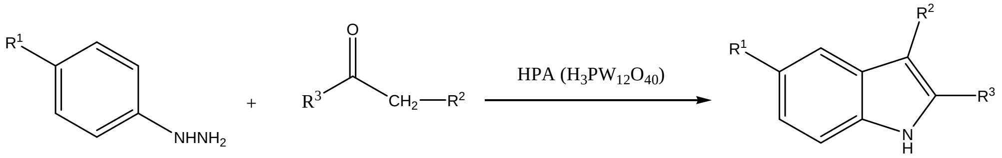
The indole ring system is probably the most ubiquitous heterocycle that represents an important structural component in many pharmacologically active compounds. Although many methods have been developed for the synthesis of indoles [1-3], Fischer indole synthesis is still one of the most versatile and widely employed methodologies for the preparation of indole intermediates and biologically active compounds [4,5].

In this work, a simple, efficient and green procedure one-pot Fischer indole synthesis approach has been developed by using the $H_3PW_{12}O_{40}$ heteropolyacid as a green and reusable heterogeneous catalyst. Yields of 60–93% were obtained after reaction in heteropolyacid catalysts at 70–100 °C in 0.5–2 h, and exclusive formation of 2,3-disubstituted indoles was observed in the reaction of alkyl methyl unsymmetrical ketones. This procedure offers several advantages including mild reaction condition, high yield of products, short reaction time, recyclability of the catalyst and easy work-up procedure. The indoles produced could be conveniently separated from the reaction mixture without any volatile organic solvents.



R^1: H, Cl, NO_2
R^2: alkyl
R^3: H, alkyl

References:

[1] Van Order, R. B.; Lindwall, H. G.; *Chem. Rev.* **1942**, *30*, 69.
[2] Gribble, G. W.; *J. Chem. Soc., Perkin Trans. 1* **2000**, 1045.
[3] Cacchi, S.; Fabrizi, G. *Chem. Rev.* **2005**, *105*, 2873.
[4] Robinson, B. *Chem. Rev.* **1963**, *63*, 373.
[5] Linnepe, P.; Schmidt, A. M.; Eilbracht, P. *Org. Biomol. Chem.* **2006**, *4*, 302.

Direct synthesis of $[TBA]_4[PW_{11}FeO_{39}].nH_2O/SiO_2$ composite and its catalytic performance in oxidation of sulfides with H_2O_2

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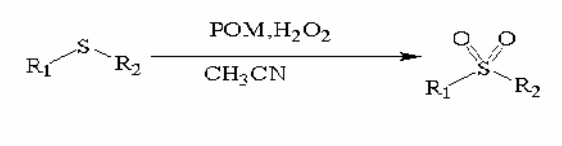
Oxidation of sulfides to sulfoxides or sulfones has been the subject of many studies. Organo sulfur compounds are useful intermediates in organic synthesis. Some oxidizing agents that used for this purpose including nitric acid, MnO_2, hydrogen peroxide, O_2 and so on[1,2].

The development of heterogeneous catalysts for the liquid phase oxidation of organic compounds is a challenging goal [3]. Transition metal substituted polyoxometalates (POM) have attracted much attention as oxidation catalysts due to their unique physical–chemical properties such as thermal and hydrolytic stability, motile acidities and red-ox potentials[4,5]. One of the disadvantages of POMs utilization as homogeneous catalysts is the difficulty of their separation from reaction mixture and their inevitable loss during recycling. Substantial efforts for the incorporation of POMs into the suitable inorganic solids have been reported as an effective method to overcome the mention problems [6–8].

In this work a polyoxometalates – composite was prepared by sol-gel technique and characterized by IR , UV, TG, SEM and XRD. The characterization results reveal that the $[TBA]_4[PW_{11}FeO_{39}]nH_2O$ disperse in the silica matrix and its structure remained intact after formation of the composite. This composite was used as an efficient heterogeneous catalyst for oxidation of sulfide by H_2O_2. it has been shown high to excellent yields and high reusability in oxidations of various sulfides with hydrogen peroxide.



References:

[1] C.L. Hill, C.M. Prosser-McCarthy, Cord. Chem. Rev. **1995**, 143, 407.
[2] R. Neumann, Prog. Inorg. Chem. **1998**, 47, 317.
[3] (a) R.C. Larock, Comprehensive Organic Transformations, Wiley–VCH, New York, **1999**.
[4] J. March, Advanced Organic Chemistry, John Wiley, New York, **1992**.
[5] Sheldon, R.A. Arends, I.W.C. Eten Brink, G.J. Dijksman, A. Acc. Chem. Res. **2002**, 35 , 774.
[6] Velusamy, S. Punniyamurthy, T. Org. Lett.**2004**, 6, 217.
[7] Zhan, B.Z. Thompson, A. Tetrahedron Lett.**2004**, 60, 2917.
[8] Mallat, T. Baiker, A. Chem. Rev.**2004**, 104, 3037.

Diphenylphosphorylated pegs (DPPPEGs) as new ligands and media for palladium-catalyzed carbon-carbon bond formation

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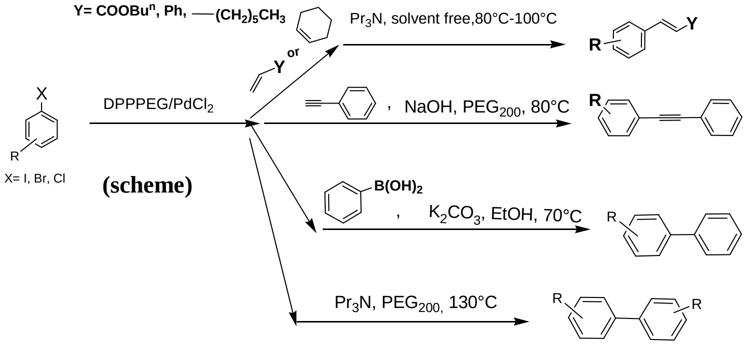
Cross-coupling reactions for carbon-carbon bond formation are among the most valuable synthetic methods developed over the past decade [1]. Apart from commonly used triarylphosphine ligands, and development of methods with non-phosphine ligands [2], great progress has been achieved in the field of catalytic reactions and new phosphine ligands have been developed [3-5]. The commercial availability of many PEG derivatives with two –CH_2OH end groups make it easy to prepare a variety of PEG supported ligands and catalysts [6]. Herein, we report on the use of easily prepared diphenylphosphorylated PEGs as media and also as bidentate ligands for Pd(II)-catalyzed carbon-carbon bond formation. For example, palladium–DPPPEG complexes have been employed as catalysts for the Mizoroki–Heck, Suzuki–Miyaura, Sonogashira and homocoupling reactions (Scheme). This method offers a very simple work-up procedure. DPPPEGs can be easily recovered for further use, because of their facile preparation methods.



(scheme)

References:

[1] (a) Beletskaya, I. P.; Cheprakov, A. *Chem. Rev*. **2002**,*100*, 3009-3066. (b) Yin, L.; *Chem. Rev*. **2007**, *107*, 133.

[2] Mino, T.; Shirae, Y.; Sasai, Y.; Sakamoto, M.; Fujita, T.; *J. Org. Chem.* **2006**, *71*,6834

[3] (a) Iranpoor, N.; Firouzabadi, H.; Azadi, R. *Eur. J. Org. Chem*. **2007**, *13,* 2197. (b) Iranpoor, N.;Firouzabadi, H.; Azadi, R.; *J. Organomet. Chem*, **2008**, *693*, 2469. (c) Safavi, A.; Maleki, N.; Iranpoor, N.; Firouzabadi, H.; Banazadeh, A. R.; Azadi, R.; Sedaghati, F.; *Chem. Commun*. **2008**, *14*, 6155. (d) Zotto, A. D.; Prat, F. I.; Baratta, W.; Zangrando, E.; Rigo, P. *Inorg. Chim. Acta*.**2009**, *362*, 97. (e) Iranpoor, N.; Firouzabadi, H.; Gholinejad, M. *Tetrahedron* **2009**, *65*, 7079.

[4] (a) Zheng, P.; Zhang, W. *J. Catal*. **2007**, *250,* 324. (b) Durgan, G.; Aksin, O.; Artok, L. *J. Mol. Catal. A* **2007**, *278*, 189. (c) Turkmen, H.; Pape, T.; Hahn, F. E.; Centinkaya, B. *Eur. J. Inorg. Chem***.** **2009**, *2*, 285. (d) Shang, Y-j.; Wu, J-W.; Fan, C-l.; Hu, J-S.; Lu, B-Y. *J. Organomet. Chem***.** **2008**, *693*, 2963.

[5] Littke, A. F.; Fu, G. C. *J. Am. Chem. Soc*. **2001**, *123*, 6989.

Cellulose sulfuric acid (CSA) as a bio-supported and recyclable solid acid catalyst for the synthesis of 2*H*-indazolo[2,1-b]phthalazine-triones and acetalization of carbonyl compounds as bis(cyclic acetals)

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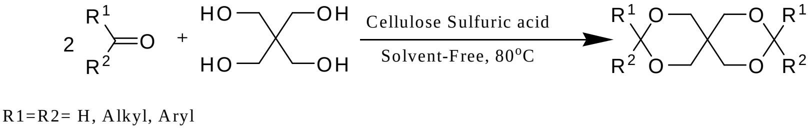
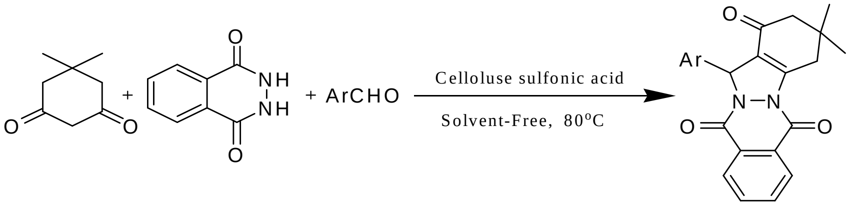
Cellulose and its derivatives have some unique properties such as inexpensive, extremely inert, and environmentally benign, which make them attractive alternatives for conventional organic or inorganic supports for catalytic applications. Recently, CSA has emerged as a promising biopolymeric solid support acid catalyst for various acid catalyzed reactions [1].

Pentaerythritol acetals in general are applied as plasticizers and vulcanizers, as physiologically active substance and as potential protective groups for aldehydes and ketones [2]. Herein, we report an efficient, green method for the acetalyization of carbonyl compound under solvent-free conditions with simple work-up and excellent yield in the presence of cellulose sulfuric acid as a reusable, biodegradable catalyst using pentaerythritol with aldehydes and ketones (Scheme 1).



Scheme 1

In addition, we reported an efficient method for the preparation of 2*H*-indazolo[2,1-b]phthalazine-trione derivates by the three-component condensation reaction of phthalhydrazide, dimedone, and aromatic aldehydes under solvent-free conditions in good to excellent yields and short reaction times using cellulose sulfuric acid as catalyst (Scheme 2).



Scheme 2

References:

[1] Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Rezazadeh, F. *Appl. Catal. A: Gen.* **2009**, *358*, 146.

[2] Rabindran Jermy, B.; Pandurangan, A. *Catal. Commun.* **2006**, *7*, 921. (b) Netherton, M. R.; Fu, G. C. *Org. Lett.* **2001**, *3*, 4295. (c) Liu, J.; Zhao, Y.; Zhao, Y.; Li, L.; Zhang, T. Y.; Zhang, H. *Org. Biomol. Chem.* **2003**, *1*, 3227.

[3] Bergbreiter, D. E.; Tian, J.; Hongfa, C. *Chem. Rev.* **2009**, *109*, 530.

Heteropoly acid encapsulated in polymer as an efficient catalyst for tetrahydropyranylation of alcohols and phenols

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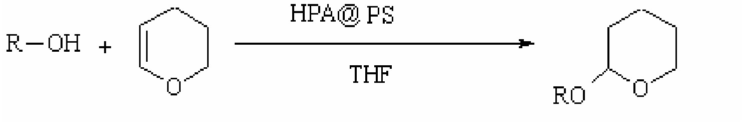
The protection of hydroxyl groups has found widespread application especially in steroids, sugars, glycerides and natural products. It is also useful for multi-step organic syntheses. The tetrahydropyranylation is one of the most frequently employed methods to protect hydroxyl group of alcohols and phenols. The THP ethers are attractive because they are less expensive and are stable enough to a variety of condition. A wide variety of catalysts already been applied for tetrahydropyranylation of alcohols and phenols including the use of protic acids, Lewis acids, ion exchange resins and etc. In this work heteropoly acid encapsulated in polymer was prepared and characterized by FT-IR, thermal gravimetry (TG), SEM techniques. This catalyst was used for tetrahydropyranylation of alcohols and phenols at room temperature.

In this catalytic system primary, secondary and tertiary alcohols and phenols were converted to their corresponding tetrahydropyranyl ether in excellent yield. At the end of each reaction, the catalyst was filtered and washed. No appreciable loss in the catalytic activity of the catalyst was observed after reusing the catalyst for four consecutive runs.



Reference:

[1] M. Moghadam, S. Tangestaninejad, V. Mirkhani, R. Shaibani, *Tetrahedron* **2004,** *60*, 6105.

[2] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, S.A. Taghavi, *J. Mol. Catal. A: Chem.* **2007**, *274*, 217.

[3] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, S.A. Taghavi, *Catal. Commun.* **2007**, *8*, 2087.

[4] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, S. Gharaati, *Polyhedron* **2010**, *29*, 212.

Cu-catalyzed addition of Grignard reagent to nitriles

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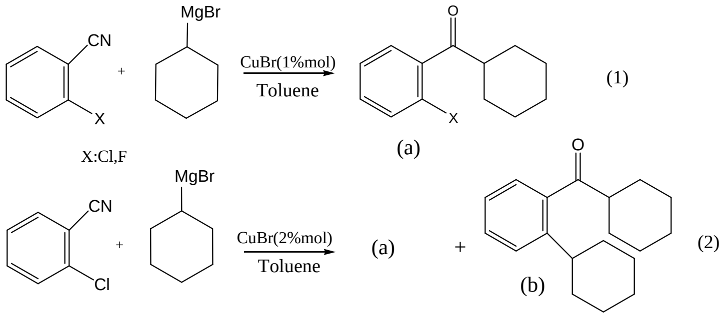
Reaction of Grignard reagents with nitriles is one of the most attractive and useful procedures in the formation of ketones. Although the addition of Grignard reagents to nitriles has been known for a long time [1], synthetically useful preparations using bulky reactants usually requires harsh conditions such as refluxing in high boiling solvents or under heating by microwave irradiation [2]. The nucleophilic addition of Grignard reagents to nitriles, especially when using sterically demanding components, is effectively catalyzed by copper(I) salts [3]. During the course of our studies on Cu-catalyzed reactions for the preparation of ketones, we realized that the reaction products depend on the nature of solvent and the percentage of CuBr catalyst. When the reaction is performed in THF in the presence of 2% catalyst the expected ketone (a) was obtained in a very low yield. When the same reaction was performed in toluene using 1% CuBr catalyst, 85% yield was achieved (eq. 1). Upon change of the percentage of catalyst to 2%, the expected ketone as well as product (b) was obtained(eq. 2). This is the first report of a coupling reaction between halobenzonitriles and Grignard reagent in the absence of additives such as 1,3-butadiene and NMP.



References:

[1] Kharasch M.S., Reinmuth.O. Prentice-Hall: New York, **1954**, 767.
[2] Gregg B.T., Golden K.C., Quinn J.F., Wang Hong-Jun, Zhang W., Wang R., Wekesa F., Tymoshenko D.O. *Tetrahedron Lett*. **2009**, 50, 3978.
[3] Weiberth F.J., Hall S.S. *J.Org. Chem*. **1987**, 52, 3901.

Free radical scavenging activity of various *Hyssopus Officinalis* extracts

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Hyssopus officinalis (Lamiaceae) is one of the most important pharmaceutical herbs that is extensively used as a food flavor and in sauce formulations [1]. It is used in tea blends for cough relief, for antispasmodic effects, and to relieve catarrh [2]. Hyssop possesses antifungal and anti-bacterial properties, insecticidal, antiplatelet and α-Glucosidase inhibitory activities [3].

Free radicals are created when cells use oxygen to generate energy. These by-products are generally reactive oxygen species (ROS) such as super oxide anion, hydroxyl radical and hydrogen peroxide that result from the cellular redox process. At low or moderate concentrations, ROS exert beneficial effects on cellular responses and immune function but at high levels, free radicals generate oxidative stress, a deleterious process that can damage cell structures, including lipids, proteins, and DNA [4].

In this study, various parts of *Hyssopus Officinalis* (leaf, stem and flower) were successively extracted with ethyl acetate, acetone, methanol and ethanol using a soxhlet extractor for 8 h each. The crude extracts were screened for free radical scavenging and reducing power activities. The data obtained in this study clearly establish the antioxidant potency of all extracts.

Refrences:

[1] Kazazi, H.; Rezaei, K.; Ghotb-Sharif, S. J.; Emam-Djomeh, Z.; Yamini, Y. *Food Chem.* **2007,** *105*, 805.
[2] Khazaie, H. R.; Nadjafi, F.; Bannayan, M. *Industrial Crops and Products*. **2008,** 27, 315.
[3] Tognolini, M.; Barocelli, E.; Ballabeni, V.; Bruni, R.; Bianchi, A.; Chiavarini, M.; Impicciatore, M. *Life Sci.,* **2006**, 78, 1419.
[4] Pham-Huy, L. A.; He, H.; Pham-Huyc, C. *International Journal of Biomedical Science,* **2008,** 4, 89.

Synthesis of novel benzimidazopiperazinone derivatives by Ugi 3CC reactions using bifunctional starting material

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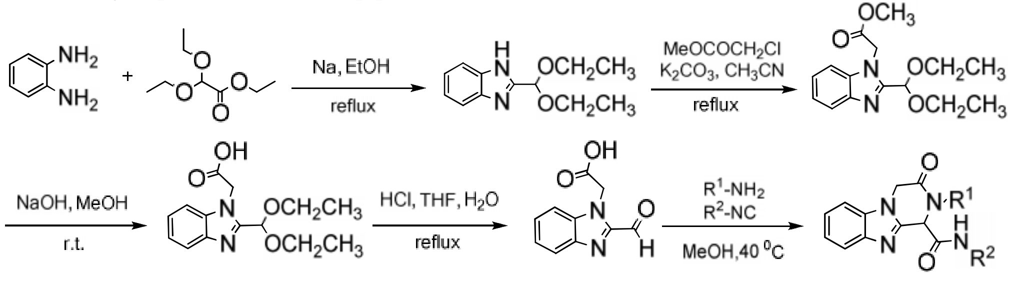
Piperazines, and their keto analogs are among the most important backbones in today's drug discovery [1]. Piperazines are the unique class of compounds with the privileged structures in molecules involved in the regulation of a wide variety of biological processes [2]. Ketopiperazines, the interesting examples of conformationally rigid cyclic peptidomimetics [3], are fragments of natural products of diverse structural complexity and biological activities [4]. Moreover, benzimidazoles with the known extensive biochemical and pharmacological properties [5], we envisioned that fusion of these moieties could rapidly identify new novel pyrazino[1,2-*a*]benzimidazole-3-one heterocycles.

In this poster, We have carried out the synthesis of 2-(2-formyl-1*H*-benzoimidazol-1-yl)acetic acid in four steps in order to use it as a formyl-acid bifunctional starting material with isocyanides and primary amines in Ugi 3CC. We have obtained the novel benzimidazole-fused 6-oxo-pyrazine-2-carboxamides. The structure of the products were elucidated using spectroscopic data.

In conclusion, by using a bifunctional starting material that have aldehyde and carboxylic acid functional groups in a Ugi 3CC reaction, novel heteroaryl-fused pyrazinones were prepared. The method offers several advantages including moderate to high yields of products and an easy experimental work-up procedure.



References:

[1] Thorp, D. S. *Pharmacogenomics J*. **2001**, *1*, 229.

[2] L_opez-Rodr_ıguez, M. L.; Ayala, D.; Benham_u, B.; Morcillo, M. J.; Viso, A. *Curr. Med.Chem*. **2002**, *9*, 1867.

[3] Gonz_alez, J. A.; Garc_ıa-L_opez, M. T.; Herranz, R. *J. Org. Chem*. **2005**, *70*, 3660.

[4] Govek, S. P.; Overman, L. E. *J. Am. Chem. Soc*. **2001**, *123*, 9468.

[5] Ansari, K. F.; Lal, C. *Eur. J. Med. Chem*. **2009,** *44*, 4028.

A convenient ultrasound-promoted regioselective synthesis of fused 6-amino-3-methyl-4-aryl-1H-pyrazolo [3,4-b]pyridine-5-carbonitrile

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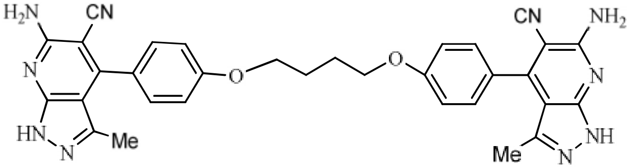
Pyrazolopyridines have received more and more attention in the recent years. Pharmaceutical researches of this kind of compounds have been reported, such as a potent cyclin dependent kinase 1 (CDK1) inhibitor, HIV reverse transcriptase inhibitors, CCR1 antagonists, protein kinase inhibitors, and inhibitors of cGMP degradation, together with several herbicidal and fungicidal activities [1].

Numerous methods for the synthesis of pyrazolopyridines in the last twenty years have been reported with respect to their different structures. The main disadvantages of most of these procedures are harsh reaction condition, tedious workup, low yield, high reaction time, multi-step reaction, use of large quantity of volatile organic solvents and low regioselectivity. Therefore, development of an efficient and versatile method is still required.

Our continued interest in the development of efficient and environmentally friendly procedure for the synthesis of pharmaceutical compound [2, 3] and removing the difficulties involved in the synthesis of pyrazolopyridine promoted us to evaluate the ultrasound assisted multicomponent synthesis of pyrazolopyridine-5-carbonitrile from malononitrile, substituted benzaldehyde and 3-methyl-5-aminopyrazole.



References:

[1] Quiroga, J.; Cruz, S.; Insuasty, B.; Abonia, R. *Heterocyclic Commun.* **2000**, *6*, 272.
[2] Mahmoodi, N.O., Tabatabaeian, K., Kosari, M., Zarrabi, S, *Chin. Chem. Lett*. **2008**, *12*, 1431.
[3] Kiyani, H.; Mahmoodi, N. O.; Tabatabaeian, K.; Zanjanchi, M. A. *Mendeleev Commun.*, **2009**, *19*, 203.

Photocatalytic ring opening of α-epoxyketones by DDQ in acetone

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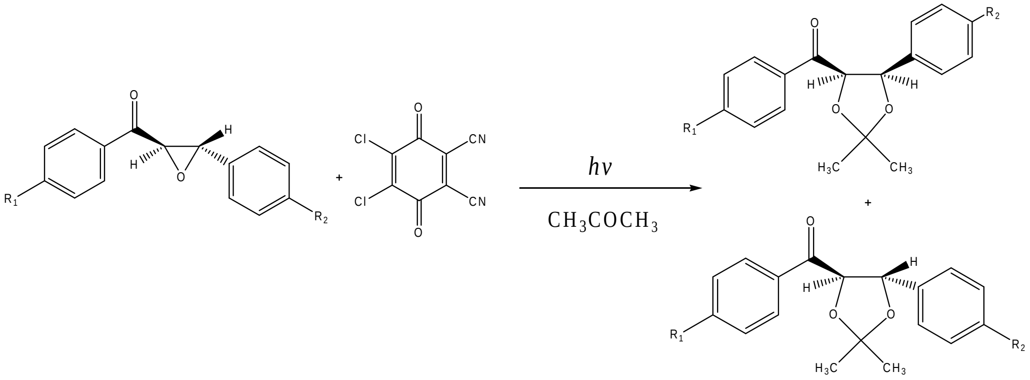
Polarized epoxides, due to their facile formation and higher reactivity toward nucleophiles, are of the most versatile building blocks in organic synthesis. Ring opening of epoxides and α-epoxyketones in the presence of various nucleophiles has received considerable attention in recent years. The ring opening of these compounds in the presence of various nucleophiles leads to the formation of some interesting compounds such as ethers, dioxolanes, and trioxolanes, partially owing to current interest in single electron transfer (SET) process and also because of potential application in organic synthesis. Such reactions have been recognized as important processes not only in thermal but also in photochemical transformations.

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) is a well-known electron-acceptor species and its interaction with a variety of electron donors has been the subject of several investigations. Photocatalytic ring opening reactions of α-epoxyketones by various photocatalysts in the presence of different nucleophiles have been extensively investigated to clarify the effect of the substituent on α-epoxyketones and also the nucleophilicity of solvent (acetic acid, acetone, cyclohexanone and methanol) on the rate and diastereoselectivity of reaction [1]. In continuation to these works, we were interested to investigate the behavior of these compounds towards electronically excited DDQ in acetone solution. The results will be presented.



References:

[1] Memarian, H. R; Saffar-Teluri, A. *J. Mol. Catal. A: Chem.* **2007**, *274*, 224.

Bronsted acidic ionic liquid catalyzed one-pot synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones under solvent-free conditions

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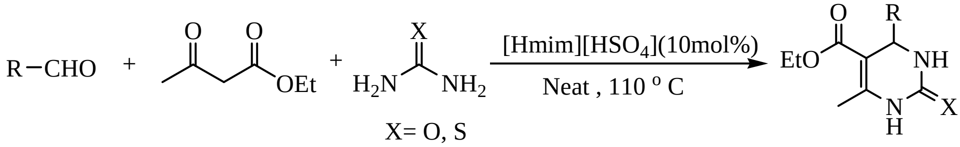
Using ionic liquids (ILs) is increasing with a very fast rate because of their beneficial properties such as undetectable vapor pressure, non-inflammability, wide liquid range, reusability and high thermal stability [1]. A subdivision of ILs is protic ionic liquids (PILs), which are produced through the combination of a Brønsted acid and Brønsted base [2]. These acidic ionic liquids have widely been applied in electrochemistry, synthesis of nanostructure materials, reaction media and catalyst [2]. Furthermore, Brønsted acidic ionic liquids can be designed to replace traditional mineral liquid acids such as sulfuric acid and hydrochloric acid in organic synthesis. There are various Brønsted acidic ionic liquids applied in organic synthesis. However, the majority of these ionic liquids are synthesized with a time-consuming and expensive procedure. Methyl imidazolium hydrogen sulfate [Hmim][HSO_4] has easily been synthesized and used as an efficient, inexpensive and reusable catalyst in organic synthesis [3]. Moreover, the present ionic liquid is halogen free and because of less carbon numbers, this ionic liquid has less toxicity. Herein we report, an efficient and convenient procedure for the synthesis of 3,4- dihydropyrimidin-2(1*H*)-ones and thiones by the one-pot three-component condensation of aldehydes, ethylacetoacetate and urea or thiourea in the presence of catalytic amount of methyl limidazolium hydrogen sulfate ([Hmim]HSO_4) as a Brönsted acidic ionic liquid under solvent-free conditions.



References:

[1] Welton, T. *Chem. Rev.* **1999**, *99*, 2071.
[2] Greaves, T. L.; Drummond, C. J. *Chem. Rev.* **2008**, *108*, 206.
[3] Hajipour, A.R.; Khazdooz, L.; Ruoho, A.E. *Catal. Commun.* **2008,** *9,* 89.

Synthesis of *N*-unsubstituted β-lactams from *N*-alkoxyphenyl-*β*-lactams with Cobalt(III) Fluoride or Argentic oxide

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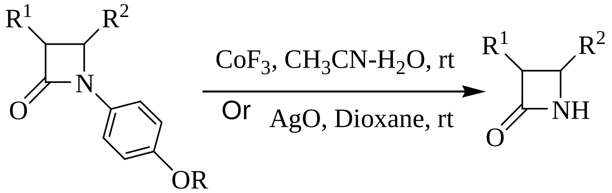
2-Azetidinones (β-lactams) have been of interest to the synthetic and medicinal chemists, as they are a structural part of the penicillin antibiotics, which have proved to be useful to the human health. In addition, there are many important non-antibiotic biological activities for 2-azetidinones [1]. They are also being used increasingly as valuable starting materials to develop new synthetic methodologies [2].

N-Unsubstituted β-lactams have been used as intermediates in the synthesis of β-lactam antibiotics and the glutamine synthase inhibitor, tabtoxin. The importance of *N*-unsubstituted β-lactams for the semisynthesis of the novel anticancer agents Taxol and Taxotere is also well documented [3]. *N*-Unsubstituted *β*-lactams have been prepared by several methods [4] but some of these methods are expensive and in some cases the yields of products were low.

Cobalt(III) fluoride has been used previously in preparation of quinones [5]. The argentic oxide has been used as an oxidizing agent in chemical reactions. It is commercially available and it has been used in some organic reactions [6]. Based on these arguments, we report herein the first example of oxidative *N*-dearylation of β-lactams using CoF_3 or AgO in mild reaction.



References:

[1] (a) Morin, R. B.; Gorman, M. *Chemistry and Biology of β-Lactam Antibiotics*, Academic Press, New York **1982**. (b) Jarrahpour, A.; Zarei, M. *Tetrahedron* **2009**, *65*, 2927.
[2] (a) Alcaide, B.; Almendros, P.; Aragoncillo, C. *Chem. Rev.* **2007,** *107*, 4437. (b) Jarrahpour, A.; Zarei, M. *Tetrahedron Lett.* **2007**, *48*, 8712.
[3] (a) Turos, E.; Heldreth, B.; Long, T. E.; Jang, S.; Reddy, G. S. K.; Dickey, S.; Lim, D. V. *Bioorg. Med. Chem.* **2006**, *14*, 3775. (b) Jarrahpour, A.; Zarei, M. *Synlett* **2008**, 381.
[4] (a) Jarrahpour, A.; Zarei, M. *Phosphorus Sulfur Silicon* **2009**, *184*, 1738. (b) Page, M. I. *The Chemistry of β-lactams*; Chapman and Hall, London, 1992.
[5] Tomatsu, A.; Takemura, S.; Hashimoto, K.; Nakata, M. *Synlett* **1999**, 1474.
[6] (a) McMillan, J. A. *Chem. Rev.* **1962**, 62, 65. (b) Sisko, J.; Henry, J. R.; Weinreb, S. M. *J. Org. Chem.* **1993**, *58*, 4945.

Reaction between pyrridin carbaldehyde derivativs and acetylenic esters the presence of triphenylphosphine

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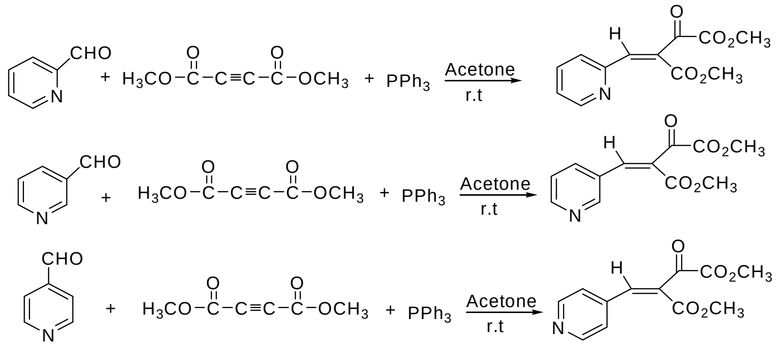
The carbon-carbon bond forming reaction involving the addition of nucleophiles to acetylenes is of great significance in organic synthesis.

The addition of triphenylphosphine to dimethylacetylenic di carboxylate in the precense of electron-defficient aromatic aldehydes such as pyrridin carbaldehyde derivatives leading to (Z)-dimethyl 2-oxo-3-(pyridin-2-ylmethylene) succinat , and (Z)-dimethyl2-oxo-3-(pyridin-3- ylmethylene) succinat , and (Z)-dimethyl2-oxo-3-(pyridin-4-ylmethylene) succinat. This product exist as a mixture of two geometrical isomers.



References:

[1] Nair, V.; Sreekanth, R.; Vinod, U.; *Organic letters*. **2001**, *3,* 3495.
[2] Yavari, I.; Alizadeh, A.; Anary-Abbasinejad, M . *Phosphorus, sulfur and silicon,* **2002**, *177,* 81.

New recoverable and reusable microencapsulated Bi(OTf)$_3$ catalyst for methoxymethylation of alcohols

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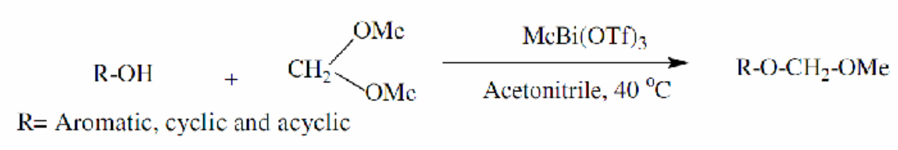
Functional group protection protocols play a very important role in synthetic organic chemistry [1]. The most commonly encountered functional groups for protection in organic synthesis are alcohols, carboxylic acids, and amines. For alcohols, protection sequences involving tetrahydropyranyl(THP) ethers [2] and methoxymethyl(MOM) ethers are frequently used.

Over the past few years, Bi(OTf)$_3$ has been reported as a new and efficient catalyst for organic synthesis, which exhibits, in numerous cases, a stronger activity than other known metal triflates, in particular those of transition elements[3]. In this direction, use of active homogeneous catalysts as well as heterogenized catalysts in an inert matrix has been widely explored. One of the major advantages associated with such heterogeneous catalysts is that they are reusable, and the expensive catalysts can be recovered from the reaction medium by simple filtration. There are several different ways by which active homogeneous catalysts have been heterogenized for use in organic synthesis. Perhaps a most attractive method known to date is microencapsulation of active catalysts in an inert organic polymer matrix [4].

Herein we report microencapsulation of Bi(OTf)$_3$ with poly(o-phenylenediamine) and use it as efficient catalysts for methoxymethylation of alcohols. We are particularly interested in Bi(OTf)$_3$ because it is inexpensive and can be easily prepared in laboratory from commercially available bismuth(III) oxide and triflic acid. Protection of aromatic, cyclic and acyclic alcohols was achieved by this method.



References:

[1] Greene, T.W. *Protective Groups in Organic Synthesis, Wiley, New York*, **1981**, 10.
[2] Parham, W.E.; Anderson, E. l. *J. Am. Chem. Soc.* **1948**, *70*, 4187.
[3] Vidal, S. *Synlett* **2001**, *7*, 1194.
[4] Donbrow, M. *Microcapsules and Nanoparticles in Medicine and Pharmacy, CRC Press, BocaRaton*, **1992**.

Synthesis of 2-amino-4H-chromene derivatives catalyzed by $ZrCl_4$

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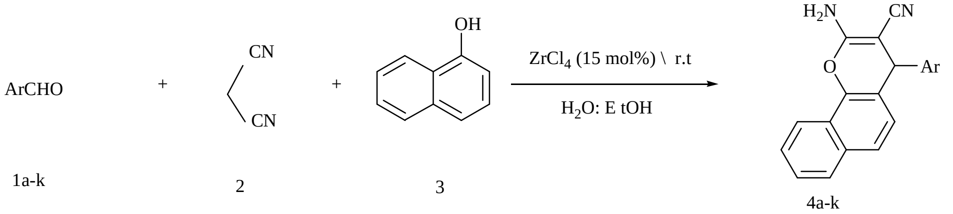
Polyfunctionalized naphth[b]pyrans and their derivatives are important classes of oxygenated heterocycles, which have attracted much interest because of the biological activities of naturally occurring representatives[1]. In addition, they can be used as cosmetics, pigments and utilized as potential biodegradable agrochemicals [2]. Zirconium(IV) chloride was founded as a useful catalyst resulting in higher selectivity, milder reaction conditions and easier work-up for many reactions.

The main methods for preparing these heterocycles consist of reaction between arylaldehyde, malononitrile and 1-naphthol as a one–pot synthesis. The continuous efforts have been devoted to the development of more general and versatile synthetic methodologies to this class of compounds[3].

Herein we wish to report the synthesis of 2-aminochromene derivatives catalyzed by $ZrCl_4$. The 2-amino -4H-naphth[b] chromene derivatives were obtained in slightly high yields (95–98%) .



1a-k:Ar=C_6H_5, 4-Br-C_6H_4,4-ClC_6H_4,4-CNC_6H_4,2,3-$Cl_2C_6H_3$, 2,4-$Cl_2C_6H_3$, 3OH-C_6H_4, 2NO_2-C_6H_4, 3-NO_2-C_6H_4, 4-$CF_3C_6H_4$, 3-ClC_6H_4

References:

[1] Issa Yavari, I.; Djahaniani, H.; Nasiri,F. *Tetrahedron Lett.* **2003**, *59*, 9409.
[2] Maggi, R.; Ballini, R.; Sartori, G. *Tetrahedron Lett*. **2004**, *45*, 2297.
[3] Abdolmohammadi, S.; Balalaie, S. *Tetrahedron Lett.* **2007**, *48*, 3299.

Synthesis of 7-nitro -5-(2'-fluorophenyl)-1, 3-dihydro-2H-1,4-benzodiazepin-2-one using hexamethylenetetramine (hexamine)

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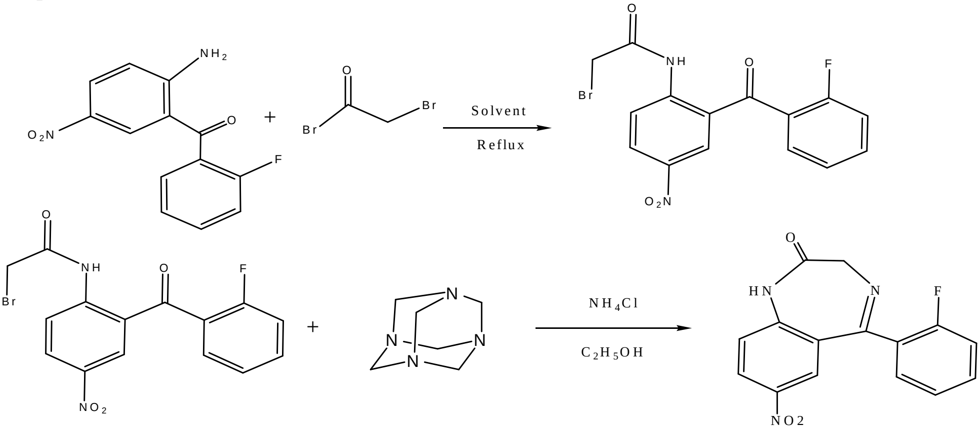
7-Nitro-1-methyl-5-(2'-fluorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one (Flunitrazepam) is a drug from family of 7-membered heterocyclic compounds 1,4-benzodiazepinones. Although a number of methods for synthesis of flunitrazepam have been reported in the literature but they suffer because of using anhydrous liquid ***ammonia*.**

In this research work the new method for synthesis of 1,4-benzodiazepin-2-one (II) an from 2-bromoacetamido-2,-fluoro-5-nitrobenzophenone, hexamethylenetetramine(**hexamine) and ammonium chloride in ethanol** will be reported.

2-Bromoacetamido-2,-fluoro-5-nitrobenzophenone starting material was prepared from reaction of 2amino-2’-fluoro-5-nitrobenzophenone and bromoacetyl bromide in DCM at reflux temperature.



The results indicate that the best yield cyclisation reaction obtained when the mole ratio of the components acetamide: NH_4C l: hexamine in order was as 1.0: 2.5: 3.0.
The structure of product was evaluated by melting point, ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, GC-Mass and IR spectroscopy techniques.

References :

[1] H.Boemches. *Ger. Offen. 2334273,(***1974**) .
[2] R.I. Freyer. *US Patent No. 3247187(***1966***).*
[3] V. N. Anikeev,1 A. I. Petrunin,2 M. T. Kilin,3 and F. V. Guss4 NITRAZEPAM SYNTHESIZED BY, Pharmaceutical Chemistry Journal Vol. 38, No. 5, **2004**, 261.
[4] I. Panderi a, H. Archontaki b, E. Gikas a, M. Parissi-Poulo; Journal of Pharmaceutical and Biomedical Analysis, 17 (**1998**) 327.

Direct synthesis of novel thermally stable and optically active poly(ester-imide)s derived from α-amino acids

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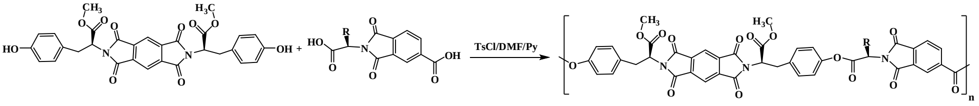
Materials that incorporate α-amino acids have generated significant interest because they offer certain advantages over conventional polymer systems [1]. The resulting polymers are optically active and have special chemical activities such as catalytic properties that exist in genes, proteins and enzymes [2]. Since amino acids are naturally occurring compound, synthetic polymers based on these materials are expected to be biodegradable and are therefore classified under environmentally friendly polymers [3]. Poly(ester imide) (PEI) is known as an important type of high-performance polymers because of its outstanding properties, such as excellent mechanical properties, thermal stability, chemical resistance, and low melting viscosity [4-5].

Herein, for the first time, we wish to report the synthesis and characterization of novel PEIs which have two different types of amino acids in the main chain. Direct polymerization reactions of different chiral diacids derived from L-phenylalanine, L-leucine, L-methionine, L-valine and L-Isoleucine with nontoxic diphenolic monomer of L-tyrosine were performed in a system of tosyl chloride, pyridine and *N,N*-dimethylformamide as a condensing agent. The synthesized polymers were characterized by means of FT-IR, ^{1}H-NMR, elemental and thermogravimetric analysis techniques. These PEIs show optical rotation and are readily soluble in various organic solvents and have moderate thermal stability.



R: $PhCH_2$-, $(CH_3)_2CHCH_2$-, $CH_3CH_2CH(CH_3)$-, $CH_3SCH_2CH_2$-, $(CH_3)_2CH$-

References

[1] Nair, L.; Laurencin, C. T. *Prog. Polym. Sci.* **2007**, *32*, 762.
[2] Wang, B.; Yao, Y., Peng, J.; Lin, Y.; Liu, W.; Luo, Y.; Xiang, R.; Wu, D. *J. Appl. Polym. Sci.* **2009**, 114, 883.
[3] Guo, K.; Chu, C.C. *Biomacromolecules* **2007**, *8*, 2851.
[4] Huang X, Xu, Y, Zong, L, *Polymer,* **2009**, *50*, 2793.
[5] Mallakpour, S.; Tirgir, F.; Sabzalian, M. R. *J. Polym. Res*. In Press **2010**.

N-heterocyclic carbene–palladium complex immobilized on silica for Suzuki coupling reaction

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N-Heterocyclic carbenes (NHCs) have been known to be outstanding ligands for a variety of organometallic complexes that are key components in catalysis.These system provide very effective ligands for supported catalysis showing enhanced stability and functioning at low loading levels of catalyst.

In particular, the support of Pd–NHC complexes is of utmost importance because of the high activity of these complexes in coupling chemistry [1]. Different supporting materials and approaches have been exploited for the immobilization of palladium precursors which include polymer supported NHC–Pd[2], silica coated nanoparticle supported NHC–Pd [3], NHC–Pd complex/ionic liquid matrix onto silica and NHC–Pd complexes immobilized onto clays [4].

This letter reports a method for preparing a novel silica-support *N*-Heterocyclic carbene–palladium complex. NHC-Pd/silica exhibited excellent performance in the Suzuki reaction of various aryl halide derivatives with phenylboronic acid in the aqueous phase. These heterogenous catalysts can be recycled >>5 times with no loss of activity.

References:

[1] William, J.; Sommer.; M, Weck. *Coordination chemistry. Rev.* **2007**, 251, *860*, 873.
[2] Steel, P. G.; Teasdale, C. W. T. *Tetrahedron Lett*. **2004,** *45*,7789.
[3] Stevens, P. D.; Li, G.; Fan, J.; Yen M., Gao ,Y. *J. Chem. Soc. Chem. Commun*. 2**005,** 3544.
[4] Mas-Marz´a, E. A. M. Segarra, C. Claver, E. Peris, E. Fernandez, *Tetrahedron Lett.* **2003,** *44,* 6595.

Esterification of 9-anthracenecarboxylic acid with 2-hydroxyethyl methacrylate

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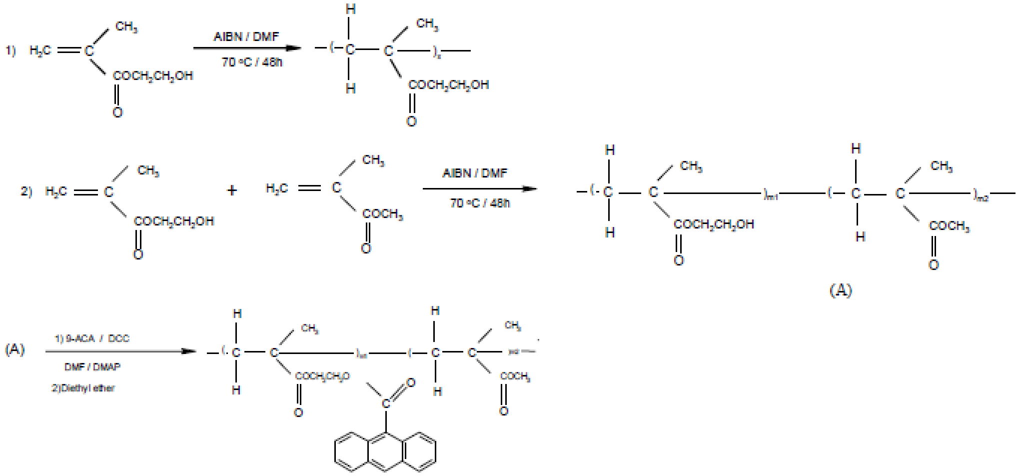
It is well known that N,N'-dicyclohexylcarbodiimide (DCC) plays a vital role in organic chemistry and that it is widly used as an activating/dehydrating agent in the synthesis of various organic compounds. A widly used and promising method for esterification is the carbodiimide coupling approach, invovling interaction between the acid and alcohol in the presence of (DCC) and 4-(dimethylamino) pyridine (4-DMAP) as catalysts [2]. In this work the homopolymer of 2- hydroxyethyl methacrylate (HEMA) and its random copolymers with methyl methacrylate (MMA) (in 1:1 mole ratio) were synthesized by free radical polymerization method in N,N-dimethyl formamide (DMF) solution, utilizing a,a,-azobis (isoboutyronitrile) (AIBN) as initiator at the temperature range of 65- 70°C. Then, homopolymer and copolymers of HEMA have been modified by incorporation of 9-anthracenecarboxylic acid (9-ACA) in of polymers in presence of (DCC), (4-DMAP), and (DMF) [1]. It was found that the molar ratio acid/ alcohol/ catalyst is eguालts 0.02: 0.02: 0.002, optimal for preparation of the ester. The results show that, with the incorporation of the(9-ACA) in the polymer side chains, a series of novel modified polymer containing new properties are obtained that can find some applications in polymer industry[3]. The obtained polymers were characterized by FT-IR and 1H-NMR.



References:
[1] Tsvetkova, B.; Tencheveva, J.; Peikov, P. *Acte Pharm*. **2006,** 56, 251.
[2] Babazadeh, M.; Edjlali,L.; Rashidian,L. *J.Polym.* **2007,** 14, 207.
[3] Safa, K. D.; Nasirtabrizi, M.H., *Eur. Polym. J*. **2005**, 4, 2310.

Polyoxazoline-β-cyclodextrin hyperbranched copolymers as drug delivery

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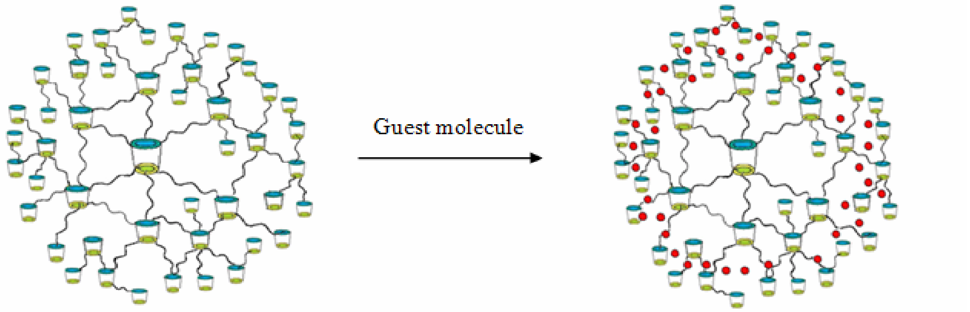
A novel class of biodegradable hyperbranched polymers containing poly (2-ethyle-2-oxazolines) (PEOz) and β-cyclodextrin (β-CD) were synthesized for drug delivery system. In this synthetic strategy tosylated β-CD was prepared and it used as macroinitiator for ring opening polymerization of oxazoline monomer and poly(CD-EOz) was obtained. Polymerization was quenched using different molecules and hyperbranched polymers with different properties, such as solubility and loading capacity were obtained [1,2]. Congo red and Ag nanoparticle were encapsulated by poly(CD-EOz) hyperbranched polymers and were characterized by ^{1}H NMR, FTIR , UV, differential scanning calorimetric (DSC) and transmission electron microscopy (TEM) [3,4]. The controlled release of guest molecule from hyperbranched polymer / guest molecule complex in vitro condition also investigated.



References:

[1] Santander-Ortega, M.J.; Stauner, T.; oretz, B. ; Ortega-Vinuesa , J.L.; Bastos-González, D. ; Wenz, G.; Schaefer, U.F.; Lehr, C.M. *Journal of Controlled Release.* **2010,** 141, 85.
[2] Kumari, A.; Kumar Yadav, S.; Yadav, S.C. *Colloids and Surfaces B: Biointerfaces.* **2010,** 75, 1.
[3] Liu, J.; Pang,Y.; Huang, W.; Zhu, X.; Zhou, Y.; Yan, D. *Biomaterials* .**2009**, doi:10.1016/j. biomaterials. 2009.10.021.
[4] Aryal, S.; Prabaharana, M.; Pilla, S.; Gonga, S. *International Journal of Biological Macromolecules* .**2009,** 44, 346.

Synthesis of new derivatives of pH sensitive fluorescine

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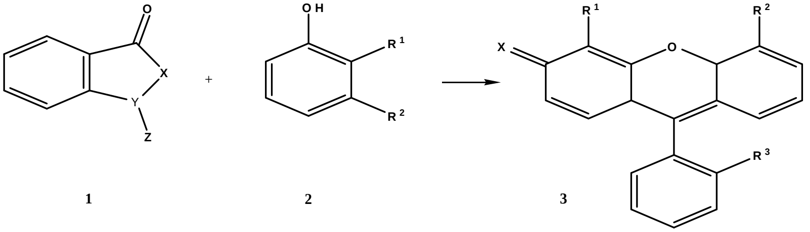
The recent explosion in new fluorescence applications is accelerating the pace of research and development in basic and applied life science, including genomics, proteomics, bioengineering, medical diagnosis and industrial microbiology. [1-2]

In this study, we try to report the synthesis of new derivatives of fluorescine using phethalic anhydride or sodium saccharin (**1**) and phenol derivatives (**2**) in the presence of $ZnCl_2$. The structures of products (**3**) were elucidated by IR, UV and NMR spectroscopy. The fluorescence properties were studied by fluorometry. Also the effect of pH on the fluorescent properties was investigated. The results indicated that all of synthesized compounds had proper fluorescence properties at 200-550 nm. These compounds were better fluorescent agents in acidic media.



1	**X**	**Y-Z**
a	O	C=O
b	NH	SO_2

2	**R_1**	**R_2**
a	H	OH
b	CH_3	OH
c	H	NH_2

3	**X**	**R_1**	**R_2**	**R_3**
a	O	H	H	CO_2H
b	O	CH_3	CH_3	CO_2H
c	NH	H	H	CO_2H
d	O	H	H	SO_2NH_2
e	O	CH_3	CH_3	SO_2NH_2

References:

[1] Hibbert . E. J. Soc. Dyes Colour **1927**, 44, 292.
[2] Clarke. E. A .Int. Dyer. **1981**, 165, 5,250.

Antimicrobial activities of fused 2-amino-4*H*-pyranes derived from TOSMIC and acetylenic esters in the presence of cyclic *CH*-acids

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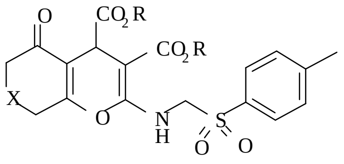
During the last twenty years, the study the biological activity of chromene derivatives has been the aim of many scientists [1]. Fused chromenes are interested due to their significant antibacterial and novobiocin activity. The chemistry of poly functionalized 4*H*-pyranes are also an ongoing area of interest because of their wide range of applications [2]. We have perversely reported the reaction between cyclic and acyclic CH-acids with acetylenic esters in the presence of alkyl isocyanides to produce highly functionalized 2-amino-4*H*-pyranes [3,4]. In this work we wish to report the antimicrobial activities of fused 2-amino-4*H*-pyrane derivatives **1** and **2** derived from the reaction of TOSMIC and acetylenic esters in the presence of cyclic CH-acids against Gram-positive and Gram-negative bacteria. These activities were tested *in vitro* using two reference bacteria strains. e.g. *Staphylococcus aureus* and *Escherichia coli.* These compounds were active against both strains tested by disk diffusion method in ranging 6 to 17 mm per 1000 µg disk.



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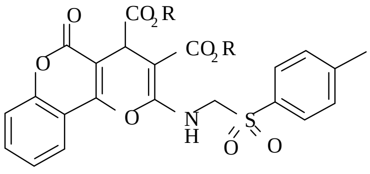

2

X: CH_2, CMe_2; R: Me, Et

References:

[1] Vaccaro, W.; Yang, B.; Kim, S.; Huynh, T.; Leavitt, K.; Li, W. *Wo Patent* 2004, 4009017.
[2] Elnagdi, M. H.; Elfaham, H. A.; Elgemeie, G. E. H. *Heterocycles,* **1983**, *20*, 519.
[3] Nasiri, F.; Nazem, F.; Pourdavaei, K. *Mol. Div*ers. **2007**, *11*, 101.
[4] Maghsoodlou, M. T.; Yavari, I.; Nasiri, F.; Djahaniani, H.; and Razmjoo, Z. *Monats Chem.*, **2003**, *134*, 1585.

$PVP\text{-}(H_2SO_4)_n/NH_4NO_3$: As an efficient system for the first *mono* and *di*-nitration of Bisphenol A as well as nitration of the other phenols

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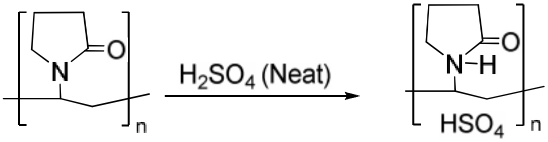
Solid acids have many advantages such as simplicity in handling, decreased reactor and plant corrosion problems, and more environmentally safe disposal. Also, wastes and by-products can be minimized or avoided by developing cleaner synthetic routes [1]. On the basis of our experiences in the application of solid acids [2], we found that poly vinyl pyrrolidone (PVP) reacts with concentrated sulfuric acid to give $PVP\text{-}(H_2SO_4)_n$. It is interesting to note that this exothermic reaction is easy and clean without any required work-up procedure (Scheme 1).



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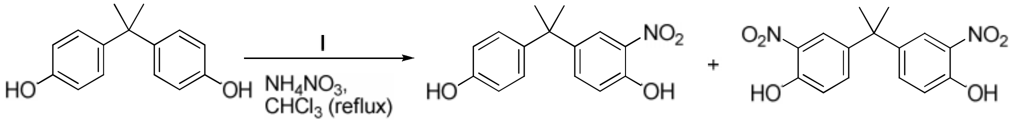
Scheme 1.

In continuation of our studies on the nitration of phenols [3], we were interested in using the $PVP\text{-}(H_2SO_4)_n$ for the *in situ* generation of NO_2^+ in combination with NH_4NO_3 and wet SiO_2 and eventually nitration of phenols. Herein, we wish to report a simple, economical and effective method for the first *mono* and *di*-nitration of Bisphenol A as well as nitration of the other phenols (Scheme 2).



Scheme 2.

References:

[1] Shirini, F.; Zolfigol, M. A.; Salehi, P.; Abedini, M. *Curr. Org. Chem.* **2008**, *12*, 183.
[2] Zolfigol, M. A.; Ghaemi, E.; Madrakian, E.; Ghorbani Choghamarani, A. *Mendeleev Commun.* **2006**, 41.

Synthesis of *β*-acetamido ketones *via* one pot multicomponent reaction catalyzed by *L*-pyrrolidine-2-carboxylic acid-4-hydrogen sulfate

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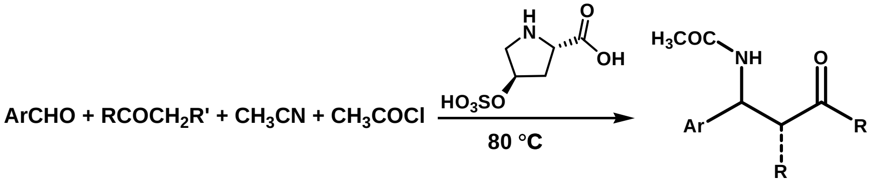
During the last few years, multi-component reactions (MCRs) have proved to be remarkably successful in generating molecular complexity in a single synthetic operation [1]. Multicomponent reactions (MCRs) are important for the achievement of high levels of diversity, as they allow more than two building blocks to be combined in practical, time-saving one-pot operations, giving rise to complex structures by simultaneous formation of two or more bonds, according to the domino principle. *β*-Acetamido ketones are versatile intermediates in that their skeletons exist in a number of biologically or pharmacologically important compounds. These compounds are important building blocks for the synthesis of molecules such as 1,3-amino alcohols and structural scaffolds found in natural nucleoside peptide antibiotics such as nikkomycins or neopolyoxins [2].

In continuing of our investigation on the application of new catalysts or reagents in organic functionalization [3-4], we became interested to introduce a new acidic catalyst for the preparation of *β*-acetamido ketones. In a typical procedure, the reaction of enolisable ketones, acetyl chloride, acetonitrile with various aromatic aldehydes in presence of 0.65 mol% of *L*-pyrrolidine-2-carboxylic acid-4-hydrogen sulfate proceeded smoothly at 80 °C in 4 h to afford reasonable yields of *β*-acetamido ketones (Scheme 1).



Scheme 1

References:

[1] Bora, U.; Saikia, A.; Boruah, R. C. *Org. Lett.* **2003**, *5*, 435.
[2] Enders, D.; Moser, M.; Geibel, G.; Laufer, M. C. *Synthesis* **2004**, 2040.
[3] Ghorbani-Choghamarani, A.; Zolfigol, M. A.; Rastegar, T. *Chin. J. Catal.* **2009**, *30*, 273.
[4] Ghorbani-Choghamarani, A.; Nikoorazm, M.; Goudarziafshar, H.; Tahmasbi, B. *Bull. Korean Chem. Soc.* **2009**, *30*, 1388.

Conformational analysis and experimental single crystal X-ray of *N,N'*-dibenzylideneethylenediamine derivatives

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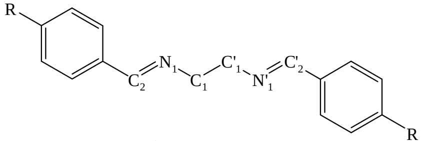
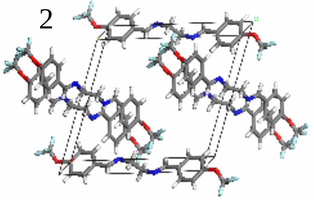
Schiff base derivatives of *N,N'*-Dibenzylideneethylenediamine **1** ($RC_6H_4CHNCH_2CH_2NCH$-C_6H_4R, R=H) have been widely studied in the literature [1-4]. Two derivatives of **1** including *N,N'*-bis(4-trifluoromethoxybenzylidene)ethylenediamine **2** ($R=OCF_3$), and *N,N'*-bis(4-dimethylamino-benzylidene)ethylenediamine **3** ($R = N(CH_3)_2$), compounds were prepared and characterized by X-ray crystallography. The molecule **2** is anti, while the molecule **3** has gauche conformation in solid state. To determine conformational stability, molecular energy profile of each of these compounds were obtained by B3LYP/6-31++G** and HF/6-31++G** levels of theory. Based on the calculations, there are seven minima in the calculated potential energy curves. A gauche conformer has the lowest energy minimum (gas phase) among the other conformers. This is in contrast to X-ray finding (solid phase) of compounds **1** and **2** but complements the X-ray result of compound **3**. These results were analyzed by natural bond orbital (NBO) and molecular orbital (MO) to determine the role of intra- and intermolecular interactions in the crystal structures.



Compound	1	2	3
R	-H	$-OCF_3$	$-N(CH_3)_2$

2



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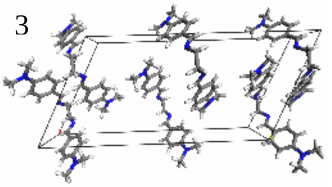

References:

[1] Unaleroglu C.; Temelli B.; Hokelek T. *J. Mol. Struct.* **2001**, *570*, 91.

[2] Habibi M. H.; Montazerozohori M.; Lalegani A.; Harrington R. W.; Clegg W. *J. Fluor. Chem.* **2006**, *127*, 769.

[3] Habibi M. H.; Montazerozohori M.; Barati K.; Harrington R. W.; Clegg W. *Analytical Sciences* **2007**, *23*, x47.

[4] Habibi M.H.; Montazerozohori M.; Barati K.; Harrington R.W.; Clegg W.; Choi J.H. *Analytical Sciences* **2007**, *23*, x117.

Conjugated dienes: the Effects of substitutional group

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The chemical reactivity and the distinguished electronic structure of many unsaturated molecular systems were of a great interest for many years [1-4]. When the conjugation of diene is absent in other saturated analogues, it was found that the rotation around the C-C or the C-N single bond is less hindered with relatively lower energetic barriers as compared to unsaturated ones [1,2]. Additionally, the torsional potential is considered as a sensitive probe of the electronic structure of molecules leads to interesting conclusions on interactions between the double bond and the substituent, such as destabilizing steric perturbations and electronic conjugation [1]. A diene system tends to be planar for maximizing the conjugation. Firstly for understanding the effect of dihedral angle and the degree of conjugation on single C-C bond strength, the length of this bond that represents the bond strength were calculated. This was seen that the planar form of it minimized the energy but in *cis* configuration, the steric eclipsing decreases the stability of it. For understanding the effect of substitutional group on the structure of dienes, the structure of several substituted conjugated diene (C=C-C=C) systems were optimized with the HF and MP2 methods and the 6-311++G** basis set. It was predicted that the planar form of dienes (180 degree for *trans* and zero for *cis* configuration) in which the conjugation of two double C=C bond is maximized, have more stability in comparison with other dihedral angle. But in some cases, the spatial problem lowers the stability of *cis* configuration. On the other hand the steric crowding is minimum in *trans* configuration so the dihedral angle of the dienes tend to be equal to 180. But in unusual cases the interaction of substitution to diene makes the non-planar dienes more stable. As a other considerable result, the energy difference between *cis* and *trans* configuration is small in some cases. For instance the energy difference between two configuration in $(OH)_2C{=}CH{-}CH{=}C(NH_2)_2$ and $(NH_2)_2\,C{=}CH{-}CH{=}CF_2$ are considerably low. This might be consequence of intramolecular hydrogen bonding.

References

[1] H.M. Badawi, *J. Mol. Struct. (Theochem)*, 343 (**1995**) 117.
[2] H.M. Badawi, A. Al-Rayyes, *J. Mol. Struct. (Theochem)*, 428 (**1998**) 247.
[3] W. Forner, H.M. Badawi, *Asian J. Spectrosc.*, 2 (**1998**) 72.
[4] A. Al-saadi and H. M. Badawi, *J. Mol. Model.*, Vol. 582, 153(**2002**).
[5] H.M. Badawi, *J. Mol. Struct. (Theochem)*, 336 (**1995**) 21.
[6] H.M. Badawi, A.A. Al-Rayyes, *J. Mol. Struct. (Theochem)*, 397 (**1997**) 51.
[7] H.M. Badawi, W. Forner, *Asian J. Spectrosc.*, 3 (**1999**) 169.

Nanocasted and supported $Cu_{3/2}PMo_{12}O_{40}$: Efficient catalysts for the synthesis of amides from benzylalcoholes and nitriles

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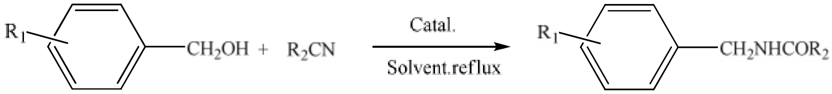
Heteropoly acids (HPAs) with the Keggin structure are the most studied class within polyoxometalates because they possess relatively high thermal stability and acidity. Supported HPAs are important for many applications because bulk HPAs have low specific structure areas (1–10 m^2/g). It is important to increase the surface area or even better to increase the number of accessible acid sites of the HPAs. This can be achieved by dispersing the HPAs on a solid support with a high surface area [1]. In a heterogeneous system, it is possible to control the solid strength by supporting HPAs on different carriers. Immobilization of HPAs on a number of porous supports such as silica, active carbon, montmorillonite K-10, and zeolite was therefore extensively studied SiO_2, which is relatively inert towards HPAs, is the most often used [2, 3].

The discovery of many types of mesoporous silicas, such as SBA-15, KIT-6, FDU-12 and SBA-16, porous crystalline transition metal oxides have been synthesized using the mesoporous silicas as hard templates. The elimination by HF of the silica matrix from the composites obtained by the two-step reaction deposition of $Cu_{3/2}PMo_{12}O_{40}$ salt nanocrystal [4]. We have used 2D hexagonal SBA-15 silicas as templates for the nanofabrication of $Cu_{3/2}PMo_{12}O_{40}$ nanoparticles.

Herein, we wish to report a mild and efficient method for the preparation of amides from benzyl alcohols and nitriles in the presence of a catalytic amount of $Cu_{3/2}PMo_{12}O_{40}/SiO_2$ and $Cu_{3/2}PMo_{12}O_{40}$ nanocrystal.



References:

[1] Dias, J. A.; Caliman, E.; Dias, S. C. L.; Paulo, M.; de Souza, A. T. C. P. *Catal Today*, **2003**, *85*, 39.
[2] Kozhevnikov, I. V. *Catal. Rev. Sci. Eng.* **1995**, *37*, 311.
[3] Kozhevnikov, I .V.; Sinnema, A.; Jansen, R. J. J.; Pamin, K.; Van Bekkum, H. *Catal Lett*, **1995**, *30*, 241.
[4] Madhusudhan Rao, P.; Goldberg-Oppenheimer, P.; Kababya, S.; Vega, S.; Landau, M.V. *J. Mol. Catal. A: Chem.* **2007**, *275*, 214.

Synthesis and characterization of nano-sized iron oxide as a catalyst in the organic reactions

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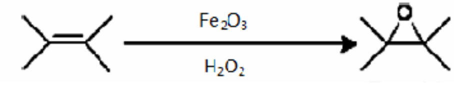
The synthesis and characterization of nano-structured Iron oxide is of immense interest in current research because of fundamental and technological advantages. A wide variety of applications such as catalysis involving nanoparticles is now an industrial reality [1]. Nanoparticles of metals and metal oxides have been extensively used as catalysts in many organic reactions because of their high surface area and facile separation [2]. Nanoparticles are intrinsically unstable and often tend to form agglomerates to reduce the energy associated with the high surface area/volume ratio because of their small particle size. In the past decade, the synthesis of superparamagnetic nanoparticles has received increased attention not only for its fundamental scientific interest, but also for many technological applications: such as magnetic storage media [3], biosensors, medical applications [4], and magnetic ink for printing. Amongst iron oxide nanoparticles, maghemite (ϒ-Fe_2O_3) is ferromagnetic and characterized by the superparamagnetic relaxation phenomenon, which is strongly affected by particle size, shape and various surface effects. Recently, several methods for the preparation of ϒ-Fe_2O_3 nanoparticles have been developed, e.g. thermal decomposition of lepidocrocite, co-precipitation from solution and laser pyrolysis , microwave plasma, electrochemical synthesis, sol–gel method, and mechanical activation. Several magnetic oxide nanoparticles including ϒ-Fe_2O_3 and magnetite have also been synthesized by using microemulsion and other methods [5]. In this paper, nano-sized iron catalyst prepared by microemulsion method. Sodium dodecyl sulfate (SDS) as a surfactant and a solution contained 1-butanol and chloroform used as an organic solvent. The precipitate was washed with water and acetone and gathered from filter. The precipitate was dried in an oven at 120 ^oC for 16 hour then calcinated in flowing dry air at 300 ^oC for 2 hours. The nano iron oxide was characterized by XRD, TEM and BET techniques. Applications of nano-sized iron oxide was investigated as catalyst in the organic reactions. One of these applications is epoxidation of olefins which is widely used in the synthesis of many commodity and fine chemicals as well as pharmaceuticals and agrochemicals.



Resrences

[1] H. Cao, S.L. Suib, *J. Am. Chem. Soc*. **1994,** *116*, 5334.
[2] I.W.C.E. Arends, *Angew. Chem.* **2006,** *118*, 6398.
[3] Q. Guo, X. Teng, S. Rahman, H. Yang, *J. Am. Chem. Soc*. **2003,** *125*, 630.
[4] Y.-M. Huh, Y.-W. Jun, H.-T. Song, S. Kim, J.-S. Choi, J.-H. Lee, S. Yoon, K.-S. Kim, J.-S. Shin, J.-S. Suh, J. Cheon, *J. Am. Chem. Soc.* **2005,** *127*, 12387.
[5] T. Hyeon, S.S. Lee, J. Park, Y. Chung, B.N. Hyon, *J. Am. Chem. Soc*. **2001,** *123*, 12798.

Chemical modification of polyaniline by graft reaction of polyaniline on poly (styrene alternative -maleic anhydride) copolymer

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Polyaniline (PANI) is one of the most important conducting polymers discovered in the past decades.To improve the solubility of PANI in organic solvent and its processability, many approaches have been employed, such as the copolymerization of aniline (ANI) with its derivatives [1] and suitable substitutions of the emeraldine base, either at the N sites or on the phenyl rings of the PANI backbone [2]. The substitutions on the PANI backbone can cause large torsional effects that reduce the conjugation length and hence the conductivity. Synthesis methods through modifications of the PANI backbone have also been employed to prepare water-soluble PANI.

Herein a new *N*-substituted PANi is synthesized by insertion of polyaniline on to poly(styrene-alt-maleic anhydride) back bone. The poly(styrene-alt-maleic anhydride) was synthesized by radical copolymerzation of styrene and maleic anhydride in 1:1 molar ratio polyaniline was synthesized by chemical oxidation reaction of aniline by ammonium persulfate in prescnce of ultrasonic irradiation. The complet UV-vis studyies were done for obtaind graft copolymers in various pH.

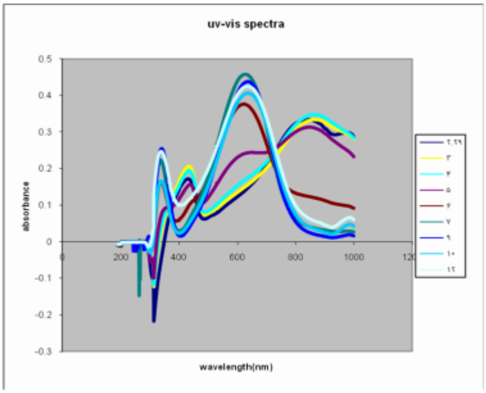

Figure: Absorption spectra of grafted polyaniline on poly (styrene alt -maleic anhydride) copolymer in the pH range of 2–12

References:

[1] J. Libert and J. L. Bredas, *Synth. Met.,* **1995**, 69, 121.

[2] (a) Kilmartin, A. P.; Wright, G. A. Synth Met, **1997**,88, 153; (b) Kilmartin, A. P.; Wright, G. A. Synth Met **1997**, 88, 163; (c) Kinlen, P. J.; Liu, J.; Ding, Y.; Graham, C. R.; Remsen, E. E. Macromolecules **1998**, 31, 1735; (d) Roy, B. C.; Gupta, M. D.; Bhoumik, L.; Ray, J. K. Synth Met , **2002**, 130, 27.

Preparation and investigation of poly(vinyl butyral)(PVB)-carbon nanotubes (CNT) nanocomposites

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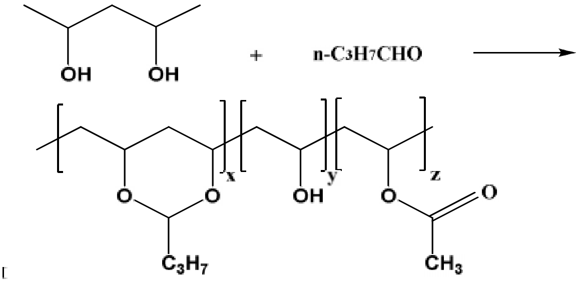
Polymer nanocomposites constitute a new class of materials in which the polymer matrix is reinforced by uniformly dispersed particles having at least one dimension in the nanometer scale. Nanocomposites exhibit improved properties when compared to pure polymer or conventional composites, such as enhanced mechanical and thermal properties [1].

Since their discovery, carbon nanotubes (CNT) have attracted tremendous attention due to their unique properties such as high mechanical strength and high electrical conductivity [2]. One of the most promising applications of CNT is polymer/CNT nanocompositesCombination of their superb physical properties with the high aspect ratio makes CNT an excellent reinforcing material for high-performance and multifunctional polymer nanocomposites [3].

The poly(vinyl butyral) (PVB) was prepared by acetalization of poly(vinyl alcohol) (PVA) via aqueous method. Then, films of PVB-CNT nanocomposites with different CNT loading were produced. Structure, morphology and thermal properties of samples were characterized by scanning electron microscopy (SEM), TGA and FT-IR.



References:
[1] Meneghetti, P.; Qutubuddin, S. *Chem. Eng. Commun.* **2001**, *188*, 81.
[2] Baughman, R. H.; Zakhidov, A. A.; De Heer, W. A. *Science.* **2002**, *297*, 787.
[3] Kodjie, S. L.; Li, L.; Li, B.; Cai, W. W.; Li, C. Y.; Keating, M. *J. Macromol. Sci. Phys*. **2006**, *45*, 231.

Ultrasound-promoted highly chemoselective reduction of aromatic nitro compounds to the corresponding *N*-arylhydroxylamines using stannous chloride

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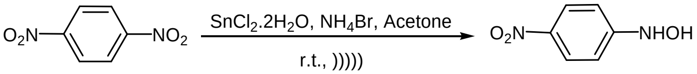
Arylhydroxylamines are an important class of compounds frequently used as key intermediates in the construction of numerous fine chemicals, many natural products and other useful biologically active compounds. For these reasons, several methods have been developed for the preparation of arylhydroxylamines, including catalytic transfer hydrogenation and metal-mediated reduction of the corresponding nitro compounds [1].

Stannous chloride is amongst the popular reducing agent used for reduction of aromatic nitrocompounds [2]. In order to improve this reduction procedure in terms of selectivity, generality and reaction time, we were interested in studying the effect of ultrasounds on the reaction. As well as Energy efficient, ultrasounds can also enhance the rate of the reactions and, in many cases, improve product yields and sometimes can replace phase-transfer catalyst [3].

We reported here an approach for the preparation of *N*-arylhydroxylamines from the corresponding aromatic nitro compounds using the $SnCl_2$. $2H_2O/NH_4Br$/Acetone system under ultrasound. This method was mild, exceedingly efficient, highly chemoselective, and especially simple compared to the traditional method in which the careful manipulation was needed.



References:

[1] a) Srivastava, R. S.; Nicholas, K. M. *J. Am. Chem. Soc.* **1997**, *119*, 3302. b) Cui, J.; Qian, X.; Li, F. *Chem. Commun.* **2004**, 2338.
[2] Bellamy, F. D.; Ou, K. *Tetrahedron Lett.* **1984**, *25*,839.
[3] Ung, S.; Falguieres, A.; Guy, A.; Ferroud, C. *Tetrahedron Lett.* **2005**, *46*, 5913.

Study hydrogen bond by Ab initio and NBO computational method of phthalic, Iso phthalic , Tere phthalic acid and hydroxy nitro benzoic

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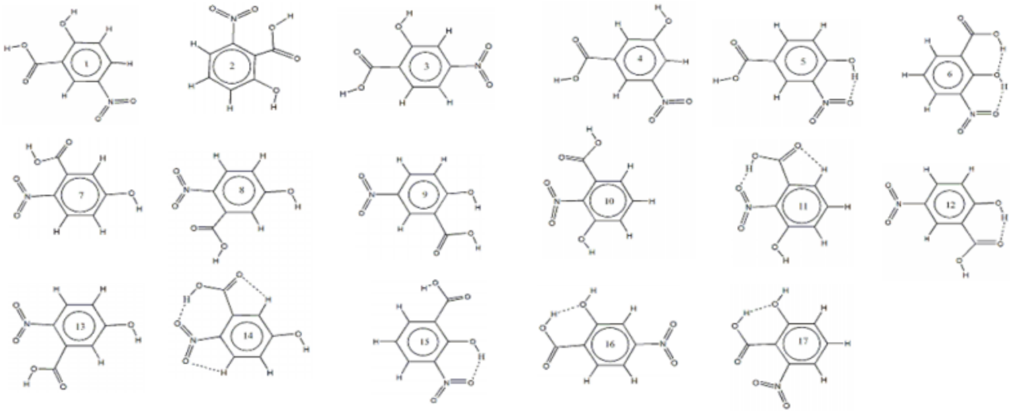
Ab initio quantum chemistry method can be helpful for study molecule and discover property . Density Functional Theory (DFT) is benefit method of computational quantum chemistry for Phthslic acid and Hydroxy nitro benzoic[1]. In this paper study energy hydrogen bond of Phthalic and Hydroxy nitro benzoic[2] . At first we study Hydrogen bond of phthalic acid in gas phase and compare this bond in polar and non-polar solvent . We used DMSO , Methanol , THF and water as polar solvent and CCl_4 and Benzene as non-polar solvent . Observation by Ab initio and NBO analysis showed the stability phtalic acid in polar solvents than non-polar that data attune with experimental data accordingly level of stability by theoretical chemistry have been conclude. Hydrogen bond of seventeen structure of hydroxy nitro benzoic acid by computational chemistry in gas phase . After optimized , structure twelve showed stability of all molecule[1,3] . All structure optimized geometrical by (Density Functional Theory) B3LYP and (Hartree-Fock) HF method by 6-311++G** level of standard basis set . Used by Gaussian 03w package of program for Ab initio and NBO calculate[4].



References:
[1] A.D. Becke, J. Chem. Phys. 98 (**1993**) 5648.
[2] C. Lee, W. Yang, R.G. Parr, Phys. Rev. B 37 (**1988**) 875.
[3] J. Emsley, Struct. Bonding (Berlin) 57 (**1984**) 147.
[4] M.J. Frisch , Gaussian ’03, in: Revision B-0.3, Gaussian Inc., Pittsburgh, PA, **2003**.

Synthesis of some novel thiazoloquin, azolinone derivatives via one-pot three component reaction

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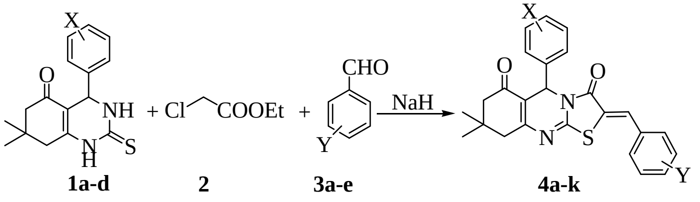
Multicomponent reactions (MCRs), an important subclass of tandem reactions [1], are one-pot processes in which three, four or five easily accessible component react to form a single product, which incorporates essentially all the carbon atoms of the starting materials [2]. MCRs are a promising field of chemistry because the synthesis of complicated molecules can be achieved in a very fast, efficient, and time-saving manner without the isolation of any intermediate [3].

In the present study, we report our results on a new type of multicomponent reaction where three organic components react to form novel compounds. The starting thioxoquinazolinones **1a-d** were synthesized by the reaction of 5,5-dimethylcyclohexane-1,3-dion (dimedone) and corresponding aromatic aldehyde with thiourea in the presence of a catalytic amount of silica sulfuric acid (SSA) [4]. Further reaction of compounds **1a-d** with aromatic aldehydes **3a-e** and ethyl chloroacetate **2** in the presence of sodium hydride in refluxing ethanol afforded the corresponding thiazoloquinazolinone derivatives **4a-k**, as shown in Scheme.



X= H, 4-Me, 4-OMe, 4-Cl, 3,4-OMe
Y= H, 4-Me, 4-Cl, 4-NO_2, 4-OMe

References:

[1] Tietze, L. F. *Chem. Rev.* **1996**, *96*, 115.
[2] Ramon, D. J.; Yus, M. *Angew. Chem. Int. Ed.* **2005**, *44*, 1602.
[3] Chetia, A.; Saikia, C. J.; Lekhok, K. C.; Boruah, R. C. *Tetrahedron Lett.* **2004,** *45*, 2649.
[4] Shaabani, A.; Sarvary, A.; Rahmati, A.; Rezayan,A. H. *Lett. Org. Chem.* **2007**, *4*, 68.

One-step synthesis of desyl chloride

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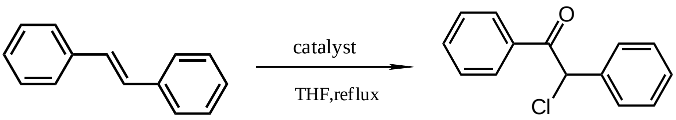
Desyl chloride [1-8] has been prepared by the action of thionyl chloride on benzoin, and on *l*-benzoin. It has also been prepared by the action of hydrogen chloride on azibenzil. Investigation of the literature revealed Other examples, such as : the addition of nucleophiles to Weinreb amides, palladium-catalyzed acylations of arylboronic acids and arylzinc compounds, iron-catalyzed cross-couplings of acyl chlorides and Grignard reagents,6 acylation of arylcuprates, and cobalt, rhodium, vanadium-catalyzed coupling reactions, all suffered from similar shortcomings and Pd-catalyzed coupling of an Rchloro thiol ester with an aryl boronic acid; however, this route was unattractive due to the necessity of preparing the thiol ester, the added expense of the boronic acid, and the use of a stoichiometric copper reagent. Here in, we report the direct synthesis of Desyl chloride in one step from (E)-Stilbene.



References:

[1] Liebeskind, L. S.; Srogl, J. *J. Am. Chem. Soc*. **2000**, *122*, 11260.
[2] (a) Tillyer, R.; Frey, L. F.; Tschaen, D. M.; Dolling, U. H. *Synlett* **1996**, 225. (b) Peese, K. M.; Gin, D. Y. *J. Am. Chem. Soc*. **2006**, *128*, 8734.
[3] (a) Gooâen, L. J.; Winkel, L.; Do¨hring, A.; Ghosh, K.; Paetzold, J. *Synlett* **2002**, 1237. (b) Haddach, M.; McCarthy, J. R. *Tetrahedron Lett.* **1999**, *40*, 3109. (c) Bumagin, N. A.; Korolev, D. N. *Tetrahedron Lett.* **1999**, *40*, 3057. (d) Urawa, Y.; Ogura, K. *Tetrahedron Lett.* **2003**, *44*, 271. (e) Chen, H.; Den, M. *Org. Lett.* **2000**, *2*, 1649.
[4] (a) Faul, M. M.; Winneroski, L. L. *Tetrahedron Lett*. **1997**, *38*, 4749. (b) Grey, R. A. *J. Org. Chem.* **1984**, *49*, 2288.
[5] (a) Scheiper, B.; Bonnekessel, M.; Krause, H.; Fu¨rstner, A. *J. Org. Chem.* **2004**, *69*, 3943. (b) Fiandanese, V.; Marchese, G.; Martina, V.; Ronzini, L. *Tetrahedron Lett.* **1984**, *25*, 4805.
[6] (a) Sapountzis, I.; Dube, H.; Lewis, R.; Gommermann, N.; Knochel, P. *J. Org. Chem.* **2005**, *70*, 2445. (b) Dieter, R. K.; Sharma, R. R.; Yu, H.; Gore, V. K. *Tetrahedron* **2003**, *59*, 1083.
[7] Fillon, H.; Gosmini, C.; Pe´richon, J. *Tetrahedron* **2003**, *59*, 8199.
[8] Frost, C. G.; Wadsworth, K. J. *Chem. Commun.* **2001**, 2316.

Six-membered P-heterocyclic silylenes: A survey of stability

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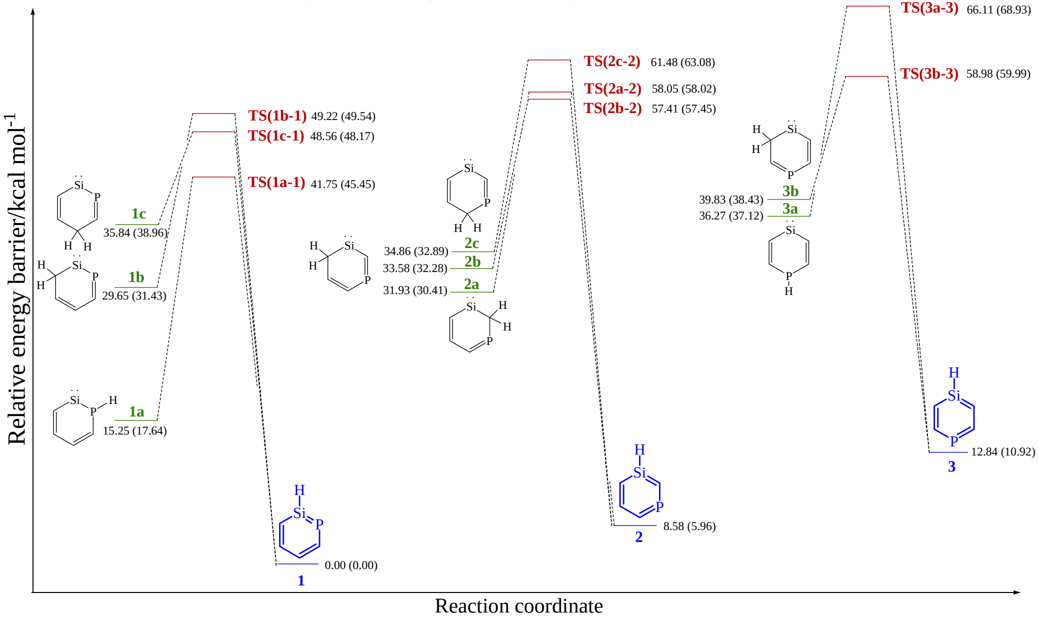
Silylenes are divalent, dicoordinate silicon species which, until recently, were only observable at low temperatures. The reactivity of silylenes is linked to the presence of both a 3*s* lone pair and a vacant 3*p* orbital at the silicon atom [1-2]. Research on silylenes has developed rapidly since the synthesis of the first isolable one reported by Denk *et. al* [3].

P-heterocyclic silylenes are a novel brand of intermediates whose scrutiny required comparison of the following eight spices (Figure), at B3LYP/AUG-cc-pVTZ//B3LYP/6-31+G* and MP2/6-311++G**//B3LYP/6-31+G* levels of theory. From a thermodynamic point of view, **1a** and **3a** are relatively the most stable with singlet-triplet energy gaps ($\Delta E_{\text{S-T}}$) of 37.0 and 28.1 kcal/mol, respectively. The calculated energy barrier for a 1,2-*H* shift of **1a** to **1** is 26.5 kcal/mol compared to 28.8 kcal/mol for the 1,4-*H* shift of **3a** to **3**. This study signifies the thermodynamic and kinetic stabilities of P-heterocyclic silylenes along with their silylenic species.



References:

[1] R. Becerra, R. Walsh, *Res. Chem. Kinet,*.**1995**, 263.
[2] J. Belzner, H. Ihmels, *Adv. Organomet. Chem.* **1998**, *1*, 43.
[3] Denk, M.; Lennon, J. R.; Hayashi, R.; West, R.; Belyakov, A. V.; Verne, H. P.; Haaland, A.; Wagner, M.; Metzler, N. *J. Am. Chem. Soc.* **1994**, *116*, 2691.

Diketene-based multicomponent reactions

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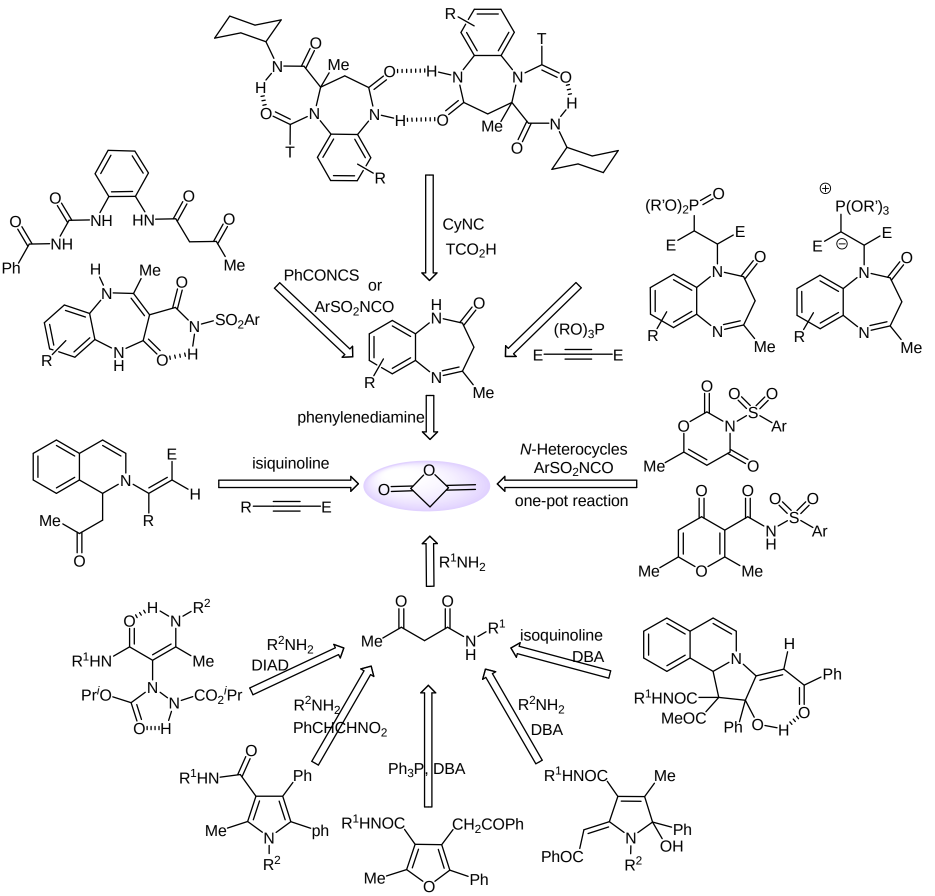

References:

[1] Zohreh, N.; Alizadeh, A.; Bijanzadeh, H. R.; Zhu, L. G. *J. Comb. Chem.* **2010** (in press) and references 20a-g sited there.

[2] Alizadeh, A.; Zohreh. N. Helv. Chem. Acta. 2010 (in press).

[3] (a) Alizadeh, A.; Rezvanian, A.; Bijanzadeh, H. R. *Synthesis* **2008**, 725. (b) Alizadeh, A.; Rezvanian, A.; Zhu, L. G. **2008**, *64*, 351.

PPA-SiO$_2$: A new and efficient catalyst for one-pot multi-component synthesis of 3,4-dihydropyrimidin-2(1H)-ones and -thiones

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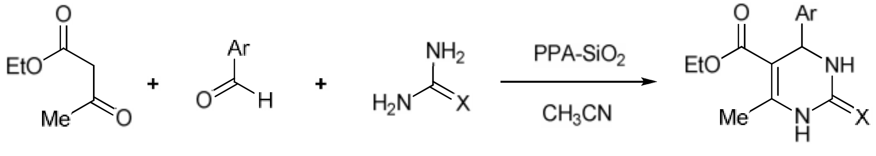
Dihydropyrimidinones and -thiones have attracted considerable interest recently because of their wide range of biological activities such as antibacterial, antitumor, anticancer, and anti-inflammatory properties [1, 2]. The first procedure for the synthesis of dihydropyrimidinones reported by Biginelli in 1893, involves acid catalyzed one-pot three-component condensation of β-dicarbonyl compounds with an aromatic aldehyde and urea derivatives [3]. There are several improved methods for the synthesis of these compounds using various Brønsted acid and Lewis acid catalysts such as alcoholic HCl [4], dry acetic acid [5], boric acid [6], *p*-TsOH [7], etc. However, many of these methods are associated with expensive and highly acidic catalysts, long reaction times, unsatisfactory yields, and difficult product isolation.

Thus, herein we wish to report the new efficiently synthesis of 3,4-dihydropyrimidin-2(1H)-ones and -thiones through one-pot three-component reaction of ethyl acetoacetate, an aryl aldehyde, and urea or thiourea in acetonitrile using PPA-SiO$_2$ as catalyst.



References:

[1] Kappe, C. O.; Fabian, W. W. *Tetrahedron,* **1997**, *53*, 2803.
[2] Kappe, C. O. *Eur. J. Med. Chem.*, **2000**, *35*, 1043.
[3] Biginelli, P. *Gazz. Chim. Ital.*, **1893**, *23*, 360.
[4] Gupta, R.; Gupta, A. K.; Paul, S.; Kachroo, P. L. *Indian J. Chem. Sect B,* **1995**, *34B*, 151.
[5] Yadav, J. S.; Reddy, B. V. S.; Reddy, E. J.; Ramalingam, T. *J. Chem. Res. (S),* **2000**, 354.
[6] Tu, S.; Fang, F.; Miao, C.; Jiang, H.; Feng, Y.; Shi, D.; Wang, X. *Tetrahedron Lett.*, **2003**, *44*, 6153.
[7] Jin, T.; Zhang, S.; Li, T. *Synth. Commun.*, **2002**, *32*, 1847.

Synthesis of carbon nano sheets (Buckypapers) by functionalized multi-walled carbon nano tubes

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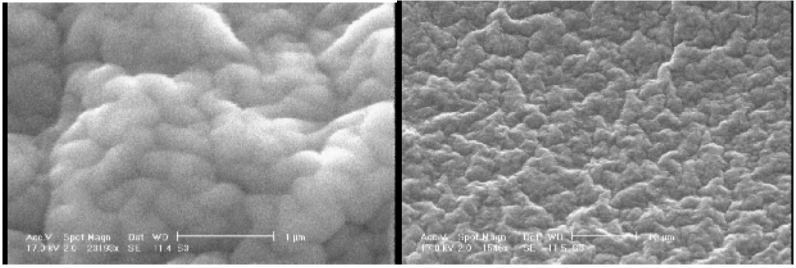
Carbon nanotubes (CNTs) have attracted worldwide attention due to their unique mechanical, thermal and electronic properties [1]. Among various their engineering applications, potential fillers in polymer matrices have been widely considered to improve mechanical, rheological and electrical properties of nanocomposites [2,3] due to their high aspect ratio, mechanical strength, and electrical and thermal conductivity [4,5] in the areas of automobile industry, aerospace technology and energy storage.

We report the syntheses of carbon nano sheets (buckypapers) by end and side wall functionalized of multi-walled carbon nano tubes (MWCNTs). MWCNTs were refluxed in HNO_3 to introduce carboxylic acid groups. Then MWCNTs-COOH reacts with Oxalyl Chloride until lead to MWCNTs-COCl. This product adds to diamine compound to achieve MWCNTs-CO-NH-R-NH_2. The products in each step were characterized utilizing Fourier transform Infrared Spectra, Raman Spectra, Nuclear Magnetic Resonance, Scanning Electron Microscopy, Ultraviolet / Visible Absorbance Spectra. The results show that the final macro molecules are easily dispersed in organic solvent. The buckypapers demonstrated very high specific surface areas and good roughness factors.



References:

[1] N. Grossiord, J. Loos, O. Regev, C. E. Koning, *Chem. Mater*, **2006**, *18*, 1089.
[2] A. Maity, M. Biswas, J. Ind. Eng. Chem. **2006**, 12, 311.
[3] S. T. Kim, J.Y. Lim, B. J. Park, H. J. Choi, *Macromol. Chem. Phys*, **2007**, *208*, 514.
[4] E. N. Konyushenko, J. Stejskal, M. Techova, J. Hradil, J. Kovarova, J. Prokes, M. Cieslar, J. Y. Hwang, K. H. Chen, I. Sapurina, *Polymer*, **2006**, *47*, 5715.
[5] M. K. Yeh, N. H. Tai, J. H. Liu, *Carbon*, **2006**, *44*, 1.

Synthesis of *O*-vinylic salicylaldehydes as precursor for intramolecular 1,3-dipolar cycloaddition reaction

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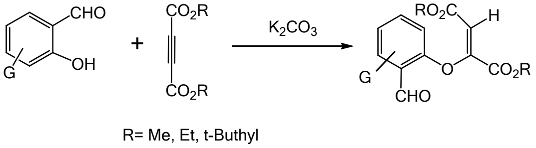
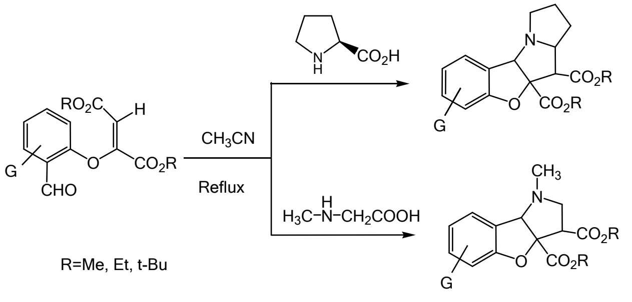
Intramolecular [3 + 2]-cycloaddition of azomethine ylides has the power to construct complex cyclic systems from relatively simple precursors [1]. This important aspect of 1,3-dipolar cycloaddition chemistry has been well studied in recent years. *O*-allyl or *O*-propargyl salicylaldehydes [2], and several other systems [3] have been developed for the synthesis of bicyclic, tricyclic, and even more complex ring skeletons.

Several methods have been reported in the literature for the synthesis of *O*-vinylic salicylaldehydes whose protocols are multi-step in nature [4].

We herein report a simple method for stereoselective synthesis of *O*-vinylic salicylaldehydes and using these products as precursor for intramolecular 1,3-dipolar cycloaddition reaction that form a novel tetracyclic system.





References:

[1] *Synthetic Application of 1,3-Dipolar Cycloaddition Chemistry toward Heterocycles and Natural Products;* Padwa, A.; Pearson, W. H., Eds.; Wiley: Hoboken, NJ, **2003**.

[2] Bashiardes, G.; Safir, I.; Mohamed, A. S.; Barbot, F.; Laduranty, J. *Org. Lett.* **2003**, *5*, 4915.

[3] Zhang, Wei.; Lu, Y.; Geib, S. *Org. Lett.* **2005**, *7*, 2269.

[4] Guo,Y-W.; Shi,Y-L.; Li, H-B.; Shi, M. *Tetrahedron* **2006**, *62*, 5875.

Synthesis of alkylhalydes from tetrahydropyranyl ethers in ionic liquids as reagent and medium of reaction

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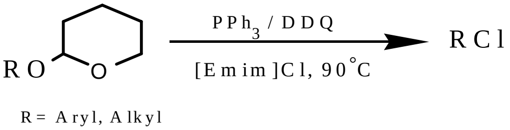
The tetrahydropyranylation is one of the methods to protect hydroxyl group in a multistep organic synthesis, Because of the remarkable stability of tetrahydropyranyl ethers toward a variety of conditions [1].

Organic molecules containing halogen atoms are found in many products, such as pharmaceuticals, agrochemicals, and materials for advanced technologies. In organic synthesis, they are important intermediates in reactions [2]. Bromination and chlorination are straightforward processes. Iodination is frequently more difficult because the reaction proceeds very slowly and is often reversible under standard conditions [3]. Solvents are high on the list of damaging chemicals. Some more recent reviews showing an overview of the potential of ionic liquids as solvents for synthesis and catalysis [4].



THP ether was prepared by previously reported method [5]. To a flask containing a stirring mixture of 2, 3-dichloro-5, 6-dicyano-p-benzoquinone (DDQ) and triphenylphosphine (PPh3) in 1-ethyl-3-methylimidazolium chloride or bromide as Ionic Liquid was added THP ether in an oil bath at 90 degree centigrade (scheme). A wide variety of THP ether underwent smooth reaction to give the corresponding alkylhalyde in good to excellent yield.

Neutral medium of reaction and high yield of product are the two advances of this method.

References:

[1] Brindaban, C.; Saha,R.; Saha, M . *J. Org. Chem.* **1994,** *59,* 8269.

[2] Cristiano, R.; Ma, K.; Pottanat, G.; R,Weiss. *J. Org. Chem.* **2009**, *74,* 9027.

[3] Ho,M.; Flynn, A.; Ogilvie, W. *J. Org. Chem.* **2007**, *72,* 977.

[4] Welton, W. *Chem. Rev*. **1999**, 8, 2071.

[5] Shirini, F.; Zolfigol, M.; Abri, A. *Chinese Chemical Letters.* **2007**, *18,* 803.

Conformational study on the protected dipeptide HCO-Gly-L-Leu-NH$_2$ by using Ab initio and DFT calculations

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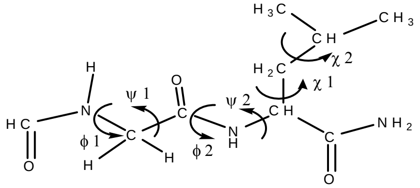
Ab initio and DFT calculations were carried out for determining various conformations and Ramachandran maps of HCO-Gly-L-Leu-NH2 dipeptide .At first the effect of Leucine's side chain angles (χ_1,χ_2) on the conformational stability was considered, for χ_1 and χ_2 at 30 intervals from 0° to 360° were changed and their geometries optimized. Three minima were found that Anti-Anti (χ_1=180, χ_2=180),trans-Gauche(-) (χ_1=210, χ_2=300) and Gauche(+)-trans (χ_1=60, χ_2 =210) that the Anti-Anti conformer has the lowest energy. And then for Anti-Anti the ramachandran map were investigated at the RHF/6-31G* level .The $\beta_L\beta_L$ and $\gamma_D\beta_L$ conformers existed in the HCO-Gly[x]-L-Leu[β_L]-NH2 when the Leucine residue was restrained to β_L and varying glycine residue for each of the nine optimized conformations and $\beta_L\alpha_D$, β_L γ_L, $\beta_L\beta_L$, $\beta_L\gamma_D$,$\beta_L\delta_D$, $\beta_L\alpha_L$ conformers existed in HCO-Gly[β_L]- L-Leu[x]-NH2 when glycine the residue was restrained to β_L and varying Leucine for each of the nine optimized conformations.And then DFTcalculations (at the B3LYP/6-31G* level of theory) were carried out for determining various conformations caused from changing dihedral angles (Ψ, φ) of backbone skeleton for anti-anti of side chain.In this state, Ψ and φ dihedral angles were changed and with using frequency calculations at the same level thermodynamic properties such as E, H, G and S were obtained.

RESULTS:In this study at Ramachandran map Investigation 7 stable conformers were found that $\beta_L\gamma_L$ conformer is the most stable And also our calculations at B3LYP/6-31G* level show that when dihedral angles Ψ1, φ1, Ψ2 and φ2 are180, 180, 150 and 210 respectively ,the conformer has maximum stability.



References :

[1] Souvik Mondal ,Durga Sankar Chowdhuri ,Soumen Ghosh ,Ajay Misra ,Sudipta Dalai THEOCHEM (**2007**)
[2] Peter Hudaky , Andras Perczel. .THEOCHEM **2004**.

Clean procedure for the synthesis of bis (indolyl) methanes under thermal conditions by $FePO_4$

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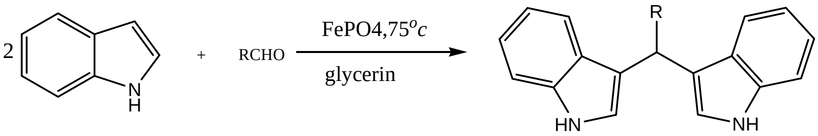
Bis(indolyl) methanes and its derivatives are known as an important class of hetrosyclic compounds and bioactive intermediates in R&D and pharmaceutical industry[1].In resent years, synthesis of this class of molecues under mild conditions have been reported with promoters such as montmorilloite clay k-10 [2], trichloro-1,3,5-triazine [3], sodium dodecyl sulfates (SDS) [4], amino sulfonic acid [5], and metal hydrogen sulfates [6],

However, most of the existing methods involve toxic metal ions and solvent, high cost, and cumber some work-up procedures.

Consequently new procedures that address these drawbacks are desirable,performing a simple, clean and highly efficient green protocol has been glycerin and $FePO_4$ are successfully use of indoles with aldehydes. The product was simply extracted with ethyl acetate(15 ml). catalytic system for the synthesis of bis(indolyl) in good to excellent yields through the reaction



Refences:

[1] The chemistry of indoles.Academic press, *New york Sundberg*(**1996)**
[2] Chakrabarty, M.; Ghosh, N.; Basak, R.; Harigaya, Y.A.; *synth commun* **(2004)** *34:421-434*
[3] Sharma, G.V.M.; Reddy, j.j.; Lakshmi, P.S.; Krishna, P.R.A.; *Tetrahedron* ***Lett*** **(2004**) *45:7729-77*
[4] Deb, M.L.; Bhuyan, P.J.; *Tetrahedron Lett* (**2005**)*.34:1441-1443.*
[5] Ji,Tai li.; Hong,Guang,Dai.; (*Hebi Province Baoding* ***071002,***PRChaina)
[6] Niknam, K.; Zolfigol, M.A.; j *Iran chem. SOC:3:318-322*

Operationally simple and selective michael addition under in water in the presence of organocatalyst

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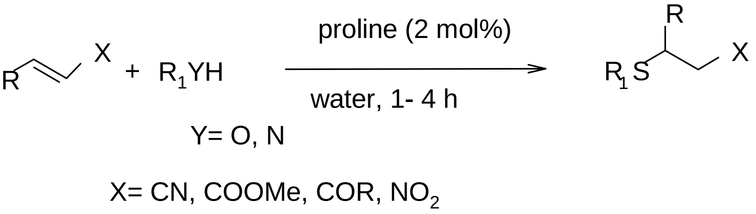
The rapid and very simple conjugate addition of thiols and amines to α,β-unsaturated carbonyl compounds under solvent free conditions in the presence of organocatalyst at room temperature is reported. The reaction of aryl, alkyl, aliphatic and hindered thiols and amines with chalcone, enone and nitrostyrene gave the corresponding Michael adducts with significant advantages such as high conversions, short reaction time, mild reaction conditions, low cost, simple catalyst and high to quantitative yields with excellent chemoselectivity.



References:

[1] Azizi, N. Saidi, M. R. *Tetrahedron*, **2004**, 60, 383.

[2] Liu M.; Sibi. M.P. *Tetrahedron* **2002**, 58, 7991.

[3] Younes Abrouki, Mohamed Zahouily,Ahmed Rayadh, Bouchaib Bahlaouan and Saïd Sebti, *Tetrahedron,43,49*, **1951**.

[4] Cheng, S. Comer, D. D. *Tetrahedron Lett.* **2002**, 43, 1179

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University of Mazandaran,
Babolsar,Iran 13-15 October 2010

۲۱ تا ۲۳ مهرماه ۱۳۸۹
بابلسر- دانشگاه مازندران
دانشکده شیمی

Three-component reaction between triphenylphosphine, acetylenic esters and *N*'-[2-(phenyl)-acetyl]-formic acid hydrazide

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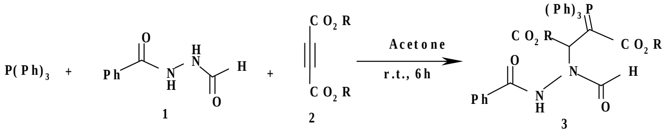
Phosphorus ylides are reactive systems, which take part in many reactions of value in organic synthesis [1]. Several methods have been developed for the preparation of phosphorus ylides. These ylides are usually prepared by treatment of an appropriate phosphonium salt with a base; the corresponding phosphonium salts are usually obtained from the phosphine and an alkyl halide. Phosphonium salts are also prepared by Michael addition of phosphorus nucleophiles to activated olefins [2]. Reaction of acetylenic esters with triphenylphosphine in the presence of an organic compound possessing an acidic-hydrogen has been recently reported to produce phosphorus ylides [3]. In continuation of our previous works on the reaction between triphenylphosphine and acetylene esters in the presence of organic N-H, O-H or C-H acids [4,5].

Herein we have described a simple, and one-pot, three-component reaction between dialkyl acetylenedicarboxylate, triphenylphosphine and N'-[2-(phenyl)-acetyl]-formic acid hydrazide for the preparation of functionalized phosphoranes in good yields.



3	R	% Yield*
a	CH_3	93
b	C_2H_5	91
c	*t*-Bu	93

* Isolated yields

The structures of **3a-c** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:
[1] Maryano, B. E.; Reits, A. B. *Chem. Rev*. **1989**, 89, 863.
[2] Engel, R. *Synthesis of Carbon-Phosphorus Bonds* (CRC Press, Boca Raton, FL.1988).
[3] Yavari, I.; Karimi, E. *Phosphorus, Sulfur and Silicon Relat. Elem*, **2007,** 182, 595.
[4] Anary-Abbasinejad, M.; Mosslemin, M. H.; Hassanabadi, A.; Tabatabaee, M. *Synth. Commun*. **2008**, 38, 3700.
[5] Mosslemin, M. H.; Anary-Abbasinejad, M.; Hassanabadi, A.; Bagheri, M.A. *J. Sulfur, Chem*. **2010**, 31, 135.

One-pot synthesis of thermally stable ketenimine derivatives by three component reaction of alkyl isocyanides, dialkyl acetylenedicarboxylates and different hydrazide acids

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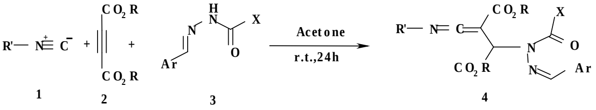
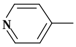
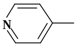
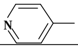
Ketenimines are important reactive intermediates that occur as transient compounds in many thermal and photochemical reactions [1,2].In recent years, the synthetic applications of multifunctional heteroallenes have been widely investigated [3].In spite of extensive developments in the chemistry of modified ketenes and isocyanates [4], little attention has been paid to the synthesis of ketenimines [5].The trapping of the 1:1 intermediate formed between dialkyl acetylenedicarboxylates and isocyanides with OH, NH, and CH acids has been widely studied [6,7]. Herein we have described a simple, and one-pot, three-component reaction between alkyl isocyanides, dialkyl acetylenedicarboxylates and different hydrazide acids for the preparation of thermally stable ketenimine derivatives in good yields.



4	Ar	X	R	R'	*%Yield
a	phenyl	Me	Me	Cy	89
b	phenyl		Me	t-Bu	90
c	p-Cl-phenyl	Me	Me	Cy	94
d	p-Cl-phenyl		Et	Cy	93
e	p-Cl-phenyl	Me	t-Bu	Cy	87
f	p-Cl-phenyl		Me	t-Bu	88

*isolated yields

The structures of **4a-e** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:

[1] Tidwell , T.T. *Ketenes*. Wiley, New York, 1995.
[2] Chiang , Y.; Grant, A. S.; Guo, H-X.; Kresge, A.J.; Paine, S. W. *J. Org. Chem*. **1997**, 62, 5363.
[3] Reichen, W. *Chem. Rev*. **1978**, 78, 569.
[4] Ishida, M.; Minami, T.; Agawa, T. *J. Org. Chem*. **1979**, 44, 2067.
[5] Krow, G. *Angew. Chem*. Int. Ed. Eng. **1971**, 10, 435.
[6] Mosslemin, M. H.; Nateghi, M. R.; Hassanabadi, A.; Zare, M. *J Chem. Res*. **2010**, 3, 178.
[7] Anary-Abbasinejad, M.; Kamali-Gharamaleki, M.; Hassanabadi, A. *J. Chem. Res*. **2007**, 170.

One-pot synthesis through the reaction of 4-substituted benzoic acid derivatives with dimethylacetylen dicarboxylate in the presence of PPh_3

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[b] *Drug design and development research center Tehran university of medical scinces Tehran, Iran.*
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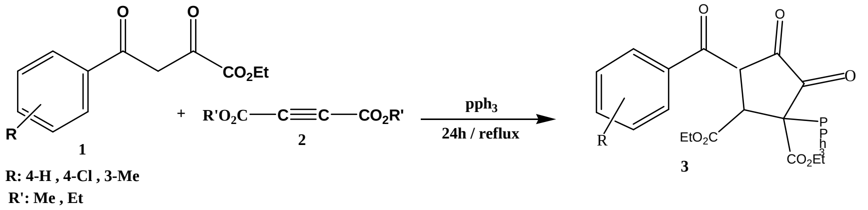
In recent years there has been increasing interest in the synthesis of organophosphorus compounds, that is, those bearing a carbon atom bound directly to a phosphorus atom. There have been many studies on reactions between trivalent phosphorus nucleophiles and α,β-unsaturated carbonyl compounds in the presence of a proton source such as an alcohol or a CH-acid [1].

The intramolecular Wittig reaction is useful for cycloalkene synthesis. The common five-, six-, and seven-membered ring cycloalkenes are produced easily by intramolecular Wittig reactions [2].

we report a simple on-pot three-compounents from reaction of triphenylphosphine and dimethylacetylendicarboxylate in the presence ethyl 2,4-dioxo-4-phenyl butanoate derivatives and under conditions reflux lead to 3.



References:

[1] Yavari , I.; Alizadeh, A.; Anary-Abbasinejad , M.; *Tetrahedron* Letters 44 **(2003)** 2877.
[2] Yavari, I.; Mohtat, B.; Zare, H.; Alborzi A.R.**;** *Mendeleev commun***., 2005**, 15(6), 250.

3-Aminopropylated silica gel as an efficient catalyst for the reaction of 1-phenyl-3-methyl-5-pyrazolone with aldehydes

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Use of heterogeneous solid base catalysts is of current interest in chemistry and industry because solid bases offer many advantageous such as simplicity in handling, more environmentally safe disposal and less plant corrosion problems [1]. Amine functionalized silica gel such as 3-aminopropylated silica gel (AP-SiO_2) is one of the organic-inorganic hybrid materials that have been applied as effective solid base catalyst in organic transformations. In these types of solid base catalysts, the reactive centers are highly mobile similar to that of homogeneous catalysts and at the same time these species have the advantage of being recyclable in the same fashion as heterogeneous catalysts.

As part of our ongoing program directed toward the development of new methods in organic reactions [2], herein, we introduced 3-aminopropylated silica gel (AP-SiO_2) (Figure 1) as an efficient catalyst for tandem Knoevenagel-Michael reaction of two equivalents of 1-phenyl-3-methyl-5-pyrazolone with various aldehydes.

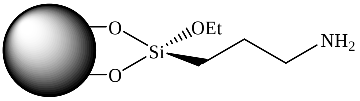

FIGURE 1.

Ease of recovery and catalyst reusability make this method an economic and waste-free chemical process for the efficient synthesis of a variety of bis(pyrazolyl)methanes. Short reaction times, simple work-up and mild reaction conditions are the other advantageous of the present methodologies.

References:

[1] a) Ballini, R.; Bosica, G.; Livi, D.; Palmieri, A.; Maggi, R.; Sartori, G. *Tetrahedron Lett.* **2003**, *44*, 2271; b) Macquarrie, D. J.; Maggi, R.; Mazzacani, A.; Sartori, G.; Sartorio, R. *Appl. Catal. A: Gen*. **2003**, *246*, 183.

[2] a) Sobhani, S.; Faal Maleki, M. *Synlett* **2010**, 383; b) Sobhani, S.; Tashrifi Z. *Tetrahedron* **2010**, *66*, 1429.

BSA: As a novel, efficient and recyclable catalyst for the synthesis of quinoxalines at room temperature

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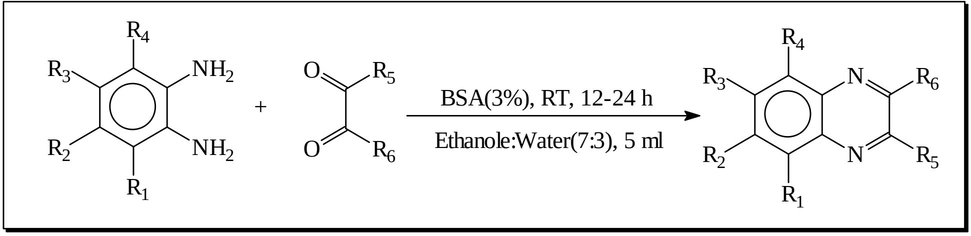
The reaction of boronic acid and chlorosulfonic acid in dichloromethane produced boronsulfunic acid (BSA), which was used as a novel, efficient and recyclable catalyst in presence of ethanole: water (9:1, 5 ml) for the room temperature synthesis of quinoxalines derivatives from 1,2-diamino compounds and 1,2-dicarbonyl compounds in high yield(›95%).



In recent year, the research for environmentally begin chemical processes or methodologies has received much attention, and the development of heterogeneous catalysts for fine chemical synthesis has become a major area of research. The potential for incorporation in continuous reactors and micro reactors) could lead to navel environmentally benign chemical procedures for academia and industry [1-8].

References:

[1] Peyman, S.; Zolfigol, M., A.; Shirini, F.; Baghabanzadeh, M. *Current Organic Chemistry* **2006**, *10*, 2171.
[2] Sajjadifar, S.; Vahedi, H.; Massoudi, A.; Louie, O. *Molecules* **2010**, *15*, 2491.
[3] Niknam, K.; Saberi, D.; Mohgheghnejad, M. *Molecules* **2009**, *14*, 1915.
[4] Kiasat, A. R.; Fallah-Mehrjardi, M; *J. Braz. Chem. Soc.* **2008**, *19*, 1595.
[5] Wen-Xue, G. *et al*; *J. Braz. Chem. Soc.* **2009**, 1.
[6] Dabiri, H. R. *et al*; *J. Braz. Chem. Soc.* **2008**, *19*, *8*, 1646.
[7] Hasaninejad, A. *et al*; *ARKIVOK* **2008**, (xiii), 28.
[8] Heravi, M. M. *et al*; *ARKIVOK* **2006**, (xvi), 16.

Oxidative coupling of thiols to the corresponding disulfides and chemoselective oxidation of sulfides into sulfoxides by poly(4-vinylpyridinium nitrate)

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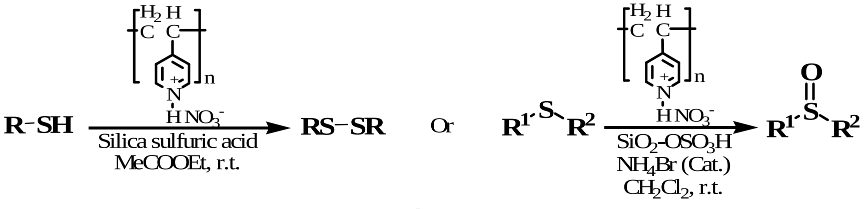
Sulfoxides are both useful elements of stereocontrol in asymmetric synthesis and important targets of pharmaceutical interest [1]. Sulfoxides are generally prepared via oxidation of the corresponding sulfide; however, it is often very difficult to stop the oxidation at the sulfoxide stage. Also disulfide bonds play crucial roles in biology and chemistry. Oxidation of thiols is the most exploited method for disulfide synthesis mainly because a large number of thiols are commercially available and/or are easily synthesized [2]. There are lots of reagents and oxidizing media available for the preparation of sulfoxides and disulfides [3-4]. However, most of them are not satisfactory because of several reasons such as the formation of environmentally unfavorable by-products, over-oxidation, low yields of products, tedious work-up, toxicity or expensive reagents.

Therefore to improve mentioned limitations we decide to design a new system for these transformations. In continuing of our studies on the application of new reagents or reagent systems in organic reactions [5] we became interest to explore a new methodology for the fine and selective conversion of thiols into disulfides also sulfides into sulfoxides. Consequently herein we report the oxidative coupling of a variety of aliphatic and aromatic thiols into disulfides using poly(4-vinylpyridinium nitrate) and silica sulfuric acid, and chemoselective oxidation of different types of sulfides into sulfoxides with same reagent and acid catalyzed by NH_4Br (Scheme).



Scheme

References:

[1] Russo, A.; Lattanzi, A. *Adv. Synth. Catal.* **2009**, *351*, 521.
[2] Alam, A.; Takaguchi, Y.; Tsuboi, S. *Synthetic Commun.* **2005**, *35*, 1329.
[3] Ghafuri, H.; Hashemi, M.M. *J. Sulfur Chem.* **2009**, *30*, 578.
[4] Dilsha, K.M.; Kothari, S. *J. Chem. Sci.* **2009**, *121*, 189.
[5] Ghorbani-Choghamarani, A.; Goudarziafshar, H.; Nikoorazm, M.; Yousefi, S. *Can. J. Chem.* **2009**, *87*, 1144.

1,3-Dipolar cycloaddition of nitrile oxide with alkenes; synthesis of new isoxazolines

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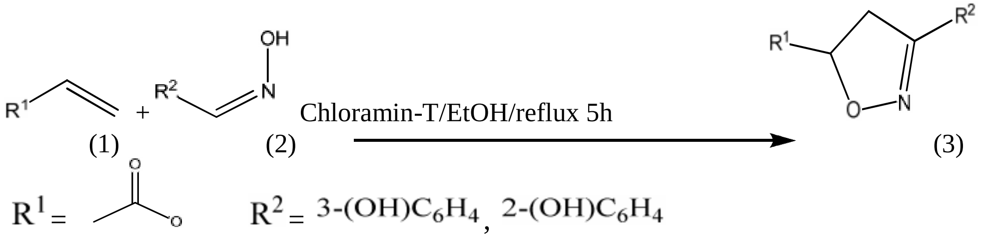
Heterocycles are an important class of compounds, not only because of their natural abundance, but also because of their chemical, biological,in this context isoxazole is one of the most useful compounds and pharmacentical importance which is as an important unit in many biologically active compounds [1].

The 1,3-dipolar cycloaddition reactions (1,3-DCRs), have been largely studied as useful synthetic strategy to obtain various heterocyclic systems [2]. 1,3-Dipolar cycloaddition reaction using nitrile oxides is one of the versatile methods for the preparation of synthetically useful intermediates isoxazolines and isoxazoles [3].

It is known that 1,3-dipolar cycloaddition is the powerful method for the synthesis of five membered rings [4].

Herein we report the use of N-chloro-N-sodio-4-methylbenzene-sulfonamide known as chloramines-T to affored new of 2-isoxazolines during cycloadditions to olefins. Typically, the cycloadditon is carried out by heating an equimolecular of an alkene 1, aldoxime 2, and chloramines-T trihydrate in ethanol under reflux for 5 h in general, 2-isoxazolines 3.



References:

[1] Weissberger, A. *Chem. Herterocycle.Compd*. **1962**.
[2] Aversa, M.C.; Bonaccorsi, P.; Giannetto , P. *J. Heterocycl. Chem*. **1989**, 26, 1619. and Grubert, L.; Patzel, M.; Jugelt, W.; Riemer, B.; Liebscher, J. Liebigs. *Ann. Chem* **1994**, 1005.
[3] For reviews,see a) Kozikowski, A.P., *Acc. Chem. Res*., **1984**, 17, 410. b) Baraldi,P.G., Barco, A., Benetti,S., Pollini, G.P., Simoni,D., *Synthesis*, **1987**, 857. c) Caramella,P., Grunanger,P.,in:" *1,3-Dipolar Cycloaddition Chemistry*, " Padwa , A.(ed.),Vol.1, chapter3, John Wiley&Sons,New York, **1984**.
[4] Carruthers, W. *Cycloaddition Reaction in Organic Synthesis*, Pergamon Press, Oxford, **1990.**

Synthesis of pyrano[3,2-*d*]isoxazole derivatives *via* multicomponent reactions

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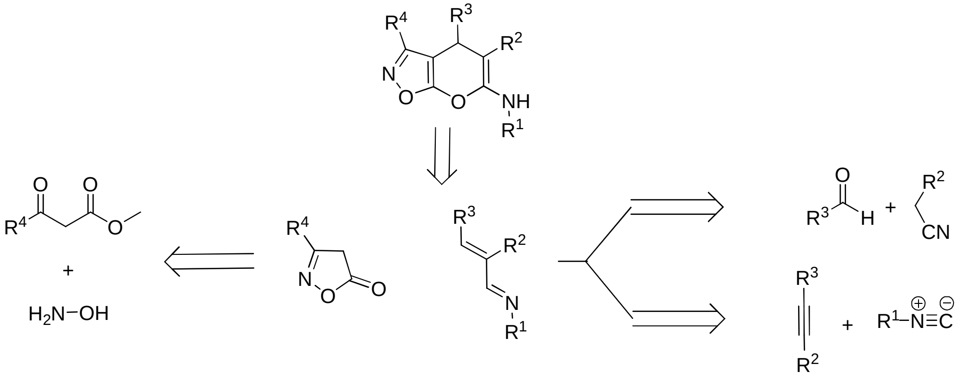
Many isoxazole derivatives are known to possess a variety of biological activities for medicine and agriculture. For example isoxazolylmethanols have anti-inflammatory and analgesic activity, haloisoxazolylureas have acaricidal and insecticidal properties, and 3-hydroxy-5-methylisoxazole shows highly fungicidal activity [1-2].

Following our studies towards the development of new routes to the synthesis of organic compounds and our interest in multicomponent reactions (MCRs) [3-5], herein we wish to describe two new synthetic methods for the synthesis of pyrano[3,2-*d*]isoxazole including: *i*) using isoxazol-5(4*H*)-one, dialkyl acetylenedicarboxylates and isocyanides in CH_2Cl_2 at room temperature and *ii*) using isoxazol-5(4*H*)-one, aldehyde and malononitrile in EtOH at room temperature.



References:

[1] Abdel-Rahman, A. H.; Keshk, E. M.; Hannab, M. A.; El-Badyb S. M. *Bioorg. Med. Chem.* **2004**, *12* 2483.

[2] Kim, H. J.; Jang, J. Y.; Chung, K. H.; Lee, J. H. *Biosci. Biotechnol. Biochem.* **1999**, *65*, 494.

[3] Shaabani, A.; Ghadari, R.; Sarvary, A.; Rezayan, A. H. *J. Org. Chem.* **2009**, *74*, 4372.

[4] Shaabani, A.; Sarvary, A.; Rezayan, A. R.; Keshipour, S. *Tetrahedron* **2009**, *65*, 3492.

[5] Shaabani, A.; Rezayan, A. R.; Keshipour, S.; Sarvary, A.; Ng, S. W. *Org. Lett.* **2009**, *11*, 2581.

Copper catalyzed arylation of ureas

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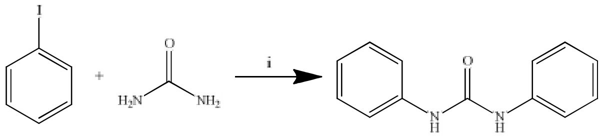
Arylureas have numerous applications such as drugs [1], pesticides [1], selective anion-binding receptors [2] and polymer materials [3]. Common methods for the synthesis of arylureas include the reactions of arylamines with isocyanates or phosgene [1]. Alternative routes to these substances include the reductive carbonylation of Nitroarenes [4] or oxidative carbonylation of amines [5]. It is evident that most of these methods utilize hazardous and toxic reagents.

Recent developments in the palladium and copper catalyzed amination of aryl halides dramatically simplified classical amination reactions such as the Ullmann and Goldberg reactions, which require very high temperatures and toxic reagents [6]. Among these the palladium catalyzed reactions are very sensitive to functional groups such as –OH, $–NH_2$, exogenous air or moisture and also very expensive compared to the copper reagent [7]. We report a simple and mild copper catalyzed amidation of aryl halides with urea. A preliminary screening of ligands showed that both 2-amino pyridine and 2-carboxilic pyridine afforded products in the coupling reactions, with the latter giving low yields. Efforts to use other ligands such as ethylenediamine, 1,2-ethanediol, etc. were not successful. We chose 2-amino pyridine as the preferred ligand for the coupling reactions.



(i) : CuI, 2-Aminopyridine, KOH, DMF, 90°C, 24h

References:

[1] Vyshnyakova, T. P.; Golubeva, I. A. *Russ. Chem. Rev.* (*Engl. Transl.*) **1985**, 54, 249 261.
[2] Schmidtchen, F. P.; Berger, M. *Chem. Rev.* **1997**, 97,1609–1646.
[3] Okaniwa, M.; Takeuchi, K.; Asai, M.; Ueda, M.*Macromolecules* **2002**, 35, 6224–6231.
[4] Tafesh, A. M.; Weiguny, J. *Chem. Rev.* **1996**, 96, 2035–2052.
[5] Mulla, S. A. R.; Rode, C. V.; Kelkar, A. A. *J. Mol. Cat. A. Chem.* **1997**, 122, 103– 109.
[6] Wolfe, J. P.; Wagaw, S.; Marcoux, J. F.; Buchwald, S.L. Acc. *Chem. Res.* **1998**, *31*, 805–818.
[7] Kwong, F. Y.; Klapars, A.; Buchwald, S. L. *Org. Lett***. 2002**, *4*, 581–584.

New and convenient approach to heterotetracyclic benzoxazocines *via* unique tandem 1,3-dinucleophilic addition of bifunctional nucleophiles to quinolinium salts

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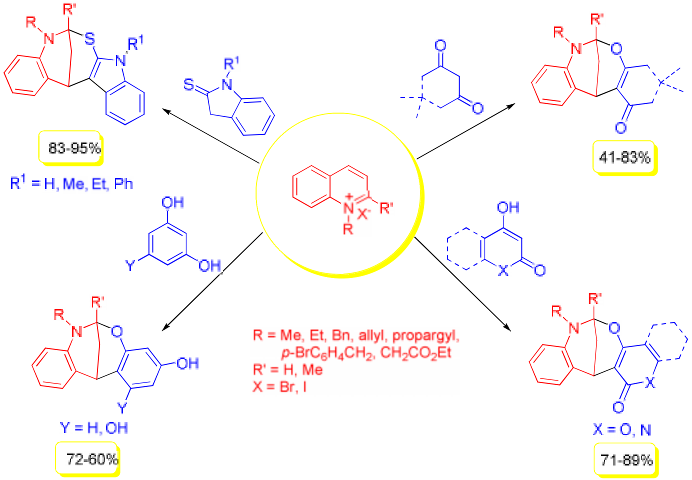
Benzoxazocines have received considerable attention because of their pharmacological properties including antidepressant, antithrombotic, antipsychotic along activity against breast cancer [1]. The construction of medium-ring heterocycles especially eight-membered rings, remains a significant synthetic challenge goal in modern organic synthesis because of entropy reasons and ring strain. However, limited attention has been given to the synthesis of medium-ring heterocycles, examples include cycloadditions, ring closing metathesis, ring expansion, Mitsunobu reactions, and metal-mediated ring cyclization [2]. We herein reported the novel and efficient synthesis of a broad spectrum of polycyclic benzoxazocines via unique tandem 1,3-dinucleophilic addition of different bifunctional nucleophiles to quinolinium. The reaction generally involves the initial addition of nucleophiles to quinolinium salts to form enamine intermediate which can be trapped by intramolecular *O/S*-alkylation of nucleophiles. The procedure is a very mild, efficient and the substrates are easily available (Scheme 1).



References:

[1] Mishra, J. K.; Samanta, K.; Jain, M.; Dikshit, M.; Panda, G. *Bioorg. Med. Chem. Lett*. **2010**, *20*, 244.

[2] Pflantz, R.; Sluiter, J.; Krička, M.; Saak, W.; Hoenke, C.; Christoffers, J. *Eur. J. Org. Chem*. **2009**, 5431.

Boron sulfonic acid, $B(HSO_4)_3$, in organic synthesis: Friedel-Crafts alkylation, synthesis of ethers and synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones

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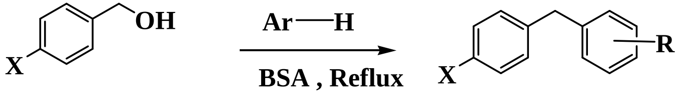
Heterogeneous solid acid catalysts for the synthesis of fine chemicals have attracted considerable attention from both environmental and economical points [1]. In this project we wish to report $B(HSO_4)_3$ as an efficient solid acid catalyst in:

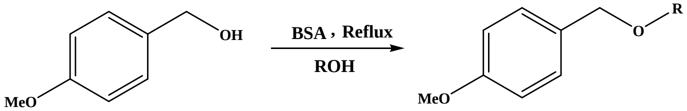
A: Friedel-Crafts Alkylation



R = CH_3, H

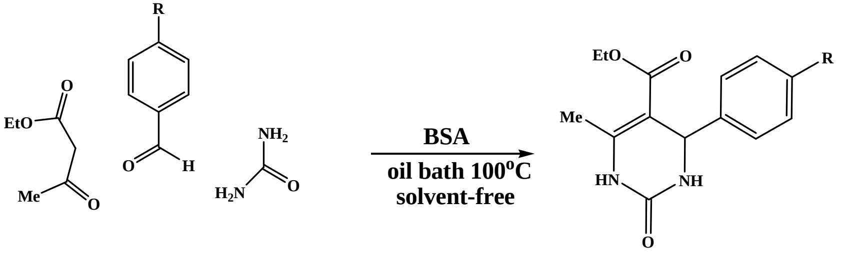
ArH = benzene or toluene

B: Synthesis of ethers



R=Me,Et,1-Pr,2-Pr,2-Bu,t-Bu

C: Synthesis of 3,4-Dihydropyrimidin-2(1*H*)-ones



References:

[1] Kiasat, A. R.; Fallah-Mehrjardi, M. *J. Braz. Chem. Soc*. Vol 19. No. 8. **2008**

The bioactive and volatile compositions of Achillea millefolium by GC/MS

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Essential oils can be extracted using a variety of methods, although some are not commonly used today. Currently, the most popular method for extraction is steam distillation, but as technological advances is made more efficient and economical methods being developed.

Essential oils are generally extracted by distillation. Other processes include expression, or solvent extraction. They are used in perfumes, cosmetics, soap and other products, for flavoring food and drink, and for scenting incense and household cleaning products.

The genus Achillea is widespread in Iran, mainly in north and west flora, and is represented by more than 19 species; seven of them could be endemic plants in Iran. According to literature, this species was not the subject of research until now; therefore, its chemical composition is not well known. Achillea millefolium ssp. elbursensis Hub. Mor. is a rare endemic subspecies of A. millefolium found in the alpine part of the Elburse mountain chain [3]. It is unlike A. millefolium ssp. millfolium, which is a weed often found growing at the margin of cultivated fields or gardens. An oil of millefolium ssp. The essential oil Achillea millefolium subsp. millefolium Afan. (Asteraceae) were investigated. GC-MS analysis of the essential oil resulted in the identification of 21 compounds constituting 94.8% of the total oil. Eucalyptol (2.93%), neryl acetate (17.48%), linalool (3.15%), β-pinene (2.53%), 1,8-cineol(1.93%) benzyl benzoate (6.08%) and geraniol(33.43%)were the principal components comprising 67.53% of the oil [3].

References:

[1] K.H. Rechinger. Flora Iranica, pp. (**1986)** . No. 158**.** 1 -44, Akademische Druck-u. Verlagsanstalt.

[2] Rahimmalek, M. ; Tabatabaei, B.E. S.; Etemadi, N.; Goli, S. A. H.; Arzani, A.; Zeinali, H. Industrial Crops and Products**. 2009,** 29(2-3), 348.

[3] Candan, F.; Unlu, M.; Tepe, B.; Daferera, D.; Polissiou, M.; Sökmen, A.; Akpulat, H. A. J. of Ethnopharmacology. **2003**, 87, 215.

[4] Rahimmalek, M. ; Tabatabaei, B.E. S.; Etemadi, N.; Goli, S. A. H.; Arzani, A.; Zeinali, H. Industrial Crops and Products. **2009**, 29(2-3), 348.

Highly efficient cyanosilylation of carbonyl compounds and preparation of α-aminonitriles by $SbCl_3$ under solventless conditions

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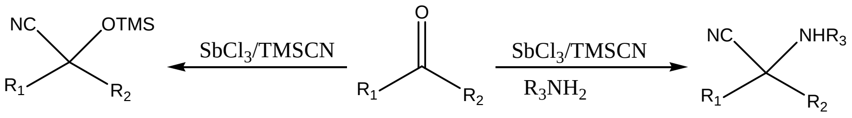
$SbCl_3$ is a mild Lewis acid, which has attracted attention as a catalyst in promoting various organic transformations.[1] However no report has described so far the catalytic properties of $SbCl_3$ for cyanosilylation reactions and the preparation of α-aminonitriles. Cyanosilylation of carbonyl compounds is one of the most efficient methods for the synthesis of silyated cyanohydrins. It is well known that cyanohydrins are important intermediates in organic synthesis.[2]

We wish to report an efficient method for the synthesis of silylcyanoethers in presence of catalytic amount of $SbCl_3$ at rt in solvent free conditions (Scheme). A series of carbonyl compounds react with trimethylsilyl cyanide (TMSCN) in the presence of $SbCl_3$ under solvent-free conditions at rt to give the cyanation products.

α-Aminonitriles are useful intermediates for the synthesis of amino acids. [3] α-Aminonitriles are generally prepared by the nucleophilic addition of cyanide ion to imines (Strecker synthesis).[4] Application of $SbCl_3$ as catalyst was extended for the conversion of aldehydes into α-aminonitriles. The reaction is efficient and proceeds at room temperature by the addition of a primary amine to a mixture of aldehyde/TMSCN in the presence of a catalytic amount of $SbCl_3$ under solvent free conditions (Scheme). A wide range of aldehydes were converted to the corresponding α-aminonitriles in high yield.



R_1, R_2 =Alkyl, Aryl Or H

R_3 = Alkyl, Aryl

Scheme

In conclusion, we have demonstrated highly efficient and convenient methods for cyanosilylation of carbonyl compounds and the preparation of α-aminonitriles in the presence of $SbCl_3$ under solventless conditions without the need for an inert atmosphere. The procedures include simple workup and shorter reaction periods and afford excellent yields of the product.

References:

[1] Francom, P.; Janeba, Z.; Shibuya, S.; Robis, M. *J. Org. Chem.* **2002**, *67*, 6788.
[2] Gregory, R. J. H. *Chem. Rev.* **1999**, *99*, 3649.
[3] Dalko, P. I.; Moisan, L. *Angew. Chem. Int. Ed.* **2004**, *43*, 5138.
[4] Tian, S. K.; Deng, L. *J. Am. Chem. Soc.* **2001**, *123*, 6195.

Multicomponent reactions of enaminones under solvent-free conditions: Facile Synthesis of thiazole derivatives

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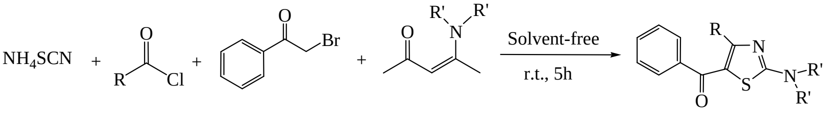
Thiazoles play a prominent role in Nature. For example, the thiazolium ring present in vitamin B1 serves as an electron sink and its coenzyme form is important for the decarboxylation of α-keto-acids [1]. Several pesticides possessing a thiazole nucleus are known in agriculture. Large numbers of thiazole derivatives have emerged as active pharmaceutical ingredients in several drugs for their potential anti-inflammatory [2,3], anti-tumour [4] anti-hyperlipidemic, anti-hypertensive, anti-HIV infections [5], and several other biological properties.

As part of our continuing interest in the development of new synthetic methods in heterocyclic chemistry, we wish to present an efficient synthetic route to functionalized thiazoles. Thus, the reaction of ammonium thiocyanate **1**, acid chlorides **2**, and phenacyl bromide **3** in the presence of enaminone **4** produced 1,3-thiazoles **5** in good yields.



1 **2** **3** **4** **5**

5	R	R'	Yield (%)
a	Ph	CH_3	84
b	Ph	$(CH_2)_2O(CH_2)_2$	80
c	Ph	$(CH_2)_4$	82
d	*p*-NO_2-C_6H_4	CH_3	90
e	*p*-NO_2-C_6H_4	$(CH_2)_5$	80

References:

[1] Breslow, R. *J Am Chem Soc* **1958**, *80*, 3719-3726.
[2] Miwatashi, S.; Arikawa, Y.; Kotani, E.; Miyamoto, M.; Naruo, K. I.; Kimura, H.; Tanaka, T.; Asahi, S.; Ohkawa, S. *J Med Chem* **2005**, *48*, 5966-5979.
[3] Papadopoulou, C.; Geronikaki, A.; Hadjipavlou-Litina, D. *Il Farmaco* **2005**, *60*, 969-973
[4] Kumar, Y.; Green, R.; Borysko, K. Z.; Wise, D. S.; Wotring, L. L.; Townsend, L. B. *J Med Chem* **1993**, *36*, 3843-3848.
[5] Bell, F. W.; Cantrell, A. S.; Hoberg, M.; Jaskunas, S. R.; Johansson, N. G.; Jordon, C. L.; Kinnick, M. D. *J Med Chem* **1995**, *38*, 4929-4936.

Novel optically active poly (ester-imide)s: biodegradation study in soil

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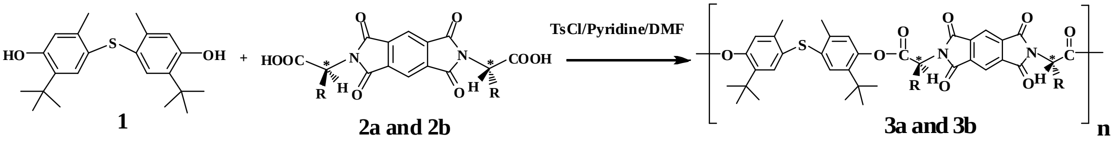
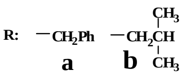
Synthetic biodegradable polymers nowadays have been found as promising biomaterials with increasing applications in pharmaceutical, biomedical and tissue engineering. A tremendous amount of work has been done at international level during the last decade to study the behavior of the biodegradable polymers when exposed to different environments [1, 2]. Chirality is a main concern in the current pharmaceutical industry, because each enantiomer of the chiral drugs shows great differences in pharmacodynamic, pharmacological, and toxicological behavior [3].

In the present work, we successfully prepared a series of optically active poly(ester-imide)s (PEI)s having excellent thermal stability and good solubility in common organic solvent by direct polycondensation of optically active diacids (2a and 2b) with aromatic diol (1) using TsCl/DMF/Py as a condensing agent. All of the polymers were fully characterized by ^{1}H-NMR, FT-IR, elemental analysis and specific rotation. In addition, biodegradability behavior of the synthetic polymers was investigated under soil conditions. The results showed that the synthesized polymers are nontoxic and therefore classified as environmentally friendly polymers.



1 2a and 2b 3a and 3b

Polycondensation reaction of diacids (2a-2b) with diol 1



$R: \; -CH_2Ph \quad -CH_2CH(CH_3)_2$

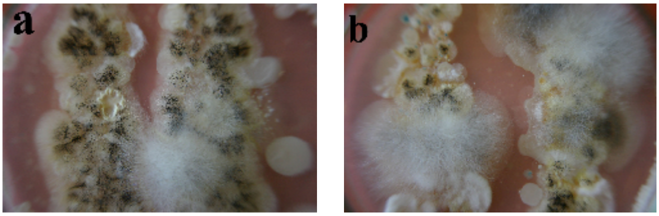


Fig. 1. Investigation of PEIs biodegradability behavior; PEI3a (a), PEI3b (b)

References:

[1] Guo, K.; Chu, C.C. *Biomacromolecules* **2007**, *8*, 2851.
[2] Kolitz, M.; Cohen-Arazi, N.; Katzhendler, J.; Domb, A.J. *Macromolecules* **2009**, *42*, 4520.
[3] Mallakpour, S.; Sepehri, S. *J. Appl. Polym. Sci.* **2008**, *110*, 2942.

Influence of functional monomer nature on morphology and binding properties of molecularly imprinted nanoparticles for galantamine

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Galantamine (GLM) is one of the major drugs used for the treatment of mild to moderate Alzheimer's disease. Because of its low concentration in blood, serum, urine or other biological fluids, in clinical studies it is necessary to extract this drug by a highly selective solid phase [1]. The molecular imprinting technique has emerged as a powerful approach for the creation of recognition sites in highly cross-linked polymeric matrices.

In this research we want to reveal the influence of a functional monomer nature on morphology and binding properties of molecularly imprinted particles so, uniformly sized MIPs for GLM have been prepared by precipitation polymerization method using methacrylic acid (MAA) as a functional and methyl methacrylate (MMA) as a non functional monomer [2].

In this research, uniformly sized molecularly imprinted nanospheres were prepared using methacrylic acid (MAA) as a functional monomer, methyl methacrylate (MMA) as a non-functional monomer and ethylene glycol dimethacrylate (EGDMA) as a cross-linker agent, GLM as a template molecule and azobisisobutyronitrile (AIBN) as initiator. In this study, we will focus on the effect of functional monomer nature used (methacrylic acid and methylmethacrylate) in the morphology and in the binding of template [3,4].

The results showed that the binding the target drug to the template was increased by increasing amount of MAA units. An important result obtained is the possibility of modulate the binding and recognition performance by varying of the percentage of MAA and MMA units in the copolymer. The obtained results were also revealed good selectivity for MIP in extraction of GLM and it can be found from very good selectivity factor which was up to 8.4 in a number of synthesized MIPs. Particle size of synthesized nano particles has been shown by SEM images and there have been substantial differences in the morphology of imprinted and non-imprinted polymer nanospheres in shape and size.

References:

[1] Tas, C.; Ozkan, C.K.; Savaser, A.; Ozkan, Y.; Tasdemir, U.; Altunay, H. *Eur. J. Pharm. Biopharm.* **2006**, *64*, 246.
[2] Yoshimatsu, K.; Reimhult, K.; Krozer, A.; Mosbach, K.; Sode, K.; Ye, L. *Analytica Chimica Acta* **2007**, *584*, 112.
[3] Javanbakht, M.; Namjumanesh, H.; Akbari-Adergani, B. *Talanta* **2009**, *80*, 133.
[4] Javanbakht, M.; Shaabani, N.; Akbari-Adergani, B. *J. Chromatogr. B* **2009**, *877*, 2537.

Electron-transfer induced dehydrogenation of 2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxamides under thermal condition and microwave irradiation

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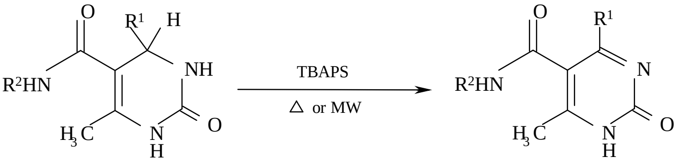
Dehydrogenation of 2-oxo-1,2,3,4-tetrahydropyrimidines (THPMs) to their corresponding 2-oxo-1,2-dihydropyrimidines (DHPMs) is one of the reactions which can affect the biological activities of these compounds. Recent investigations concerning the biological activities of these compounds indicate that this activity is dependent on the C4 absolute configuration of these compounds [1], which can be easily lost upon dehydrogenation and converting them to the corresponding 1,2-dihydropyrimidinones.

In contrast to 1,4-dihydropyridines and 1,4-dihydropyrimidines which are easily dehydrogenated to their corresponding pyridines and pyrimidines either by thermal or photochemical procedures, 2-oxo-1,2,3,4-tetrahydropyrimidines are resistant to dehydrogenation by using various oxidizing agents [2]. However, in recent years, some procedures were reported for the dehydrogenation of 5-carboethoxy- and 5-acetyl-2-oxo-1,2,3,4-tetrahydropyrimidines [3].

In continuation to these works, we were interested to investigate the behavior of various carboxamide groups instead of the acetyl and carboethoxy groups towards tetrabutylammonium peroxydisulfate (TBAPS) as oxidant under thermal condition and microwave irradiation. The results will be presented.



R^1 and R^2: alkyl and aryl

References:

[1] Rovnyak, G. C.; Kimball, S. D.; Beyer, B.; Cucinotta, G.; Dimarco, J. D.; Gougoutas, J.; Hedberg, A.; Malley, M.; McCarthy, J. P.; Zhang, R.; Moreland, S. *J. Med. Chem.* **1995**, *38*, 119.

[2] Vanden Eynde, J. J.; Audiart, N.; Canonne, V.; Michel, S.; Van Haverbeke, Y.; Kappe, C. O. *Heterocycles* **1997**, *45*, 1967.

[3] Memarian, H. R.; Farhadi, A.; Sabzyan, H.; Soleymani, M. *J. Photochem. Photobiol. A: Chem.* **2010**, *209*, 95 and references cited therein.

One-pot synthesis of 2,4,5-trisubstituted and 1,2,4,5-tetrasubstituted imidazoles catalyzed by *N, N, N', N'*-tetrabromobenzene-1,3-disulfonamide

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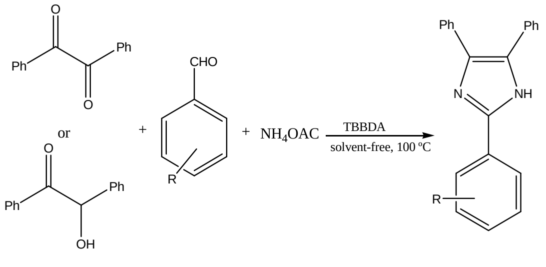
The imidazole ring system is one of the most important substructure found in a large number of natural products and pharmacologically active compounds and the members of this class of compounds are known to possess NO synthase inhibition and antifungal, antimycotic, antibiotic, antiulcerative, antibacterial, antitumour, and CB1 receptor antagonistic activities. Various substituted imidazoles act as inhibitors of p38 MAP kinase and B-Raf kinase, glucagon receptors, plant growth regulators, therapeutic agents, and also pesticides [1]. The various catalysts that have been developed for synthesis of substituted imidazoles include Lewis acids such as $InCl_3.3H_2O$ [2].

Herein, we wish to report a facile and improved protocol for preparation of substituted imidazoles under solvent-free conditions using *N,N,N',N'*-tetrabromobenzene-1,3-disulfonamide [TBBDA] [3] as catalyst. This method offers several advantages such as inexpensive catalyst, short reaction time, easy synthetic procedure, free of organic solvent, high yields, simple work up procedure and easy isolation.



References:

[1] Sivakumar, K.; Kathirvel, A.; Lalitha, A. *Tetrahedron Lett.* **2010**,doi:10.1016/j.tetlet.2010.04.013

[2] Sharma, S. D.; Hazarika, P.; Konwar, D. *Tetrahedron Lett.* **2008**, *49*, 2216.

[3] Ghorbani-Vaghei, R.; Jalili, H., *Synthesis,* **2005**, 1099.

A novel and efficient method for diazotization and azo dyes synthesis from aromatic amines at room temperature under solvent free condition

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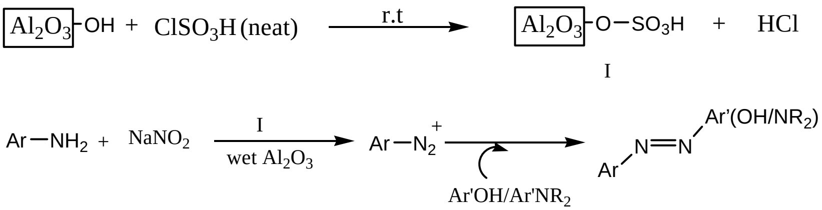
It is well known that azo compounds are the most widely class of industrial synthesized organic dyes due to their versatile application in various fields, such as dyeing textile fiber, biological–pharmacological activities and advanced application in organic synthesis [1,2]. Optical switching and image storage can be made by azobenzene liquid crystal film [3]. Generally, solid state reactions tend to occur with minimal atomic/molecular motion [4]. Thus they have many advantages such as high efficiency and selectivity. Easy separation and purification, mild reaction conditions [5]. Therefore we would like to report a simple and convenient solid state reaction, using of alumina sulfuric acid for the diazotization and coupling reaction for the synthesis of azo dyes.

Some amines and phenols were subjected to diazotization and coupling reactions in the presence of alumina sulfuric acid (I), $NaNO_2$ and wet Al_2O_3 in the absence of any solvent at room temperature. The azo dyes were performed in good to excellent yields.



Scheme

References:

[1] F. Karci, A. Demircali, I. Sener, *Dyes & Pigm*. **2006**,*71*, 90.

[2] M.R. Yazdanbakhsh, A. Ghanadzadeh, E. Moradi, *J. Mol. Liq*. **2007,** *136*, 165.

[3] Campbell, D.; Dix, L. R.; ostron, P. *Dyes & Pigm*. **1995**, *29* (1), 77-83

[4] Singh, N. B.; Singh, R. J.; Singh, N. P. *Tetrahedron* **1994**, *50*, 6441

[5] Rasmussem, M. O; Alexon. O; Tanner, D. *Synthe. Commun*. **1997**, *27*, 4027

A new, simple and efficient method for the pyrazoles Synthesis in water at room temperature

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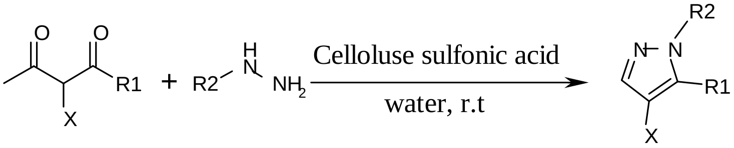
Synthesis of heterocyclic nitrogen containing compounds has attracted interest of many organic chemists, due to their therapeutic and pharmacological properties. Among them, pyrazoles and their derivatives are precursors for a wide variety of bioactive compounds including anti-inflammatories, antipyretics, analgesics, bactericides and fungicides [1]. On the other hand cellulose and its derivatives have some unique properties which make them potent as conventional organic supports for catalytic applications [2].

In this research we report the preparation of a series of pyrazoles by condensation of hydrazine ⁄ hydrazides with various 1,3-diketones in the presence of catalytic amount of celloluse sulfonic acid in water as a green solvent. Green chemistry approach, Mild reaction condition which proceeds at room temperature, readily prepared catalyst, high selectivity, reduced by-products and waste, using friendly processes easy work up procedure and good to excellent yields (80-95%) are the merits of our method[3].



References:

[1] Longhi, K.; Moreira, D. N.; Marzari, M. R. B.; Floss, V. M.; Bonacorso, H. G.; Marcos, N. Z. And Martins, A. P. *Tetrahedron Letters* 51, **2010,** 3193–3196.

[2] Shaabani,A.; Seyyedhamzeh,M.; Maleki,A.; And Rezazadeh, F. *Applied Catalysis A: General* 358, **2009**, 146–149.

[3] (a) Clarke, J. H. *Green Chem*. **1999**, 1, 1; (b) Anastas, P. T. and Warner, J. C. *Green Chemistry, Theory and Practice*; Oxford University Press, **1998**.

Prediction of $p56^{lck}$ protein Tyrosine Kinase inhibitory activity of flavonoid derivatives using QSAR method

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The quantitative structure-activity relationship (QSAR) research field provides medicinal chemists with the ability to predict drug activity by mathematical equations which construct a relationship between the chemical structure and biological activity [1].These mathematical equations are in the form of y=Xb+e that describe a set of predictor variables (X) with a predicted variable (y) by means of a regression vector (b) [2].

In a QSAR study, we proposed the method of substituent electronic descriptors (SED) as an alternative to both substituent constants and molecular descriptors [3]. Herin, this method was used to discover a quantitative relationship between molecular structure and $p56^{lck}$ Protein Tyrosine Kinase Inhibitory activity. Substituents were considered as radical molecule. Hyperchem software (Hypercube, Inc., version 7) was used to build the substituent radical structures into computer. Molecular structures were optimized utilizing Guassian 98. The structures of the substituents were obtimized with 6-31G basis set for all atoms, except for iodine, for which we used LanL2Dz Pseudo method as basis set. Considering no molecular symmetry constraint all bond lengths and angles optimization were carried out at level of UHF/6-31G and RHF/6-31G for singlet state of molecules, respectively. The calculated descriptors can be classified into three different electronic categories including local charges, dipoles, and orbital energies. The quantum chemical indices of hardness (HD), softness (SOF), electronegative (EN), and electrophylicity (EPH) were calculated according to the method proposed by Thanikaivelan et al. [4]. We used the aforementioned quantum descriptors and applied them to find a reasonable relationship between molecular quantum indices and $p56^{lck}$ Protein Tyrosine Kinase inhibitory activity. Although we have found that these SED parameters have an impact on protein tyrosine kinase inhibitory activity of compounds, results show a poor improvement than literatures. So we used new quantum descriptors derived from potential energy surfaces (PES) using guassian 98 with employing Cube (100, potential) keyword. In this manner we found that the PES quantum descriptors besides the previously defined descriptors have an excellent promise in describing QSAR of flavonoid derivatives as $p56^{lck}$ protein tyrosine kinase inhibitors than those provided previously.

Reference:

[1] Hansch, C.; Hoekman, D.; Gao, H., *Comparative QSAR. Chem. Rev.,* **1996**, *96*,1045.
[2] Hemmateenejad, B.; *Chemom. Intell. Lab. Syst.* **2005,** 75, 231.
[3] Hemmateenejad, B.; Sanchooli, M., *Chemometrics,* **2007,** 21, 96.
[4] Thanikaivelan, P.; Subramanian, V.; Rao, JR. BU. Nair. *Chem. Phys. Lett*. 323 (**2000**) 59.

Synthesis, characterization and applications of molecular imprinted polymer as extractant for preconcentration and determination of Baclofen

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Molecular imprinted polymers (MIPs) were prepared from methacrylic acid and Allyl glycidil ether/ iminodiacetic acid as the functional monomer and N, N methylene-diacrylamid as the cross-linker in methanol solution using baclofen as the template molecule and 2,2-azobis-isobutyronitrile as the initiator. The polymer was by elemental analysis, IR and thermogravimetric analysis (TGA) and studied for preconcentration and determination of baclofen using high performance liquid chromatography for drug monitoring. The effects of amount of the cross-linker, the ratio of template molecule and functional monomer, amount of solvent and amount of the radical initiator on the polymerization were examined. The polymerization also was performed in presence of Cu (II) which can coordinate the drug and retain it in polymer. Clearly, in the last polymerization manner, the polymer first was doped with Cu (II) then acted as a sorbent. The synthesized polymer was successfully applied for drug determination from tablet matrix.

Reference:

[1] V . M . Biju , j . Mary Gladis , T prasada Rao . Ion imprinted polymer particles : synthesis , characterization and dysprosium ion uptake properties suitable for analytical applications . *Analytical chemical Acta* **2003,** *478,* 43.

[2] Natalia Perez – Moral , Andrew G . Mayes . Direct rapid synthesis of MIP beads in SPE cartridges . *Biosensors and Bioelectronics,* **2006,** *21,* 1798.

[3] Li-Qin Lin , Jing Zhang , Qiang fu , Lang- Chong He , Ying-Chun Li .Concentration and extraction of sino menine from herb and plasma using a molecularly imprinted polymer as the stationary phase . *Analytical chemical Acta,* **2006,** *561,* 178.

In situ preparation of new polyamideimide/titania nanocomposite thin film

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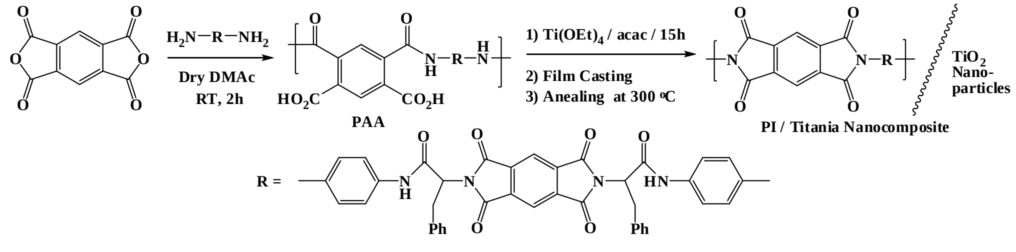
Recently, organic/inorganic nanocomposite materials fabricated via the sol-gel process have attracted a great deal of attention in material science because of their multi-purpose applications [1]. TiO_2 (titania) is one of the most vital inorganic component for the synthesis of nano hybrid materials because of the versatility, availability, non toxicity, excellent optical property, etc [2]. Polymer/titania nanocomposites have been used in production of several high-tech materials such as interference filter, antireflective coating, and optical waveguides [3].

Polyimides (PI)s with excellent heat resistance and outstanding mechanical properties are exceptional candidates as nanocomposite matrixes and may be prepared through the polymerization of diamines and dianhydrides [4]. In the presented study, the reaction performed at room temperature and poly(amic acid) (PAA) was prepared in a dry aprotic solvent. In following, the thermal imidization process condensed the PAA to the PI quantitatively. Water generated from this condensation reaction hydrolyzed the titanate agent to the titania nanoparticles in a sol-gel manner. Considering the fact that the existence of additional functional groups with capability to coordinate to titania would improve the particle dispersion chiefly, herein, we have synthesized a diamine monomer containing additional amide groups which are able to construct the strong H-bond lattice with titania nanoparticles. Using this strategy we have fabricated a new series of well-dispersed PAI/titania nanocomposites with different percentage of titania contents.

On the other hand the introduction of L-amino acid moieties in the structure of diamine monomer may increase the bioactivity and biocompatibility of thin nanocomposite films potentially.



References:

[1] Tsai, M.; Chang, C.; Chen, P.; Ko, C. *Thin Sold Films* **2008**, *516*, 5654.
[2] Tsai, M. ; Liu, S. ; Chiang, P. *Thin Solid Films* **2006**, 515, 1126.
[3] Que, w.; Zhou, Y.; Lam, Y. L.; Chan, Y. C.; Kam, C. H. *Thin Solid Films* **2000**, *358*, 16.
[4] Liaw, W.; Chen, K.; *Eur. Polym. J.* **2007**, **43**, 2265.

Diketene-based multicomponent reactions

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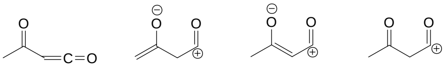
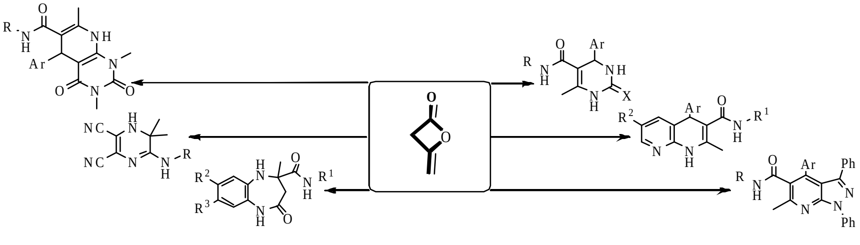
Multicomponent reactions (MCRs), are powerful synthetic tools which have changed the landscape of organic and medicinal chemistry because of environmental concerns, atom economy and their ability to generate large libraries of compounds in one synthetic step or two synthetic steps [1,2].

Diketene is a strained molecule (E_{strain}=22.5 kcal/mol), which is readily ring-opened and therefore frequently appears to react as acetylketene **I** or one of its dipolar tautomers (**II** and **III**). It is important to note that each of dipolar tautomers is equal to a β-dicarbonyl synthon. On the other hand diketene is a reagent for synthon **IV** [3].



I **II** **III** **IV**

In view of our current interest on diketene-based multicomponent reactions (MCRs) herein, we report diketene as an alternative substrate for one-pot synthesis of new compounds under multicomponent reactions strategy [4].



References:

[1] Zhu, J.; Bienayme, H. Multicomponent Reactions; Wiley-VCH: Weinheim, 2005.
[2] Dömling, A.; Ugi, I. *Angew. Chem., Int. Ed.* **2000**, *39*, 3168.
[3] Mansson, M.; Nakase, Y.; Sunner, S. *Acta Chem. Scand.* **1968**, *22*, 171.
[4] (a) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Rezazadeh, F.; Behnam, M. *J. Comb. Chem.* **2009**, *11*, 375. (b) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Behnam, M.; Rezazadeh, F. *Tetrahedron Lett.* **2009**, *50*, 2911. (c) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Behnam, M. *Tetrahedron Lett.* **2009**, *50*, 6355. (d) Shaabani, A.; Maleki, A.; hajishaabanha, F.; Mofakham, H.; Seyyedhamzeh, M.; Mahyari, M.; Ng, S. W. *J. Comb. Chem.* **2010**, *12*, 186. (e) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Hajishaabanha, F. *Tetrahedron* **2010**, *66*, 4040.

Reductive acetylation of carbonyl compounds to acetates with $NaBH_4$ in the presence of catalytic amounts of Co(dimethylglyoxime) dichloride complex

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Acetylation of carbonyl compounds is generally achieved via reduction followed by the acetylation. However, the literature review shows that direct reductive acetylation of such compounds was rarely studied. Zn/Ac_2O/tertiary amines, Zn/Ac_2O/pyridine, $Zn/Ac_2O/NaOAc$, CH_3COCl/Bu_3SnH, and lanthanide complexes/isopropenyl acetate [1] are the methods which have been reported for this transformation. Moreover, the combination systems of borohydrides have been also reported for one-pot reductive acetylation of carbonyl compounds. The protocol of $NaBH_4/EtOAc$ [2] was the first report in this subject; however, the method described reductive acetylation of few carbonyl compounds to their acetates in moderate yields. Moreover, this method was accompanied with the reduction, producing carbinols as side products. Tamami *et al*. developed the title reaction by the application of poly (4-vinylpyridine) supported $Zn(BH_4)_2$ for chemoselective reductive acetylation of aldehydes over ketones [3]. Though the method is successful in its chemoselectivity, however, long reaction times and moderate yields of products are disadvantages of this method [4].

In the line of the outlined strategies, herein, we wish to report a combination system of $NaBH_4$ with $Co(dmg)Cl_2$ [5] as a bench-top protocol for reductive acetylation of a variety of carbonyl compounds such as aldehydes, ketones, α,β-unsaturated aldehydes and ketones, α-diketones and acyloin in ethyl acetate under reflux condition. The corresponding esters were obtained in high to excellent yields. Observation of the obtained results shows that this method in view point of simplicity, efficiency and faster reduction rates could be worth for addition to the current methodologies.

References

[1] Nakano, Y.; Sakaguchi, S.; Ishii, Y. *Tetrahedron Lett.* **2000**,*41*, 1565.
[2] Rao, B. R.; Nambudiry, M. E. N. *Synth. Commun.* **1991**,*21* , 1721.
[3] Tamami, B.; Goudarzian, N.; Kiasat, A. R. *Eur. Polym. J.* **1997**, *33*, 977.
[4] Zeynizadeh, B.; Setamdideh, D.; Faraji, F. *Bull. Korean Chem. Soc.* **2008**, *29*, 76.
[5] Nayak, S. C.; Das, P. K.; Sahoo, K.K. *Chem. Pap.* **2003**, *57*, 91.

The synthesis of aromatic α-diketones from cyanide catalyzed condensation of aromatic aldehydes

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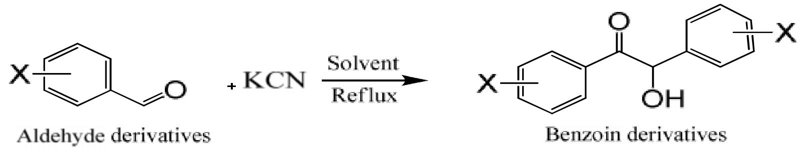
Benzil derivatives are important synthons for the synthesis of natural products, Industrial materials, and pharmaceutical materials [1]. α- diketones are versatile building blocks for the synthesis of biologically active and photoresponsive compounds [2]. Several methods for the synthesis of benzils are reported in the literature which include acyloin condensation of esters with sodium metal and subsequent oxidation [3], coupling of acid chlorids [4], oxidation of 1,2-Diols [5].

Several other methods, including the oxidation of alkenes or methylene ketones and non-oxidative methods, have also been reported [6].

However cyanide catalyzed condensation of aromatic aldehydes is a simply and efficient method for preparation of benzoin derivatives which could be oxidized to their relative benzils. In this study, we have surveyed the effects of temperature and substituents on the yields of benzoins. In addition, we have developed a catalytic system based on ammonium nitrate and copper (II) acetate for oxidation of resulted benzoins to their relative benzils. Our studies revealed that this reaction is promoted by protic solvents and higher temperatures.



References:

[1] SIwamoto, K. ; Hamaya, M. ; Hashimoto, N. ; Kimura, H. ; Suzuki, Y. *Tetrahedron Lett*. **2006**, *47*, 7175.

[2] (a) Rong, F.; Chow, S.; Yan, S.; Larson, G.; Hong, Z. *J. Bioorg. Med. Chem. Lett*. **2007**, *17*, 1663. (b) Ams, M, R.; Wilcox, C, S.; *J. Am. Chem. Soc.* **2007**, *129*, 3966.

[3] Mc Elvain, S, M.; *Org. React*. **1948**, *4*, 256.

[4] Gotard. P.; Coultgoal, R.; Kagan, H, B. *Tetrahedron Lett*. **1981**, *22*, 3959.

[5] Uyanik, M.; Akakura, M.; Ishihara, K. *J. Am. Chem. Soc*. **2009**. *131*, 251.

[6] Katritzky, A, R.; Zhang, D.; Kirichenko, K. *J. Org. Chem*. **2005**, *70*, 3271.

Diastereoselective synthesis of fused [1,3]thiazolo[1,3]oxazins and[1,3]oxazino[2,3,b][1,3]benzothiazoles

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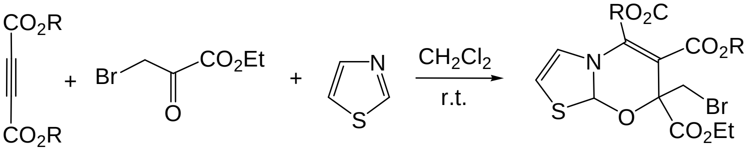
In general, multi-component reactions (MCRs) are perfectly suited for combinatorial library syntheses, thus are finding increasing use in the discovery process for new drugs and agrochemicals[1].In this respect, several studies involved sulfur-containing compounds because they present good conduction in organic materials [2] or are relevant biologically. Also, sulfur containing anions have found extensive use as versatile reagents in organic synthesis. Some heterocyclic compounds containing a thiazole ring in their structures offer important applications in pharmaceutical as well as in agrochemical chemistry For example, ritonavir, an anti-HIV drug contains the thiazole moiety. These products, which contain N and S atoms, are bridged easily with other molecules or can coordinate several metal ions. For example, they could be used to entrap mercury in the environment [3] and as a new inhibitor for copper[17]. Herein, we describe an efficient procedure for direct synthesis of 7-ethyl 5,6-dialkyl 7*H*-[1,3]thiazolo[2,3-*b*][1,3]oxazin-5,6,7-tricarboxylate or 2-ethyl 3,4-dialkyl 2*H*-[1,3]oxazino[2,3-*b*][1,3]benzothiazol-2,3,4-tricarboxylate is described. This involves a reaction of activated acetylenic compounds with Pyruvates in the Presence of Thiazol or Benzothiazol in dichloromethane at room temperature.



References:

[1] Domling, A.; Ugi, I. *Angew Chem Int Ed.* **2000**, *39*, 3169.
[2] Hansen, TK.; Becher, J. *Chem Soc Rev*. **1994**, *23*, 41.
[3] Yavari , I.; Sabbaghan, M.; Hossaini, Z. *Mol Divers.* **2007**, *11*, 1.

Preparation of new co-polyamides based on 4-(4-methoxyphenyl)urazole

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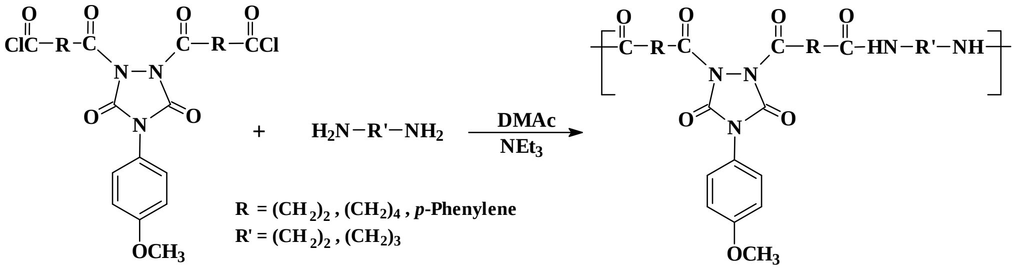
Heterocyclic nitrogen-containing molecules constitute the largest portion of chemical entities, which are part of many natural products, fine chemicals, and biologically active pharmaceuticals vital for enhancing the quality of life [1]. Among a large variety of nitrogen-containing heterocyclic compounds, urazole (1,2,4-triazolidine-3,5-dione) is interesting because it has many industrial uses. It is used in the manufacture of automobile air bags, as a blowing agent in plastics, as a stabilizer in milk [2], and in the production of herbicides, antifungal compounds, and anti-tumor drugs [3]. It is also used as a laboratory reagent for the synthesis of novel heterocyclic and organometallic compounds [4]. In this work, we present synthesis of new co-polymers based on 4-(4-methoxyphenyl)-1,2,4-triazolidine-3,5-dione.

We have recently synthesized and identified some new diacid chlorides based on 4-phenylurazole or 4-(4-methoxyphenyl)urazole with succinoyl chloride, adipoyl chloride or terphthaloyl chloride. Herein, we wish to report the synthesis of new co-polyamides based on 4-(4-methoxyphenyl)-1,2,4-triazolidine-3,5-dione. For this goal, 4-(4-methoxyphenyl)urazole was reacted with two moles of aliphatic or aromatic diacid chlorides in dimethylacetamide (DMAc) in the presence of triethylamine as a scavenger. The resulting diacid chlorides were reacted with 1,2-diaminoethane or 1,3-diaminopropane without separation. Some physical properties and spectroscopic data of the resulting co-polymers were reported.



References:

[1] Domling, A.; Ugi, I. *Angew. Chem. Int. Ed.* **2000**, *39,* 3168.
[2] Wakabayashi, O.; et al, Ger. Offen. **1976**, 2,526,358.
[3] Wakabayashi, O.; et al, *Japan. Kokai,* **1976,** 7632,586.
[4] Jikihara, T.; et al, *U.S.* **1981,** 4,249,934.

Facile synthesis of the new derivatives of 3-alkylsulfanyl-5-chloro-7-methyl-[1,2,4]triazolo[4,3-c]pyrimidine

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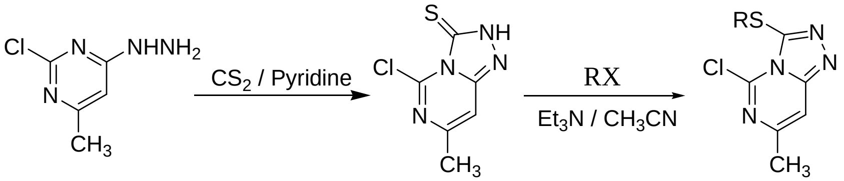
Triazolopyrimidines are of interest not only for the synthesis of heterocyclic systems but also as compounds having biological activity and exhibiting, in particular, hypotensive, antiseptic, antiarrhythmic, and antiasthmatic properties[1,2]. Some methods for the preparation of these heterocyclic system are involves treatment of hydrazinopyrimidines with carbon disulfide or sodium nitrite in the presence of acetic acid [3] or condensation of the hydrazinopyrimidines with either formic acid or its orthoester [4] and also by the Dimroth rearrangement of imino derivatives of some pyrolopyridines in the presence of NaOH to obtain the hydrazinopyrimidine which were transformed into [1,2,4]triazolo[4,3-c]pyrimidines by treatment with acylhalides[5].

In this study, the reaction of 2-chloro-4-hydrazino-6-methylpyrimidine with carbonedisulfide in boiling pyridine led to the synthesis of 5-chloro-7-methyl-[1,2,4]triazolo[4,3-c]pyrimidine-3(2H)-thione. Subsequently, this precursor was alkylated by various alkyl halides in CH_3CN and in the presence of triethylamine to give the corresponding 3-alkylsulfanyl-5-chloro-7-methyl- [1,2,4]triazolo[4,3-c]pyrimidine derivatives.



References:

[1] Brown, D. J.; Grigg, G. W.; Iwai, Y.; McAndrew, K. N.; Nagamatsu, T.; Van Heeswyck, R. *Aust. J. Chem.*, **1979**, 32, 2713.
[2] Dlugosz, A. *Pol. J. Chem.*, **1992**, 66, 131.
[3] A. Sh. Oganisyan, A. S. Noravyan, and M. Zh. Grigoryan, *Chemistry of Heterocyclic Compounds,* **2004**, Vol. 40.
[4] Oganisyan1, A. S.; Noravyan1, A. S., Karapetyan, A. A.; Aleksanyan, M. S.; Struchkov, T. *Chemistry of Heterocyclic Compounds,* **2001**, Vol. 37, No. 5.
[5] Vorobev, E. V.; Kurbatov, E. S.; Krasnikov, V. V.; Mezheritskii, V. V.; Usova, E. V. *Rus. Chem. Bull.*, **2006**, 55, 1492.

Ab initio molecular orbital study of organic four-membered cyclic compounds containing heteroatom

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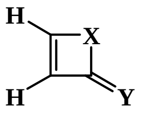
Recently, experimental and computational studies are carried out on organo-sulfur compounds and/or conjugated systems containing heteroatom, examples: 1,2,4,6-tetrathiepane [1] and lenthionine (1,2,3,5,6-pentathiepane) [2], organic six-membered Cyclic sulfoxides [3], etc. Organo-sulfur compounds are considered in biochemistry, atmospheric cycle, polymer and rubber chemistry, anti-oxidant and anti radiation processes, etc [4].

Herein we report energy, geometrical parameters and zero-point vibrational energy (ZPVE) for 2*H*-thiete-2-thione, 2*H*-oxete-2-thione, 2*H*-thiet-2-one, 2*H*-thiete-2-selenone, 2*H*-selenete-2-thione, 2*H*-selenete-2-selenone, 2*H*-oxet-2-one, 2*H*-selenet-2-one and 2*H*-oxete-2-selenone have been calculated by the HF/6-31+G*, B3LYP/6-31+G* and MP2/6-31+G* methods. Also, energy of cyclic structures compares with liner structures that those are structural isomers.



X= O, S, Se Y= O, S, Se

References:

[1] Yavari, I.; Jabbari, A.; Moradi, Sh. *Lect. Notes Comput. Chem.*, **2004**, 403.
[2] Yavari, I.; Jabbari, A.; Moradi, Sh. *J. Mol. Struct. (Theochem)*, **2003**, *225*, 631.
[3] Yavari, I.; Haghdadi, M.; Amiri, R. *Phosphorus, Sulfur, and Silicon and the Related Elements*, **2006**, *181(7)*, 1693-1705.
[4] Radriquez, E. *J. Am. Chem. Soc*. Washington, DC, **1988**.

Synthesis and characterization of A_4+ B_2- type nanostructure hyperbranched polymers with carboxy and amine end groups

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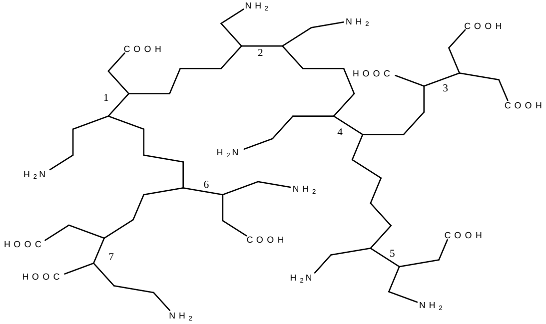
In the last two decades, researchers both from academia and industry showed high interest on hyperbranched polymers due to their unique chemical and physical properties [1-3]. The overall aim of this research is to describe the synthesis of nanostructure branched poly (amide-imide)s containing amino acid residue in an A_4 + B_2 approach. Desired tetrafunctional monomer was synthesized from L-cysteine in a three–step reaction procedure. The characterization of the hyperbranched structure of the polymers was facilitated by the study of a model reaction of ethylenediamine- ettraacetic acid (EDTA) with different diamines. Direct polycondensation using triphenylpho- sphite was utilized to synthesize all of the branched polymers. Reaction parameters such as temperature, reaction time, monomer concentration and stirring speed were such optimized to get a soluble material before the gel point. Different functional conversions to reach the gel point of polymerization were obtained for different diamines. The structures of monomer and polymers were confirmed by IR, NMR, CHN analysis and optical rotation measurements. Property investigations revealed ion that the polymer had good solubility in common organic solvents, and reduced solution viscosity compared to linear similar polymers. Scanning electron microscopy (SEM) was used to analyze the morphology of the synthesized poly(amide – imide)s in view of size distribution homogeneity and particle dimensions.



References

[1] SCHOLL, M., KADLECOVA, Z., KLOK, H.A. Dendritic and hyperbranched polyamides. Prog. Polym. Sci., **2009**, *34*, 24-61 .

[2] WANG, H., et al. Synthesis and property investigations: A partially conjugated hyperbranched polymer for light-emitting application. *Synth. Met.*, **2008**, *185*, 437-441.

[3] SCHOLL, M., et al. The Thermal polymerization of Amino Acids Revisited; *Synthesis* and Structural Characterization of Hyperbranched Polymers from L-Lysine. J. Polym. Sci. Part A: Polym. Chem., **2007**, *45*, 5494-5508.

An efficient method for one-pot three-component synthesis of amidoalkyl naphthols

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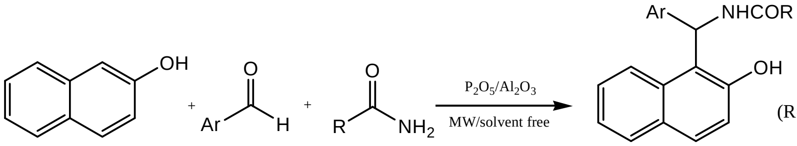
Compounds bearing 1,3-amido oxygenated functional groups are ubiquitous to a variety of biologically important natural products [1]. It is noteworthy that 1-amidoalkyl-2-naphthols can convert into important biological active 1-aminoalkyl-2-naphthol derivatives by hydrolysis reaction [2]. The importance of amidoalkyl naphthols for their synthesis has attracted renewed attention and various improved procedures have been reported. Many of these reported methods employ catalysts. [3-4]

In continuation of our interest in finding new environmentally benign methods for organic transformation and use of silica gel supported solid acid [5]. We want to report here the rapid and efficient preparation of amidoalkyl naphthols by a multicomponent reaction of 2-naphthol, aromatic aldehyde and amide using P_2O_5/Al_2O_3 as catalyst under microwave irradiation and solvent free conditions (Scheme).



(R=CH_3, CH_2Cl, $CHCl_2$, Ph)

Scheme

In all cases, aromatic aldehydes with substituents carrying either electron-donating or electron-withdrawing groups reacted successfully and gave the products in high yields. A series of amidoalkyl naphthols were prepared in high to excellent yields.

References:

[1] Dingermann, T.; Steinhilber, D.; Folkers, G. *In Molecular Biology in Medicinal Chemistry*; Wiley VCH: Weinheim, 2003 Gregory, R. J. H. *Chem. Rev*. **1999**, *99*, 3649.
[2] Shen, A. Y.; Tsai, C. T.; Chen, C. L. *Eur. J. Med. Chem.* **1999**, *34*, 877.
[3] Shaterian, H. R.; Hosseinian, A.; Ghashang, M. *Tetrahedron Lett*. **2008**, *49*, 5804.
[4] Khodaei, M. M.; Khosropour, A. R.; Moghanian, H. *Synlett* **2006**, *916*.
[5] Pourmousavi, S. A. Zinati Z. *Turk J Chem.* **2009,** *33*, 385.

HPA/ SBA-15 as a nonoreactor for the synthesis of 3-(2'-benzothiazolyl)-2,3-dihydroquinazolin-4(1*H*)-ones under solvent-free conditions

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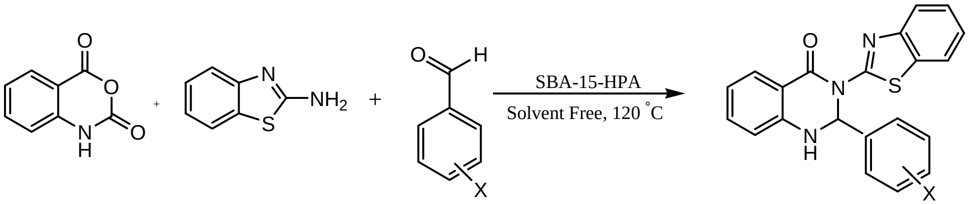
Dihydroquinazolinones and their derivatives are important heterocyclic compounds which influence numerous cellular processes. They are analgesic, diuretic and vasodilating agents while display a broad range of biological, medicinal, and pharmacological properties [1].

Heterogeneous phase reactions are of significant importance in organic chemistry. Compared to the polymers, inorganic mesoporous materials are an excellent support for the heterogenization of molecular catalysts due to its excellent thermal and chemical stability. SBA-15 is a newly discovered mesoporous silica molecular sieve with uniform tubular channels whose pore diameter is variable from 50 to 300 A°. SBA-15 has large pore diameter, thick pore wall and high hydrothermal stability. There are a few papers about the modification and application of SBA-15 with heteropolyacid [2].

Hence, we have designed a three-component one-step synthesis of 3-(2'-Benzothiazolyl)-2,3- dihydroquinazolin-4(1*H*)-ones, in which HPA/SBA-15, is used as a nanoreactor, non-toxic and inexpensive catalyst. (Scheme1)



Scheme1

References:

[1] Rueping, M.; Antonchick, A. P.; Sugiono, E.; Grenader, K. *Angew. Chem. Int. Ed*. **2009**, *48*, 908.

[2] Satish Kumar, G.; Vishnuvarthan, M.; Palanichamy, M.; Murugesan, V. *Journal of Molecular Catalysis A: Chemical*, **2006**, *260*, 49.

Study of chemical constituents and antimicrobial activity of essential oil of Thymus caucasicus

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The genus thymus, consisting of about 350 species, is one of the most important genera belonging to the lamiaceae. *Thymus caucasicus* is one of the 14 thymus species in iran. *Thymus caucasicus* distributed in iran mostly at north-west (Ardabil) [1].

Thymus caucasicus at the flowering stage were collected, from Ardabil province (No. 41 at Central Herbarium of Institute of Medicinal Plants, ACECR).

The essential oil aerial parts of *T. caucasicus* were collected by Hydrodistillation in a Clevenger type apparatus and Steam distillation method. The essential oils were dried over anhydrous sodium sulphate and after filtaration, stored at +4˚C until tested and GC/MS analyzed.

The essence of T. *caucasicus* which was collected by hydrodistillation, 44 compounds were identified which most important ones were Nerolidol (52.31 %), Geraniol (7.02 %), Geranyl acetone (5.64 %).

In steam distillation essence of *T. caucasicus*, 58 compounds were identified which most important ones were Nerolidol (53.58 %), Geranyl acetone (6.57 %), Geraniol (7.02 %).

In vitro antimicrobial activities of *T. caucasicus* was performed against eight standard bacterial strains using agar dilution method .Result showed that was effective against *Staphylococcus aureus*, *Staphylococcus epidermidis*, *Bacillus subtilis*, *Escherichia coli*, *Klebsiella pneumonia*, *Pseudomonas aeruginosa* and Meticillin Resistant Staphylococcus aureus.

Reference:

[1] Jalas, J. 1982. Jn: K.H. Rechinger (ed). Akademische Druck und Verlagsanstalt. Graz, Austria. 150: 550-551.

[BMIM][BF_4] A novel and recyclable medium for synthesis of diketopyrrolopyrroles

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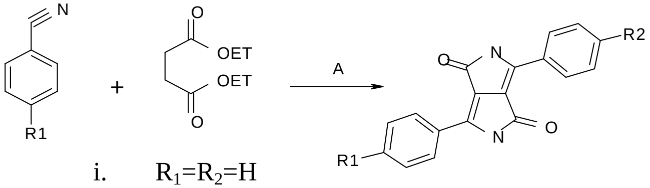
Ionic liquids have recently attracted increasing interest in the concept of green synthesis. Although ionic liquids were initially introduced as an alternative green reaction media because of their unique chemical and physical properties such as non-flammability, thermal stability, and selective miscibility, today their use has been stretched far beyond this border, showing their significant role as catalysts.

A task-specific ionic liquid, [bmim][BF_4], has been introduced as a catalyst and as a reaction medium in the synthesis of diketopyrrolopyrrole (DPP) pigments under basic conditions and at room temperature. [bmim][BF_4] was regenerated successfully and re-used. In this paper, [bmim][BF_4] is employed as a useful and novel reaction media for the synthesis of DPPs in the peresence of an organic base such as sodium-tert-amyl oxide(t-amyl-ONa), at room temprature.



i. $R_1=R_2=H$
ii. $R_1=R_2=Cl$
iii. $R_1=R_2=Br$
iv.

Figure1: Scheme of synthesis of pigments, A: [bmim][BF_4] and base(t-amyl-ONa), 60°C.

FTIR, particle size distribution, SEM and ^{1}H-NMR have been employed for monitoring of the process. In comparison to traditional organic solvents, [bmim][BF_4] is preferred as a novel and green solvent due to higher yield as well as smaller particle size distribution of products.

References

[1] Brindaban C. Ranu**,**Organic letter,**2005**,vol7,No14,3049-3052
[2] J.S.Yadav,**2003**,WIELY-VCH, 948.
[3] I.yavari,Tetrahedron Letteres, ,**2007**,48,3753.

Sodium ion bond dimer of amino acids: structure, stability and enthalpy of formation

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The metal ions have important rules in structure and function of proteins and other biomolecules [1]. They act as cofactor in activation of enzymes[1-4], and other bioreactions. The sodium ion is undoubtedly much abundant ions in biological systems and act in generating ionic gradients across membranes and for the maintenance of osmotic balance [**Error! Bookmark not defined.**]. On the other hand the sodium pomp in which sodium ions is transferred, has a critical rule in nervous system. Therefore understanding the nature of sodium ion interaction with amino acids helps the scientists to make their insight about sodium pomp clearer and to find ways to regulate their action. The importance of Na^+ in biology has prompted many studies about its intrinsic binding modes and affinities to simple model systems, mainly amino acids and small peptides [1-3]. In this research as well as calculation the sodium affinity of amino acids, the structure, enthalpy of formation and stability of sodium ion bond dimer of twenty three numbers of amino acids were calculated. All calculations were performed by HF and MP2 method, 6-311++G** basis set and gaussian03 package. Interactions may be considered to be exist between sodium ion and two forms of amino acids and its zwitterions. All calculations were performed to study the structure of sodium ion bond dimer for these forms of amino acids. As a result of this research, the structure of amino acid strongly affected in presence of sodium ion. Additionally by calculation of infrared spectrum for the complex of sodium ion with amino acid and sodium ion dimer of them it was shown that they are all stable and their enthalpy of formation is negative (their formation are energetically favored) while the sodium bond dimer of zwitterions of amino acids is much stable than other form of it.

References:

[1] Robert R. Crichton, Biological Inorganic Chemistry an Introduction, Elsevier, 1st edition. **2008**.
[2] Z. Rappoport and I. Marek, The chemistry of organomagnesium compounds, **2008** John Wiley & Sons, Ltd
[3] R.B. Davies and E.P. Abraham, Biochem. J., (**1974**) 143, p.129.
[4] J. A. Cowan, Chem. Rev. **1998**, 98, p.1067.
[5] Russ Hille, Chem. Rev., **1996**, 96, p.2757.
[6] Zahra Aliakbar Tehrani, Alireza Fattahi, Ali Pourjavadi, Carbohydrate Research, 344, (**2009**) p.771.
[7] Frank Jensen, J. Am. Chem. Soc., **1992**, 114, p.9533.
[8] Milan Remko, and Bernd Michael Rode, J. Phys. Chem. A, **2006**, 110, p.1960.

Enantioselective addition of trimethylsilyl cyanide to aldehydes induced by a new chiral schiff bases

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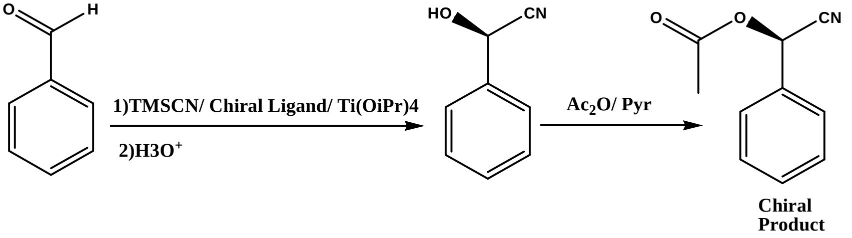
Enantiomerically pure cyanohydrins are valuable building blocks for pharmaceuticals and fine chemicals, and their synthesis has been the subject of several reviews and symposiums. Existing methods for the preparation of chiral cyanohydrins include both enzymatic and chemical processes.[1,2] Chemically, several efficient methods have been developed.

*C*1 and *C*2-symmetric chiral Schiff bases derived from the condensation of salicylaldehydes with suitable chiral amines are among the most successful types of ligands in organic synthesis, such as enantioselective addition of trimethylsilyl cyanide to aldehydes.



We now describe a new chiral Ti(IV) catalyst with chiral imino alcohol Schiff bases as the ligand**,** which effects the enantioselective addition of trimethylsilyl cyanide to aldehydes.

References:

[1] For a review, see North, M. *Synlett* **1993**, 807.
[2] (a)Effenberger, F.; Ziegler, T.; Forster, S. *Angew. Chem., Int. Ed. Engl.* **1987**, *26*, 458. (b) Ognyanov, V. I.; Datcheva, V.K.; Kyler, K. S. *J. Am. Chem. Soc.* **1991**, *113*, 6992.

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Formation of thiazol-2(3*H*)-imines by reaction of *α*-amino acids, aroylisothiocyanates, and *α*-bromoketones in an ionic liquid

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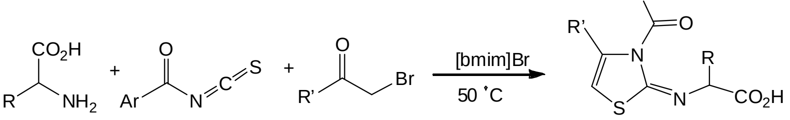
Thiazoles are an important group of heterocyclic compounds, several derivatives of which have been found to possess useful biological activity such as anti-tumor, anti-fungal, anti-inflammatory, and anti-microbial [1, 2]. In recent years, thiazole derivatives have attracted considerable attention because of their bioactivity and many applications in organic and medicinal chemistry [3]. Although the Hantzsch process, in which an *α*-halocarbonyl compound is condensed with a thioamide, has been for decades the method of choice for the synthesis of thiazoles, great effort has been dedicated to more flexible procedures, and particularly to that of thiazole ring formation in novel reaction media.

As part of our current studies on the development of new routes in heterocyclic synthesis [4], we report an efficient one-pot synthesis of functionalized thiazole-2(3*H*)-imines by a three-component reaction between aroylisothiocyanates, *α*-amino acids, and *α*-bromoketones in 1-butyl-3-methylimidazolinium bromide ([bmim]Br) as a green solvent. In conclusion, we have developed a convenient, practical, and one-pot method for the synthesis these new compounds.



1	R
a	H
b	Me
c	*i*-Pr

2	Ar
a	Ph
b	*p*-Tolyl

3	R'
a	CO_2Et
b	4-$MeOC_6H_4$
c	4-BrC_6H_4

4	R	Ar	R'	Yiled (%)
a	H	Ph	CO_2Et	76
b	H	Ph	4-$MeOC_6H_4$	79
c	H	Ph	4-BrC_6H_4	86
d	Me	Ph	CO_2Et	96
e	Me	Ph	4-$MeOC_6H_4$	94
f	Me	Ph	4-BrC_6H_4	97
g	*i*-Pr	Ph	CO_2Et	92
h	*i*-Pr	Ph	4-$MeOC_6H_4$	89
i	*i*-Pr	Ph	4-BrC_6H_4	96
j	Me	*p*-Tolyl	CO_2Et	80
k	Me	*p*-Tolyl	4-$MeOC_6H_4$	85
l	Me	*p*-Tolyl	4-BrC_6H_4	83

Scheme 2. Synthesis of functionalized thiazole-2(3*H*)-imines**.**

References:

[1] Pereira, R.; Gaudon, C.; Iglesias, B.; Germain, P.; Gronemeyer, H.; de Lera, A. R. *Bioorg. Med. Chem. Lett.* **2006**. *16*, 49.

[2] Franklin, P.X.; Pillai, A.D.; Rathod, P.D.; Yerande, S.; Nivsarkar, M.; Padh, H.; Vasu, K.K.; Sudarsanam, V. *Eur. J. Med. Chem.* **2008**, 43, 129-134.

[3] Zhou, G.B.; Guan, Y.Q.; Shen, C.; Wang, Q.; Liu, X.M.; Li, L.L. *Synthesis* **2008**, 13, 1994-1996.

[4] Yavari, I.; Hossaini, Z.; Shirgahi-Talari, F.; Seyfi, S. *Synlett* **2008**, 11, 1631-1632.

Synthesis and properties of poly(vinyl alcohol)/nanoclay bio-nanocomposites

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Poly(vinyl alcohol) (PVA) is a hydrophilic polymer with fascinating characteristic such as superior chemical resistance, processability, biocompatibility and biodegradability that play an significant role on the industrialized of pharmaceutical and biomedical devices [1].

Polymer/layered-silicate hybrids-nanocomposites have attracted interest in today's materials research, as it is possible to achieve impressive enhancements of material properties compared to the pure polymers. Especially when these properties depend on the surface area of the filler particles, small amounts of nanometer-thin layered inorganic fillers give rise to the same level of mechanical and thermal improvements as are typically achieved with loadings of 30-50% of micron-sized fillers [2]. Since polymer/MMT nanocomposites frequently exhibit excellent properties including reduced gas permeability, improved solvent resistance, and enhanced thermal stability and flame-retardant properties, different polymer/MMT nanocomposites have been successfully synthesized by incorporating MMT in various polymer matrixes [3].

The present study describes the modification of nanoclay to organophilic nanoclay with the ion exchange of a reactive organic cation such as ammonium salt of L-leucine amino acid. Then PVA/organo-nanoclay nanocomposites were prepared with different amount of clay and were characterized by X-ray diffraction and fourier transformation infrared. The morphology observation was performed by scanning electron microscopy and transmission electron microscopy that indicate the flake structured organo-modified MMT is homogeneously dispersed in PVA matrix.

References:

[1] Strawhecher, K. E.; Manias, E. *Chem. Mater*. **2000**, *12*, 2943.
[2] Paranhos, C. M.; Soares, B. G.; Olivera, R. N.; Pessan, L. A. *Macromol. Mater. Eng*. **2007**, *292*, 620.
[3] Zhang, J.; cheng, X.; Liu, H.; Lu, W. *Chin. J. Chem*., **2009**, *27*, 1611.

New procedure for the synthesis of N- benzylbenzimidazole catalyzed by $ZrCl_4$ on nanosilica

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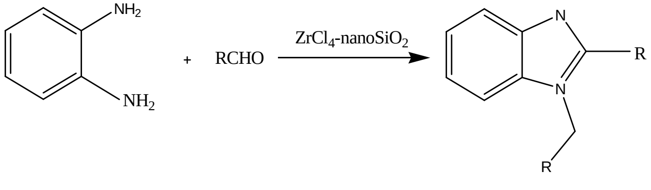
Benzmidazoles and their derivatives exhibit a number of important pharmacological properties, such as antihistaminic, anti-ulcerative, anti-allergic, and anti-pyretic. In addition, benzimidazole derivatives are effective against the human cytomegalovirus (HCMV) and are also efficient selective neuropeptide Y Y1 receptor antagonists [1].

Most of the previous methods for the synthesis of benzimidazoles involved the use of volatile organic solvents and based on the solid-phase synthesis via *o*-nitroanilines or the condensation of *o*-phenylenediamines with carboxylic acid derivatives, aldehydes, and aryl halides [2].

However, most of these protocols use expensive and toxic reagents and/or have long reaction times in high temperature and are limited to aromatic carbonyl compounds [3].

Herein we wish to report efficient one-pot synthesis, for the synthesis of 1,2-disubstituted benzimidazole derivatives under solvent-free condition by the reaction of *o*-phenylenediamine and different aldehydes in the presence of nanosilica supported $ZrCl_4$ (Scheme 1). The products were obtained in high purity and excellent yields beside the very simple and effective workup. Beside of all mentioned advantages, the high reuseability of the catalyst is another unique feature of this method to develop the synthesis of 1,2-disubstituted benzimidazole.



References:

[1] Barker, H. A.; Smyth, R. D.; Weissbach, H.; Toohey, J. I.; Ladd, J. N.; Volcani, B. E. *Bio. Chem.* **1960**, *235*, 480.

[2] (a) Reddy, G. V.; Rao, V. V. V. N. S. R.; Narsaiah, B.; Rao, P. S. *Synth. Commun.* **2002**, *32*, 2467. (b) Perumal, S.; Mariappan, S.; Selvaraj, S. *Arkivoc* **2004**, *8*, 46. (c) Rao, A.; Chimirri, A.; Ferro, S.; Monforte, A. M.; Monforte, P.; Zappalà, M. *Arkivoc* **2004**, *5*, 147.

[3] Ma, H. Q.; Wang, Y. L.; Li, J. P.; Wang, J. Y. *Heterocycles* **2007**, *71*, 135.

Cyclization reaction of anthranilic acid derivatives with potassium cyanate: A novel synthetic route to quinazoline-4-one dimer derivatives

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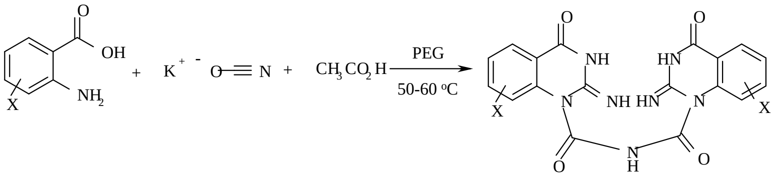
Anthranilic acid derivatives as simple and available compounds have been widely used in heterocyclic synthesis [1-3]. Quinazoline-4-ones and quinazoline-2,4-diones are remarkable and interesting heterocyclic compounds due to their pharmacological and biological properties [4]; thus, considerable attention has been focused on their synthesis [5].

Here, we have found a simple and interesting route to the synthesis of some dimeric quinazoline-4-ones. The ring closure reaction of anthranilic acid derivatives **1** in the acidic solution of potassium cyanate in PEG proceeds to the synthesis of compounds **2** with good yields and simple work-up. The whole reaction sequence runs in one-pot, without separation of the intermediates and without use of any catalyst.



1 **2**

References:

[1] Cainelli, G.; Panunzio, M.; Andreol, M.; Martelli, G.; Spunta, G.; Giacomin, D.; Bandin, E. *Pure & Appl. Chem.* **1990**, *62,* 605.

[2] Nikpour, F.; Sheikh, D.; Saraji, M. *Chem. Lett.* **2007**, *36*, 1074.

[3] Nikpour, F.; Sheikh, D. *Chem. Lett.* **2007**, *36*, 858.

[4] a) Buckley, G. M.; Davies, N.; Dyke, H. J.; Gilbert, P. J.; Hannah, D. R.; Haughan, A. F.; Hunt, C. A.; Pitt, W. R.; Profit, R. H.; Ray, N. C.; Richard, M. D.; Sharpe, A.; Taylor, A. J.; Whitworth, J. M.; Williams, S. C. *Bioorg. Med. Chem. Lett.* **2005**, *15,* 751; b) Colotta, V.; Catarzi, D.; Varano, F.; Calabri, F. R.; Filacchioni, G.; Costaglib, C.; Galli, A. *Bioorg. Med. Chem. Lett.* **2004**, *14*, 2345.

[5] a) Mizuno, T.; Iwai, T.; Ishino, Y. *Tetrahedron Lett.* **2004**, *45*, 7073. b) Schwinn, D.; Glatz, H.; Bannwarth, W. *Helv. Chim. Acta* **2003**, *86*, 188; c) Makino, S.; Suzuki, N.; Nakanishi, E.; Tsuji, T. *Synlett* **2001**, 333; d) Makino, S.; Suzuki, N.; Nakanishi, E.; Tsuji, T. *Synlett* **2001**, 333.

SCF-MO Calculation of electrophilic aromatic reactions of azulene

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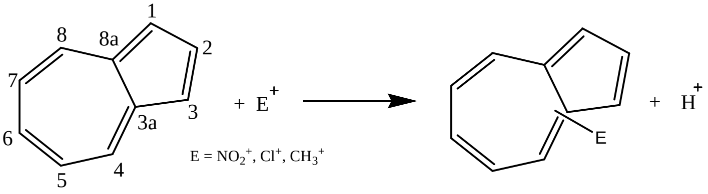
Azulene not only has a beautiful deep blue color, but also has a large dipole moment (μ=0.8-1.08D) and unusual photo physical properties, the excited states and electronic spectrum of azulene are of interest for theoretical and spectral studies and fluorescence properties [1, 2].

In this study the reactivity of different positions of azulene against common electrophils, like NO_2^+, Cl^+, CH_3^+,were investigated. The structures of cationic intermediates and products of the reaction were optimized at HF/6-31+G* level of theory. Then, the relative stabilities of intermediates and products were calculated. The results indicated that the position 1 was the best for electrophilic aromatic reactions. Although isomers containing substituent at position 2 were the most stable isomers.



References:

[1] P.M Kozlowski, G. Raunhut, and P. Pulay. *J. Chem. Phys*. **1995**, *103(13)*, 5650.
[2] J. Michel and E.W. Thulstrup. *Tetrahedron,* **1976**, *32*, 205.

Guanidine hydrochloride as a highly efficient catalyst for modified Ritter reaction in water

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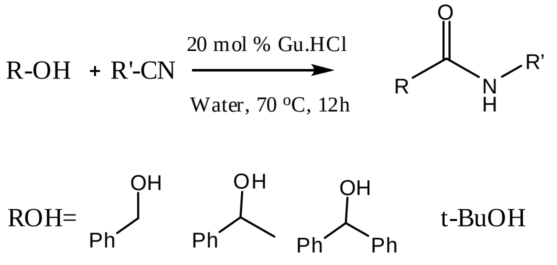
The Ritter reaction [1], the reaction of nitrile with a substituted alkene or alcohols using a stochiometric amount of sulfuric acid to the corresponding amide, is an important transformation in organic synthesis. The reaction is especially useful for the preparation of bulky amides, which may be hydrolyzed to yield hindered amines. This method works well only under strongly acidic conditions, thus limiting its applicability to compounds containing functional groups stable to acid.

Since recognized as a major concept, organic catalysis has attracted much attention and has been applied extensively in non-asymmetric and asymmetric reactions due to its determined scientific significance and its huge potential in organic chemistry [2]. Among them, guanidine hydrochloride in water was selected.

In conclusion, we have established an efficient and simple method for preparation of *N*-*tert*-butyl and *N*-alkyl amides with bulky substituents *via* Ritter reaction using 20 mol% guanidine hydrochloride catalyst. Easily available and low-price catalyst, easy work up, water as solvent and excellent yields were the advantages of the proposed method.



R'= Ph, CH_2=CH_2, CH_3

References:

[1] (a) Benson, F. R.; Ritter, J. J. *J. Am. Chem. Soc.* **1949**, *71*, 4128; (b) Krimen, L. I.; Cota, D. J. *Org. React.* **1969**, *17*, 213.Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.

[2] (a) Jarvo, E.J.; Miller, S.J. *Tetrahedron* **2002**, 58, 2481; (b) Basavaiah, D.; Rao, A.J.; Satyanarayana, T.; *Chem. Rev.* **2003**,103, 811.

Synthesis of compound 5-(3, 4, 5-trimethoxyphenyl)-4-(1,3,5-triphenyl-1H-1,2,4-triazol-4(5H)-yl)-2H-1,2,4-triazole-3(4H)-thione under basic conditions

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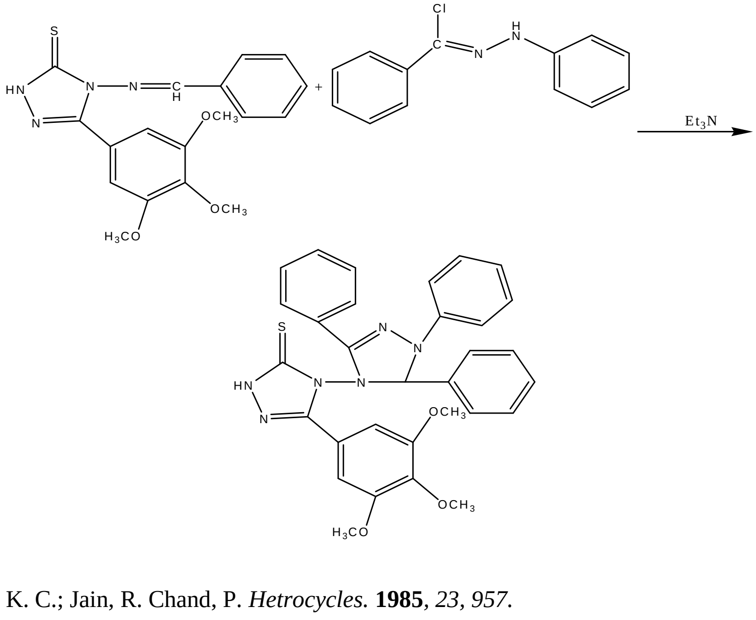
1,3-Dipolar cycloaddition reactions are important in construction of five-membered hetrocycles [1]. In this research 1,3-Dipolar cycloaddition reaction has been studied. At the first, by using of suitable appropriate materials nitrilimine compound was obtained.Then by using of 5-amino triazole and reaction with benzaldehyde the compound 4-(benzylidenamino)-5-(3,4,5-trimethoxyphenyl)-2H-1,2,4-triazole-3(4H)-thione was obtained [2]. At the last stage corresponding imine as 2 with nitrilimine as 3 in a suitable solvent in base media in situ reacted together and the compound that called 5-(3,4,5-trimethoxyphenyl)-4-(1,3,5-triphenyl-1H-1,2,4-triazol-4(5H)-yl)-2H-1,2,4-triazole-3(4H)-thione and use in farming field and producing kinds of toxic drugs with excellent yield was obtained [3].The structure 5-(3,4,5-trimethoxyphenyl)-4-(1,3,5-triphenyl-1H-1,2,4-triazol-4(5H)-yl)-2H-1,2,4-triazole-3(4H)-thione were confirmed on the basis of their IR, ^{1}HNMR, ^{13}CNMR and MASS spectra data.



References:

[1] Joshi, K. C.; Jain, R. Chand, P. *Hetrocycles.* **1985**, *23, 957.*

[2] Ansari, K. F.; Lal, C. *J. Med. Chem.* **2009**, *44*, *2294*.

[3] Aly, A. A.; El-Sayed, R. *Chem. Pop.* **2006**, *60, 56*

A green synthesis of aryl-14*H*-dibenzo[*a, j*]xanthenes

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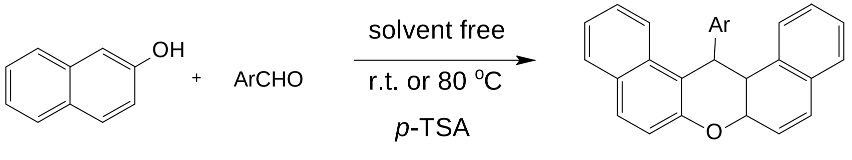
The synthesis of xanthenes, especially benzoxanthenes, has been of considerable interest to chemists because their oxygen heterocycles may contribute to potential antibacterial, antiviral,[1] and anti-inflammatory activities.[2] Furthermore, these compounds can be used as dyes, [3] in laser technology, and pH-sensitive fluorescent materials for the visualization of biomolecular assemblies. For the synthesis of benzoxanthenes, various methods have been reported including the reaction of b-naphthol with formamide, 2-naphthol-1-methanol, and carbon monoxide. However, these methods have drawbacks such as poor yields, prolonged reaction time, using of toxic organic solvents, excess reagents/catalysts, and harsh reaction conditions. Due to these disadvantages, several reactions have been improved by the condensation of b-naphthol with aldehydes in the presence of a catalyst, such as sulfamic acid, AcOH/H2SO4, iodine, K5CoW12O40-3H2O, cyanuric chloride, LiBr.

However, searching another environmentally friendly catalyst and green solvents is still highly desirable. As a result of our ongoing interest in green chemistry and acid catalyzed organic reactions, we wish to report a solvent free reaction for the preparation of benzoxanthenes by the condensation reaction of aromatic aldehydes with β-naphthol in the presence of *p*-TSA at room temperature or 80 ^{o}C. Most substituted benzaldehydes reacted with β -naphthol completely and afforded the corresponding products of aryl-14*H*-dibenzo[*a*,*j*]xanthene in high yields. The products could be easily identified by the singlet peak (about 6.4–6.6 ppm) in ^{1}H NMR spectrum.



Reference:

[1] Hideo, T. Jpn. Tokkyo. Koho. JP 56005480, 1981; *Chem. Abstr.* **1981**, *95*, 80922.
[2] Poupelin, J. P.; Saint-Rut, G.; Foussard-Blanpin, O.; Narcisse, G.; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.* **1978**, *13*, 67.
[3] Banerjee, A.; Mukherjee, A. K. *Stain Technol.* **1981**, *56*, 83.

New procedure for the synthesis of 1-thiocarbamoyl-3,5-diaryl-4,5-dihydro-1H-pyrazoles

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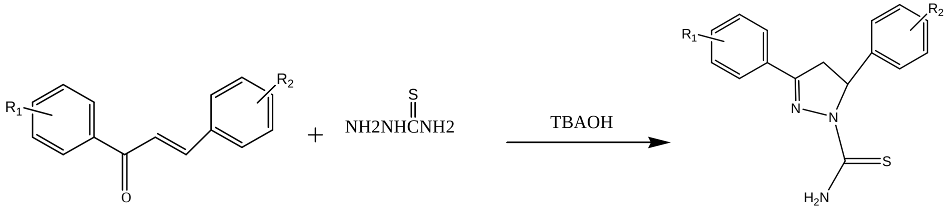
Pyrazoles possess a broad spectrum of important biological and pharmaceutical activities such as antimicrobial, antihypertensive, antitumor, antiinflammatory, antidepressant and anticonvulsant activities [1-2].Recently reported that 1-thiocarbamoyl-3,5-diaryl-4,5-dihydro-1H-pyrazoles are selective monoamine oxidase inhibitors that may have promising features in the treatment of Parkinson’s and Alzeheimer’s diseases.They are also useful intermediates for important pharmaceutical products, such as Rimonabant and Celecoxib [3-4].

Recently, some procedures have been published for the synthesis of pyrazoles.However, some of these preparations require relatively expensive reagents and have low yields, long reaction times in high temperature and sometimes tedious work-up with using of toxic reagents or solvents [5-8].

Herin We wish to report an efficient, green and facile method for the synthesis of 1-thiocarbamoyl-3,5-diaryl-4,5-dihydro-1H-pyrazoles under solvent-free condition by the reaction of thiosemicarbazide and chalcone derivatives in the presence of basic ionic liquid.

This method has many advantages over existing methods, including high yields, simple work-up, short reaction times, no side reactions and easy work-up.



References:

[1] Özdemir, A.; Turan-Zitouni, G.; Kaplancıklı, Z. A.; Revial, G.; Güven, K. *Eur. J. Med. Chem.* **2007**, *42*, 403.

[2] Palanska, E.; Aydin, F.; Uçar, G.; Erol, D.; *Arch. Pharm. Chem. Life Sci.* **2008**, *341*, 209–215.

[3] Donohue, S. R.; Halldin, C.; Pike, V. W. *Tetrahedron Lett*. **2008**, *49*, 2789

[4] Chimenti, F.; Carradori, S.; Secci, D.; Bolasco, A.; Bizzarri, B.; Chimenti, P.; Granese, A.; Ya´n˜ez, M.; Orallo, F. *Euro. J. Med. Chem*. **2009**, 1-5.

[5] Pizzuti, L.; Piovesan, L.; Flores, A.; Quina, F.; Pereira, C.*; Ultrason. Sonochem.* **2009**, *16*, 728–731.

[6] Langer, P.; Freiberg, W. *Chem. Rev*. **2004**, *104*, 4125–4149.

[7] Matsumura, N.; Kunigihara, A.; Yoneda, S. *Tetrahedron Lett*. **1984**, *25*, 4529–4532.

An efficient coupling reaction of 2,3-dihydro-3-aryl-2-thioxoquinazolin-4(1*H*)-ones

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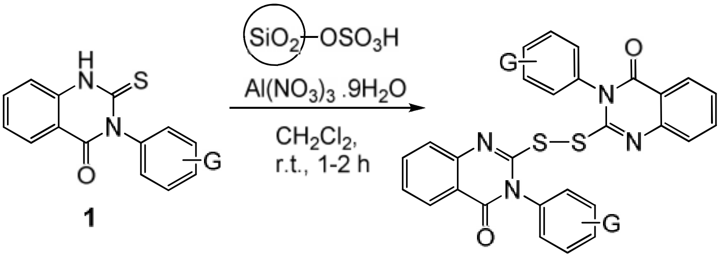
Conversion of thiols to disulfides is important from biological points of view [1]. Thiols and disulfides are important in living cells being a structural feature of many biomolecules such as; cysteine, methionine amino acids and proteins [2]. In biological systems, thiols are oxidized by flavins, cytochromes and dehydroascorbic acid to control the cellular redox potential and prevent oxidative damage [3-5]. This paper describes an efficient coupling reaction of 2,3-dihydro-3-aryl-2-thioxoquinazolin-4(1*H*)-ones (**1**) {aryl = 2-CH_3-C_6H_4- (**a**), 3-CH_3-C_6H_4- (**b**), 4-CH_3-C_6H_4- (**c**), C_6H_5- (**d**), 4-Br -C_6H_4- (**e**), 4-Cl-C_6H_4- (**f**)} and ethyl 2-cyano-3-(arylamino)-3-thioxopropanoate (**1g**) in the presence of $Al(NO_3)_3.9H_2O$ catalyzed by silica sulfuric acid at room temperature in excellent yield.



2 (90-99%)

G = *o*-CH_3 (**a**), *m*-CH_3 (**b**), *p*-CH_3 (**c**), H (**d**), *p*-Br (**e**), *p*-OCH_3 (**f**)

Scheme 1.

References:

[1] Jocelyn, D. C. *Biochemistry of the Thiol Group*, Academic Press: New York, **1992**.
[2] Capozzi, G.; Modena, G. *The Chemistry of Thiol Group*, Part 2; S. Patai, Ed., pp. 785, Wiley: New York, **1974**.
[3] Pe'er, I.; Felder, C. E.; Man, O.; Silman, I.; Sussman, J. L. *Proteins* **2004**, *54*, 20.
[4] Bardwell, J. C. *Mol. Microbiol.* **1994**, *14*, 199.
[5] N. Kharasch and A.S. Arora, *Phosphorus and Sulfur 2*, 1 ,**1976** .

Synthesis of *N*- alkyl or arylidene-2-(2-phenoxyphenyl)-acetohydrazides as anti-inflammatory agents

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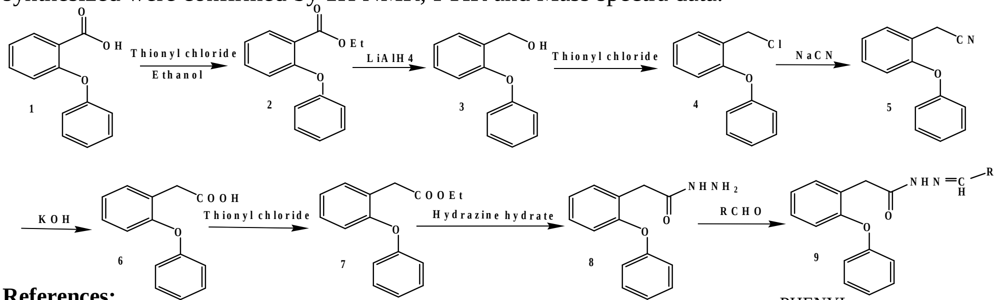
Non-steroidal anti-inflammatory drugs (NSAIDs) are widely used for the treatment of pain and inflammation, particularly for different types of arthritis [1–3] (Diclofenac sodium). The pharmacological activity of NSAIDs is related to the suppression of prostaglandin biosynthesis by inhibiting the enzyme prostaglandin endoperoxidase (COX-1,2) [4,5]. Local irritation by the direct contact of carboxylic acid (–COOH) moiety of NSAIDs with GI mucosal cells (topical effect) and decreased tissue prostaglandin production in tissues which undermines the physiological role of cytoprotective prostaglandins in maintaining GI health and homeostasis [6]. Several studies have described the derivatization of the carboxylate function of representative NSAIDs with amide or N-acylarylhydrazone having less acidic amide hydrogen resulted in an increased anti-inflammatory activity with reduced ulcerogenicity [7,8].

In our attempt to discover new, safer and potent agents for treatment of inflammatory diseases, we synthesized a series of N-substituted-2-(2-phenoxyphenyl)-acetohydrazides (9a-j) by reacting the amino group of 2-(2-phenoxyphenyl)-acetohydrazide (8) with a variety of aldehydes in order to obtain new compounds with potential analgesic and anti-inflammatory activity. The starting material (8) was synthesized from 2-phenoxy benzoic acid (1). The structure of synthesized were confirmed by 1H NMR, FTIR and Mass spectra data.



R
- **a.** PHENYL
- **b.** 4-METHYL - PHENYL
- **c.** 4-METHOXY- PHENYL
- **d.** 4-CHLORO - PHENYL
- **e.** 4-DIMETHYL- AMINO - PHENYL
- **f.** 4-NITRO - PHENYL
- **g.** 2,4-DIMETHOXY - PHENYL
- **h.** 2-PYRIDYL
- **i.** 3-PYRIDYL
- **j.** 4-PYRIDYL

References:

[1] Palomer, A.; et al. *J. Med. Chem*. **2002**, *45*, 1402–1411.
[2] Sorbera, L. A.; et al. *Drug Future* **2001**, *26*, 133–140.
[3] Talley, J. J.; et al. *J. Med. Chem.* **2000**, *43*, 775–777.
[4] Almasirad, A.; et al. *J. Pharm. Pharm. Sci.* **2005**, *8*, 419.
[5] Hawkey, C.; et al. *J. Arthritis Rheum.* **2000**, *43*, 370–377.
[6] Duarte, C. D.; et al. *Bioorg. Med. Chem.* **2007**, *15*, 2421.
[7] Lima, P. C.; et al. Eur. *J. Med .Chem.* **2000**, *35*, 187.
[8] Figueiredo, J. M.; et al. *Bioorg. Med. Chem.* **2000**, *8*, 2243.

Effect of different parameters on the removal of Tartrazine as an organic pollutant by Ag doped TiO_2 photocatalyst

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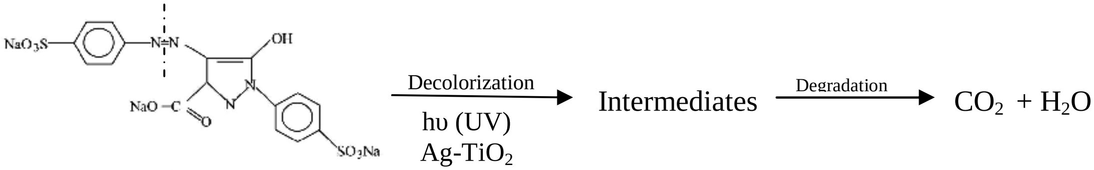
Wastewaters generated by textile, paper, food and some other industries are known to contain considerable amounts of toxic aromatic dyes, especially azo dyes. One of them, Tartrazine (also known as: Acid Yellow 23, C.I. No.19140, Food Yellow No. 4) is principally the trisodium 5-hydroxy-1-(4-sulfonatophenyl)-4-(4-sulfonatophenylazo)-H-pyrazol-3-carboxylate [1].

Many studies indicate that the azo dyes are toxic or carcinogenic. Thus, appropriate treatment of dye wastewaters to remove color and the dye compounds is clearly an important issue. Recently, chemical treatment methods, based on the generation of hydroxyl radicals, known as advanced oxidation processes (AOPs) has been developed. Among AOPs, TiO_2 mediated semiconductor photocatalysis is gaining more importance due to its high production of hydroxyl radicals. Earlier studies have revealed that the photocatalytic activity of TiO_2 can be improved significantly by doping with noble metals such as Pt, Au, Ag, etc. [2,3].

Herein we report an efficient method for the removal tartrazine in water in the presence of aqueous suspensions of TiO_2 and Ag doped TiO_2 (Ag/TiO_2) nanoparticles, under UV-C light irradiation. Silver doped TiO_2 nanoparticles were prepared by photodeposition (PD) method. In the PD method Ag metal doped on TiO_2 was prepared by photoreducing Ag^+ ions to Ag metal on the TiO_2 surface. The presence of silver in TiO_2 was found to enhance the removal of tartrazine. The higher activity of $Ag\text{-}TiO_2$ is due to the enhancement of electron-hole separation by the electron trapping of silver particles [4]. The effects of the influencing factors on the removal of tartrazine, such as doping content of silver, photocatalyst dosage, and pH were evaluated, showing the optimum values of 1wt% Ag, 600 mgl^{-1} and 9.5, respectively, for these factors. A complete decolorization of 0.05 mM tartrazine dye solution under UV irradiation at optimum conditions on Ag/TiO_2 was observed in 15 minutes.



References:

[1] Tanaka, T.; Takahashi O. ; Oishi S. ; Ogata A. *Reprod. Toxicol.* **2008**, *26,* 156.

[2] Behnajady, M.A., Modirshahla, N., Shokri, M., Elham, H., Zeininezhad, A. *J. Environ. Sci. Health A.* **2008**, *43,* 460.

[3] You, X.; Chen, F., Zhang, J.; Anpo, M. *Catal. Lett.* **2005**, *102,* 247.

[4] Sobana, N.; Muruganadham, M.; Swaminathan, M. *J. Mol. Catal. A.* **2006**, *258,* 124.

Photocatalytic ring opening of α-epoxyketones by 2,4,6-triphenylpyrylium tetrafluoroborate in cyclopentanone

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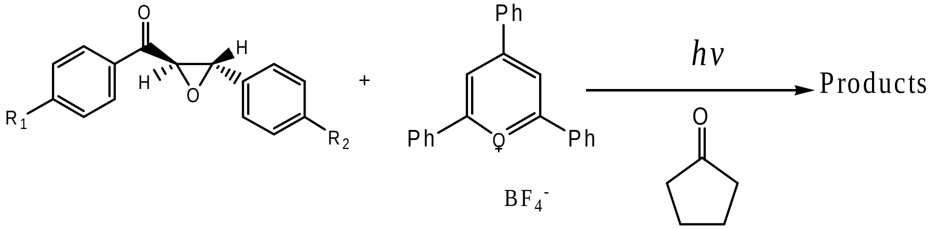
Single electron transfer (SET) induced ring opening of epoxides and α-epoxyketones has been of great interest for several years and is still under intensive investigation [1]. Such reactions have been recognized as important processes not only in thermal but also photochemical transformations. Polarized epoxides, due to their facile formation and high reactivity toward nucleophiles, are of the most versatile building blocks in organic synthesis. Ring opening of epoxides and α-epoxyketones in the presence of various nucleophiles has received considerable attention in recent years. The ring opening of these compounds in the presence of various nucleophiles leads to the formation of some interesting compounds such as ethers, dioxolanes, and trioxolanes,partially owing to current interest in single electron transfer (SET) process and also because of potential application in organic synthesis.

Light-induced electron transfer reaction of some α-epoxyketones as electron donor molecule by 2,4,6-triphenylpyrylium tetrafuoroborate (TPT) as electron acceptor species in the presence of various nucleophilic solvents has been investigated [2]. The observed higher diastereoselectivity of reaction in cyclohexanone solution led us to investigate this reaction in cyclopentanone to elucidate the effect of the smaller size of the nucleophile compared with cyclohexanone on the rate and diastereoselectivity of reaction. The results will be presented.



References:

[1] Masaki, Y.; Miura, T.; Ochiai, M. *Bull. Chem. Soc. Jpn*. **1996**, *69,* 195-205.

[2] Memarian, H. R.; Nikpour, F. *Molecules* **2002**, *7*, 63-71and references cited therein.

Four components reaction in synthesis of phosphorus compounds from reaction between isocyanat, phenols, diamethylacetylenedicarboxylate in the presence of triphenylphosphine and triphenylphosphite

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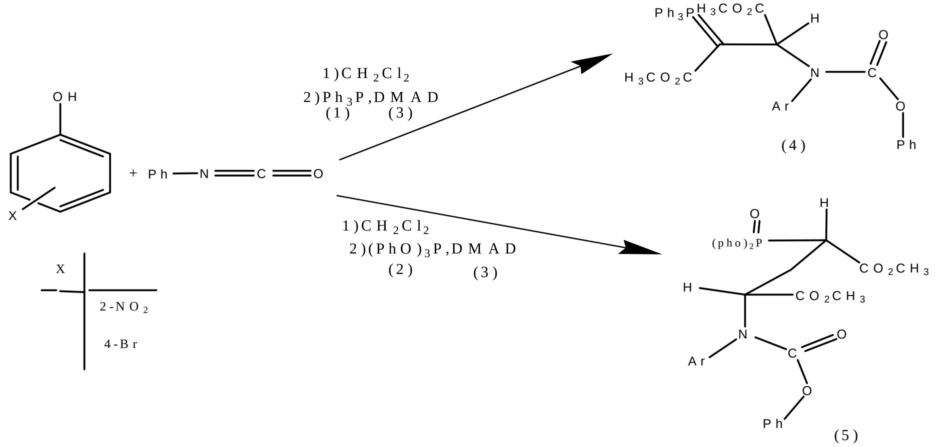
Development of simple synthetic routes for widely-used organic compounds from readily available reagents is one of the major tasks in organic chemistry [1]. Phosphorus compounds are of great interesting compounds because pharmaceutical and biological activities that include anti-inflammatory, cardiotonic, inotropic, antihypertensive, antimicrobial propreties [1-5]. We wish to describe an efficient synthetic route to carbamat containing stable phosphorus ylides. This route consists of steps, approaching through the condensation of strong O-H acids with phenyl isocyanate according to a reported Method producing the desired carbamat. In the one according media reactions the carbamat was brought into reaction with triphenylphosphine (1) and triphenylphosphite (2) and dimethylacetylenedicarboxylate (3) leads to the corresponding stable phosphorus ylides (4) and phosphonato esters (5) in excellent yield.



References:
[1] Johnson, A.W. *Ylide chemistry* (Academic press, London, **1966.**
[2] P.laszlo, *Organic Reaction: Simplicity and Logic* (Wiley, New york, **1995**)
[3] J.I.G.Cadogan, *Organo phosphorus Reagents in organic synthesis* (Academic press, New York, **1979**.
[4] Maghsoodlou,M.T;HabibiKhorassani,S.M;Rofouei,M.K;Adhamdoust,S.R;Nassiri,M.*Arkivoc* **2006**,xii,1, 45.
[5] Sheldrick, G.M.*Acta Cryst A* **2008**, 64,112.

$H_2O_2/TiCl_4$: A valuable reagent system for the conversion of thioamides to amides

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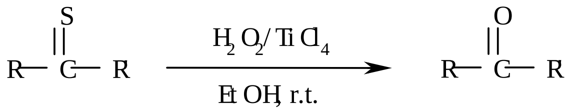
Amides are important commercial and biological compounds. Because amides constitute the backbone of protein molecules, their chemistry is of extreme importance.

The conversion of thioamides to their oxygen analogues has received considerable attention. This transformation has been accomplished in a variety of ways [1-3]. However, many of these suffer from limitations such as high toxicity, vigorous reaction conditions, unsatisfactory yields, tedious work up and use of large excess of reagents. Thus, a need for a practical, efficient and greener alternative for this important transformation is desirable.

Aqueous hydrogen peroxide (30%) is an ideal oxidant in view of its high effective-oxygen content, its eco-friendly byproduct (water), its relative safety in storage and operation, and its comparatively low cost of production and transportation.

As part of our continuing studies on the use of hydrogen peroxide in organic synthesis [4]. we now wish to report a reasonably simple and efficient method which enables one to economically desulfurise thioamides to their oxo analogues using H_2O_2 in the presence of $TiCl_4$ in excellent yields.



$$R-\overset{\overset{S}{\|}}{C}-R \xrightarrow[EtOH,\ r.t.]{H_2O_2/TiCl_4} R-\overset{\overset{O}{\|}}{C}-R$$

References:

[1] Suto, Y.; Yamagiwa, N.; Torisawa, Y. *Tetrahedron Lett*. **2008**, *49*, 5732.
[2] Polshettiwar, V.; Varma, R. S. *Tetrahedron Lett*. **2008**, *49*, 2661.
[3] Olah, C. A.; Arvanaghi, M.; Ohannesian, L.; Surya, P. G. K. *Synthesis* **1984**, 785.
[4] (a) Bahrami, K. *Tetrahedron Lett.* **2006**, *47*, 2009. (b) Bahrami, K.; Khodaei, M. M.; Kavianinia, I. *Synthesis* **2007**, 547. (c) Bahrami, K.; Khodaei, M. M.; Naali, F. *J. Org. Chem.* **2008**, *73*, 6835; (d) Bahrami, K.; Khodaei, M. M.; Tirandaz, Y. *Synthesis* **2009**, 369.

Three-component reaction between triphenylphosphine, dialkyl acetylenedicarboxylates and arylglyoxal or 3-(3,5-dimethyl pyrazol- 1- yl)- 3-oxo propionitrile

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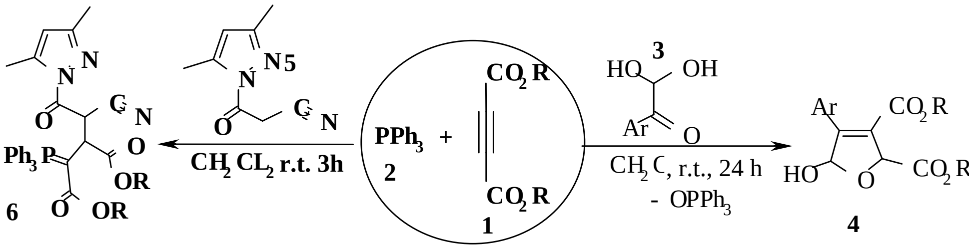
Three-component reaction between tripenylphosphine, dialkyl acetylenedicarboxylates (DAAD's) and organic acidic compounds is well known to produce phosphorus ylides[1]. If the starting acidic compound posseses a carbonyl group in an appropriate position, these ylide intermediates may be converted to cyclic compounds by intramolecular Wittig reaction[2]. This strategy has been recently utilized for the synthesis of a variety of heterocyclic and carbocylic compounds. In continuation of our previous work on the reaction between trivalent phosphorus nucleophiles and acetylene diesters in the presence of acidic organic compounds [3], here we wish to report that the reaction between dialkyl acetylenedicarboxylates**1**, triphenylphosphine **2** and arylglyoxalmonohydrates **3** afforded 2,5-dihydrofuran derivatives in good yields. Also we report three-component reaction between dialkyl acetylenedicarboxylates1, triphenylphosphine**2** and 3-(3,5-dimethyl pyrazol- 1- yl)- 3-oxo propionitrile **5** leads to phosphorus ylides **6** in good yields.



References:

[1] Corbridge, D. E. C. Phosphorus: An Outline of the Chemistry, Biochemistry, and Uses, 5th ed.; Elsevier: Amsterdam, **1995**.
[2] Engel, R. Synthesis of Carbon-Phosphorus Bonds; CRC Press: Boca Raton, FL, **1988**.
[3] Anary-Abbasinejad. M, Mosslemin M. H, Hassanabadi A, Tabatabaee M, *Synth. Commun*. **2008**, *38*, 3700.

One pot synthesis of bis-thiazolidinedione derivatives

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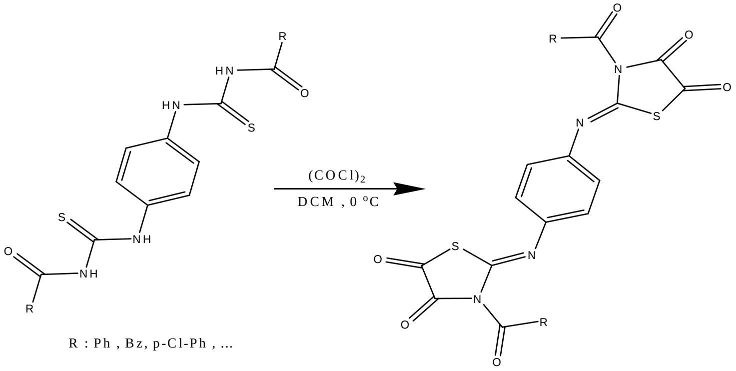
Thiazolidinediones are an important class of heterocyclic compounds having important biological activities [1]. One of the most important methods for the synthesis of these compounds is one pot reaction of thioureas with oxalylchlorid [2]. The aim of this research is synthesis of new derivatives of bulky bis thiazolidinedione derivatives [3].

Herein as a part of our ongoing research program, we wish to report an efficient and facial method for the synthesis of thiazolidinedione derivatives. In this work bis-1,4-phenyl thioureas derivatives were synthesized and then reacted with oxalylchloride in 0°C and DCM. These new compounds were fully characterized by spectroscopic means and their purities were established by elemental analysis.



References:

[1] Dominguez, J. N.; Leon, C.; Rodrigues, J.; Dominguez, N. G.; Gut, J.; Rosenthal, P. J. *J. Med. Chem.* **2005**, *48*, 3654.

[2] Zhang, Q.; Guan, J.; Sacci, J.; Ager, A.; Ellis, W.; Milhous, W.; Kyle, D.; Lin, A. J. *J. Med. Chem.* **2005**, *48*, 6472.

[3] N. Sunduru , K. Srivastava , S. Rajakumar , S. K. Puri, J. K. Saxena, P. M. S. Chauhan, *Bio. Med. Chem. Lett.* **2009,** *19*, 2570.

Catalytic oxidative conversion of Hantzsch 1,4-dihydropyridines and 3,4-dihydropyrimidine-2(1H)-ones to corresponding pyridines and pyrimidinones using NaI/AcOH-H_2O_2 system

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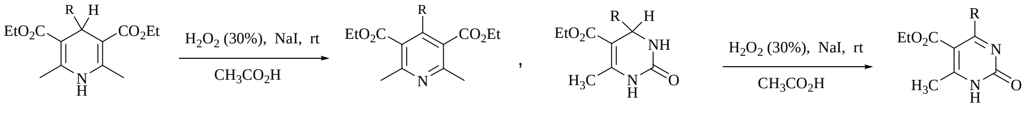
The oxidation of 1,4-dihydropyridines (1,4-DHPs) **1** and 3,4-dihydropyrimidine-2(1H)-ones **3** provide an easy access to pyridine **2** and pyrimidinones **4** derivatives which are widely used as intermediates of organic synthesis. Pyridine and pyrimidinone skeleton also exists in many natural or synthetic biologically active materials, and its derivatives are applied in various pharmaceutical and biochemical fields [1]. So, these findings make considerable attention to develop an efficient method for the synthesis of pyridine and pyrimidinone derivatives.

Numerous reagents and procedures have been developed for these purposes [2]. Recently, attention has been paid to more efficient and environmentally benign reagents or methods [3]. However, most of these reactions require an extended period of time for completion utilize strong oxidants in large excess and afford only modest yields of the products. In order to find a milder and environmentally benign oxidant for the dehydrogenation of 1,4-DHPs and 3,4-dihydropyrimidine-2(1H)-ones, we wish to report in this paper that hydrogen peroxide as an environmentally safe oxidant, can serve an efficient oxidant catalyst by NaI/AcOH to reduce the time of oxidation, mild and highly efficient reagent for oxidation of 1,4-DHPs and 3,4-dihydropyrimidine-2(1H)-ones (Scheme 1).



1 (a-k) **2** (a-k) **3** (a-k) **4** (a-k)

R (a-k) = Ph, 2-Pyridil , 3-Pyridil , 4-Pyridil , 2-OH-C_6H_4 , 3-OH-C_6H_4 , 4-OH-C_6H_4 , 2-NO_2-C_6H_4 , 3-NO_2-C_6H_4 , 4-NO_2-C_6H_4 , 4-OMe-C_6H_4

Scheme 1

References:

[1] Kuppe, E.O.; Fabian, W.M.F.; Semones, M.A. *Tetrahedron*. **2004**, *53,* 2803.
[2] Huaxuetongbao, X.H.Yi. **2003**, *66*, 211.
[3] Yadav, J.S.; Reddy, B.V.S.; Sabitha,G. et al. *Synthesis*. **2000**, 1532.

MP2, DFT and ab initio conformational analysis of methyl-3-methoxy salicylate

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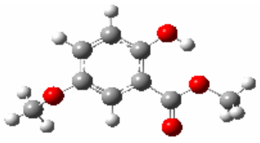
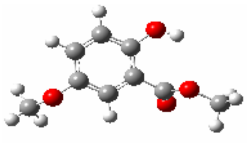
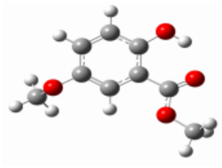
Nowadays, the synthesis of benzoic acids for example salicylates have become attractive due to their biological, pharmaceutical and industrial widely applications. Salicylic acid and its derivatives are anti-inflammatory, antiseptic and antipruritic drugs used in the treatment of wounds and parasitic skin diseases like corns, warts and acne. The best-known derivative of salicylic acid is acetylsalicylate commonly known as aspirin, is used as an analgesic, anti-inflammatory and anti-pyretic drug. It is known to inhibit the enzyme cyclooxygenase, that promotes blood clotting and, as such, it may reduce heart attacks and strokes. A number of attempts have been made to develop prodrugs of aspirin in order to depress its side effects involving gastric irritation and bleeding, as well as to improve transport characteristics [1-4].

The different spatial arrangements that a molecule can adopt due to rotation about σ bonds are called conformations and hence conformational isomers or conformers. The study of the energy changes that occur during these rotations is called conformational analysis. This is important because the structure of a molecule can have a significant influence on the molecular properties, including dictating the outcome of a reaction. Although the ideas are developed for the simplest functional groups, the alkanes, the same principles can be expanded and applied to other functional groups [5].

Herein we report quantum chemical conformational analysis of methyl-3-methoxy salicylate with employment of computational chemistry. The conformational analysis of this compound was done by performing HF, DFT and MP2 levels of theory using the standard 6-31G basis set to study most stable and unstable conformer and intramolecular hydrogen bonding. The optimized geometries, total energies and Hydrogen bonding lengths of methyl-3-methoxy salicylate conformers were calculated.







References:

[1] Humbert, B., Alnot, M., Quiles, F., Spectrochim. Acta A, **1998**, 54, 465.
[2] Sobolewski, A.L., Domcke, W., J. Phys. Chem, **2004**, 108, 10917.
[3] Boczar, M., Boda, L., Wojcik, M.J., Spectrochim. Acta A, **2006**, 64, 758.
[4] H. A. Dabbagh et al, Spectrochim. Acta A , **2008**, 69, 449.
[5] http://www.chem.ucalgary.ca

Bromination of 1,3-dicarbonyl compounds with *N*-bromosaccharin in the presence of $Mg(ClO_4)_2$ as a catalyst in acetonitrile or solvent free

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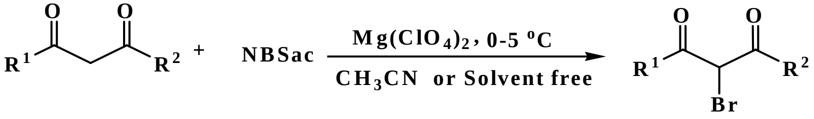
The regioselective α-bromination of β-keto esters and 1,3-diketones is a useful transformation in organic synthesis [1]. These brominated products serve as valuable building blocks for the synthesis of both natural and non-natural products [2].

Bromination of dicarbonyl compounds has been accomplished with various reagents, such as molecularbromine [3], NBS/Amberlyst-15 [4], and ethylenebis(*N*-methylimidazolium) ditribromide [5]. Nevertheless, selective monobromination of 1,3-diketones and β-keto esters remains a challenge since these reactions in many cases result in a mixture of mono and dibrominated products [6].

N-Bromosaccharin is a strong oxidizing and brominating agent that used for halogenation of aromatic compounds, co-halogenation of alkenes and oxidation of alcohols [7].

Herein we report an efficient and regioselective method for α-monobromination of β-keto esters and 1,3-diketones using *N*-bromosaccharin in the presence of catalytic amount of $Mg(ClO_4)_2$ in acetonitrile or solvent free conditions



R^1= Alkyl, Aryl, Alkoxy

R^2= Alkyl, Aryl, CF_3

References:

[1] Larock, R. C. ComprehensiVe Organic Transformations, 2nd ed; VCH Publishers Inc.: New York, **1999**; pp 717.
[2] Coats, S. J.; Wasserman, H. H. *Tetrahedron Lett*. **1995**, *36*, 7735.
[3] Hakam, K.; Thielmann, M.; Thielmann, T.; Winterfeldt, E. *Tetrahedron* . **1987**, *43*, 2035.
[4] Meshram , H.; Reddy, P.; Sadashiv, K.; Yadav, J. *Tetrahedron Lett*. **2005,** *46*, 623.
[5] Hosseinzadeh, R.; Tajbakhsh, M.; Mohadjerani, M.; Lasemi, Z. *Monatsh chem*. **2009**, *140*, 57.
[6] Pravst, I.; Zupanab, M.; Stavber,S. *Green Chem*. **2006**, *8*, 1001.
[7] Pandey, K. *Synlett*. **2008**, *6*, 947.

Melamine-formaldehyde resin as an efficient and recoverable catalyst for the synthesis of tetrasubstituted imidazoles

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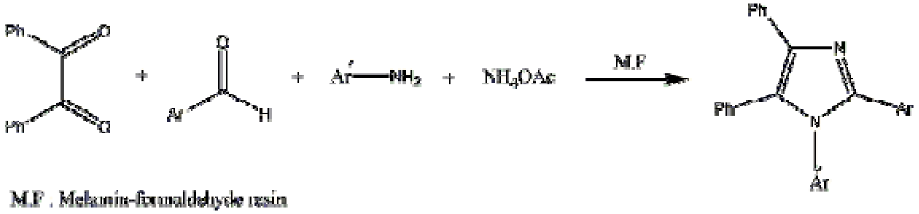
Imidazole and its derivatives play an important role in the fields of biology and pharmacology as well as chemistry [1]. Imidazole ring systems are frequently found in numerous naturally accuring and synthetic molecules. There are many methods for the synthesis of highly substituted imidazoles [2].

Multi-component reactions have proved to be remarkably successful in generating products in a single synthetic operation [3]. In four-component condensation methods imidazoles could be obtained with varying levels of purity. In addition, highly functionalized synthesis of polar imidazoles in solution requires laborious work-up and purifications [4].

Here we report the four-component condensation of benzyl, benzaldehyde derivatives, primary amines and ammonium acetate catalyzed by Melamine-formaldehyde resin as an efficient and facile one-pot synthesis of tetrasubstituted imidazoles.



M.F , Melamin-formaldehyde resin

References:

[1] Zhong, J.; *Nat. Prod. Rep,* **2005***, 22, 196*.

[2] Khalili, B.; Tondro, T.; Hashemi, M. M.; *Tetrahedron*, **2009***, 65, 6882*.

[3] Bara, U.; Saikita, A.; Boruah, R. C.*; Org. Lett.* **2003**, *5, 435*.

[4] Maduskuie, T. P.;Wilde, R. G.; Billheimer, J. T.; Gromley, D. A.; Germain, S.; Gillies, P. J.; Higley,C. A.; Johanson. A. L.; Pennev, P, *J. Med. Chem,* **1995***, 38, 1067.*

An efficient one-pot synthesis of amides from imines using triethylsilane in the presence of Zinc and carboxylic anhydride

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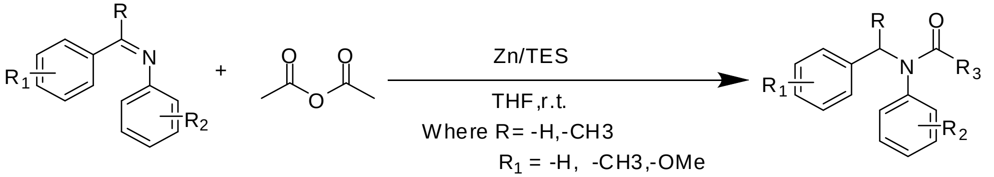
The amide functional groups found in the chemical structures of polymers, natural products, and pharmaceuticals [1]. Thus, the development of a new mild and versatile method for amide formation is important and valuable. The most common way to form an amide bond is the reaction of amines with activated carboxylic acid derivatives, such as acyl chloride or anhydride [2,3].Three is no any direct methods for thesynthesis ofamidesfrom the corresponding imines. Now we reported direct conversion of imine functional groups (which is obtained easily by the reaction of carbonyl compounds with various amines) to amide groups for first time.

In this context low-cost zinc is employed as a catalyst along with triethylsilane (TES) in THF solvent for a simple, straightforward, chemo-selective reduction and tandem amidationof various aldimines and ketimines to the corresponding amides at room temperature and ambient pressure.



Where R= -H,-CH3
R_1 = -H, -CH3,-OMe
R2 = -H, -CH3,-OMe
R3 = -CH3,-CH2 -CH3

References:

[1] Humphrey, J. M.; Chamberlin, A. R. *Chem. Rev*. **1997**, *97*, 2243

[2] Larock R. C. Comprehensive Organic Transformation; VCH: New York, **1999**.

[3] (a) Dawson, P. E.; Muir, T. W.; Clark-Lewis, I.; Kent, S. B. *Science* **1994**, *266*, 776; (b) Beller, M.; Cornils, B.; Frohningm, C. D. *J. Mol. Catal. A: Chem*. **1995**, *104*, 17; (c) Saxon, E.; Bertozzi, C. R. *Science* **2000**, *287*, 2007; (d) Ln, Y.-S.; Alper, H. *Angew. Chem., Int. Ed*. **2001**, *40*, 779.

Synthesis of nocistatin as an opioid peptide

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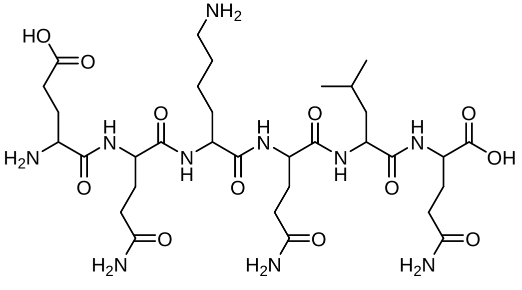
Nocistatin is a new biologically active peptide produced from the same precursor as nociceptin and tests indicate that these two peptides may play opposite roles in pain transmission. Nocistatin blocks nociceptin-induced allodynia and hyperalgesia, and attenuates pain evoked by prostaglandin E_2. It is the carboxy-terminal hexapeptide of nocistatin (Glu-Gln-Lys-Gln-Leu-Gln), which is conserved in bovine, human and murine species, that possesses allodynia-blocking activity. Furthermore, intrathecal pretreatment with anti-nocistatin antibody decreases the threshold for nociceptin-induced allodynia. Although nocistatin does not bind to the nociceptin receptor, it binds to the membrane of mouse brain and of spinal cord with high affinity [1-3].

The synthesis of nocistatin was done according to solid phase peptide synthesis on the surface of 2-chlorotritylchloride resin also using fmoc-protected amino acids in the presence of TBTU as a coupling reagent. The product was purified by preparative HPLC and structure was confirmed base on HR-ESI mass spectrometric data.



Glu-Gln-Lys-Gln-Leu-Gln

References:

[1] Okuda-Ashitaka, E.; Minami, T.; Tachibana, S.; Yoshihara, Y.; Nishiuchi, Y.; Kimura, T.; Ito, S. *Nature***, 1998,** 392, 286.

[2] William, J.; Martin, A. B.; Malmberg and Allan, I.; Basbaum. *Current Biology*, **1998**, 8, R525.

[3] Okuda-Ashitaka, E.; Minami, T.; Ito, S. *J. Biol. Macromol*. **2002**, 2, 3.

Ab Initio and DFT calculations on physical organic aspects of the cationic phosphorus ligand –Ru (II) halide complexes

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The increasing demand to produce enantio-pure pharmaceuticals, flavors, and other fine chemicals has advanced the field of asymmetry catalytic technologies. Among all asymmetry catalytic methods, catalytic enantioselective hydrogenation of unsaturated bonds such as olefins, ketones, and imines, which employs dihydrogen and small amounts of transition-metal complexes modified intrinsically by chiral ligands, is now recognized as being the most promising strategy for the synthesis of large amounts of enantiomerically pure products [1], and enormous progress has been achieved in this area.

Among these transition metal complex, rhodium (I) and ruthenium (II) complexes and, most often, diphosphine-based chiral ligands have been extensively employed in asymmetric hydrogenation. Experimental results have shown the reaction of ruthenium complexed with diphosphine-based chiral ligands catalyzed asymmetric hydrogenation of β-ketoesters are mild. So it has been used for the synthesis of a large variety of biologically or pharmaceutically important chiral compounds [2].

In studying the θ, some chemists have used MM2 method [3, 4], a molecular mechanism method which eliminates the change of electronic structures with lower precise especially when system containing transition metals. Based on this reason, density functional theory (DFT) method have been performed on the cationic phosphorus ligand - Ru (II) halide [4].

The full-parameter geometry optimization of cationic (S) – BINAP – Ru (II) halide complex was performed by DFT method using B3LYP with several basis sets. 3-21G / SDD basis sets is found to be the most suitable method with consideration of both precision and efficiency. The dihedral angles (θ) of the binaphthyl or biphenyl with different phosphorus ligand – Ru (II) halide complexes were found changing from 59.9 to 79.3 degree, while the natural bite angle (n) of those complexes only changes from 87.4 to 90.3 degree. It is different from the common view of asymmetric organic chemists' that θ directly influences βn.

References:

[1] Brown, J. M. *Comprehensive Asymmetric Catalysis*, **1999**, *Vol. 1,* Chap.5.1.
[2] Ohkuma,T.; Kitamura,M.; Noyori, R. *Catalytic Asymmetric Synthesis,* 2nd Ed., **2000**, 1.
[3] Zhang, Z. *J. Org. Chem.*, **2000**, *65*, 6223.
[4] Duprat de Paule S.; *et al. Tetrahedron Lett.,* **2003**, *44,* 823.

Synthesis and characterization of aqueous cationic hybrid nano-SiO_2/TiO_2 urethane dispersion

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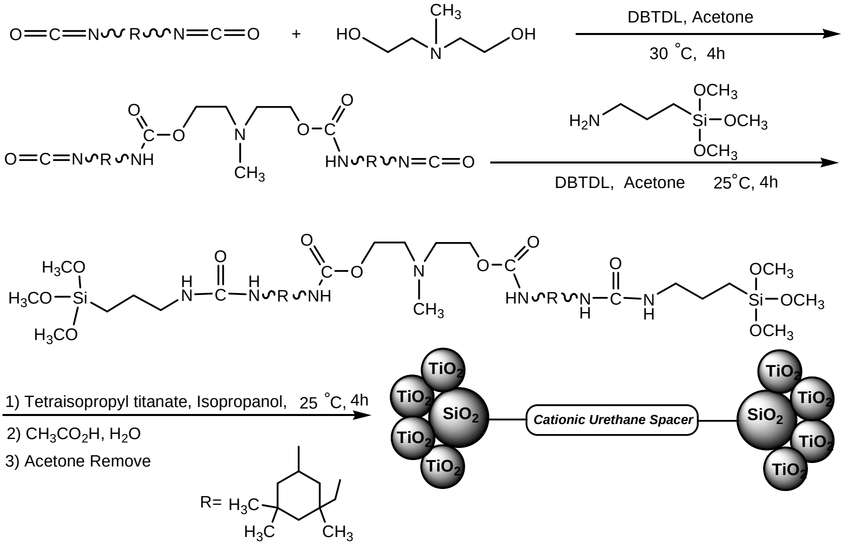
The aqueous cationic hybrid nano-SiO_2/TiO_2 urethane dispersions are water base white composite materials that used in inkjet printers. These were synthesized in four steps. In the first step, macromonomer diisocyanate having amine group was prepared by isophorone diisocyanate (IPDI) and N-methyldiethanolamine in presence of acetone as solvent and dibutyldtin dilaurate (DBTDL) as catalyst. Then, urethane bis(trimethoxysilyl) was prepared by reaction of amine functionalized macromonomer diisocyanate and 3-aminopropyl trimethoxysilane. Next, hybrid nano-SiO_2/TiO_2 urethane was synthesized by tetraisopropyl titanate in presence of isopropanol as solvent. The last step involved neutralization and dispersion in water, where amine functional polyurethane was neutralized by addition of acetic acid. The cationic hybrid nano-SiO_2/TiO_2 urethane dispersions have been characterized with ^{1}H-NMR, FT-IR and SEM.



References:

[1] Ming Y.; Yao C.; Hsieh C.; Yang H.; Wu C. *European Polymer Journal,* **2008**, *44*, 2777.
[2] Chen J.; Zhou Y.; Nan Q.; Sun Y.; Ye X.; Wang Z. *Applied Surface Science,* **2007**, *253*, 9154.
[3] Mishra A.; Mishra R.; Narayan R.; Raju K. *Progress in Organic Coatings*, **2010**, *67*, 405.

Preparation of L-leucine anhydride from L-leucine cyclization reaction in the mixture of ethylene glycol/Ionic liquid as recation solvent

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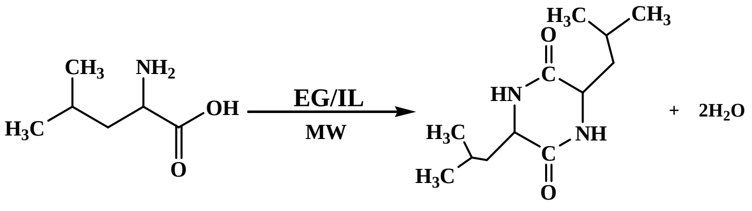
Room temperature ionic liquids (RTILs) consisting of N-alkylimidazolium cations and various anions, have attracted wide attention as reaction media or catalysts in organic reactions and polymerization due to their polar nature, and as substitutes for conventional volatile organic solvents. They possess intriguing properties such as nonvolatility, low toxicity, ease of handling, nonflammability and high ionic conductivity [1]. Even though piperazines have been known for more than a century, only recently have 2,5-diketopiperazines attracted attention due to their biological properties.1 Their peculiar heterocyclic system found in several natural products constitutes a rich source of new biologically active compounds.

A novel and convenient microwave-assisted dimerization of an active peptide compound L-leucine in mixer of ethylene glycol and ionic liquid (EG/IL) as solvent is described. The key reaction giving rise to the amino acid is the intermolecular coupling. Synthesis by microwave irradiation in mix solvent(EG/IL) gave the desired compounds in compariable yields and in shorter reaction times than those obtained by EG as solvent alone.ratio of EG/IL impressed on yield of product.



L-leucine

L-leucine anhydride

Reference

[1] Mallakpour, Sh; Rafiee, Z, *Polym Deg and Stab*, **2008**, 93, 753.

[2] Long, D. D.; Tennant-Eyles, R. J.; Estevez, J. C.; Wormald, M. R.; Dwek, R. A.; Smith, M. D.; Fleet, G. W. J. J. *Chem. Soc., Perkin Trans*. **2001**, 1, 807.

Synthesis and characterization of environmentally degradable poly(ether-urethane)s derived from L–leucine cyclopeptide

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Conventional polyurethanes (PU)s are among biomaterials not intended to degrade but are susceptible to hydrolytic, oxidative and enzymatic degradation in vivo. While the susceptibility of PUs to such degradation is a problem for long lasting biomedical implants, it can be deliberately exploited to design (bio) degradable PUs. Molecular weight and chemical compositions can be explored to prepare PUs with specific properties [1,2].

(Bio)degradable polyurethanes are typically prepared from polyester polyols, aliphatic diisocyanates and chain extenders. In this work we have developed a degradable chain extender based on α-amino acid cyclopeptide to accelerate hard segment degradation. Thus a new class of optically active degradable poly(ether-urethane)s (PEUUs) was synthesized via direct reaction of 4,4’-methylene-bis(4-phenylisocyanate), L-leucine anhydride cyclopeptide and polytetrahydrofuran as polyether soft segment. The reaction was performed via solution polymerization under graduate heating in the presence of different catalyst. The resulting polymers have inherent viscosities in the range of 0.18–.41 dL/g. Decomposition temperatures for 5% weight loss occurred above 300 ^{o}C by TGA in nitrogen atmospheres. These polymers are optically active, environmentally degradable, thermally stable and soluble in amide-type solvents. Different properties of these polymers were studied by SEM, XRD, TGA, DSC and FTIR.

References:

[1] Tataiam ,L.; Moore, T. G.; Adhikari, R.; Malherbe, F.; Jayasekara, R.; Griffiths, I.; Gunatillake, P. A. *Biomaterials* **2007**, *28,* 5407.

[2] Rafiemanzelat, F.; Abdollahi, E.; *polym. Deg. Stabl.* **2010**, *95*, 901.

Synthesis and characterization of various substituted s-triazines and its derivatives

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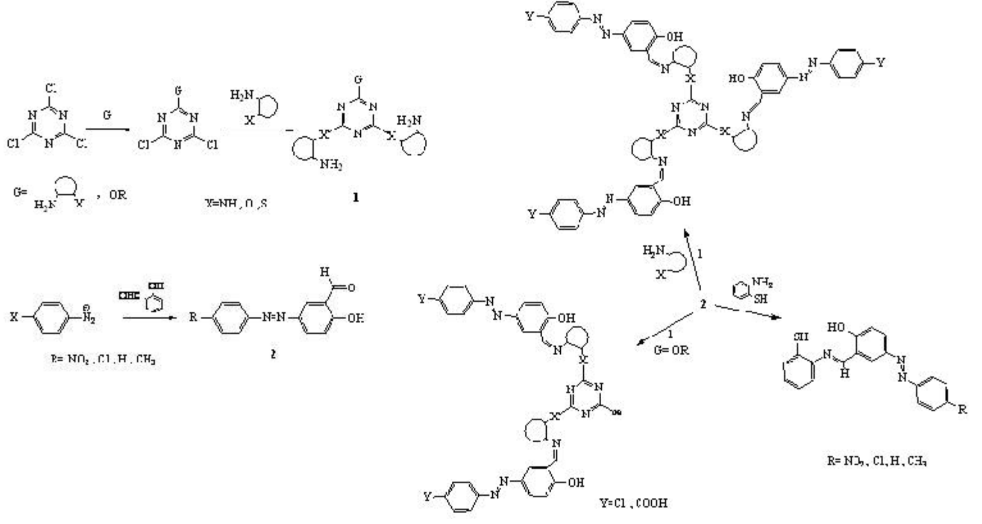
1, 3, 5-triazine derivatives have been known for a long period of time. They have found widespread applications in the pharmaceutical, textile, plastic and are used as pesticides, dyestuffs, optical bleaches, explosives, and surface active agents. All of the s-triazine derivatives that have wide practical applications are 2, 4, 6-mono, di- or tri-substituted, symmetrical and nonsymmetrical compounds bearing different constituents [1]. In other hand, the Azo compounds have been applied to photo responsive molecular switches and materials. They have found broad application in nonlinear optics, optical storage media, chemo sensors and optical switches [2].In this study, the synthesis of new 2, 4, 6-derivatives of 1, 3, 5-triazine together with novel applications of cyanuric chloride and its derivatives, will be presented. The aim of this study was to Introduction of some functional groups such as carboxyl, amine, hydroxyl and azo dyes on the 1, 3, 5-triazine scaffold under various conditions. In combination, our results suggest that this compound may be useful for reactive dyes.



References:

[1] Meier.H.; Lehmann.M.*Tetrahedron* **2004**, *60*, 6881.

[2] X. Xia, L. Huat Gan , *Dyes and Pigments.* **2009,** *83*, 291.

Synthesis, characterization and antimicrobial activities of some novel Bis-chalcones

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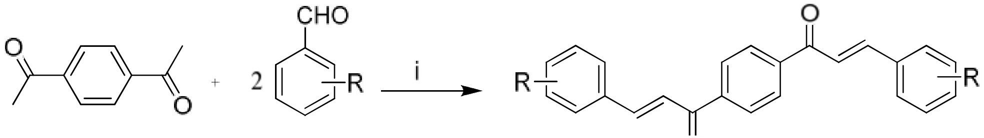
Chalcones are widely distributed in nature and considered as the precursors for flavonoid synthesis in plants. They also with proper substitution have recently been isolated from *Broussonetia papyrifera*, known to selectively inhibit enzymes like protein tyrosine phosphatase 1B (PTP1B) and aldose reductase [1]. Besides, compounds with a chalcone-based structure have shown an impressive array of pharmacological activities including anticancer, antimicrobial [2], anti-HIV and antitumor [3] activities.

These compounds are not only a segment of biologically important but also a versatile intermediate for the synthesis of heterocyclic compounds [4].

In view of aforesaid points, we decided to extend our research in synthesis of biological active compounds [5] and have synthesized some novel Bis-chalcones (**1-14**) in excellent yields by condensation reaction of 1,4-diacetylbenzene with various aldehydes in ethanol 96% and aqueous NaOH at room temperature. The biological activities of these compounds also are investigated against some bacteria and fungus.



i: NaOH/ EtOH/RT

(1-14)

References:

[1] a) Chan, R. M.; Hu, L. H.; An, T. Y.; Li, J.; Shen, Q. *Bioorg. Med. Chem. Lett.* **2002**, *12*, 3387; b) Severi, F.; Benvenuti, S.; Constantino, L. C.; Vampa, G.; Antolini, L. *Eur. J. Med. Chem.* **1998**, *3*, 859.

[2] a) Modzelewska, A.; Pettit, C.; Achanta, G.; Davidson, N. E.; Huangb, P.; Khana, S. R. *Bioorg. Med. Chem.* **2006**, *14*, 3491; b) Nowakowska, Z. *Eur. J. Med. Chem.* **2007**, *42*, 125.

[3] a) Gschwendt, M.; Kisttstein, W.; Furstenberg, G.; Mark, F. *Cancer Lett.* **1984**, *25*, 177; b) Artico, M.; Santo, R. D.; Costi, R.; Novellino, E.; Greco, G.; Massa, S.; Tramontano, E.; Marongiu, M. E.; Montis, A. D.; Colla, P. L. *J. Med. Chem.* **1998**, *41*, 3948.

[4] Nagaraj, A.; Reddy, C. S. *J. Iran. Chem. Soc.* **2008**, *5*, 262.

[5] Mobinikhaledi, A.; Foroughifar, N.; Kalhor, M.; Mirabolfathy, M. *J. Heterocycl. Chem.* **2010**, *47*, 77.

Guanidine hydrochloride: An active and simple catalyst for Mannich type reaction in solvent-free condition

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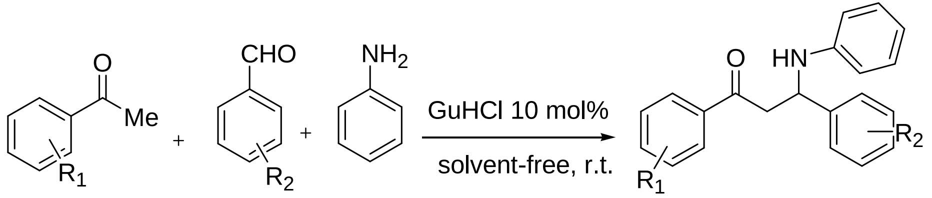
A Mannich-type reaction is a multicomponent reaction of a non-enolizable aldehyde, a primary or secondary amine, and an enolizable carbonyl compound to afford the corresponding β-amino carbonyl compound [1]. These β- amino carbonyl compounds are important synthetic intermediates for various pharmaceuticals and natural products [2] and have found wide application in organic synthesis. Commercially available guanidine hydrochloride (GuHCl) has been found to be a highly efficient catalyst for the Mannich reaction. β-amino carbonyl compounds were obtained in reasonable yields when the Mannich reaction was carried out at room temperature under solvent-free conditions. Simple experimental conditions and product isolation procedure makes this protocol potential for the development of clean and environment-friendly strategy for the synthesis of β-amino-ketones. Guanidine hydrochloride (H2NC NHNH2·HCl, GuHCl) is a dry, nonvolatile, odorless and white crystalline solid with outstanding physical property and stability. The crystals can be kept in the laboratory for many years without change.



References:

[1] Mannich, C.; Krosche, W. Ueber ein Kondensationsprodukt aus Formaldehyd, Ammoniak und Antipyrin. *Arch. Pharm*. **1912**, *250*, 647–667.

[2] Davis, F.; Zhang, A.; Anilkumar, Y., G. Asymmetric Synthesis of the Quinolizidine Alkaloid (−)-Epimyrtine with Intramolecular Mannich Cyclization and N-Sulfinyl δ-Amino β-Ketoesters. *J. Org. Chem*. **2003**, *68*, 8061–8064.

Conversion of alcohols into alkyl thiocyanates with *N*-thiocyanatosuccinimide (NTS) as a highly efficient reagent

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N-Thiocyanatosuccinimide (NTS) is a reactive electrophilic sulfur species [1] which can be easily prepared by the reaction of *N*-bromosuccinimide with thiocyanate. This reagent has been employed in diverse organic transformations such as thiocyanation of electron-rich aromatic compounds [2], ringexpansion– thiocyanation of 1,3-dithiolanes and 1,3-dithianes [3], and α-thiocyanation of N-acyl carboximides [4]. Organic thiocyanates are important sulfur-containing compounds which have wide application in synthetic and medicinal chemistry [5]. Alkyl thiocyanates are prepared directly from alcohols. Phosphine-based reagents have been used for the activation of the hydroxy group of alcohols. These reagents include $Ph_3P(SCN)_2$ [6], $Ph_3P(Br)_2/NH_4$ SCN [7], Ph_3P/dichlorodicyanoquinone/Bu_4NSCN [8], Ph_3P/diethyl azodicarboxylate/NH_4SCN [9], diphenylphosphinite ionic liquid (IL-$OPPh_2$)/Br_2/NH_4SCN [10] and cyanuric chloride/N,N-dimethylformamide/ KSCN [11]. However, these methods have certain limitations arising from the use of expensive and explosive reagents, long reaction times, and tedious work-ups. We report here, a new, mild, and efficient procedure for the one-pot conversion of primary, secondary, and tertiary alcohols into their corresponding alkyl thiocyanates or alkyl isothiocyanates using in situ-generated NTS and NH_4SCN in acetonitrile at room temperature.

$$\text{ROH} \xrightarrow[\text{CH}_3\text{CN, r. t., 0.25-2 h}]{\text{NTS, NH}_4\text{SCN}} \text{RSCN or/and RNCS}$$

70-95%

$R = 1^o, 2^o, 3^o$ alkyl

References:

[1] Ashby, M. T.; Aneetha, H. *J. Am. Chem. Soc.* **2004**, *126*, 10216.
[2] Toste, F. D.; De Stefano, V.; Still, W. J. *Synth. Commun.* **1995**, *25*, 1277–1286.
[3] Firouzabadi, H.; Iranpoor, N.; Garzan, A.; Shaterian, H. R.; Ebrahimzadeh, F. *Eur. J. Org. Chem.* **2005**, 416–428.
[4] Falck, J. R.; Gao, Sh.; Prasad, R. N.; Koduru, S. R. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 1768–1771.
[5] Mohanazadeh, F.; Aghvami, M. *Tetrahedron Lett.* **2007**, *48*, 7240.
[6] Tamura, Y.; Kawasaki, T.; Adachi, M.; Tanio, M.; Kita, Y. *Tetrahedron Lett.* **1977**, 4417.
[7] Iranpoor, N.; Firouzabadi, H.; Shaterian, H. R. *J. Chem. Res. (S)* **1999**, 676.
[8] Iranpoor, N.; Firouzabadi, H.; Akhlaghinia, B.; Azadi, R. *Synthesis* **2004**, 92.
[9] Iranpoor, N.; Firouzabadi, H.; Nowrouzi, N. *Tetrahedron* **2006**, 62, 5498.
[10] Iranpoor, N.; Firouzabadi, H.; Azadi, R. *Tetrahedron Lett.* **2006**, *47*, 5531.
[11] Mokhtari, B.; Azhdari, A. Azadi, R., *J. Sulfur Chem.*, **2009**, *30*, 585-589.

Nano-ordered B-MCM-41: As an efficient catalyst for Strecker reaction and Fries rearrangement

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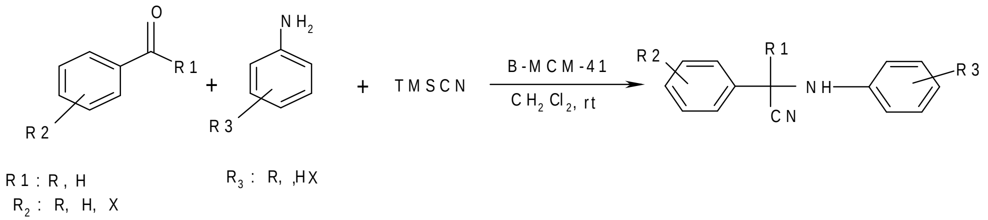
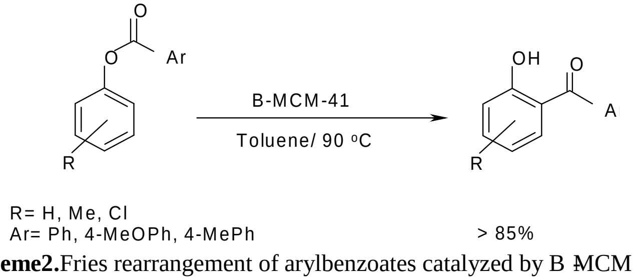
Ordered mesoporous materials are very attractive as heterogeneous solid catalysts for fine chemicals synthesis because attractive feature of mesoporous materials is their high surface areas, which provide a high concentration of active sites often introduced by incorporating metal ions into the siliceous framework [1].

We wish herein to report that mesoporous boronsilicate (B-MCM-41) efficiently catalyzed the three-component Strecker-type reaction associating an carbonyl compound, an amine and a cyanide source to afford the corresponding a-aminonitrile in excellent yields (up to 97%) [2] (**Scheme 1**) Furthermore The catalytic performance of B-MCM-41 was evaluated for the Fries rearrangement of phenyl benzoate **(Scheme2).**



Scheme1. Three-component Strecker-type reaction of various carbonyl compounds and amines catalyzed by B-MCM-41



Scheme2. Fries rearrangement of arylbenzoates catalyzed by B-MCM-41

References:
[1] Xiu, T.; Liu, Q.; Wang, J. *Mat .Chem .Phys* .**2007,***105*, 10.
[2] Iwanami, K.; Seo, H.; Choi, J.c.; Sakakura, T.; Yasuda,H. *tetrahedron lett***. 2010**, 66, 1898.

Synthesis of symmetrical 1,4-diketones in ionic liquids

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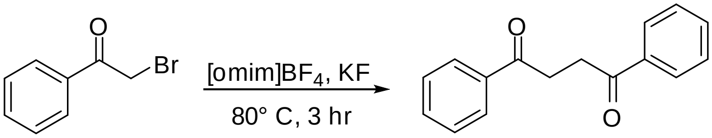
1,4-Diketones are important intermediates in the synthesis of five-membered carbocyclic and heterocyclic compounds. For example they are used for the preparation of derivatives of terthiophene and other conjugated five-membered heterocycles being intensively employed as monomers for the synthesis of electroconductive polymers [1].

A number of methodologies for the synthesis of 1,4-dicarbonyl compounds have appeared so far in the literature [2]. Most of these methods are reported to utilize metals such as Zn, Ni, and Fe as condensation agents in volatile and toxic solvent.

Recently ionic liquids are known as green solvents for many chemical reactions. Therefore, they have found particular importance in organic synthesis. In this work, we present a new, simple and environmentally benign procedure for the generation of 1,4-diketones, directly from the corresponding α-halo ketones. The commercially available phenacyl bromide condenses in the presence of half mole of KF in [omim]BF_4 ionic liquid at 80 ºC within 3 h with moderate yield.



References:

[1] Ceylan, M.; Gürdere, M. B.; Budak, Y.; Kazaz, C.; Seçenbne, H. *Synthesis* **2004,** *11*, 1750.
[2] Sato, T.; Okazaki, H.; Otera, J.; Nozaki, H. *J. Am. Chem. Soc.* **1988**, *110*, 5209.

Improved synthesis of substituted 2- aminobenzothiazoles

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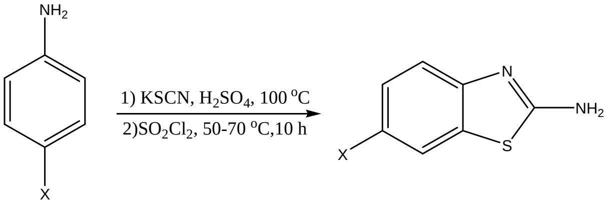
The chemistry of 2-aminobenzothiazoles has gained increased interest in both synthetic organic chemistry and biological fields, since a large number of developments in the use of such compounds seem to be of considerable value. These compounds broadly found with applications in drug discovery and development of the treatments of diabetes, epilepsy, inflammation, amyotrophic lateral sclerosis, analgesia, tuberculosis and viral infection [1-2]. Azo dyes derived from 2- aminobenzothiazoles produce a pronounced bathochromic shift as compared to the corresponding benzoid compounds [3].

Looking at the importance of these compounds, in this study, substituted 2-aminobenzothiazoles **1-4** were synthesized from corresponding aniline derivatives in moderate temperature and conditions. The structures of these were confirmed by FT-IR, ^{1}H and ^{13}C NMR and elemental analysis.



(**1**):X= -OCH_3 (**2**):X= -CH_3
(**3**):X= -H (**4**):X= -Cl

References:

[1] He, Y., Benz, A., Fu, T., Wang, M., Covey, D. F., Zorumski, C. F. and Mennick, S., *Neuropharmacology* **2002**, *42*, 199.
[2] Srivastava, S. D.; Shukla, D. K. *J. Indian Chem. Soc*. **2008,** *85,* 306.
[3] Moradi-e-Rufchahi, E. *Chinese Chemical Letters,* **2010,** *21,* 542.

Efficient synthesis of perfluorinated hetrocyclic systems from pentafluoropyridine and mono and bidentent nucleophiles by ultrasonic irradiation

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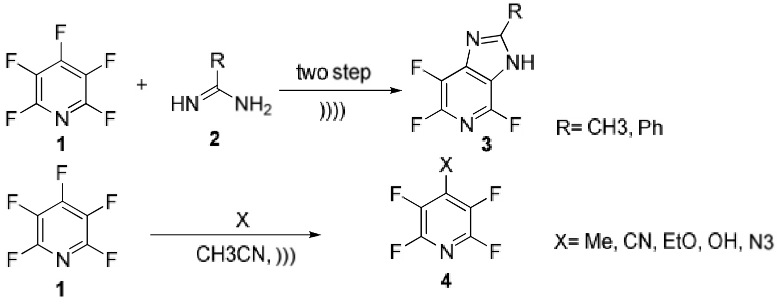
Syntheses of fluorinated heterocyclic systems are important in life science industries and pharmaceutical investigation [1]. Pentafluoropyridine has attracted considerable interest due to its synthetic utility. Various multi-functional pyridine derivatives and construction of new heterocyclic and macrocyclic systems could be accessed from simple reaction conditions [2]. These include reaction of various nucleophiles with pentafluoropyridine. All five fluorine atoms in pentafluoropyridine may be substituted by an appropriate nucleophile due to its highly electron efficient aromatic ring system.

As a part of our investigation concerning of pentafluoropyridine [3], Herein we would like to report synthesis of some pentafluoropyridine derivatives in very short reaction times and high yield by reaction of appropriate nucleophile with pentafluoropyridine in the perecens of ultrasonic irradiation. Also here we report syntheses of fluorinated imidazopyridine scaffolds by reaction of pentafluorop-yridine or 4-phenylsulfonyl tetrafluoropyridine substrates and various amidines. We will describe an effective method for the synthesis of perfluorinated hetrocyclic systems. Reaction of pentafluoropyridine with various bidentent nucleophiles gave imidazopyridine system wich is a major structure for the synthesis of several derivatives. By use of perfluoro aromatic system, we have very susceptible system towards nucleophilic attack.



References:

[1] Joule, J.A.; Mills, K.; *Heterocyclic Chemistry*; Blackwell: Oxford, **2000**.
[2] Amii, H.; Uneyama, K. *Chem. Rev*. **2009**, 109, 2119
[3] Ranjbar-Karimi, R.; Mousavi,M. *J. Fluorine Chem*. **2010**, *131*, 587.

Oxidative deprotection of trimethylsilyl ethers to corresponding carbonyl compounds by trichloroisocyanuric acid

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The oxidation of trimethylsilyl ethers is an important transformation in organic synthesis. Several methods have been explored to accomplish such a conversion. Some of these methods involve the use of cobalt (II) tetrasulfophthalocyanine [1], ionene supported peroxodisulfate [2], calcium hypochlorite [3], HIO_3 in the presence of $NaHSO_4.H_2O$ [4] and etc. However, a lot of drawbacks may be encountered in using some of these reagents such as low yields, harsh reaction conditions, tedious work-up procedures and some limitations. Therefore, introduction of new methods and reagents for such functional group transformation is still in demand. Trichloroisocyanuric acid (TCCA) is a stable and inexpensive reagent used as an excellent oxidant. Some recent application of the utilization of TCCA in organic synthesis include: Oxidation of bisnaphthols to spironaphthalenones [5], synthesis of benzimidazoles [6], dihydropyrimidinones [7] and 2,5-disubstituted-1,3,4-oxadiazoles [8]. In this research, we wish to report an eco-friendly method for direct oxidation of trimethyl silyl ethers to the parent ketones and aldehydes using TCCA as an efficient oxidant Under mild an heterogeneous conditions. This transformation can be carried out by either a one-pot procedure in the presence of wet SiO_2 at room temprature. The use of one-pot method to establish such a transformation will increase the overall efficiency.

$$\mathbf{RR^1CHOTMS} \xrightarrow[\text{wet SiO}_2\text{, r.t}]{\text{TCCA}} \mathbf{RR^1CO}$$

R: Alkyl

R^1: H, Alkyl

References:

[1] Shaabani, A.; Rezayan, A. H.; Heidary, M.; Sarvary, A. *Catal. Commun.* **2008**, *10*, 129.
[2] Lakouraj, M. M.; Tajbakhsh, M.; Ramzanian-Lehmali, F.; Ghodrati, K. *Monatsh. Chem.* **2008**, *139*, 537.
[3] Mojtahedi, M. M.; Abaee, M. S.; Abbasi, H. *Chemicke Listy* **2008**, *102*, 975.
[4] Shirini, F.; Khademian, M.; Abedini, M. *ARKIVOC* **2008** (xv), 71.
[5] Khoramabadi-Zad, A.; Yavari, I.; Shiri, A.; Bani, A. *J. Heterocyclic Chem.* **2008**, *45*, 1351.
[6] Bigdeli, M. A.; Dostmohammadi, H.; Mahdavinia, G. H.; Nemati, F. *J. Heterocyclic Chem.* **2008**, *45*, 1203.
[7] Bigdeli, M. A.; Jafari, S.; Mahdavinia, G. H.; Hazarkhani, H. *Catal. Commun.* **2007**, *8*, 1641.
[8] Pore, D. M.; Mahadik, S. M.; Desai, U. V. *Synth. Commun.* **2008**, *38*, 3121.

A rapid and new multicomponent route to 4,4’-(arylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ols)

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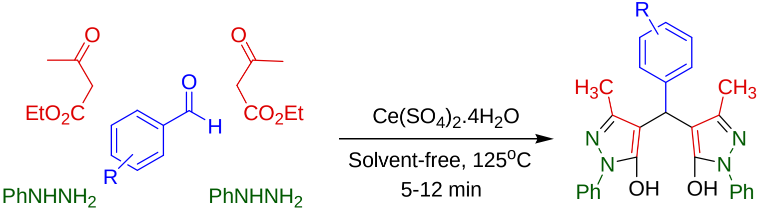
Nitrogen heterocycles containing pyrazol moiety are of special interest because they show some biological and pharmacological activities such as antidepressant [1], antibacterial and antitumor [2].

The conventional chemical approach to titled compound involves the successive Knoevenagel synthesis of the corresponding arylidenepyrazolones and its basepromoted Michael reaction and also one-pot tandem Knoevenagel-Michael reaction of arylaldehydes with two equivalents of 5-methyl-2-phenyl-2,4-dihydro-3*H*pyrazol-3-one performed under a variety of reaction conditions [3]. However, there are disadvantages to these mentioned methods such as low yield, prolonged reaction time and use of toxic organic solvents, harsh reaction conditions or tedious workup procedures.

Thus, a search for new reagents and the development of new methods are still of practical importance. Herein, the one-pot multicomponent synthesis of 4,4'-arylmethylene-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) was reported by effective tandem Knoevenagel-Michael reaction of aryl aldehydes, phenyl hydrazine and ethyl acetoacetate in the presence of catalytic amount of $Ce(SO_4)_2.4H_2O$ (1.2 mol%) as reusable and environmentally friendly catalyst at 125°C in solvent-free conditions. All of the obtained compounds were characterized by FT IR, ^1H and ^{13}C NMR. This new methodology is of interest due to minimizing the cost operational hazards and environmental pollution, high yields, short reaction time, cost effective, simple work-up and reusability of catalyst.



References:

- [1] Bailey, D.M.; Hansen, P.E.; Hlavac, A.G.; Baizman, E.R. J. Pearl, A.F. Defelice, M.E. Feigenson, *J. Med. Chem.* **1985,** *28*, 256.
- [2] Mahajan, R.N.; Havaldar, F.H.; Fernandes, P.S. *J. Indian Chem. Soc*. 68 (1991) 245.
- [3] Chauhan,P.M.S.; Singh, S.; Chatterjee, R.K.; *Indian J. Chem. Sect. B: Org. Chem. Incl. Med. Chem.* **1993**, *32*, 858.

A mild, efficient and one pot synthesis of 2-substituted benzimidazoles using anhydrous $AlCl_3$

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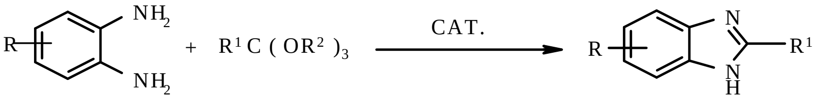
A large number of benzimidazole derivatives exhibit diverse biological and pharmacological activities [1]. They exhibit significant activity against several viruses including HIV, RNA influenza, antimicrobial agents and inhibitors of HCMV replication, potentional antitumour agents [2]. They can also act as ligands to transition metals for modeling biological systems [3].

In view of the importance of benzimidazoles, many classical methods for the synthesis of 2-substituted benzimidazoles have been reported in the literature. Usually, phenylenediamine and carboxylic acids or carboxylic acid derivatives [4], are the starting materials for the synthesis of 2-substituted benzimidazoles under vigorous dehydrating conditions [5].

In this study, for the synthesis of benzimidazoles we threated phenylendiamine with orthoesters such as orthoformate and orthoacetate in the presence of $AlCl_3$ as a catalyst under solvent-free conditions.

Ecofriendly, solvent-free methodology has been employed at 80°C, and compared with the conventional method, The solvent-free method showed the advantages of excellent yield and shorter reaction time.



R = H , Me , NO_2 , CO_2H
R^1 = H , Me
R^2 = Me , Et

References:

[1] Kumar, D,; Jacob, M. R,; Reynolds, M. B & Kerwin S. M. *Bioorg Med chem*., **2002**, *10*, 3991.
[2] Zhang, Z. H,; Yin L,; Wang, Y.M. *Catalysis Communications.* **2007,** *8*, 1126.
[3] Fgekner,T,; Gallucci J,; Chan, M. K. *J. A. Chem. Soc*. **2004**, *126*, 223.
[4] Liu J,; Yang, B. Q & Bai, Y. J. *Synth Commun.*, **2002**, *32*, 3703.
[5] Phillips, M. A. *J. Chem. Soc*., **1928**, 2393.

Facile synthesis of acridine derivatives under solvent-free conditions

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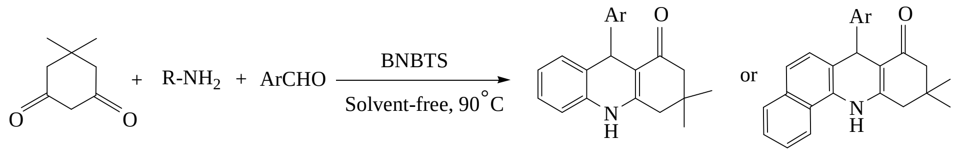
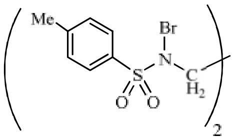
Acridines and its derivatives inhibit HIV-1 reverse transcriptase by intercalating the template-primer hybrid [1]. They are also well known as antimicrobials [2-3], used for the treatment of urinary incontinence [4] and as potential *bis*-intercalating agents has been extensively studied. Moreover, new acridine (naphthalene-quinolines) skeleton fused with a five or six membered ring yields polycyclic derivatives, which also plays an important role as some DNA-intercalating anticancer drugs [5].

Thus, the synthesis of acridine derivatives is an important and useful task in organic chemistry. Herein we report a convenient method for the synthesis of acridine derivatives from different anilines and naphthalene-1-amine, dimedone and various aldehydes in the presence of BNBTS [6] under solvent-free conditions gave products with good to high yields.



R = naphthyl, aryl



BNBTS

References:

[1] Cellai, L.; Di Filippo, P.; Iannelli, M. A.; Antonini, I.; Martelli, S.; Benedetto, A.; Di Caro, A.; Cholody, W. M. *Pharm. Pharmacol. Lett.* **1994**, *3*, 198.

[2] Al-Ashmawi, M. I.; El-Sadek, M. A.; El-Bermawy, M. A.; Mohamed, A. K.; Al-Sabbagh, O. L .Zagazig. *J. Pharm. Sci.* **1994**, *3*, 144.

[3] Demeunynck, M.; Charmantray, F.; Martelli, A. *Curr. Pharm. Design.* **2001**, *7*, 1703.

[4] Ohnmacht, C. *J. Eur. Pat. Appl.* EP 539, 153; *Chem Abstr.* **1993**, *119*, 117144.

[5] Antonini, I.; Polucci, P.; Magnano, A.; Cacciamani, D.; Konieczny, M. T.; Lukowicz, J. P.; Martelli, S. *Bioorg. Med. Chem.* **2003**, *11*, 399.

[6] Ghorbani-Vaghei, R.; Khazaei, A. *Tetrahedron Lett.* **2003**, *44*, 7525.

One-pot synthesis of xanthenes derivatives under solvent-free conditions

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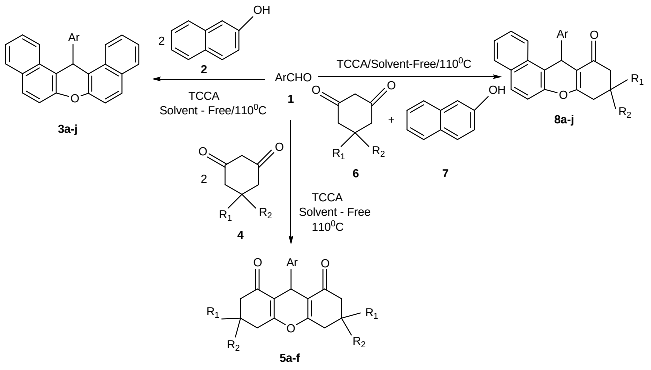
The development of new methods for the synthesis of xanthene derivatives is an important area of synthetic research because of the broad spectrum of their biological and pharmaceutical properties such as antibacterial, antiviral and anti-inflammatory activities as well as phototoxicity and antagonist activity [1-3]. Some xanthene derivatives are used in industry, such as florescent material for visualization of biomolecules, in laser technologies due to their useful spectroscopic properties and as dyes [4-6].

Herein, we report an efficient, mild, and environment friendly method for the synthesis of 14- aryl-14H-dibenzo[a,j]xanthenes, 1,8-dioxo-octahydroxanthene and 12-aryl -8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one derivatives using trichloroisocyanuric acid as neutural catalyst under solvent-free conditions [7].



References:

[1] Wang, H.; Lu, L.; Zhu, S. Y.; Li, Y. H.; Cai, W. M. *Curr. Microbio.* **2006**, *52*, 1.
[2] Zhang, Z. H.; Tao, X. Y. *Aust. J. Chem.* **2008**, *61*, 77.
[3] Naya, A.; Ishikawa, M.; Matsuda, K.; Ohwaki, K.; Saeki, T.; Noguchi, K.; Ohtake, N. *Bioorg. Med. Chem.* **2003**, *11*, 875.
[4] Knight, C. G.; Stephens, T. *Biochem. J.* **1989**, *258*, 683.
[5] Pohlers, G.; Scaiano, J. C. *Chem Mater.* **1997**, *9*, 3222.
[6] Hilderbrand, S. A.; Weissleder, R. *Tetrahedron Lett.* **2007**, *48*, 4383.
[7] Mohammadpour Amini, M.; Seyyedhamzeh, M.; Bazgir, A. *Appl. Catal. A: Gen.* **2007**, *323*, 242.

High termal stability ionic liquids as tamplate in synthesis silica nanopours materials

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With the developmentof porous materials, the porous silica have received wide interest in view of their important applications in bioengineering, catalysis,environmental engineering, sieving, and sensor system[1]. In recent years, the advantages of the ILs in nanopours material synthesis procedures as template have been realized and received more and more intention [2].

In this paper, the prpous is prepreation silica porous material with use of the some of ionic liquids based N,N-dimethyl aminopyridinium cation (DMAP) with high termal stability.

First according to a proper sol-gel method, various RTILs (R$^+$, X$^-$; R$^+$ = R DMAP , X$^-$ = Br, BF$_4$ as a new kind of recyclable templates in present TMOS as the sol-gel precursor and deionized water were employed. Then ILs was removed from the silica matrix by calcination method[3].

The resulting gels were characterized by using thermogravimetric analysis, differential scanning calorimetry, infrared spectroscopy and calcined gels were analyzed using scanning electron microscopy and variation of ILs on porous material in shape and pores size were investigated.

In the countinuous, reaction was fallowed under acidic conditions at temperature above the melting point of the functional IL such as; 2–ethoxyethyl-4-(N,N-dimethyl amino) pyridinum tetrafluoroborate in a so-called nanocasting sol-gel technique, that a mesoporous silicas with highly ordered monolithic was obtained.

References

[1] Kruk, M.; Jaroniec, M. *Chem. Mater*. **2001**, 13, 3169.
[2] K.R. Seddon, *Nat. Mater*. **2003**, 2, 363.
[3] Marc A. Klingshirn, Scott K. Spear, John D. Holbreyc and Robin D. Rogers,*Chem. Mater*., **2005**, 15, 5174.

Ab initio study of conformational peroperties of some ketenimine and bis (ketenimine) derivations

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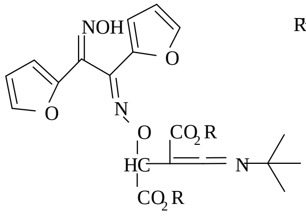
Although ketenimines were first reported by Staudinger and Meyer [1] in the 1920, significant development in the chemistry of these materials is of relatively recent origin. These compounds, which can formally be regarded as imine derivatives of ketenes, are isoelectronic with allenes and indeed the reaction and conformational peroperties of these compounds parallel the reaction and conformational features of allenes, where the two planes π bonds and, thus, the substituents attached to the terminal atoms, are in orthogonal planes.

In spite of developments in the chemistry of ketenimines, little attention has been paid to the synthesis and properties investigations of bis (ketenimines) [2].

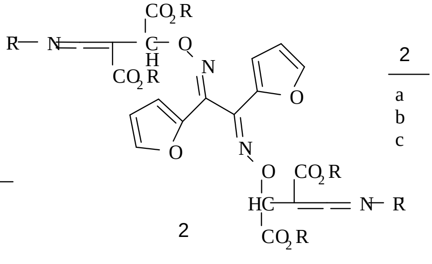
In recent years, with the development of computer hardware, computional chemistry – including molecular dynamics- has become a popular too for chemists studying molecular structures, properties and chemical reactions [3].

We recently synthesized the stable ketenimine bis (ketenimines) (**1, 2**) and examined their Daynamic NMR properties at high temperatures. Now, we wish to calculate the barrier energy for restricted rotation around the C-N bond with ab initio method, B3LYP/6-311G*, and compare with D NMR data.

1	R
a	Me
b	Et
c	t-Bu



1



2

2		R’
a	Me	t-Bu
b	Et	Cy
c	t-Bu	t-Bu

Refrences:

[1] Staudinger,H.; Meyer, *G. Helvetica Chimica Acta.* **1919**, *2*, 619.
[2] Johnson, R. P. *Chemical Reviews* **1989**, *89*, 1111.
[3] Hirst,D.M. *A Computational Approach to Chemistry, Black well Scientific, Oxford*. **1990**.

Silica supported $AgNo_3$: a very cheap, safe and heterogeneous catalyst for synthesis of xanthene derivatives in water

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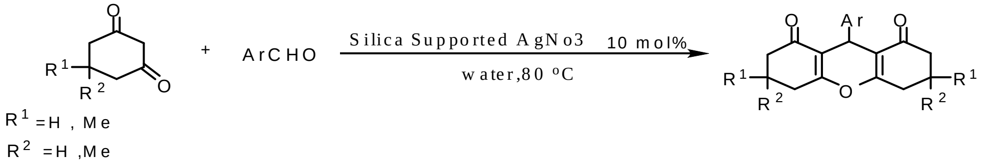
xanthene derivatives have various biological activities such as tranquilizing, antimycobacterial, cardio tonic, antidepressant and antitumor [1]. They have also many applications in dyes, pharmaceuticals and efficient electroluminescent materials [2]. In this article, an easy effective, cheap and environmentally adapted method for synthesis xanthene derivatives by condencation reaction between dimedon with aromatic aldehyds in water as solvent in the presence of Silica Supported $AgNo_3$ is explained as an effective and reusable catalyst. The remarkable features of this new procedure are high conversions, shorter reaction times, cleaner reaction profiles and simple experimental and work-up procedures [3,4].



References

[1] J.-J. Li, X.-Y. Tao, Z.-H. Zhang, *Phosphorus. Sulfur. Silicon*. **2008**, *183*, 1672.
[2] X. Fan, X. Hu, X. Zhang, J. Wang, *Can. J. Chem*. **2005**, *83*, 16.
[3] Abhijit P. Chavan, *J. Korean. Chem. Soc,* **2009**, *53*, 4.
[4] Kerstin Rohr, Rainer Mahrwald. *Bioorganic & Medicinal Chemistry Letters* **2009**, *19,* 3949.

Synthesis and characterization of polyurethane clay-nanocomposite by solution method

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Thermoplastic polyurethane due to its versatile properties is used as an engineering polymer in numerous applications. This is mostly due to combinations of hard and soft segments in polyurethane chain which leads to a two phase structure. A wide range of properties could be attained by different members of PU family which are synthesized using different isocyanates and polyols as monomers [1].

Nanocomposites are a new class of material. During recent decade stress has been put on examining nanocomposites of different polymers and their unusually good properties when compared to composites filled with common micro-sized reinforcing fillers. Nanocomposites have attracted great attention among researchers since they improve several important properties of polymers and make them applicable in new fields while maintaining their cost effectiveness [2-4].

In this study polyurethane nanocomposites were prepared by using several types of organoclay and their thermal and mechanical properties were examined. Samples were prepared via solution method and DMF was used as solvent. TDI (Toluene Di-isocyanate) as isocyanate, CAPA 4000(M_w = 4000) as polyol and 1,4-Butanediol as chain extender were used in this study. Nocomposites containing five types of Italian clay known as Dellite series namely, Dellite 67G, Dellite 72T, Dellite HPS, Dellite 43B and Dellite LVF were synthesized and compared. Some important properties like thermal stability and tensile modulus were found to be improved and improvement was highly dependent on surface modification of organoclay and dispersion of organoclay in polymer matrix [5-6].

References:

[1] Fu, M.H. *Polyurethane Elastomer and its Application,* Chemical Industry Impress, Beijing, **1994**, 10.
[2] Novak, B. M., *Adv. Mater*., **1993**; 5:422.
[3] Torre, L.; Frulloni, E.; Kenny, J. M.; Manferti, C.; Camino, G., *J. Appl. Polym. Sci*., **2003**, 90, 2532.
[4] Bauera ,F.; Glasela, H-J.; Hartmanna, E.; Langgutha, H.; Hinterwaldner, R., *Int. J. Adh.. Adhes*. **2004**, 24, 519.
[5] Esposito Corcionea,C.; Prinari, P.; Cannolettaa, D.; Mensitierib, G.; Maffezzoli, A., *Int. J. Adh. Adhes*., **2008**, 28, 91.
[6] Mishra, A. K.; Nando, G. B.;Chattopadhyay ,S., *J. Polym. Sci., Part B: Polym. Phys.*, **2008**, 46, 2341.

The synthesis of 1,3,4,5-tetrahydro-2H-imidazolo[4,5:5,6]cycloocta[1,2-b] quinoxalin-2-one

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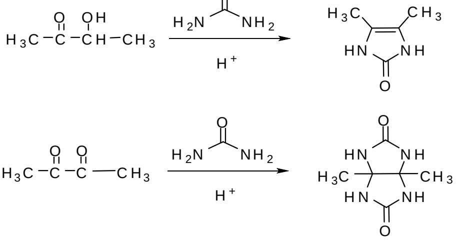
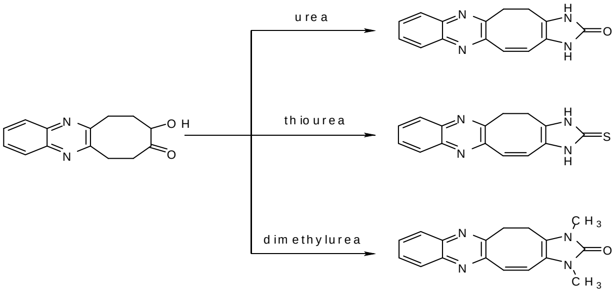
From reaction of alpha-ketol with urea or thiurea is produced imidazolone and thioimidazolone that they are in equilibrium with their enol tautomers, while from reaction of alpha-diketone with urea and thiourea is prepared glycoluril and thioglycoluril



As a consequence, imidazolone must be obtained from reaction of alpha-ketol with urea. In spite of that the reaction does not completely in progress in the same manner. The elimination reaction of a hydrogen molecule and formation double bond is not for aromaticity as similar reactions. The proton shift occurs on cyclooctane ring for transition double bond to joined together imidazolone and quioxaline. Notice that the Cisoid–cyclooctatriene is more stable than transoid-cyclooctatrienethe, energy calculation indicate the present of cisoid isomer and coupling constant (J_3H-H=12.9) two protons of double bond. As expected, in imidazolone and thioimidazolone rings can occurs keto-enol tautomerization but ^{1}HNMR spectrum and theoretical data specifically show that keto-tautomer predominate at equilibrium.



References:

[1] Butler R. Hussain, L. *Journal.Chemical.Society. Perkin II*, **1981**, 310.
[2] Contreras J. G. Madariaga, S. T. J. Phys. Org. Chem. **2003**; 16: 47.

Adsorption of heavy metal ion from waste water by chemically modified polyacrylonitrile grafted bagasse

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Toxic heavy metals water is a global problem that is growing threat to the human health and environment. Therefore, the removal and separation of toxic and environmentally relevant heavy metal ions are a technological challenge with respect to industrial and environmental application[1].

The methods commonly used to remove toxic heavy metal from municipal and industrial wastewater are based on the adsorption of ions onto insoluble compounds and the separation of the sediments formed[2].

Graft copolymerization of acrylonitrile monomer onto bagasse gives the polyacrylonitrile grafted bagasse. Conversion of obtained graft copolymer nitrile groups to oxazoline groups was carried out by reaction with ethanolamine. It was observed that after the modification reaction, the color of sample became dark yellow. IR spectra of un-modified and modified resins were carried out to certify that the modification reaction has produced the desire pendant groups on the resin.The modified and unmodified resins were evaluated on fixing different metal ions, Hg(II), Cu(II), Cd(II), Zn(II), Co(II), Cd(II), Ni(II) and Pb(II); from aqueous solution. These results have shown that the chemical modifications of resin based on acrylonitrile grafted bagasse have provoked an increase of metal ion fixing capacity depending upon the pH employed.

References

[1] Bernabe L. Rivas, Carla Munoz. *Journal of Applied Polymer science,Vol.114,* 1587. *(2009)* .

[2] Lynda H. Wartelle , Wayne E. Marshall. *Water Research 39, 2869 (2005).*

[3] Umesh K. Garg, M.P. Kaur, Dhiraj Sud. *Journal of Hazardous Materials,140,* 60 (2007).

Synthesis and application of modified silica sulfuric acid (MSSA) as a solid acid heterogeneous catalyst in michael addition reactions

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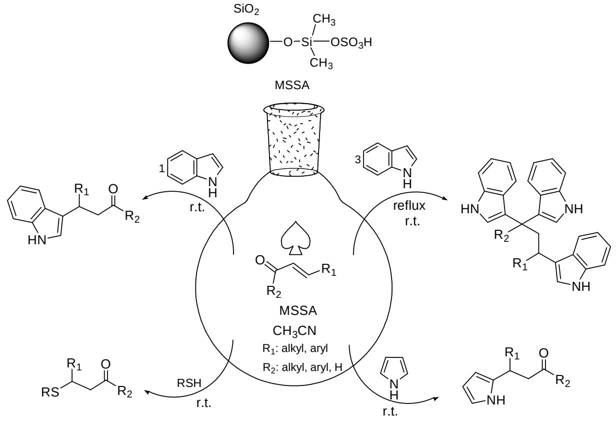
Michael additions promoted by Lewis acid catalysts are one of the most important carbon–carbon bond-forming reactions in organic synthesis. Addition reactions of indoles, amines and thiols to α,β-unsaturated compounds have received much interest due to a number of their derivatives occur in nature and possess a variety of biological activities [1,2]. As a part of our ongoing research program to develop new synthetic methodologies [3,4], we found that modified silica sulfuric acid (MSSA) as a stable solid acid heterogeneous catalyst, non-volatile, inexpensive and safe reagent for conjugate addition of indoles, pyrroles and thiols to Michael acceptors under solvent conditions.



References:

[1] Sundberg, R. J. The Chemistry of Indoles: Academic Press: New York, **1969**; p. 113.
[2] Staunton, B.; Wilkinson, Top. *Curr. Chem*. **1998**, *195*, 49.
[3] Zolfigol, M. A. *Tetrahedron*, **2001**, *57*, 9509.
[4] Veisi, H. *Tetrahedron Lett.*. **2010**, *51*, 2109.

Synthesis of novel Diels-Alder adducts prepared via cycloaddition of styrylcyclohex-2-enone dienes with maleic anhydride dienophile

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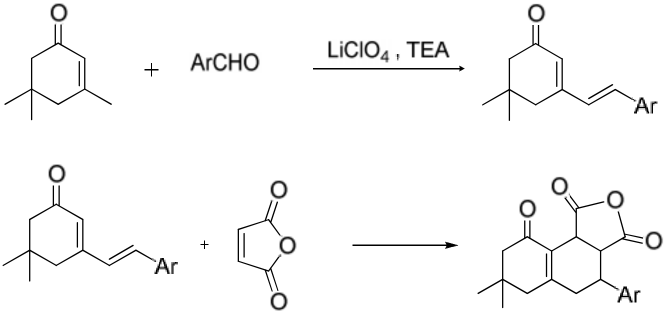
Diels–Alder cycloaddition is one of the most versatile and synthetically useful reactions in which up to four stereogenic centers can be generated in a single step [1]. In connection with our investigations on Diels–Alder reaction [2] and in regard with our previous work on the synthesis of styrylcyclohex-2-enone dienes, we decided to use these dienes for their cycloaddition with dienophiles.

In this work, a variety of dienes are prepared and subjected to react with maleic anhydride as the dienophile under thermal conditions. Products are obtained in high yields and characterized by spectroscopic methods. Reactions are *endo* stereoselective.



References:

[1] Mojtahedi, M. M., Abaee, M. S., Zahedi, M. M., Jalali, M. R., Mesbah, A. W., Yaghoubi, R., Forouzani, M. *Monatsh. Chem.* **2008**, *139*, 917.

[2] Ward, D. E., Abaee, M. S. *Org. Lett.* **2000**, *2*, 3937.

Chemical composition of essential oils of leaf and flower from two *Eucalyptus* species

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Eucalyptus (family *Myrtaceae*) is a genus of tall, evergreen and magnificent trees cultivated world over for its oil, gum, pulp, timber, medicine value [1]. The essential oil found in its foliage is the most important one and use in food, perfumery and pharmaceutical industries [2,3]. In this study, the leaves and flower essential oils of two species of *Eucalyptus* from Zahedan (*E. microtheca* and *E. viminalis*) have been submitted to hydrodistillation and have been subjected to *GC-MSS* analysis. Identification of oils components was achieved based on their retention indices and by the comparison of their mass spectral fragmentation patterns and the *MSS* library database.

A total of 99 compounds were identified from the essential oil of *E. microtheca*, with the dominant compounds beings *α-phellandrene* (16.5%), *aromadendrene* (12.7%), *α-pinene* (6.7%), *globulol* (6%) and *p-cymene* (5.2%). For *E. viminalis* 65 compounds were identified with *1,8-cineole* (57.7%), *α-pinene* (13.4%), and *limonene* (5.4%). In addition, the chemical compounds of the flower essential oil were also analyzed. There are a few reports on the composition of volatiles chemical compositions from flowers [4]. The major components in the flower were *α-pinene* (16.2%), *β-pinene* (11.1%), *o-cymene* (8.1%), *aromadendrene* (7.4%), *α-phellandrene* (7%), *globulol* (5.4%). There are 27 components which are in common in three samples analyzed in this work. So, one can use the flower of *E. microtheca* instead of its leaf.

References:

[1] Diazy R. Batish, Harminder Pal Singh, Ravinder Kumar Kohli, Shalinder Kaur. *Forest Ecology and Management*. **2008**, *256*, 2166.
[2] Martin Gilles, Jian Zhao, Min An, Samson Agboola. *Food Chemistry*. **2010**, *119*, 731.
[3] Sen-Sung Cheng, Chin-Gi Huang, Ying-Ju Chen, Jane-Jane Yu, Wei-June Chen, Shang-Tzen Chang. *Bioresource Technology*. **2009**, *100*, 452.
[4] Andreas Giamakis, Ourania Kretsi, Ioanna Chinou, Caroline G. Spyropoulos. *Phytochemistry*. **2001**, *58*, 351.

Solvent-free and efficient conversion of epoxides to *vic*-dichlorides using chlorodiphenylphosphine/ hexachloroacetone as a new and neutral system

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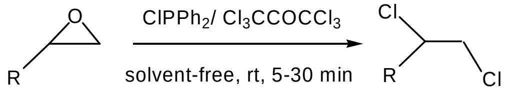
The elimination of volatile organic solvents in organic syntheses is a most important goal in ‘green’ chemistry. The development of solvent-free organic synthetic methods has thus become an important and popular research area [1]. On the other hand, although there are many methods reported for the conversion of epoxides into β-halohydrins, their conversion to vicinal dihalides as other important halogenated compounds is rarely found in the literature. In this connection, the use of reagents such as PPh_3/CCl_4 [2], PPh_3/X_2 (X= Cl, Br) [3] and also PPh_3/ N-halo imides in acetonitrile under reflux conditions [4] have been reported for the preparation of *vic*-dihalides from epoxides. Recently, we have reported on the application of PPh_3/DDQ/ tetraalkylammonium halides in refluxing acetonitrile in the conversion of the epoxides to β-halohydrins and *vic*-dihalides [5] and also the application of chlorodiphenylphosphine in the solvent-free conversion of epoxides to chlorohydrins under mild conditions [6]. In continuation of these works, we now report on a new, more facile and milder method for the efficient and solvent-free conversion of epoxides to *vic*-dichlorides using chlorodiphenylphosphine and hexachloroacetone ($ClPPh_2/Cl_3CCOCCl_3$) in low molar ratio (1.2:0.25) under neutral conditions at room temperature in good to excellent yields (Scheme).



R= $PhOCH_2$, $CH_2=C(CH_3)CO_2CH_2$, Ph, $(CH_3)_2CHOCH_2$,
$CH_2=CHCH_2OCH_2$, $C_{12}H_{25}$, p-Cl-$PhOCH_2$ or epoxide= cyclohexene oxide

Under these reaction conditions, activated aromatic ring, carbon-carbon double bonds and ethereal bonds as functional groups that are present in the epoxide molecules remain intact. In conclusion, the present investigation has demonstrated that the use of $ClPPh_2$ and hexachloroacetone offers an environment-friendly solvent-free, simple and convenient method avoiding the use of molecular halogen with respect to its harsh handling for the mild conversion of epoxides to their corresponding *vic*-dichlorides. Commercial availability, short reaction times, ease of handling and inexpensive of the reagent, the use of reagent in low molar ratio, reduced pollution, easy work up, high yields and operation at room temperature in neutral media are considered as other advantages of this method. Further studies toward the other applications of this reagent in organic synthesis are in progress in our laboratory.

References:

[1] Tanaka, K.; Toda, F. *Chem. Rev.* **2000**, *100*, 1025.
[2] Isaacs, N. S.; Kirkpatrick, D. *Tetrahedron Lett.* **1972**, *13*, 3869.
[3] Sonnet, P. E.; Oliver, J. E. *J. Org. Chem.* **1976**, *41*, 3279.
[4] Iranpoor, N.; Firouzabadi, H.; Azadi, R.; Ebrahimzadeh, F. *Can. J. Chem.* **2006**, *84*, 69.
[5] Iranpoor, N.; Firouzabadi, H.; Aghapour, G.; Nahid, A. *Bull. Chem. Soc. Jpn.* **2004**, *77*, 1885.
[6] Aghapour, G.; Afzali, A.; Salek, F. *Indian J. Chem.* **2009**, *48B*, 231.

Synthesis of organosoluble and thermal polyamides from novel aliphatic-aromatic diacid

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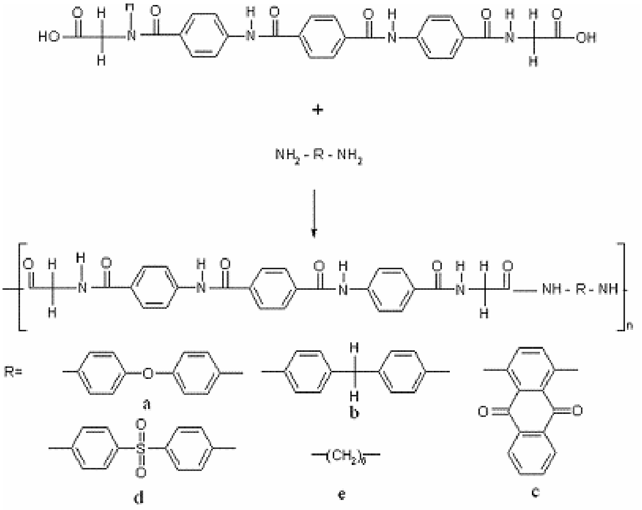
Aromatic/aliphatic polyamides (PAs) were synthesized from a new diacid monomer, aminohippuricterephthaloyl diacid, with various commercial aliphatic and aromatic diamines. The diacid and the prepared polyamides were characterized by elemental analyis, FTIR, and ^{1}HNMR. The PAs were all soluble in common organic solvents such as dimethylsulfoxide (DMSO), N,N-dimethylformamide (DMF), and N-methylpyrolidone (NMP). The PAs showed inherent viscosity in the range of 0.3-0.35 dl/g in NMP at 25 °C and good thermal stability with the char yield in the range of 24-85% at 650 °C in nitrogen atmosphere [1-3].



References:

[1] Abadie, M.J.M.; Voytekunas, V.Y.; Rusanov, A.L. *Iran. Polym J.* **2006,** *15*, 65.
[2] Cassidy, P.E. *Therm. Stab. Polym.*Dekker, New York, **1980.**
[3] Mallakpour, S.; Kowsari, E. *Polym. Adv. Technol.* **2005,** *16*, *732*.

Water soluble Calix[4]arene as a new ligand for speration Inidium from Cadmium

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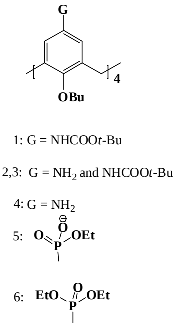
In is one of the most used radio nuclides for nuclear medical applications, both in therapeutic and diagnostic nuclear medicine because of their short half –live, 2.8 days. An the other hand the preparation of high-purity ^{111}In solutions from irradiated targets, especially ^{112}Cd targets, is one of the most important topics in medicinal chemistry[1].
We have recently illustrated SPE a fast and convenient way for further purification of ^{111}In solutions shortly before their use [2].

The synthesis and complexive abilities of different derivatives of functionalized calix[4]arene which can bind selectively Cd^{+2} ans In^{+3} were studied is this paper. We have prepared various type of calix[4]arene ligands which have different functional groups at the upper rim of Calix[4]arene such as tetraaminocalix[4]arene(**1**) Tri-BOC-calix[4]arene(**2**), Tetra-BOC-calix[4]arene(**3**), DiBOCcalix[4]arene(**4**), tetrakis(dimethoxyphosphoryl methyl)calix[4]arene(**5**), and tetrakis(hydroxyphosphorylmethyl)calix[4]arene(**6**) and then the complexation of ligands (**1** to **6**) with Cd^{+2} and In^{+3} in water or methanol/water (20%) have been evaluated at 25° C, using UV-Vis spectrophotometric techniques. The results showed that the water soluble ligand (**5**) which have the phosphonate groups at the upper rim of calix[4]arene could separate Cd^{+2} from In^{+3} in water.

Table 1. Association constants between metal ions and various calix[4]arene ligands

Entry	Ligand	(solvent)	K_a [M^{-1}] for Cd^{2+}	K_a [M^{-1}] for In^{3+}
1	**1**	MeOH/ Water (10%)	21000	35000
2	**2**	MeOH/ Water (20%)	15000	33000
3	**3**	MeOH/ Water (10%)	45000	32000
4	**4**	MeOH/ Water (20%)	14000	16600
5	**5**	MeOH/ Water (20%)	**5900**	**42000**
6	**5**	Water	**63000**	**12500**
7	**6**	MeOH	19000	________



References:
[1] Tolmachev, V.; Bernhardt, P.; Forssell, E.; Lundqvist, H.; *Nuclear Medicine & Biology* **2000**, *27*, 183.
[2] Ebrahimi, F.; Jungclas, H.; Happe, S.; Ensinger, W.; Bombard, A., Zadmard, R.; *Solvent Extraction and Ion Exchange*, **2010**, *28*, 109.

Synthesis and characterization of diorganomorpholinometalates of gallium and indium using morpholine as ambident ligand

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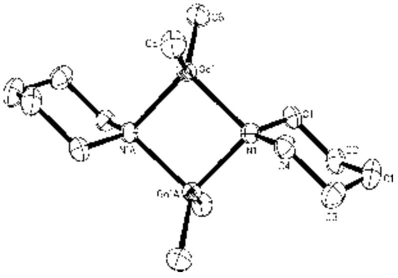
Organometallic compounds with metal-nitrogen bonds were studied intensively in the previous years, where the metal was an alkali-cation [1-3].

In this work we wanted to examine the cyclic amine morpholine and its ability to make µ-bridge.

The reaction of $Li[N(CH_2CH_2)_2O]$ (LiMorpholinate) with Me_2GaCl and Me_2InCl gives by salt-elimination the diorganoamidometalates $Me_2M(Morph)$ (M=Ga:**1**; M=In: not shown). These were characterized by NMR and vibrational spectroscopy as well as by X-ray structure determinations. According to this, centrosymmetrical dimmers are present in the solid state while a monomer-dimer equilibrium was assumed for the THF-solution. Cryoscopic molecular weight determination confirmed our assumptions.

The reaction of $MeInCl_2$ with Li-morpholinate at 20° C gave after work-up and recrystallization from diglyme the salt $[Li(Diglyme)\{In_3Me_2Cl_4(Morph)_4\}]$. In another reaction, the treatment of the mixture of $MesInCl_2/Li(Morph)$ with wet THF yield as only isolated compound the coordination polymer $[Li_6Cl_6(HMorph)_3]$ (**2**).



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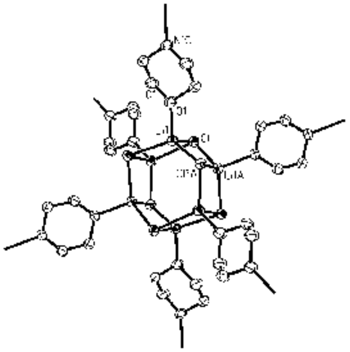

(2)

References:

[1] J. Pauls ; Neumueller, B. *Inorg. Chem.* **2001**, *40*, 121.
[2] J. Pauls ; Neumueller, B. *Z. Anorg. Allg. Chem.* **2001**, *627*, 583.
[3] J. Pauls ; S. Chitsaz ; Neumueller, B. *Z. Anorg. Allg. Chem.* **2001**, *627*, 1723.

Novel conjugates of 5-aminosalicylic acid with non-steroidal anti-inflammatory drugs

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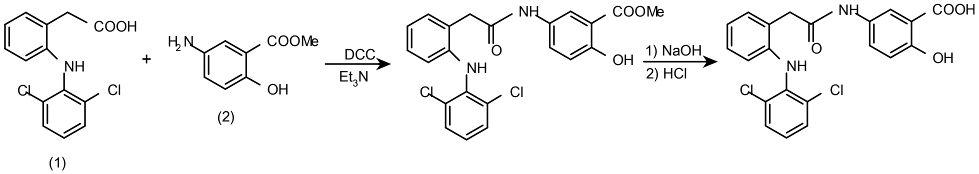
Non-steroidal anti-inflammatory drugs (NSAIDs) such as diclofenac (**1**), ibuprofen, indomethacin, and many others are important in treatment of inflammatory diseases, e.g. rheumatoid arthritis. But, prolonged administration of high doses appears serious gastrointestinal side effects, such as gastric ulcerations and intestinal perforations [1-3]. Sulfasalazine, by contrast, has a therapeutic effect on inflammatory diseases with releasing 5-aminosalicylic acid (5-ASA) in the lower intestine as an antioxidant which may contribute to systemic anti-inflammatory activity if absorbed in sufficient quantities. Therefore, it is interesting to attempt to combine both types of activity by synthesizing stable 5-ASA conjugates of NSAID via an amide bond [4].

This research work describes synthesis and characterization of a series of novel 5-ASA conjugates of various NSAIDs. First, 5-ASA was reacted with dry methanol in the presence of H_2SO_4 and neutralized by Na_2CO_3 solution to give methyl-5-aminosalicylate (**2**). A solution of NSAID and methyl-5-aminosalicylate in dry dichloromethane was cooled, and triethyl amine and *N*,*N*-dicylohexyl carbodiimide (DCC) were slowly added with stirring. After 15 h, the organic phase was extracted with 1M HCl. On standing overnight, the corresponding compound precipitated from the cooled organic solution in high yield. Then, a suspension of the obtained compound in methanol was adjusted to pH 11.5 with 1N NaOH and the resulting solution was refluxed for several days. The reaction mixture was then cooled to 0 °C and treated dropwise with concentrated HCl. The precipitate was collected by filtration and dried in vacuum at room temperature. The structure of all the synthesized compounds was characterized and confirmed by FT-IR, NMR and elemental analyses techniques. The pharmacological of the novel conjugates is under investigation.



References:

[1] Babazadeh, M.; Mosanejhad, T. *Iran. Polym. J.* **2009**, *18*, 179.
[2] Babazadeh, M. *Int. J. Pharm.* **2008**, *356*, 167.
[3] Babazadeh, M. *J. Appl. Polym. Sci.* **2007**, *104*, 2403.
[4] Babazadeh, M.; Edjlali, L.; Rashidian, L. *J. Polym. Res.* **2007**, *14*, 207.

p-Toluene sulfonyl chloride: A recyclable catalyst for the synthesis of bis-indolyl methanes and coumarins

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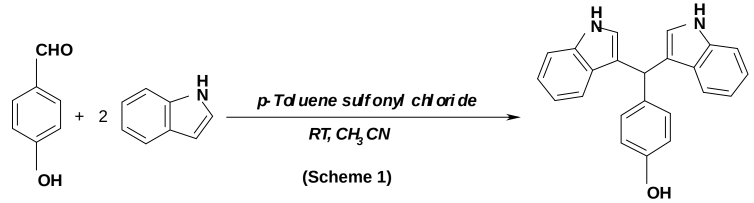
Indole and its derivatives are important intermediates in organic synthesis and exhibit arious physiological properties and pharmacological activities. [1] Therefore the preparation of these intermediates has received increased attention from synthetic organic chemists and biologists.

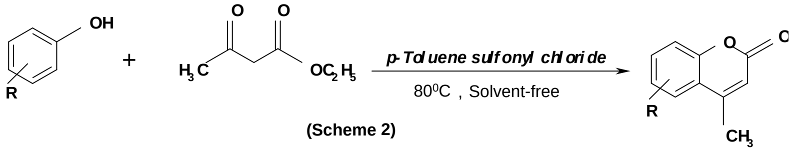
p-Toluene sulfonyl chloride an efficient catalyst for the preparation of bis(indolyl)methanes at room temperature.These condensations were accomplished by the mixing of indole with aromatic aldehydes in the presence of this catalyst at room temperature in good to excellent yields.(scheme 1)

Coumarins and their derivatives form an elite class of compounds, occupying an important place in the realm of natural products and synthetic organic chemistry. Their applications range from additives in food, perfumes, cosmetics, pharmaceuticals and in the preparation of insecticides [2] optical brighteners and dispersed fluorescent and tunable laser dyes.[3]

p-Toluene sulfonyl chloride an efficient catalyst for the Pechmann condensation reaction of phenols and β-ketoesters under solvent-free conditions. The reaction protocol is simple and is followed by aqueous work-up leading to the formation of the corresponding coumarin derivatives in good yield and high purity.(Scheme 2)



(Scheme 1)



(Scheme 2)

References:

[1] Sundberg, R. J.; *The C hemistry of Indoles* ,Academic Press: New York, **1970**.

[2] Kennedy, R. O.; Zhorenes, R. D. *Coumarins: Biology, Applications and Mod e of Action;* John Wiley and Sons: Chichester, **1997 .**

[3] Zabradnik, M. *The Production and Application of Fluorescent Brightening Agents;* John Wiley and Sons: New York, **1992.**

One -pot synthesis of tri- and tetra-substituted imidazoles using NaH_2PO_4 under solvent-free conditions

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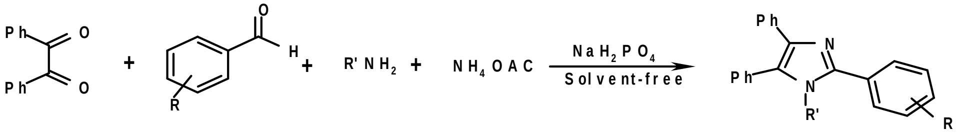
Sodium dihydrogen phosphate (NaH_2PO_4) efficiently catalyzes the condensation reaction of benzil, aldehydes, amines and ammonium acetate in a four-component reaction under solvent-free conditions. The reaction proceeds rapidly and affords the corresponding tetra-substituted imidazoles in high yields. Also an efficient route was developed for the synthesis of tri-substituted imidazoles from condensation of benzil, aldehydes and ammonium acetate using NaH_2PO_4.

Multicomponent reaction (MCR) condensations involve three or more compounds reacting in a single event, but consecutively to form new products, which contains the essential parts of all the starting materials [1].

The developing of new MCRs, and improving known multi-component reactions are an area of considerable current interest [2]. One such reaction is the synthesis of imidazoles. The prevalence of imidazoles in natural products and pharmacologically active compounds has instituted a diverse array of synthetic approaches to these heterocycles [3].

There are several methods for the synthesis of highly substituted imidazoles [4] Following our systematic studies directed towards the development of practical, safe, and environmentally friendly procedures for several important organic transformations in this paper we report a simple and environmentally benign methodology for the synthesis of tetrasubstituted imidazoles via direct four-component condensation reaction between aldehydes, 1,2-diketones, amines, and ammonium acetate using catalytic amounts of NaH_2PO_4 under solvent-free conditions.



References:

[1] Domling, A.; Ugi, I. *Angew Chem Int Ed* **2000**, *39*, 3168.

[2] Eilbracht, P.; Barfacker, L.; Buss, C.; Hollmann, C.; Kitsos-Rzychon, B. E.; Kranemann, C. L.; Rische, T.; Roggenbuck, R.; Schimdt, A. *Chem. Rev.* **1999**, *99*, 3329.

[3] Sisko, J. *J. Org. Chem.* **1998**, *63*, 4529.

[4] Katritzky, A. R.; Boulton, A. J. (Eds.), Advances in Heterocyclic Chemistry; Academic: New York, **1980**; Vol. *27*.

Silica supported zinc bromide: A reusable and highly efficient heterogeneous catalyst for the coupling reaction of acid chlorides with terminal alkynes

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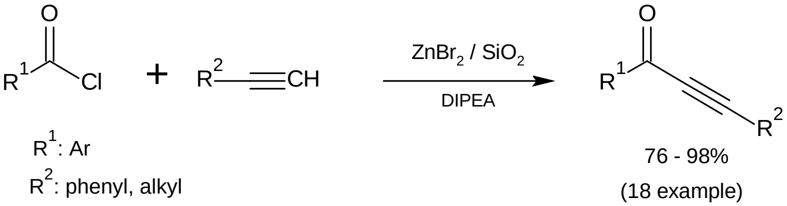
Ynones are compounds of considerable synthetic interest because of their occurrence in a wide variety of biologically active molecules and as key synthetic intermediates [1].

As a part of our continuing interest in palladium catalyzed carbon–carbon cross-coupling reactions, we recently reported use of heterogeneous Pd-catalyst for coupling reactions at ambient temperature under copper free condition [2].

Herein we report an efficient method for synthesis of ynones by cross-coupling of acid chlorides with terminal alkynes in the presence of recyclable silica supported zinc bromide ($ZnBr_2$-SiO_2) under sovent free condition.



References:

[1] Weber, L.; *Curr. Med. Chem.* **2002***, 9, 1241.*
[2] Bakherad, M.; Keivanloo, A.; Bahramian B, Rajaei, M. *Tetrahedron Lett*. **2010**, *51*, 33.

New experimental strategies in conversion of thiocarbonyls to their carbonyl compounds

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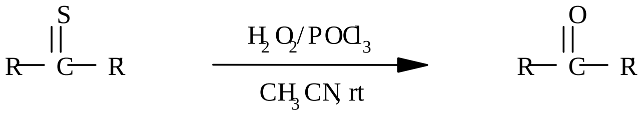
The formation of amide bonds constitutes a widely used process for both synthetic organic chemists and biologists. Amide linkages are present in many biologically active molecules and key natural products and hence, a variety of methods for the synthesis of this functionality have been developed to date [1-3]. However, the different reagents used for this conversion have varying degree of success as well as limitations due to side reactions. To circumvent these problems, alternative strategies toward the preparation of amides have been explored for years.

With our continuous investigation on the methodology of green synthesis [4], we now wish to report a simple and efficient method which enables one to economically desulfurise thiocarbonyls to their carbonyls using H_2O_2 in the presence of $POCl_3$ in excellent yields (Scheme 1).



$$R-\overset{\overset{\displaystyle S}{||}}{C}-R \xrightarrow[CH_3CN,\ rt]{H_2O_2/POCl_3} R-\overset{\overset{\displaystyle O}{||}}{C}-R$$

Scheme 1.

References:

[1] Mohammadpoor-Baltork, I.; Memarian, H. R.; Bahrami, *Monatsh. Chem.* **2004**, 135, 411.
[2] Gao, J.; Wang, G.-W. *J. Org. Chem.* **2008**, *73*, 2955.
[3] Hashimoto, M.; Obora, Y.; Sakaguchi, S.; Ishii, Y. *J. Org. Chem.* **2008**, *73*, 2894.
[4] Bahrami, K.; Khodaei, M. M.; Tirandaz, Y. *Synthesis* **2009**, 369.

Heteropolyacids: An efficient catalyst for synthesis of CL-20

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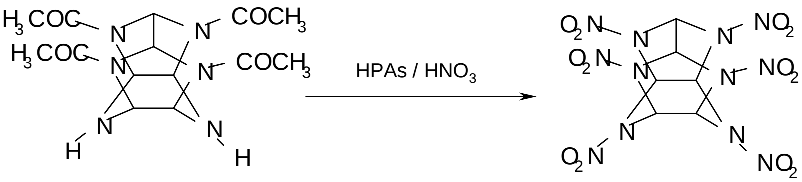
The search for new energetic materials as potential replacements for currently used explosive and propellant formulations (used in gun and rocket propellants) is an area of intense investigation in military and industrial applications [1–2]. There are three propellant compounds currently attracting much interest:2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12 hexaazaisowurtzitane (HNIW), also known as CL-20. Many reports have been published on its physical characteristics; these are reviewed in a recent article by Nielsen et al.1 All known methods of producing 2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane are based on the same starting material, 2, 4, 6, 8, 10, 12-hexabenzyl 2, 4, 6, 8, 10, 12-hexaazaisowurtzitane, which is first reductively acylated to form 2, 6, 8, 12-tetraacetyl-4, 10-dibenzyl-2,4,6,8,10,12-hexaazaisowurtzitane [4].

Heteropolyacids (HPAs), catalyze a wide variety of reactions in homogeneous or heterogeneous (liquid–solid, gas–solid, or liquid–liquid biphasic) systems, offering strong options for more efficient and cleaner Processing compared to conventional mineral acids. Our interest in the study of the explosive and thermal characteristics of 2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane prompted us to develop an acceptable synthetic procedure for this material. In this article a study was undertaken to determine effect of heteropolyacids in nitration of TAIW.



References:

[1] Nielsen, A.T. US Patent 5,693,794, **1997**.

[2] Panikov, N.S.; Sizova, M.V.; Ros, D.; Christodoulatos, C.; Balas, W.; Nicolich, S. *Biodegr. Springer Sci*. **2007**, *18*, 317.

[3] Agrawal, J. P.; Hodgson, R. D. John Wiley & Sons Ltd, the Atrium, Southern Gate, Chichester, England, **2007**.

[4] Misono, M. *Chem Commun*. 1141, **2001**.

Synthesis of new imidazo[1,2-a]pyrimidines from arylaminoisoxazol-5(2H)-ones

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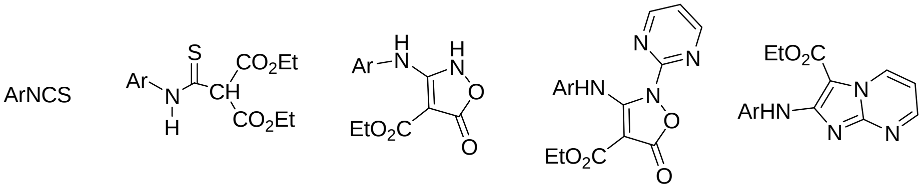
The synthesis of ethyl 3-phenylamino-5-oxo-2,5-dihydroisoxazol-4-carboxylate has been reported by Worrall [1]. The reaction of 2-pyridyl-3-arylaminoisoxazolones with triethylamine leads to the formation of indoles and carbon dioxide [2], an outcome that is formally the same as that achieved by photolysis [3].

Reaction of isothiocyanate **1** with sodium salt of diethylmalonate at room temperature gave the corresponding derivatives of sodium diethyl arylthiocarbamoylmalonate (**2**) in good yield. Treatment of these compounds **2** with hydroxylamine under reflux conditions gave 3-arylaminoisoxazol-5(2H)-ones (**3**) in high yield, which were converted to *N*-substituted derivatives **4**. The rearrangements of compounds **4** in TEA gave the corresponding imidazo[1,2-a]pyrimidines **5.** These rearrangements of 2-heterocyclyl isoxazolones appear to be generally applicable to the synthesis of heterocycles which are suitable synthetic intermediates for a series of new polycyclic heterocycles with possible pharmaceutical applications and could be expected to intercalate with DNA [4-6].



1 **2** **3** **4** **5**

Ar = 3-BrC_6H_4 , 3-MeC_6H_4 , 4-MeC_6H_4 , 4-BrC_6H_4

References:

[1] Worrall, D. E. *J. Am. Chem. Soc.* **1923**, *45*, 3092.
[2] Khalafy, J.; Prager, R. H. *J. Sci. I. R. Iran.* **2000**, *11*, 32.
[3] Khalafy, J.; Prager, R. H.; Smith. *J. Chem. Res (M).* **1999**, 518.
[4] Pham, T.-N; Tuteja, R.; Ocham, A.; Falaschi, A. *Biochem. Biophys. Res. Commun*. **1997**, *236*, 636.
[5] Stiborova, M.; Bieler, C, A.; Wiessler, M.; Frei, E. *Biochem. Pharmacol.* **2001**, *62*, 1675.
[6] Ajay Babu, P.; Laxmi Narasu, M.; Srinivas, K. *Arkivoc.* **2007**, *ii,* 247.

Heck coupling reaction using a new monomeric ortho-palladated complex

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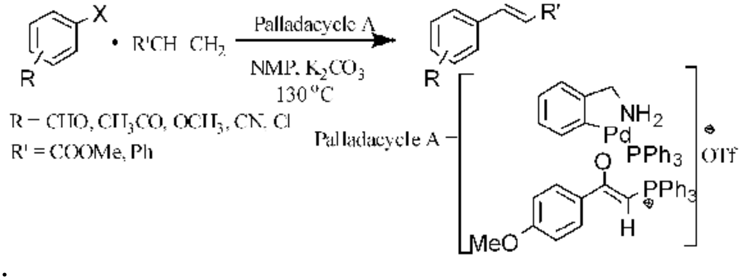
Due to many vast application of carbon-carbon bond formation [1], over the past few years, the C-C coupling reactions have become a versatile tool in organic synthesis [2]. One of the most efficient methods in this field entitled Heck reaction, in which a palladium catalyzed reaction is carried out between an olefin and an aryl or alkenyl halide in the presence of a base. This reaction was discovered by Heck [3] and Mizoroki [4] about 40 years ago. Among the new methods for efficient performing of these reactions, application of palladacycle catalysts in the Heck reaction of activated and non-activated aryl halides using very low catalyst concentration is well known today.

After 1996, that the first application of microwave irradiation in organic synthesis was reported by Gedye and Giguere [5], this technique was used in different types of reactions and its results clearly showed that the required time for completion of the reactions can be decreased in this manner.

In this article, we want to report a new catalytic system for the Heck reaction of various aryl halides under both conventional heating and MW irradiation conditions. Reactions were performed under the optimized conditions. Under both heating conditions, full conversion of reactants to products was obtained and resulted yields were very excellent.



References:

[1] Bong Park, S.; Alper, H. *Org. Lett.* **2003**, *5,* 3209.
[2] Hamza, K.; Abu-Reziq, R.; Avnir, D.; Blum, J. *Org. Lett.* **2004**, *6*, 925.
[3] Heck, R.F.; *Acc. Chem. Res*. **1979**, *12*, 146.
[4] Mizoroki, T.; Mori, K.; Ozaki, A.; *Bull. Chem. Soc. Jpn.* **1971**, *44*, 581.
[5] Giguere, R.J.; Bray, T.L.; Duncan, S.M.; Majetich, G.; *Tetrahedron Lett*. **1986**, *27,* 4945.

Serendipitous one-pot stereoselective synthesis of brand-new fluorescent dyes

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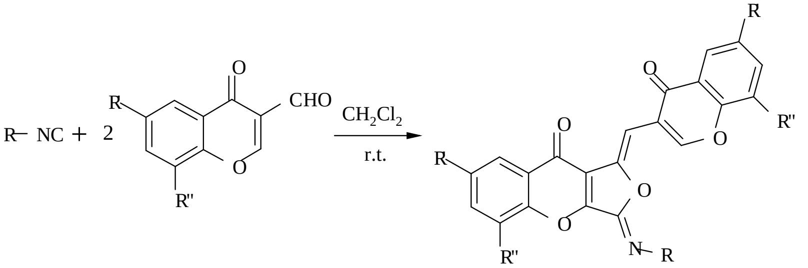
Fluorescence is the emission of electromagnetic radiation light by a substance that has absorbed radiation of a different wavelength. In most cases, absorption of light of a certain wavelength induces the emission of light with a longer wavelength [1].

Synthesis of fluorescent dyes with extended π-conjugation continues to arouse strong interest because of their applications as sensors and biosensors, electroluminescent materials, lasers, copy-preventing inks, solar energy collecting materials, and other optoelectronic devices [2-4]. So far, many strategies and various classes have been adopted to reach this goal [5,6]. However, it is very important to design and develop new fluorescent chromophores which have special functionalities as new dye materials.

Following our recent works [7,8] on the application of isocyanide-based multicomponent reactions in functionalized dyes synthesis, in the present work, we describe the stereoselective synthesis of novel (1*Z*)-3-(alkylimino)-1-[(4-oxo-4*H*-chromen-3-yl)methylene]-1,3-dihydro-9*H*-furo[3,4-*b*]chromen-9-one blue-emitting fluorescent dyes from the reaction of 3-formylchromone derivatives with alkyl isocyanides in CH_2Cl_2 at room temperature.



References:

[1] Lakowicz, J. R. “Principles of fluorescence spectroscopy”, 3rd ed., New York: Springer, **2006**.
[2] Kido, J.; Okamoto, Y. *Chem. Rev.* **2002**, *102*, 2357.
[3] Thompson, M. A.; Forrest, S. R. *Nature* **2000**, *403*, 750.
[4] McQuade, D. T.; Pullen, A. E.; Swager, T. M. *Chem. Rev.* **2000**, *100,* 2537.
[5] Valeur, B. “Molecular Fluorescence”, Wiley-VCH: Weinheim, **2002**.
[6] Chen, C. H.; Shi, J. *Coord. Chem. Rev.* **1998**, *171*, 161.
[7] Teimouri, M. B.; Khavasi, H. R. *Tetrahedron* **2007**, *63*, 10269.
[8] Teimouri, M. B.; Bazhrang, R. *Monatsh. Chem.* **2008**, 139, 957.

Synthesis and electrochemical study of novel dopamine derivative using modified multi-wall carbon nanotubes paste electrode

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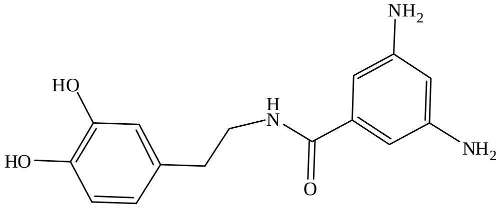
Catechol, formerly recognized as 1, 2-dihydroxybenzene is an organic compound with the molecular formula of $C_6H_4(OH)_2$. Several industrially important flavors and fragrances are prepared starting from catechol. It is a common building block in organic synthesis [1,2]. In continuation of our efforts to synthesize novel monomers [3], in this study, we wish to describe the synthesis and characterization of 3,5-diamino-*N*-(3,4-dihydroxyphenethyl)-benzamide (3,5-DAB) as a new diamine compound. 3,5-DAB was prepared from the reaction of 3,5-dinitrobenzoylchloride and 3-hydroxytryaminum chloride in *N*,*N*-dimethylacetamide as a solvent in the presence of propylene oxide as an acid scavenger and then reduction in hydrazine hydrate in the presence of palladium activated carbon.

For the electrochemical investigation of 3,5-DAB we prepared a mixture of 3,5-DAB with graphite powder and carbon nanotubes in a mortar and pestle. Then, paraffin was added to the mixture and was mixed well until a uniformly-wetted paste was achieved. Electrical contact was made by pushing a copper wire down the glass tube into the back of the mixture. The unmodified carbon nanotubes paste electrode was prepared in the same way without adding 3,5-DAB to the mixture to be used for comparison purposes.



References:

[1] Nematollahi, D.; Rafiee, M. *J. Electroanal. Chem*. **2004**, *31*.566.
[2] http://en.wikipedia.org/wiki/Catechol. 07, April, 2010.
[3] Mallakpour, S.; Moghaddam, E. *Iran. Polym. J*. **2006**, *15*, 547.

Preparation of nanoflake magnetic polypyrrole composite based on $SrFe_{12}O_{19}$ and strontium ferrite coated with Fe_3O_4

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Nanoflake composite $SrFe_{12}O_{19}$/Polypyrrole and composite core–shell $SrFe_{12}O_{19}/Fe_3O_4$/Polypyrrole were synthesized by in situ polymerization method. In this paper, the synthesized of $SrFe_{12}O_{19}$ nanoflake as first core by sol-gel method. Than fabricated a shell layer from magnetic nanoparticles of Fe_3O_4, which synthesized by co-precipitation technique, onto the $SrFe_{12}O_{19}$ nanoflake. Than nanoflake $SrFe_{12}O_{19}$ and core – shell $SrFe_{12}O_{19}/Fe_3O_4$ was used as template for the preparation of $SrFe_{12}O_{19}$/Polypyrrole and $SrFe_{12}O_{19}/Fe_3O_4$/Polypyrrole nanocomposites. Final nanocomposites respectively have a conductive property $4.23*10^{-2}$ sem^{-1} and $4.12*10^{-2}$ sem^{-1} and is magnetic property of nanoflake $SrFe_{12}O_{19}$ and $SrFe_{12}O_{19}$/Polypyrrole and $SrFe_{12}O_{19}/Fe_3O_4$/Polypyrrole nanocoposites respectively equal with M_s=57 emu/g, Ms= 3.22 emu/g and Ms= 2.99emu/g. Also Final nanocomposites in soluble at organic solvent such as DMF and DMSO and has a flake structure. Conductivity and magnetic property respectively determine by instrument forth points and vibrant sample magnetometer (VSM), morphology and particle size determined by FE-SEM, XRD and TEM.

References:

[1] Zheng, Z., Chen, Y., Shen Z., Ma, J., Sow, C. H., Huang, W., Yu, T., *Appl. Phys. A*, **2007**, *89*, 115.
[2] Tang, Q., Sun, X., Li, Q., Wu, J., Lin, J., Huang, M. ,*Materials Letters*, **2009**, *63*, 540.
[3] Li, Q., Zhang, C., Wang, Y., Li, B., *Synthetic Metals*, **2009**, *159*, 2029.

Tert-Butylation of *p*-cresol with MTBE in presence of acids as catalyst

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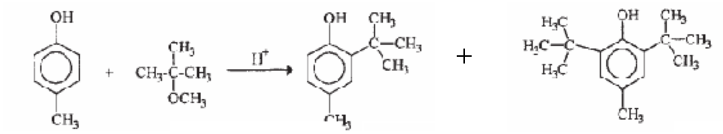
It is well recognized that the presence of stabilizers are of primary importance in industry for the long term durability of materials, such as solid rocket propellants, plastics and rubbers. A novel synthesis method is performed for the synthesis of butylated hydroxyl toluene (BHT), used as an important chemical intermediate and a well known commercial antioxidant in food industrials, pharmaceuticals, and the basic raw material for the manufacture of bis-phenolic antioxidants, and oil-soluble phenol-formaldehyde resins [1,2]. Selective liquid phase *tert*-butylation of *p*-cresol with Methyl tert-butyl ether (MTBE) has been conducted to produce 2-*tert*-butyl *p*-cresol (2-TBC) over three types of acids including, Toluene 4-sulphonic acid, tri-flouro methane sulponic acid and chlorosulponic acid. Thus, MTBE is a good source for the generation of pure isobutylene and the by-product, methanol, is also a very important raw material in chemical industry [3]. The effect of various parameters, namely, temperature, reactant mole ratio, catalyst to *p*-cresol mole ratio and time of reaction on the conversion of *p*-cresol and yield and selectivity of 2-TBC were systematically optimized as well. The catalytic results are also compared with those obtained using other catalysts such as: Ion-exchange resins, clays, zeolites, heteropoly acids and sulfated zirconia [4]. Based on catalytic results, the three acids in this work are found to be a highly active catalyst for the synthesis of 2-*tert*-butyl *p*-cresol with high selectivity. Fig. below shows the reaction scheme for alkylation of *p*-cresol with MTBE.



Catalyst 2-TBC 2, 6 DTBC

References:

[1] Dumitriu, E.; Meloni, D.; Monaci, R.; Solinas, V. *Laboratory of Catalysis, Technical University of Iasi, 71 D. Mangeron Ave, 70050-Iasi, Romania.* **2000**.

[2] Sarish,S.; Devassy, Biju M.; Halligudi, S.B. *Cochin University of Science and Technology, Kochi 682 022, India Inorganic Chemistry and Catalysis Division, National Chemical Laboratory, India.* **2005.**

[3] Kirthivasan, N. *Heterogeneous Catalysis: Preparation, Characterization and Application, Ph.D.* (chemistry) thesis, University of Bombay, Bombay (Mumbai), Dec. **1995**.

[4] Yadav, G. D.; Pujari, A. A. and Joshi, A. V. *Chemical Engineering Division, University Department of Chemical Technology (UDCT), University of Mumbai, Matunga, MUMBAI-400 019, India.***1999**.

Synthesis and characterization of 2-amino-7-(dimethylamino)-4-methylthiophenyl-4*H*-chromene-3-carbonitrile derivatives as potential apoptosis inducers

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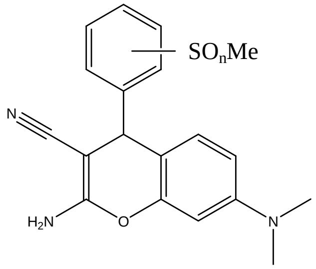
Apoptosis or programmed cell death is the normal process of cellular suicide that proceeds with characteristic biochemical and cytological features, including nuclear condensation and fragmentation. Apoptosis enables organisms to control their cell numbers and to eliminate unneeded cells that may threaten their survival [1].

Since many cancer cells exhibit abnormal inhibition of apoptosis [2]. We are interested in the development of inducers of apoptosis as potential anticancer agents.

Herein we report the synthesis and characterization of 2-amino-7-(dimethylamino)-4-methylthiophenyl-4*H*-chromene-3-carbonitrile derivatives as potential apoptosis inducers. They were synthesized by one-pot reactions of methylthiobenzaldehyde, 3-dimethylaminophenol, and malonitrile in good yields.

The purity of the synthesized compound was confirmed by chromatography. The structure of compound was characterized using IR, ^{1}HNMR spectra.



References:

[1] O ’Driscoll, L.; Linehan, R.; Clynes, M. Survivin: Role in Normal Cells and in Pathological Conditions. *Curr. Cancer Drug Targets* **2003**, *3*, 131.

[2] Reed, J. C. Dysregulation of Apoptosis in cancer. *J. Clin. Oncol.* **1999**, *17*, 2941.

An efficient one-step synthesis of polyhydroquinoline via a TiO_2 nanoparticle-catalyzed four-component Hantzsch reaction

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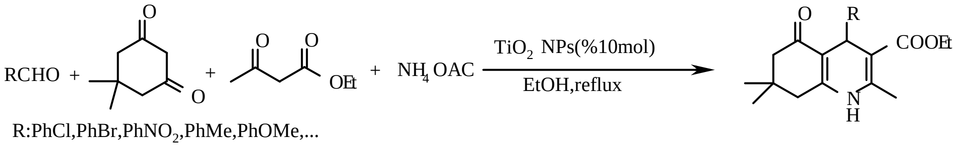
One-pot multi component coupling reactions (MCRs), where several organic moieties are coupled in one step, for carbon-carbon and carbon–heteroatom bond formation is an attractive synthetic strategy for the synthesis of small–molecule libraries with several degrees of structural diversities [1].

Nanocrystalline metal oxides have found excellent applications as active adsorbents for gases, for destruction of hazardous chemicals [2] and as catalysts for various organic transformations [3]. Their high reactivity is due to high surface areas combined with unusually reactive morphologies.

In continuation of our work on the application of nano oxides in organic methodologies, here we report an effective four-component condensation of aldehyde, dimedone, ethyl acetoacetate and ammonium acetate to give the corresponding polyhydroquinoline derivatives in good to high yields using TiO_2 nanoparticle catalyst.



References:

[1] a) Hantzsch, A.; *Justus Liebigs. Ann. Chem*. **1882**, *215*, 1. b) Bossert, F.; Vater, W.; *Med. Res. Rev*. **1989**, *9*, 291.
[2] Schlogl, R.; Abd Hamid, S B.; *Angew. Chem. Int. Ed*. **2004**, *43*, 1628.
[3] Kantam, M L.; Mahendar, K.; Sreedhar, B.; Vijay Kumar, K.; Choudary, B M.; *Synth. Commun*. **2008**, 3919.

Synthesis of highly functionalized α,β-unsaturated γ-butyrolactones from activated carbonyl compounds and dialkyl acetylenedicarboxylates in the presence of triphenylphosphine

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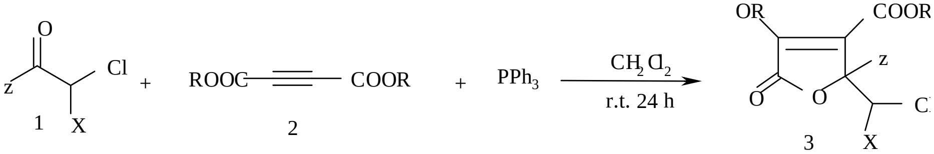
The reaction of 1:1 zwitterionic species, generated in situ by the addition of triphenylphosphine to suitably active π-systems such as acetylenic esters has been investigated in detail [1]. α-keto esters and α-keto nitriles have electron-withdrawing groups directly bound to their ketonic carbonyl groups. The strong electrophilic nature of their ketonic groups is expected to facilitate various kinds of nucleophilic addition [2]. We became interested in the use of activated carbonyl compounds such as α-halo ketones as trapping reagents for the produced zwitterionic intermediates from addition of triphenylphosphine to acetylenic esters. Here, we report reactions of α-halo ketone derivatives **1** with acetylenic esters **2** in the presence of triphenylphosphine that lead to highly functionalized α,β-unsaturated γ-butyrolactones **3** in moderate to good yields.



1, 2	*R*	*Z*	X	Yield of **3** (%)
a	CH_3	CH_3	H	60
b	CH_3CH_2	CH_3	H	55
c	CH_3	CH_2Cl	*H*	*50*
d	CH_3CH_2	CH_2Cl	*H*	*45*
e	CH_3	*Ph*	Cl	*54*
f	CH_3CH_2	*Ph*	Cl	*50*

References:

[1] (a) Johnson, A. W. Tebby , J. C. *J. Chem. Soc*. **1961**, 2126; (b) Zhang, C.; Lu, x. *J.Org. Chem*. **1995**, *60*, 2906; (c) Nair, v.; Mathen, J. s.; Viji, s., Sriniras, R; Nandar kumar, M. V.; Vorma, L. R. *Tetrahedron*, **2002**, *58*, 8113; (d) Yavari, I.; Djahaniani, H.; Nasiri, F. *Synthesis*, **2004**, 679.
[2] Hunig, s.; Schaller, K. *Angew. Chem. Int. Ed*. **1982**, *21*, 36.

Carbon-based solid acid as an efficient and reusable catalyst for one-pot synthesis of 1,8-dioxodecahydroacridines

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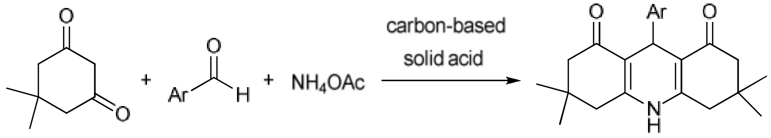
The 1,4-dihydropyridine (DHP) ring system is found in a variety of compounds including dyes, organic materials and pharmaceuticals. Among the pharmaceuticals, 1,4-dihydropyridines have been employed for the treatment of platelet antiaggregatory activity and Alzheimer’s disease [1]. 1,8-Dioxodecahydroacridines, with a 1,4-dihydropyridine parent nucleus, have received less attention than other 1,4-dihydropyridine derivatives. These compounds have been shown to have very high lasing efficiencies and used as photoinitiators [2, 3]. Very few methods are known in the literature for the synthesis of acridinediones. The most straightforward synthesis of this compounds involve the three-component condensation of an aldehyde, dimedone, and ammonium acetate or appropriate amines in the presence of several catalysts such as [Hmim]TFA , [$B(C_6F_5)_3$] and $Zn(OAc)_2.2H_2O$ [4-6]. However, some of these methodologies encounter some limitations, such as long reaction times, unsatisfactory yields, harsh reaction conditions, requirement of expensive catalysts and tedious work-up procedure.

Thus, in this work, we wish to report a simple, efficient, and eco-friendly method for the synthesis of 1,8-dioxodecahydroacridines via three-component condensation of an aldehyde, dimedone, and ammonium acetate using carbon-based solid acid as catalyst. The catalyst can be reused after a simple work-up. Other advantages of these protocols are high yields, relatively short reaction times and easy work-up.



References:

[1] Bretzel, R. G.; Bollen, C. C.; Maeser, E.; Federlin, K. F. *Drugs Future,* **1992**, *17*, 465.
[2] Shanmugasundaram, P.; Murugan, P.; Ramakrishnan, V.T.; et. al. *Heteroat. Chem.*, **1996**, *7*, 17.
[3] Tu, S.; Miao, C.; Gao, Y.; Fang, F.; Zhuang, Q.; Feng, Y.; Shi, D. *Synlett*, **2004**, 255.
[4] Dabiri, M.; Baghbanzadeh, M.; Arzroomchilar, E. *Catal. Commun.*, **2008**, *9*, 939.
[5] Chandrasekhar, S.; Rao, Y.S.; Sreelakshmi, L.; et. al. *Synthesis*, **2008**, *11*, 1737.
[6] Balalaie, S.; Chadegani, F.; Darviche, F.; Bijanzadeh, H. R. *Chin. J. Chem.*, **2009**, *27*, 1953.

Synthesis of novel mediate for reversible addition fragmentation chain transfer (RAFT) polymerization

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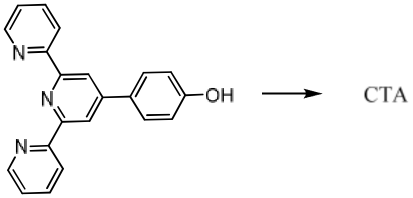
Radical polymerization with reversible addition-fragmentation chain transfer (RAFT polymerization) is a reversible deactivation polymerization and one of the most versatile processes for conferring living characteristics on radical polymerization [1]. The polymerization of most monomers that are polymerizable by radical polymerization can be controlled by the RAFT process. However, the RAFT agent [ZC(=S)S-R) must be selected according to the monomer(s) used [2]. Thus, RAFT agents such as dithioesters (Z = aryl, alkyl) or trithiocarbonates (Z = alkylthio) suitable for controlling polymerization of “more-activated” monomers (MAMs), such as styrene, methyl acrylate (MA), and methyl methacrylate (MMA).

The terpyridine as R-group increase heat stability of the polymer. The hydroxy containing terpyridine was synthesized via ring assembly procedure reported by Hanabusa [3]. The terpyridine containing thiocarbonyl-thio RAFT agent, with terpyridine as R group was synthesized by hydroxy functionalized terpyridine.

All of the materials were characterized by FT-IR and H-NMR spectroscopy.



CTA= chain transfer agent

References:

[1] Moad, G.; Rizzardo, E.; Thang, S. H. *Polymer* **2008**, *49*, 1079.
[2] Chong, Y. K.; Krstina, J.; Le, T. P. T.; Moad, G.; Postma, A.; Rizzardo, E.; Thang, S. H. *Macromolecules* **2003**, *36*, 2256.
[3] Hanabusa, K.; Hirata, T.;Inoue, D.; Kimura, M.; Shirai, H. *Coll. Surf. A: Physicochem. Eng*. 2000, *169*,307.

Theoritical study for reaction between triphenylphosphine and activated acetylenic esters in the presence of theophylline compound

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In the present work, the stability of the Z and E isomers was undertaken for the two isomers of a phosphorus ylide by means of atoms in molecules (AIM) analysis. Phosphorus ylides are important reagents in synthetic organic chemistry, especially in the synthesis of naturally occurring products and compounds with biological and pharmacological activity [1-6]. Most of the phosphonium salts are usually made from the reaction of phosphine and an alkyl halide [4-6], though they can be obtained by Michael addition of phosphorus nucleophiles to activated olefins [2,3]. A facile synthesis of the reaction between triphenylphosphine **1**, dialkyl acetylendicarboxylates **2** and teophylline **3** (as a heterocyclic compound) has been earlier reported [7]. The reaction is shown in Figure 1. The Z and E isomers were optimized for all ylide structures at HF/6-31G(d,p) level of theory by gaussian03 package program. The energy of both isomers have been calculated at B3LYP/6-311++G** level. Atoms in molecules (AIM) analysis at HF/6-31G(d,p) level of theory have been performed in order to gain a better understanding of most geometrical parameters in both E-4(a,b) and Z-4(a,b) of phosphorus ylides. The numbers of critical points and intramolecular hydrogen bonds as well as the charge of atoms that constructed on the Z and E isomers have been recognized. The results altogether reveal the effective factors on stability of the Z- and the E- ylide isomers.

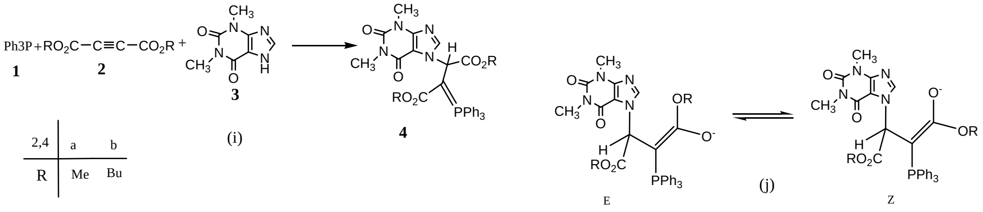

Figure 1: (i) The reaction between triphenylphosphine **1**,dialkyl acetylenedicarboxylate **2** (2a or 2b) and theophylline **3** for generation of stable phosphorus ylides **4** (4a or 4b), (j) Two isomers (Z)-4a and (E)-4a (major and minor) of ylide 4a.

References:

[1] Wittig, G. *Science*, **1980**, *210*, 600.
[2] Johnson, A. W. *Ylide Chemistry*, Academic Press, New York, **1979**.
[3] Cadogan, *J. I. G. Organophosphorus reagents in organic synthesis*, Academic Press, New York, **1979**.
[4] I. Yavari, L. Ahmadian-Razlighi, *Phosphorus, Sulphur and Sillicon*, **2006**, *181*, 771.
[5] M. T. Maghsoodlou, N. Hazeri, G. Afshari, U. Nroumand, *Phosphorus, Sulphur and Sillicon*, **2006**, *181*, 2681.
[6] S. M. Habibi-Khorassani, M. T. Maghsoodlou, H. Roohi, M. Zakarianejad, M. Moradian, *Progress in Reaction Kinetics and Mechanism*, **2005**, *30*, 127-144.
[7] S. M. Habibi-Khorassani, A. Ebrahimi, M. T. Maghsoodlou, H. Saravani, M. Zakarianezhad, M. Ghahramaninejat, M. A. Kazemian, M. Nassiri, Z. Khajehali, *Progress in Reaction Kinetics and Mechanism*, **2009**, *34*, 301.

Synthesis of a new series of novel chromeno[4,3-e][1,4]thiazepin-6(5*H*)-one coumarin derivatives

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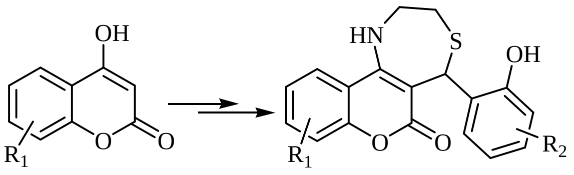
Thiazepinones, benzothiazepines and other thiazepine derivatives are moieties whose biological activity has received much attention [1].

Benzothiazepines and Coumarin derivatives play a unique role in drug discovery programs, as they display a wide spectrum of biological activities such as antibacterial, antifeedant [2], analgesic [3] and calcium antagonism [4]. Therefore, both the coumarins and the thiazepins possess worthy and imperative bioactivities, which render them useful substances in drug research.

In view of these observations and in continuation of our research program on the synthesis of heterocyclic compounds, we report herein the synthesis of some new thiazepin analogues fused with coumarin derivatives in two step, which have been found to possess an interesting profile of cytotoxic activities.



R_1=H, OH
R_2=H, 3-OMe, 5-OMe, 5-Br

References:

[1] (a) Strzelczyk, M.; Matyjewska, H.; Strozynski, H. Pol. *J. Pharmacol. Pharm.* **1990**, *42*, 377; (b) Ueyama, N.; Wakabayashi, S.; Tomiyama, T. Yakugaku Zasshi **1996**, *116*, 106.
[2] Reddy, R. J.; Ashok, D.; Sarma, P.N. *Indian J. Chem.* 32B **1993**, 404. Raev, L.; Voinov, E.; Ivanov, I.; Popov, D. **1990**, *Antitumor activity of some coumarin derivatives, Pharmazie*, 45: 696.; *Chem. Abstr.* **1990**, 114, 74711 B.
[3] K. Satyanarayanan, M.N. Rao, *Indian J. Pharm. Sci.* **1993**, *55*, 230.
[4] M. Chaffman, R.N. *Brogden, Drugs* **1985,** *29*, 387.

The first report on preparation of siloxane containing poly(amide-imids) in the presence of ionic liquids as green media under microwave heating

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A main driving force of synthetic organic chemistry is the sustainable development of efficient and cleaner technologies to decrease the consumption of traditional toxic and volatile organic solvents (VOCs) in academic and industrial laboratories. The exploit of ionic liquids (ILs) as reaction media to synthesize various polymers has been explored in recent years [1]. Microwave heating has been shown to dramatically reduce reaction times, increase product yields, and enhance product purities by reducing unwanted side reactions compared to conventional heating methods [2]. ILs are outstanding microwave-absorbing agents owing to their high ionic conductivity and polarizability; so, combining the properties of ILs with microwave heating should afford a rapid and eco-friendly technique for the production of polymers. The advantages associated with the green solvent aspect of ILs and the green chemistry aspect of microwave irradiation have been very recently accentuated in highly improved methods for polymer synthesis [3]

In this paper, we wish to report a convenient, cost effective and environmentally benign green chemical method for the synthesis of poly(amide-imide-siloxane)s (PAIS)s by using tetrabutyl ammonium bromide (TBAB), and phosphonium bromide, under microwave irradiation condition. In this paper a new class of poly(amide-imide-siloxane)s (PAIS)s was synthesized via direct polycondensation reaction of a diacid incorporating siloxane and imide moiety with 4,4’-methylene-bis(4-phenylisocyanate) affording amide linkage via isocyanate route. The resulting polymers have inherent viscosities in the range of 0.16–0.29 dL/g. These polymers are crystalline and thermally stable. The presence of siloxane linkage in poly(amide-imide) backbone lead to improved solubility while maintaining good thermal properties. Decomposition temperatures for 5% weight loss (T5) occurred above 220 ^{o}C by TGA. Some structural characterization and physical properties of these new PAIs are reported. This environmentally-friendly green technique is a fast, high yielding and simple manipulation route, which avoids the usage of volatile organic solvents and catalyst.

References:

[1] Minami, H.; Yoshida, K.; Okubo, M. *J. Macromol. Rapid Commun*. **2008**, *29*, 567.
[2] Zhang, C.; Liao, L.; Gong, S. *J. Green Chem*. **2007**, *9*, 303.
[3] Mallakpour, S.; Taghavi, M. *Polymer*. **2008**, *49*, 3239.

Modification of Cloisite Na$^+$ using natural amino acids: Synthesis and characterization of novel organo-bionanoclays

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Nanohybrid materials prepared by the nanoscale inclusion of organic moieties into the interlayer spaces of layered inorganic hosts have received great attention in the past decade. Among these nanohybrid materials, organo-clays constitute a versatile area of investigation, which is due in particular to the availability of natural clay minerals and their ability to incorporate a large variety of functional molecules [1]. Layered silicate montmorillonites have been the inorganic material of choice because of their easy swelling in water, thus allowing subsequent surface modifications with alkyl ammonium ions [2]. In the pristine state, these montmorillonite platelets are held together by electrostatic interactions, thus leaving an interlayer between them. The modification at the polar surfaces reduces the surface energy of the platelets and renders them organophilic and partially polar, thus helping to disperse them in the polymer matrices. The modifiers used are generally long carbon chain compounds with an alkylammonium or alkylphosphonium cation [3]. Positively charged amino acids have a similarity in chemical structure with conventional modifiers with alkylammonium cations. In this work, ammonium salt of different natural amino acids was used for modification of Cloisite Na$^+$.

The intercalated materials were characterized by X-ray diffraction (XRD), thermogravimetric analysis (TGA), fourier transform infrared spectroscopy, dispersibility measurement and scanning electron microscopy and transmission electron microscopy methods. According to the XRD results the intercalation was successful as the increased basal spacing attested. TGA characterization and analysis show that the amount of organic modifier in the organo-modified clays is in good agreement with theoretically calculated stoichiometric content expected for approximately complete exchange of Na$^+$ ions by organic cations. In this method, use of volatile and toxic common organic compound will be eliminate and provide a technology which will be environmentally benign process for the synthesis of bionanocomposites in future.

References:

[1] *Handbook of Layered Materials*; Aucherbach, S.; Carrado, KA.; Dutta, P. Eds.; Marcel Dekker: New York, **2004**.
[2] Tonli, IK, Letaief, S.; Ngameni, E.; Detellier, C. J. *Mater. Chem.* **2009,** *19*, 5996.
[3] Mehta, GK.; Mark, J.; Lee, JW.; Kotov, N.; Linderman, JJ.; Takayama, S. *Adv. Funct. Mater.* **2007**, *17*, 2701.

The study of cleavage of *α,β*-epoxybis(silanes) with $LiAlH_4$

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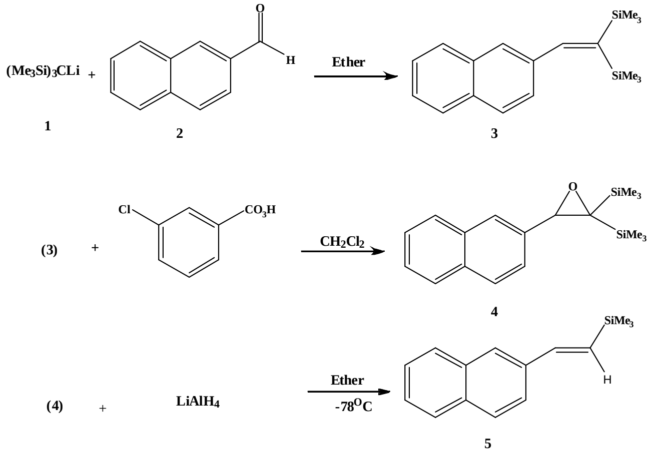
α,β-epoxybis(silanes) react with a wide variety of reagents via ring opening *α* to silicon. These reactions have been found to have a variety of uses in organic synthesis. Vinylbis(silanes) are important synthetic intermediates in stereocontrolled organic synthesis. One of the synthetically most useful transformations of vinylbis(silanes) is epoxidation. The Peterson olefination reaction of naphthaldehyde (2) with tris(trimethylsilyl)methyllithium, $(Me_3Si)_3CLi$ (1), in Et_2O gives disubstituted vinylbis(silane) (3) which reacts with MCPBA in CH_2Cl_2 at r.t. to afford disubstituted epoxybis(silane) (4).

The treatment of the resulting epoxybis(silane) with $LiAlH_4$ gives corresponding vinylsilane(5). It has been reported that the reaction of epoxybis(silane) with $LiAlH_4$ gave the *β*-hydroxybis(silane) without any formation of vinylsilane by Peterson-type reaction. However, in the case of epoxybis(silane)(4), Peterson-type olefination was found to take place after or concurrently with the addition of $LiAlH_4$, to give the corresponding vinylsilane(5) stereoselectively.



References:

[1] Hudrlik, P.F.; Agwaramgbo, E. L. 0. and Hudrlik, A. M. *J. Org. Chem.* **1989,** *54*, 5613.

[2] Safa, K.D.; Ghorbanpour, Kh.; Hassanpour, A.; Tofangdarzadeh, Sh. *J. Organomet. Chem.* **2009**, *694*, 1907.

[3] Safa, K.D.; Paymard Samani, S.; Tofangdarzadeh, Sh.; Hassanpour, A. *J. Organomet. Chem.* **2008,** *693*, 2004.

Synthesis of spiro [indene-2, 3′-pyrrolo [2, 1-a] isoquinoline]-1, 3-diones through 1, 3-dipolar cycloaddition reaction

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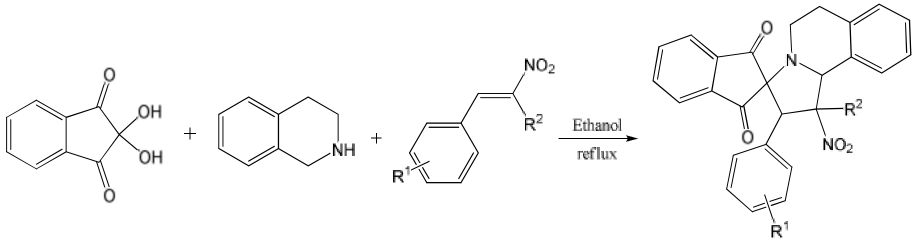
1,3-dipolar cycloaddition reactions are fundamental processes in organic chemistry, and have taken a prominent place as a synthetic strategy for the construction of a variety of five-membered heterocycles [1].

Azomethine ylides are a class of powerful reagents to utilize in the 1,3-dipolar cycloaddition reactions which generally afford arrange of pharmacologically important heterocyclic compounds [2]. Spiropyrrolidines and spiro pyrrolizidines have gained much attention in recent years due to their interesting biological activity [3].

Herein we describe a rapid, mild and efficient synthesis for spiroheterocycles which proceeds by the 1,3-dipolar cycloaddition reaction of ninhydrin, 1,2,3,4-tetrahydroisoquinoline and various derivatives of β-nitrostyrene in ethanol.



Identification of the products was carried out by spectroscopic methods.

References:

[1] Shanmugam, P.; Viswambharan, B.; Madhavan, S. *Org. Lett.* **2007**, *9*, 4095.
[2] Jayashankaran, J.; Manian, R. D.; Venkatesan, R.; Raghunathan, R. *Tetrahedron*. **2005**, 61, 5595.
[3] Poornachandran. M.; Raghunathan, R. *Tetrahedron*. **2006**, *62*, 11274.

Reaction of *N*-alkyl-3-chloroquinoxaline-2-amines with propargyl alcohol: An efficient synthesis of *N*-substituted pyrrolo[2,3-*b*]quinoxaline-2-carbaldehydes

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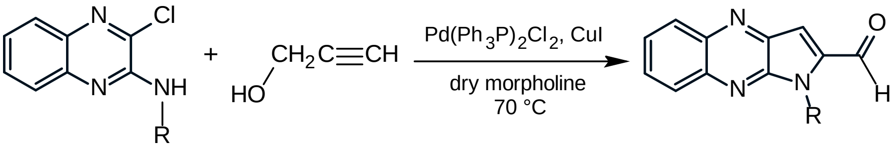
Quinoxalines and their derivatives are very important class of nitrogen containing heterocycles and show various biological activities such as anti-viral, anti-bacterial, anti-biotic, anti-inflammatory and kinase inhibitor properties [1].

In continuation of our recent studies on the Pd-catalyzed reaction of acetylenes leading to heterocyclic compounds, specially pyrrolo[2,3-*b*]quinoxalines [2], we became interested to consider the reaction of *N*-alkyl-3-chloroquinoxaline-2-amines **1a-h** with propargyl alcohol **2** in organic solvents.

When compounds **1a-h** were reacted with propargyl alcohol **2** in dry morpholine in the presence of $Pd(PPh_3)_2Cl_2$ and CuI iodide at 70 ºC, *N*-substituted pyrrolo[2,3-*b*]quinoxaline-2-carbaldehydes **3a–h** were obtained in moderate to good yields. The reactions were carried out under an argon atmosphere, and solvents were degassed prior to use.



1a-h **2** **3a-h**

R = Bn, Me, *n*-Pr, *i*-Pr, *i*-Bu, *n*-Bu, Et, $MeOCH_2CH_2$

References:

[1] Kim, Y. B.; Kim, Y. H.; Park, J. Y.; Kim, S. K. *Bioorg. Med. Chem. Lett.* **2004**, *14*, 541.
[2] Keivanloo, A.; Bakherad, M.; Rahimi, A.; Taheri, S.,A., N. *Tetrahedron Lett.* **2010**, *51*, 2409.

Investigation of some antranilic acid derivatives as excellent cadmium chelators

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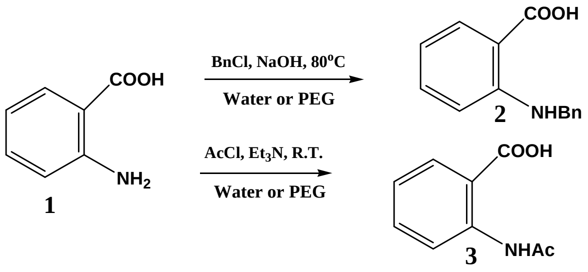
In Pharmaceutical approach, good antidotes against heavy metals are good bidental chelators that react with poisons to give a stable complex with them [1].

Based on this logic we have already introduced different phenylthiopolyoles as potentially good antidote drugs as we reported earlier [2]. We had also introduced some antranilic acids derivatives as potentially good opaque drugs by some theoretical calculations. Later we used some antranilic acid derivatives for removing lead ions without any external base addition [3].

By considering this fact that antranilic acid has been reacted as a good bidental ligand with Pb^{2+}, we synthesized some antranilic acid derivatives in green conditions. We used water or PEG as solvent. Then we treated them with some Cd^{2+} as poison. Our results show that a very strong complex created by both N-benzyl **(2)** and N-acyl **(3)** derivatives of antranilic acid. Where for some other ions we needed to a base to remove H^+ as driving force, in the case of Cd^{2+} no base was necessary. This fact shows that there is a strong complexation between Cd^{2+} (as Pb^{2+}) and **2**, **3** and based on pharmaceutical approach, they would be good antidote drugs for lead removing.



References:

[1] Catzung, Pharmakology, Translated by N. Ghotbi and E. Esfandiary, Arjomand Pob., 1374.
[2] A. Amoozadeh, *et al.* The 4th National Biotechnology Congress, 15-17 August 2005, International Center for Science and high Technology and Environmental Science, Kerman. p. 43.
[3] A. Amoozadeh, *et al.* 6th Iranian Biophysical Chemistry Conference, 27-29 Aug. 2008, Razi University of Kermanshah, p.78.

Three-component reaction of trimethylphosphit, benzaldehyde, and glycine: An efficient one-pot synthesis of phosphonato esters

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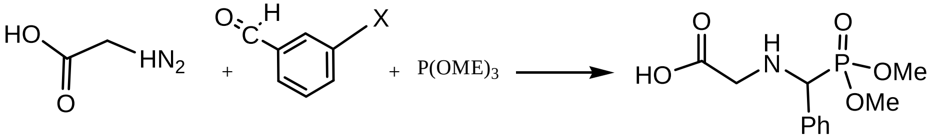
In recent years, there has been an increasing interestin the synthesis of organophosphorus compound.This interest has resulted from the recognition of the value of such compounds in a wide range of industrial,biological, and chemical synthetic aspects.

In this study phosphonato esters were obtained in excellent yields from the 1:1:1addition reaction between benzaldehyde **2**, glycine **1** in the presence of thrimethylphosphite **3** leads to posphonato esters. These reactions proceeded smoothly at ambient temperature and are completed within 24 h in high yield. TLC and 1H NMR spectra of the crude products clearly indicated formation of phosphonate esters **4** (see Scheme 1).The essential structures of the products **4a–c** were deduced from elemental analysis, IR, 1H, 13C, 31P NMR, and mass spectra.



(Scheme 1)

Entry	Product	X	Yield %
A	4a	H	87%
B	4b	OMe	90%
C	4c	NO2	93%
D	4d	Cl	92%

References:

[1] Maghsoodlou , M. T., Rostami Charati, F., Habibi Khorassani, S. M., Ghasemzadeh, Makha, M. *Chem Res* **2008**, 55.

[2] Rostami Charati, F, Maghsoodlou , M. T, Habibi Khorassani, S. M, Makha, M, *Tetrahedron Lett* **2008,** *49,* 343.

Metaborosulsuric acid catalyzed highly efficient alkylation of 1,3-dicarbonyl compounds with benzylic alcohols

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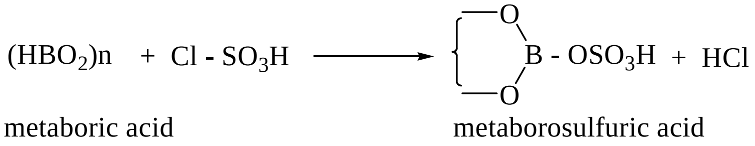
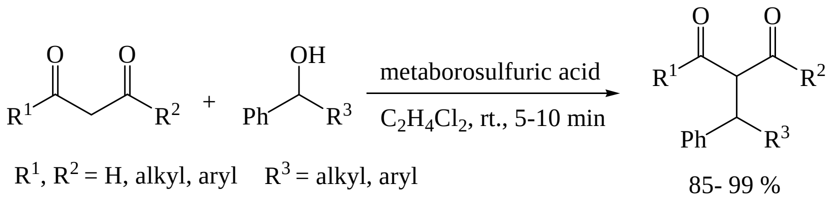
The alkylation of 1,3-dicarbonyl compounds usually requires not only the transformation of 1,3-dicarbonyl compounds into more reactive species, such as enolates by reacting the 1,3-dicarbonyl compounds with base, but also the use of alkyl halides, since the hydroxyl group is not a good leaving group and 1,3-dicarbonyl compounds do not have high nucleophilicity.

Therefore, the development of a practical and economical process for carbon–carbon bond formation between active methylene compounds and unmodified substrates is an important task. In this regard, carbon–carbon single bond formation between an active methylene compound with an alcohol would be an attractive salt-free and atom-economic process with water being the only by-product.

Herein, we report a new Bronsted acid catalyzed alkylation of 1,3-dicarbonyl compounds under mild reaction conditions at room temperature that proceeded in good to excellent yields. The present protocol is applicable to a variety of 1,3-dicarbonyl compounds and benzylic alcohols. However, little has been explored on direct carbon–carbon bond formation using alcohols [2-3].





References:
[1] Ma, S.; Yu,S.; Peng, Z.; Guo, H. *J. Org. Chem.* **2006**, *71*, 9865.
[2] Bisaro, F.; Pretat, G.; Vitale, M.; Poli, G. *Synlett*. **2002**, 1823.
[3] Yasuda, M.; Somyo, T.; Baba, A. *Angew. Chem.* **2006**, *45*, 793.

Silica gel promotes cascade synthesis of 2-(heteroaryl)acetamide derivatives from isocyanides, dialkylamines and heteroarylcarbaldehydes

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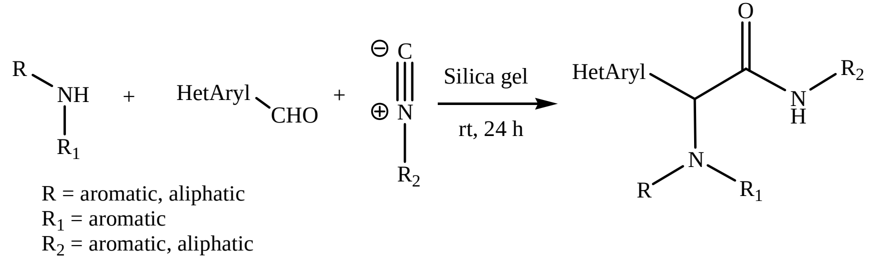
The ability of an isonitrile to undergo easy R-addition with a nucleophile and an electrophile under mild conditions has made them popular reactants for the development of novel MCRs. Isocyanides, regarded for many years as compounds with unpleasant odor and with very few chemical and pharmaceutical applications, are now looked upon as useful synthons, attributed primarily to the renaissance of the isocyanide based multicomponent for Passerini three-component (P-3CR) and more importantly the Ugi four-component reaction (U-4CR) [1,2]. As part of our ongoing program to develop efficient and robust methods for the preparation of organic compounds [1,2], we sought to develop an efficient route for the one-pot synthesis of sterically congested 2-(heteroaryl)acetamide derivatives from simple and readily available isocyanides, heteroarylcarbaldehydes and secondary amines in the presence of silica gel at ambient temperature.

In the absence of silica gel, the yields were only *ca.* 15% at room temperature after 24 hours and in each case several by-products were observed. The structures of the products were deduced from their IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. In summary, we have found a new and efficient method for the synthesis of sterically congested 2-(heteroaryl)acetamide derivatives. We believe the reported method offers a simple and efficient route for the preparation of the 2-(heteroaryl)acetamide derivatives. Its ease of work-up and the acceptable yields make it a useful method.



References:

[1] Ramazani, A.; Rezaei, A. *Org Lett*. **2010**, *12*, 2852.
[2] Ramazani, A.; Mahyari, T. M.; Rouhani, M.; Rezaei, A. *Tetrahedron Lett.* **2009**, *50*, 5625.
[3] Souldozi, A.; Ramazani, A. *Tetrahedron Lett.*, **2007**, *48*, 1549.
[4] Kazemizadeh, A. R.; Ramazani, A. *J. Braz. Chem. Soc*. **2009**, *20*, 309.

Heck coupling reaction using dimeric orthopalladate complex of homoveratrylamine in ionic liquid

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Cyclopalladated complexes are important starting materials in organometallic chemistry. Palladacycles have acquired great interest due to their applications in many areas including organic synthesis in carbon-carbon bond formation, material science and as biologically active compounds [1]. One of the most efficient methods in the formation of $C_{(sp^2)}$-$C_{(sp^2)}$ bond entitled Heck reaction in which a palladium catalysed reaction is carried out between an olefin and an aryl or alkenyl halide in the presence of a base. Cyclopalladated complexes allowed the Heck reaction to be performed with activated and non-activated aryl halides using very low amount of catalyst [2]. The use of ionic liquids as reactions medium may offer a convenient solution to both the solvent emission and catalytic recycling problem. Ionic liquids containing imidazolium cations can be used as powerful media in some catalytic organic reactions not only for the facilitation of catalyst recovery but also for the acceleration of the reaction rate and improvement of selectivity [3].The Heck reaction has been studied extensively in ionic liquids, where Pd^{II} complexes or Pd^0 nanoparticles act as catalysts [4].

The $[Pd\{C_6H_2(CH_2CH_2NH_2)\text{-}(OMe)_2,3,4\}\ (\mu\text{-}Br)]_2$ complex had been demonstrated to be active and efficient catalyst for the Heck reaction of aryl iodides, bromides and even chlorides in ionic liquid. The cross-coupled products were produced in excellent yields in a short reaction time using catalytic amounts of complex at 130 °C in 1-butyl-methyl imidazolium chloride.

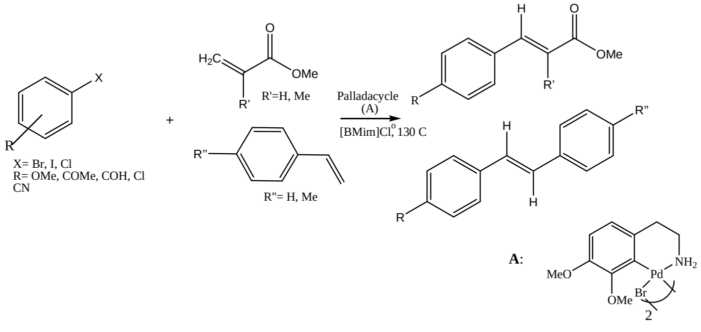

Figure 1

References:

[1] Hajipour, A. R.; Karami, K.; Pirisedigh, A. *Appl. Organometal. Chem.* **2009,** *23*, 504.

[2] Hajipour, A. R.; Karami, K.; Pirisedigh, A.; Ruoho, A. E. *Organomet. Chem*. **2009**, *694,* 2548.

[3] Hajipour, A. R.; Rafiee, F. *J. Iran. Chem. Soc.* **2009**, 6, 647.

[4] Consorti, C. S.; Flores, F. R..; Dupont, J. *J. Am. Chem. Soc*. **2005**, *127,* 12054.

Synthesis of a new thiazole and thiazolidin-4-one derivatives with use of monothiosemicarbazone derivatives of 1, 3-bicarbonyl compounds

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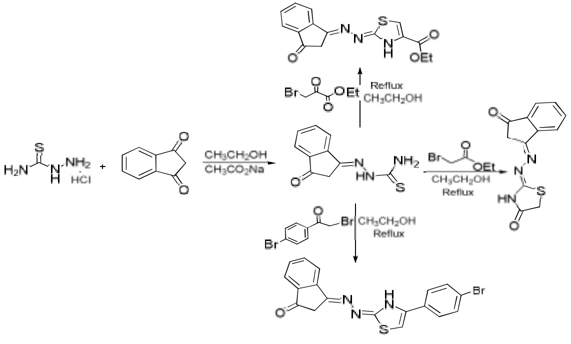
Thiazole and its derivatives are very useful compounds in various fields of chemistry including medicine and agriculture. For example, the thiazolium ring present in vitamin B1 serves as an electron sink, and its coenzyme form is important for the decarboxylation of a-keto acids.[1] this heterocyclic system has found broad application in drug development for the treatment of inflammation [1], hypertension,bacterial [2],and HIV infections.Thiazoles are also synthetic intermediates and common substructures in numerous biologically active compounds. Thus the thiazole nucleus has been much studied in the field of organic and medicinal chemistry. In this investigation first we synthesis a series of monothiosemicarbazone derivatives of 1,3-bicarbonyl compounds as a intermediate, then these compounds are used for synthesis of thiazole and thiazolidin-4-one derivatives in ethanol as a solvent. The results of ^{1}H NMR, ^{13}C NMR, FT-IR and UV spectra confirmed the formation of these products.



References:

[1] Haviv, F.; Ratajczyk, J. D.; DeNet, R. W.; Kerdesky, F. A.; Walters, R. L.; Schmidt, S. P.; Holms, J. H.; Young, P. R.; Carter, G. W. *J. Med. Chem*. **1988**, *31*, 1719.

[2] Tsuji, K.; Ishikawa, H. *Bioorg. Med. Chem. Lett*. **1994**, *4*, 1601

Substituent effect in photocatalytic dehydrogenation of 2-oxo-1,2,3,4-tetrahydropyrimidines using nano-TiO_2

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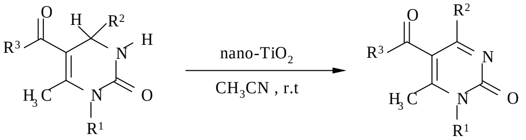
2-Oxo-1,2,3,4-tetrahydropyrimidines (THPMs) are an important classes of compounds which possess wide spectral pharmacological properties [1]. Oxidation of THPMs are important because of formation of core 2-oxo-1,2-dihydropyrimidines which are important for the pharmacological activity such as pyrimidine MKS-442 one of the most important classes of drugs for the treatment of the HIV virus [2].

Recently, we have reported thermal oxidation of THPMs by potassium peroxydisulfate under various experimental conditions [3] or by UV irradiation [4]. In contrast to the proposed radical mechanism for the thermal oxidation, an electron-transfer induced photooxidation is proposed in chloroform solution.

TiO_2 a well-known photocatalyst has been used as an electron-acceptor species for various organic transformations [5].

In continuation to our previous studies, we were interested to investigate the effect of the nature of the substituents on 1-, 4-, and 5-positions of THPM ring on the electron donating ability of these compounds towards excited nano-TiO_2. The results will be presented.



References:

[1] Kappe, C. O. *Eur. J. Med. Chem*. **2000** *35*, 1043.
[5] Zhou, W.; Gumina, G.; Chong, Y.; Wang, J.; Schinazi, R. F.; Chu, C. K. *J. Med. Chem*. **2004**, *47*, 3399.
[2] Memarian, H. R.; Farhadi, A.; Sabzyan, H. *Ultrason. Sonochem.* **2010**, *17*, 579 and references cited therein.
[3] Memarian, H. R.; Farhadi, A.; Sabzyan, H.; Soleymani, M. *J. Photochem. Photobiol. A.* **2010**, *209*, 95 and references cited therein.
[4] Yogo, K.; Ishikawa, M. *Catal. Surv. Jpn*. **2000**, *4*, 83.

Syntesise some fluorinated thiazolopyridine derivatives from pentafluoropyridine

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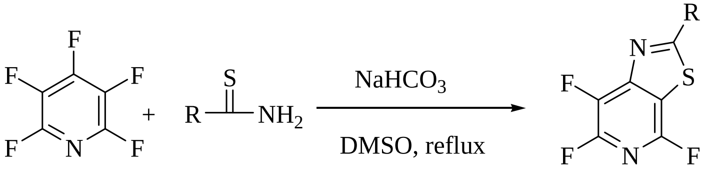
Thiazolopyridines have been reported to furnish various biological activities such as antimicrobial, bactericidal, coronary dilating, antihypertensive and muscle relaxing [1]. In addition, bis-heterocyclic compounds exhibit various biological activities and exert much higher antibacterial activity than heterocyclic compounds [2]. Pentafluoropyridine has attracted considerable interest due to its synthetic utility. Various construction of new heterocyclic and macrocyclic systems could be accessed from simple reaction conditions. These include reaction of various bifunctional nucleophiles with pentafluoropyridine. All five fluorine atoms in pentafluoropyridine may be substituted by an appropriate nucleophile due to its highly electron efficient aromatic ring system [3].

In view of the above facts and in continuation of our work on the preparation of fluorinated heterocyclic and macrocyclic compounds from pentafluoropyridine [4], we report here the synthesis of some novel fluorinated thiazolopyridine starting from pentafluoropyridine.

Annelation processes involving the reaction between pentafluoropyridine and some thioamide derivatives in the presence of sodium bicarbonate and also in DMSO solution were studied (Table 1). Thioamide derivatives reacted efficiently with pentafluoropyridine to give 4,6,7-trifluoro-2-substituted-thiazolo[5,4-c]pyridine systems by substitution at the 4-position of the pyridine ring followed by intermolecular ring closure at the geometrically accessible 3-position.



References:

[1] Shiba, S. A.; El-Khamry, A. A.; Shaban, M. E.; Atia, K. S. *Pharmazie*, **1997**, *52*, 189.
[2] Holla, B. S.; Gonsalves, R.; Shenay, S. *Eur. J. Med. Chem.* **2000**, *35*, 267.
[3] Amii, H.; Uneyama, K. *Chem. Rev.* **2009**, *109*, 2119.
[4] Ranjbar-Karimi, R.; Mousavi,M. *J. Fluorine Chem.* **2010**, *131*, 587.

One-pot reductive mono-*N*-alkylation of aniline and nitroarene derivatives using aldehydes

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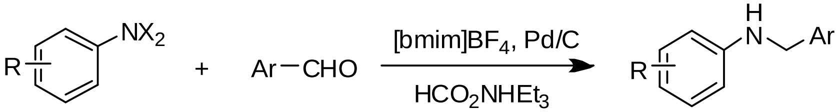
Amines and their derivatives are highly versatile building blocks for various organic substrates and are essential precursors to a variety of biologically active compounds. Amines also serve other purposes in the fields of bioorganic, industrial, and synthetic organic chemistry. With this growing repertoire of applications, developing efficient methods for the synthesis of amines draws much attention. The reductive amination reaction remains one of the most powerful and widely utilized transformations that allow the direct conversion of carbonyl compounds into amines using simple operations [1].

Additionally, one-pot transformations are economically and ecologically highly intriguing for developing efficient new synthetic processes in a domino fashion, generating a suitable reactive functionality en route [2].

Herein, we report an efficient, facile, mild, and environmentally benign one-pot reductive mono-*N*-alkylation of aniline and nitroarene derivatives using aldehydes by Pd/C catalyst in [bmim][BF4] ionic liquid as the solvent with triehtylammonium formate as the in situ hydrogen donor. After completion of the reactions and separation of the products, the ionic liquid is recovered and successfully reused in the next reactions.



X= H, O

Reference:

[1] Sydnes, M. O.; Kuse, M.; Isobe, M. *Tetrahedron*, **2008**, *64*, 6406.
[2] Byun, E.; Hong, B.; De Castro, K. A.; Lim, M.; Rhee, H. *J. Org. Chem.*, **2007**, *72,* 9815.

α-Bromination of arylcyclohexyl ketone and oxidation-bromination of corresponding phenyl alcohol

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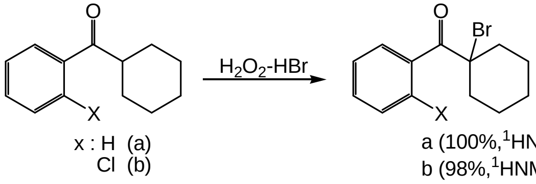
α-Bromination of carbonyl compounds is an important reaction in organic synthesis as the resulting α-bromo-ketones are used in the synthesis of variety of organic compounds. A number of various bromination protocols of carbonyl compounds have been developed, including the used of molecular bromine in the presence protic or lewis acid [1], N-bromosuccinimide (NBS) with natural catalyst [2], tetralkylammonium tribromides [3] and aqueous H_2O_2-HBr [4]. The use of molecular bromine has several drawbacks arising out of its hazardous nature, difficult handing, low atom efficiency and the formation of HBr as a by-product. We examined various bromination reagents under different reaction conditions for bromination of cyclohexyl phenyl ketones, a and b, to obtain the corresponding α-bromocyclohexyl phenyl ketones in high yield. The best yield was obtained when H_2O_2-HBr was used at room temperature in 2:1 H_2O_2 to HBr molar ratio in the absence of solvent for 30h.(eq. 1). Then, the same aqueous H_2O_2-HBr system was used for a tandem oxidation-bromination of alcohol (c) to prepare α-bromo-ketone (d) in high yield (eq. 2).



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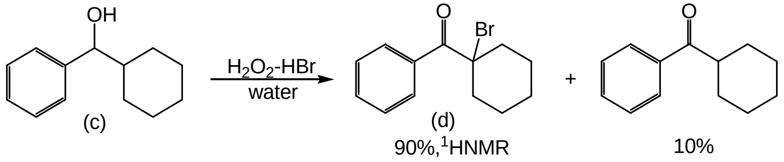

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References:

[1] Garbisch., E. W. *J. Org. Chem*. **1965**, 30, 2109.

[2] Tanemura, K. Suzuki, T. Nishida, Y. Satsumabayashia, K. Horaguchi., T. *Chem Commun*. **2004**, 470.

[3] Kavala, V. Naik, S. Patel., B. K. *J. Org. Chem*. **2005**, 70, 6556.

[4] Podgorsek, A. Stavber, S. Zupanab, M. Iskra., J. *Green Chem*. **2007**, 9, 121.

Ultrasound-promoted regio and chemoselective synthesis of pyridazinones and phthalazinones

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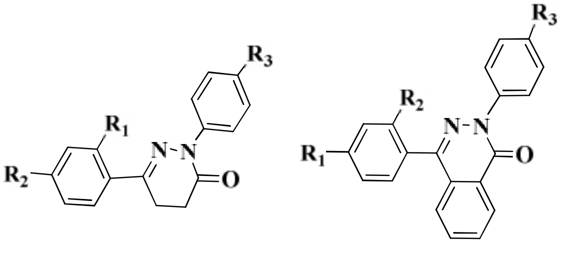
Pyridazinones are useful compounds with a broad array of biologically activities. They possessed notable, platelet aggregation inhibiter, phosphodiesterase, antiasthmatic, anticsecretory and antiulcer , antidepressant, antibacterial, antifongic, α-adrenoceptor antagonists, analgesic, antiinflammatory anticancer, pesticidal and herbicidal properties[1].

Previously reported synthetic routes to synthesis of pyridazinones includes reaction of γ-ketoacids and their derivatives with alkylhydrazines or phenyl-hydrazines, condensation of wittig reagents with arylhydrazones or condensation of α-ketoesters with hydrazinocarbonyl-acetic acid esters, catalytic reactions of alkynes with arylhydrazines (hydrohydrazination), condensation of hydrazine with appropriate substituted lactones.

Our continued interest in the development of efficient and environmentally friendly procedure for the synthesis of pharmaceutical compound [1,2] and removing the disadvantages involved in the previous methods for the synthesis of these compounds promoted us to evaluate the ultrasound assisted multicomponent synthesis of pyridazinones and phthalazinones from Arene, cyclic anhydride and Arylhydrazine.



References:

[1] Betti, L., Floridi, M.; Giannacini,G.; Manetti, F.; Strappaghetti, G. ; Tafi, A. ; Botta, M. *Bioorg. Med. Chem. Lett.* **2003**,*13*, 171
[2] Mahmoodi, N.O., Tabatabaeian, K., Kosari, M., Zarrabi, S, *Chin. Chem. Lett*. **2008**,*12*, 1431.
[3] Kiyani, H.; Mahmoodi, N. O.; Tabatabaeian, K.; Zanjanchi, M. A. *Mendeleev Commun.*, **2009**, *19*, 203.

Reaction between naphthalene diole derivativs and acetylenic esters the presence of triphenylphosphine

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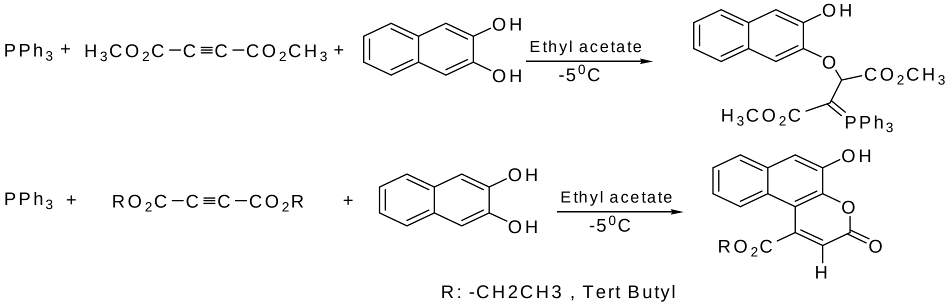
Protonation of the reactive 1;1 intermediate produced in the reaction between triphenylphosphine and acetylenic esters by naphthalene diole derivatives leads to vinyl triphenylphosphonium salt , which undergoe Michael addition with the conjugate base to produce highly functionalized 2-oxo-2H-chromene derivatives in good yields [1,2,3]. The reaction of 2,3-naphthalene diole with DMAD in the presence of PPh3 leads to stable dimethyl-2-(3-hydroxynaphtyl)-3-(1, 1, 1-triphenyl- **λ^5**-phosphanylidene)-succinate and the reaction of 2,3-naphthalene diole with DEADand DTAD, in the presence of PPh$_3$ leads to stable alkyl 5-hydroxy-3-oxo-3H-benzo[f]chromene-1-carboxylate.



References:

[1] Yavari, I .; Adib ,M .; Hojabri ,L .; *Tetrahedron*, **2001** , 57 ,7537.
[2] Ramazani, A.; Soldozi .;A.; *phosphorus and silicon*, **2003** ,178 ,1329.
[3] Soldozi, A.; Ramazani ,A .; Noshiranzadeh ,N.; *phosphorus and silicon* ,**2006**, 181, 587.

Novel and efficient catalysts for the one-pot synthesisof 4H-pyran derivatives

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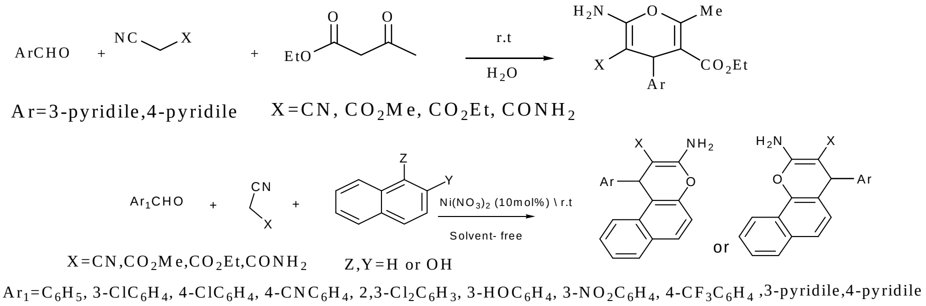
The 4H-pyran derivatives are important structural component of many naturally occurring compounds. A particularly interesting group of 4H-pyrans are 2-amino-4*H*-chromenes since they are used as cosmetics and pigments, spasmolytic, diuretic, anticoagulant, antianaphylactic, antibacterial , anticancer agents and as potent apoptosis inducers[1]. Development of 4-Hpyrans synthesis has been of considerable interest in organic synthesis, because of their wide biological and pharmaceutical activities.

The combination of solvent-free and MCR reactions represents a very powerful method from both economical and synthetic points of view since the isolation of the intermediates is skipped, the overall reaction time is significantly decreased, higher yields of products are obtained, and due to less use of solvent and reagents the costs are lowered. For these reasons and in our continuing we report herein our results for the synthesis of 2-amino-4*H*-chromene using $Ni(NO_3)_2$ as an efficient catalyst for the three-component solvent-free condensation of an aldehyde, malononitrile and an activated phenol with excellent yield and we wish to disclose a green protocol for the synthesis of a variety of biologically important 4H-pyrans .



References:

[1] Yavari, I.; Djahaniani, H.; Nasiri,F. *Tetrahedron Lett.* **2003**, 59, 9409.
[2] Peng, Y.; Song, G. *Catal Commun* . **2007**, 111, 114.
[3] Abdolmohammadi, S.; Balalaie, S. *Tetrahedron Lett.* **2007**, 48, 3299.

Versatile conversion of alcohols into alky formates and trimethylsilyl ethers catalyzed by polyvinylpolypyrrolidonium tribromide (PVP-Br_3)

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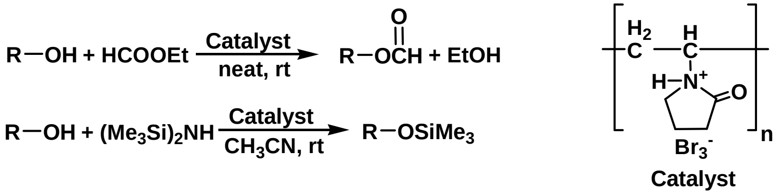
In the last few years, supported reagents on the organic polymers have become increasingly used in organic functional group transformations [1]. Protection and deprotection of functional groups are indispensable in gradients of the synthesis of poly functional compounds. Silyl ethers are the most popular and useful protecting groups of the hydroxy function in synthetic organic chemistry and various types of silyl ethers have been developed [2]. Also the formylation of hydroxyl group is one of the most widely use transformation in organic synthesis. Formylation of alcohols is an important transformation in organic synthesis and provides an efficient method for the protection of OH groups. A variety of catalysts and reagents have been developed for the trimethylsilylation and formylation of alcohols, which include mainly protic acids, Lewis acids, heterogeneous catalysts and others [3-4].

In continuation of our studies on the organic transformation [5-6], we were interested to find an appropriate catalytic system for the formylation and trimethylsilylation of alcohols under nearly neutral conditions. Herein we report a mild and efficient method for trimethylsilylation and formylation of alcohols using 1,1,1,3,3,3-hexamethyldisilazane and ethyl formate in the presence of catalytic amounts of phenyltrimethylammonium tribromide (PVP-Br_3), as a neutral and heterogeneous catalyst at room temperature (Scheme 1).



Scheme 1

References:

[1] Ghorbani-Choghamarani, A.; Chenani, Z.; Mallakpour, S. *Synth. Commun.* **2009**, *39*, 4264.
[2] Suzuki, T.; Watahiki, T.; Oriyama, T. *Tetrahedron Lett.* **2000**, *41*, 8903.
[3] Upadhya, T.T.; Daniel, T.; Sudalai, A.; Ravindranathan, T.; Sabu, K.R. *Synth. Commun.* **1996**, *26*, 4539.
[4] Niknam, K.; Zolfigol, M. A.; Saberi, D.; Khonbazi, M. *Chin. J. Chem.* **2009**, *27*, 1548.
[5] Ghorbani-Choghamarani, A.; Zeinivand, J. *J. Iran. Chem. Soc.* **2010**, *7*, 190.
[6] Ghorbani-Choghamarani, A.; Rezaei, S. *J. Chin. Chem. Soc.* **2009**, *56*, 251.

The influence of carbon nanotube and montmorillonite (MMT) on thermal degradation and mechanical properties of poly(vinyl butyral)(PVB)

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Poly(vinyl butyral) (PVB) is a sturdy and flexible polymer. Especially, it is known for its high impact strength at low temperatures. Furthermore, PVB has excellent properties with many materials such as glass, metal, plastics and wood. Thus, PVB is widely used as paint, adhesive agent, printing paste and a film sandwiched in a safety glass for automobiles [1].

Dispersion at a nanoscale of MMT clays in polymers is well-known to enhance the mechanical, barrier, flammability properties as well as the thermal stability of the polymer matrix, even at low loadings [2-3]. Because of the platelet like structure of this kind of nanofiller, significant effects can be also observed if good exfoliation and dispersion of the filler in the matrix are ensured. Carbon nanotubes possess high flexibility, low mass density and large aspect ratio [4]. CNT have a unique combination of mechanical, electrical, and thermal properties that make nanotubes excellent candidates to substitute or complement the conventional nanofillers in the fabrication of multifunctional polymer nanocomposites.

In this work, at first CNT/MMT/ PVB nanocomposites were prepared. Then, Characterization of these new materials was performed by scanning electron microscopy (SEM). Also, thermal gravimetric analysis (TGA) and tensile tester were used for thermal and mechanical properties.

References:

[1] Blomstrom, T. P.; Kroschwitz, J. I. *Concise encyclopedia of polymer science and engineering*. New York, Wiley, **1990**, 270.
[2] Okada, A.; Usuki, A. *Macromol. Mater. Eng.* **2007**, *291*, 1449-1476.
[3] Utracki, LA.; Sephr, M.; Boccaleri, E. *Polym. Adv. Technol.* **2007**, *18,* 1-37.
[4] Cooper, C. A.; Young, R. J.; Halsall, M. *Composites, Part A.* **2001**, *32*, 401-411.

PPA-SiO_2: A mild, efficient and reusable catalyst for the synthesis of 1,5-benzodiazepines

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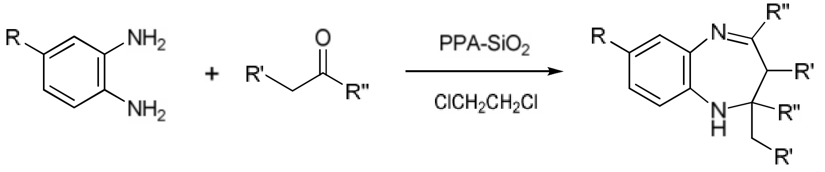
Benzodiazepines are an important class of bioactive molecules, widely used as anticonvulsant, antianxiety and hypnotic agents [1, 2]. Some benzodiazepine derivatives are used as dyes for acrylic fibers in photography and also as anti-inflammatory agents [3, 4]. Particularly, 1,5-benzodiazepines are useful precursors for the synthesis of some fused ring benzodiazepine derivatives such as triazolo-, oxadiazolo-, oxazino- or furanobenzodiazepines [5, 6]. Despite their wide range of pharmacological activity, industrial, and synthetic applications, the synthesis of 1,5-benzodiazepines has received little attention. Also, there is no report on the use of silica-supported polyphosphoric acid (PPA-SiO_2) as a heterogeneous catalyst for the synthesis of these compounds.

Thus, in this work, we wish to report a green, simple and eco-friendly procedure for the synthesis of 1,5-benzodiazepines by the condensation of *o*-phenylendiamines with ketones in the presence of PPA-SiO_2 as catalyst. The catalyst can be reused after a simple work-up. Other advantages of this method are high yields, relatively short reaction times and easy work-up.



References:

[1] Schutz, H. *Benzodiazepines*, Springer, Heidelberg, **1982**.
[2] Landquist, J. K. in, *Comprehensive Heterocyclic Chemistry*, ed. Katritzky, A. R.; and Rees, C. W. Pergamon, Oxford, **1984**, *1*, 166–170.
[3] Haris, R. C.; and Straley, J. M.; *US Pat.* 1,537,757, **1968**; *Chem. Abstr.*, **1970**, *73*, 100054w.
[4] De Baun, J. R.; Pallos, F. M.; Baker, D. R. *US Pat.* 3,978,227, **1976**; *Chem. Abstr.*, **1977**, *86*, 5498d.
[5] Essaber, M.; Baouid, A.; Hasnaoui, A.; Benharref, A.; Lavergne, J. P. *Synth. Commun.*, **1998**, *28*, 4097.
[6] Reddy, K. V. V.; Rao, P. S.; Ashok, D. *Synth. Commun.*, **2000**, *30*, 1825.

An improved procedure for preparation of carbapenem antibiotic: meropenem

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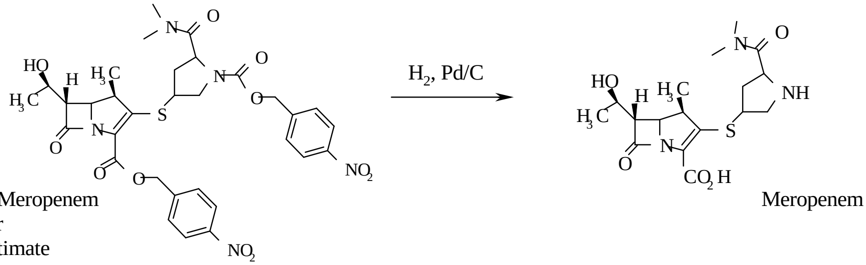
Meropenem is a semisynthetic, broad spectrum carbapenem antibiotic for parenteral administration [1,2]. It is used in the treatment of a wide range of serious infections such as intra-abdominal infections, urinary tract infections, and lower respiratory tract infections [3,4]. There are several methods reported in literature for the preparation of Meropenem [5]. This process required chromatographic purification and concentration of the aqueous solution by reverse osmosis to give meropenem.

We herein report a cost-effective and commercial process for preparation of meropenem with improved yield and shorter reaction time.



Protected Meropenem
or
Penoltimate

Meropenem

The protected meropenem is subjected to hydrogenolysis on 10% Pd/C in mixture solvent water –Tetrahydrofuran at 20-25 °C for 7 h (~ 3bar of H_2 gas). After hydrogenation, the reaction mixture is filtered and the layers are separated. To the aqueous layer activated carbon was added for further purification. After filteration, to the aqueous layer acetone and seed sample of meropenem were added at 5-10 °C. The suspension was stirred for 2 h at 0-5 °C. The precipitate was collected by filtration and dried to give Meropenem as a nonsterile solid (yield=63% and assay by HPLC ≥98%).

References:

[1] Pfaller, M. A.; Jones, R. N. *Diagn. Microbiol. Infect. Dis.* **1997**, *28*, 157.
[2] Blumer, J. L. *Int. J. Antimicrob. Agents* **1997**, *8*, 73.
[3] Wiseman, L. R.; Wagstaff, A. J.; Brogden, R. N.; Bryson, H. M. *Drugs* **1995**, *50*, 73.
[4] Bradley, J. S. *Pediatr. Inject. Dis. J.* **1997**, *16*, 263.
[5] (a) Nadenik, P.; Storm, O.; Kremminger, P. (Sandoz) WO 05/118586, **2005**; (b) Surulichamy, S.; Sekar, S.; Deshpande, P. N.; Ganpathy, P.; Sarangdhar, R. J.; Henry, S. S.; Karale, S. N.; Jangale, A. A.; Kaldale, R. D. (Orchid) WO 05/ 118586, **2007**.

Rapid and efficient synthesis of 2-aminobenzophenone derivatives under ultrasonic irradiation

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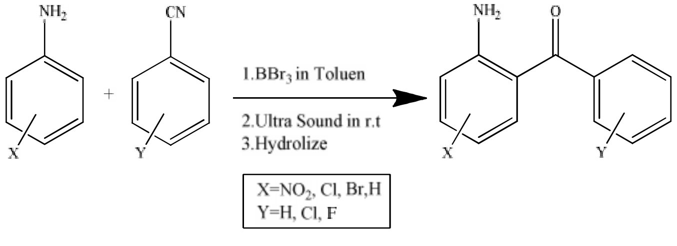
Developing of new methodology in organic synthesis such as application of ultrasonic, microwave irradiation, ionic liquids and solvent free conditions is the best approach for organic chemists. On the other hand, 2-aminobenzophenone derivatives are important compounds in organic chemistry because of their application in heterocyclic synthesis and pharmaceutical compounds[1] . These compounds have been used as starting material for the synthesis of a wide variety of heterocyclic systems such as 1,4 benzodiazepines. There are some general methods for the preparation of 2- aminobenzophenons, such as Friedel-Crafts reaction of anthranilic acid derivatives with aryl compounds [2], Friedel-Crafts acylation of para substituted anilines [3] and reaction of aryl-Grignard reagents with 2-nitro or 2-aminobenzaldehydes[4]. These methods are common, but contain several additional steps, such as protecting and deprotecting of the amino group. Herein we report an efficient method for the preparation of 2-aminobenzophenone derivatives under ultrasonic irradiation. We used aniline derivatives and benzonitrile derivatives as reactant and boron tribromide as an efficient Lewis acid in our method and in all reactions we saw good yields.



References:

[1] Walsh, D.A. *Synthesis*. **1980**, 677.
[2] Scheifele, H.J.; Detarr, D.F. *Org. Synth.* Coll. 4, **1963**, 34.
[3] Sternbach, L.H.; Fryer, R.I.; Metlesics, W.; Sach, G. J. Org. Chem. **1962**, *27*, 3781.
[4] Liou, J.P.; Chang, J.Y.; Chang C.Y.; Hsieh, H.P. *J. Med. Chem***. 2004**, *47*, 2897.

Comparison of methods of HD , SDE and MWCNT for identification and extraction of volatile components of medicinal herbal

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Essential oils are widely used in the cosmetic industry, most especially, in the production of various cologne waters, bathing lotions, hair lotions, shampoos, and as components of disinfectants and insecticides [1] reported antimicrobial activity of essential oils obtained from oregano, thyme, sage, rosemary, clove, coriander, garlic and onion against both bacteria and fungi [2]. Also, Essential oils can be extracted using a variety of methods, although some are not commonly used today. Currently, the most popular method for extraction is steam distillation, but as technological advances are made more efficient and economical methods being developed.

Among the several techniques that have been developed to isolate volatile compounds, simultaneous distillation–extraction (SDE), Multi-walled Carbon nanotubes (MWCNT). simultaneous distillation–extraction (SDE),introduced in 1964 by Likens and Nickerson, is one of most widely employed. This method has been successfully applied in the extraction of essential oils [3], aroma compounds [4], and other volatile products from numerous matrices. In the flavour area, this technique is usually considered to be superior to classical ones, such as distillation or solvent extraction. This technique combines steam distillation together with continuous extraction with a solvent or a mixture of solve.

Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, optics, materials science, and architecture.Multi-walled nanotubes (MWNT) consist of multiple rolled layers (concentric tubes) of graphite [5].

References:

[1] Boelens, M. H. Essential oils and aroma chemicals from Eucalyptus globules Labill. Perfumer and Flavorist, **1985**, 9, 1–14.
[2] Godefroot, M. Sandra, P. Verzele, M. *J. Chromatogr.* **1981,** 203**,** 325.
[3] Blanch, G. P. Reglero, G. Herraiz, M. *Food Chem.* **1996,** 56, 439.
[4] Careri, M. Mangia, A. Mori, G. Musci, M. *Anal. Chim. Acta* **1999,** 386, 169.
[5] Wang, X.; Li, Q.; Xie, J.; Jin, Z.; Wang, J.; Li, Y.; Jiang, K.; Fan, S. *Nano Lett.* **2009**, **9**

Ultrasound assisted dehydrogenation of 2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxamides

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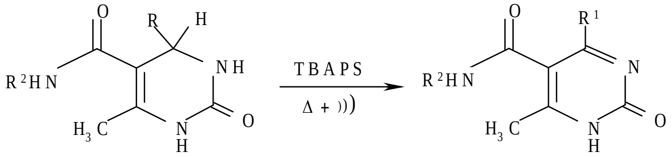
Application of ultrasound technique in organic synthesis has been increasingly progressed because of its advantages such as shorter reaction times, milder reaction condition and higher yields in comparison to the classical methods. Since in this technique the reaction is carried out normally at lower temperature relative to the usually thermal methods, therefore the possibility of occurrence of undesired reactions is reduced and as a result of a cleaner reaction, the workup is easier. The generation of many cavities and increasing of temperature and pressure during collapse of cavities is the important effect of ultrasound [1].

Six-membered heterocyclic compounds are important constituents which often exist in biologically active natural products and also in synthetic compounds of medicinal interest. Among them, pyrimidine cores are important classes of drugs. The pyrimidine derivative, MKC-442, is one of the most important classes of drugs to inhibit the HIV virus [2]. Oxidation of 2-oxo-1,2,3,4-tetrahydropyrimidines is an important method for the preparation of pyrimidine derivatives.

Although various methods for the oxidation of specific 1,4-dihydropyridines exist, 2-oxo-1,2,3,4-tetrahydropyrimidines are highly stable toward mild and powerful oxidants. However in recent years some procedures were reported for oxidation of these compounds [3].

Herein we report a simple method for oxidation of various 2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxamides by tetrabutylammonium peroxydisulfate as an efficient oxidizing agent to their corresponding 2-oxo-1,2-dihydropyrimidine-5-carboxamides under sono-thermal condition. The results will be presented.



R^1 and R^2 : alkyl and aryl

References:

[1] Mason,T. J.; Luche, J. L.; Van Eldik, R.; Hubband, C. D. (Eds.) *Chemistry under extreme or non-classical conditions,* Wiley and Spectrum, New York and Heidelberg, **1997**, 317.

[2] Zhou, W.; Gumina, G.; Chong, Y.; Wang, J.; Schinazi, R.F.; Chu, C. K. *J. Med. Chem.* **2004**, *47,* 3399.

[3] Memarian, H. R.; Farhadi, A.; Sabzyan, H. *Ultrason. Sonochem.* **2010**, *17,* 579. and references cited therein.

Synthesis of new highly optical active advanced polyamideimides with enhanced organosuability and thermal stability

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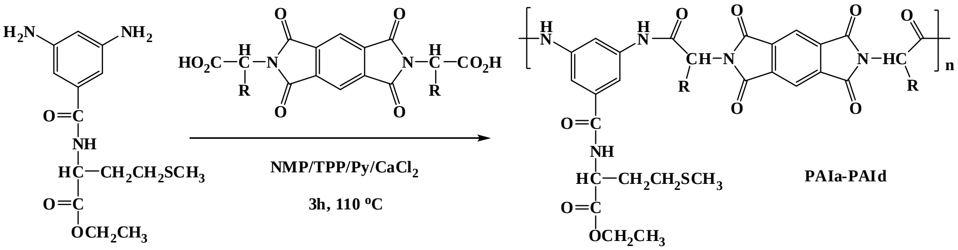
During the last decade, resolution of racemic compounds attracted great attentions in analytical chemistry, especially in pharmaceutical analysis, because each enantiomer of the chiral drugs exhibits great differences in pharmacological, pharmacodynamic, and toxicological manners [1]. High performance liquid chromatography using a chiral stationary phase is one of the most popular methods for the direct separation of chiral compounds [2].

Polyamideimides (PAI)s are among the most significant engineering macromolecules due to the elevated heat resistance, low dielectric constant and small thermal expansion coefficient and seems to be the powerful materials as chairal stationary phases [3]. However, the high melting or glass-transition temperatures and restricted solubility in organic solvents, have limited the processability of PAI for chromatographic purposes [3]. Consequently exertion of a useful strategy for the improvement of solubility and processability of PAIs without significant decrease of thermal properties is indispensable. Herein we wish to report the design and synthesis of a bulky diamine monomer containing L-metionine moiety in the pendant group as well as its polycondensation with several optically active diacids, to produce a series of novel optically active PAIs with superior processability without the lose of their high thermal stability.



R: a = $-CH_3$, b = $-CH_2Ph$, c = $-CH_2CH(CH_3)_2$, d = $-CH_2CH_2SCH_3$

References:

[1] Chen, Y.; Yang, Y.; Su, J.; Tan, L.; Wang, Y. *React. Funct Polym.* **2007**, 67, 396.
[2] Xiao Kanazawa, H.; Ayano, E.; Sakamoto, C.; Yoda, R.; Kikuchi, A.; Okano, T. *J. Chromatogr. A* **2006**, 1106, 152.
[3] Radosz, M.; Hu, X. ; Cong, H.; Shen, Y. *Ind. Eng. Cem. Res.* **2007**, *46*, 1547.

Application of Al_2O_3/NaOH in the preparation of Semicarbazone under microwave irradiation

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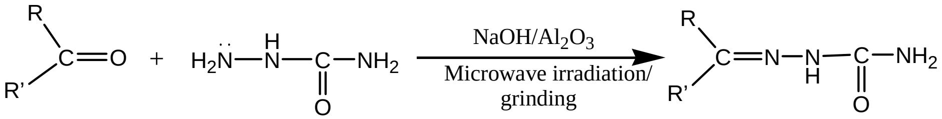
Somewhat we need to do chemical reaction with more selectivity specifically when the compound has several active groups. For this goal we use protecting group to inactive other groups that may do trade in reaction, in the ending of reaction it transform to primal shape by deprotection. One of the best protective groups is semicarbazons.

Semicarbazones and thiosemicarbazones are of considerable pharmacological interest since a number of derivatives have shown a broad spectrum of chemotherapeutic properties [1]. The most common method for production of semicarbazon is reaction between aldehyde/ketone and semicarbazide in the present of one acidic or basic catalyst.

Herein we report application of NaOH supported on Alumina in the facile preparation of semicarbazones from carbonyl groups in solvent free condition and under microwave irradiation. The products were obtained in high isolated yields and in short reaction times. The reaction is very clean and the products were obtainrd in high isolated yields in short reaction conditions.



R' : H, alkyl or aryl

References:

[1] De Oliveira, R. B.; de Souza-Fagundes, E. M.; Soares, R. P. P.; Andrade, A. A.; Krettli, A. U; Zani, C. L. *E. J. Medic. Chem.* **2008**, *43*, 1983.

Photocatalytic oxidative degradation of an organic azo dye: The preparation of photocatalysts and investigation of their performance

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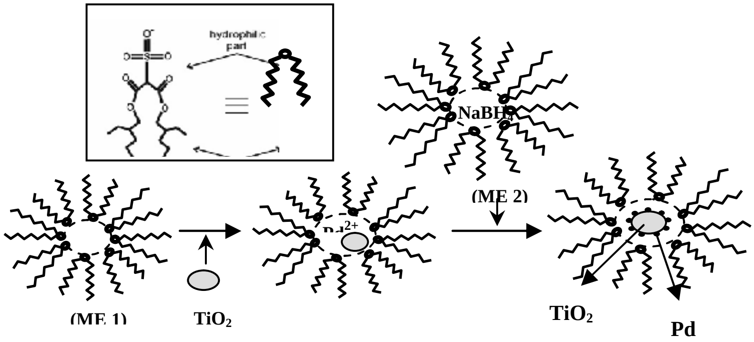
A “water-in-oil” (w/o) microemulsion is formed by solubilizing water in a oily phase using a surfactant [1]. The resulting homogeneous mixture contains small aggregates (reversed micelles with size of 5-50 nm) consisting of tiny water droplets surrounded by surfactant molecules. These aggregates can contain and solubilize water soluble reactants in oil matrix, hence can act as nano-reactors [2]. Mixing two w/o microemulsions with at least two inorganic reactants, which can form water insoluble product, have been widely used for preparation of the inorganic nanoparticles [3].

In the first part of this contribution, the preparation of Pd-loaded TiO_2 photocatalysts using two microemulsion method, namely, metal precursor containing (*n*-heptane (oil phase)/AOT (sodium bis(2-ethylhexyl) sulphosuccinate)/water/ $PdCl_2$) and reducing microemulsion (*n*-heptane/ AOT/ water/$NaBH_4$) is reported. Then the results of studying photocatalytic degradation of an organic azo dye (Acid Yellow 23) on the prepared Pd/TiO_2 nanaoparticles under UV-irradiation in distilled water are presented. The effect of different parameters affecting the performance of the resulting photocatalysts was investigated. The highest photocatalytic efficiency was observed for the photocatalyst containing 0.75wt% Pd doped on TiO_2 and using of 400 mgL^{-1} of the catalyst.



References:

[1] Najjar, R., Stubenrauch C. *J. Coll. Interf. Sci.* **2009**, 331, 214-210.
[2] Uskokovic, V.; Drofenik, M. *Surf. Rev. Lett.* **2005**, *12,* 239.
[3] Boutonnet, M.; Lögdberg, S.; Svensson, E. E. *Curr. Opin. Coll. Interf. Sc.* **2008**, *13,* 270.

One-pot synthesis of highly functionalized 1-H pyrazoles by pseudo four-component reaction of cyclohexyl isocyanide, dialkyl acetylenedicarboxylates and hydrazide acids

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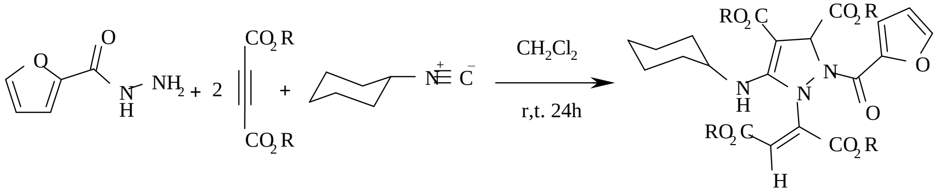
Multi-component condensation reactions (MCRs) occupy an advantageous position because of high atom economy, their convergent character and simple procedures. Therefore, the development of novel MCRs are of interest for chemists [1].

A large and important class of MCRs are the isocyanide based multicomponent reactions (IMCRs), first of them was introduced in 1921 by Passerini. One of the most utilized multicomponent reactions is Ugi reaction. Synthesis of α-acylamino amides is achieved by reacting aldehydes, primary amines, carboxylic acids and isocyanides [2]. Recently, three-component reaction between isocyanides, electron-deficient acetylenic esters and organic compounds containing at least one acidic NH, OH or CH group have been reported [3]. These reactions usually passe through a zwiterionic intermediate to produce keteneimines which may be isolated as stable products or cyclize to heterocyclic compounds.

Herein we report an efficient method for synthesis of 1-H pyrazoles by pseudo four-component reaction between cyclohexyl isocyanide, dialkyl acetylenedicarboxylates and hydrazide acids.



References:

[1] Zhu J.; Bienayme, H. *Multicomponent Reactions*. Eds.; Wiley-VCH: Weinheim, 2005.
[2] Ugi, I.; Werner, B.; Domling, A. *Molecules* **2003**, 8, 53.
[3] Anary-Abbasinejad, M.; Mosslemin, M. H.; Tahan, S.; Anaraki-Ardakani, H. *J. Chem. Res*, **2006**, 170.

Enantioselective synthesis of new substituted of [1,2,4]triazino[3,4-b][1,3,4] thiadiazine

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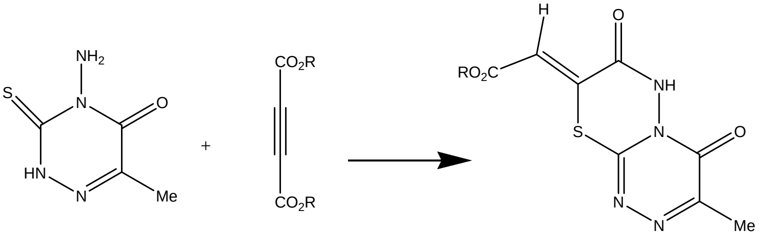
Fused rings of triazino thiadiazine are a class of heterocyclic compounds with interested biological activity [1,2]. Several methods have been reported for the preparations of this compounds [3]. In this research we reported a convenient and efficient rout to synthesized new derivatives of [1,2,4]triazino[3,4-b][1,3,4]thiadiazine **3** by reaction between substituted [1,2,4] triazine **1** with electron deficient esters**2** as DMAD and DEAD,… . The structure of products was deduced from its elemental analyses and its IR, ^{1}H and ^{13}C-NMR spectra. The ^{1}H-NMR spectra for compounds **2** exhibited the methylidene proton signals near 6.8 ppm, which is also consistent with Z-configuration.



1 **2** **3**

References:

[1] Witvrouw, M.; Arranz, M. E.; Pannecouque, C.; Declercq, R.; Jonckheere, H.; Schmit, J.-C.; Vandamme, A. M.; Diaz, J. A.; Ingate, S. T.; Desmyter, J.; Esnouf, R.; Van Meervelt, L.; Vega, S.; Balzarini, J.; De Clercq, E. Antimicrob. *Agents Chemother*. **1998**, *42*, 618.

[2] El Bialy, S. A. A.; Abdelal, A. M.; El Shorbagi, A. N.; Kheria, M. M. *Arch. Pharm. Pharm. Med. Chem*. **2005**, *338*, 38.

[3] Fotouhi, L. Mosavi, M. Heravi, M. M. Nematollahi D. *Tetrahedron Lett.* **2006,** *47*, 8553.

Synthesis of some water-soluble 3,5-dihydroxymethyl-4-aryl substituted pyridines

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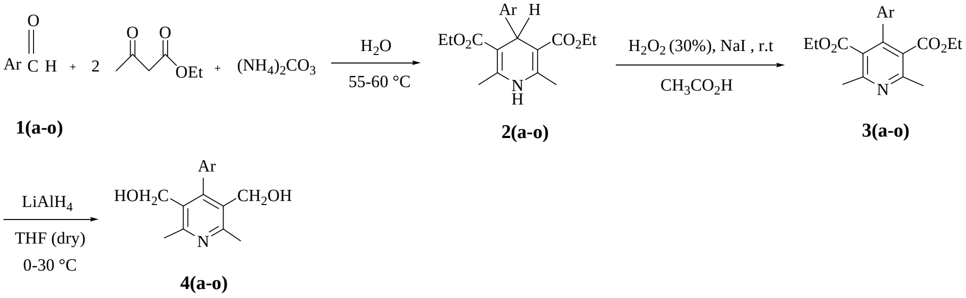
It has been interested in whether organic compounds can regulate biological processes aiming at application setups. It was founded some 4-arylpyridine derivatives could function as an organic solvent-free solution. Hence, they could play a significant role in biological systems. These premise result in this statement that 4-arylpyridine derivatives can regulate biological processes under physiological conditions [1]. The results obtained here demonstrate the synthesis of some water-soluble of 4-arylpyridine derivatives.

At the first step of this research the Hantzsch 1,4-dihydropyridines were synthesized from the respective aromatic aldehydes [2] and then oxidation of 1,4-DHP to corresponded pyridines were prepared by H_2O_2-AcOH/NaI that already reported by us. In the next step reduction of diethyl 2,6-dimethyl-4-arylpyridine-3,5-dicarboxylate to the respective 3,5-dihydroxymethyl-2,6-dimethyl-4-arylpyridnes **4(a-o)** were carried out with lithiumaluminiumhydrid **4(a-o)** (scheme 1).



Ar (a-o) = C_6H_4, 2-F-C_6H_4, 3-F-C_6H_4, 4-F-C_6H_4, 4-CF_3-C_6H_4, 4-MeO-C_6H_4 , 2-Pyridil , 3-Pyridil , 4-Pyridil , 2-HO-C_6H_4 , 3-HO-C_6H_4 , 4-HO-C_6H_4 , 2-NO_2-C_6H_4 , 3-NO_2-C_6H_4 , 4-NO_2-C_6H_4

Scheme 1

References:

[1] Sambongi, Y.; Nitta, H. et al. *J. Org. Chem.*2002, *67*, 3499.
[2] Tamaddon, F.; Razmi, Z.; Jafari, A.A. *Tetrahedron Lett.* **2010**, *51*, 1187.

Metaborosulfric acid: A novel catalyst to conversion of alcohols into diphenylmethyl (DPM) ethers

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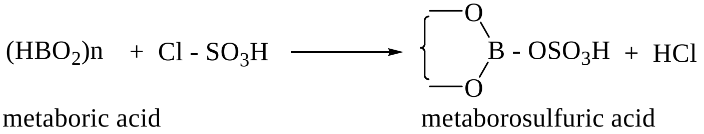
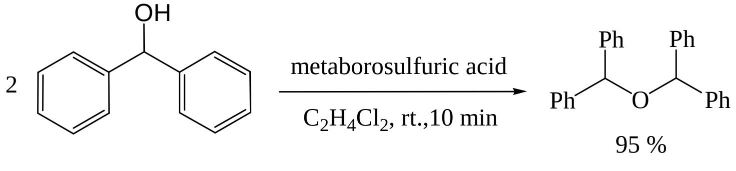
The preparation of DPM ethers is one of the popular methods in view of their low cost and high stability towards a variety of reagents. Additionally, DPM ethers and DPM groups are found as part of the structure of pharmacological active compounds [1].

A wide variety of reagents are available for the preparation of DPM ethers such as diphenylmethyl chloride or bromide in the presence of a base, diphenylmethanol- sulfuric or *p*-toluenesulfonic acids, diphenylmethylphosphate-trifluoroacetic acid, ytterbium triflate-ferric chloride, Nafion-H and 12-Tungstophosphoric acid supported on inorganic oxides [2].

Herein, we describe a novel and efficient method for the synthesis of diphenylmethyl (DPM) ethers by the condensation of diphenylmethanol with alcohols in the presence of metaborosulfuric acid (MBSA) as a novel catalyst in dichloroethane at room temperature. The present method offers several advantages such as high yields, short reaction times and a simple work-up procedure.





Reference:

[1] a) Namboodiri, V.; Varma, R. *Tetrahedron Lett.* **2002,** *43*, 4593.

[2] a) Dobson, D.; Todd, A.; Gilmore, J. *Synth. Commun.* **1991,** *21*, 601; b) Sugsawa, S.; Fujiwara, K. *Org. Synth. Coll.* **1963,** *4*, 72; c) Parades, R.; Perez, R. *Tetrahedron Lett.* **1998,** *39*, 2037; d) Lapatsanis, L. *Tetrahedron Lett.***1978,** *19*, 3943; f) Sharma, G; Prasad, T.; Mahalingam, A. *Tetrahedron Lett.* **2001,** *42*, 759; e) Stanescu, M.; Varma, R. *Tetrahedron Lett.* **2002,** *43*, 7307. f) Mohammadpoor-Baltork, I.; Moghadam, M.; Tangestaninejad, Sh.; Mirkhani, V. *Polyhedron* **2008,** *27*, 2612.

Determination of fatty acids of wild Pear’s fruit from Mazandaran’s forest

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The objective of the present study is focused on the chemical composition of the organic compound from wild Pear's fruit of Iran (savadkooh, Mazandaran).Organic compound were extracted through solvent extraction in the soxhlet apparatus using n-Hexan. The dense extracts had greenish color with week smell. The extracts of fruit analyzed by gas chromatography system. A bonded phase, open tubular fused silica capilari column was employed (30m* 0.25 mm i.d.).The result of essential oils analysis from Pear’s fruit indicated the presence of 14 compounds.The result of fatty acids analyzed showed that the main fatty acid was linolelaidic acid with percentages of 56.16 in the Pear's fruit. Other acids found in these fruit were oleic acid with 24.54% and palmitic acid with 11.40%.

One-pot, three-component synthesis of new tetrahydroindeno[1,2-b] pyrrolo-3-carboxylates

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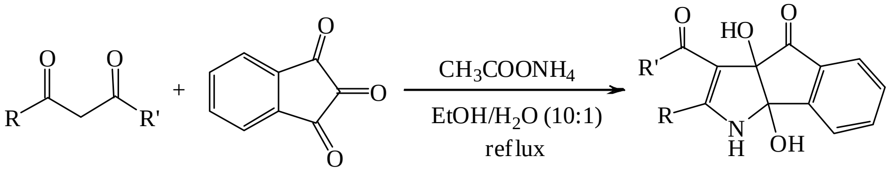
MCRs are perfectly suited for combinatorial library synthesis, and thus are finding increased use in the discovery process for new drugs and agrochemicals .They provide a powerful tool toward the one-pot synthesis of diverse and complex compounds as well as small and drug-like heterocycles [1].

Polysubstituted pyrroles are molecular frameworks having immense importance in material science [2]. They have been also employed as antioxidants , antibacterial , ionotropic, antitumor, anti-inflammatory, and antifungal agents. Moreover, they are a highly versatile class of intermediates in the synthesis of natural products as well as in heterocyclic chemistry .

As part of our research on the development of new synthetic methods in heterocyclic chemistry [3,4], herein, we describe an efficient synthesis of functionalized tetrahydroindeno [1,2-b]pyrrole-3-carboxylate 3 via the reaction of 1,3-dicarbonyls 1 and ninhydrin 2 in the presence of ammonium acetate in EtOH/H_2O as a solvent .



1 2 3

References:

[1] Weber, L.; Curr Med Chem . **2002**, 9, 2085.
[2] Baumgarten, M.; Tyutyulkov, N .; Chem Eur J. **1998**, 4, 987.
[3] Azizian , J.; Karimi, AR.; Kazemizadeh, Zahra.; Mohammadi, A.; Mohammadizadeh, MR. The Journal of organic chemistry .**2005**,70 (4), 1471.
[4] Ji S, J.; Wang, S. Y.; Zhang, Y.; Loh, T P.; Tetrahedron. **2004**, 60, 2051.

Synthesis of 1,3-dimethyl pyrimidine-2,4(1H,3H)-dione and xanthenes derivatives in reaction dimedone with benzylidene and benzylidene -1,3-dimethylbarbituric acid

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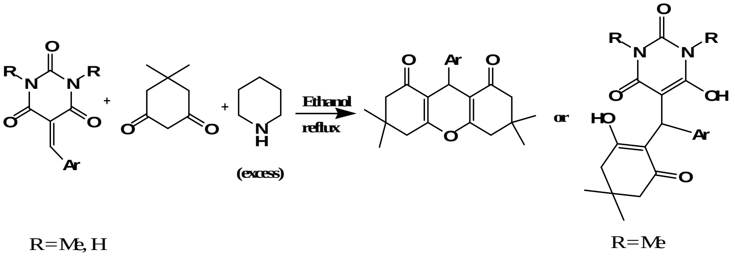
Benzylidenebarbituric acids are potential organic oxidizers [1]. These compounds are also used in preparation of oxadeazaflavines [2], in unsymmetrical synthesis of disulphides [3], as antibacterial agents [4] and in synthesis of Merocyanine dyes [5]. The nucleophilic attack at the electron-deficient double bond of Michael acceptors has long been a field of great interest in physical organic chemistry [6]. Benzylidenebarbituric and thiobarbituric acids are characterized by their strongly polarized exocyclic double bond with a positive partial charge on the arylidene carbon[7].

The reaction of benzylidenebarbituric acid and 1,3-dimethylbenzylidene barbituric acid with dimedone in piperidine is investigated. A different behavior is observed. Reaction with benzylidenebarbituric acid yields xanthenes, where as reaction with benzylidene-1,3-dimethylbarbituric acid gives 6-hydroxy-5-((2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-enyl)(aryl)methyl)-1,3-dimethyl pyrimidine-2,4(1H,3H)-dione derivatives. The ^{1}H NMR spectrum of pyrimidine derivatives supported the finding by showing a broad singlet at δ 10.60 and a singlet at δ 12.84 for the OH protons which disappeared when shaken with D_2O.



Refrences:

[1] Tanaka, K.; Cheng, X.; Kimura, T.; Yoneda, F. *Chem. Pharm. Bull.* **1986**, 34, 3945.
[2] Figueroa-Villar, J. D.; Rangel, C. E.; Dos Santos, L. N. *Synth. Commun.* **1992**, 22, 1159.
[3] Tanaka, K.; Cheng, X.; Yoneda, F. *Tetrahedron.***1988**, 44, 3241.
[4] Tihomir, T.; Nace, Z.; Manica, M. P,; Danijel, K.; Lucija, P. M. *European Journal of Medicinal Chemistry*. **2010**, 45, 1667.
[5] Frank, W.; Sheng, Y. *J. Org. Chem.* **2003**, 68, 8943.
[6] Kaumanns, O.; Mayr, H. *J. Org. Chem.* **2008**, *73*, 2738.
[7] Kaumanns, O.; Appel, R.; Lemek, T.; Seeliger, F.; Mayr, H. *J. Org. Chem.* **2009**, 74, 75.

TMSCl Promoted selective oxidation of sulfides to sulfoxides with hydrogen peroxide

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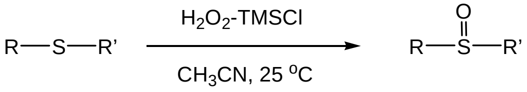
Selective oxidation of sulfides to sulfoxides is a very important reaction in organic synthesis, since they have been well known to act as useful synthetic intermediates for the construction of various chemically and biologically significant molecules [1]. The direct oxidation of sulfide is one of the most important and widely studied reactions for the preparation of sulfoxide. Although a great number of methods are available for the conversion of sulfides to corresponding sulfoxides [3], there are various limitations such as the use of strong acidic or basic conditions, elevated temperatures, long reaction times, hazardous organic solvents and reagents, transition metal catalysts, the formation of sulfones as side products from the overoxidation of sulfides and the undesired reaction occurring from other functional groups. Therefore, there still is a need for the development of new, efficient, highly selective and widely applicable methods for this transformation, as well as concerning about all the above important protocols under the mild reaction condition.

In continuation of our recent work on the oxidation of sulfides,[15] herein, we wish to report an efficient protocol in which H_2O_2 has been used as the oxidizing agent in the presence of TMSCl for the chemoselective oxidation of sulfides to their sulfoxides in excellent yields and short reaction times. The route for the synthesis of sulfoxides is shown in Scheme 1.



Scheme 1.

References:

[1] Carreno, M. C. *Chem. Rev*. **1995**, *95*, 1717.
[2] (a) Mata, E. G. *Phosphorus, Sulfur Silicon Relat. Elem*. **1996**, *117*, 231. (b) Madesclaire, M. *Tetrahedron* **1986**, *42*, 5459.
[3] (a) Bahrami, K. *Tetrahedron Lett*. **2006,** *47*. (b) Khodaei, M. M.; Bahrami, K.; Tirandaz,Y. *J. Sulfur Chem*. **2009,** *30,* 581. (c) Khodaei, M. M.; Bahrami, K.; Shiekh Arabi, M. *J. Sulfur Chem*. **2010,** *31,* 83.

Sulfamic acid functionalized hydroxyapatite-encapsulated γ-Fe_2O_3 nanoparticles: a re-usable heterogeneous superparamagnetic organocatalyst

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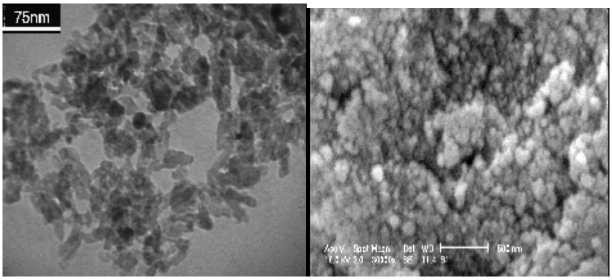
Since the discovery of organocatalysis, there have been a rapidly growing number of reports in the literature addressing the use of organic compounds or organic salts as catalysts [1-3]. The first superparamagnetic propylsulfamic acid nanoparticle supported onto hydroxyapatite [γ-Fe_2O_3@HAp-Si-$(CH_2)_3$-$NHSO_3H$] synthesized for use as a unique heterogeneous organocatalyst of wonderful activity and clean recyclability for at least 10 reaction cycles without considerable loss of reactivity. “Green” aspect achieved by facile recovery of the catalyst carried by applying an external magnet device. The catalyst fully characterized by TEM, SEM, FTIR, TGA, XRD, BET, elemental analysis (CHNOS) and VSM.



References:

[1] Book: Dalko, P.I.; Ed., Enantioselective Organocatalysis, Wiley-VCH, Weinheim (2007).
[2] List, B. *Chem. Rev*. **2007**, *107*, 5413.
[3] (a) Dondoni, A.; Massi, A. *Angew. Chem. Int. Ed.*, **2008**, *47*, 4638-4660; (b) Gruttadauria, M.; Giacalone, F.; Noto, R. *Chem. Soc. Rev*. **2008**, *37,* 1666-1688; (c) Werner, T. *Adv. Synth. Catal*. **2009**, *351*, 1469.

Gas-phase acidities of some planar hydrocarbons

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The acidities and basicities of organic compounds are expected to be different in the gas phase and in solution. Whereas in the gas phase acidity and basicity are intrinsic properties of the individual molecules, in the liquid state these properties belong to the phase as a whole due to the interaction between solute and solvent molecules. Considerable data on gas phase acidity are also available [1]. The solution and gas-phase acidities of C-H acids are of particular interest because of the wide structural variations that are possible in this class of compounds. In this study, Density functional theory (DFT) calculations at *B3LYP/6-311+G*** level have been used to compute the gas phase acidity of some hydrocarbons (**Figure 1**) and compare them with experimental values.

The relative stability of gas phase carbanions can also be assessed by the energy of their reaction with a proton, which is called proton affinity. An interesting insight into the origin of acidity is provided by the proton affinities of the corresponding anions. It is therefore of interest to consider briefly the spatial and electronic structure of the parent hydrocarbons and their anions. The most striking structural feature of the series is that they are all planar, which is indicative of the strong π-electron delocalization. Likewise, the acidities of the compounds have been used to study the aromatic character of the resulting conjugate base based on different criteria of aromaticity.

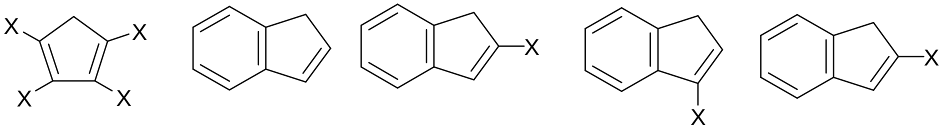

Figure 1. A set of the planar hydrocarbons studied.

References:

[1] Jinfeng, C.; Topsom, R. D.; Headley, A. D.; Koppel, I.; Mishima, M.; Taft, R. W.; Veji, S. *Theochem*, **1988**, *45*, 141.

Synthesis of novel aminopeptide derivatives similar to aminopeptidase N inhibitorse (APNIs)

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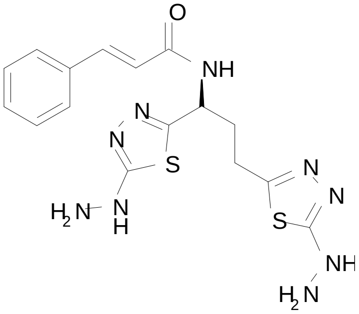
Novel aminopeptidase N (APN) inhibitors can used as medicines of anti cancer that absorb by active parts of APN and inactivate RNA parts of these enzyme , with this method can prevent from growth of cancer cells [1]. In this study, we report the synthesis novel Aminopeptidase N inhibitors via L-iso-especially anti-tumor properties [2]. This was followed by coupling with various primary amines, and produced novel Aminopeptide. These new compounds have potent inhibitory activities against APN enzyme.

In conclusion biological characterization of these compounds cause to selective inhibitory activity toward APN [3]. Develop new APN inhibitors has been useful for medical and therapeutic utilization [4]. Because of these biological activity of, we try to syntheses some novel aminopeptide derivatives by cinnamic acid as a starting chemical compound.



References:

[1] Fukasawa, K.; Fujii, H.; Saitoh, Y.; Koizumi, K.; Aozuka, Y.; Sekine, K.; Yamada, M.; Saiki, I.; Nishikawa, K. *Cancer Lett.*, **2006**, *243*, 135.

[2] Akao, Y.; Maruyama, H.; Matsumoto, K.; Ohguchi, K.; Nishizawa, K.; Sakamoto, T.; Araki, Y.; Mishima Nozawa, Y. *Biol. Pharm. Bull.* **2003**, *26*, 1057.

[3] Grzywa, R.; Oleksyszyn, *J. Bioorg. Med. Chem. Lett*. **2008**, *18,* 3734.

[4] Mina-Osorio, P. *Trends Mol. Med*. **2008**, *14*, 361.

DFT studies, NBO and NICS analysis of all fluoroanilines and chloroanilines as candidate monomer for new conducting polymers

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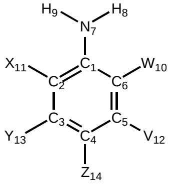
Conducting polymers because of change in theiroptical and electrical properties in nano-meteric dimension are most probable systems for nanoelectronical applications [1]. polyanilines can produce one - dimension morphologies,such as polymer nanostructure (nano - tube, - wire, -fiber, - filament, -rod, composite and -particle) the most researches is done about that [2,3]. Structural and electronic characteristics of the neutral and ionized mono -, di -, tri -, tetra - , penta - fluoroanilines and chloroanilines are studied using DFT- B3LYP method with the 6-311+ G** basis set.Vibrational frequencies,nuclear chemical shielding constants, chargeand spin-density distribution, size anddirection of the dipole moment vector, ionization potential electric polarizability, HOMO -LUMO gaps and NICS have also been calculated and analyzed.

Results of this study show that among all of these compounds 2,5-difluoroaniline as candidate monomers for intelligent polymeric nano-wires have the most suitable conditions for electropolymerization.



A: X=Y=W=V=H		aniline
B: X=F, Y=Z=V=W=H		2-fluorobenzenamine
C: Y=F, X=Z=V=W=H		3-fluorobenzenamine
D: Z=F, X=Y=V=W=H		4-fluorobenzenamine
E: X=Y=F, Z=V=W=H		2,3-difluorobenzenamine
F: X=Z=F, Y=V=W=H		2,4-difluorobenzenamine
G: X=V=F, Y=Z=W=H		2,5-difluorobenzenamine
H: X=W=F, Y=Z=V=H		2,6-difluorobenzenamine
I: Y=Z=F, X=V=W=H		3,4-difluorobenzenamine
J: Y=V=F, X=Z=W=H		3,5-difluorobenzenamine
K: X=Y=Z=F, V=W=H		2,3,4-trifluorobenzenamine
L: X=Y=V=F, Z=W=H		2,3,5-trifluorobenzenamine
M: X=Y=W=F, Z=V=H		2,3,6-trifluorobenzenamine
N: X=Z=W=F, V=Y=H		2,4,6-trifluorobenzenamine
O: Y=Z=V=F, X=W=H		3,4,5-trifluorobenzenamine
P: X=Z=V=F, Y=W=H		2,4,5-trifluorobenzenamine
Q: X=Y=Z=V=F, W=H		2,3,4,5-tetrafluorobenzenamine
R: X=Y=Z=W=F, V=H		2,3,4,6-tetrafluorobenzenamine
S: X=Y=V=W=F, Z=H		2,3,5,6-tetrafluorobenzenamine
T: X=Y=Z=V=W=F		2,3,4,5,6-Pentafluorobenzenamine
B*: X=Cl, Y=Z=V=W=H		2-chlorobenzenamine
C*: Y=Cl, X=Z=V=W=H		3-chlorobenzenamine
D*: Z=Cl, X=Y=V=W=H		4-chlorobenzenamine
E*: X=Y=Cl, Z=V=W=H		2,3-dichlorobenzenamine
F*: X=Z=Cl, Y=V=W=H		2,4-dichlorobenzenamine
G*: X=V=Cl, Y=Z=W=H		2,5-dichlorobenzenamine
H*: X=W=Cl, Y=Z=V=H		2,6-dichlorobenzenamine
I*: Y=Z=Cl, X=V=W=H		3,4-dichlorobenzenamine
J*: Y=V=Cl, X=Z=W=H		3,5-dichlorobenzenamine
K*: X=Y=Z=Cl, V=W=H		2,3,4-trichlorobenzenamine
L*: X=Y=V=Cl, Z=W=H		2,3,5-trichlorobenzenamine
M*: X=Y=W=Cl, Z=V=H		2,3,6-trichlorobenzenamine
N*: X=Z=W=Cl, V=Y=H		2,4,6-trichlorobenzenamine
O*: Y=Z=V=Cl, X=W=H		3,4,5-trichlorobenzenamine
P*: X=Z=V=Cl, Y=W=H		2,4,5-trichlorobenzenamine
Q*: X=Y=Z=V=Cl, W=H		2,3,4,5-tetrachlorobenzenamine
R*: X=Y=Z=W=Cl, V=H		2,3,4,6-tetrachlorobenzenamine
S*: X=Y=V=W=Cl, Z=H		2,3,5,6-tetrachlorobenzenamine
T*: X=Y=Z=V=W=Cl		2,3,4,5,6-Pentachlorobenzenamine

Figure 1: All possible of fluoroanilines and chloroanilines.

References:

[1] Ram , M. S.; Palaniappan, S. *J. Molecular Catalysis* **2003**,*201*, 289.
[2] Wallace ,Gordon G.; Spinks, Geoffrey M.; Leon A.P.; Kane- Maguire, Peter R. Teasda, Conductive electroactive polymers:polymer systems., CRC Press, Queensland, **2009**.

Synthesis and characterizations of anionic polyurethane dispersion (APUD)

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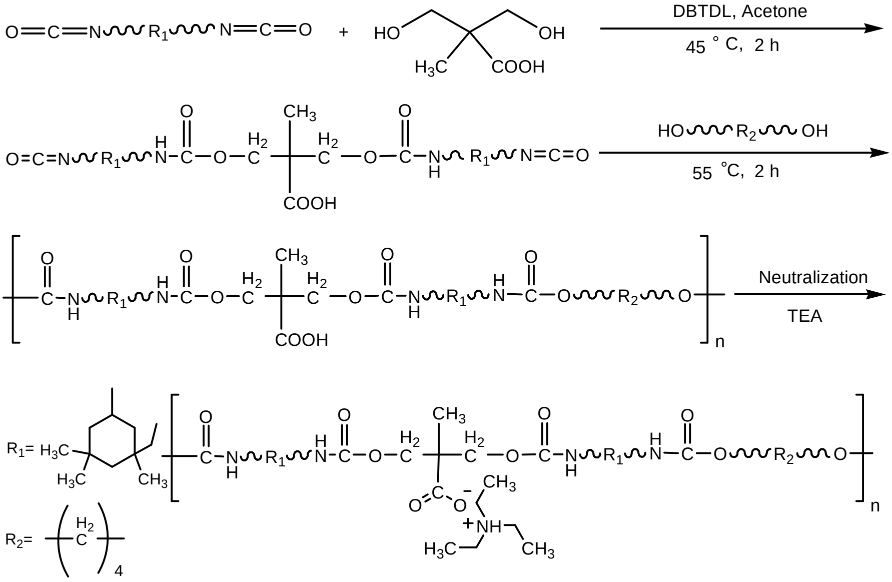
Anionic polyurethane dispersions (APUDs) were synthesized in three steps. In the first step, macromonomer diisocyanate with carboxylic acid was prepared by isophorone diisocyanate (IPDI), dimethylol propionic acid (DMPA) in presence of acetone as solvent and dibutyltin dilaurate (DBTDL) as catalyst. Then, carboxylic polyurethane was prepared by reaction of macromonomer diisocyanate with carboxylic acid and butanediol (BDO) as chain extender. The next step was involved neutralization and dispersion in water, where acidic polyurethane was neutralized by the addition of triethylamine (TEA). In this work the factors that influence synthesis of APUD were studied. Experimental data indicates factors that influence the synthesis of APUD mainly involve reaction temperature, reaction time, the concentration of catalyst, DMPA content, BDO content. The APUDs have been characterized with ^{1}H-NMR, FT-IR and GPC.



References:
[1] Madbouly S.; Otaigbe J. *Progress in Polymer Science*. **2009**, *34*, 1283.
[2] Liu S.; Zhu G. *European Polymer Journal*. **2007**, *43*, 3904.
[3] Subramani, S.; Park Y.; Lee Y.; Kim , J. *Progress in Organic Coatings*. **2003**, *48*, 71.

DBUH-Br_3 as a selective and efficient catalyst for the oxidation of sulfides to sulfoxides by H_2O_2

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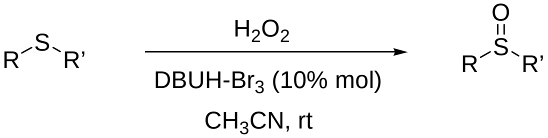
Sulfoxides are important intermediates in the synthesis of various natural products [1,2]. Syntheses of sulfoxides are usually achieved by oxidation of their corresponding sulfides. During the last years, various procedures for H_2O_2 oxidation of sulfides including the use of various heterogeneous catalyst systems have been reported [3-5]. The application of this oxidant has been developed due to its effective oxygen content, eco-friendly nature, low cost, and also safety in storage and operation [6,7]. Although, many reagents have been employed for the oxidation of sulfides to sulfoxides, the most common problem encountered during the reaction is the over-oxidation of sulfoxides to their corresponding sulfones [8].

Prompted by these reports and due to the potential oxidation of sulfur-containing compounds by H_2O_2, in the presence of catalysts, in this study we wish to report on a new and efficient method for selective oxidation of sulfides to sulfoxides by H_2O_2 as oxidant and in the presence of DBUH-Br_3 as catalyst. Chemoselectivity, easy and clean work-up, green oxidant, high yields and the easy preparation of the catalyst were the remarks of this method which could be the priority of the other existing methodologies.



References:

[1] Prilezhaeva, E.N., *Russ. Chem. Rev.* **2000**, *69*, 36.
[2] Rich, D.H.; Tam, J. P. *J. Org. Chem.* **1977**, *42*, 3815.
[3] Neumann, R., Juwiler, D. *Tetrahedron* **1996**, *52*, 8781.
[4] Gresley, N. M.; Griffith, W. P.; Laemmel, A. C. *J. Mol. Catal.* **1997**, *117*, 185.
[5] Collins, F.M.; Lucy, A. R.; Sharp, C. *J. Mol. Catal.* **1997**, *117*, 397.
[6] Bonadies, F.; De Angelis, F.; Locati, L. *Tetrahedron Lett.* **1996**, *37*, 7129.
[7] Kaczorowska, K.; Kolarska, Z.; Mitka, K. *Tetrahedron* **2005**, *61*, 8315.
[8] Venkataramanan, N. S.; Kuppuraj, G.; Rajagopal, S. *Coord. Chem. Rev.* **2005**, *249*, 1249.

Study of proper hydrogen bonding between thymine tautomers and some important biological anions using NBO analysis

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One of the possible molecule mechanisms for the formation of spontaneous mutations is conditioned by the tautomerism of DNA bases. The tautomerism of bases can play an important role in formation of the Watson-Crick-like mismatched base pairs [1]. In the last 30 years many studies have evaluated the influence of environmental and chemical agents such as PH, metal cations, anions and alkylating compounds on the tautomerization of nucleobases. The presence of anions near bases can strongly affect the electron distribution in the bases via hydrogen bonding and thus also the tautomeric equilibria. In other words, the effect of the anions can favor the formation of the rare tautomers, which are believed to be involved in various biochemical processes including point mutation [2].

In the present study, we consider the interaction of the selected anions (F^-, Cl^-, CN^-, OH^- and $NO3^-$) with tautomers of thymine nucleobase. Ab initio calculations have been carried out with the Spartan 06 software. The structures are calculated at the density functional theory (DFT) level, employing the B3LYP exchange-correlation functional and the 6-311++G(d,p) basis set. Vibrational frequencies are calculated for all structures to verify that no negative frequencies are present for local and global minimum structures on the potential energy surface.

References:

[1] Danilov, V. I.; Anisimov, V. M.; Kurita, N.; Hovorun, D.; *Chemical Physics Letters*. **2005**, *412*, 285.
[2] Kabelac, M.; Hobza, P.; astry, G. ; *J. Phys. Chem. B*. **2006**, *110*, 14515.

Iron (III) phosphate: a novel and recoverable catalyst for the synthesis of 2-aryl-oxazolines and 2- aryl -imidazolines under solvent-free conditions

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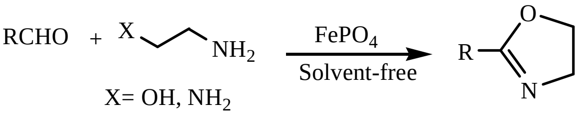
2-oxazolines and 2- imidazolines are employed in a wide variety of biologically active natural products and enzyme inhibitors. They also contribute to the flavors of a variety of foods [1]. They are also found in the structure of optically active polymers which attracted much attention due to their unique function [2].

2-Substituted oxazolines and imidazolines are an important class of heterocyclic componds with an astonishingly wide rang of applications in synthetic organic chemistry [3]. The variety protocol for preparation oxazolines reported which suffer problems such as long reaction times, low yield, using toxic catalyst and hard extraction method [4].

Iron (III) phosphate has limitedly been employed in transformation of organic compounds such as the selective oxidation of CH_4 to CH_3OH [5], benzene to phenol [6] and one-pot synthesis of dihydropyrimidinones and thiones [7].

Herein, iron (III) phosphate was found as highly efficient catalyst for the synthesis of oxazolines and imidazolines from the condensation of various aromatic aldehydes with amino alcohols and ethylenediamine respectively (Scheme 1).



Scheme 1

References:

[1] Maga, J. A.; Crit, R. C. Rev. *Food Sci. Nutr.* **1981,** *14*, 295.
[2] Cwik, A.; Hell,; Hegedus, A.; Finta, Z.; Horvath, Z. *Tetrahedron Lett.* **2002**, *43*, 3985.
[3] G ant, T. G.; Meyers, A. I. *Tetrahedron* **1994**, *50*, 2297.
[4] Mohammad poor-Baltork, I.; Moghadam, M.; Tangestaninejad, S.; Mirkhani, Hojati, SF.; *Polyhedron*, **2008**, *27*, 750.
[5] Otsuka, K.; Wang, Y. *Appl. Catal. A: Gen*. **2001**, *222*, 145.
[6] Ren, T.; Yan, L.; Zhang, X.; Suo, J. *Applied Catal. A: General* **2003**, *244*, 11.
[7] Heravi, M. M; Behbahani, F. K; Zadsirjan, V, Hossien A. Oskooie. *Heterocycles Commun*. **2006**, *12*, 369.

One-pot synthesis of 1, 4-Dihydropyridine using active carbon sulfuric and Silica sulfuric acid as an efficient and reusable catalysts

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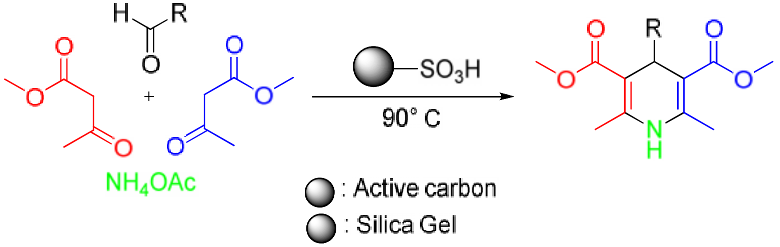
Catalysts have played a vital role in chemistry in the 20th century. As we enter the 21st century, the drive towards clean technology brought about by public, legislative and corporate pressure will provide new and exciting opportunities for catalysis and catalytic processes [1]. Chemical clean technology or green chemistry has at its heart the utilization of methods that reduce or eliminate the use or generation of hazardous substances [2, 3]. This embraces the principle of clean synthesis which involves improvements in process selectivity, high atom efficiency and easy separation with re-use of non-product components. The efficient use of solid catalysts can go a long way towards achieving these goals. Product isolation is simplified compared to homogeneous reactions and reactions often run under milder conditions and achieve higher selectivity. Catalysts based on high surface area inorganic support materials offer the additional advantage of high thermal and mechanical stabilities. Herein, we report the synthesis of a carbon based solid acid with a high density of sulfonic acid groups (SO_3H) and discuss its performance as a novel strong and stable solid acid.In this study besides active carbon sulfuric acid we have tested silica sulfuric acid [4] in order to show the activity of these catalysts in production of 1, 4-Dihydropyridine compounds.



References

[1] Clark J. H., *Green Chem.* **1999**, *1*, 1.
[2] Tundo P., Anastas P.T. Eds., Green Chemistry: Challenging Perspectives, Oxford Science, Oxford, **1999**.
[3] Clark J. H., Chemistry of Waste Minimisation, Chapman and Hall, London, **1995**.
[4] Zolfigol, M. A. *Tetrahedron*, **2001**, 9509.

L-Proline catalyzed one-pot synthesis of fused 1,4-dihydropyridines

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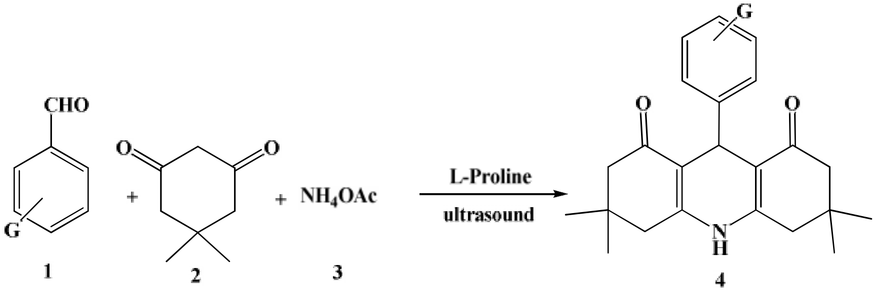
In recent years, an increasing interest has been focused on the synthesis of 1,4-dihydropyridine compounds owing to their significant biological activity such as vasodilator, bronchodilator, anti-atherosclerotic, antitumor and antidiabetic activity. In particular, dihydropyridine drugs such as nifedipine, nicardipine, amlodipine and others are effective cardiovascular agents for the treatment of hypertension [1].

Numerous synthetic methods have been reported for the preparation of 1,4-dihydropyridine derivatives under classical or modified conditions [2]. However, these methods suffers from several disadvantages such as longer reaction times, excess of organic solvent, lower product yield, harsh refluxing condition, use of high temperatures, extensive reagents, occurrence of several side products and difficulty in recovery and reusability of the catalyst.

In continuation of our recent interest in the synthesis and derivatization of 1,4-dihydropyridines [3], Herein we report an effective and versatile procedure for the synthesis of 1,4-dihydropyridines derivatives by a multi-components reaction using L-proline (Scheme 1).



References:

[1] Shan, R.; Velazquez, C.; Knaus, E. E. *J. Med. Chem.* **2004**, *47*, 254.
[2] Ko, S.; Sastry, M. V. N, Lin, C, Yao, C. F. *Tetrahedron. Lett.* **2005**, *46*, 5771.
[3] Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K. *Molecules* **2009**, *14*, 1468.

Synthesis and application of acylated polyacrylic acid/SBA-15 composite for acylation of alcohols and amines

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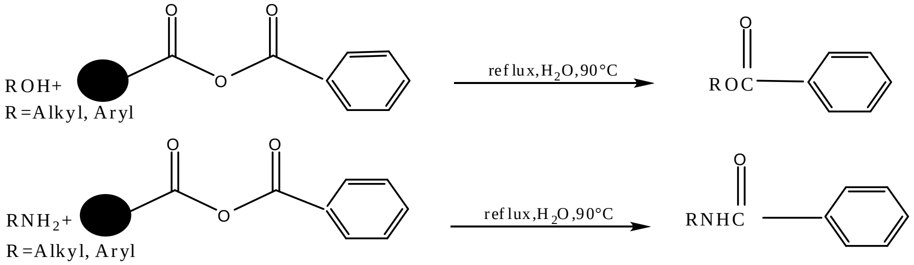
Acylation of alcohols and amines is of enormous interest in organic synthesis since it provides a useful and efficient protection protocol in a multi step synthesis process. Many of the chemical reaction involved in the synthesis of drugs frequently use acylation reactions in the preparation of drug candidates molecules [1]. Moreover, due to high importance of the acylation reactions in industry a search for new methods is demanded. Acylation is usually done by anhydride in the presence of an acid or base catalyst in a suitable organic solvent [2]. For instance the various catalysts developed for the activation of anhydride include nucleophilic agents such as Bu_3P and lewis acids such as $Sc(OTF)_3$, $Sc(NTF_2)_3$ TMSOTF, $Bi(OTF)_3$, $Cu(OTF)_2$, $TaCl_5$, Zeolites, Clays, Nafion –H, Yttria – Zirconia , and $LiClO_4$.

However, Bu_3P is flammable and undergoes aerial oxidation. Triflates are costly and moisture sensitive. Other major disadvantages of the existing protocols are harsh condition, harmful organic solvent and tedious workup procedures and formation of unwanted side products [3]. To over come such drawbacks and to make the reactions both economically and enviromentally advantagous a series of amides and esters and thio esters were prepared in moderate to good yields using acylated polyacrylic acid / SBA- 15 composite, as a heterogeneous acylating agent in H_2O. The results showed that when the aryl group in the substrate was a phenyl or a phenyl substituted by an electron donating group, the yields and rate of reaction drastically increased. All of the reaction products and polymeric composite were characterized with different methods such as FT-IR, H-NMR and XRD techniquos.



References:

[1] Streedhar, B.; Arunbhathi, R.; Amaranth Reddy, M.; Parthas, G, *Appl. Clay. sci*. **2009**, *43*, 425.
[2] Rajabi, F, *Tet. Let*. **2009**, *50*, 395.
[3] Chakraborti, A. K.; Gulhane, Jesh, *Tet. Let*. **2003**, *44*, 6749.

The study and interpretation of the effects of three different fillers (sillis, barite, calcium carbonate) over the chemical strength and the mechanical properties of the floor-coating carpets with the base of acrylic copolymer.

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The study and interpretation done on the basis of the effects of three different fillers on the acrylic carpets indicates that, the Barite Filler had the most type of strength, elasticity and some percentages of height expedition and above all the increase in vulnerability on the said carpets. However, Sillis Filler has the capacity to become quite appropriate in chemical strength, the over-range of elastic strength, and be the main cause of co-stricken strength, while the Calcium Carbonate Filler will decrease the above-mentioned chemical strength and the rest of mechanical properties of carpets with the acrylic basis. It is necessary to state that, the effect of the amount of PVC would have also been studied and the optimum sign has already been determined within the field. These kinds of covers include those resins with Poly Methyl-Meta basis, Fillers and Pigments; they also stand as the initiation into per-oxide and can be the cause of expedition. The Two-Part used resin of these systems is in-solvable and under-combined which needs the per-oxide initiation to be activated [1].

The Main Goal: the on-going project has studied the effects of different parameters such as Tensile strength and Filler Types (Barite, Silicon-Calcium-Carbonate) over chemical strength and also the Physical-Mechanical Properties such as thickness, co-stricken strength, elastic strength and vulnerability, the surface qualities of the carpets with the base of Acrylic Polymers has been interpreted within the field as well.

C0ncolution: improving Properties of the Floor-Coating .with high hardness and chemical strength

نسبتS-400/B-400	۱/۱	۱/۲	۲/۱
اجزاءرنگ	g	g	g
Tio_2	۱۵	۱۵	۱۵
$Baso_4$	۲۴/۵	۳۲/۶	۱۶/۴
Sio_2	۲۴/۵	۱۶/۴	۳۲/۶
RM-965	۳۶	۳۶	۳۶

References:

[1] Bassi r.roy S.K.Hand book of coating for concrete Scotland: whittles.pub, **2002**.
[2] Coyard H.Deligny P.Resins for surface coatings, vol.1, **2001**.
[3] Wypych eorge, Hand book of fillers, Canada: chem. tec. pub, **1999**.

Studies on graft copolymerization of 2-hydroxypropylemethacrylate onto CMC initiated by ceric ammonium nitrate

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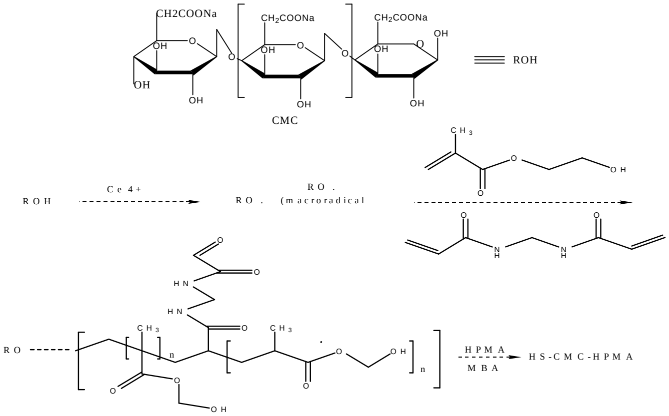
The Chemical modification of polysaccharide fibers by graft copolymerization of vinyl monomers with various initiators has received considerable attention during the past decades [1]. Depend on the nature of vinyl monomer used in the grafting onto polysaccharide, chemical and physical properties of initial polymer can be changed extensively.

The main goal of this paper is to use this method for improving property of a Carboxymethyl celloluse . The monomer used in this work is 2-hydroxypropylmetacrylate (HPMA).This monomer is grafted onto Carboxymethyl celloluse by using Ceric ammonuim nitrate (CAN) as an initiator by a free-radical mechanism.

The effect of various factors such as monomer, polysaccharide and initiator concentration, the temperature and the time of the reaction on the polymerization process were investigated. Optimization of these factors yield CMC grafted copolymer of with high percent of grafting [2].



References:

[1] P.A. Sandford. Chitosan and alginate: new forms of commercial interest. *Am. Chem. Soc. Div. Polym. Chem.* **1990**, *3*, 628.

[2] T. Lindmark, Y. Kimura, P. Artursson. Absorption enhancement through intracellular regulation of tight junction permeability by medium chain fatty acids in Caco-2 cells. *J. Pharmacol. Exp. Ther.***1998**, *284*, 362.

Silica sulfuric acid nanoparticles: An efficient and versatile reagent for synthesis of dihydropyrimidinone and triazole derivatives

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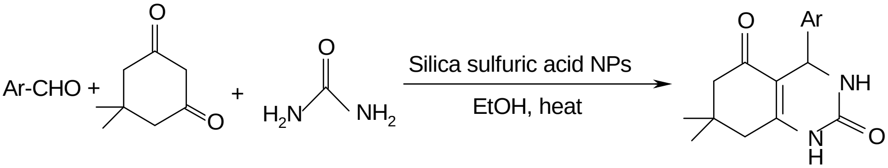
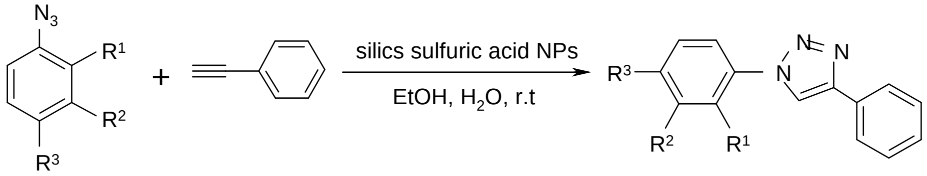
Dihydropyrimidinones have attracted increasing attention due to their significant pharmaceutical and therapeutic properties [1] such as antiviral, antitumor, antibacterial and anti-inflammatory activities.



The cycloaddition of azides to alkynes is one of the most important synthetic routs to 1H-[1,2,3]triazoles. N-heterocyclic compounds such as [1,2,3]-triazoles may display biological activities like anti-HIV, anti microbial activity and more [2].



The use of solid acides has many advantages over liquid acides such as ease of handling, decreasing reactor and environmentally safe disposal [3]. High surface area of porous solids makes them a good candidate for reagent support in heterogeneous reactions since the catalytic reactions take place on or near the catalyst's surface. In conclusion, we have successfully developed an efficient nano catalyst with 100-120nm particle size, for the synthesis of dihydropyrimidinone and triazole derivatives with improved yields.

References:

[1] Kappe, C. O. *Tetrahedron*, **1993**, *49*, 6937.
[2] Velazquez, S.; Alvarez, R.; Perez, C. *Antivir. Chem. Chemother*. **1998**, *9*, 481.
[3] Corma, A.; Garcia, H. *Catal.Today*. **1997**, *38*, 257.

Opening of epoxides with amines promoted by Silica bonded S-sulfonic acid: a mild and efficient method for the synthesis of *β*-amino alcohols

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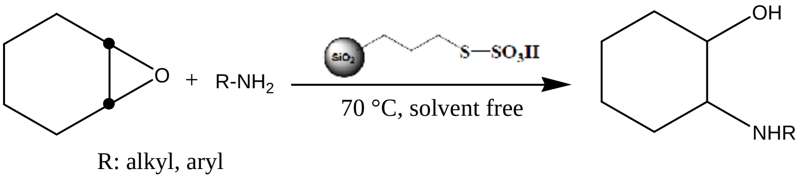
β-Amino alcohols are an important class of organic compounds due to their high occurrence in nature and their use as intermediates in the synthesis of natural products and pharmaceuticals [1]. The classical synthesis of β-amino alcohols involves the ring opening of epoxides with amines [2]. However, these reactions, which are generally carried out with large excess of amines at elevated temperatures, often fail when poorly nucleophilic amines or sterically crowded amines/epoxides are concerned. A variety of activators or promoters such as metal amides, metal triflates and transition metal halides have been developed to perform the epoxide ring opening reactions with amines under mild conditions [3]. However, many of these methods often involve the use of expensive and stoichiometric amounts of reagents, poor regioselectivity especially with metal amides derived from primary amines, extended reaction times and also entail undesirable side reactions such as rearrangement of the oxiranes to allyl alcohols under basic conditions [4] or polymerization in strongly acidic conditions resulting in low yields of the desired products.

In this article we introduced a new method for the preparation of β-Amino alcohols , by the reaction of epoxides with amines in the presence of Silica-bonded *S*-sulfonic acid (SBSSA) as catalyst at 70 °C in good to excellent yields.



Refrences:
[1] Joossens, J.; Van der Veken, P.; Lambeir, A. M.; Augustyns, K.; Haemers, A., J. *Med. Chem.* 2004, 47, 2411.
[2] Hodgson, D. M.; Gibbs, A. R.; Lee, G. P. *Tetrahedron* 1996, 52, 14361.
[3] Das, U.; Crousse, V.; Kesavsn, V. Daniele, B. D. Begue, J. P. *J. Org. Chem*. 2000, 65, 6749.
[4] Yamada, J.; Yumoto, Y.; Yamamoto, Y. *TetrahedronLett*. 1989, 30, 4255.

ZnO Nanoparticles: A highly efficient nanocatalyst for *N*-formylation of primary and secondary amines under solvent free condition

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Nanoscale oxide particles are gaining increasing technical importance for classic areas of application such as catalysts, passive electronic components, or ceramic materials [1,2]. Zinc oxide nanoparticles are certainly one of the most interesting multifunctional of metal oxides, because it has surface properties which suggest that a very rich organic chemistry may occur there.

Formamides are important intermediates in the synthesis of carbonyl compounds. A number of methods have been reported for the formylation of amines [3]. Many of these methods have disadvantages such as expensive and toxic reagents and catalysts, long reaction times, high temperature, side products formation, tedious work-up procedure and difficult accessibility to reagents.

Here we describe the use of ZnO nanoparticles (NAP-ZnO) as a simple and efficient heterogeneous eco-friendly catalyst for *N*-formylation of different amines (Scheme 1). Our protocol avoids the use of expensive reagents and the reaction performed under solvent free condition serves as an efficient method. We believe that the present methodology could be an important addition to the existing methodologies.

$$R^1R^2NH \quad + \quad HCO_2H \xrightarrow[70\ ^{o}C,\ \text{Solvent-free}]{\text{ZnO nanoparticles (2 mol\%)}} R^1R^2NCHO$$

R^1 = H, alkyl, aryl
R^2 = alkyl, aryl

References:

[1] Feldmann, C.; Jungk, H. *Angew. Chem. Int. Ed.* **2001,** *40*, 359.

[2] Wang, Y.; Ma, C.; Sun, X.; Li, H. *Inorg. Chem. Commun.* **2002**, *5*, 751.

[3] (a) Chandra Shekhar, A.; Ravi Kumar, A.; Sathaiah, G.; Luke Paul, V.; Sridhar, M.; Shanthan Rao, P. *Tetrahedron Lett.* **2009**, *50*, 7099; (b) Desai, B.; Danks, T. N.; Wagner, G. *Tetrahedron Lett.* **2005**, *46*, 955.

Synthesis and application of novel functionalized silica bonded calix in heterogeneous and acid catalytic reactions

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From the "Green Chemistry" point of view, it is essential to develop new catalysts which can be recovered after the reaction and re-used several times.In this context, heterogeneous catalyst is emerging as an alternative to homogeneous process, because of their high efficiency, low toxicity and reusability[1].One strategy to transform a homogeneous into heterogeneous process is to anchor the active site onto a large surface solid carrier provided that the anchoring methodology maintains the intrinsic activity and selectivity of the catalytic center[1].Among various inorganic solid support, silica is usually preferred since it displays many advantageous properties-excellent stability(chemical, thermal), high surface area, good accessibility and organic groups can be robustly anchored to the surface, to provide catalytic centers[2].

Calixarenes as a macrocyclic molecule are receiving increasing attention because of their application in diverse areas such as host-gust chemistry, selective ion transport, sensors and catalysis[3].In the calixarene family, calix[4]arenes are the most popular because of their rigid structures which make them candidates complexation studies with ions and neutral molecules[4].

The main objective of the present work is the synthesis the new heterogeneous catalyst based on functionalized calix[4]arene.The covalently bonding of chlorosulfonated calix[4]arene directly on to the silica surface is schematically illustrated in figure 1.

Solide state NMR, elemental analysis , XRD, TGA, BET, TPR, TPD can be used to characterize catalyst.The catalytic activity of obtained silica bonded calixarene was investigated for the heterogeneous acid catalyst reactions such as phenol formaldehyde condensation, ester and amide hydrolyses.

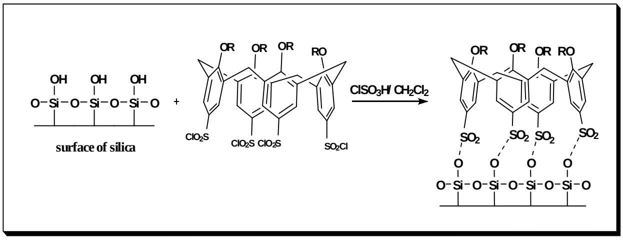

Figure 1

Reference:
[1] Choudhary, D.; Paul, S.; Gupta, R.; Clark, J. H. Green Chem. **2006**, 8, 479.
[2] Gupta, Raman ; Paul, S.; Gupta Rajive, J. Mol. Cata. A: Chem. **2007**, 266, 50.
[3] Patra, S.; Suresh, E.; Paul, P. Polyhedron, **2007**, 26, 4971.
[4] Notestein, J. M.; Iglesia, E.; Katz, A. J. Am. Chem. Soc. **2004**, 126, 16478.

Regiospecific reduction of triarylpyrylium salts using task specific ionic liquid [bmim]BH_4 as a new hydride donor

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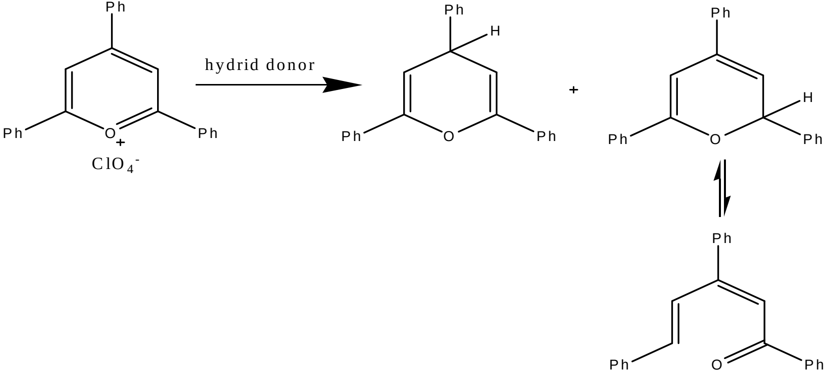
The heteroaromatic pyrylium ions are fundamental heterocyclic systems .Owing to their high reactivity towards nucleophiles and the biological importance of the reduction products, a number of reductions of this compound carried out in the present of some hydride donors [1]. Typically hydride donors can attack pyrylium salts either in α-position or in γ-position and leading to corresponding 2H-pyrans (I) and 4H-pyrans (II) respectively (Scheme) [2].



(Scheme)

According to special properties of ionic liquids as reagent [3].we decided to study the reduction of triarylpyrylium salts in the presence of new hydride donor [bmim]BH_4. The results revealed regio-specificity and good yield for products.

References:

[1] Balaban, A. T.**;** Fischer, G. W. *Advances in Heterocyclic Chemistry* **(1982)**. In: A. R. Katritzky (Ed). *Pyrylium salts: syntheses, reactions, and physical properties*. Academic Press. Inc. (London) LTD., 30-35.
[2] A.T. Balaban, G. Mihai,and T. Mukai, *Heterocycles*, 4,739,**(1976).**
[3] Wang, J.**;** Song, G.**;** Peng, Y. *Tetrahedron Lett*. (**2008).**

The investigation of the synthesis possibility of 5-phenyl-2-alkyl-2H-tetrazole

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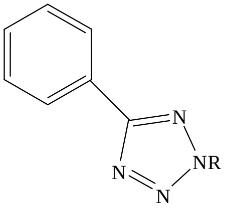
A number of tetrazole derivatives exhibit biological activities and have found applications as carboxylic surrogates [1]. The development of tetrazole chemistry during the past 20 years can be ascribed to their diverse applications in medicine, biochemistry, agriculture, photography information recording systems, explosives and others [2,3]. Various modifications of the structure of tetrazoles have been carried out in order to obtain compounds with different physicochemical properties and subsequently with different pharmacodynamic and pharmacokinetic properties [4]. Novel methods of synthesis of substituted tetrazoles have been developed in recent years, including a simple and effective alkylation method for the synthesis of mono - and di -substituted tetrazoles with various frameworks [5].

In this research work, we described the synthesis of new compounds of these families. Therefore benzaldehyde **(1)** was converted to benzaloxime **(2)**, by using NH_2OH, dehydration of compound **(2)** with acetic Anhydride obtained benzonitrile**(3)**. The 5-phenyl-2H-tetrazole **(4)** was synthesized by [3 + 2] cycloaddition reaction between compound **(3)** and NaN_3. The alkylation of tetrazole **(4)** with alkyl halids , produced the 5-phenyl-2alkyl-2H- tetrazole **(5)**. Also, the reaction of tetrazole **(4)** with epichlorohydrin resulted 1-chloro-3-(5-*p*-tolyl-2H-tetrazol-2-yl)propan-2-ol **(6)**.

The structures of all the synthesized compounds were confirmed by FT- I R and ^{1}HNMR spectroscopies.



References:

[1] Herr, R. J. J. *Bioorg. Med. Chem.* **2002**, *10,* 3379.
[2] Sosnowska, N. S. J. *Org. Chem.* **2001**, *66*, 8737.
[3] Koldobskii, G. I. Ostrovskii, V. A. *Russ. Chem. Rev.* **1994**, *63,* 797.
[4] Hrabalek, A. Myznikov, L. Kunes, J. Vavrova, K. Koldobskii, G. *Tetrahedron Lett.* **2004**, *45*, 7955.
[5] Couri, M. R. Luduvico, I. Santos, L. Alves, R. Prado, M. A. Gil, R. F. *Carbohydrate Reserch,* **2007**, *342*, 1096.

Experimental measurement of diffusion coefficient of volatile organic compounds

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Molecular diffusion is a mass transport process. The diffusion is generally governed by molecular size, shape and mass of permeant [1]. Diffusion coefficient is important for many industrial and research areas, as for example, extraction of essential oils, membrane manufacture, distillation, de-volatilization and and the effectiveness of reactors at high conversion [2,3].

The aim of this work is to measure the diffusion coefficient of acetone at 313.15 K by using the evaporation method in a capillary T-shaped tube by using Fick's law [4]. Acetone was placed in a 100 mm height, 2mm ID tube. The height of acetone in tube was 35 mm. The tube was mounted in a gland on top of the water batch and connected to the air pump. The volume rate of air that passed over the test tube was 95 ± 5 mL/min. The amount of air volume rate was assumed to be adequate so as to ensure that the concentration of the acetone at the top of the tube was zero. The diffusion occurred over a period six hours, with readings taken each half-hour by catheometer.

The diffusion coefficient was calculated to be 0.1733 ± 0.005 cm2/s at T = 313.15 K. Our results were compared using the Chapman-Enskog equation as well as the Fuller et al method. The diffusion coefficient calculated by the Chapman-Enskog [5]. Was 0.1107 cm2/s and the result of the Fuller et al method [5]. was 0.1196 cm2/s. The literature value found in references was 0.125 ± 0.004 cm^2/s [6]. The agreement of our method with the other methods available for calculating the diffusion coefficient was reasonable and also agreed well with the literature value found. This led to a conclusion that this method of determining the diffusion coefficient of acetone into air can be aconsiderrd a reliable method.

References:

[1] Khayet, M.; Cojocarub, C., Separation and Purification Technology, **2008**, *63*, 303.
[2] Reisa, R.; Nobregab, R., Chemical Engineering Science, **2005**, *60*, 4581.
[3] George D. Verros, Journal of Membrane Science **2009**, *328*, 31.
[4] Christie J. Geankoplis; Transport Processes and Unit Operations (3th Edition), **1998**, 432.
[5] Poling; Bruce E; Prausnitz, Properties of Gases and Liquids (5th Edition), **2001,** 623.
[6] Richard G. Griskey, Transport Phenomena and Unit Operations, **2002**, 252.

Environmentally friendly one-pot synthesis of benzimidazoles in the presence of $Fe(HSO_4)_3$ under aqueous conditions

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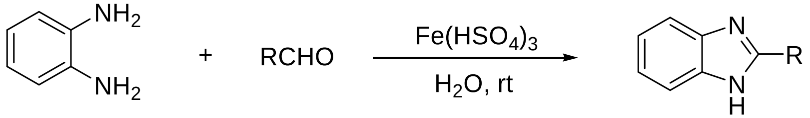
Benzimidazoles and their derivatives are the important intermediates for pharmaceutical and biological fields. They have been used as antiulcerative, antihypertensives, antivirals, antifungals, anticancers, antitumor, antihistamines and antihelminithic agents [1]. The most popular method for synthesis of benzimidazoles is the coupling of phenylendiamines derivatives with carbonyl compounds like carboxylic acid, nitriles, imidates, orthoesters and aldehydes which often requires strong acidic conditions and sometimes very high temperatures [2].

Various catalysts which also act as oxidative reagent have been used for this purpose like sulfamic acid, DDQ, Oxone, $FeCl_3.6H_2O$, $In(OTf)_3$, Yb(OTf), $Sc(OTf)_3$ and $KHSO_4$ [3].

In this work we used a versatile method for the synthesis of benzimidazoles from the reaction of *ortho*-phenylendiamin with different aldehydes in presence of $Fe(HSO_4)_3$ as an oxidative catalyst. All the reactions were preceded in water as an environmentally benign solvent with high yields and easy isolation of products at room temperature.



References:

[1] Niknam, K.; Fatehi-Raviz, A. *J. Iran. Chem. Soc.*, **2007**, *4,* 438.
[2] Lin, S.; Yang, L. *Tetrahedron Lett.* **2005**, *46*, 4315.
[3] Xiangming, H.; Huiqiang, M.; Yulu, W. *ARKIVOC*, **2007**, 150.

Atom transfer radical polymerization and nitroxide mediate radical polymerization of styrene onto poly(ethylene terephthalate)

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Poly(ethylene terephthalate) (PET) is a semi-crystalline thermoplastic polyester used in many fields. For a variety of applications, however, it is necessary to impart desired properties by introducing specific functional groups on the surface. A simple method for growing polymer brushes by Atom Transfer Radical Polymerization (ATRP) on PET was devised. The PET surface was first reacted with 1,3-diaminopropane by aminolysis reaction to incorporate primary amino and alcohol functions on the surface (PET-NH_2). Then, in a second step, α-phenyl chloro acetyl chlorid was grafted with aminated PET (PET-Cl) [1]. The efficiency of these reactions was confirmed by using ATR-FTIR spectra.

Surface-initiated ATRP was performed using styrene monomer with CuCl/b.pyridine (PET-g-PS).

For Nitroxide Mediate Radical Polymerization (NMRP) method 1-hydroxy-2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO-OH) was coupled with acetylated PET (PET-TEMPO). The graft copolymerization of styrene was initiated by PET-TEMPO carrying TEMPO groups as a macroinitiator [2,3].

References:

[1] Loïc Bech; Tamara Elzein; Thierry Meylheuc; Arnaud Ponche; Maurice Brogly;Bénédicte Lepoittevin; Philippe Roger **.** *Eur. Polym. J.* **2009**, *45*, 246.
[2] Abbasian, M., Namazi, H., Entezami, A., *Polym. Adv. Technol.* **2004**, *15,* 606.
[3] Entezami, A.; Abbasian, M, *Iranian Polymer Journal (review)* **2006**, *15*, 583.

Investigation the reductive elimination from platinum(IV) structures by B3LYP method

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The reductive elimination reaction leading to formation of C-C, C-H, and C-X bonds is one of the most fundamental steps in many catalytic reactions. The importance of reductive elimination has prompted numerous researchers to study this process [1]. In this regard, much attention has been paid to the reductive elimination from d^6 octahedral complexes particularly from Pt(IV) complexes. The reductive elimination from Pt(IV) complexes gives the Pt(II) d^8 complexes adopting square planar geometries[2]. In this study, we have used the B3LYP method to investigate the reductive elimination from platinum(IV) structures of the form L_2PtR_4 where L = PMe_3, PH_3, PF_3, PC_{l3}, CO, NH_3 and R = vinyl, Me. We conclude that reductive elimination occurs via the L-predissociation pathway for R = Me, irrespective of ligand L. But when R = vinyl, direct elimination is the preferred pathway if the L ligand is PMe_3; otherwise both pathways are competitive for R = vinyl. We also note that if L is more electron withdrawing and less electron donating, the reductive elimination from the six coordinate complexes L_2PtR_4 will be more rapid. Reductive elimination from the five coordinate complexes $LPtR_4$ proceeds more easily if the ligand trans to the two R groups being coupled is more electron donating and the ligands cis to the two R groups are more electron withdrawing.

References:

[1] Ariafard, A.; Brian F. Yates. *Journal of Organometallic Chemistery* . **2009**, *10*, 1016.
[2] Ejei, Z.; M. Sc. Thesis, Azad University, Iran, **2009**.

An efficient and practical synthesis of new derivatives of indoles catalyzed by starch-sulfuric acid under ultrasonic irradiation

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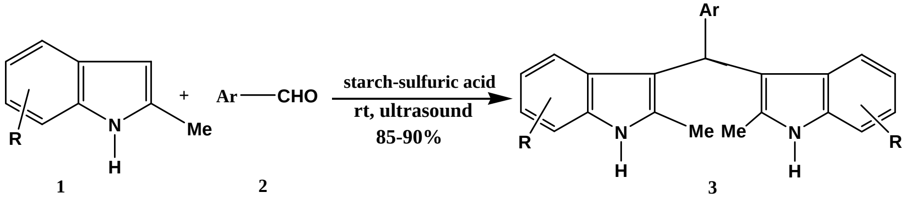
Indole derivatives are found abundantly in a variety of natural plants and exhibit various physiological properties and are potentially bioactive compounds. Bis(indolyl)methanes (BIM) are the most active cruciferous substances for promoting beneficial estrogen metabolism in woman and men [1]. They are also effective in the prevention of cancer due to their ability to modulate certain cancer causing estrogen metabolites [2,3].

In recent years, several synthetic methodologies have been devised for the synthesis of bis(indolyl)methanes [4] and some of them employ expensive reagent or harsh reaction conditions. Herein we wish to report an efficient method for the synthesis of new derivatives of bis(indolyl)methanes catalyzed by starch-sulfuric acid, under ultrasonic irradiations (Scheme 1). Starch-sulfuric acid a newly introduced [5] biosupported solid acid catalyst in the presence ultrasonic irradiation furnished the desired bis(indolyl)methanes in excellent yields (85-90%) and short reaction times (5-10 min) (Scheme 1).



R = alkyl, Cl, Br, etc.

Scheme 1

References:

[1] Zeligs, M. A. *J. Med. Food* **1998**, *1*, 67.

[2] Michnovicz, J. J.; Bradlow, H. L. *Food Phytochemicals for Cancer Prevention*, in: M.J. Huang, T. Osawa, C. T. Ho, R. T. Rosen (Eds.), American Chemical Society, Washington, DC, **1994**, 282.

[3] Banerji, J; Dutta, U.; Basak, B.; Saha, M.; Budzikiewicz, H.; Chatterjee, A. *Indian J. Chem. B* **2001,** *40*, 981.

[4] Babu, G.; Sridhar, N.; Perumal, P. T. *Synth. Commun.* **2000**, *30*, 1609; Shun-Jun, J.; Min-Feng, Z.; Da-Gong, G.; Shun-Yi, W.; Teck-Peng, L. *Synlett* **2003**, 2077; Bandgar, B. P. ; Shaikh, K. A. *Tetrahedron Lett.* **2003**, *44*, 1959.

[5] Shaabani, A.; Rahmati, A.; Badri, Z. *Catal. Commun*. **2008**, *9*, 13.

Three-component synthesis of dialkyl 2-((cyclohexylimino)methylene)-3-(arylsulfonylamino)succinate

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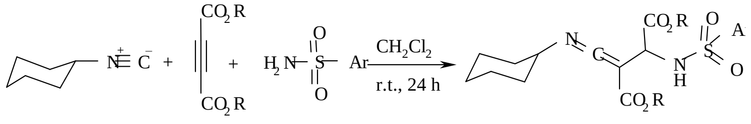
Multi-component reactions (MCR) have been received great attention from chemists because they can be widely employed for the rapid assembly of arrays with high molecular diversity [1].

Ketenimines are important reactive intermediates that occur as transient compounds in many thermal and photochemical reactions. There has been intense interest in their addition reactions, such as cycloaddition, nucleophilic, and electrophilic addition [2]. Ketenimines have been extensively used in organic synthesis as versatile building blocks for the preparation of a large variety of cyclic compounds via inter- or intramolecular cycloaddition reactions.

Although the trapping of the 1:1 intermediate formed between dialkyl acetylenedicarboxylate and isocyanides with OH, NH, and CH acids has been widely studied,[3] trapping of the initially formed 1:1 intermediate with arylsulfonamides has not been reported. In the course of our works on the reaction between isocyanides and acetylenic esters, [4] here we wish to report a simple one-pot three-component reaction between cyclohexyl isocyanides, **1** dialkyl acetylenedicarboxylates **2** and arylsulfonamide **3** leading to dialkyl 2-((cyclohexylimino)methylene)-3-(arylsulfonylamino) succinate derivatives **4.**



1 **2** **3** **4**

References:

[1] Ugi, I.; Werner, B.; Domling, A. *Molecules*. **2003**, *8*, 53.
[2] Fromont, C.; Masson, S. *Tetrahedron* **1999**, *55*, 5405.
[3] Anary-Abbasinejad, M.; Moslemine, M. H.; Anaraki-Ardakani, H. *J. Fluorine. Chem.* **2009**, *130*, 368.
[4] Anary-Abbasinejad, M.; Mosslemin, M. H.; Anaraki-Ardakani, H. *Synlett.* **2009**, *16*, 2676.

Coupling of thiols to disulfides by urea-hydrogen peroxide (UHP) in the presence of Manganese and Iron Schiff base complexes

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Disulfide bond formation is important in organic synthesis, in biologically active molecules and for protein stabilization and in peptides [1]. Industrially, they find wide application as vulcanizing agent for rubber and elastomers, imparting them excellent tensile strength [2].

There are several oxidative methods for the synthesis of disulfides from thiols and protected thiols. Recently many mimic biological systems for their high efficiency and mild condition have been investigated. In this direction, metalloporphyrines and metal tetradentate Schiff base complexes are systems that have been used as efficient catalysts in the presence of different oxidants [3-6]. Between the different oxidants, urea-hydrogen peroxide (UHP) has many advantages for oxidation reaction because it is an adour-less, safe, non-toxic and easy to use.

In this work at first step, bis(2-hydroxybenzylidene)-4-methyl-1,2-benzenediamine and their Mn(III) and Fe(III) Schiff base complexes are prepared and catalytic activity of these complexes for oxidative coupling of thiols to disulfides was investigated. Various parameters for reactions such as axial ligand, solvent, amount of oxidant and catalyst amount were optimized. The results showed good catalytic activity of Mn(III) Schiff base complex with respect to Fe(III) complex for the oxidation of a variety of aromatic thiols in high to excellent yields within 5-90 minutes.

$$2RSH \xrightarrow[\text{Imidazol, CH}_3\text{OH}]{\text{Mn(III) or Fe(III)complexes/UHP}} RSSH$$

References:

[1] a) Ogawa, A.; Nishiyama, T.; Kambe, N.; Murai, S.; Sonada, N. *Tetrahedron Lett.* **1987**, 28, 3271. b) Jahnson, J. R.; Bruce, W. F.; Dutcher, J. D. *J. Am. Chem. Soc.* **2005**, 65, 1943
[2] Ramados, K.; Srinivasan, N. *Synth. Commun.* 1995, 25, 227.
[3] Karami, B.; Montazerozohori, M.; Moghadam, M.; Habibi, M. H.; Niknam, K. *Turk. J. Chem.* **2005**, 29, 539.
[4] Karami, B.; Montazerozohori, M.; Habibi, M. H. *J. Chem. Res.* **2006**, 490.
[5] Golchoubian, H.; Hosseinpoor, F. *Catal. Commun.* **2007**, 8, 697.
[6] Karami, B.; Montazerozohori, M.; Nasr-Esfahani. M. *Hetrocycles.* **2005**, 65, 2181.

Copper catalyzed cross-coupling of vinyl halides with aromatic and aliphatic thiols in the presence of KF/Al_2O_3

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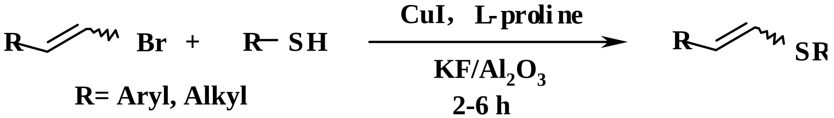
Aryl and alkenyl sulfides are important building blocks present in a great number of natural and/or medicinal products and versatile reagents in organic synthesis [1]. Various methods for their syntheses have been explored. Among them the addition of thiols to alkynes by free radical conditions or by anionic addition conditions is one of the most straightforward methods to obtain vinyl sulfides [2]. The valuable protocol to gain the vinyl sulfides is the cross-coupling of thiols with the alkenyl halide under the catalysis of transition metal complex in a stereospecific manner [3-4].

Here we wish to report cross-coupling of vinyl bromides with thiols catalyzed by CuI/L- proline in presence of KF/Al_2O_3 (Scheme 1).



Scheme1

In this report, various vinyl sulfides were prepared by the reaction of appropriate aryl and alkyl thiols with vinyl halides under optimum conditions. Yield of the reactions were excellent and all the products were characterized by ^{1}HNMR spectra, melting point and comparison with authentic samples.

Reference:

[1] (a) Hynes, J. Jr.; Nasser, T.; Overmann, L.; Watson, D.A.; *Org. Lett.* **2002,** 4, 929. (b) Ogawa, A.; Ikeda, T.; Kimura, K.; Hirao, T. *J. Am. Chem. Soc*. **1999**, 12, 5108.
[2] (a) Benati, L.; Capella, L.; Montevecchi, P. C.; Spagnolo, P. *J. Chem. Soc., Perkin Trans*. **1995**, 1, 1035. (b) Griesbaum, K. *Angew. Chem., Int. Ed. Engl*. **1970**, 9, 273.
[3] Bryan. C. S; Braunger. J. A; Lautens. M. *Angew. Chem. In. Ed*. **2009**, 48, 7064.
[4] Guo. S. R; Yuan. Y. Q. *Synthetic Commun*. **2008**, 38, 2722.

A facile, environmentally benign method for the solvent-free synthesis of *N,N*-dialky sulfonamides under microwave irradiation

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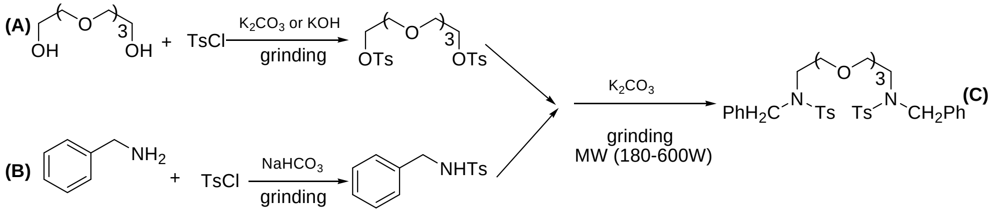
Sulfonamides have long been a research area as a result of their pharmaceutically importance widely used as antibacterials, diuretics, anticonvulsants, hypoglycemic, and HIV protease inhibitors [1]. In addition, *N,N*-dialkylated sulfonamides constitute a class of pharmaceutically important [2] compounds and can be use for synthesis of secondary amines by subsequent desulfonation.

Herein, an easy and convenient solvent-free method for *N*-alkylation of *N*-monosubstituted sulfonamides has been developed. In this way, reaction of primary and secondary alcohols **(A)** [3] and primary amines **(B)** [4] by tosylchloride under grinding condition, has been carried out which led to tosylated starting materials and thereafter the reaction of tosylated amines and alcohols under microwave irradiation have produced the variety of *N,N*-dialkyl sulfonamides **(C)** containing two various *N*-substituents alkyl or aryl groups in high yields.



References:

[1] Hansch, C.; Sammes, G.; Taylor, J. B. *In Comprehensive Medicinal Chemistry;* Pergamon Press: Oxford, **1990**; Vol. 2, Chapter 7.1.
[2] Huang, Z. H.; Lin, Z. L.; Huang, J. L. *Eur. J. Med. Chem.* **2001**, *36*, 863.
[3] Kazemi, F.; Massah, A. R.; Javaherian, M. *Tetrahedron.* **2007**, *63*, 5083.
[4] Massah, A. R.; Kazemi, F.; Alizadi, D.; Shakiba, F.; Aliyan, H.; Javaherian Naghash, H.; Momeni, A. R. *Letters in Organic Chemistry,* **2006**, *3*, 253.

Multicomponent synthesis of pyrano[2,3-c]pyrazol-6-one derivatives under aqueous and ultrasonic conditions

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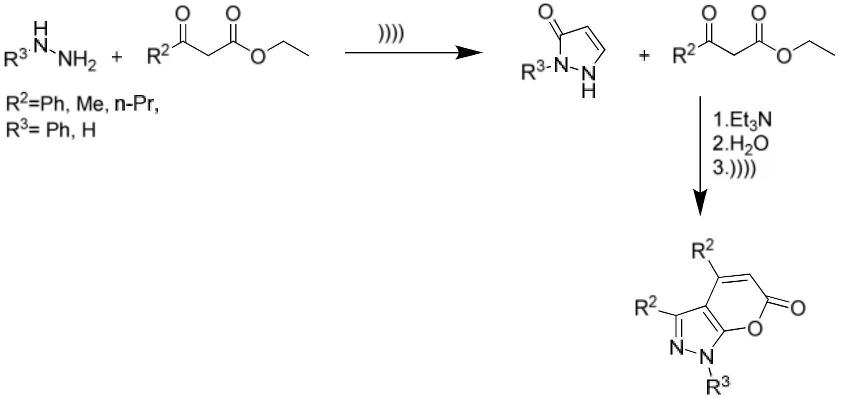
Heterocyclic derivatives containing the pyrazolone core are of particular importance in pharmaceutical chemistry [1] due to their numerous applications as analgesic, antipyretic, antiarthritic, uricosuric, antiinflammatory, and antiphlogistic properties. Particularly, the 3-methyl-1-phenyl-2-pyrazolin-5-one derivative (edaravone) [2] acts as a radical scavenger to interrupt the preoxidative chain reactions and membrane disintegrations associated with ischemia [3]. In addition, these compounds are appropriate precursors for industrial preparation of herbicides products [4].

In the framework of our investigations on the development of green chemical procedures [5], we would like to herein report a novel and environmentally safe procedure for rapid preparation of various derivatives of the title compounds using aqueous triethylamine ultrasound irradiation.



References:

[1] T. Ueda, H. Mase, N. Oda, I. Ito, Chem. Pharm. Bull. **1981,** 29, 3522.
[2] H. Nakagawa, R. Ohyama, A. Kimata, T. Suzuki, N. Miyata, Bioorg. Med. Chem. Lett. **2006**, 16, 5939.
[3] H. Kawai, H. Nakai, M. Suga, S. Yuki, T. Watanabe, K.I. Saito, J. Pharmacol. Exp. Ther. **1997**, 281, 921.
[4] C. Cativiela, J.L. Serrano, M.M. Zurbano, J. Org. Chem. 60 (**1995**) 3074.
[5] M.M. Mojtahedi, E. Akbarzadeh, R. Sharifi, M.S. Abaee, Org. Lett. 9 (**2007**) 2791.

An efficient synthesis of 2-mercaptopyrimidine containing dialkyl 2-(alkyl- or arylcarbamothioyl)-2-butenedioates via a multicomponent reaction

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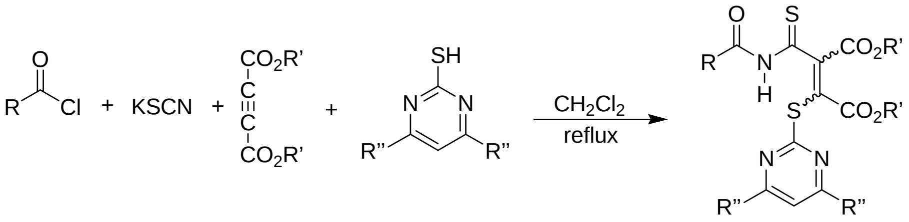
When conducting multicomponent reactions (MCRs) an organic chemist tries to combine three or more reactants in an in situ method. The resulting target molecule has all reactants incorporated in the molecular structure [1-3]. Pyrimidine derivatives have been employed in a wide range of medicinal chemistry because of their diverse biological activities [4-5]. Owing to the increasing importance of entitle structures, we wish to describe an efficient synthetic route of the dialkyl 2-(acetyl- or benzoylcarbamothioyl)-3-(pyrimidin-2-ylthio)-2-butenedioate derivatives. All compounds have been characterized by IR, ^{1}H- NMR, ^{13}C-NMR and Mass spectroscopy.



R: Me, Phenyl
R': Me, Et, *t*-butyl
R": H, Me

References:

[1] Armstrong, R. M.; Combs, A. P.; Tempest, P. A.; Brown, S. D, Keating, T. A. *Acc. Chem. Res.*, **1996**, *29*, 123.
[2] Ganem, B. *Acc. Chem. Res.* **2009**, *42*, 463.
[3] Yavari, I.; Hossaini, Z.; Sabbaghan, M.; Ghazanfarpour-Darjani, M. *Mol. Diverse.* **2009**, 13, 295.
[4] Wolf, J. F.; Ratham, T. L.; Sleevi, M. C.; Campbell, J. A.; Greenwood, T. D. *J. Med. Chem.* **1990**, *33*, 161.
[5] Sikora, E.; Jakcman, A. L.; Newell, D. R.; Calvert, A. H. *Biochem. Pharmacol.* **1988**, *37*, 4047.

Sesquiterpene lactones from centaurea golestanica

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The large genus *Centaurea* (Asteracea) comprises about 500 species, which are predominately distributed around the Mediterranean area and in West Asia.

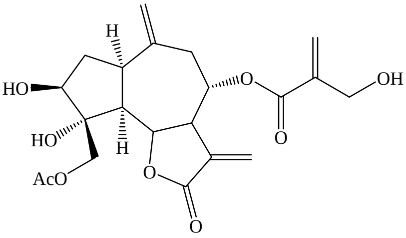
Centaurea golestanica, is an Iranian endemic species distributed in Golestan province of Iran. No previous phytochemical study has been performed on *C. golestanica*.

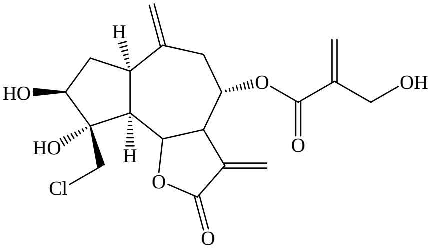
Characteristic constituents of Centaurea species, which are used in folk medicine, are by order of their abundance, guaianolides, germacranolides, elemanolides and eudesmanolides [1].

In the continuation of our work on Iranian medicinal plants [2, 3], herein we isolated main chemichal constituents of *Centaurea golestanica* and elucidated their structures.

From the acetone extract of the aerial parts of Centaurea golestanica two sesquiterpene lactones, belonging to the guaiane class, were isolated by chromatographic methods (on silicagel and sephadex LH-20 column) and identifed, together with two known flavanoids and two Sterols.

All structures were elucidated by spectroscopic methods including one- and two-dimensional homo- and heteronuclear NMR experiments.





References:

[1] Matloubi-Moghaddam, F.; Moridi Farimani M.; Salahvarzi S., Amin G. *eCAM,* **2007,** *4(1),* 95, *4*, 199.

[2] Matloubi-Moghaddam, F.; Moridi Farimani M.; Amin G. *Iranian Journal of DARU,* **2000**, No.3&4..

[3] Bermejo, J.; Creche, J.; Bentamene, A.; Benayache, S.; Benayache1, F. *Chemistry of Natural Compounds* **2007**, *43*, 749.

Aerobic oxidation of alcohols catalyzed by copper nanoparticles-polyacryl amide/SBA-15 composite

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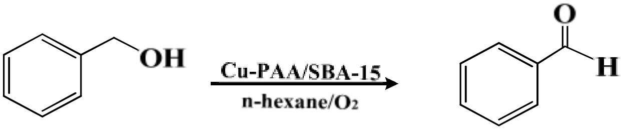
Selective oxidation of alcohols to the corresponding aldehydes or ketones with molecular oxygen has attracted much attention from the viewpoint of establishing green chemical processes for the synthesis of carbonyl compounds, which are important and versatile intermediates for the production of fine chemicals. Many homogeneous catalysts, especially palladium, ruthenium and copper complexes or compounds, could efficiently catalyze the aerobic oxidation of alcohols [1,2]. Heterogeneous catalysts possess obvious advantages in product isolation and catalyst recycling use, and have thus received growing interest in the past years. On the other hand, owing to their extraordinary size and shape dependant properties, numerous nanomaterials based on various metals and metal complexes have been synthesized and characterized during the past few years [3]. There are many polymer/nanoparticle composite materials, and optimal control over the structure of the composite could be achieved by preassembling the inorganic nanoparticles with the organic polymer [4].

In this study, we presented a novel method to synthesis and characterization of a new heterogeneous hybrid polymer-inorganic catalyst in which the copper nano-particles are highly dispersed and grafted on the polymer/SBA-15. Copper nanoparticles-polyacrylamide (PAA)/SBA-15 composite catalyst have been prepared by in situ polymerization and tested for liquid-phase oxidation of alcohols with molecular oxygen. The physical and chemical properties of Cu-PAA/SBA-15 were investigated using FT-IR, XRD, BET, SEM and TGA techniques. The effects of reaction temperature, solvent and the amounts of catalyst as well as recyclability of the catalyst were investigated. The catalyst was very stable and could be reusable for more than six times without losing activity.



References:

[1] Stahl, S. S. Angew. *Chem. Int. Ed.* **2004**, *43*, 3400.
[2] Caspi, D. D.; Ebner, D. C.; Bagdanoff, J. T.; Stoltz, B. M. *Adv. Synth. Catal.* **2004**, *346*, 18. Ali, S.R.; Bansal, V.K.; Khanb, A.A.; Jainc, S.K.; Ansarid, M.A. *J. Mol. Catal. A. Chem.* **2009**, *303*, 60.
[3] Wei, Qing-Bo.; Luo, Yan-Ling.; Zhang, Chang-Hu.; Fan, Li-Hua.; Chen, Ya-Shao. *Sen. Act. B*. **2008**, *134*, 49.

A greener rout for the one pot synthesis of five-membered heterocycl rings based on imidazole and imidazoline derivatives using Iron(III) phosphate

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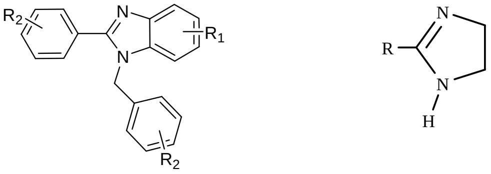
Benzimidazoles are important biologically active heterocycles possessing selective neuropeptide YYI receptor antagonists and so on [1-3]. Consequently, a variety of methods have been developed for the preparation of substituted benzimidazoles [4]. Since benzimidazole drivatives are useful and important in the field of drugs and harmaceuticals, the development of simple, convenient, high yielding and environmentally benign protocols is desirable. Therefore, the search continues for a better catalyst for the synthesis of benzimidazoles, in terms of operational simplicity, economic viability and selectivity. Also, imidazoline derivatives are of great importance because they exhibit significant biological and pharmacological activities.

In this study, 2-Aryl-1-arylmethyl-1H-benzimidazoles and 2substituted-imidazolines are selectively synthesized in high yields under extremely mild conditions via the condensation of 1,2-diamines with aromatic and aliphatic aldehydes and nitriles using catalytic amount of Iron(III) phosphate under solvent free conditions (Scheme 1). The use of readily available Iron (III) phosphate as a reusable and recyclable catalyst makes this process quite simple, convenient, and environmentaly-friendly.



Scheme 1

References:

[1] Zarrinmayeh, H.; Nunes, A.M.; Ornstein, P.L.; Zimmerman, D.A.; Gackenheimer, S.L.; Bruns, R.F.; Hipskind, P.A.; Britton, T.C.; Catrell, B.E.; Gehlert, D.R. *J. Med. Chem.* **1998**, *41*, 2709.

[2] Nakano, H.; Inoue, T.; Kawasaki, N.; Miyataka, H.; Matsumoto, H.; Taguchi, T.; Inagaki, N.; Nagai, H.; Satoh, T. *Bioorg. Med. Chem.* **2000**, *8*, 373.

[3] Kohara,Y.; Kubo, K.; Imamiya, E.; Wada, T.; Inada, Y.; Naka, T. *J. Med. Chem.* **1996**, *39*, 5228.

[4] Wu, Z.; Rea, P.; Wickam, G. *Tetrahedron Lett.* **2000**, *41*, 9871.

Efficient hydration of nitriles to amides in the presence of $FeCl_3$/montomorrilonitril

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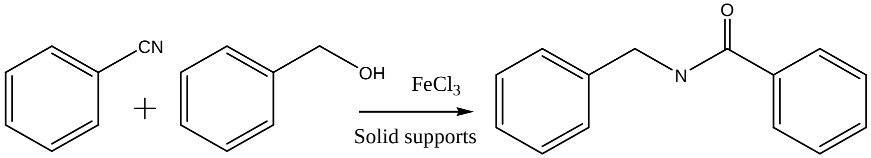
Hydration of nitriles to the corresponding amides is an important reaction in academia and industry because of their usefulness in a wide variety of applications such as intermediates in organic syntheses and as raw materials for engineering plastics, detergents, and lubricants. For example, hydration of acrylonitrile produces annually more than 2 × 10^5 tons of acrylamide and is the most important technology for the production of this chemical. Homogeneous hydration of nitriles is traditionally carried out with acids and bases such as H_2SO_4 and NaOH. However, carboxylic acids are formed as undesirable by-products by hydrolysis of the starting nitriles and amide products, especially under strongly basic conditions.



We herein report a facile and efficient synthetic strategy for the hydration of nitriles to the corresponding amides in good to excellent yield using heterogenous[1] $FeCl_3$ under solvent-free conditions. The results of TG-DTA and BET indicated that dispersed $FeCl_3$ coordinates with surface hydroxyl groups leading to formation –O-Fe-Cl as stable Lewis acid sites under the reaction condition. To confirm the role of $FeCl_3$, the reactions were carried out in the presence of various metal chlorides.

References:

[1] H. R. Darabi, K. Aghapoor, F. Mohsenzadeh, F. Taala, N. Asadollahnejad, A. R. Badiei, *Catal let*, **2009**, 133:84 -89.

Simple synthesis of *NH*- and *NR*-phthalimide derivatives in mild conditions

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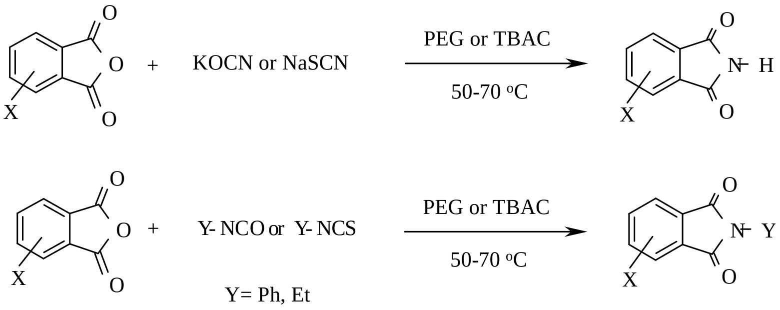
Phthalimides are considerably interesting as versatile intermediates in the synthesis of heterocycles [1] and their wide pharmacological and biological properties such as anticonvulsant, anti-inflammatory and antitumor activity [2]. Because of their remarkable applications, considerable attention has been focused on their synthesis [3-5].

Here we have described a simple and convenient method for the one-pot synthesis of *NH*- and *NR*-phthalimide derivatives from the reaction of phthalic anhydride derivatives with potassium cyanate, sodium thiocyanate, phenyl and ethyl isocyanate and isothiocyanate in PEG or TBAC in mild conditions. High yields of products obtained in neutral media without use of any catalyst and with very simple work-up.



TBAC: tetra-*n*-buthylammonium chloride

References:

[1] Martin, B.; Sekljic, H.; Chassaing, C. *Org. Lett.* **2003**, *5*, 1851.
[2] a) Chun-Jiang, W.; Xianfeng, S.; Xumu, Z. *Angew. Chem. Int. Ed*. **2005**, *44*, 4933; b) Lima, L. M.; Castro, P.; Machado, A. L.; Fraga, C. A.; Lugnier, C.; Moraes, V. L.; Barreiro, E. J. *Bioorg. Med. Chem.* **2002**, *10*, 3067.
[3] Khajavi, M. S.; Nikpour, F.; Hajihadi, M. *J. Chem. Res.(s)*,**1996**, 96.
[4] Nikpour, F.; Kazemi, S.; Sheikh, D. *Heterocycels* **2006**, *68*, 1559.
[5] Nikpour , F.; Mohammadi-Mogaddam, B. *Heterocycels* **2008**, *75*, 2289.

A facile synthesis of bridged polycyclic naphthooxazocines skeletons; eight membered ring constructions *via* tandem dinucleophilic addition of naphthols to quinolinium salts

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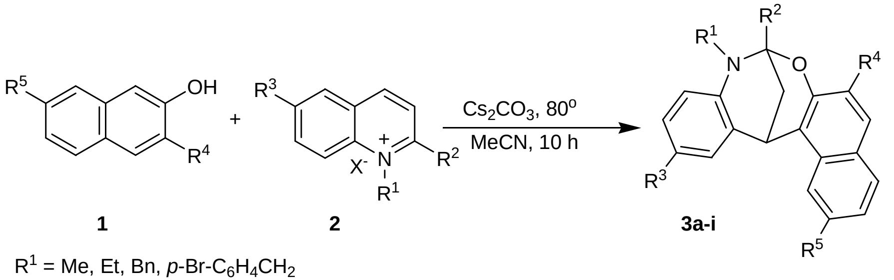
In recent years, many researches in organic chemistry have focused on discovering new methodologies for ring construction [1]. In this respect, methodologies leading to the synthesis of bridgehead heterocycles containing an eight membered ring are particularly appealing because these molecules with functional groups having cleft-like shapes have recently emerged as useful tools in the molecular recognition studies [2]. Among the members of this family, benzoxazocines have received considerable attention because of their pharmacological properties such as antidepressant, antithrombotic, antipsychotic for the central nervous system (CNS), and antibreast cancer [3]. On the other hand, the quinoline skeleton is found in a large number of naturally occurring and synthetic biologically active heterocyclic compounds. Notably, bicyclic *N/O*-acetals are present in a number of natural products, such as quinocarcin, tetrazomine and the bioxalomycins, showing good antitumour or antimicrobial activity [4].We herein reported the tandem process for the construction of heterotetracyclic naphthooxazocines. The reaction generally involves the initial addition of naphtols **1** to quinolinium salts **2** to form enamine intermediate which can be trapped by intramolecular cyclization of naphthols . The procedure is a very mild, efficient and the substrates are easily available (Scheme 1).



R^1 = Me, Et, Bn, p-Br-$C_6H_4CH_2$
R^2 = R^3 = H, Me R^4= R^5 = H, OH   X = Br, I

References:

[1] (a) B. K. Mehta; K. Yanagisawa; M. Shiro; H. Kotsuki, *Org. Lett*. **2003**, *5*, 1605
[2] M. Demeunynck; A. Tatibouet, *Recent Developments in Tröger's Base Chemistry, In Progress in Heterocyclic Chemistry,* Vol. *11;* G. W. Gribble; T. L. Gilchrist, Eds.; Pergamon: Oxford, UK, **1999**, 1;
[3] J. K. Mishra; K. Samanta; M. Jain; M. Dikshit; G. Panda, *Bioorg. Med. Chem. Lett*. **2010**, 20. 244.
[4] M. E. Flanagan; R. M. Williams, *J. Org. Chem*. **1995**, *60*, 6791.

Synthesis and application of task- specific ionic liquids (1, 1'-bis-methyl-3, 3'-methylene-bisimidazolium) for nucleophilic substitution in room temperature

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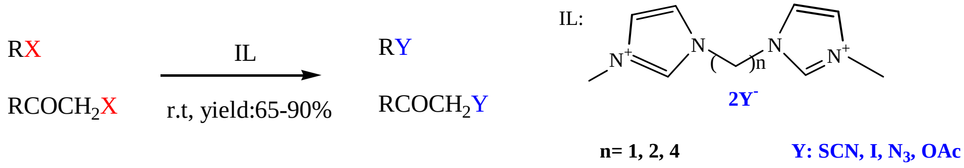
It is well-known that in the tune up of a synthetic method a crucial role is played by solvent. The possibility to change solvent nature as a function of the studied reaction is very important. This justifies the growing interest in ionic liquids (ILs) shown by the scientific community in the past decade. Besides their low vapour pressure and nonflammability, for which they have been claimed green solvents for industrial applications, their peculiar characteristic is the ionic nature [1].

Ionic liquids based on imidazolium cations have been extensively studied with a variety of structural modifications leading to differences in the physical and chemical properties of the liquid. Moreover, most attention has been focused on modification of the cation, particularly by incorporating hydroxyl, nitrile and carboxylic acid functionalities [2]. On the other hand, not much attention has been directed toward the preparation of ILs with useful anions. A functionalized anion could not only influence the physical and chemical properties of the IL but also may function as a catalyst. There are very few examples where ILs have been employed as reaction media and as the nucleophile in an organic transformation [3]. Also, the application of task specific ionic liquids (TSILs) enhances the versatility of classical ionic liquids. Herein, we describe a synthesis of TSILs containing a methylene bridged bisimidazolium cation combined with different anions. Furthermore, these TSILs have been applied as the reagent for the nucleophilic substitution reactions of *α*- halo ketones and alkyl halides.



References:

[1] Tavares, A. P. M.; Rudreguez, O.; Macedo, E.; Biotechnol. Bioeng. 101, 201-207; **2008**.

[2] Predel, T.; Schlücker, E.; Wasserscheid, P.; Arlt, W.; Chem. Eng. Technol. 30, 1475-1480; **2007**.

[3] Keskin, S.; Kayrak-Talay, D.; Akman, U.; Hortacsu, O.; J. Supercrit. Fluids. 43, 150-180; **2007**.

Synthesis of novel peptides *via* combination of α- and unusual γ- amino acids; structure survey and reactivity

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The insertion of additional atoms into the backbone of synthetic polypeptides greatly enhances the repertoire of stable, internally hydrogen-bonded folded structures. The creation of new classes of foldamers has been facilitated by the use of conformational constrained residues.

Backbone substitution restricts the stereochemically allowed conformations generated by rotation structural diversity in protein structures is generated by using two different secondary structural elements, helices and extended strands.

The formation of amyloid protein deposition is associated with major human diseases. A partial list includes Alzheimer’s disease, Parkinson’s disease, Type II diabetes, and many more. Variations in the mode of arrangement of the constituent structural units lead to a remarkable range of three-dimensional arrangements or folds. The synthesis of novel peptides could affect the formation of amyloid is an interesting subject in this area. In continuation of our research program for the synthesis of novel pharmaceutical peptides, we wish to report herein the synthesis of some novel peptides which is combination of phenylalanine as an α-amino acid with two different γ- amino acids and capacity of the desired peptides for the formation of fibril structure.

Phenylalalanine was selected as an α-amino acid for its interesting structure role and its capacity for the formation of amyloid structure. Two γ- amino acids were selected as starting materials and formation of peptide bond between them and phenylalanine was studied. The selected unusual amino acids were 1) Gabapentin [2] has been introduced as an anti-convulsant agent that is useful for the treatment of epileptic seizures. 2) Baclofen is a γ- amino acid which can help reduce muscle spasm [3]. In all cases, the synthetic peptides contained one unusual amino acids with different sequences. The peptides were synthesized in solution phase using coupling reagent. The structures of the products were deduced using spectroscopic data and High resolution Mass spectrometry (HR-ESI) data. Investigation about the biological activities and potential for the formation of fibril structure is under investigation.

References:

[1] Reches, M.; Gazit, E. *Science* **2003**, *300*, 625.
[2] Chatterjee, S.; Shamala, N.; Balaram, P. *Acc. Chem. Res.* **2009**, *42*, 1628.
[3] Bowery, N. G.; Hill, D. R.; Hudson, A. L.; Doble, A.; Middlemiss, D. N.; Shaw, J.; Turnbull, M. *Nature*, **1980**, *283*, 92.

Polyvinylpolypyrrolidonium tribromide (PVP-Br_3) as new polymeric reagent for the oxidation of organic compounds

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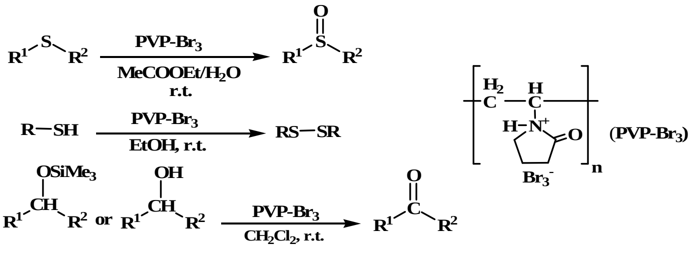
In the last few years, supported reagents on the organic polymers have become increasingly used in organic functional group transformations [1], mainly because the reactions are carried out under mild conditions and the organic products are easily isolated from the reaction media. The selective oxidation of primary and secondary alcohols into corresponding aldehydes and ketones is undoubtedly one of the most important and challenging transformations in organic chemistry both at the laboratory and industrial synthetic chemistry. On the other hand the protection of certain functional groups and the deprotection of the protected derivatives constitute important processes in synthetic organic chemistry of polyfunctional molecules, including the total synthesis of natural products [2]. Controlled oxidative coupling of thiols into disulfides are of interest from synthetic, biological and industrial points of view [3]. Also the chemoselective oxidation of sulfides to the corresponding sulfoxides is of great importance. In continuing of our studies about application of polymeric supported reagents [4-5] in functionalization of organic compounds, we became interested to use polyvinylpolypyrrolidonium tribromide for the oxidation of different types of organic compounds such as alcohols, trimethylsilyl ethers, sulfides and thiols (Scheme).



Scheme

Oxidation of these compounds were performed easily by mixing with appropriate amounts of polyvinylpolypyrrolidonium tribromide in the presence of two drops of water (except for thiols) in an organic solvent; then stirring of this mixture at room temperature.

References:

[1] Zakavi, S.; Abasi, A.; Pourali, A.R.; Rayati, S. *Bull. Korean Chem. Soc.* **2008**, *29*, 866.
[2] Tajbakhsh, M.; Alinezhad, H.; Urimi, A.G. *Phosphorus, Sulfur, and Silicon* **2008**, *183*, 1447.
[3] Fukuzawa, S.; Shimizu, E.; Atsuumi, Y.; Haga, M.; Ogata, K. *Tetrahedron Lett.* **2009**, *50*, 2374.
[4] Ghorbani-Choghamarani, A.; Nikoorazm, M.; Goudarziafshar, H.; Shiri, L.; Chenani, Z. *Bull. Korean Chem. Soc.* **2009**, *30*, 972.
[5] Ghorbani-Choghamarani, A.; Chenani, Z.; Mallakpour, S. *Synth. Commun.* **2009**, *39*, 4264.

Efficient synthesis of heptapeptides with anti-cancer activities

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An oncogene is a gene that, when mutated or expressed at high level, may help to turn a normal cell into a tumor cell. Defected cells normally undergo cell programmed death (apoptosis) in healthy individuals. Some muted and/or overexpressed oncogenes can cause defected cells to survive, proliferate and produce tumors [1]. Since 1970s, many oncogenes have been identified that are involved in human cancers and many cancer drugs have been developed that target either genetic sequences and/or their products [2, 3].

Synthesis of novel biologically active peptides is an attractive field in peptide pharmaceutical technology. Therefore we are pleased to report herein, the efficient synthesis of two heptapeptides using solid phase peptide synthesis strategy. The synthesized peptides were purified using preparative HPLC with C-18 column and the structures were assigned according to high resolution mass spectrometry (HR-ESI) data.

These synthesized heptapeptides have shown significant anti-cancer activities in our preliminary experiments but their mechanism of actions is not known yet. The investigation is underway to address their specificity, toxicity and mode of actions.

References:

[1] Brenner, S.; Horvitz, H. R.; Sulston, J. E.; *The Nobel Prize in Physiology or Medicine,* **2002**.
[2] Yokota J.; *Carcinogenesis,* **2000**, *21*, 497.
[3] Croce, C. M.; *N. Engl. J. Med.* **2008**, *358* (5), 502.

Sulfuric acid-([3-(3-silicapropyl)-sulfanyl]-propyl)-ester: An efficient and recyclable solid acid catalyst for the synthesis of 4,4'-(arylmethylene)-bis-(1*H*-pyrazol-5-ols)

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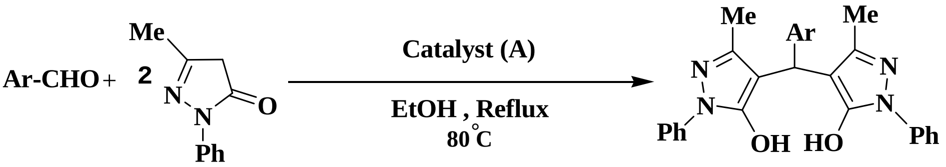
Pyrazoles are an important class of bio-active drug targets in the pharmaceutical industry, as they are the core structure of numerous biologically active compounds. For example, they exhibit anti-anxiety, antipyretic, analgesic and anti-inflammatory properties. 4,4’-(arylmethylene)-bis-(1*H*-pyrazol-5-ols) have antiviral activity against peste des petits ruminant virus (PPRV) [1].

The conventional chemical approach to 4,4'-(arylmethylene)-bis-(3-methyl-1-phenyl-pyrazol-5-ols) involves the successive Knoevenagel synthesis of the corresponding arylidenepyrazolones and its base-promoted Michael reaction and also one-pot tandem Knoevenagel-Michael reaction of arylaldehydes with two equivalents of 5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one performed under a variety of reaction conditions [2,3].

Sulfuric acid-([3-(3-silicapropyl)-sulfanyl]-propyl)-ester (**A**) is employed as a recyclable catalyst for the condensation reaction of aromatic aldehydes with 3-methyl-1-phenyl-5-pyrazolone . This condensation reaction was performed in ethanol at refluxing conditions giving 4,4'-(arylmethylene)-bis-(1*H*-pyrazol-5-ols) in 75–90 % yields [4].



References:

[1] Sujatha, K.; Shanthi, G.; Selvam,N. P.; Manoharan, S.; Perumal, P. T.; Rajendran, M. *Bioorg.Med. Chem. Lett.* **2009,** *19,* 4501.
[2] Hamama, W. S. *Synth. Commun*. **2001,** 31, 1335.
[3] Li, X.-L.; Wang, Y.-M.; Tian, B.; Matsuura,T.; Meng, J.-B. *J. Heterocycl. Chem.* **1998**, 35, 129.
[4] Niknam, K.; Sabri, D. *Applied Catalist A; Gen*. **2009,** 366, 220.

Investigation of functionalization and doping effects on a selective graphene: Electronic properties and NMR study

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Graphene has been becoming a new star in many fields after its successful fabrication [1-3]. The term "graphene" should be used to designate the individual carbon layers in graphite intercalation compounds [4]. The interest stems from the particular electronic properties of graphene as well as the promising perspectives for future technological applications [5].

In this research, NMR parameters consisting of isotropic and anisotropic chemical shielding parameters have been calculated to investigate the properties of electronic structures of the boron (B) and nitride (N) doped considered graphene, in addition, using density functional theory (DFT) we have investigated alteration of functional groups on the geometry and electronic structures of selective graphene. Optimization of structures and calculation of NMR parameters performed using B3LYP exchange-functional and 6-31G* standard basis set. The quantum chemical calculations yield the CS tensors in the principal axis system (PAS) with the order of $\sigma_{33} > \sigma_{22} > \sigma_{11}$ .Therefore, eqs. (1) and (2) are used to convert the calculated CS tensors to the isotropic (CS^I) and anisotropic (CS^A) parameters. All DFT calculations have been performed by the Gaussian 98 program.

$$\mathrm{CS}^{I}\,(\mathrm{ppm}) = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}) \qquad (1) \qquad ; \qquad \mathrm{CS}^{A}$$

$$(\mathrm{ppm}) = \sigma_{33} - \frac{1}{2}(\sigma_{11} + \sigma_{22}) \qquad (2)$$

Our results indicated that the doping of C atom by B atom, the properties of the electronic structures were less influenced regarding to the pristine model (fig 1) than the case of doping C atom by N atom. Furthermore, NMR parameters have been calculated to investigate the properties of the electronic structures. The changes of the calculated CS tensors in two different functional groups, regarding to the pristine model are also shown by changes of the structural properties.

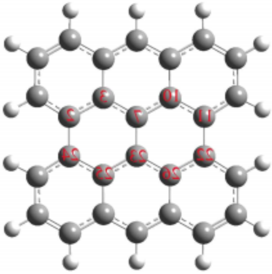

Fig 1: The pristine model of graphene

References:

[1] Novoselov, K. S. Geim, A. K. Morozov, S. V. Jiang, D. Zhang, Y. Dubonos, S. V. Grigorieva, I. V. Firsov, A. A. *Science* **2004**, *306*, 666.
[2] Geim A. K. Novoselov, K. S. *Nat. Mater. **2007***, 6, 183.
[3] Castro Neto, A. H. Guinea, F. Peres, N. M. R. Novoselov K. S. Geim, A. K. *Rev. Mod. Phys.* **2009,** 81, 109.
[4] Boehm, H. P.; Setton, R. Stumpp, E., **1994**.
[5] Geim A K, *Science* **2009**, 324, 1530.

Synthesis and characterization of new composites of poly (*ortho*-methoxyaniline) with silica sulfuric acid under solvent free condition

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Conducting polymers and silica (SiO_2) are very important materials for a wide range of technological applications. Enormous works on conducting polymers have been performed to enhance conductivity of conducting polymers by doping with inorganic and organic acids. Electrical properties of polymers are modified by adding inorganic particles within the polymer matrix. Composites containing organic polymers and inorganic particles regime provide a completely new class of materials with novel properties. Among them, many PANI/inorganic polymer composites have been prepared recently. These composites based on polyaniline have been harvesting several intriguing properties within themselves due to the mutual influence of the individual constituents and synergism of their properties [1].

It has been found that ring-substituted (alkyl and alkoxy) and *N*-alkyl-substituted PANI are more soluble than unsubstituted PANI [2]. They can be synthesized both chemically and electrochemically. The most common method of chemical synthesis includes oxidation of the monomer with an oxidizing agent, e.g. ammonium peroxydisulfate, which is added to monomer solution [3].

In this work we prepared a new composite of silica with poly (*ortho*-methoxyaniline) (POMA) by two methods and in solvent free condition. The first one uses in-situ polymerization of monomer in the presence of an oxidant and solid dopant acid (silica sulfuric acid) [4,5]. In another method, POMA was synthesized separately [6] and then grinded with silica sulfuric acid in solid state.

Conductivity measurements of pressed pellets of the composites were performed using the four-probe technique. The UV-Vis absorption spectra were obtained from the polymers dissolved in *N*-methyl-2-pyrrolidinone (NMP). The FT-IR spectra of the polymers were obtained in the base powdery form (compressed KBr pellets) and morphology of the composites were investigated by SEM.

References:

[1] Hesheng, X.; Qi, W. *J. Appl. Polym. Sci.*, **2003**, *87*, 1811.

[2] Mazur, M. *Eur. Phys. J. E.*, **2007**, *22*, 67.

[3] Jamal, R.; Abdiryim, T.; Nurulla, I. *Polym. Adv. Technol*. **2008**, *19*, 1461.

[4] Modarresi-Alam, A. R.; Khamooshi, F., etal, *ARKIVOC* **2007**, *xvi*, 238.

[5] Modarresi-Alam, A. R. et al. *Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications, Ottawa, Ontario, Canada*, 4-6 August **2010.**

[6] Wei, Y.; Foeke, W. W.; Wnek, G. E.; Ray, A.; Macdiarmid, A. G. *J. Phys. Chem.*, **1989**, *93*, 495.

A novel synthesis of aryl mesylates via one-pot demethylation-mesylation of aryl methyl ethers using a mixture of phosphorus pentoxide in methane-sulfonic acid

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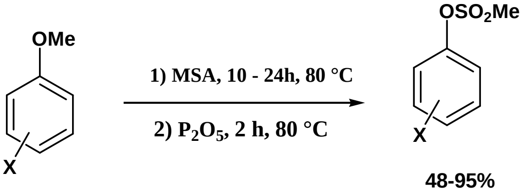
Sulfonate esters are valuable intermediates in organic synthesis. Among of sulfonate esters, aryl mesylates are useful intermediates in organic synthesis with applications in agrochemicals [1], polymers and recently Suzuki-type cross-coupling reaction [2]. Although there are many classical methods for synthesizing of aryl mesylates, these involve either long reaction times, expensive reagents, or the use of very toxic reagents.

Methyl ethers have been employed as protecting group; however, this is generally avoided because of requiring harsh reagents or conditions for its removal that are often at odds with other functionality [3].

Herein, we report one-pot demethylation-mesylation aryl methyl ethers in the presence of a mixture of phosphorus pentoxide in methanesulfonic acid as an efficient reagent. Treatment of a broad range of aryl methyl ethers with a mixture of methanesulfonic acid and phosphorus pentoxide at 80 °C furnishes the corresponding mesylates in 48-95% yield. Both electron-rich and electron deficient aryl methyl ethers participate in the reaction.



References:

[1] Giles, D. P.; Kerry, J. C.; Kozlik, A.; Palmer, B. H.; Shutler, S. W.; Willis, R. J. Eur. Patent 26040, **1981**

[2] Buchwald, S. L.; Munday, R. H.; Martinelli, J. R. *J. Am. Chem. Soc*. **2008**, *130*, 2754.

[3] Zuo, L.; Yao, S.; Wang, W.; Duan, W. *Tetrahedron Lett*. **2008**, *49*, 4054.

The structure and mechanical properties of Silver / low density polyethylene (Ag /LDPE) nanocomposites as antibacterial agent for medical and food industrial applications

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In the past decade, nanocomposites based on polymer matrix have received considerable attention in both fundamental research and industry exploitation due to their unique physical and/or chemical properties. Low density polyethylene (LDPE) possesses excellent biocompatibility with human body and usually used as a kind of implantable material. It can be potentially used as antibacterial material when it is incorporated by antimicrobial agents such as silver nanoparticles.

In this study, Silver/low-density-polyethylene (Ag/LDPE) nanocomposites have been prepared using a melt-blending technique with 1.0, 2.0, 3.0, 4.0 and 5.0 wt.% of silver nanoparticles and the effect of adding Ag on structural and some mechanical properties of LDPE was investigated. The structure characteristics of nanocomposite characterized by using X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray energy dispersive spectroscopy (EDS). The results of XRD, SEM and SEM–EDS Ag-mapping show that the nanocomposites are a hybrid of the polymer and the silver nanoparticles, in which the silver.

The influences of the silver nanoparticle's loading, varied from 1 to 5 wt. %, and the silver nanoparticle's size, 50 nm, on the Young's modulus, yield strength, tensile strength and elongation at break point were investigated. The mechanical properties of pure LDPE and Ag/LDPE composites were measured by tensile tests. Increasing the silver nanoparticle's loading caused an increase in Young's modulus for the nanocomposite, while decreasing the yield strength. But the yield strength for this nanocomposite increased when the silver nanoparticle's loading was less than 2 wt.% .It was also found that there was a decrease in tensile strength and elongation at break point for this nanocomposite.The antibacterial properties of the new synthesized nanocomposites are being evaluated for further applications.

Puckering energy 1,3-Halo-1,3-dibora-cyclobot-2-ylidenes

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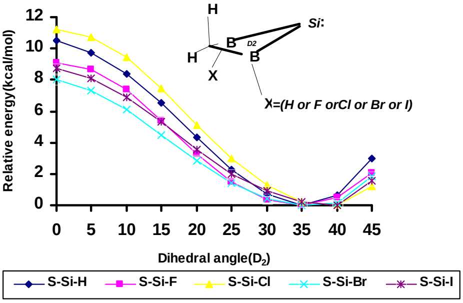
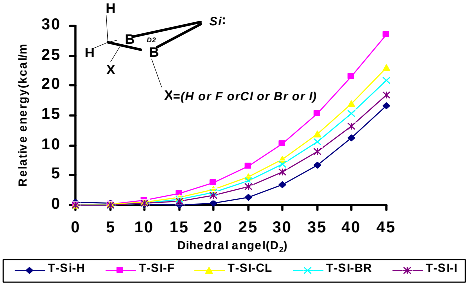
The 1,3-dibora-cyclobot-2-ylidene [1] is one of the most intriguing organoboron compounds, and its unique bonding situation has stimulated much activity in synthesis [2] and theoretical chemistry [3]. Puckering energy of 1,3-dibora-cyclobot-2-ylidene and its heavier analogues is studied in B3LYP/6-311++G** level of theory.

In order to confirm global minima, for each diboretane, energy surface studies are necessary, since puckering of 1,3-dibora-cyclobot-2-ylidene rings may alter positions of the global minima. Puckering energy surfaces are sketched for both singlet and triplet states of diboretane rings as a function of dihedral angle C-B-M-B (M=C, Si). The magnitude of puckering energy barriers for triplet states is higher than Singlet state.





References:

[1] Klusik H., Berndt A. *Angew. Chem.* **1983,** *95,* 895; *Angew. Chem., Int. Ed. Engl.* **1983**, *22,* 877.
[2] Berndt A. A*ngew. Chem.* **1993**, *105,*1034; *Angew. Chem., Int. Ed. Engl.* **1993**, *32*, 985.
[3] McKee M. L. *Inorg. Chem.* **1999,** *38,* 321.

Synthesis and characterization of new aromatic poly(amide-ether-imide)s derived from a new imide-containing aromatic dicarboxylic acide

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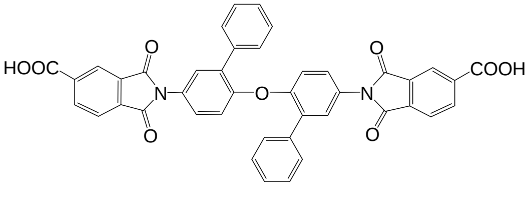
Rigid-rod aromatic polyimides and polyamides constantly attract wider interest because of their unique mechanical and thermal properties [1]. Synthesis and processing of these materials are generally more difficult due to their limited solubility and infusibility. One of the successful approaches to increase solubility and processability of these polymers is the introduction of bulky lateral substituents, flexible alkyl side chains, unsymmetric, alicyclic, and kinked structure. To develop easily processable high-performance materials, modifications that increase the solubility while maintaining the rigid-rod character and the thermal stability are of particular interest [2-4].

In this work, we report the synthesis of a series of new poly(amide-ether-imide)s based on a new diacid namely 2,2'-diphenyl-4,4'-bis(N-trimellitoyl)diphenyl ether **(I)** using Yamazaki phosphorylation polycondensation. Some characteristics of the polymers prepared such as organo-solubility, inherent viscosity, thin film quality, thermal stability, and crystallinity will also be reported.



(I)

References:

[1] Ghosh, M. K.; Mittal, K. L. *Polyimides: Fundamentals and Applications*, Marcel Dekker: New York, 1996.

[2] Liaw, D. J.; Liaw, B. Y. *Macromoel. Symp.* **1997**, *122*, 343.

[3] Liaw, D. J.; Liaw, B. Y.; Hsu, P. N.; Hwang, C. Y. *Chem. Mat.* **2001**, *13*, 1811.

[4] Glatz, F. P.; Mulhaupt, R. *Polym. Bull*. **1993**, *31*, 137.

An industry guide for the prevention and control of odors at organic wastes processing facilities

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Composting is the process by which organic waste materials are decomposed in the presence of oxygen, through the action of bacteria and other microorganisms. The microorganisms consume oxygen while feeding on organic matter, which generates heat, carbon dioxide and water vapor. These products are released into the atmosphere. The composting process reduces both the volume and mass of the raw materials while transforming them into a composted organic material as fertilizer [1]. Odor is one of the most common, immediate and potentially damaging emissions at composting sites. It should not come as a surprise that it is also one of the most widespread sources of public complaint about their environment. The nature of the odor emitted from the composting process will depend on the type of material being processed and the stage within the composting cycle. Due to the necessary reliance on microorganisms to degrade the organic wastes, there will always be some odor emitted at each stage of the process. The key to good composting is to manage the process to avoid excessive odor emissions. The aim of this study was to investigate pathways for generation odors in the composting process. The types of odorous substances emitted from the starting phase based on a fresh feedstock will include the following: Aldehydes; Alcohols; Carboxylic acids; Esters; Ketones; Sulphides; nd Terpenes and the types of odorous substances emitted from the mesophillic phase will include: Organic sulphides; Terpene; and Ammonia [2]. This report reviews the application of physical and chemical controls such as: moisture, temperature, pH and C/N ratio, to provide the prevention and control of odors at organic wastes processing facilities and improving compost process efficiency [3].

References:

[1] Good Practice and Regulatory Guidance on Composting and Odour Control for Local Authorities, Department for Environment, Food & Rural Affairs, Queen's Printer and Controller of HMSO 2007, Nobel House 17 Smith Square London SW1P 3JR, Website: www.defra.gov.uk
[2] An industry guide for the prevention and control of odours at biowaste processing facilities, Jeremy Jacobs1, Nick Sauer and E. Jane Gilbert, The Composting Association, Environment Agency ,2007.
[3] Improving Compost Process Efficiency by Controlling Aeration, Temperature and pH, Cecilia Sundberg, Faculty of Natural Resources and Agricultural Sciences, Department of Biometry and Engineering Uppsala, Acta Universitatis Agriculturae Sueciae, 2005.

A new synthetic method for preparing iodohydrins and iodoethers from aromatic alkenes using $Hg(BF_4)_2.SiO_2$

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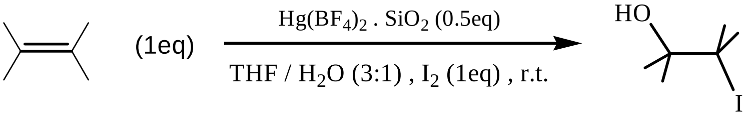
The regioselective functionalization of alkenes with the functional groups such as hydroxy or alkoxy and halogen finds application in various useful organic transformations [1].

These halo derivatives are widely applicable in industrial process for the synthesis of drugs, pharmaceuticals, agrochemicals, pigments and photographic material [2].

The formation of chlorohydrins and bromohydrins from alkenes is a well-established preparative procedure. However, the direct synthesis of iodohydrins from olefins is usually difficult to achieve by the same procedure because of ready reversibility of the addition of IOH to olefins in a dilute aqueous solution of iodine [3].

A new simple method for preparation iodohydrin and iodoether from aromatic alkenes is described.

Iodohydrin and iodoether were prepared in excellent yield using Mercury(II) tetrafluoroborate ($Hg(BF_4)_2$. SiO_2), I_2 in aqueous THF or alcohols (methanol, *iso*-propanol and *tert*-butanol). The reactions take place at room temperature within short reaction times and with high regioselectivity, following Markovnikoff fashion.



References:

[1] (a) Tenaglia, A.; Pardigon, O.; Buono, G. *J. Org. Chem.*, **1996,** 61, 1129; (b) Dolenc, D.; Harej, M. *J. Org. Chem*. **2002**, *67*, 312.
[2] Cabanal-Duvillard, I.; Berrier, J. F.; Royer, J.; Husson, H. P. *Tetrahedron Lett*., **1998**, *39* 5181.
[3] (a) Cornforth, J. W.; Green, T. D. *J. Chem. Soc. C* **1970**, 846. (b) Cambie, R. C.; Noall, W. I.; Potter, G. J.; Rutledge, P. S.; Woodgate, P. D. *J. Chem. Soc., Perkin Trans. 1* **1977**, 226.

DFT study on the structural properties and the strength of watson-crick base pairing of the boron analogues of Uracil

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The field of biochemistry revolves around studying the structure, function, and interactions of nucleic acids, which store and transmit genetic information, and proteins which are biological catalysts. Although hydrogen bonds are among the weakest chemical interactions, they occupy a key position in biochemistry and biology**.** The synthesis of modified versions of DNA is an area that is receiving much attention. The replacement of the nitrogen atom on the nucleobases with boron atom has provided insight into DNA and RNA stability, recognition, and replication at the atomic level. What would be the implication if nitrogen atom is replaced by boron atom? It should be noted that borauracils, borathymines or boracytosines, and their derivatives, should be interesting compounds to be considered in search for new inhibitors of enzymes involved in nucleotide metabolism [1].

Boron analogues of biologically active compounds show unique properties that may promote enzyme inhibition [2,3]. In the present research, we investigated a detailed density functional theory study of the structural, tautomeric, base-pairing ability to adenine nucleobase and electronic properties of two the boron analogues of uracil nucleobase and effects of these modifications on theirs base-pairing and acid-base properties. Our goal is to gather data to help elucidate the structure and electronic properties of boron analogues of uracil.

References:

[1] A. H. Soloway, W. Tjarks, B. A. Barnum, F. G. Rong, R. F. Barth, I. M. Codogni, J. G. Wilson, *Chem. Rev.* **1998***, 98*, 1515.
[2] V. J. Reddy, S. Chandra, M. V. Ram Reddy, *Org. Biomol. Chem.* **2007***, 5*, 889.
[3] W. Yang, X. Gao, B. Wang, *Med. Res. Rev*. **2003**, *23*, 346.

Dynamic stereochemistry of Rutin (vitamin P) in solution: Theoretical approaches and experimental NMR validation

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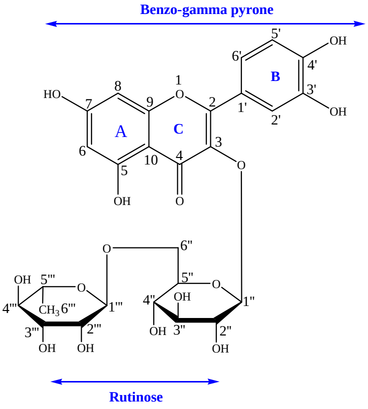
Bioflavonoids are benzo-γ-pyrone derivatives of plant origin with a wide range of physiological activities such as antioxidant, antimicrobial, anti-inflammatory, antiallergenic, antiviral, and anti-tumor properties [1]. Rutin (Figure 1) is a non-toxic bioflavonoid composed of the flavonol quercetin and the disaccharide rutinose that is found in more than 70 plant species. It is used clinically in therapeutic medicine, especially in humans for the treatment of lymphoedema following axillary lymph node excision [2]. It has less toxicity in the human body and has the potential to be a novel therapeutic agent. In this report, conformational studies of the exocyclic hydroxymethyl group in the disaccharide rutinose in rutin have relied heavily on the use of $^3J_{HH}$ values to estimate rotamer populations in solution. The strategy was to obtain experimental results from extracted rutin from *Salvia Macrosiphon*, and then these data were used to test the ability of DFT methods to estimate the chemical shifts and coupling constants. Good agreement between experimental NMR and theoretical data confirms the accuracy of the $B_3LYP/6\text{-}311G^{**}$ method for calculation of chemical shifts and coupling constants of saccharides.



References:

[1] Aron, P. M.; Kennedy, J. A. *Mol. Nutr. Food Res.*, **2008**, *52*, 79-104.
[2] Sun, W.Q.; Sheng, J. F. *Handbook of natural active constituents*; Chinese Medicinal Science and Technology Press: Beijing, **1998**, pp 2241-2316.

Direct reductive amination of aldehydes and ketones by $NaBH_4$ using MWCNTs-SO_3H as catalyst

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Amines are ubiquitous functionalities in current drugs and active pharmaceutical intermediates. Reductive amination of aldehydes and ketones is an important direct transformation of carbonyl compounds into amines. In this important carbon–nitrogen bond forming process, aldehydes or ketones are reacted with ammonia, primary or secondary amines in the presence of a reducing agent to produce primary, secondary and tertiary amines, respectively [1].

The transformation of amines from aldehydes and ketones is an important method in organic synthesis because of their versatile utility as intermediates for synthesis of pharmaceuticals and agrochemicals. For the transformation, the two synthetic methods are commonly used. One is the reductive amination, which is termed as a direct reaction.

Several reagents which effect reductive amination have been developed, including: catalytic hydrogenation, $Et_3SiH–CF_3CO_2H$, Zn–AcOH, Bu_3SnH–DMF, $NaBH_3CN$, $NaBH(OAc)_3$, pyridine– BH_3, $ZnCl_2–NaBH_4$, silica gel–$Zn(BH_4)_2$, $Ti(O\text{-}i\text{-}Pr)_4–NaBH_4$, $NiCl_2–NaBH_4$, $NaBH_4–ZrCl_4$, $NaBH_4–H_2SO_4$, $NaBH_4$–wet clay-microwave and borohydride exchange resin. In terms of functional group tolerance, side reactions and reaction conditions, most of these reagents have one or more drawbacks [2].

Herein, we studied the direct reductive amination of aldehydes and ketones with primary or secondary amines in the presence of MWCNTs-SO_3H which afforded the corresponding imine which was then reduced with $NaBH_4$ to give amines in high yields.

References:

[1] Burkhardt, E. R.; Coleridge, B. M. *Tetrahedron. Lett*. **2008**, *49*, 5152.
[2] Heydari, A.; Khaksar, S.; Akbari, J.; Esfandyari, M.; Pourayoubi, M.; Tajbakhsh, M. *Tetrahedron. Lett.***2007**, *48*,1135.

Synthesis of new symmetrical metal free [1,4,8,11]-tetraaza[14]annulene derivatives

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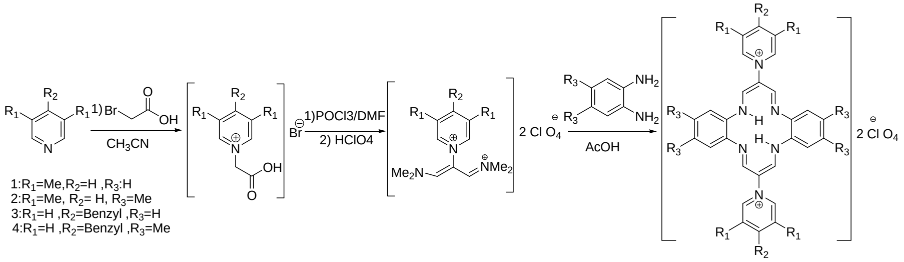
Tetraaza [14]annulene macrocycles have been studied by many workers because of the utility to model porphyrins and corrin rings in biological systems [1–2].

In this study we used heteroaromatic molecules such as pyridine derivatives as an starting material to synthesis of new [1,4,8,11]-tetraaza[14]annulene derivatives in excellent yields, We have been focusing our attention on synthesis of symmetrical tetraazaannulenes having tow same N- heteroaromatic groups at the position 6 and 13 of the macrocyclic ring and fused aromatic group at the 2,3 and 9,10 position of the tetraazaannulene ring.The structure and purity of the prepared compounds were confirmed by IR, NMR, Mass spectroscopy and elemental analysis.



References:

[1] Fairbank. M. G. McAuley. A. *Inorg. Chem*. **1986**, *25*, 1233.
[2] Chapman. K. D, Davies.M, Vuik. C. P, *J. Am. Chem. Soc*. **1984**, *106*, 2692.

$BiCl_3/SiO_2$ as a highly effective catalyst for the synthesis of benzimidazoles

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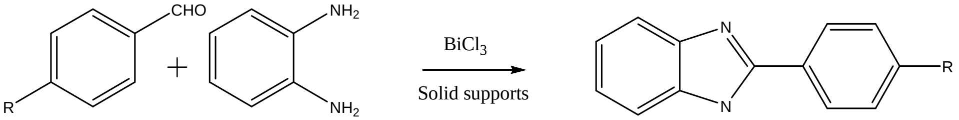
The development of simple, efficient and environmentally benign chemical processes or methodologies for widely used organic compounds from readily available reagents is one of the major challenges for chemists in organic synthesis. The importance of imidazoline and benzimidazole units arises, because they are found in many biologically active compounds.[1] In organic synthesis, imidazoline units are also used as synthetic intermediates, chiral auxiliaries, chiral catalysts and ligands for asymmetric catalysis. In addition, the benzimidazole moiety is found in various synthetic pharmaceuticals displaying a broad spectrum of biological activity including anti-ulcer, anti-tumour and anti-viral effects. A number of methods have been reported for the synthesis of imidazolines and benzimidazoles. However, many of the synthetic protocols reported so far suffer from disadvantages. Therefore, the development of a cost effective, safe and environment friendly reagent system is desirable.



Here, we would like to report as a full form for the preparation of Benzimidazoles from aldehydes using $BiCl_3/SiO_2$ at room temperature. The BET analysis showed an remarkable reduction in surface area and pore volume of $SbCl_3/SiO_2$ as compared to support material, attributed to surface coverage by reagent molecules ($SbCl_3$) on the surface of silica gel.

The effect of amount of active species $BiCl_3$ for the synthesis of Benzimidazoles was studied by varying the catalyst amount. To investigate the role of $BiCl_3/SiO_2$, the same reaction was carried out in the absence or presence of silica gel. In both cases, low yield of product was obtained, which indicates that catalyst is obviously necessary for the reaction.

References:

[1] Grimmett, M. R. In *Comprehensive Heterocyclic Chemistry*; Katrizky, A. R., Rees, C. W., Scriven, E. F. V., Eds.; Pergamon: Oxford, **1996**; Vol. 3, pp 77–220;

Synthesis, characterization and in vitro drug-release study of ibuprofen polymeric prodrugs based on 2-hydroxypropyl methacrylate

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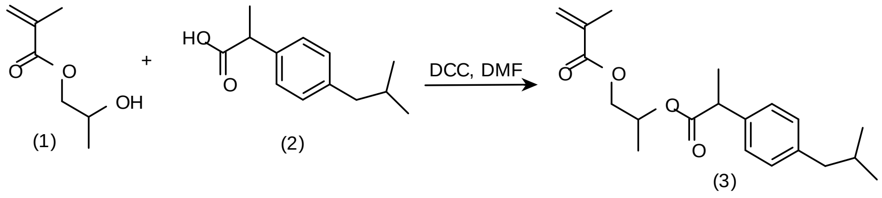
One field of application that has attracted polymer chemist's attention from the late 1960s onwards is the need for advanced drug delivery systems to improve drug efficacy. Polymeric prodrug is a conjugation of a drug with a polymer, which has several advantages such as control the rate of drug release, administrate at low dosage, improve site-specificity and increasing therapeutic benefit [1-4].

In this research work, ibuprofen (**1**) as a non-steroidal anti-inflammatory drug (NSAID), was linked to 2-hydroxypropyl methacrylate (**2**) by activated ester methodology in the presence of *N,N*-dicyclohexyl carbodiimide (DCC) agent. The resultant methacrylic derivative of ibuprofen (**3**) was then copolymerized with 2-hydroxyethyl methacrylate and methyl methacrylate by free radical polymerization method to give the related polymeric prodrugs. FT-IR, ^{1}HNMR, and elemental analysis data confirmed the structure of the compounds. The average molecular weights and the polydispersity indices of the prodrugs were determined by gel permeation chromatography.

In vitro drug-release study was performed into cellophane membrane dialysis bag by hydrolysis of polymeric prodrugs in various buffered solutions (pH 1, 7.4 and 10) at physiological conditions. Detection of the hydrolyzed solutions by UV spectroscopy at selected intervals showed that the drug can be released by selective hydrolysis of the ester bond at the side of drug moiety. The release profiles indicated that the hydrolytic behaviour of polymeric prodrugs is strongly based on the polymer hydrophilicity and the pH value of the hydrolysis solution. The results suggested that these polymeric prodrugs could be useful for releasing ibuprofen in controlled release systems.



References:

[1] Babazadeh, M.; Mosanejhad, T. *Iran. Polym. J.* **2009**, *18*, 179.
[2] Babazadeh, M. *Int. J. Pharm.* **2008**, *356*, 167.
[3] Babazadeh, M. *J. Appl. Polym. Sci.* **2007**, *104*, 2403.
[4] Babazadeh, M.; Edjlali, L.; Rashidian, L. *J. Polym. Res.* **2007**, *14*, 207.

Preparation and electrochemical properties of silyl derivatives of ferrocene

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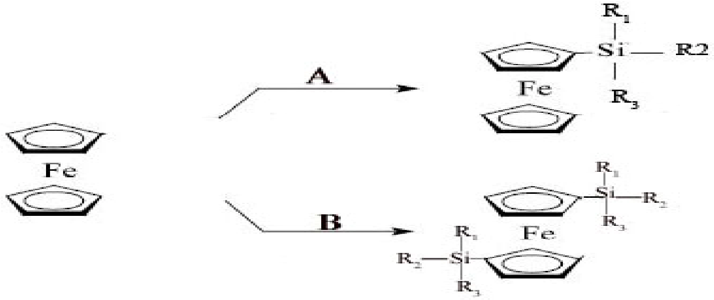
Ferrocene is a starting material for the preparation of numerous derivatives used in many areas of chemistry and in recent years, the applications of them have been widespread in many fields of chemistry such as material science [1], asymmetric catalysis [2], and biologically active compounds [3,4], enzyme based sensors [5]. One of the properties of ferrocene derivatives that has been widely examined is the redox potential of the iron center in ferrocene derivatives.

In this paper we want to prepared some silyl-substituted ferrocene derivatives and then report the electrochemistry behavior of them by simple and modified electrode in different conditions. This substituted groups changes physical state of ferrocene from solid to liquid and also cause the potential shift in cyclic voltametry.



A :t-BuLi /THF, $R_2R_2R_3SiCl$ / n-hexane => product monosubstituted
B :n-BuLi / TMEDA, $R_1R_2R_3SiCl$ / n-hexane => product disubstituted

References:

[1] liu, J.; Castro, R.; abboud, K .A.; Kaifer, A.E. *J.Org.Chem*. **2000,** *65*, 6973.
[2] Argyropoulos, N.; argyropoulou, E.C. *J.Organomet.Chem.* **2002**, *654*, 117.
[3] Kelly, P.N.; Pretre, A.; Devoy, S.; O'Rielly, I.; Devery, R A.; J.F. Goel, Gallagher, A.J . Lough, P.T.M. Kenny, J .Organomet .Chem .692 (**2007**) 1323 .
[4] M.F.R .Fouda, M.M .Abd-Elzaher, R.A .Abdelsamaia, A.A .Labib, Appl .Organometal . Chem 21 (**2007**) 613 .
[5] V.B. Kandimalla, V.S. Tripathi, H. Ju, Biomaterials 27 (**2006**) 1167.

Synthesis of novel heterocyclic compounds such as pyrimidine derivatives using tri-component reaction of 1,3-diimino isoindoline with acetylenic esters in the presence of tert-butyl isocyanide.

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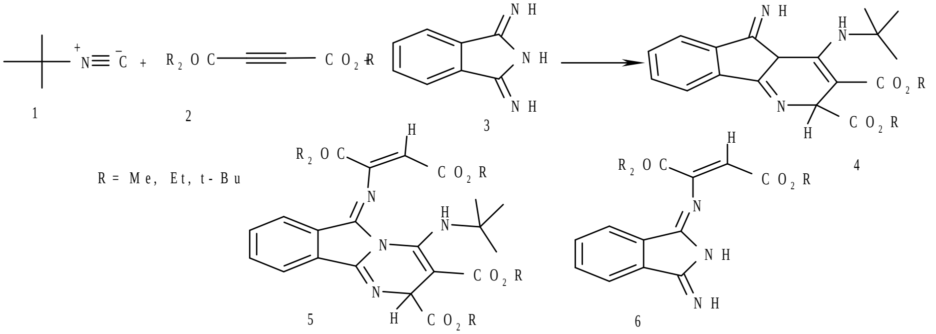
The pyrimidine heterocyclic core is an important subunit because of its widespread abundance in the basic structure of numerous natural products. A number of synthetic pharmacophores based upon the pyrimidyl structure exhibit antibacterial, antimicrobial, anticancer, anti-HIV-1 and antirubella virus activities [1]. Pyrimidines are considered to be important not only because they are on integral part of genetic materials viz. DNA and RNA as nucleotides and nucleosides but also they have important numerous biodynamic properties and biological activities [2].

Multi-component reactions (MCRs) have emerged as an efficient and powerful tool in modern synthetic organic chemistry due to their valued features. MCRs, leading to interesting heterocyclic scaffolds, are particularly useful for the construction of diverse chemical libraries of 'drug-like' molecules [3].

Herein we report multicompounent reaction of tert-butyl isocyanide (1) with dialkyl acetylenedicarboxylates (2) and 1,3-diimino isoindoline (3). The reaction proceeded in tetrahydrofuran and afforded (4),(5) and (6) in moderate yields. The structure of products was deduced from their ^{1}H NMR, ^{13}C NMR, IR products and Mass spectral data.



Refrences:

[1] Barthakur, MG.; Gogoi,S.; Dutta, M.; Boruah, RC. *Steroids*. **2009** , *74, 730.*

[2] Rabio, UM.; Mohamed, RA.; Abou-El-Wafa, MH. *Spectrochimica Acta part A*. **2007**, *68, 605.*

[3] Adib, M.; Mahdavi,M.; Ansari,S.; Malihi,F. *Tetrahedron lett*. **2009**, *50, 7246.*

Poly(4-vinylpyridinium tribromide) promoted oxidative conversion of thiols to the corresponding disulfides

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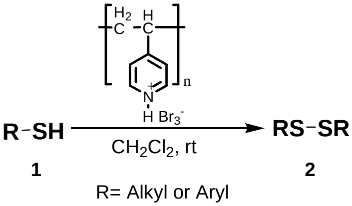
The conversion of thiols to disulfides is of considerable interest in chemical, biological, and industrial points of view. The classical procedures for this type of reaction use reagents such as silica-PCl_5/$NaNO_2$ [1], $NaBrO_3$/NaBr [2], 1-chlorobenzotriazole [3] and etc. There are a variety of reports on the functionalization of organic compounds with molecular bromine. In order to decrease the toxicity of molecular bromine, a variety of organic tribromide reagents were reported and applied in different functional group transformations. In this light we decided to prepare a new and reusable tribromide reagent.

In continuing of our attempt to introduce new methodologies for organic functional group transformations [4-5], we became interested to prepare poly(4-vinylpyridinium tribromide). Consequently, a variety of aliphatic and aromatic thiols **1** converted into corresponding disulfides **2** using poly(4-vinylpyridinium tribromide) in dichloromethane at room temperature (Scheme 1).



Scheme 1

In summary, in this research project we introduce a new type of tribromide reagent with polymeric structure. This insoluble, powdery reagent allows a simple recovery procedure.

References:

[1] Pathak, U.; Pandey, L.K.; Mathur, S. *Synth. Commun.* **2009**, *39*, 2923.
[2] Joshi, G.; Bhadra, S.; Ghosh, S.; Agrawal, M.K.; Ganguly, B.; Adimurthy, S.; Ghosh, P.K.; Ranu, *Eng. Chem. Res.* **2010**, *49*, 1236.
[3] Stellenboom, N.; Hunter, R.; Caira, M.R. *Tetrahedron* **2010**, *66*, 3228.
[4] Goudarziafshar, H.; Ghorbani-Choghamarani, A.; Nikoorazm, M.; Naserifar, Z. *Chin. J. Chem.* **2009**, *27*, 1801.
[5] Ghorbani-Choghamarani, A.; Nikoorazm, M.; Goudarziafshar, H.; Tahmasbi, B. *Bull. Korean Chem. Soc* , **2009**, *30*, 1388.

An efficient one-pot synthesis of alkyl 2-(bromomethyl) 2- (4-aryl) 4-alkoxy 2,5-dihydro 5-oxofuran 3-carboxylate

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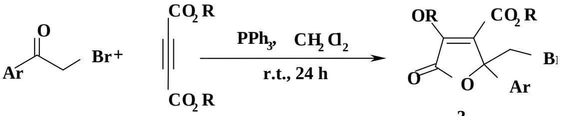
Dihydrofurans are the most important hetrocycles commonly found in a large variety of naturally occurring substances [1]. The development of new and efficient methods for their synthesis remains an area of current interest and a whole series of new synthetic methods have appeared in literature [2]. Herein we have described a simple, and one-pot, three-component reaction between different phenacyl bromides and dialkylacetylenedicarboxilates was carried out with triphenylphosphin and functionalized dihydro oxofuran derivatives in excellent yields.



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3	Ar	R	%Yield*
a	4-Cl C_6H_5	CH_3	88
b	4-Cl C_6H_5	C_2H_5	86
c	4-Cl C_6H_5	*t*-Bu	92
d	4-Br C_6H_5	CH_3	85
e	4-Br C_6H_5	C_2H_5	80
f	4-Br C_6H_5	*t*-Bu	90

* Isolated yields

The structures of **3a-f** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:

[1] Lipshutz, B. H. *Chem. Rev*. **1986**, *86*, 795.
[2] Heiba, E. I.; Dessau, R. M. *J. Org. Chem*. **1974**, *39*, 3456.

One-pot synthesis of 12-aryl-8,9,10,12-tetrahydrobenzo[a]xanthen-11-ones

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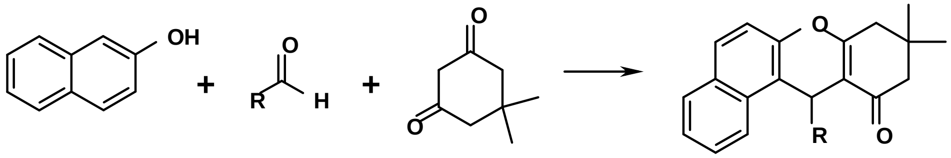
Xanthenes and benzoxanthenes are important heterocycles that are known to possess multiple biological activities. Although not widely found in nature, xanthenes and compounds based on these core templates exhibit a broad spectrum of pharmaceutical activities. Thus a broad utility range has made xanthenes prime synthetic candidates thereby accentuating the need to develop newer synthetic routes for scaffold manipulation of xanthene derivatives. The synthesis of tetrahydrobenzo[a]xanthen-11-ones has been reported in the presence of a acidic catalyst [1-2].

As a consequence of our interest in the synthesis of heterocycle systems and application of solid acid catalysts in organic synthesis [3], herein, we report a facile, three-component one-pot synthesis of tetrahydrobenzo[a]xanthen-11-one derivatives by one-pot three-component condensation reaction strategy of β-naphthol with aldehydes and dimedone using catalytic amounts of boric acid under solvent-free conditions.



R = C_6H_5,4-ClC_6H_4, 4-Me C_6H_4, 4-$OMeC_6H_4$,
3-$NO_2C_6H_4$, 2,4-$Cl_2C_6H_4$, 4-$NO_2C_6H_4$, 4-FC_6H_4
2-$NO_2C_6H_4$, 2-ClC_6H_4,3-$OMeC_6H_4$, 2-$OMeC_6H_4$

Operational simplicity, mild reaction conditions, enhanced rates, low cost and solvent-free conditions are significant advantages of the protocol presented here.

References:

[1] Shaterian, H. R.; Yarahmadi ,H. *Tetrahedron Lett.* **2008,** *49*, 1297.
[2] Nagarapu, L.; Baseeruddin, M.; Apuri, S.; Kantevari, S. *Catal. Commun.* **2007**, *8,* 1729.
[3] Karimi-Jaberi, Z.; Keshavarzi, M. *Chin. Chem. Lett.* **2010**, *21*, 547.

Simple synthetic strategy for preparation of quinoxaline and pyridopyrazine derivatives

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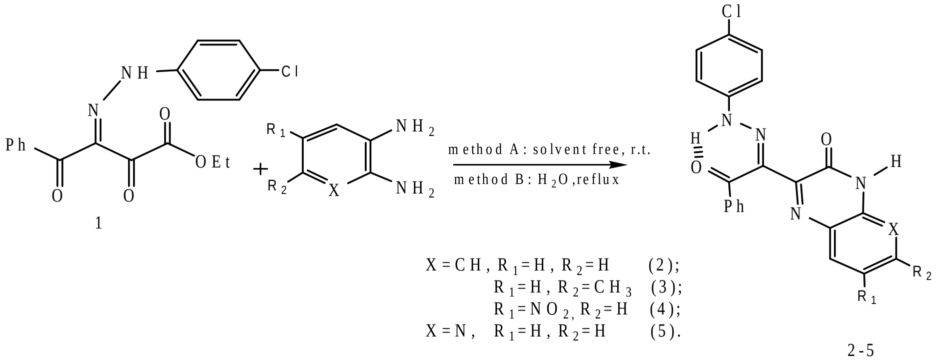
3-arylhydrazono-2,4-dioxo-4-phenylbutanoates have been prepared by the coupling of benzoyl pyruvic ester with aryldiazonium chlorides [1]. 3-arylhydrazono-2,4-dioxo-4-phenylbutanoates were used for the synthesis of the following heterocycles and react with dinucleophiles as substituted analogues [2].

We introduced a simple, quick, efficient and green synthesis for preparation quinoxaline and pyridopyrazine derivatives under solvent free conditions at room temperature (method A) [3] and in water was refluxed (method B) [4]. Structure of this compounds which has been conformed by the IR, ^{1}H-NMR and ^{13}C-NMR spectroscopy will be reported. Substituted quinoxaline derivative are pharmacologically important compounds [5].



References:

[1] Mitchell A. and Nonhebel D. C.; *Tetrahedron*; **1979,** 35, 2013.
[2] Fokin A. S., Burgart Ya. V., and Saloutin V. I.; Russ. *J. Org. Chem.*; **2006,** 42, 906.
[3] Issa Yavari,Anvar Mirzaei and Gholamhossein Khalili; *J. Helvetica Chimca Acta* **2010**, 93, 654.
[4] Prakasam Thirumurugan, Durasamy Muralidharan, Paramasivan T.perumal *J dyes and pigments* **2009,** 81,245.
[5]Montana, M.; Terme, T.; Vanelle, P. *Tetrahedron Lett*. **2005**, 46, 8373.

Solvent-free synthesis of pyrido[2,3-*d*]pyrimidine derivatives over ZrO_2 nanoparticles catalyst

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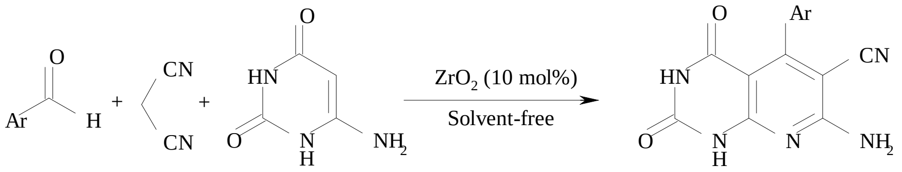
The fused pyrimidines have been studied for over a century due to a variety of chemical and pharmacological efficiency. In continuation of our previous works on the development of novel and efficient catalytic methods for the synthesis of heterocyclic compounds [1-3], herein has been reported a novel and highly efficient solvent-free protocol for the synthesis of pyrido[*d*]pyrimidine derivatives **4** via a three-component reaction of aromatic aldehydes, malononitrile and 4(6)-aminouracil in the presence of ZrO_2 nanoparticles az an efficient, inexpensive, moisture stable, commercially available and environmentally benign catalyst.

The method we have presented here in addition to its simplicity of operation has the advantages of high yields, easy work-up, short reaction time and recyclability of the catalyst. A reasonable mechanism has also been proposed for the courses of reactions.



1 **2** **3** **4**

References:

[1] Abdolmohammadi, S.; Balalaie, S. *Tetrahedron Lett*. **2007**, *48*, 3299.
[2] Balalaie, S.; Abdolmohammadi, S.; Bijanzadeh, H. R.; Amani, A. M. *Mol. Divers*. **2008**, *12*, 85.
[3] Balalaie, S.; Abdolmohammadi, S.; Soleimanifard, B. *Helvetica Chem*. Acta **2009**, *92*, 932.

Effect of structural constituents and curing agents on thermal stability and flammability of novel epoxy modified polyurethanes

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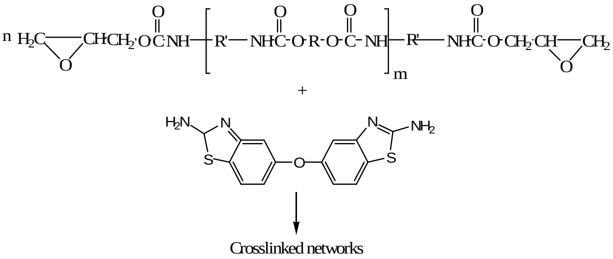
Polyurethanes are one of the most versatile products in the group of engineering polymers possess high tensile modulus, high abrasion resistance, and resistance to oil and many solvents [1]. However, their low service temperature limits their wide range application as high performance materials. Chemical modification of polyurethane backbone through the introduction of heterocyclic structures is an acceptable rout to tackle this drawback [2-4]. The presence of free isocyanate groups is another problem that some commercial polyurethane may have. Functional group transformation of isocyanates to non-moisture sensitive but highly reactive epoxy groups is a way to overcome this difficulty [5].

In the present work a series of polyurethane prepolymers with terminal epoxy groups were synthesized and fully characterized by spectroscopic methods. For these polyurethanes the molecular weight of polyols and the structure of diisocyanates were changed to find their effects on final properties of obtained polymers. These prepolymers then transformed to crosslinked networks via reaction with a hetrocyclic diamine containing benzthiazole moieties. The thermal, mechanical and viscoelastic properties of this polymer were studied and compared with non heterocyalic and aliphatic diamines. Considerable improvement in thermal, mechanical and viscoelastic properties were detected via introduction of benzothiazole moieties.



References:

[1] Szycher, M. Szycher Handbook of Polyurethanes, CRC Press, BocaRaton, FL, **1999**.
[2] Yeganeh, H.; Atai, M.; Hojati Talemi, P.; Jamshidi, S. *Macromol. Mater. Eng*. **2006**, *291*, 883.
[3] Yeganeh, H.; Mehdipour-Ataei, S.; Ghaffari, M. *High Perform. Polym*. **2008**, *20*, 126.
[4] Yeganeh, H.; Razavi-Nouri, M.; Ghaffari, M . *Polym. Adv. Tech.* **2008**, *19*, 1024.
[5] Yeganeh, H.; Hojati Talemi, P.; Jamshidi, S. *J. Appl. Polym. Sci*. **2007**, *103*, 1776.

Investigation of hydrolysis properties of new segmented poly(urethane urea)s based on environmental friendly diisobutyl-2,5-diketopiperazine

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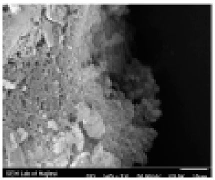
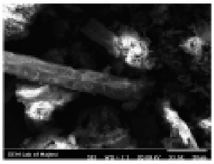
Diketopiperazines are the smallest cyclic peptides known, which are commonly biosynthesized from amino acids by different organisms, and are considered to be secondary functional metabolites or side products of terminal peptide cleavage. Cyclic dipeptides are extensively obtained by extraction from natural sources, and may also be easily synthesized [1]**.** A large number of degradable polymers have been used in biomedical applications, or as environmental friendly polymers. In addition in response to public concern about the effects of plastics in the environment and damaging effects of plastic wastes on animals and birds, it has become a widely accepted opinion that (bio)-degradable polymers have a well-grounded job in solving waste problem [2,3]**.**

In this work anhydride cyclodipeptide (LAC) was prepared through a green method under microwave irradiation with good yield. Then a new class of hydrolysable poly(ethereurethaneeurea)s (PEUUs) was synthesized via two-step polymerization method. In the first step, 4,40-methylene-bis-(4-phenylisocyanate) (MDI) was reacted with LAC to produce isocyanate-terminated poly(imide-urea) oligomers (hard segment). Reaction of the resulting pre-polymer with different molecular weights (MW) of polyethyleneglycols (PEG)s such as PEG-400, PEG-600, PEG-1000 and PEG-2000 was the second step to furnish a series of new PEUUs. The resulting multiblock copolymers have inherent viscosities in the range of 0.4e1.8 dL/g. These multiblock copolymers are hydrolysable, thermally stable and soluble in amidetype solvents. Polymers containing different molecular weights of PEGs soft segments show different thermal stability, phase separation, hard segment cohesiveness and hydrolysis rate. Some structural characterization and physical properties of these PEUUs are reported.



(1) Scanning electron micrographs of PEUUs surface before degradation



(2) Scanning electron micrographs of PEUUs surface after degradation

References:

[1] Delaforge M, Bouill'e G, Jaouen M, Jankowski CK, Lamouroux C, Bensoussan C. Recognition and oxidative metabolism of cyclodipeptides by hepatic cytochrome P450. *Peptides*. **2001**, 22 (4), 557.

[2] Rutkowska M, Krasowska K, Heimowska A, Steinka I, Janik H. Degradation of polyurethanes in sea water. *Polym Degrd Stab*. **2002**, 76 (2), 233.

[3] Okada M. Chemical syntheses of biodegradable polymers. *Prog Polym Sci*. **2002**, 27 (1), 87.

Melamine sulfonic acid as a novel, green and ecofriendly catalyst for one-pot synthesis of aryl-14H-dibenzo[a.j]xanthenes under solvent-free conditions

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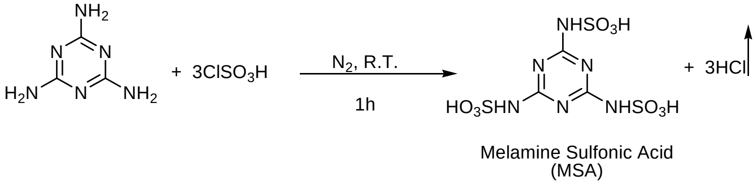
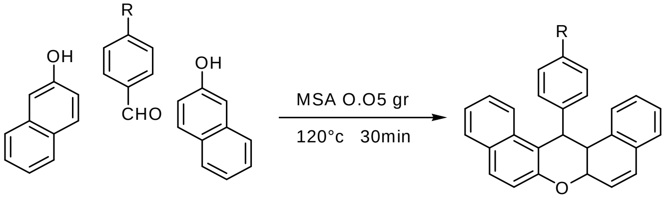
The synthesis of xanthenes, especially benzoxanthenes has attracted interest due to their biological and pharmaceutical properties such as antiviral, antibacterial, and antiflammatory [1]. Furthermore, these compounds represent a very important class of leuco-dyes .Various methods are available for the construction of xanthenes and benzoxanthenes. In this methods use different liquid catalysts has been reported.

Homogeneous acidic catalysts are commonly used for organic synthesis carried out in laboratories and industries. However, the above-mentioned catalysts have several disadvantages because they are corrosive, toxic or volatile, and generate large amount of waste. In order to overcome all the drawbacks in the use of environmentally hazardous homogeneouse catalysts,solid acids have been tested. Each catalyst has its own advantages and disadvantages. It is always interesting to develop a new environmental benign catalyst for organic transformation.

In this project Melamine Sulfonic Acid has been used as an efficient heterogeneous acidic catalyst in the aryl-14-H-dibenzo[a , j] xanthenes preparation.





References:

[1] Poupelin J. P.; Saint-Ruf, G., Foussard-Blanpin, O., Narcisse, G.; Uchida-Ernouf , G., Lacroix, R. *Eur J Med Chem.* **1978**, 1125.

Oxidative aromatization of some 3, 5-diacetyl-1, 4-dihydropyridine derivatives with supported ammonium chlorochromate on silica gel under microwave irradiation

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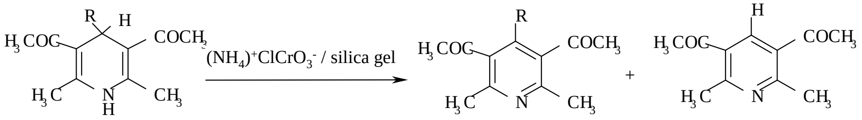
The 1,4-dihydropyridine (DHP) derivatives which contain the 1,4-dihydropyridine structure of the natual reduced nicotinamide adenine dinucleotide [NAD(P)H] coenzyme play a vital role in many bioreductions and possess a high biological activity as a class of useful drugs [1].

The oxidative aromatization of dihydropyridines provides an efficient method for the preparation of pyridine derivatives. In recent years, much attention has been paid to the use of microwave irradiation in organic synthesis due to added advantage like reduction in reaction time. So, in connection with our previous research on the chemistry of 1,4-dihydropyridines [2, 3], we wish to report the results obtained from a study of the oxidation of some 3,5-diacetyl 1,4-dihydropyridines with ammonium chlorochromate absorbed on the silica gel under microwave irradiation with high yield in short reaction time.

Chromium (VI) is established as oxidant for many types of compounds [4]. In recent years ammonium chlorochromate was used for oxidation of some organic compounds [5, 6]. The solid-phase synthesis under microwave irradiation has several advantages because solvents are often expensive, toxic, difficult to remove and are environmentally polluting. In conclusion, this method leads to a benign and attractive procedure for the oxidation of 1,4-dihydropyridines.



References:

[1] Brewster, M. E.; Simay A.; Czako, K.; Winwood, D.; Farag. H.; Bodor, N. *J. Org. Chem.* **1989**, *54*, 3721.
[2] Memarian, H. R.; Abdoli-Senejani, M.; Dopp, D. *J. Chin. Chem. SOC.* **2007**, *54*, 13.
[3] Memarian, H. R., Abdoli-Senejani, M., *Ultrason. Sonochem.* 2008**,** *15***,** 110 and references cited therein.
[4] Patel S.; Mishra B.K. *Tetrahedron* **2007**, *63*, 4367.
[5] Heravi M.M.; Beheshtiha, Y.S.; Oskooi, S. H. A.; Shoar, R. H.; Khalilpoor, M. *Phosphorus Sulfur.* **2000**, *161*, 251.
[6] Zhang, G.-S.; Shi, Q.-Z.; Chen, M.-F.; Cai, K. *Synth. Commun.* **1997,** *27***,** 3691.

Synthesis and spectral study of some new *N*-cyclohexane carboxyl phosphoramidate derivatives

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The chemistry of carbacylamidophosphates with –C(O)NHP(O)- moiety in their molecular core units are recently developed due to their biological activity and their applications as O,O-donor ligands for metal complexation. Here, two new compounds with general formula $C_6H_{11}C(O)NHP(O)R_2$, with R=2-ClC_6H_4NH (**1**), $C_6H_{12}NH$ (**2**) were prepared and characterized by IR, ^1H, ^{13}C and ^{31}P NMR spectroscopy and elemental analysis. The stating reactant, $C_6H_{11}C(O)NHP(O)Cl_2$, was prepared by the reaction of PCl_5 and cyclohexane carboxamide in CCl_4 and treating with formic acid. Compounds **1** and **2** were synthesized by the reaction of $C_6H_{11}C(O)NHP(O)Cl_2$ with corresponding amine in a 1:4 molar ratio. IR spectrum of $C_6H_{11}C(O)NHP(O)Cl_2$ exhibits the characteristic band of carbonyl group (C=O) in 1719 cm^{-1}. This band is shifted to lower frequencies in the IR spectra of **1** and **2**, (1679 and 1661 cm^{-1} respectively). In compounds **1** and **2**, as we observed earlier for phosphoramidate analogues, the $P–N_{amine}$ stretching vibrations appear at higher frequencies than the $P–N_{amide}$ vibrations. The ^{31}P NMR chemical shifts are observed for **1** and **2** at about 8.64 and 7.01 ppm respectively. In ^1H NMR spectra of **1** a broad peak is observed for the proton of NH_{amidic} at δ= 8.99, but for **2** a doublet signal at δ= 8.51 ($^2J_{PNH}$ = 6.2 Hz) was obtained for this proton.

$SbCl_3$ as an efficient catalyst for synthesis of benzimidazole derivatives

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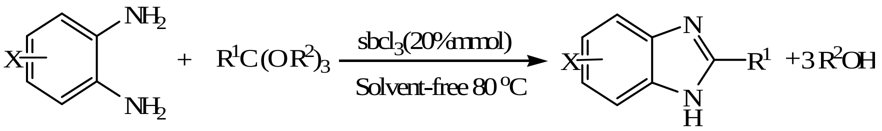
These heterocycles have shown different pharmacological activities such as: antiviral, anti microbial , antifungal , anti Parkinson , anti cancer and antibiotic properties [1].

Synthesis of benzimidazole derivatives by reaction of o-phenylendiamines with ortho-esters in presence of a catalytic amount of lewis acid ($SbCl_3$) under solvent –free conditions is report .

Recently, several methods have been introduced, where aldehydes , acid chloride, o-dinitrobenzene and 2-nitroanilines are used as starting materials for this synthesis [2]. Although, some of these methods suffer from one or more of the following drawbacks such as long reaction time , low yields of products in some cases, tedious work- up, corrosive reagents and large amounts of solid support [3]. This new protocol has the advantages of high yields, solvent-free reaction conditions, easy handling and suitable temperature.



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R_1= H, Me,Et R_2= Me, Et
X= H, Cl, Me, NO_2

References:

[1] Iraj Mohammadpoor _ Baltork ; Ahmad Reza Khosropour ; Seyedeh Fatemeh Hojati , *Catal. Commun* 8, **2007**, 1865.
[2] Zhan – Hui Zhang ; Liang Yin ; Yong - Mei Wang , *Catalysis Communications* 8 , **2007** , 1126.
[3] Majid M. Heravi ; Samaheh Sadjadi ; Hossein A .Oskooie ; Rahim Hekmat Shoar ; Fatemeh F . Bamoharram , *Catal. Comun* , **2008** , 504 .

Synthesis, characterization and investigation swelling behavior of co-polymeric gels based on *L*-Cysteine

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Synthetic polymeric gels with chiral recognition ability or functionalized sites are interesting materials for separation [1-2]. Also, gels in swollen state absorb and envelop a large amount of a suitable solvent that cause to diffuse some solute molecules [3-4]. In this report, Diacid (781) was prepared by a successive two-step process from *L*-Cysteine. This compound containing four functional groups produced a network gel(781781) in the reaction conditions of thiol and carboxylic acid groups. For studying of the effect of the flexibility on gel structural parameters,Co-polymeric gels (781781781) were synthesized by nonlinear polymerization of monomer (781) with adipic acid and diamine in the molar ratio of 1:0.5:0.5, 1:1:1, 1:2:2 and 1:3:3. The amount of gel formation and the the extent of swelling by solvent were considered by calculating the gel fraction and swelling ratio of synthetic gel. Morphology of outer surface and cross-section of prepared films from synthesized gels was considered by scanning electron microscopy (SEM). The images indicate microparticals with dimensions about of .25µm. Thermo-analytical methods DSC and TGA/DTG were used to investigate the thermal stability of gels. The formation of new functional groups which connect monomer unites for gel construction was confirmed by infrared spectroscopy and elemental analysis. The chirality of monomer and polymeric gels is shown by optical activity measurements in solution and suspension.

References:

[1] Habaue, S.; Nakano, T.; Okamoto, Y.; *Polymer* **2004**, *45*, 5095
[2] Khan, A.; Mahmood, F.; Khokhar, M.; Ahmed, S.; *Reactive& Functional Polymer* **2006**, *66*, 1014.
[3] Spizzirri, U.G.; Peppas, N.A.; *Chem Mater*. **2005**, *17*, 6719.
[4] Hiratani, H.; Mayer, J.M.; *Langmuri* **2001**. *17*, 4431.

Synthesis of benzylidene chromene deriviatives

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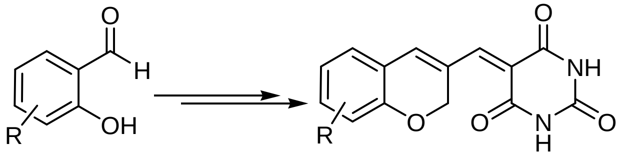
Chromenes are gregarious of natural compounds that exist in plants, which are heterocyclic compounds receptacle oxygen in whorl pyrane conjunct with benzene. The molecular with chromene structure have several biological activities [1]. These have utilization in synthesis of drug compounds as primer material [2]. Recently a context about synthesis of benzelidene chromene derivatives is reported that shows these compounds display antileishmanial and antiviral activity [3]. Leishmaniasis has a major and increasing impact on global public health and is endemic in many tropical and subtropical regions of the world, particularly in Africa, Asia, and Latin America. It found in 88 countries and affects around 12 million people of the world and 350 million people are at risk of infection with Leishmania [4].

Therefore, in continuation and improvement of the antileishmania effects our aim in this paper is study of synthesis of novel chromenes derivatives based on coupling chromenes derivatives with barbitoric acid and other benzilydene chalcones.



R= 3-OMe, 4-OH, 5-Brom

References

[1] Hirano, R.; Sasamoto, W.; Matsumoto, A.; Itakura, H.; Igarashi, O.; kondo, K. *J. Nutr. Sci. Vitamins.* **2001**, *47*, 357.
[2] (a) Goodman, L.; Benitez, A.; Anderson, C. D.; Baker R. B. *J. Am. Chem. Soc.* **1958**, *80*, 6582. (b) Condreay L, D.; Condreay J, P.; Jansen R, W.; Paff M, T.; Averett D, R. *Agents Chemothe.* **1996**, *40*, 520.
[3] Nazarian, Z.; Emami, S.; Heydari, S.; Ardestani, S.; Nakhjiri, M.; Poorrajab, F.; Shafiee, A.; Foroumadi, A. *European Journal of Medicinal Chemistry*. **2010**, *45*, 1424.
[4] Desjeux , p. Microbiology and infectious diseases**.** **2004**, *27(5)*, 305.

Three-component one-pot synthesis of α-carbamato-alkyl-β-naphthol and 2*H*-indazolo [2,1-b]phthalazine-trione derivatives

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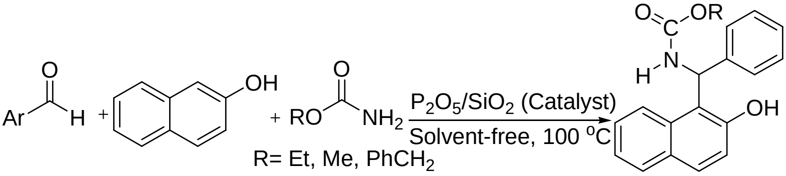
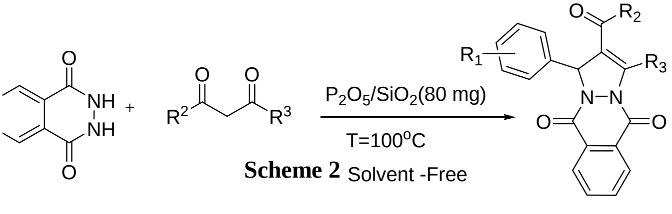
P_2O_5 supported on SiO_2 as an inexpensive, heterogeneous stable catalyst, free flowing, and white powder was prepared from mixing of dangerous and corrosive P_2O_5 with thin layer chromatography silica gel. It has the advantage of being easily removed from the organic product by filtration and also this reagent is improved storage stability in moisture in comparison to P_2O_5, which is very sensitive to moisture and also it showed much more reactivity than unsupported P_2O_5 [1].

In continuation of our research on application of heterogeneous catalysts in organic reactions [2], we have employed silica supported P_2O_5 in preparation of α-carbamato-alkyl-β–naphthols from three-component reactions of aromatic aldehydes, β–naphthol, and (ethyl, methyl, benzyl) carbamate under solvent-free conditions at 100 °C (Scheme 1).



Scheme 1

We also report a mild and highly efficient procedure for the synthesis of 2*H*-indazolo [2,1-b]phthalazine-triones using the optimize amount of P_2O_5/SiO_2 (80 mg) under solvent-free conditions. Three-component, one-pot condensation of phthalhydrazide, aromatic aldehydes and 1,3-dicarbonyl compounds cause to synthesis a series of 2*H*-indazolo[2,1-b]phthalazine-triones in presence of P_2O_5/SiO_2 under thermal solvent-free conditions (Scheme 2).



Scheme 2

References:

[1] Eshghi, H.; Rafei, M.; Karimi, M. H.; *Synth. Commun.* **2001**, *31*, 771.

[2] Shaterian, H. R.; Hosseinian, A.; Ghashang, M. *Tetrahedron Lett.* **2008**, *49*, 5804.

Highly efficient mannich reaction of aldehydes, secondary amines and naphthols catalyzed by nano-ordered B-MCM-41

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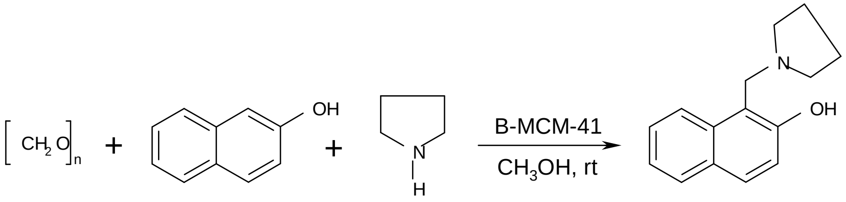
The Mannich reaction is one of the most important basic carbon–carbon bond-forming reactions in organic synthesis for preparation of different valuable synthetic intermediates such as β-amino carbonyl compounds and 1,2-amino alcohol. Lewis acids, Lewis bases, Bronsted acids, rare metal salts, and some organocatalsts have been investigated as the catalysts for this reaction over the past decades [1,2].

On the other hand, ordered mesoporous materials are very attractive as heterogeneous solid catalysts for fine chemicals synthesis. Mesoporous materials provide high surface areas which a high concentration of active sites often by incorporating metal ions into the siliceous framework is produced. Herein, we wish to report mesoporous boronsilicate (B-MCM-41) as an efficient nano-ordered solid acid catalyst for the three-component mannich reaction of aldehydes, secondary amines and naphthols at room temperature to afford the corresponding products in good to excellent yields [3].

In the initial experiments, different solvents were screened for Mannich reaction of paraformaldehyde, pyrrolidine and 2-naphthol at room temperature. Among the others, methanol was found to be the most efficient solvent for this reaction. The product can be separated easily from the reaction system.



References:

[1] Dong, F.; Kai, G.; Dai-zhen, Z.; Zu-liang, L. *Monatsh. Chem*. **2009**, *140*, 1325.
[2] Dong, F.; Jun, Z. Xin-Li; Zu-liang, L. *Catal. Lett*. **2007**, *116*, 76.
[3] Iwanami, K.; Seo, H.; Choi, J.c.; Sakakura, T.; Yasuda,H. *Tetrahedron Lett*. **2010**, 66, 1898.

Synthesis of 1, 2 bis(2-hydroxybenzylideneamino)benzene new derivatives as novel tetradentate Schiff bases and their complexes with Cobalt

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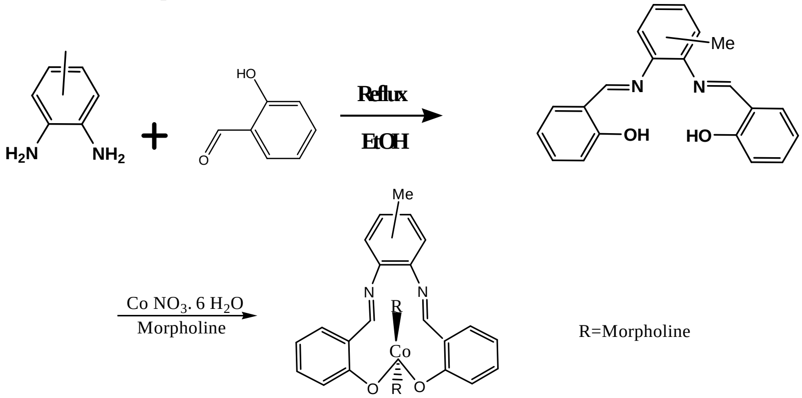
Schiff bases are capable of forming coordinate bonds with many of metal ions through both azomethine group and phenolic groups [1]. A large number of Schiff bases and their complexes are significant interest and attention because of their biological activity including anti-tumor, antibacterial, and anti-carcinogenic properties [2].

Tetradentate Schiff bases are well known to coordinate with various metal ions forming stable compounds and some of these complexes are recognized as oxygen carriers [3].

In this project all the Schiff base ligands were prepared by condasations between diaminotoluenes and salicylaldehyde in ethanol. The crude product was re-crystallized from dichloromethane/hexane (1:2) mixed solvent, after that some pail yellow crystal was resulted.

Herein we report synthesis and characterizations of novel Cobalt (*II*) Schiff base complexes in ethanol solution in presence of excess morpholine base. The purity of the synthesized compound was confirmed by recrystallization. The structure of compound was characterized using IR, ^{1}HNMR and spectra.



References:

[1] S.A. Sadeek, M.S. Refat, J. Korean Chem. Soc. 50 (2) (**2006**) 107.
[2] N. Raman, A. Thangaraja, C. Kulandaisamy, Trans. Met. Chem. 28 (**2003**).
[3] C. Floriani, F. Calderazzo, *J. Chem. Soc.* A (**1969**) 946.

Catalyst-free synthesis of 2-amino-3,5-dicarbonitrile-6-thio-pyridines in ionic liquid, [bmim]Br, as an efficient promoting medium

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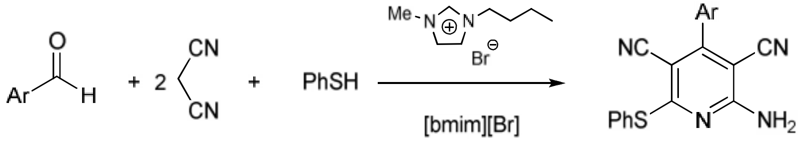
The presence of the pyridine ring system in a number of natural products, vitamins, and pharmacologically significant molecules [1] has made it a prime target for scientific research. In particular, 2-amino-3,5-dicarbonitrile-6-thio-pyridines exhibit diverse pharmacological activities and are useful as anti-prion [2], anti-hepatitis B virus [3], and anti-cancer [4] agents.

These compounds are generally synthesized via one-pot three-component condensation of an aldehyde, malononitrile and a thiol in the presence of several catalysts such as DABCO or triethylamine [5], piperidine [6], DBU [7], etc. However, some of these methodologies encounter some limitations, such as long reaction times, unsatisfactory yields, harsh reaction conditions, requirement of expensive catalysts and hazardous organic solvents.

Herein we wish to report a green and rapid methodology for the synthesis of 2-amino-3,5-dicarbonitrile-6-thio-pyridines by one-pot multi-component reaction of a variety of aryl aldehydes with malononitrile and thiophenol in ionic liquid [bmim]Br as an efficient promoting medium without the use of any catalyst.



References:

[1] Balasubramanian, M.; Keay, J. G. **1996**. Comprehensive Heterocyclic Chemistry II. In: Katritzky AR, Rees CW, Scriven EVF, Eds, Pergamon Press: London Vol. *5*, Chapter 6, pp 245–300, and references cited therein.
[2] Reddy, T. R. K.; Mutter, R.; Heal, W.; Guo, K.; Gillet, V. J.; Pratt, S.; Chen, B. *J. Med. Chem.*, **2006**, *46*, 607.
[3] Chen, H.; Zhang, W.; Tam, R.; Raney, A. K. PCT Int. Appl. WO 2005058315 A1 20050630, **2005**.
[4] Cocco, M. T.; Congiu, C.; Lilliu, V.; Onnis, V. *Eur. J. Med. Chem.*, **2005**, *40*, 1365.
[5] Evdokimov, N. M.; Magedov, I. V.; Kireev, A. S.; Konienko, A. *Org. Lett.*, **2006**, *8*, 899.
[6] Guo, K.; Thompson, M. J.; Reddy, T. R. K.; Mutter, R.; Chen, B. *Tetrahedron*, **2007**, *63*, 5300.
[7] Mamgain, R.; Singh, R.; Rawat, D. S. *J. Heterocycl. Chem.*, **2009**, *46*, 69.

Design and synthesis of 2-allyl-1-alkoxy-4-methoxybenzene as potent 15-lipoxygenase inhibitors

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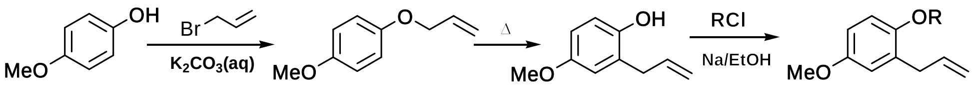
Mammalian lipoxygenases (LOs) are heterogeneous families of enzymes distributed widely throughout the plant and animal kingdoms, and are responsible for the oxidation of polyunsaturated fatty acids and esters to hydroperoxy derivatives [1]. These are non-heme iron-containing enzymes and named according to the position at which a key substrate, arachidonic acid (AA), is oxidized. There is reasonable homology between soybean enzyme (SLO) and the human one [2]. This homology becomes more identical (50%) within 8Å in the active site pocket. Obviously SLO is much more accessible than the human one. Therefore, one can expect that the results can be extendable to the human LO.

In this study, on the basis of recently report on inhibitory potency of eugenol and esteragol compounds [3], a group of 2-allyl-1-alkoxy-4-methoxybenzene were designed, synthesized and evaluated as potential inhibitors of soybean 15-lipoxygenase (SLO). Some compounds showed best IC_{50}s in SLO inhibition. All compounds were docked in SLO active site and the SAR (structure activity relationship) studies suggested that the inhibitory activity of these molecules largely depends on the orientation of allyl group toward the Fe^{III}–OH moiety in the active site of enzyme and also, it is resulted that long and volume lipophilic chain of the alkyl part of the ethers would effect on inhibitory potency variation of the synthetic compounds. So it is assumed that lipophilic interaction of ligand–enzyme would be in charge of inhibiting the enzyme activity.



References:

[1] Brash, A. R. *J. Biol. Chem.* **1999**, *274*, 23679.
[2] Sadeghian, H.; Seyedi, S. M.; Saberi, M. R.; Arghiani, Z.; Riazi, M. *Bioorg. Med. Chem.* **2008**, *16*, 890.
[3] Seyedi, S. M.; Sadeghian, H.; Jafari, Z.; Attaran, N.; Sadeghian, H.; Saberi, M. R.; Riazi, M. *Bioorg. Med. Chem.* **2009**, *17*, 1614.

Reaction of *N*1-phenyl-3-oxo-4-benzoylsuccinimide with hydrazines

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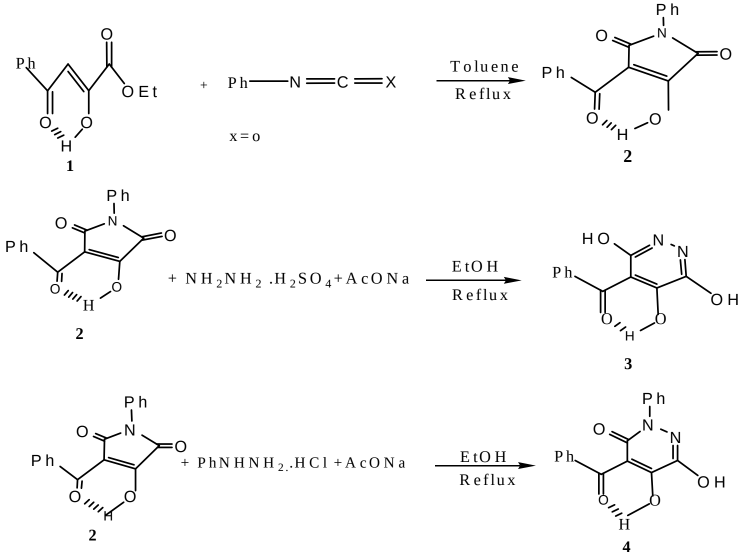
4-Phenyl-2,4-dioxobutanoate is formally derivative of pyruvic acid and it is as such trivially referred to as benzoylpyruvate.Having multiple functionalities, it is important synthesis precursor capable of interacting with both electrophilic as well as nucleophilic reagents. Research showed that pharmaceutical point of heterocyclic compounds based on benzoylpyruvate chemistry is interesting, also have some biological activity [1].

Reaction of benzoylpyruvate (**1**) with phenylisocyanate in toluene produced N1-phenyl-3-oxo-4- benzoylsuccinimide (**2**) [2].

Compound **2** react with hydrazonium sulfate and phenylhydrazonium chloride in ethanol containing AcONa to form the corresponding pyridazine derivatives.

The structures of products were confirmed by determination of the melting point and spectrophotometric techniques such as IR, ^{1}H-NMR and^{13}C-NMR.



References:

[1] Nolsoe, J. MJ.; Weigelt, D. *J.Heterocyclic Chem*. **2009**, *46*, 1.
[2] Fadda, A. A.; Abdel-Latif, E.; El-Mekawy, R.E. *Eur. J. Med. Chem*. **2009**, *44*, 1250.

Synthesis and characterization of the smallest members of pinacolophanes

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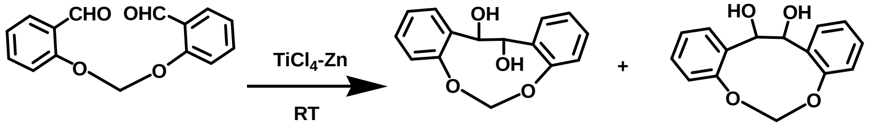
The novel short bridged pinacolophanes were synthesized by intramolecular reductive coupling in the presence of low-valent titanium at room temperature. The stereochemistry of each product was determined by NMR spectral data as well as X-ray structure analyses. The crystal structure of the molecules has some intramolecular hydrogen bonding which plays an important role in holding their configuration. The molecules in crystal are arranged in designed shapes that result from the short and various intermolecular hydrogen bondings of the molecules.



1 trans-2 cis-2

The assignment of *cis*- and *trans*- geometries was based on ^{1}H NMR. The *cis*- geometry was assigned to the isomer with lower chemical shift values for the aromatic protons. The ^{1}H NMR of the *cis*- and *trans*-diols showed symmetrical aromatic rings (two doublets and two triplets) and a single signal for both the CH(OH) methyne groups. However, the methylene groups, except for *cis*-2, appeared as two doublets to show that both groups are non-equivalent. In the ^{13}C NMR spectrum, eight signals were observed, which is in agreement with a time-averaged C2v symmetry in solution.

The molecular structure of *trans*-2 and *cis*-2 were established by X-ray crystallographic analysis. The ORTEP drawing is shown in Figure 1.

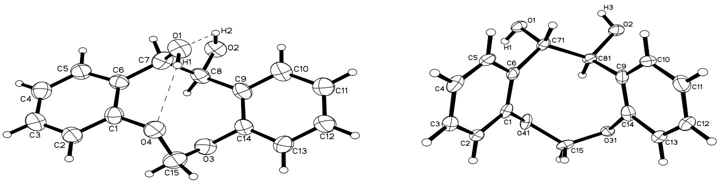


Figure 1. ORTEP drawing of *trans*-2 and *cis*-2 (major specimen) at 100 K.

References:

[1] Darabi, H. R.; Jadidi, K.; Mohebbi, A. R.; Faraji, L.; Aghapoor, K.; Shahbazian, S.; Azimzadeh Arani, M.; Nasseri, S. M. *Supramolecular Chem*. **2008**, *20*, 373.

[2] Darabi, H. R.; Mohebbi, A. R.; Bolourtchian, M. *Supramolecular Chem*. **2003**, *15*, 465.

Three-component Synthesis of alkyl 2-[4-oxopyridin-1(4H)-yl]acrylates by nucleophilicaddition of alkyl propiolates catalysed by Ph_3P

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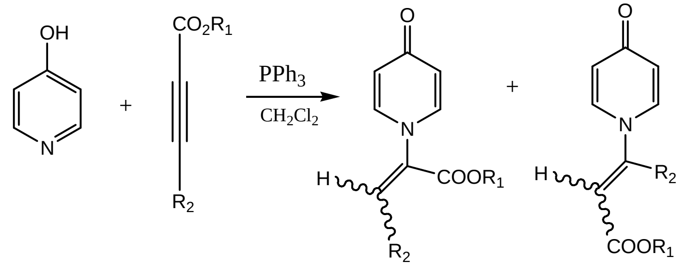
Organophosphorus compounds have been used in organic synthesis as useful reagents as well as legends of a number of transition catalysts. The phosphine induced isomerization of alkynoates and addition to the α-substituted alkyl acrylates [1].

An important point is the ability of the nucleophile to undergo Michael addition in preference to the α-attack since phosphines could also serve as general base catalysts for conjugate addition [2]. Thus the addition of 4-hydroxy pyridine (4-pyridinol) to alkyl propiolates proceeds under neutral conditions in the presence of triphenylphosphine to give a corresponding α-substituted alkyl acrylates in fairy good yields.

The products are commercially available multifunctional system, which is apparently completely enolized in liquid phase, as indicated by ^1H, ^{13}C, NMR, IR and mass spectroscopy.



	R_2	R_1
a	Me	H
b	Et	H
c	Et	ph

In conclusion the reaction of 4-hydroxy pyridine with alkyl propiolates in the presence of Ph_3P provides a simple one-pot entry into the synthesis of compounds of potential interest, and may be considered as potentially useful synthetic intermediates because they possess carbon atoms with different oxidation states.

Reference:

[1] Trost ,B. M., Dake, G. R., *J. Am. Chem. Soc.* **1997**, *119*, 7597.
[2] B. Mohtat, S. Jabbar, A. Ghasemi, I. Yavari, *J. Chem. Res*, **2008,** 601.

A green new method for synthesis of Cu (Π) phthalocyanine derivatives using catalysts under solvent-free condition

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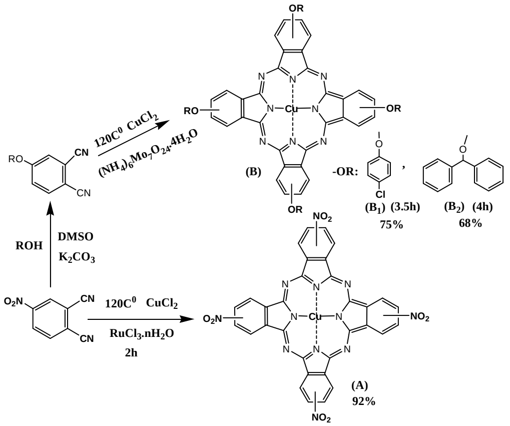
Phthalocyanines (Pcs), one of the best known synthetic porphyrin analogues, are highly versatile and stable chromophores with unique physicochemical properties that make them, alone or in combination with many other electro- and photoactive moieties, ideal building blocks for the construction of molecular materials with special electronic and optical properties [1]. Pcs have macrocyclic 18π electron systems that are known to be the source of semiconductor characteristics, and they are characterized by high thermal and reasonable chemical stability [2] [3]. In this paper we synthesized derivatives of Cu (II) phthalocyanines from 4-nitro phthalonitrile that it was prepared from phthalimide. For synthesis of derivatives of Cu (II) phthalocyanine we mixed 4mmol intermediates of phthalonitrile and 1mmol $CuCl_2$ and 5% w ruthenium choloride or ammonium molybdate as catalysts and heated with stirring to 120 ^{0}C and the mixture was washed with boiling water and filtered. The products were dark green. In conclusion we synthesized of these derivatives without solvent that is compatible with invironment. These products were identified by IR, Uv- Vis, MS. The peak at 640–690 nm (Q-band) attributed to the π–π* transition and the peak at 330–380 nm (S-band). IR spectra showed elimination of peak of CN in (2230cm^{-1}) and appearance of peak of C=N in (1640cm^{-1}).



References:
[1] Bilgin, A.; Yagcı, C.; Yıldız, U. *macp*, **2005**, 2257.
[2] Wohrle, D.; Schulte, B. *Makromol. Chem.*, **1985**, *186*, 2229.
[3] Alemdar, A.; Ozkaya, A.R.; Bulut, M. *Polyhedron*, **2009**, *28*, 3788.

Melamine-$(H_2SO_4)_3/NH_4NO_3$: As an efficient system for the first *mono* and *di*-nitration of bisphenol A as well as nitration of the other phenols

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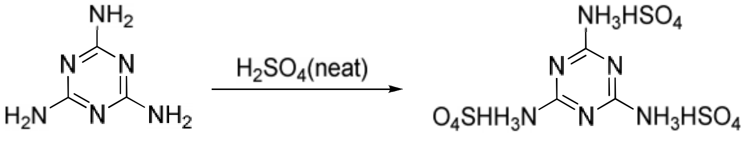
Solid acids have many advantages such as simplicity in handling, decreased reactor and plant corrosion problems, and more environmentally safe disposal. Also, wastes and by-products can be minimized or avoided by developing cleaner synthetic routes [1]. On the basis of our experiences in the application of solid acids [2], we found that melamine reacts with concentrated sulfuric acid to give Melamine-$(H_2SO_4)_3$. It is interesting to note that this exothermic reaction is easy and clean without any required work-up procedure (Scheme 1).



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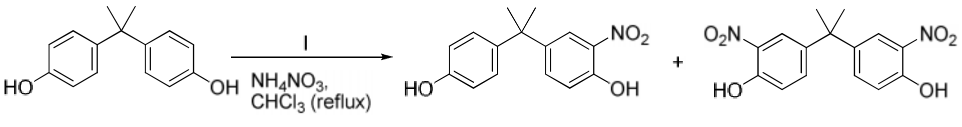
Scheme 1.

In continuation of our studies on the nitration of phenols [3], we were interested in using the Melamine-$(H_2SO_4)_3$ for the *in situ* generation of NO_2^+ in combination with NH_4NO_3 and wet SiO_2 and eventually nitration of phenols. Herein, we wish to report a simple, economical and effective method for the first *mono* and *di*-nitration of Bisphenol A as well as nitration of the other phenols (Scheme 2).



Scheme 2.

References:

[1] Shirini, F.; Zolfigol, M. A.; Salehi, P.; Abedini, M. *Curr. Org. Chem.* **2008**, *12*, 183.
[2] Zolfigol, M. A.; Ghaemi, E.; Madrakian, E.; Ghorbani Choghamarani, A. *Mendeleev Commun.* **2006**, 41.

$Mg(BF_4)_2$ doped in [BMIM][BF_4]: A task-specific ionic liquid-catalyst for efficient synthesis of 1,8-dioxo-decahydroacridines and bis-coumarins

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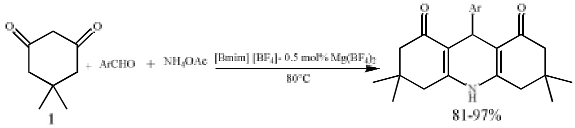
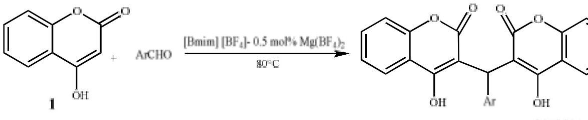
During recent two decades ionic liquids (ILs) have proved themselves as new generation of solvents having exclusive physical and chemical properties suitable for affecting the efficiency and selectivity of numerous reactions. High polarity and non-coordinative nature of ILs made them promised media for enhancing the catalytic activity of metal catalysts. In these media cationic metal catalysts are not tethered and so are more effective even in lower concentrations [1]. 1,4-Dihydropyridines represent an important class of compounds which are found in many biologically active compounds, such as vasodilator, bronchodilator, anti-atherosclerotic, antitumor, calcium channel blockers, geroprotective, hepatoprotective, and antidiabetic agents [2].



Ar= 2-Cl/ 4-Cl/ 4-NO_2/ 3-NO_2/ 4-CH_3/ 4-OCH_3/ 4-F/ 4-OH/ 4-NMe_2

On the other hand, 4-hydroxycoumarin derivatives are of interest because of their anticoagulant, spasmolytic, and rodenticidal activities. Some coumarin derivatives are known for their antifungal and anti-HIV activities. They are also extensively used as analytical reagents [3].



Ar= 2-Cl/ 4-Cl/ 4-NO_2/ 3-NO_2/ 4-CH_3/ 4-OCH_3/ 4-F/ 4-OH/ 4-NMe_2

Figure 1

Herein we report an efficient method for synthesis of some bis-coumarin derivatives and 1,8-dioxo-decahydroacridines in the presence of [Bmim][BF_4]-[0.5mol% $Mg(BF_4)_2$] at 80˚C. In all cases the reactions gave solely the desired products in good yields and devoid of problems which mainly associate with using solvents such as handling, safety, and difficulties of recycling. The present methodology also offers the advantages of excellent yields, short reaction time, and milder reaction conditions.

References:

[1] Welton, T. *Chem. Rev.* **1999**, *99*, 2071.
[2] Shan, R.; Velazquez, C.; Knaus, E. *J. Med. Chem.* **2004**, *47*, 254.
[3] Sen, K.; Bagchi, P. *J. Org. Chem.* **1959**, *24*, 316.

Antioxidant activity of various *Thymus kotschyanus* aerial part extracts

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The genus *Thymus* L. (Labiatae) consists of about 215 species of herbaceous perennials and subshrubs. The Mediterranean region can be described as the center of the genus. This genus is represented in Iranian flora by 14 species, four of which (*T. carmanicus, T. daenensis* subsp. *Daenensis* and *T. daenensis* subsp. *lancifolius*, *T. persicus* and *T. trautvetteri*) are endemic [1]. The Persian name of the genus is ‘‘Azorbeh’’ and/or ‘‘Avishan’’[2]. *Thymus* species are commonly used as herbal tea, flavoring agents and medicinal plants. Among the species grown in Iran, *T. daenensis* Celak. and *T. kotschyanus* Boiss. and Hohen. are more widely used for these purposes. Infusion and decoction of aerial parts of *Thymus* species are used as tonic, carminative, digestive, antispasmodic, anti-inflammatory, antitussive, expectorant and for the treatment of colds in Iranian traditional medicine [3].

In this investigation, *Thymus kotschyanus* aerial parts were successively extracted with chloroform, ethyl acetate, acetone and ethanol using a soxhlet extractor for 8 h each. The crude extracts were screened for antioxidant activity. The reducing power and antioxidant activities evaluated in various in vitro models (DPPH, FTC, TBA) showed the highest activity for ethanolic extract. The content of total phenolic compounds and flavonoids were also measured in the plant extracts. The data obtained in the in vitro models clearly establish the antioxidant potency of all extracts.

Refrences:

[1] Rechinger, K. H. *Flora Iranica Graz*: Akademische Druck- und Verlagsanstalt **1982** (Vol. *152*).
[2] Mozaffarian, V. *Dictionary of Iranian plants names*. Tehran: Farhang Moaser Publishers, **1998**.
[3] Amin, G. *Popular medicinal plants of Iran* p. 39. Tehran*:* Research Deputy of Health Ministry, **1991** (Vol. *1)*.

Stereoselective reaction between N^1-benzyl-4-methyl-1-benzenesulfonamide derivatives with dimethyl acetylenedicarboxylate and antimicrobial activities of related *N*-vinylated products

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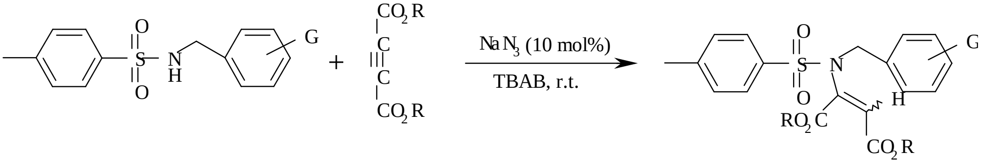
Sulfonamides receive considerable attention in the literature, as a consequence of their exciting biological properties [1]. We have perversely reported the stereoselective reaction between phenols and dimethyl acetylenedicarboxylate (DMAD) [2]. In this work we wish to report the stereoselective *syn* addition of sulfonamides **1** to dimethyl acetylenedicarboxylate in the presence of tetrabutylammonium bromide (TBAB) and sodium azid at room temperature to produce *N*-vinylated products **2**.

Gram-positive and Gram-negative bacteria are a significant cause of hospital acquired and community infections and may induce diseases associated with serious levels of morbidity and mortality. Moreover, antibiotic resistance of Grampositive pathogens, such as *Staphylococcus aureus*, *Escherichia coli*, *Enterobacter earogenes*, and *Pseudomonas aeruginosa* has become one of the major worldwide health problems [3]. The activity against Gram-positive and Gram-negative bacteria of vinylated products **2** were tested in *vitro* using two reference bacterial strains. e.g. *Staphylococcus aureus* and *Escherichia coli.* These compounds were active against both strains tested by disk diffusion method in ranging from 10 to 15 mm per 2 µg disk.



1 **2**

G: H, 2-Chloro, 4-Fluoro, 2-Methoxy R: Me, Et (E)-Isomer: 80-98%

References:

[1] Kumare, M.; Panda, G.; Srivastava, K.; Kumar.; S. *Bioorg. Med. Chem. Lett*. **2008**, *18*, 776.
[2] Nasiri, F.; Atashkar, B. *Monatsh Chem*. **2008**, *139*, 1223.
[3] Kuhn, I. ; Iversen, A. ; *Int. Antimicrob Agent*, **2000**, *14*, 337.

The study of synthesis of aceanthrylenes and their derivatives

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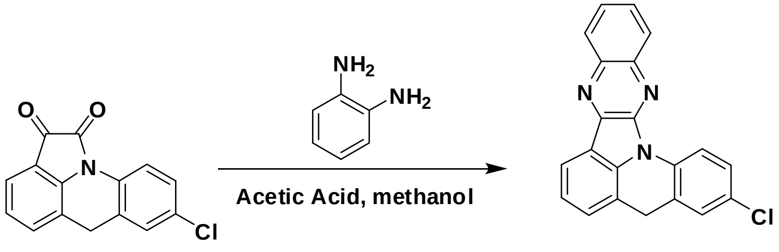
The structural diversity and biological importance of nitrogen containing heterocycles have made them attractive synthetic targets over many years and they are found in various natural products [1]. Considering to earlier synthesized compounds, we expect that our novel synthesized derivatives from Aceanthrylenes would be have critical characteristics. Among the various classes of nitrogen containing heterocyclic compounds, Aceanthrylenes derivatives are important components of several pharmacologically active compounds. They are well known in the pharmaceutical industry and have been shown to possess a broad spectrum of biological activities including antiviral, antibacterial, anti-inflammatory and as kinase inhibitors [2].

In this study, 2-chloro-9,10-dihydroacridine was treated with sodiuom in butanol at 110°C to produced in excellent yields. The 2-choloro-9,10-dihydroacridine under Fridel-Crafts reaction [3] Produced 8-chloro-6H-pyrrolo[1,2,3-de]acridine-1,2-dione in high yields.

Finally, 8-chloro-6H-pyrrolo[1,2,3-de]acridine-1-2-dione **(1)** was reacted with ortho-phenylen diamine under specific conditions to produce heterocyclic aceanthrylene derivative **(2)** in quantitatively yield. The structure of synthesized compound was characterized and confirmed by FT-IR and NMR spectroscopy techniques.



(1) **(2)**

References:

[1] Pozharskii AF, Soldatenkov AT, Katritzky AR. Heterocycles in life and society.Chichester, UK: John Wiley and Sons; **1997.**

[2] Rajesh S. Bhosale,a Swapnil R. Sarda,a Suresh S. Ardhapure,a Wamanrao N. Jadhav,a Sudhakar R. Bhusareb and Rajendra P. Pawara, *Tetrahedron Let*. **2005**, 4, 7183.

[3] Heinz Langhalas, Gertrud Schonmnann, Kurt Poilborn. *Chem. Eur. J.* **2008**, *14*, 5290.

Brønsted acidic ionic liquid as the efficient and reusable catalyst for the synthesis of coumarins via Pechmann condensation under solvent-free conditions

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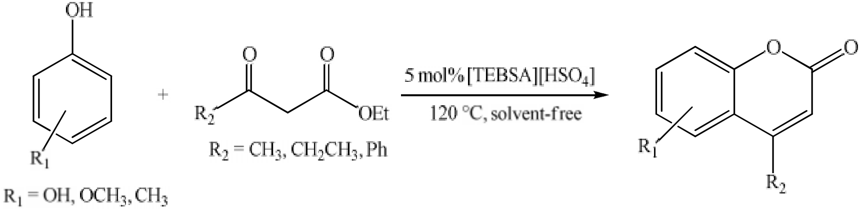
Coumarins and their derivatives represent an important class of natural products that possess significant biological and pharmaceutical properties. They act as anticancer [1], antibacterial [2], inhibitors for platelet aggregation [3]. These heterocyclic compounds are also used in perfumes [4], dispersed fluorescent and laser dyes [5]. Various methods have been used to obtain coumarins.

Among them, the Pechmann reaction was extensively used for the synthesis of coumarins. This method includes the reaction of phenols with *β*-ketoesters or malic acid or alkynoates [6] in the presence of acidic catalysts.

Herein we report a mild and efficient method for the preparation of substituted coumarins from reaction of various phenols with different *β*-ketoesters in the presence of Brønsted acidic ionic liquid ([TEBSA][HSO_4]) as an effective catalyst under thermal solvent-free conditions. High yields, short reaction times, easy work-up, reusability of the catalyst and green conditions are the most advantages of this procedure.



References:

[1] wang, C. J.; Hsieh, Y. J.; Chu, C. Y.; Lin, Y. L.; Tseng, T. H. *Cancer Lett.* **2002**, *183*, 163.
[2] Maxwell, A. *Mol. Microbiol.* **1993**, *9*, 681.
[3] Cravotto, G.; Nano, G. M.; Palmisano, G.; Tagliapietra, S. *Tetrahedron: Asymmetry.* **2001**, *12*, 707.
[4] Kennedy, R. O.; Tharnes, R. D.; Coumarins: *Biology, Application and Mode of Action; Wiley & Sons: Chichester,* **1997**.
[5] Maeda, M.; Laser Dyes; *Academic: New York*, 1994.
[6] Trost, B. M.; Toste, F. D.; Greenman, K. J. *Am. Chem. Soc.* **2003**, *125*, 4518.

A green procedure for one-pot synthesis of 1-amidoalkyl 2-naphthols using PEG-SO_3H as an efficient and reusable catalyst under solvent-free conditions

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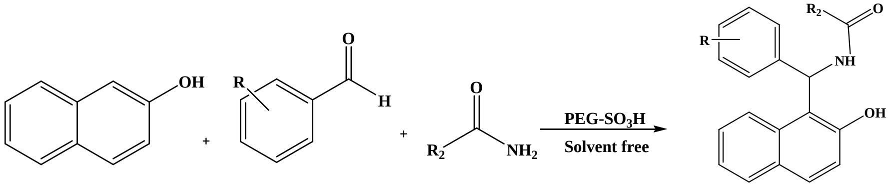
Multicomponent reactions (MCRs) are special types of synthetically useful organic reactions in which three or more different starting materials react to give a final product in a one-pot procedure [1,2].

On the other hand, solid acids have many advantages in both industry and laboratory such as simplicity in handling, decreasing reactor and plant corrosion problems, and more environmentally safe disposal in chemical processes. Furthermore, wastes and by-products can be minimized or avoided by developing cleaner synthesis routes. Poly (ethylene glycol)-bound Sulfonic acid (PEG-SO_3H) is a solid acid which can be used for different organic functional group transformations as catalyst under heterogeneous and homogenous conditions [3,4].

In this research, we report a new, simple, mild, and effective procedure for the one-pot synthesis of amidoalkyl naphthol derivatives via a multi-component condensation reaction between aryl aldehydes, 2-naphthol and amide in the presence of PEG-SO_3H as catalyst with high yields (78-94%). In conclusion we have developed a facile, convenient and environment-friendly multicomponent protocol for the synthesis of amidoalkyl naphthols under green conditions.



References:

[1] Shanthi, G.; Perumal, P. T. *Tetrahedron Lett*. **2009**, *50*, 3959.
[2] Li, K. T.; Dai, C. L.; Kuo, C. W. *Catal. Commun*. **2007**, *8*, 1209.
[3] K. Wilson, J. H. Clark, *J. Pure Appl. Chem*. **2000**, *72*, 1313.
[4] H.R. Shaterian, M. Ghashang, M. Feyzi, *Appl Catalysis A. General*. **2008**, *354*, 128.

IBr, $SnCl_2.2H_2O$ and $Ni(OAc)_2.4H_2O$ as a new and highly efficient catalyst for formation of acylals at room temperature under solvent-free conditions

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Acylals are important starting materials in organic synthesis, especially for the preparation of dienes [1] and chiral allylic esters [2] and also act as cross linking reagents for cellulose in cotton [3]. They are among the most popular protecting groups for carbonyl compounds due to their stability under neutral and mild conditions [4].

Usually, they are prepared from aldehydes and acetic anhydride using strong protic acids such as sulfuric [5], methanesulfonic [6], although the yields in many cases are poor. Many of the reported methods, however, involve strongly acidic or oxidising conditions, corrosive reagents, high temperature, high catalyst loading, longer reaction time and cumbersome procedures.

In continuation of our research, we herein report the results of IBr, $SnCl_2.2H_2O$ and $Ni(OAc)_2.4H_2O$ catalysed expedient, simple and cost effective, selective conversion of aldehydes to acylals. nor ketones react under the same conditions.

$$\mathrm{RCHO} \xrightarrow[\mathrm{Ac_2O\ (2ml)\ ,\ RT}]{\substack{\mathrm{SnCl_2\ (0.1mmol)\ or} \\ \mathrm{Ni(OAc)_2.4H_2O\ (0.15mmol)} \\ \mathrm{or\ \ IBr\ (0.05mmol)}}} \mathrm{RCH(OAc)_2}$$

References:

[1] (a) Snider, B. B.; Amin, S. G. *Synth. Commun*. **1978**, *8*, 117.
[2] Trost, B. M.; Lee, C. B. *J. Am. Chem. Soc*. **2001**, *123*, 3687.
[3] Frick, J. G.; Harper, R. J. *J. Appl. Polym. Sci*. **1984**, 29, 1433.
[4] (a) Greene, T. M.; Wuts, P. G. M. *Protective Groups in Organic Synthesis*, 3rd ed.; Wiley: New York, **1999**; p 306; (b) Gregory, M. J. *J. Chem. Soc. B* **1970**, 1201.
[5] Tomita, M.; Kikuchi, T.; Bessho, K.; Hori, T.; Inubushi, Y. *Chem. Pharm. Bull*. **1963**, *11*, 1484.
[6] Freeman, I.; Karchefski, E. M. *J. Chem. Eng. Data* **1977**, *22*, 355.

Reduction of oximes and imines with LiAlH4 under solvent-free conditions

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Reduction of imines and oximes is an important method of preparing amines. Many of the methods for this purpose involve the use of expensive and stoichiometric amounts of catalysts and organic solvents, and may suffer from poor chemoselectivity and require extended reaction times and the necessity of chromatographic workup [1]. In continuation of our interest on solvent-free reactions, we have investigated a new process without using organic solvents using ball-milling. Solvent-free organic synthesis has great value and expansive prospects. The main advantages of this economical and environmentally friendly protocol are the use of the non-expensive LiAlH4, solvent-free conditions and high yields. Lithium aluminium hydride, as a kind of common reductant, has been used widely in organic synthesis. Lithium aluminium hydride or retouched Lithium aluminium hydride can efficiently reduce imines[3].

In this work, we synthesized amines from imines and oximes by ball-milling with LiAlH4 at room temperature, followed by aqueous workup. The starting materials were also synthesized by ball- milling under solvent-free conditions.

$$\mathrm{Ar{-}CH{=}N{-}Ar} \xrightarrow[\text{ball-milling}]{\mathrm{LiAlH_4}} \mathrm{Ar{-}CH_2{-}NH{-}A}$$

References:
[1] Kazemi, F.; Kiasat**,** A. R.; Sarvestani**,** E. *Chinese Chemical Letters* **2008,** *19*, 1167
[2] Naimi-Jamal, M. R.; Mokhtari, J.; Dekamin, M. G.; Kaupp, G . *Eur. J. Org. Chem*, **2009**, 3567- 3572.
[3] Cao, Yu-Qing.; Dai, Zhi.; Chen, Bao-Hua.; Liu, Rui. *J Chem Technol Biotechnol*, **2005**, 80, 834- 836.

Solvent-free synthesis of new benzimidazoles catalyzed by a Brønsted-acid ionic liquid as a green and reusable catalyst

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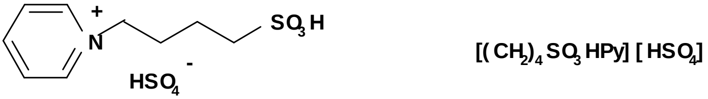
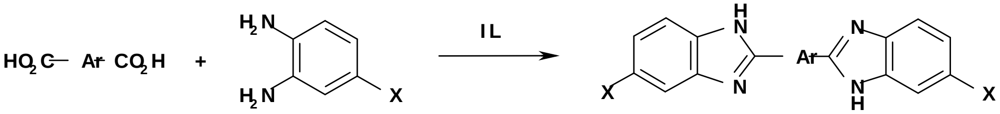
Benzimidazoles constitute an important class of heterocyclic compounds that possess a wide spectrum of biological properties [1]. and find wide applications as antifungal, antibacterial, antihelminthic, and 5-HT receptor antagonist agents. There are also literature reports on the use of benzimidazoles as corrosion inhibitors in oilfields[2,3]. The classical method for the synthesis of benzimidazoles is the Phillips reaction, which involves condensation of o-phenylenediamine with carboxylic acid or its derivatives in the presence of dilute mineral acid at elevated temperature. Although this method of condensation works well for the preparation of 2-alkyl-substituted derivatives, it frequently fails or gives low yields in the preparation of 2-aryl-substituted benzimidazoles. Polyphosphoric acid has been reported to be a highly effective, convenient reagent for promoting this type of condensation [4].

In this paper we wish to report an efficient approach to the synthesis of new dibenzimidazoles using 4-sulfonylbutyl pyridinium hydrogensulfate $[(CH_2)_4SO_3HPy][HSO_4]$, a Brønsted-acid ionic liquid (IL), as a green and reusable catalyst.





References:

[1] Spasov, A. A.; Yozlitsa, I. N.; Bagaeva, L. I.; Anisimova, V. A. *Pharm. Chem.* **1999**, *33*, 232.
[2] Mc Mohan, A. J. Colloids Surf. 1991, 59, 187.
[3] Klenerman, D.; Joseph, M. *J. Electroanalyt. Chem.* **1992**, *340*, 301.
[4] Hein, O. W.; Alcheim, R. J.; Leavitt, J. J. *J. Am. Chem. Soc.* **1957**, *79*, 427.

Characterization of by-products in amiton synthesis

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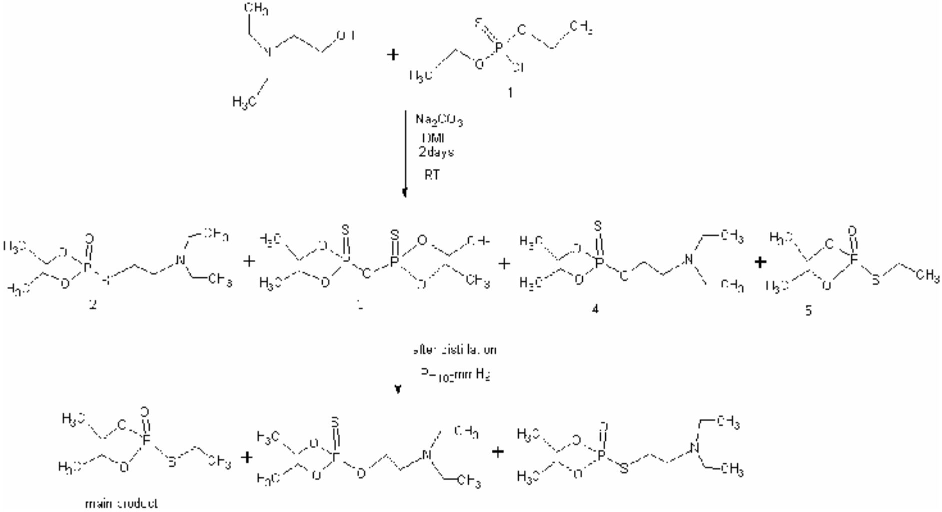
Amiton, *O*,*O*-diethyl S-[2-(diethylamino)ethyl] phosphorothiolate, is an organophosphorous compound that has been known as an insecticide and also a nerve agent called " VG" [1]. Amiton was originally developed during the early 1950s as an insecticide, but because of its toxicity has only limited applications [2]. We have synthesized Amiton by the reaction of 2-diethylamino ethanol with diethylchloro thio phosphate in dimethyl formamide in presence of sodium carbonate under reflux condition [3,4]. The compositions of the reaction mixture have been identified by ^{31}P NMR and GC-MS and compound 2, 3, 4 and 5 appeared as the principle constituent of the reaction mixture. Distillation under 100 mmHg of pressures has offered different components at different temperatures. Surprisingly we have observed that main pure product after distillation was *O,O,S*-triethyl thiophosphate (5) that was reached at 185˚ C. It seems that amiton decomposes at this temperature and it should be worked under 1 mmHg of pressures to separate amiton at temperatures lower than 185˚C.



References:

[1] Veronica T. Borrett, Robert J. Mathews, *Journal of Chromatography A*, **2003,** 1003, 143.
[2] Edgar, E. C. *Outlook Agr.* **1956**, *1*,16.
[3] Ghosh, R. J. F. Newman, *Chem. Ind.* **1955**, 118.
[4] Shafik, M. T. Enos, H. F. Agric. J. *Food Chem.* **1969,** *17,* 1186.

Preparation of carbon flake nanocomposite based on urea-formaldehyde (UF) resins

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Graphite is some of carbon derivation that approximately has electrical conductive in any dimensions. It causes that the graphite can be used as suitable composite for conductivity induction. Because of flake structure in expanded graphite, it has more light and high crystalline. This carbon form can be dispersed in aqueous and organic phases, easily. Research indicates that it can be used as reinforcements, conductive additives in composite or coating materials. In addition, graphite nanoflake can also enhance the mechanical properties, corrosion resistance and lighten the weight of materials [1]. Polymer composites are mixtures of polymer with inorganic or organic additives having certain geometries (flakes, fibers, particles). The additives embedded in the polymer in regular geometric arrangement. The electrically conductive polymeric composites can be utilizes in light emitting devices, batteries, electromagnetic shielding, anti-static, corrosion, resistant coating and functional applications [2].

In this work, nanocomposite urea-formaldehyde/nanographite was successfully synthesized by in-situ polymerization method. The modified graphite nanoflake was prepared during the several steps. Then a mixture containing graphite nanoflake and resin of urea-formaldehyde was put in ultrasonic system at the room temperature. At the second step the benzyl peroxide as initiator agent was added to prepared mixture. The result compound was gently dispersed by toluene. Eventually, a thin film was prepared from the production.

Then, average grain size, crystalline structural, morphological and electrical conductivity properties confirmed by X-ray diffraction (XRD), scanning electron microscopic (SEM), Fourier-transform infrared spectroscopy (FT-IR) and four-probe measurement, respectively.

References:

[1] Sun, G.; Li, X.; Qu, Y.; Wang, X.; Yan, H.; Zhang, Y. *Materials Letters.* **2008**, *62*, 703.
[2] Zhao, Y.F.; Xiao, M.; Wang, S.J.; Ge, X.C.; Meng, Y.Z. *Composites Science and Technology***.** **2007**, *67*, 2528.

Synthesis, characterization and applications of molecular imprinted polymer as extractant for pre concentration and determination of Atenolol

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Molecular imprinted polymers (MIPs) were prepared from methacrylic acid and Allyl glycidil ether/ iminodiacetic acid as the functional monomer and N, N methylene-diacrylamid as the cross-linker in methanol solution using atenolol as the template molecule and 2,2-azobis-isobutyronitrile as the initiator. The polymer was by elemental analysis, IR and thermogravimetric analysis (TGA) and studied for preconcentration and determination of atenolol using high performance liquid chromatography for drug monitoring. The effects of amount of the cross-linker, the ratio of template molecule and functional monomer, amount of solvent and amount of the radical initiator on the polymerization were examined. The polymerization also was performed in presence of Cu (II) which can coordinate the drug and retain it in polymer. Clearly, in the last polymerization manner, the polymer first was doped with Cu (II) then acted as a sorbent. The synthesized polymer was successfully applied for drug determination from tablet matrix.

Reference:

[1] V . M . Biju , j . Mary Gladis , T prasada Rao . Ion imprinted polymer particles : Analytical chemical Acta 478(2003)43-51.
[2] Natalia Perez – Moral , Andrew G . Mayes . Biosensors and Bioelectronics 21 (2006) 1798 – 1803.
[3] Li-Qin Lin , Jing Zhang , Qiang fu , Lang- Chong He , Ying-Chun Li . Analytical chemical Acta 561 (2006) 178-182.

Synthesis of *N*-aryl isatin derivatives using CuI and KF/Al_2O_3

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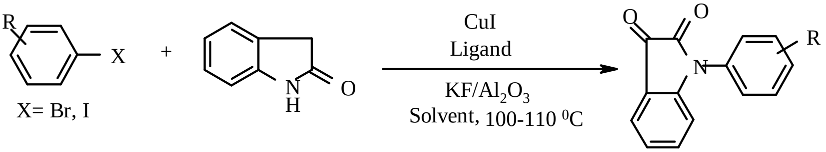
Oxindoles and isatins are familiar for their manifold biological activity. Different derivatives of compounds represent an important motif in a number of natural products and pharmaceutical targets. They display biological activity against a variety of neurodegenerative disorders and exhibit anti-tumor and anti-HIV properties [1]. Although oxindoles and isatins are ubiquitous within the pharmaceutical industry only a few examples of the Ullmann-type coupling of oxindole and isatin derivatives have been reported. Such procedures employed relatively harsh conditions (e.g., NMP, 200 °C, 24 h) or required stoichiometric amounts of copper reagents [2]. It was speculated that Buchwald's conditions for the Ullmann-type coupling reaction could be extended to the preparation of *N*-aryl oxindoles and this would serve as a valuable synthetic tool for the preparation of functionalized oxindole and isatin targets. Hudsun and et al. [3a] and Buchwald and co-work [3b] reported the coupling of oxindoles to aryl halides using a copper-diamine complex.

In our procedure we have used a stable and suitable catalytic system CuI/KF/Al_2O_3, and diamine ligand for synthesis of *N*-aryl isatin derivatives through *N*-arylation of oxindole with aryl iodides and aryl bromides. To find optimum conditions we have reacted 4-iodotoluene with oxindole in the presence of ligand, KF/Al_2O_3, CuI in different solvents. We have then used optimum condition for coupling of aryl iodides and bromides with oxindole to prepare *N*-aryl isatin derivatives.



References:

[1] (a) Bindra, J. S. In *Alkaloids*; Manske, R. H. F., Ed.; Academic Press: New York, **1973**, *14*, 83. (b) Ding, K.; Lu, Y.; Nikolovska-Coleska, Z.; Wang, G.; Qiu, S.; Shangary, S.; Gao, W.; Qin, D.; Stuckey, J.; Krajewski, K.; Roller, P. P.; Wang, S. *J. Med. Chem.* **2006**, *49*, 3432.

[2] (a) Przheval'skii, N. M.; Grandberg, I. I. *Chem. Heterocycl. Compd.* (Engl. Transl.) **1982**, *7*, 716. (b) Coppola, G. M. *J. Het. Chem.***1987**, *24*, 1249.

[3] (a) Phillips, D. P.; Hudson, A. R.; Nguyen, B.; Lau, T. L.; McNeill, M. H.; Dalgard, J. E.; Chen, J. H.; Penuliar, R. J.; Miller, T. A.; Zhi, L. *Tetrahedron Lett*. **2006**, *47*, 7137. (b) Altman, R. A.; Hyde, A. M.; Huang, X.; Buchwald, S. L. *J. Am. Chem. Soc.* **2008**, *130*, 9613.

Efficient synthesis and characterization of some novel Schiff base ligands containing amino goup

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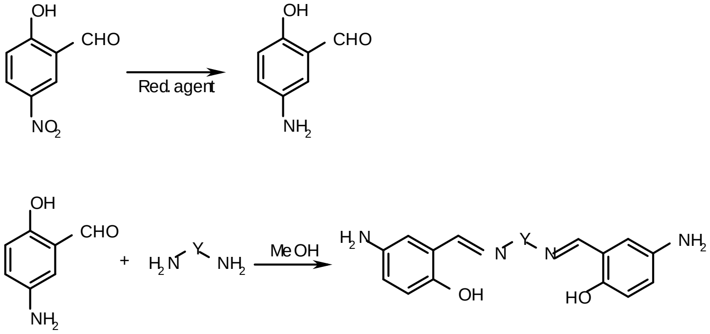
The design, synthesis and structural characterization of Schiff base complexes are a subject of current interest due to their structural, magnetic, spectral, catalytic and redox properties [1]. Chemists have reported on the chemical, structural and biological properties of Schiff bases. Schiff bases are characterized by the -N=CH- (imine) group which imports in elucidating the mechanism of transamination and rasemination reaction in biological system [2].

Metal complexes of Schiff bases are extensively studied due to synthetic flexibility, selectivity and sensitivity towards a variety of metal atoms. They are found useful in catalysis, in medicine as antibiotics and anti-inflammatory agents and in the industry as anticorrosion and sensitivity towards a variety of metal atoms [3].

Reduction of the nitro group has been one of the very important reactions in organic chemistry. In recent years, many reduction methods of the nitro group have been reported [4].

In this work, with attention to the importance of Schiff base, we report synthesis of some new Schiff bases involving amino group by reduction of nitro Schiff base ligands.



References:
[1] Venkatachalam, G.; Raja, N.; Ramesh, R.; *Spectrochimica Acta part A*. **2008**, *71*, 884.
[2] Arsalan, S.; Goglu, E.; *Sciense*. **2003**, *16*, 283.
[3] Osowle, A.; *E .J. Chem*. **2008**, *5*, 130.
[4] Seocho, Y.; *Bull Korean Chem. Soc*. **2003**, *24*, 653.

The novel synthesis of 2-(3,3,5,7-tetramethylindolin-2-ylidene)malonaldehydes And its pyrazole Derivatives

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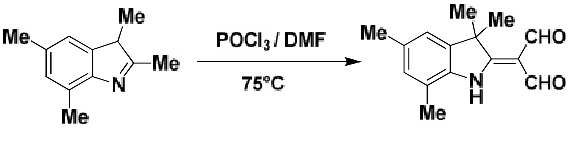
Dr. Baradarani and Co. workers described the reaction of the 2,3,3-trimethyl-Iindolenines(3H-indole) with the Vilsmeier reagent formed from dimethylformamide and phosphorylchloride to produce aminomethylene malondialdehydes [1,2].

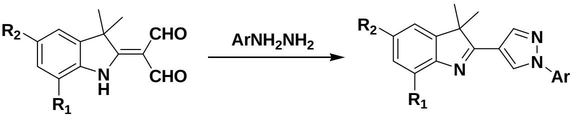
We recently described the reaction of 2,3,3,5,7-pantamethyl Indolenine (1) with the vilsmeier reagent formed from DMF and $POCl_3$ to produce aminomethylene malondialdehydes (2) (scheme 1).



(1) (2)

In view our recent finding that condensation of corresponding diformyl of 2-(3,3-dimethylindolin-2-ylidene) malonaldehydes with Hydrazine and some arylhydrazines produced 3,3dimethyl-2-(1-aryl-1H-pyrazol-4-yl)-3H-indoles in excellent yields [1,2].

In this research, we synthesized the novel diformyl compounds from (1) by the action with Vilsmeier reagent at 75 °C in excellent yields (>70%). Simply heating the diformyl (2) with hydrazines in absolute ethanol brought about a ring closure and the formation of a pyrazole ring, with a consequent migration of the double bond to regenerate an 3H-indole unit (Scheme 2).



(1) (2)

R_1=R_2= Me

References:
[1] Bradarani, M.M, Afghan, A., Zebarjadi, F., Hasanzadeh, K., and Joule,J.A., J. Heterocyclic Chem **2006**,43,1591-1595.
[2] A.Rashidi, A. Afghan, Mehdi.M Bradarani, and John A. Joule ; Heterocyclic Chem **2009**,46,428-431.

A mild and efficient one-pot synthesis of 2-dihydroimidazoles from aldehydes

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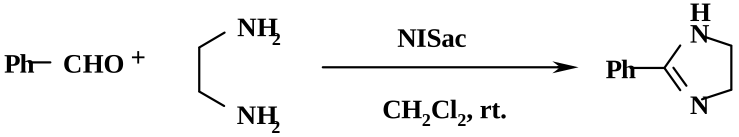
The importance of dihydroimidazole units especially in biochemistry is recently increasing, since they are found in many biologically active compounds [1]. They are also used in organic synthesis as synthetic intermediates,2 chiral auxiliaries,3 and chiral ligands.4 Therefore, several methodologies for synthesizing them have already been developed, mainly using nitriles [2] and esters [3] as the starting substrates. However, these previous methods have several drawbacks, namely the need for a high reaction temperature, acidic conditions, and the use of metal cyanide for preparation of the nitrile compounds that limit their uses. The development of mild and efficient methods is still strongly desirable.

N-iodosaccharine has been used as an oxidant and halogenating agent which is simply prepared by halogenation of saccharin [4].

Herein we have reported mild and one pot synthesis of 2-dihydroimidazoles from aldehydes and ethylenediamine in the presence of *N*-iodosaccharine at room temperature.



References:

[1] Fujioka, H.; Murai, K.; Ohba,Y.; Hiramatsu, A.; Kita, Y. *Tetrahedron Lett*. **2005**, *46,* 2197.
[2] Jung, M. E.;Huang, A. *Org. Lett*. **2000**, *2, 2659.*
[3] Jones, R. C. F.; Turner, I.; Howard, K. J. *Tetrahedron Lett*. **1993**, *34,* 6329.
[4] Menges, F.; Neuburger, M.; Pfaltz, A. *Org. Lett.* **2002**, *4,* 4713.
[5] J. M. Mitchell, N. S. Finney, *Tetrahedron Lett*. **2000**, *41,* 8431.
[6] Touzeau, F.; Arrault, A.; Guillaumet, G.; Scalbert, E.; Pfeiffer, B.; Rettori, M. C.; Renard, Merour, P.; J.Y. J. *Med. Chem*. **2003**, *46,* 1962.
[7] Soraia, S.; Jaoquim, S.; Marco, D. *Synth. Commun.* **2003**, *33,* 935.

A microwave assisted solvent and catalyst free synthesis of aminomethylene bisphosphonates

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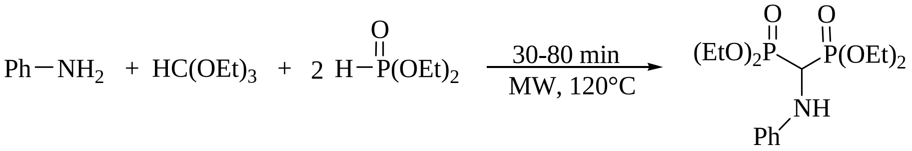
Phosphonic acids are of growing importance in understanding and modulating biological processes [1]. The synthesis of *α*-substituted phosphoryl derivatives (phosphonic and phosphinic acids) has attracted significant attention due to their biological activities with broad applications as enzyme inhibitors, antimetabolites, and antibiotics [2]. Among *α*-functionalized phosphonic acids, *α*-aminoalkylphosphonic derivatives have biological activities such as anti-bacterial, herbicidal and fungicidal.

The application of microwave energy to accelerate organic reactions is of increasing interest and offers several advantages over conventional techniques [3]. Synthesis which normally require long periods can be achieved conveniently and very rapidly in a microwave reactor. As part of our efforts to introduce novel methods for the synthesis of organophosphorus compounds, herein we report a new method for the synthesis of aminomethylene bisphosphonates. We have found that microwave-assisted one-pot reactions of amines with triethyl orthoformate and diethyl phosphite give aminomethylene bisphosphonates in good yields. A series of aminomethylene bisphosphonates have been synthesized via reactions of amines with diethyl phosphate and triethyl orthoformate. The simple work-up, mild reaction conditions, good yields, and clean reactions with no tar formation make this method an attractive and novel contribution to present methodologies.



References:

[1] (a) Engel, R. *Chem. Rev*. **1977**, *77*, 349; (b) Moonen, K.; Laureyn, I.; Stevens, C. V. *Chem. Rev*. **2004**, *104*, 6177.
[2] Collinsova, M.; Jiracek, *J. Curr. Med. Chem*. **2000**, *7*, 629.
[3] (a) Kaboudin, B.; Nazari, R. *Tetrahedron Lett*. **2001**, *42*, 8211; (b) Kaboudin, B. *Tetrahedron Lett*. **2002**, *43*, 8713; (c) Kaboudin, B. *Tetrahedron Lett*. **2003**, *44*, 1051; (d) Kaboudin, B.; aghighat, H.; Yokomatsu, T. *J. Org. Chem*. **2006**, *71*, 6604.

Monoheteroatom substituted cyclopropylcarbenes: A computational study

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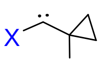
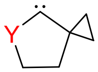
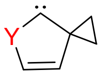
In 2005, the issue of cyclic aminoalkylcarbenes (CAACs) was introduced by preparation of a spirocyclic carbene with a cyclohexyl substituent in the position α to the carbene center [1]. Very recently, we have reported a systematic study on the effects of cyclopropyl, cyclobutyl, cyclopentyl, and cyclohexyl substituents on the stability of CAACs [2]. The results indicated higher singlet-triplet energy gap ($\Delta E_{S\text{-}T}$) for α-cyclopropyl substituted CAAC than the others due to the stabilizing interaction of the occupied Walsh orbital with the vacant *p* orbital of the carbene center.

Here, we intend to shed some light on the multiplicity, stability and reactivity of acyclic, cyclic and unsaturated cyclic alkyl, amino, phosphino, oxy, and thiocarbenes, all bearing a cyclopropyl as the second α-substituent.







$\mathbf{1_C}$: X = $C(CH_3)_3$
$\mathbf{1_N}$: X = $N(CH_3)_2$
$\mathbf{1_P}$: X = $P(CH_3)_2$
$\mathbf{1_O}$: X = OCH_3
$\mathbf{1_S}$: X = SCH_3

$\mathbf{2_C}$: Y = $C(CH_3)_2$
$\mathbf{2_N}$: Y = NCH_3
$\mathbf{2_P}$: Y = PCH_3
$\mathbf{2_O}$: Y = O
$\mathbf{2_S}$: Y = S

$\mathbf{3_C}$: Y = $C(CH_3)_2$
$\mathbf{3_N}$: Y = NCH_3
$\mathbf{3_P}$: Y = PCH_3
$\mathbf{3_O}$: Y = O
$\mathbf{3_S}$: Y = S

Based on appropriate isodesmic reactions we found: (i) the π-donor/σ-acceptor amino group stabilizes not only singlet but also the triplet states; (ii) cyclopropyl groups stabilize singlet states of all our carbenes twice or three times those of the corresponding triplet states; and (iii) the stabilizing effect of cyclopropyl group considerably decreases in the presence of heteroatoms.

References:

[1] Lavallo, V.; Canac, Y.; Präsang, C.; Donnadieu, B.; Bertrand, G. *Angew. Chem. Int. Ed.* **2005**, *44*, 5705.
[2] Kassaee , M. Z.; Momeni, M. R.; Shakib, F. A.; Ghambarian, M.; Musavi, S. M. *Struct. Chem.* **2010**, *21*, 593.

Diastereoselective synthesis of phosphonate ester through the reaction between dimethylacetylenedicarboxylate and triphenylphosphite in the presence of thiocarbamate

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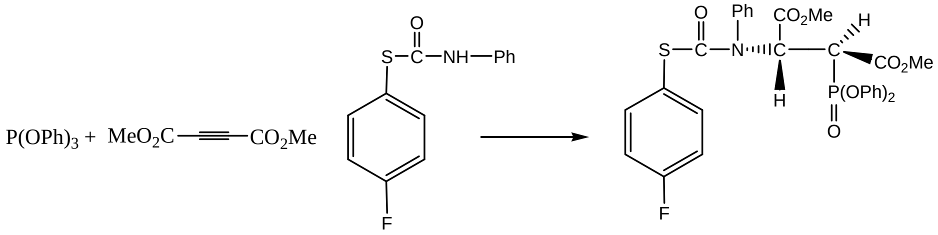
Phosphorus carbon bond formation [1] is an active and important research area, as new reactions are continuously being developed for the preparation of organophosphorus compounds such as phosphinates and phosphonates [2]. Over the last few years, the quest for the synthetic efficiency has gained remarkable importance, partly due to the need reduce waste [3]. Given the increasing industrial, biological and synthetic impact of organophosphorus compounds. The successful attack by nucleophilic trivalent phosphorus on a carbon atom is facilitated when the latter is part of, or conjugated with, a carbonyl group, or when it is part of an unsaturated bond otherwise activated [4]. Herein we wish to report a simple one-pot synthesis of phosphonate ester derivatives through the reaction between thiocarbamate and dimethylacetylenedicarboxylate in the presence of triphenylphosphite.



References:

[1] Alizaeh, A.; Bijanzadeh, H. R. *Synthesis*, **2004**, *18*, 3023.
[2] Maghsoodlou, M. T.; Hazeri, N.; Habibi-Khorassani, S. M.; Saghatforoush, L.; Rofouei, M. *Arkivoc*, **2006**, *Xiii*, 117.
[3] Maghsodlou, M. T.; Habibi-Khorassani, S. M.; Rofouei, M. K.; Adhamdoust, S. R.; Nassiri, M. *Arkivoc* **2006,** *(Xiii).*
[4] Trost, M. B. *Acc. Chem. Res*, **2002**, *35*, 695.

Solvent-free synthesis of hydroxyxanthones and hydroxythioxanthones by Heteropoly acid

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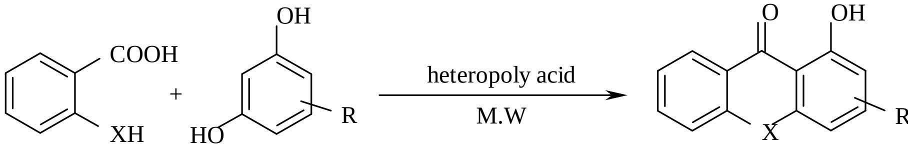
Development of methods using heteropoly acids (HPAs) as catalysts for fine organic synthetic processes related to fine chemicals, such as flavors, pharmaceuticals and food industries have been under attention in the last decade [1]. Heteropoly acids are more active catalysts than conventional inorganic and organic acids for various reactions [2].

Solid heteropoly acids have attracted much attention in organic synthesis owing to easy workup procedures, easy filtration, ease of handling, non-toxicity and experimental simplicity and minimization of cost and waste generation due to reuse [3].

In this dissertation, we describe the synthesis of some new hydroxyxanthones and hydroxythioxanthones by treatment of salicylic acid (SA) or thiosalicylic acid (TSA) with various substituted resorsinol in the presence of heteropoly acid under microwave irradiation conditions. The reaction exhibited better results in terms of the yield and rate under solvent-free condition. The catalyst was efficiently recovered from the reaction mixture and reused. Further more the results of our work confirmed that the heteropoly acids, especially tungstophosphoric acid ($H_3PW_{12}O_{40}$), are found to be an excellent catalyst for the synthesis of these interesting bioactive compounds.



X : O , S

References :

[1] Okuhara, T.; Mizuno, N.; Misono, M. *Adv. Catal.* **1996**, *41*, 221.
[2] Clark, J. H. *Acc. Chem. Res.* **2002,** *35*, 791
[3] Yadav, J. S.; Subba Reddy, B. V.; Sreedhar, R.; Shreenivas Rao, R.; Nagaiah, K. *Synthesis.* **2004,** *14*, 2381.

Deoximation of oximes to their carbonyl compounds and oxidation of thiols to disulfides by the co-naphophen/oxone catalytic system

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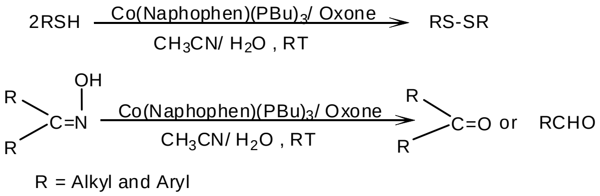
The vital role of thiols and disulfides in living systems has focused on their interconversion reactions. Oxidative conversion of thiols to disulfides is of importance from both biological and synthetic points of view, as shown by a plethora of procedures and methods that have been devised for this transformation [1].

Recovery of ketone and aldehyde from oximes is an important reaction because oxime serves as an efficient protective group for carbonyls, which are extensively used for the purification of carbonyl compounds [2].

A number of methods have been reported for deoximation of oximes and conversion of thiols to disulfides [3]. However, some of these reagents suffer from disadvantages such as long reaction times, availability, toxicity, difficult work-up, preparation and instability. To the best our knowledge potassium peroxomonosulfate (Oxone) is an inexpensive, water-soluble, and stable oxidizing reagent that is commercially available [4,5].

In this study regeneration of carbonyl compounds from the corresponding oximes and oxidation of thiols to disulfides have been performed by Oxone as an oxidizing agent, 1:1, CH_3CN/H_2O mixture as solvent, in the presente of catalytic amount of complexe (**1**). Co-Naphophen /Oxone catalytic system has the following advantages in the oxidation of thiols and oximes: (i) properly reaction time, (ii) high yields (iii) mild reaction conditions, and (iv) cheapness and stability of the oxidant.



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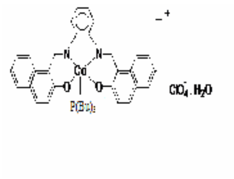

References:

[1] Karimi, B.; Zareyee, D. *Syn let.* **2002**, 346. (b) Karimi, B.; Hazarkhani, H.; Zareyee, D. *Synthesis.* **2002**, 2513.

[2] (a) Bandgar, B. P.; Lalita, B. K.; Thote, J. L. *Synth. Commun*., **1997**, 27, 1149; (b) Donaruma, L. G.; Heldt, W. Z. *Org. React*., **1960**, 11, 1.

[3] (a)Hekmatshoar, R.; Sajadi, S.; Heravi, M.M.; Bamoharram, F.F, *Molecules*. **2007**, 12, 2223-2228. (b) Karami.B.; Montazerozohori. M.; Karimipour G. R.; Habibi. M. H. *Bull. Korean Chem. Soc*., **2005**, 26, 1431.

[4] Hajipour, A. R.; Mallakpour, S. E.; Adibi, H. *J. Org. Chem.* **2002**, 67, 8666.

[5] Curran, D. P.; Brill, J. F.; Rakiewicz, D. M. *J. Org. Chem.,* **1983**; 49, 1654.

Synthesis of diaminofurazan (DAF) derivatives

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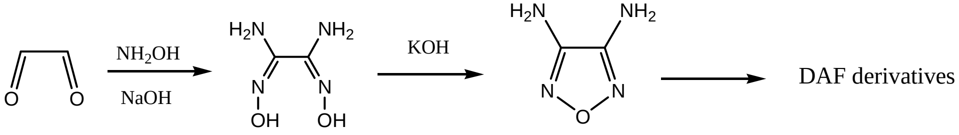
Diaminofurazans are energetic substances carrying the furazan ring. Furazans have many desirable properties for an energetic material such as dense planar structure, stabilizing aromatic nature, energetic oxygen in the ring and a high heat of formation [1]. In common procedure, DAF (3) is prepared from the base catalysed dehydration and cyclization of diaminoglyoxime (2) by aqueous sodium or preferably potassium hydroxide at 180°C in a stainless steel reactor [2]. Recently, a convenient synthesis that can be carried out efficiently at about atmospheric pressure without the need for high pressure vessel has also been reported [3]. In this study, diaminoglyoxime (2) was obtained in 2 steps from glyoxal and the one pot synthesis was also tried. Compound (2) was purified by crystallization and cyclization reaction was performed under basic condition at 180 ºC for 2h to obtain diaminofurazan (3) in 53%. In order to prepare DAF derivatives, ring opening reaction of different epoxides by DAF, as nucleophilic under silica chloride catalyst was tried and the starting material were recovered; indicating unreactive NH_2 functional group. The reaction of DAF and BuNCO was then tried and different DAF derivations were obtained. The products were analyzed by ^1H and ^{13}C NMR.



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References:

[1] Sheremetev, A. B.; Shamshina. Yu. L.; Dmitriev. D. E. *Russian Chemical Bulletin*. **2005**, 54, 1032.

[2] Boyer, J.; Gunasekaran, A. *Heteroatom Chemistry,* **1993,** *4, 521.*

[3] Baum, K; Hashmi, A. B. US patent *0137816 A1,* **2009**.

The reaction of *N*1-thiocarbamoyl-4-(p-methylphenyl)azo-3,5-dimethylpyrazole with α -halocarbonyls

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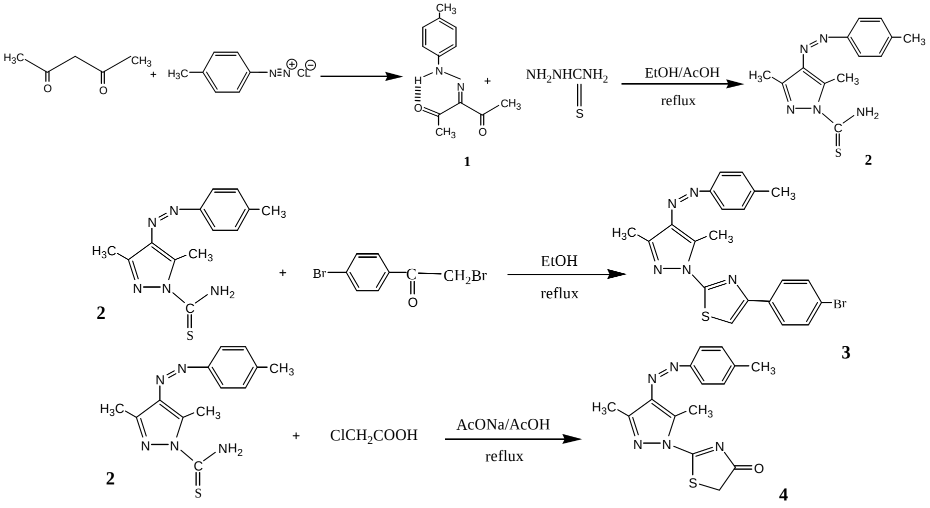
The discovery of pyrazole structure let to modern drug development via modification of main structure of drug molecule. Studies carried out with various substituted pyrazoles showed that these compounds have different biological activities [1]. The reaction of 2,4-pentanedione with aryldiazonium chlorides lead to the formation of 3-(p-methylphenyl)hydrazono-2,4-pentanedione (**1**) [2]. The N1-thiocarbamoyl-4-(p-methylphenyl)azo-3,5-dimethylpyrazole (**2**) was prepared by reacting **1** with thiosemicarbazide [3]. Pyrazole derivatives (**3,4**) were synthesized by reacting **2** with α -halocarbonyls [4,5]. The structures of the synthesized compounds were confirmed by IR, ^{1}H-NMR and ^{13}C-NMR spectral data.



Reference:

[1] Gok, S.; Murat Demet, M.; Özdemir, A.; Turan-Zitouni, G. *Med. Chem. Res.* **2010**, *19*, 94.
[2] Mitchell, A.; Nonhebel, D. C. *Tetrahedron* **1979**, *35*, 2013
[3] Burgart, Y.V.; Fokin, A.S.; Kuzueva, O.G.; Chupakin, O.N.; Salotin, V. I. *J. Fluorine. Chem.* **1998**, *92*, 101
[4] Özdemir, A.; Revial, G.; Güven, K. *Eur. J. Med. Chem.* **2007**, *42*, 403
[5] Havrylyuk, D.; Zimenkovsky, B.; Vasylenko, O.; Zaprutko, L.; Gzella, A.; Lesyk, R. *Eur. J. Med. Chem.* **2009**, *44*, 1396.

One-pot regio and stereoselective synthesis of novel 3-spiroindolizidine oxindoles through [3+2] cycloaddition

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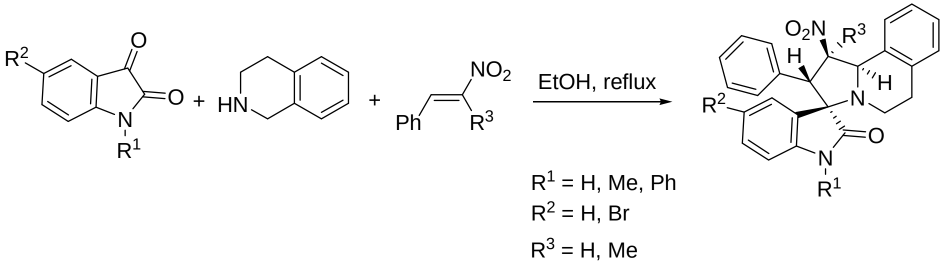
Indolizidine and pyrrolizidine alkaloids are naturally occurring N-heterocyclic metabolites which include a large number of compounds that display pronounced biological and pharmacological activities with therapeutic potential [1]. Stellettamide A, a recently discovered indolizidine alkaloid, has shown antifungal activity and cytotoxicity against K562 epithelium cells [2]. The increasing need of indolizidine and pyrrolizidine alkaloids for biological screening makes these heterocyclic compounds an attractive target in organic synthesis.

[3+2] cycloaddition of azomethine ylide has been used widely to construct complex cyclic systems from relatively simple precursors [3]. As part of our ongoing programme for the synthesis of novel heterocycles through cycloaddition reaction, herein we report an expeditious and facile protocol for the synthesis of novel indolizidines by 1,3-dipolar cycloaddition of azomethine ylides generated from isatin and 1,2,3,4-tetrahydroisoquinoline with nitrostyrenes in a one-pot reaction.



References:

[1] Harborne, J. B. *Nat. Prod. Rep.* **2001**, *18*, 361 and references therein.
[2] Pyne, S. G.; Tang, M. *Curr. Org. Chem.* **2005**, *9*, 1393.
[3] (a)Kathiravan, S., Vijayarajan, D., Raghunathan, R. *Tetrahedron Lett.* **2010**, *51*, 3065. (b) Sirisha, N., Raghunathan, R. *Tetrahedron Lett.* **2010**, *51*, 2515.

Synthesis of new derivatives of phosphonate as anti cancer prodrugs

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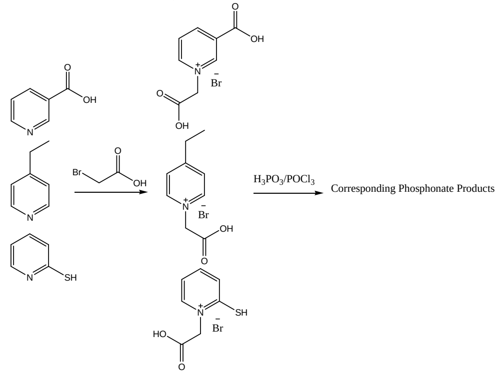
Nitrogen Containing bisphosphonate have shown a few cases to be endowed with anti cancer activity. They have also been found to have activity against the in vitro proliferation of several protozoan parasites [1, 2]. They are a class of commercial Drugs showing high affinity for bone and other calcified tissues [3, 4]. These compounds have been found to decrease levels of protein prenylation and have also been found to stimulate human T-cells[5-7] . The most potent bisphosphomates are found in the series containing hetero-aromatic moiety (with at least one nitrogen atom). Bisphosphonates are rapidly adsorbed by bone and it is of course critical for their use in treating bone-related diseases. Based upon these investigations, we synthesis new derivatives of Nitrogen containing bisphosphonates(NBPs). The synthesis of each product is shown in below schematically. The reaction mixtures in last step was neutralized in an alkaline condition at room temperature. The structure of all products in each step was characterized and confirmed by spectroscopic methods.



Reference

[1] Rodriguez, N.; Bailey, Martin, M.B.; Oldfield, E.; et.al. *J. Infect. Dis.* **2002**, *186*, 138-140
[2] Garzoni, L.R.; Waghabi, m. c.; Baptista, M, M.; et. al. Int. y. *Antimicrob. Agents.* **2004**, 23, 286.
[3] Van Beck, E. R.; Lowik, C. W. G. M.; Ebetino, F. H.; papapoulos, S. E. *Bone* **1998**, *239*, 473.
[4] Kotsikorou, E.; Oldfield, E.; *J. Med. Chem.* **2003**, *46*, 2932.
[5] Wang, L.; Kamath. A.; et.al. *J. Clin. Invest*. **2001**, *109*, 1349.
[6] Kunzaman, V.; Bauer, E.; Feurle, J; et.al, *Blood*. **2000**, *96*, 384.
[7] Kato, Y.; Tanaka, Y.; et.al, *J.Immunol*. **2001**, *167*, 5092.

Caro's acid-silica gel catalyzed promoted efficient synthesis of triheterocyclic 4*H*-pyrimido[2,1-*b*]benzazoles under solvent-free conditions

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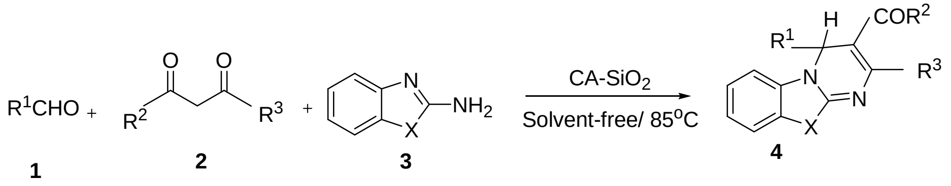
Multicomponent reactions (MCRs), an important subclass of tandem reaction,[1] are one-pot processes in which three or four easily accessible component react to form a single product, which incorporates essentially all the carbon atoms of the starting materials. Multicomponent reactions are a promising and vital field of chemistry because the synthesis of complicated molecules can be achieved in a very fast, efficient, and time-saving manner without the isolation of any intermediate.[2]

In recent years, there has been increasing interest in the design of new products for the synthesis of Biginelli and Biginell-like compounds,[3] which exhibit a wide range of biological activities.

Herein we report an efficient method for 4*H*-pyrimido[2,1-*b*]benzazoles of 2-aminobenzthiazole under solvent-free in the presence of catalytic amount of acid. Various aldehydes were converted to 4*H*-pyrimido[2,1-*b*]benzazoles derivatives in excellent yields. The reaction is versatile and also offers several advantages, such as high yields, shorter reaction times, cleaner reaction profiles and simple experimental and work-up procedures.



References:

[1] Tietz, L.F.; *Chem. Rev.* **1996**, *96*, 115.
[2] Zhu, J.; Eur. *J. Org. Chem.* **2003**, 1133.
[3] Oskooie, H.A.; Heravi, M.M.**;** Karimi N.; Monjez*y,* M. H. *Synth.Commun.* In Press.

Polyethylene glycol imidazolium bromide immobilized on silica gel as a novel phase transfer catalyst and it's application in azidolysis of epoxides

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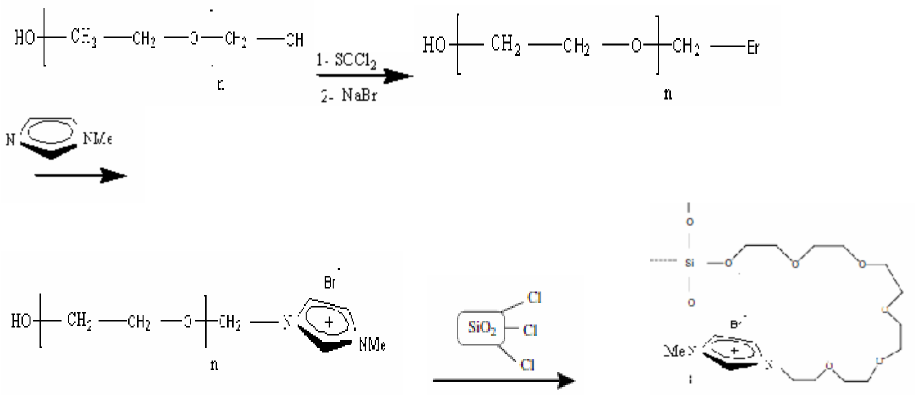
1,2-Azido alcohols are compounds of interest in organic synthesis as either precursors of vicinal amino alcohols or in the chemistry of carbohydrates, nucleosides, lactames, and oxazolines [1]. Generally, azidohydrins are prepared through the ring opening of epoxides by using different azides in suitable solvents [2]. Even though the classical protocol uses sodium azide and ammonium chloride, the azidolysis reaction requires a long reaction time (12–48 h) and the azidohydrin is often accompanied by isomerization, epimerization, and rearrangement of products.

Keeping in mind these facts as well as reports about advantages of reaction in the presence of polymer-supported catalysts, we describe here a new efficient covalent immobilization method for preparation of polyethylene glycol imidazolium bromide(Scheme1) and its successful application as a solid–liquid phase-transfer catalyst for regioselective azidolysis of epoxides using NaN_3 in water. The reactions were performed under reflux condition and in the presence of catalytic amounts (0.2 g/mmol of substrate) of polymeric catalysts and with a 2/1 molar ratio of NaN_3:epoxides. In conclusion, this methodology provides an easy, eco friendly and efficient access to highly regioselective synthesis of azidohydrine.



Scheme 1

Reference:
[1] S. W. Chen, S. S. Thakur, W. Li, C. K. Shin,R. B. Kawthekar, G. *J. Kim, J. Mol. Catal*. **2006**, *259*, 116.
[2] E. F. Scriven, K. Turnbull, *Chem. Rev*. **1988**, *88*, 297.

One-pot, three-component synthesis of functionalized dithiocarbamates

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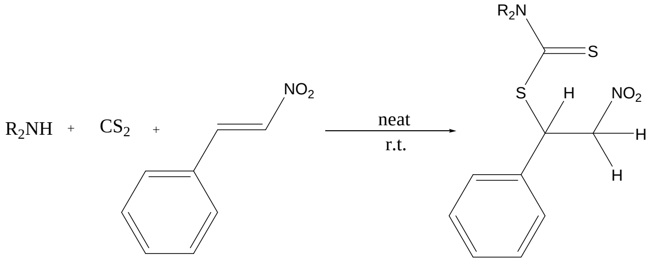
The finding of efficient reactions and environmentally benign methods, which enable the formation of Carbon-Carbon bonds and construction of different functional groups is a key part of contemporary organic synthesis.[1]Organic dithiocarbamates are valuable synthetic intermediates and many compounds with this functional group has extended biological activities.[2]We recently initiated a research program to develop efficient one-pot procedure for the synthesis of compounds which contained different functional groups in their scaffolds.

In this poster, we report three-component reaction of *β*-Nitrostyrene, secondary amines and carbon disulfide in neat condition and at room temperature for the construction of functionalized dithiocarbamates.[3]

β-Nitrostyrene was selected as a Michael-acceptor with high reactivity. The products have a Nitro group which could be used for further reactions, such as condensation, Nef reaction, cyclization after reduction of Nitro group.The structure of the products were elucidated. using spectroscopic data. Meanwhile, the details about the structure of the products will explain according to the X-ray crystallography data. Som of the products were used as starting material for the further reactions.



References:

[1] Guo, B ; Ge, Z ; Cheng, T. *Synth. Commun.* **2001**, *31*, 3021.
[2] Liu, Y; Bao, W. *Tetrahedron Lett.* **2007**, *48*, 4785.
[3] Saidi, M. R ; Aryanasab, F ; Aakbari, E ; Ebrahimi , F . *Synlett* **2007**, *18*, 2797.

Ab initio study of benzoin and benzointrimethylsilane conformers in the gas phase

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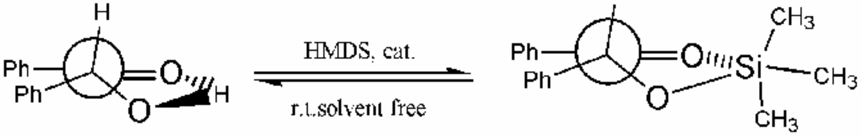
Trimethylsilylation of organic compounds [1,2] having labile hydrogen atoms is an important organic transformation. It is a frequently used protection method in multistep synthesis of natural products due to the enhanced stability under a variety of conditions, solubility in non-polar solvents, thermal stability and the ease of removal which is simply accomplished by acid or base induced hydrolysis giving only unreactive siloxane as byproduct. It is also used extensively for the derivatization of hydroxy compounds to increase their volatility for gas chromatography and mass spectrometry.

1,1,1,3,3,3-Hexamethyldisilazane (HMDS) is a stable commercially available substitute for trimethylsilylation of hydrogen-labile substrates giving ammonia as the only byproduct. Silylation using this silazane type reagent is nearly neutral and does not need special precautions and products are separated from excess HMDS using simple techniques. However, the low silylating power of HMDS is a main drawback for its application, which needs forceful conditions and long reaction times in many instances.

In the present communication we wish to report a detailed *ab initio* conformational analysis at the HF/6-31G level of benzoin and benzointrimethylsilane in gas phase. Ten conformers of benzoin and benzointrimethylsilane have been investigated using high level *ab-initio* method. Geometry optimizations and frequency calculations have been performed at RHF/6-31G level of calculation. Relative energies, rotational constants, harmonic vibrational frequencies and infrared intensities are reported. The most stable conformer are shown in **Figure 1**. The study of the conformational behavior of benzoin is important for understanding the dynamics of the α-hydroxy ketones.

Figure 1. The most stable conformers of benzoin and benzointrimethylsilane calculated at RHF/6-31G level.



References:

[1] (a) Greene, T. W.; Wuts, P. G. M. *Protective Groups in Organic Synthesis*, 3rd Edn; Wiley & Sons: New York, **1999,** 116. (b) Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem.Rev* **2004**, *104*, 199.

[2] Cooper, B. E. *Chem. Ind*. **1978**, 794 and references cited therein.

Synthesis of new ionic liquid possessing Kojic acid

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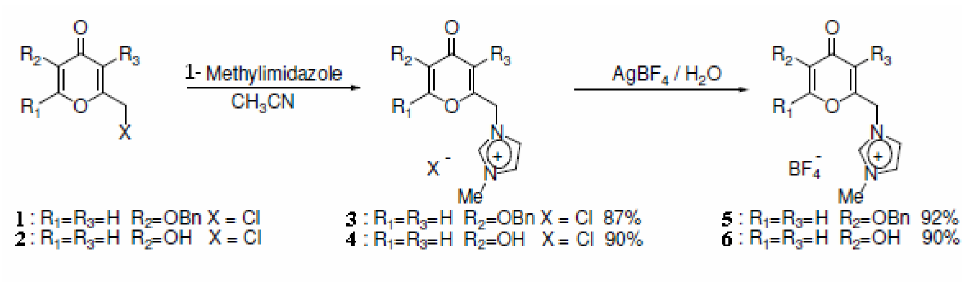
Ionic Liquids (ILs) may be defined as materials which incorporate at least one organic ion in an ion pair which is liquid at temperatures of ~100°C or lower.[1] Imidazolium-based ionic liquids have attracted considerable attention as environmentally benign solvents for various chemical reactions, dye-sensitized solar cells, electrochemical devices, wet double-layer capacitors and ion transport systems, due to their interesting properties such as thermal stability, non-flammability, very low vapor pressure and reusability.[2 -3]

On the other hand Kojic acid (5-hydroxy-2-hydroxymethyl-4*H*-pyran-4-one) is a secondary metabolic product and widely used as a food additive for preventing enzymatic discoloration of vegetable,[4] crabs and shrimps, and as a skin lightening or bleaching agent in cosmetic preparations.[5]

Herein we report synthesis of some new IL by reaction of methylimidazole wiith kojic acid. In this direction different derivatives of kojic acid (**1, 2**) reacted with methylimidazole in acetonitrile, afforded imidazolium bromides (**3, 4**) in 90% and 87% yields respectively. Then, separate solutions of imidazolium bromide and $AgBF_4$ in distilled water were prepared and mixed together to form white precipitate and filtered. By this procedure imidazolium tetrafluoroborates (**5, 6**) were obtained in 91% and 90% yields respectively.



References:
[1] Davis, Jr. J. H.; Forrester, K. J.; Merrigan, T. Tetrahedron Letter. **1998**, 39, 8955.
[2] Wasserscheid, P.; Keim, W. Angew. Chem., Int. Ed. **2000**, 39, 3772.
[3] Corma, A.; Garcia, H. Chem. Rev. **2003**, 103, 4307.
[4] Burdock, G. A.; Soni, M. G.; Carabin, I. G.Regul. Toxicol. Pharmacol. **2001**, 33, 80.
[5] Mase, M. O.; Borremans, M.; Goeyens, L. Int. J. Cosmetic Sci. **2001**, 23, 219.

Boric acid/Glycerol as an efficient catalyst for regioselective epoxide ring opening by aromatic amines in water

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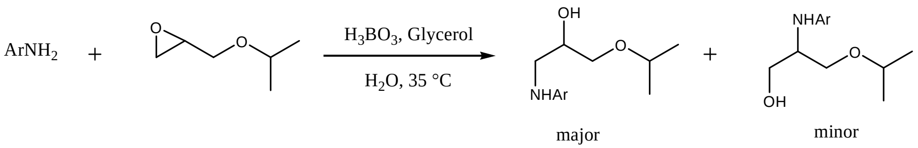
β-Amino alcohols are an important class of organic compounds which have found considerable use in medicinal as well as organic chemistry [1]. One of the most practical and straightforward synthetic procedures for the preparation of these important compounds involve the ring opening of epoxides with amines.

In recent years, boric acid have gained special attention as catalyst in organic synthesis because of many advantages such as excellent solubility in water, easy handling, inexpensiveness, commercially available and environmentally friendly [2,3]. Due to the mentioned advantages, boric acid successfully utilized in numerous reactions as catalyst [4].

Herein we wish to report an efficient procedure for epoxide ring opening with aromatic amines in order to afford β-amino alcohols in water under mild conditions by using boric acid and glycerol. Various aromatic amines were converted to their corresponding β-amino alcohols in excellent yields and considerable rigioselectivity.



References:

[1] Das U.; Crousse B.; Kesavan V.; Bonnet-Delpon D.; Be´gue J-p, *J. Org. Chem.* **2000**, 65, 6749.
[2] A. Rostami, J. Akradi. *Tetrahedron Lett.* **2010**, *51*, 3501.
[3] Sikshi, S. A.; Hultin, P. G. *J. Org. Chem.* **2006**, *71*, 5888.
[4] Kondaiah, G. C. M.; Reddy, L. A.; Babu, K. S.; Gurav, *Tetrahedron Lett.* **2008**, *49*, 106.

Synthesis and characterization of novel polyesters by reaction of bis-(4-carboxyphenyl)methylphenylsilane with different aromatic diols

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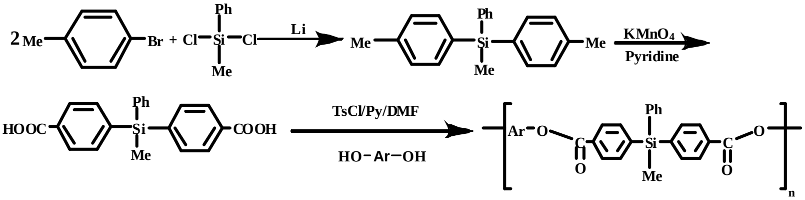
Recently, silicon-containing polymers have been extensively developed for various applications, because of their good solubility good flame retardancy, high moisture resistance, and good adhesion with semiconducting substrates [1-2]. Polyesters (PE)s are one of the most versatile polymers. PEs often have limited heat and flame resistance, so these materials are inappropriate for many important applications. Therefore, further research is needed to develop new polymeric systems, as well as to modify existing systems in order to enhance the desired properties and applications [3]. For this purpose, bis-(4-carboxyphenyl)methylphenylsilane (**1**) as a new dicarboxilic acid was prepared from the reaction of 4-bromotoluene with dichloromethylphenylsilane followed by oxidation with $KMnO_4$. A series of novel polyesters containing silane moiety were synthesized successfully by direct polyesterification of diacid **1** with several aromatic diols in tosyl chloride/pyridine/N,N-dimethylformamide (DMF) system as a condensing agent. The resulting new polymers were obtained in good yields and moderate inherent viscosities and were characterized with FT-IR, ^{1}H-NMR, elemental and thermogravimetric analysis techniques. The results show that existence of silane group in the main chain of the PEs cause to increase the thermal stability of the resulting polymers as well as their solubility.



References:

[1] Zhang, B.; Wang, Z.; Wang, Z.; Li, J.; Leng, S.; Shen, C.; Jiang, Y. *Polymer.* **2009**, *50*, 2025-2034.
[2] Tang, H.; song, N.; Chen, X.; Fan, X.; Zhou, Q. *J. Appl. Polym. Sci.* **2008**, *109*, 190-199.
[3] Mallakpour, S.; Kolahdoozan, M. *Eur. Polym. J.* **2007**, *43*, 3344-3354.

Three component synthesis of highly benzochromenes

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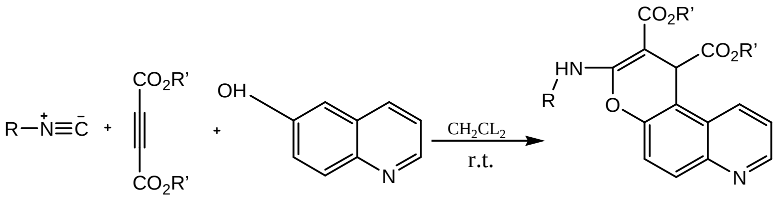
Multi component reactions (MCRs) have attracted much attention in combinatorial chemistry. Of importance in this area are the isocyanide based MCRs such as the versatile Ugi and Passerini reaction [1]. The addition of nucleophilic carbens such as isocyanides to dialkyl acetylendicarboxylates has been investigated in detail [2]. 2-Amino-4H-benzochromenes have been of interest because of their biological activity and a few methods have been reported for their synthesis. As part of our current studies on the development of few routes to hetrocyclic systems, we now report an efficient synthetic route to polysubstituted benzochromenes using alkyl isocyanides and alkyl acetylendicarboxylates in the presence of 6-quinolinol. The stracture of products was deduced from IR , ^{13}C NMR , ^{1}H NMR , Mass spectra.



	R	R`
a	***c- Hexyl***	***Me***
b	***c- Hexyl***	***Et***
c	***t- Bu***	***Me***
d	***t- Bu***	***Et***
e	***1,1,3,3 tetra methyl buthyl***	***Me***
f	***1,1,3,3 tetra methyl buthyl***	***Et***

In summary, we have found a simple and efficient method for the preparation of some highly functionalized benzochromene ring systems. The present method carries the advantage that not only is the reaction performed under neutral conditions, but also the starting materials and reagents can be mixed with out any activation or modification.

Reference

[1] (a) Ugi, I. Angew. *Chem. Int. Ed. Eng.***1982**, *21*, 810; (b) Marcaccini,S.;Torroba,T. *Org. Prep. Preced. Int.* **1993**, *25*, 141.
[2] Yavari, I.; Adib, M.; Sayahi, M. H. *Tetrahedron Lett.* **2002**, *43*, 2927.

One-pot synthesis of stable phosphorus ylides using NH- containing compounds

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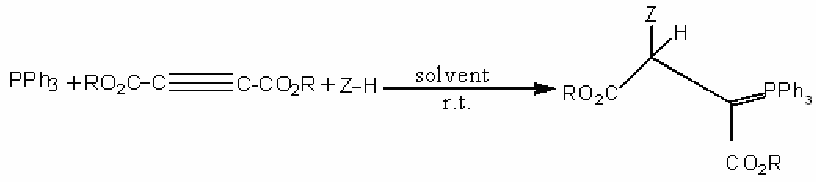
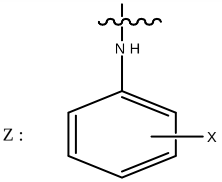
The synthesis of phosphorus ylides is important in organic chemistry because of their application in the synthesis of organic products [1-6] especially the synthesis of naturally occurring products with biological and pharmacological properties [2]. Phosphorus ylides are reactive intermediates, which take part in many valuable reactions in organic synthesis [3-6]. We report here an efficient synthetic route to phosphorus ylides using triphenylphosphine, dialkyl acetylenedicarboxylates and NH- containing compounds, these stable ylides were obtained in excellent yields. These stable ylides exist in solution as a mixture of two geometrical isomers as a result of restricted rotation around the carbon-carbon partial double bond resulting from conjugation of the ylide moiety with the adjacent carbonyl group. All known products were characterized by comparison of IR and NMR spectra with authentic samples and the new compounds were characterized by melting point, IR, NMR (^{1}H, ^{13}C and ^{31}P) spectroscopy.





	x	R
a, b, c	3-NO2	Me, Et, t-But
d	2-COCH3	Me
e	2-CL	Me

References:

[1] D. E. C. Cobridge, phosphorous. AnOutline of the Chemistry, biochemistry and uses (Elsevier, Amsterdam, **1955**), 5th ed.
[2] G. Wittig, Science, 210, 600 (**1980**).
[3] J. I. G. Cadogan, Organophosphorus Reagents in Organic synthesis (Academic press, New York, **1979**).
[4] R. Engel,synthesis of Carbon-phosphors Bonds (CRC press, Boca Raton, FL,**1988**).
[5] L. D. Quin, A Guide to Organophosphorus Chemistry (Wiley-Interscience, New York, **2000**).
[6] M. T. Maghsoodlou, N. Hazeri, S. M. Habibi-Khorassani, L. Saghatforoush, m.k.Rofouei, and M. Rezaie, Arkivoc .,(xiii),117(**2006**).

Ionic liquids-promoted synthesis of L-leucine anhydride from its amino acid: A green synthesis of amino acid anhydrides

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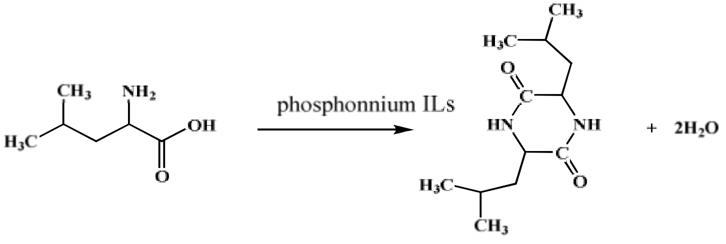
Recently amino acid anhydrides have attracted attention due to their biological properties [1]. Several methods have been reported for the synthesis of amino acid anhydrides. However, the reported methods suffer from many limitations, such as requiring multi step reactions, harsh reaction conditions, volatile and unfriendly organic solvents, yields [2]. Due to the reported synthesis limitations and as a part of our ongoing research program on the study of amino acid anhydrides [3], we developed a simple synthesis route for producing amino acid anhydrides from α-amino acids in the presence of ionic liquids (ILs) [4]. In this methodology, environmentally unfriendly organic solvents were replaced with environmentally friendly, ‘‘greener’’, ILs. The reactions in ILs have higher selectivity and conversions. Using room temperature and close to room temperature ILs, in particular those based on phosphonnium ILs, in this work L-leucine anhydride (LA) from its amino acid (LL) was prepared under microwave irradiation. The method has shown great promise as an attractive alternative to conventional solvents and heating methods.



LL

LA

References:

[1] Mc Cleland, K.; Milne, P. J.; Lucieto, F. R.; Frost, C.; Brauns, S. C.; Van De Venter, M.; Du Plessis, J.; Dyason, K. *J. Pharm. Pharmacol.* **2004**, 56, 1143.
[2] Wang, D.-X.; Liang, M.-T.; Tian, G.-J.; Lin, H.; Liu, H.-Q. *Tetrahedron Lett.* **2002**, 43, 865.
[3] Rafiemanzelat F., Abdollahi E., *J Applied polymer Sci.* Submitted for publication **2010**.
[4] Rafiemanzelat, F., Abdollahi, E., Fathollahi zonoz, A. *Monatsh Chem.* Submitted for publication **2010**.

Preparation and characterization of novel composites of poly(2-methylaniline-co-aniline) by in situ copolymerization and doping in the presence of silica-supported by sulfuric acid (SA), perchloric acid (SiO_2-$HClO_4$), camphorsulfonic acid (SiO_2-CSA) and sulfuric acid (SA, 98%) under solvent-free condition

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Polyaniline, one of the most promising conducting polymers, is inherently brittle and poor in processibility due to its insolubility in common organic solvents [1]. This problem has been overcome to some extent by using substituted derivatives of anilines such as toluidines, anisidines, *N*-methyl or *N*-ethyl anilines or copolymerization of aniline with other derivatives of aniline [2]. In recent years, composites of PANI and inorganic compounds have been synthesized in order to get new materials with modified properties and solubility in common organic solvents. The solid-state reaction has many advantages such as reduced pollution, low costs, and simplicity in process and handling. These factors are especially important in industry [3,4].

In the present work, a great success has been acquired in synthesis of new composites from silica supported by sulfuric acid (SiO_2-SO_3H), perchloric acid (SiO_2-$HClO_4$), camphorsulfonic acid (SiO_2-CSA) and sulfuric acid (SiO_2-SO_3H, 98%) with poly (2-methylaniline-co-aniline) under the solvent-free condition [4]. Firstly, we Supported silica by any of these acids [4]. Then, aniline (*AN*) and 2-methylaniline (*O*-T) copolymerization and doping were done in solid-state by using of ammonium peroxysulfate as oxidant and silica-supported by stated acids as the different solid dopants in room temperature. These different acids were made different composites with special morphological and conductivity properties.

The resulting composites were characterized and studied by using FT-IR, UV-Vis, SEM, TEM [5] and conductivity measurements.

References:

[1] Genies, E.; Boyle, M.; Lapkowski, A.; Tsintavis, M. C. *Synth. Met.* **1990**, *36*, 139.
[2] Kumar, D. *Synth. Met.* **2000**, *114,* 369.
[3] Jayakannan, M.; Annu, S.; Ramalekshmi, S. *J. Polym. Sci.* **2005**, *43*, 1321.
[4] Modarresi-Alam, A. R.; etal. *Proceedings of the International Conference on Nanotechnology: Fundamentals and Applications, Ottawa, Ontario, Canada, 4-6 August* **2010**.
[5] Wang, X.; Feng, X.; Zhao, Y.; Zhang, R.; Sun, D. *Europ. Polym. J.* **2007**, *43*.

Conformational analysis of *o*-tolyl phosphine oxide and its calcogenides by *ab initio* calculations

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The development of conformational analysis is associated primarily with the need to explain and predict the reactivity of molecules from their three-dimensional structures. Physical methods of investigating molecular structures and quantum-chemical calculations play an important role in this field of science.[1]

However, theoretical conformational analysis of organoelement compounds remains poorly developed in spite of advances in quantum-chemistry.[2] So we decided to study tri-*o*-tolyl phosphine oxide and its calcogenides ((*o*-tolyl)$_3$P=Y , Y=O, S , Se).
Geometries of the molecules are optimized using Gaussian employing Hartree-Fock method with 6-31G* basis -set.The calculated vibrational frequencies for all the molecules ensured that the geometries corresponding to the minimum energy[3]. For each of compounds four conformers (↑↑↑,↑↑↓ ,↑↓↓ ,↓↓↓) were obtained. In phosphine selenide the most conformer is ↑↑↓ and in the others (its oxide and sulphide) the most conformer is ↑↑↑.

Conformers	***o*-tolyl phosphine oxide**		***o*-tolyl phosphine** sulphide		***o*-tolyl phosphine** selenide	
	Δ_{RHF} °E	°E $_{RHF}{}^{a}$	$\Delta_{RHF}{}^{a}$ °E	°E $_{RHF}{}^{a}$	°EΔ $_{RHF}{}^{a}$	°E $_{RHF}{}^{a}$
↑↑↑	-767498.9491	0.0	-969956.9952	0.0	-2225024.3922	-0.4273
↑↑↓	-767497.0121	-1.93709	-969956.4272	-0.56795	-2225024.8195	0.0
↑↓↓	-767492.033	-4.97901	-969951.4466	-4.98067	-2225024.81۸2	-0.0013
↓↓↓	-767486.7937	-5.23933	-969946.4154	-5.0312	-222501۹.0466	-5.7729

a- °E, °EΔ(kcal.mol^{-1}

References:

[1] E Eliel, N Allinger, S Angyal, G Morrison *Conformational Analysis* (New York: Wiley, **1965**).

[2] A N Vereshchagin, S G Vul'fson, in *Konformatsionnyi Analiz Elementoorganicheskikh Soedinenii* (Conformational Analysis of Organoelement Compounds) (Ed. A N Pudovik) (Moscow:Nauka, **1983**).

[3] 98, Revision A.7, M. J. Frisch, *E. S. Replogle, and J. A. Pople, Gaussian*, Inc.,Pittsburgh PA. **1998**.

Synthesis and characterization of polyurethane organo montmorillonite nanocomposites formulated by chemically recycled polyester-polyol from PET waste

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Polyethylene terphthalate (PET) is a worldwide used polymer and packing is one of its most important applications. The continuously growing stream of wastes makes its recycling necessary. I n this study, PET flacks were chemically recycled by high functional glycols. Glycolysis of PET waste (bottle) using Trimethylol propane (TMP) and glycerin, as a binary mixture was carried out to produce suitable polyester polyol for rigid polyurethane foam fabrication. The glycolysis was carried out in atmospheric pressure and at 220˚c in the presence of Zinc acetate as transtrification catalyst. The obtained polyester polyol was characterized by FT-IR, 1HNMR and 13CNMR. It was in liquid phase and was stable for several days. The prepared polyester polyol was used as a portion of virgin polyol content (10-40%) and then was reacted with MDI to produce rigid polyurethane foams. In this study rigid polyurethane foams nanocomposits that recycled polyester polyol was used in their formulation, were obtained using different content (1-5%) of nanoclay particles. Four type of commercial nanoclay: NaMMT, 30B, 20A,15A were used. Dispertion of nanoclay particles in polymer matrix was characterized by XRD(xray diffraction) and SEM(scanning electron microscopy) and the results show the Exfoliation of nanoparticles specially 30B clay particles in polymer matrix.The thermal and mechanical properties of new nanocomposites has been characterized by thermo gravimetric analysis (TGA),thermal mechanical analysis (TMA) AND dynamic mechanical analysis (DMA).The results show that The thermal stability is increasedin the presence of the nanoclays and recycled polyester polyol , and the thermal decomposition temperature of the nanocomposites,were increased. The mechanical properties of nanocomposites were improved in the precence of both nanoparticles and recycled polyester polyol(up to 30%) and by increasing content of them ,tensile strength and the modulus were increased.The best propetis was achived using 30B nanoclays.

References:

[1] Chinnakkannu Karikal Chozhan, Muthukaruppan Alagar, Periyannan Gnanasundaram. *Acta Materialia*, February **2009**, volume 57

[2] S. Martínez-Gallegos , M. Herrero , C. Barriga , F.M. Labajos , V. Rives. *Applied Clay Science,* 45 (**2009**) 44–49.

Synthesis and study of new poly(amide-imid)/organoclay nanocomposites based on bis (4-N-trimellitylimido)diphenyl ether

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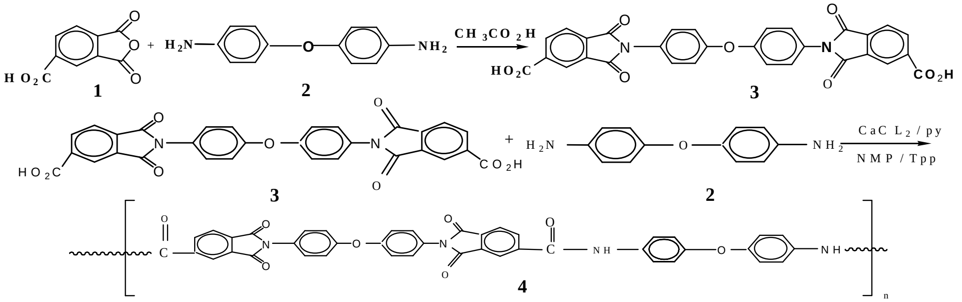
Polymer-clay nanocomposites typically exhibited mechanical, thermal and gas barrier properties, which are superior to those of the corresponding pure polymers [1-6]. A new series of poly(amide-imid)-organoclay nanocomposites (PAINC) containing ether groups were generated through solution intercalation technique of poly(amide-imid) **4** with various percent of organoclay (10-20 Wt%). Bis (4-N-trimellitylimido) diphenyl ether (**3**) as a monomer was synthesized by the reaction of trimellitic anhydride (**1**) with 4,4-diamino dipheny ether (**2**) in acid acetic solution at refluxing temperature. Then poly(amide-imide) chains **(4)** as polymer matrix were produced through polycondensation of 4,4-diamino diphenyl ether (**2**) with bis (4-N-trimellitylimido) diphenyl ether (**3**) in a medium consisting of triphenyl phosphite, *N*-methyl-2-pyrolidone (NMP), pyridine and calcium chloride. Structure and morphology of the PAINC were determined by FT-IR, X-ray diffraction (XRD) and Scanning electron microscopy (SEM). The effect of clay dispersion and the interaction between clay and polymeric chains on the properties of nanocomposites films were investigated by using Uv-Vis spectroscopy, thermogravimetric analysis (TGA) and water uptake measurements. Thermal stability of nanocomposites increased relative to the neat polyamide-imid with increasing organoclay content but water uptake of these materials decreased as compared to the neat polyamide indicating reduced permeability.



References:

[1] Giannelis, E.P.: *Polymer layered silicate nanocomposites.* Adv. Mater. **1996,** *8*, 29
[2] Yano, Y., Usuki, A., Kurauchi, T., Kamigato, O.: *J. Polym. Sci. Part Polym. Chem.* **1993,** *31*, 2493 .
[3] Zulfiqar, S., Ahmad, Z., Ishaq, M., Saeed, S., Sarwar, M.I.: *J. Mater. Sci.* **2007,** *42*, 93.
[4] Sikka, M., Cerini, L.N., Ghosh, S.S., Winey, K.I.: *J. Polym. Sci. Part B Polym. Phys.* **1996**, *34*, 1443 .
[5] Xu, R., Manias, E., Snyder, A.J., Runt, J.: *Macromolecules* **2001,** *34*, 337.
[6] Kausar, A., Zulfiqar, S., Shabbir, S., Ishaq, M., Sarwar, M.I.: *Polym. Bull.* **2007,** *59*, 457.

A highly efficient and ecofriendly procedure for the tetrahydropyranylation and deprotection of alcohols in the presence of Iron (III) phosphate as a catalyst.

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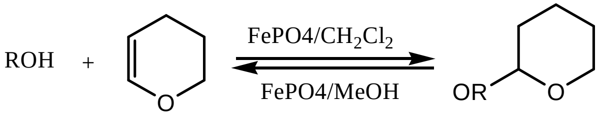
The protection of hydroxyl groups by conversion in to the corresponding tetrahydropyranyl ether is a common and extensively used transformation in organic synthesis [1]. THP ethers are stable under a variety of reaction condition such as strongly basic media, Grignard reagent, acylating agent, lithium alkyls, oxidative reagent and metal hybrids. THP groups are also the protective groups of choice in peptide, nucleotide, carbohydrate and steroid chemistry [2]. Simple, green, efficient protocol for protection of various alcohol using 2 mol% Iron(III) phosphate catalyst under mild reaction condition at room temperature are described. An efficient catalyst to perform tetrahydropyranylation in CH_2CL_2 and deprotection in MeOH (Scheme 1). The major advantages of the procedure are short reaction time, high yield, recycling catalyst, simple work up and no need for further purification [3].



References:

[1] Rostami. A; Rahmati S; Khazaei A. *Monatsh Chem.* **2009**, *140*, 663.
[2] Yang J. H.; Zhang, X.; Yi Liu, W., *Chinese Chem. Lett.* **2008**, *19*, 893.
[3] Bhujanga Rao, Ch.; Chinnababu, B.; Venkatrswarlu, Y., *J. Org. Chem.* **2009,** *74*, 8856.

Polyvinylpyridine-grafted silica containing nickel nanoparticles as a new heterogeneous catalyst for Sonogashira-Hagihara coupling reaction

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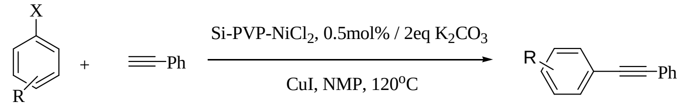
Palladium catalyzed C-C coupling reactions are one of the most employed organic transformations (1). The Sonogashira–Hagihara reaction of terminal alkynes with aryl halides is a c-c coupling reactions and is an important way for the synthesis of substituted arylated alkyne compounds, C(sp^2)-C(sp) bond (2). This reaction is catalyzed by Pd complexes in the presence of a catalytic amount of CuI and an amine base. These compounds are important intermediates in organic synthesis including natural compounds, pharmaceutical, molecular electronics, dendrimeric, oligomeric, and polymeric materials.

Recently we reported synthesis and application of palladium nanoparticles supported on a polymer [3], and polymer-grafted silica containing palladium nanoparticles[4], in cross-coupling reactions. Here we report the application of polyvinylpyridine-grafted silica containing nickel nanoparticles and its efficient use in Sonogashira-Hagihara reaction (Scheme. 1). The coupling reaction of phenylacetylene with aryl iodides, and bromides in the presence of a catalytic amount of nickel complex and CuI was successfully carried out. High efficiency of the catalyst along with short reaction time, high yields, easy purification, recyclability, large scale synthesis, simple procedure, and low cost are among the advantages of this catalytic system.



References:

[1] Metal –Catalalyzed Cross-Coupling Reactions, Diederich. F, Stang. P. J. *Wiley-VCH, Weinheim*, Germany, **1998.**
[2] Brandsma. L, Synthesis of Acetylenes, Allenes and Cumulenes: Methods and Techniques, *Elsevier, Oxford*, **2004**.
[3] Tamami. B, ghasemi. S, *J. Molecul. Catal A: Chem*., **2010,** 322, 98.
[4] Tamami. B, Farjadian. F, *J. Iran. Chem. Soc*. Accepted.

Useful intermediates for the synthesis of new derivatives of α-phenyl cycloheptanones

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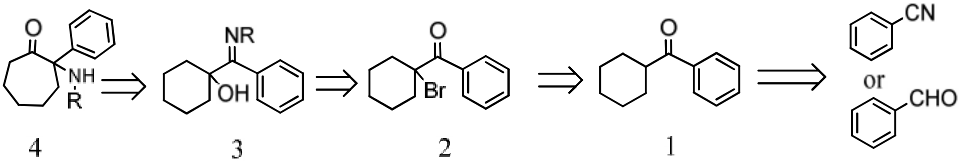
α-Phenyl ketones have proven to be a great utility in organic synthesis, pharmaceutical and in veterinary. Some of these compounds have been prepared as potential hypocholesteremic agents [1]. They also have been used to synthesize Amphetamine and Ketamine which is a short-acting parenteral anesthetic agent [2]. A search in the literature indicates that there are limited methods for the synthesis of α-phenyl cycloheptanones as a member of α-phenyl cycloalkanones, Expansion of cyclohexanones that was presented by C.D. Gutsche and oxidative rearrangements of arylalkenes are two cited methods in the literature [3].

The main objective in the current research has been the synthesis of new derivatives of α-phenyl cycloheptanones involving aryl or alkyl amines in alpha position of cycloheptanone as target molecule 4. To do this, cyclohexyl phenyl ketone 1 was prepared by two methods starting with benzonitrile or benzaldehyde. Then, the ketone 1 was brominated under two bromination conditions using HBr/H_2O_2 or NBS/ NH_4OAC to reach the corresponding α-bromo ketone 2. Products 1 and 2 were purified and analyzed by IR, ^1H NMR, ^{13}C NMR, GC and GC-MS. The bromoketone 2 is going to be used for the preparation of the corresponding hydroxyl imines 3 followed by heat treatment for ring expansion to reach target molecule 4.



4 3 2 1

References:

[1] Hewitt, L. E.; Wade, D. R.; Sinsheimer, J. E. *J. Med. Chem.* **1978**, *21*, 12.
[2] White, P. F.; Way, W. L; Trevor, A. J. *Anesthesiology* **1982**, *56*, 119.
[3] Michael, W.; Justik & Gerald F. Koser, *Tetrahedron Lett.* **2004**, *45*, 6159.

Reaction of Kojic acid with some of aromatic aldehydes in the presence of urea via Biginelli reaction

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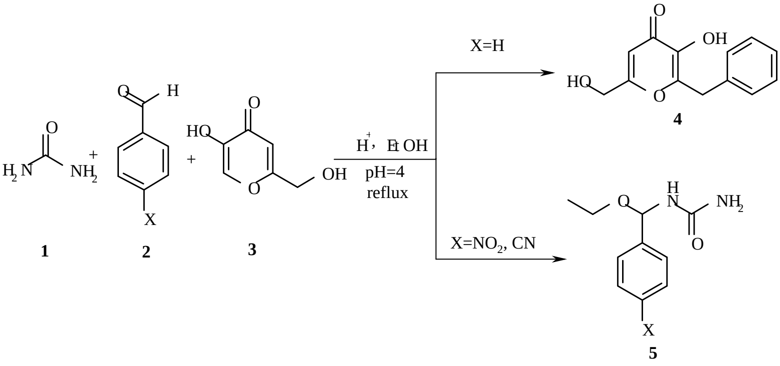
In recent years, multicomponent reactions (MCRs) have emerged as a powerful strategy to construct structurally complex molecules from simple starting materials. One of the most cited MCRs is the Biginelli reaction [1-3]. We here report the reaction of urea **1** and some of substituted aromatic aldehydes **2** in the presence of kojic acid, (2-hydroxymethyl-5-hydroxy-γ-pyrone) **3** as an *OH*-acid. These reactions lead to various functionalized aromatic compounds **4**, **5**. This reaction with benzaldehyde (X=H) leads to compound **4** that urea plays as a catalyst but these reactions with electron-deficient substituted aromatic aldehydes (X=NO_2, CN) proceed to compounds **5b-c**.



4, 5	X	yield (%) **4**	yield (%) **5**
a	H	45	-
b	NO_2	-	55
c	CN	-	55

The structures of **4** and **5** were assigned on the basis of their elemental analysis and ^{1}H, ^{13}C NMR and Mass spectra data as well as from the IR spectra.

Refrences:

[1] (a) Dömling, A. *Chem. Rev.* **2006**, *106*, 17-89; (b) Tietze, L. F.; Rackelmann, N. *Pure Appl. Chem.* **2004**, *11*, 1967.
[2] Biginelli, P. *Gazz. Chim. Ital.* **1893**, *23*, 360.
[3] Hu, E. H.; Sidler, D. R.; Olling, U. H. *J. Org. Chem.* **1998**, *63*, 3454.

DFT calculations of conformational energies, interconversion pathways and stereoelectronic interactions of 1,2,7-thiadiazepane

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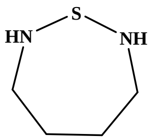
Heterocycloheptanes which are found in Alzheimer drugs, anticancer agents, antimalarials and natural products, are important compounds in many areas of science [1-2]. Contrary to the abundance of information in the synthesis and pharmacological activities of 7-membered heterocyclic compounds [3], there is relatively less information available about the conformational properties of these compounds. This study was undertaken in order to investigate the conformational analysis and stereoelectronic interactions of 1,2,7-thiadiazepane (**1**) by computational methods to determine their preference conformers. The molecular structure and conformational analysis of 1,2,7-thiadiazapane conformers have been investigated by DFT calculation at B3LYP/cc-pVDZ level of theory. Five twist-chair (**TC**), six twist boat (**TB**), three boat (**B**), four chair (**C**) and four twist (**T**) conformers were identified as minima and transition states for compound **1**. The **TC1** geometry is the most stable conformer, and the twist chair conformers are predicted to be lower in energy than their corresponding boat and chair conformations. The simplest conformational process, and the one with the lowest barrier, is the degenerate interconversion of the twist-chair 5 (**TC5**) conformation with itself *via* the C_S symmetric chair (**C2**) transition state. The NBO analysis have been carried out employing the HF/6-31G(d,p) level using B3LYP/cc-pVDZ geometries to study the stereoelectronic effects on the stability of the stereoisomers of **1** (axial-axial, equatorial-equatorial and axial-equatorial). The twist chair axial-axial (**TC1aa**) conformer is predicted to be lower in energy than their corresponding boat and chair conformations. Moreover, the results of NBO calculations showed that the axial-axial stereoisomers usually are the most stable conformers, where not only the stereoelectronic effect but also the repulsion steric is affected on the stability of them.



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References;.

[1] Jin, H.-X.; Zhang,Q.; Kim, H.-S.; Wataya, Y.; Liu, H.-H. ; Wu, Y. *Tetrahedron* .**2006**, *62, 7699*.

[2] McCullough,K.J.; Nojima,M. Curr. *Org*. *Chem*. **2001**, *5*, 601.

[3] Lebegue, N.; Gallet, S.; Flouquet, N.; Carato, P.; Pfeiffer, B.; Renard, P.; Le´once, S.; Pierre, A.; Chavatte, P.; Berthelot, P. *J. Med*. *Chem*. **2005**,*48*, 7363.

Synthesis and spectral characterization of some new thiazolyl phosphoramidates

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2-Aminothiazoles are known mainly as biologically active compounds with a broad range of activity and as intermediates in the synthesis of antibiotics and dyes [1]. Several papers have been published on the use of these compounds as antimicrobial, antifungal, anti-inflammatory activity, anesthetic and antiviral drugs [1, 2]. Although the pesticidal and herbicidal utility of phosphorus containing thiazoles and thiazolines has been reported in a patent [3], spectroscopic studies for these compounds were not investigated so far.

Herein the reaction of $X\text{-}C_6H_4OP(O)Cl_2$ (X= H, *o*-Cl and *p*-CH_3) with 2-aminothiazole in the present of triethylamine or without it was investigated. Four new compounds with formula $X\text{-}C_6H_4OP(O)RR'$ (X=H, R=R'= $NHCN(CH)_2S$ (**1**); X=H, R= $NHCN(CH)_2S$, R'=OH (**2**); X= *o*-Cl, R=R'= $NHCN(CH)_2S$ (**3**) and X= *p*-CH_3, R= $NHCN(CH)_2S$, R'=OH (**4**)) were prepared and characterized by ^{1}H, ^{13}C, ^{31}P NMR and IR spectroscopy and elemental analysis. Phosphorus chemical shifts in compounds **1**-**4** were observed in 1.35, -8.41, 2.83 and -8.64 ppm respectively. The ^{1}H NMR spectra of **2** and **4** showed characteristic broad signals of OH protons at 12.23, 11.18 ppm respectively.

References:

[1] Hang, P. C.; Honek, J. F. *Bioorg. Med. Chem. Lett.* **2005**, *15*, 1471.
[2] Geronikaki, A.; Vicini, P.; Dabarakis, N.; Lagunin, A.; Poroikov, V.; Dearden, J.; Modarresi, H.; Hewitt, M.; Theophilidis, G. *Eur. J. Med. Chem.* **2009**, *44*, 473.
[3] Melnikov, N. N.; Grapov, A. F.; Razvodovskaya, L. V.; Popov, P. V.; Sedykh, A. S.; Shapovalova, G. K.; Abelentseva, G. M.; et al. in *US Patent 4188382, Vol. US Patent 4188382*, Vsesojuzny Nauchno, Moscow, USSR, **1980**, p. 8.

A facile three-component one-pot solvent-free synthesis of 2'-aminobenzimidazolomethylnaphtols

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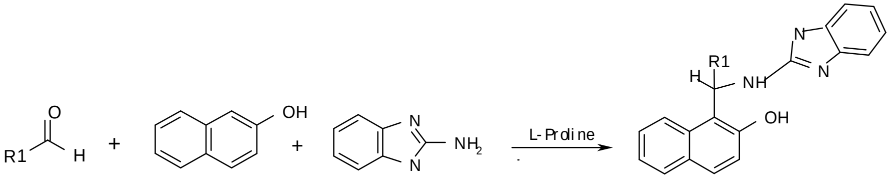
Benzimidazoles and 2-aminobenzimidazoles are privileged organic compounds due to their interesting biological properties. Many substituted 2-aminobenzimidazoles derivatives have found applications in diverse therapeutic areas including anti viral, antifungal, anthelmintic and antihistaminic to name just a few [1]. The pharmaceutical importance of benzimidazoles containing structures has prompted extensive studies for their synthesis [2].

Today, one of the major goals of synthetic organic chemistry lies in the research, discovery and exploitation of environmentally friendly methods. Recently, several techniques for the efficient use of solvent-free reactions [3] and multi-component reactions have been developed individually but when these two wings of green chemistry can be combined, an excellent green chemistry protocol is expected. Multi-component condensation reactions are a compelling method for the synthesis of organic compounds, since the products are formed in a single step and diversity can be achieved by simply varying each component.

Herein we report a facile, efficient three-component synthesis of some 2-aminobenimidazole derivatives via a one-pot grinding of 2-aminobenzimidazole with 2-naphthol and aromatic aldehydes using L-proline as catalyst under solvent-free conditions.



References:

[1] Alamgir, M.; Black, D. St. C.; Kumar, N. Synthesis, Reactivity and Biological Activity of Benzimidazoles. In *Topics in Heterocyclic Chemistry*; Springer: Berlin, Germany. **2007**, *9,* 87-118.
[2] Ozden, S.; Atabey, D.; Yildiz, S.; Goker, H. *Eur. J. Med. Chem.* **2008**, *43,* 1390.
[3] Tanaka, K.; Toda, F.*; Chem. Rev.* **2000**, *100,* 1025-1074.

The investigation of the synthesis of (3-phenyl isoxazole -5-yl)methy acetate

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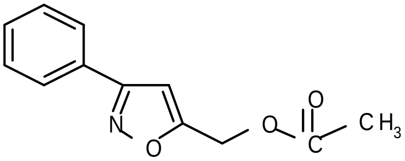
Heterocycles are widely utilized compounds in both pharmaceutical and agricultural fields. Consequently the development of methodologies useful for the assembly of molecules containing heterocyclic templates continues to attract the attention of both the academic and industrial communities. Among aromatic heterocycles, the isoxazole unit constitutes an easily accessible nucleus that is present in a number of natural and pharmacological compounds ,and displays a wide range of organic reactivities and could be used as an effective mean of preparing new molecular scaffolds.Isoxazoles have been repeatedly shown as useful synthons in organic synthesis[1]. Also, isoxazoles derivatives have been used a key intermediates in synthesis and have been investigated intensively for the last several years because of their biological activities[2].

At first benzaldeyde changed into benzaldoxime **(1)** by using hydroxylamine hydrochloride in pyridine as solvent. By increasing sodium hypochlorite, compound **(1)** changed to nitrile oxide and simultaneously a [3+2] cycloaddition reaction was carried out using propargil alcohol and nitrile oxide. The result was a mixture of two isomers: 3-phenyl-5-hydroxymethylisoxazole and 4-phenyl-5-hidroxy methyl isoxazole. Then, the mixture was separated by staying static for hours.The main isomer (3-phenyl-5-hydroxylmethylisoxazole) **(2)** was in solid phase and the isomer (4-phenyl-5-bromo methyl isoxazole) was in liquid phase.

At the rest of the research (3-phenyl isoxazole -5-yl)methyl acetate (**3**) was prepared by reaction of CH_3COOH and compound **(2)** in presence of H_2SO_4.

The structure of all the synthesized compounds was characterized and confirmed by FT-IR and NMR spectroscopy techniques.



References:
[1] Rajanarender,E., *Chin. Chem. lett.* 827, 2008.
[2] Lee, Y., Kim, B. H., Biorg. Med. Chem. Lett. 12, 1395, 2002.

Four-component reaction of cyclohexyl isocyanide, cyanoacetic acid and two equivalents of an aldehyde: Synthesis of Methyl 2-cyano-3-(aryl)-cyclohexylcarbamoyl-(aryl)- acrylate

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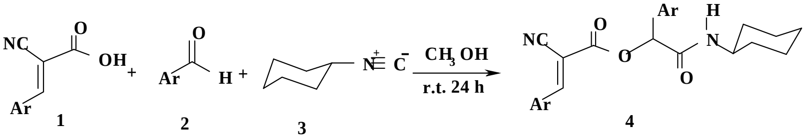
An important subject that attracted a great deal of attention from organic and bioorganic chemists during the last few decades has been the developing of new strategies for the synthesis of complex molecular structures from easily available substrates by short and effective routs [1]. Among the MCRs, isocyanide based multi-component reactions (IMCRs) have gained the most attention by the organic chemists. Ugi four component reaction(U-4CR) [2] and Passerini three component reaction (P-3CR) are among the most important IMCRs [3]. Herein we report A new and efficient one-pot synthesis by four-component reaction between of two equivalents of an aldehydes, cyclohexyl isocyanide and cyanoacetic acid at room temperature leads to Methyl 2-cyano-3-(aryl)-cyclohexylcarbamoyl-(aryl)- acrylate in good yields.



4	Ar	yield %*
a	p- NO_2-phenyl	92
b	m- CH_3O-phenyl	89
c	o- CH_3O-phenyl	90
d	p- Cl-phenyl	89

* Isolated yields

References:

[1] Domling, A. *Curr. Opin. Chem. Biol.*, **2000**, *4*, 318.
[2] Ugi, I. Werner, B. Domling, A. *Molecules*, **2003**, *8*, 53.
[3] Passerini, M. *Gazz. Chim. Ital.*, **1921**, *51* II, 126.

Synthesis of novel pyridine dicarboxylate complexes as potential superoxidismutase mimentics

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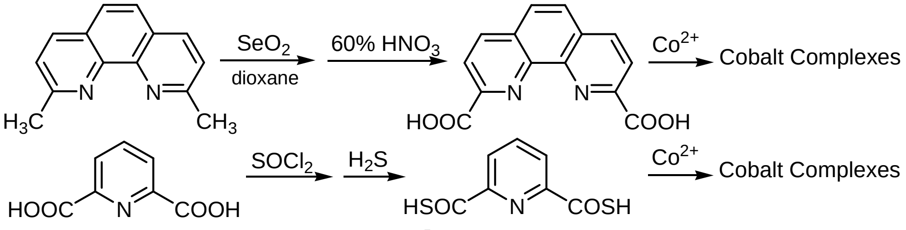
Reactive oxygen species such as superoxide O_2 and their products are credited with important roles in the oxidative stress of biological system [1]. Oxidative stress causes damage to lipid membranes, proteins, lipoproteins, nucleic acids, and many other biomolecules[2]. Accordingly, the use of superoxide dismutase (SOD) enzymes and modified SODs have been suggested as a useful therapy in combating the action of superoxide radicals in the pathogenesis of metabolic diseases [3].Most SOD mimics have been designed with a redox active metal center, similar to the active site metals of the natural SODs, that is, cobalt (II), which allows the change of metal coordination occurring during the catalytic process.

In this project two new pyridine derivatives ligands have been synthesized (scheme1) [4, 5]. Then these substances reacted with Cobalt nitrate hexahydrate to give new cobalt complexes as potential SOD-like activity.



scheme1

Reference:
[1] Halliwell, B.;Gutteridge, J. M. C. Free Radicals in Biology and Medicine, third ed.; Oxford University Press: Londone,2002.
[2] Emerit, J.; Edeas, M.; Bricaire, F. Biomed. Pharmacother. 2004, 58, 39.
[3] Henke, S. L. Expert Opin. Ther. Patents 1999, 9, 169.
[4] Sneh L.J.; Pravat B.;Heather L.M; Dalton Trans.,2004,862-871.
[5] C. J. Chandler, L. W. Deady and J. A. Reiss, J. Org. Chem. 1981, 39, 1425.

Synthesis of some new derivatives of [1,2,4]triazino[4,3-b][1,2,4,5]tetrazepin-4(6H)-one

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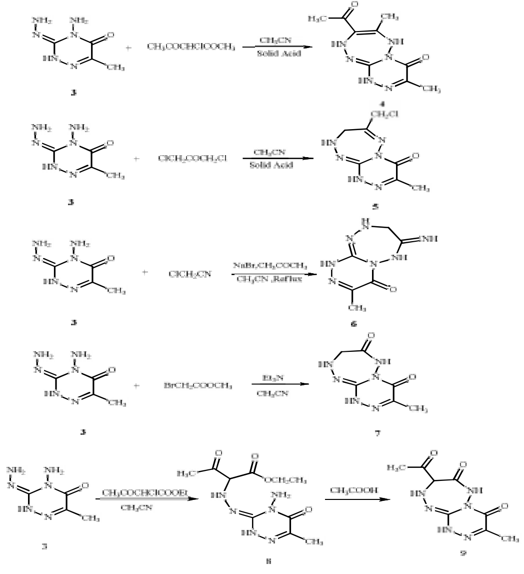
Numerous compounds containing the 1,2,4-triazine moieties are well known in natural materials and show interesting biological, pharmacological and medicinal properties. Some of the 3,5,6-trisubstituted-1,2,4-triazines can be active as blood platelet aggregation inhibitors and others exhibit antiviral inhibitory activity (against influenza viruses for example),significant activity towards leukemia and ovarian cancer, and anti-HIV activity [1].

There is varius properties for [1,2,4,5]tetrazepine such as anti-inflammatory activity agents in animals , Pharmacologic, displayed mutagenic activity in Saccharomyces cerrvisiae , and immunosuppressant activities [2].

In the present work, the synthesis of some new derivatives of [1,2,4]triazino [4,3,*b*][1,2,4,5]tetrazepine by the reaction of 4-amino-3-hydrazono-6-methyl-3,4-dihydro-1,2,4-triazin-5(4H)-one **1** with Methyl bromoacetate, 3-chloropentane-2,4-dione, ethyl-2-chloro-3-oxobutanoate, 1,3-dichloropropan-2-one and 2-chloroacetonitrile is reported.



Reference:

[1] Sztanke,K.; Pasternak,K. Rzymowska, J. Sztanke,M. Kandefer-Szerszen, M. *Eur J. Med. Chem*. **2008**, *3*, 1085. [2] Lachowicz,T. M. Konieczny,M. Witkowska,R. *Actu Microhiol*. **1974**, *147*, 6.

PPA-SiO$_2$ catalyzed one-pot multi-component synthesis of tetrahydrobenzo[*b*]pyrans

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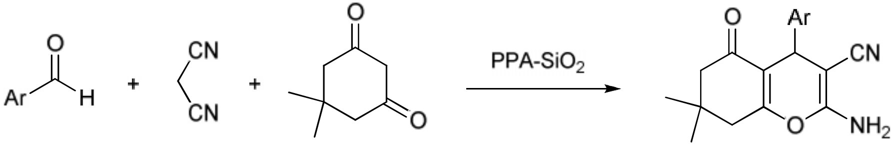
4H-Benzo[*b*]pyrans and their derivatives are an important class of compounds which have received considerable attention in recent years due to their wide range of biological activities. Compounds with these ring systems have diverse pharmacological activities such as anti-coagulant, anticancer, spasmolytic, diuretic, anti-ancaphylactia, etc [1-3]. 4H-Pyrans also constitute the structural unit of a series of natural products [4]. In the conventional reported synthesis of 4H-benzo[*b*]pyrans, the use of organic solvents like DMF/acetic acid make the work-up procedure complicated and leads to poor yields of the products besides polluting the environment [5]. These compounds have also been synthesized using methods including microwave and ultrasonic irradiation or using TBAB, (S)-proline, etc. as catalysts [6, 7]. However, many of these methods are associated with some limitations such as long reaction times, unsatisfactory yields, harsh reaction conditions, expensive or not readily available reagents, hazardous organic solvents and tedious work-up procedure.

Thus, herein we wish to report a simple, efficient, clean, high-yielding, and environmentally friendly method for the synthesis of tetrahydrobenzo[*b*]pyrans through one-pot three-component reaction of an aryl aldehyde, malononitrile and dimedone using PPA-SiO$_2$ as catalyst.



References:

[1] Green, G. R.; Evans, J. M.; Vong, A. K. In *Comprehensive Heterocyclic Chemistry II*; Katritzky, A. R.; Rees, C. W.; Scriven, E. F. V.; Eds.; Pergamon Press: Oxford, **1995**; Vol. *5*, p 469.
[2] Andreani, L. L.; Lapi, E. *Bull. Chim. Farm.*, **1960**, *99*, 583.
[3] Bonsignore, L.; Loy, G.; Secci, D.; Calignano, A. *Eur. J. Med. Chem.*, **1993**, *28*, 517.
[4] Hatakeyama, S.; Ochi, N.; Numata, H.; Takano, S. *J. Chem. Soc. Chem. Commun.*, **1988**, 1202.
[5] Wang, X. S.; Shi, D. Q.; Tu, S. J.; Yao, C. S. *Synth. Commun.*, **2003**, *33*, 119.
[6] Jin, T. S.; Xiao, J. C.; Wang, S. J.; Li, T. S.; Song, X. R. *Synlett*, **2003**, 2001.
[7] Balalaie, S.; Bararjanian, M.; Amani, A. M.; Movassagh, B. *Synlett*, **2006**, 263.

Ugi-4CC in polymer synthesis

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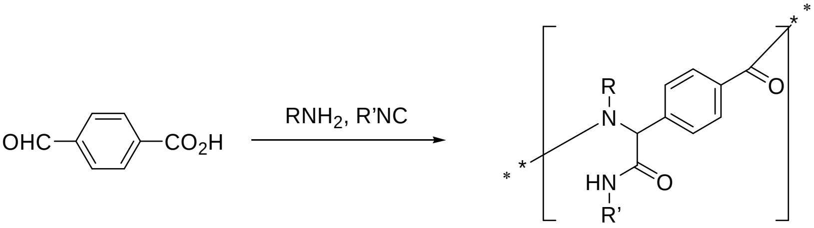
The Ugi four-component condensation (U-4CC) between an aldehyde, an amine, a carboxylic acid and an isocyanide allows the rapid preparation of α-aminoacyl amide derivatives [1]. The Ugi reaction products can exemplify a wide variety of substitution patterns, and constitute peptidomimetics that have potential pharmaceutical applications. This reaction is thus very important for generating compound libraries for screening purposes. In the base of our knowledge the utility of this reaction in the synthesis of polymer scarcely has been investigated [2,3]. We found 4-formylbenzoic acid reacted with amines and isocyanides to give polymer **1** in good yield.



1

References:

[1] Ugi, I; Meyr, R.; Fetzer, U.; Steinbrückner, C. *Angew. Chem.* **1959,** *71*, 386.
[2] Wessjohann, L. A.; Rivera, D. G.; Vercillo,O. E. *Chem. Rev*. **2009**, *109*, 796.
[3] Robotham, C. V.; Baker, C.; Cuevas , B.; Abboud, K.; Wright, D. L. *Mol. Divers*. **2003**, *6*, 237.

HPA- Catalyzed alkylation of indoles with 1,3-dicarbonil compounds: an expedient synthesis of 3- substituted indoles

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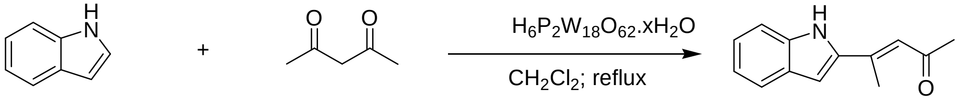
The indole nucleus is frequently found in natural products, pharmaceuticals, functional materials, and agrochemicals. Substituted indoles are capable of binding to many receptors with high affinity. Therefore, the synthesis and selective functionalization of indoles have been the focus of active research over the years.

3-Substituted indoles are important building blocks for the synthesis of various biologically active molecules. Consequently, there is a continuing interest in the development of improved methods for the synthesis of 3-substituted indoles [1].

In the past and still today, most aromatic products are prepared on the industrial level by well known classic transformations such as Friedel–Crafts alkylations, Friedel– Crafts acylations, nitrations, and halogenations. They often have major drawbacks such as drastic reaction conditions (high temperature, strong acidic conditions), low regioselectivity, and large amounts of by-products [2].

Heteropolyacids (HPAs) have many advantages finding economically and environmentally attractive in both academic and industrial significance; they are useful acids and oxidation catalysts in various reactions since their catalytic features can be varied at a molecular level Furthermore, Wells–Dawson type HPAs,[$H_6P_2W_{18}O_{62}$.x H_2O] possess super-acidity and a remarkable stability both in solution and in the solid state.

In this letter, we have report a direct $H_6P_2W_{18}O_{62}$.x H_2O, catalyzed selective 3-alkylation of Indoles with 1,3- dicarbonil compounds such as acetyl acetone under mild condition in dichloroethane, CH_2 Cl_2 , as solvent, and went to completion in 1- 2 h at reflux giving product [3].



References:

[1] Yadav, J. S.; Subba Redd, B. V.; Praneeth, K. *Tetrahedron Lett,* **2008**,. *49*, 199.
[2] Arcadi, A.; Alfonsi, M.; Bianchi, G.; D'Anniballe, G.; Marinelli, F. Adv. *Synth.Catal*. **2006**, *348*, 331.
[3] Heravi, M.; Ranjbar, L.; Derikvand, F.; Bamoharram, F. *Catal. Commun.* **2007,** *8*, 289.

Solvent-free synthesis of synthesis of benzofuro(2,3-b)benzofuran derivatives catalyzed by a Brønsted-acid ionic liquid as a green and reusable catalyst

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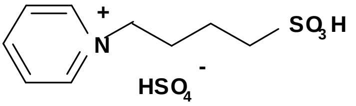
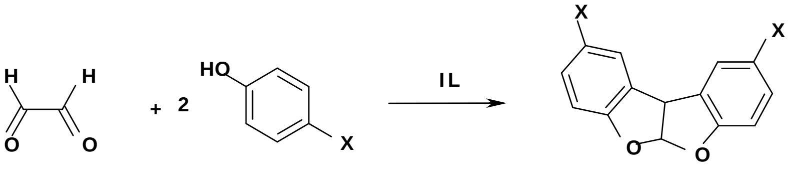
It has been reported by several investigators that the acid-catalyzed reaction of glyoxal at the ortho position of phenols has the acetal type of structure [1] and/or the ether type of structure [2]. Also the reaction of glyoxal with β-naphthols was reported by Dischendorfer [1] to produce a compound assigned as acetal structure. Coxworth [3] attempted to distinguish between several types of structures which were suggested by previous investigators who had prepared some acetal compounds by an unambiguous method [4].

Ionic liquids (ILs) have received great attention in diverse areas ranging from synthetic and catalytic chemistry to biotechnology, electrochemistry, and material science [5]. The fixation of known homogeneous catalysts on roomtemperature ionic liquids (RTILs) is an ideal combination in order to achieve the advantages of both homogeneous and heterogeneous catalysis [6].

In this paper we wish to report an efficient approach to the synthesis of Benzofuro(2,3-b)benzofuranes using 4-sulfonylbutyl pyridinium hydrogensulfate $[(CH_2)_4SO_3HPy][HSO_4]$, a Brønsted-acid ionic liquid (IL), as a green and reusable catalyst.



$[(CH_2)_4SO_3HPy][HSO_4]$



References:

[1] Discheadorfer, O. *Monauh*, **1940**, *73*, 45.
[2] Rosenthal, A.; Zainnchkovsky A. *Can. J Chem*. **1960**, *38*, 2277.
[3] Coxworth E. C. M. *Can. J. Chem.* **1967**, *45*, 1777.
[4] Riemschneider, R.; Ahrle, L.; Cohnen, W.; Heiman, E. *Chem. Ber.* **1959**, *92*, 900.
[5] Wasserscheid, P.; Keim, W. *Angew. Chem. Int. Ed.* **2000**, *39*, 3772.
[6] Greaves, T.L.; Drummond, C.J. *Chem. Rev.* **2008**, *108*, 206.

Synthesis of imidazole based Acidic Ionic Liquids bearing –SO_3H functional group

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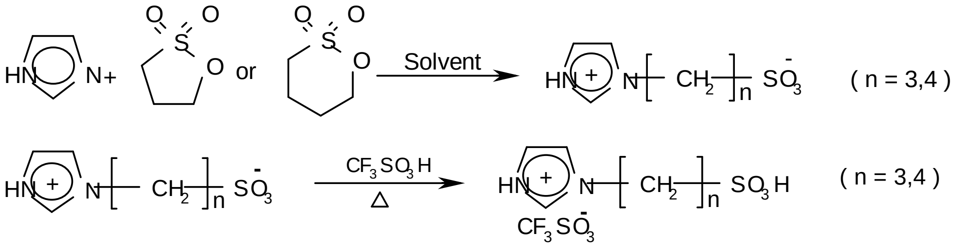
Ionic Liquids (ILs) have been one of the most rapidly growing areas of chemistry research in recent years. The room temperature ionic liquids (RTILs), a kind of environment-friendly solvent and catalyst, got broad attention of scholars from various fields such as synthesis, catalysis, separation, electrochemistry and biochemistry, due to it's adjustable physical and chemical properties such as good stability in air and moisture materials, negligible vapor pressure, high thermal and chemical stability, recyclability [1,2]. So_3H-functionalized ionic liquids show high catalytic activity and fair reusability even at very low catalyst loadings, while the conventional non-functionalized ionic liquids show poor activity [3,4]. Herein, we report the synthesis of two novel functionalized acidic ionic liquids [FAILs] of (propyl- 3- sulfonic) imidazolium trifluoromethane sulfonate [HSO_3-PIM][CF_3SO_3] and [HSO_3-BIM][CF_3SO_3] (butyl- 4- solfonic) imidazolium trifluoromethane sulfonate that were synthesized in good yields. Due to their unique structures, these novel FAILs showed noticeable hydrophilic properties and strong acidities.



References:

[1] Cole, A.C.; Jensen, J. L.; Ntai, I.; Tran, K. L. T.; Weaver, K. J.; Forbes, D. C.; Davis, J. H.; *J. Am. Chem. Soc*. **2002**, 124, 5962.

[2] Zhao, Y.; Long, J.; Deng, F.; Liu, X.; Li, Z.; Xia, C.; Peng, J.; *Catal. Commun*. **2009**, 10, 732.

[3] Liang, X.; Wanga, Y.; Gong, G.; Yang, J.; *Catal. Commun*. **2008**, 10, 281.

[4] Gui, J.; Cong, X.; Liu, D.; Zhang, X.; Hu, Z.; Sun, Z; *Catal. Commun*. **2004**, 5, 473.

Immobilized silver nanoparticles on alumina as an efficient catalyst in nitroarene reduction

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The design and synthesis of materials in nanometer size is currently the subject of intense research because their properties differ considerably from those of the corresponding bulk materials. In particular silver nanoparticles are particularly interesting due to their roles as substrates in studies of surface-enhanced Raman scattering [1], catalysis [2], *etc*.

Aromatic amines are important starting materials and intermediates for the manufacture of a great variety of chemicals, such as dyestuffs, pharmaceutical products, agricultural chemicals, polymers, *etc*. They are generally synthesized by the chemical reduction of nitroarenes [3].

In this work, stable colloidal silver was prepared by reduction of silver nitrate with $NaBH_4$. The silver nanoparticles were characterized by transmission electron microscopy (TEM) and UV-Vis spectra. For stabilization of nanoparticles and prevention of their accumulation, chemical reduction of $AgNO_3$ was done in the aqueous medium includes Alumina.

In continuation of our researches to develop green chemistry by using water as reaction medium [4], the immobilized silver nanoparticles were used in reduction of nitroarenes to the corresponding aromatic amines with $NaBH_4$ in water under MW irradiation (300 W).

$$ArNO_2 \xrightarrow[\text{water, MW (300 W)}]{NaBH_4,\ Al_2O_3\text{-}Ag(nano)} ArNH_2$$

2-5 min

References:

[1] Pileth, W.J.; *J. Phys. Chem.* **1982**, *86*, 3461.
[2] Henglein, A.; Lillie, J. *J. Phys. Chem.* **1981**, *85*, 1246.
[3] Lauwiner, M.; Rys, P.; Wissmann, J. *Appl. Catal. A: Gen.* **1998**, *172*, 141.
[4] Kiasat, A.R.; Fallah-Mehrjardi, M. *Catal. Commun.* **2008**, *9*, 1497.

Protection of carbonyl compounds using *N*-bromosaccharin

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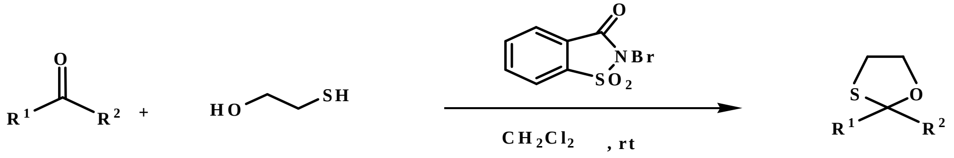
The protection of carbonyl compounds plays an important role during multiestep synthesis in
organic, medicinal, carbohydrate and drug design chemistry[1]. Among varios functional groups, protection of the carbonyl group as 1,3-oxathiolane is important for the following reason:

They can be used as acyl carbanion equvalents[2], synthesis of α-hydroxyaldehydes[3] and intermediate in organic synthesis[4]. Oxathioacetal is prepared from the corresponding carbonyl compounds on reaction with 2-mercaptoethanol by an equmolar of lewis acid such as $ZnCl_2$ [5] .

N-bromosaccharin has been proven to be a useful and alternative reagent for diverse organictransformations, such as halogenation of aromatic compounds, co-halogenation of alkenes, oxidation of alcohols, halogenation of benzylic and carbonylic position.

Herein we report an afficient method for protection of various aliphatic, aromatic aldehydes and ketons using of 2-mercaptoethanol in the presence of catalytic amount of *N*-bromosaccharin.



R^1=Alkyl,Aryl

R^2= Alkyl, H

References:

[1] Green, T. W.; Wuts, P. G. M. Protective Groups in Organic Synthesis, 3rd ed.; Wiley: New York,
1999,Chapter 4.
[2] Eliel, E. L.; Morris-Natschke, S. *J. Am. Chem. Soc.* **1984**, *106*, 2937.
[3] Lynch, J. E.; Eliel, E. L. *J. Am. Chem. Soc.* **1984**, *106*, 2943.
[4] Eliel, E. L.; Pilato, L. A.; Badding, V. G. *J. Am. Chem. Soc.* **1962**, *84*, 2377.
[5] Fallis, A. G.; Yadav, V. K. catalyst *Synlett* **2000**, *805*.

Graft copolymerization of styrene from poly(vinyl alcohol) via RAFT polymerization

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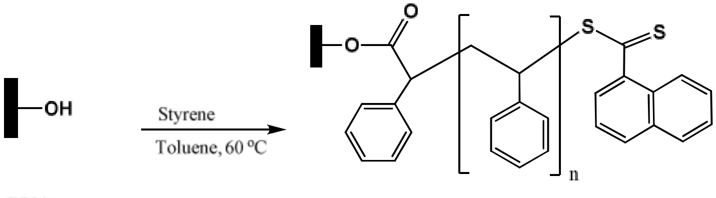
Poly(vinyl alcohol) has excellent film forming, emulsifying, and adhesive properties. It is also resistant to oil, grease and solvent [1]. Polymer grafting techniques provide a versatile tool to covalently modify the surface of materials. RAFT polymerization has been successfully applied to the controlled polymerization of various monomers under a wide range of conditions to prepare polymer materials with predetermined molecular weights, narrow polydispersities and advanced architectures [2]. The RAFT technique provides a versatile way to modify the surface of different materials with surface-attached polymers. By controlling the type, structure and graft density of the surface-attached polymers, surface hydrophobicity/hydrophilicity of substrate materials can be significantly modified, which further affects other properties including adhesion, wet ability, compatibility and solubility [3].

Poly(styrene) was grafted from Poly(vinyl alcohol) PVA backbone by reversible addition-fragmentation chain transfer (RAFT) polymerization. The structure of the graft copolymer is confirmed by FT-IR and ^{1}HNMR spectroscopy. The graft copolymer was investigated by thermogravimetric analysis, differential scanning calorimetry and X-Ray diffraction. Grafted poly(styrene) chains were cleaved from the PVA backbone by acidic hydrolysis of the PVA. The number-average molecular weight and PDI of the grafted poly(styrene) from PVA-g-PS obtained was determined by Gel Permeation Chromatography (GPC).



PVA **PVA-g-PS**

References:

[1] Miller, J. A. *Sci. News*. **1977**, *112*, 154.
[2] Andrew, B. L.; Charles, L. M. *Aust. J. Chem.* **2002**, *55*, 367.
[3] Boyes, S. G.; Granville, A. M.; Baum, M.; Akgun, B.; Mirous, B. K.; Brittain, W. J. *Surf. Sci.* **2004**, *570.*

Activation of HMDS with ionic liquids: pyridinium 2,2,2-trifluoroacetate as an efficient and reusable catalyst for the silylation of alcohols

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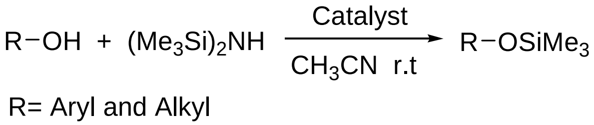
Protection of hydroxyl functional groups is an important process in multi-step synthesis.One of the popular methods for this purpose is to transfer hydroxyl groups into their corresponding silyl ethers. Hexamethyldisilazane (HMDS) which is a cheap and a commercially available compound can be used for the preparation of trimethylsilyl ethers from hydroxyl compounds. Even though, the handling of this reagent is easy, its main drawback is its poor silylating power which needs forceful conditions and long reaction times [1]. For the activation of HMDS, varieties of catalysts have been reported [2]. Most of these methods suffer from some drawbacks such as long reaction times, use of expensive reagents and catalyst, harsh reaction conditions, generation of undesired byproducts and tedious work-up.

Use of ionic liquids (ILs) as green solvents in organic reactions is in participation with some advantages such as control of product distribution, enhanced rate and/or reactivity, ease of product recovery, catalyst immobilization, and recycling.[3] Since ionic liquids are neither completely non-volatile or non-flammable, use of ILs omits the risk of combustion by replacement of volatile organic compounds widely used as solvents in organic reactions.

Considering these facts, herein we report an efficient protocol for the silylation of alcohols with activation of HMDS in the presence of catalytic amounts of pyridinium 2,2,2-trifluoroacetate as a reusable ionic liquid. (Scheme 1)



$$R{-}OH \ + \ (Me_3Si)_2NH \xrightarrow[CH_3CN\ \ r.t]{Catalyst} R{-}OSiMe_3$$

R= Aryl and Alkyl

Scheme 1

References:

[1] Bruynes, C.A.; Jurriens, T.K. *J. Org. Chem.* **1982,** *47*, 3966.

[2] (a) Tanaka, K.; Toda, F.; *Chem. Rev.* **2000**, *100*, 1025; (b) Firouzabadi, H.; Iranpoor, N.; Sobhani, S.; *Tetrahedron Lett.* **2002**, *43*, 3653.

[3] Picquet, M.; Stutzmann, S.; Tkatchenko, I.; Tommasi, I.; Zimmermann, J.; Wasserscheid, P. *Green Chem.* **2003**, *5*, 153.

A mild and efficient method for the silylation of alcohols and phenols under solvent free conditions

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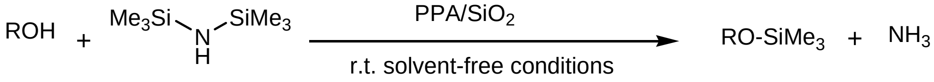
Trimethylsilyl ether formation is not only a fundamental process in the synthesis of functional organosilicon compounds but also an important technique for protection of reactive hydroxyl groups during multistep synthesis of natural products [1]. One of the most common silylating reagents used for the trimethylsilylation of hydroxyl groups is hexamethyldisilazane (HMDS), which is a stable, commercially available, cheap reagent, and is nearly neutral, so its handling does not need special precautions. The low silylating power of HMDS is the only disadvantage for this agent. Therefore, there are a variety of catalysts for activating of this reagent [2-3]. Herein, we report a new protocol for the mild and efficient trimethylsilylation of alcohols and phenols using HMDS in the presence of PPA/SiO_2 under solvent free conditions at room temperature (Scheme).



R: Alkyl, Aryl

Scheme

By using different reaction conditions for the silylation of alcohols and phenols with HMDS, we found out that best results are obtained using PPA/SiO_2 (0.05 gr), HMDS (0.8 mmol) and ROH (1 mmol) at room temperature under solvent-free conditions. A wide range of structurally diverse and functionalized phenols and alcohols underwent silylation by this process to provide the corresponding TMS ethers in good to excellent isolated yields. In addition, PPA/SiO_2 can be recovered and reused after drying.

References:

[1] Greene, T.W.; Wuts, P.G.M. *Protective Groups in Organic Synthesis*. 3rd Ed., Wiley & Sons, New York, **1999**.
[2] Karimi, B.; Golshahi, B. *J. Org. Chem*, **2000**, *65*, 7228.
[3] Akhlaghinia, B.; Tavakoli, S. *Synthesis*, **2005**, 1775.

Alumina-supported phosphorus pentoxide catalyzed preparation of trimethylsilyl ethers

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Trimethylsilylation of organic compounds having labile hydrogen atoms is an important organic transformation [1]. It is a frequently used protection method in multi-step synthesis of natural products due to the enhanced stability under a variety of conditions, solubility in non-polar solvents, thermal stability and the ease of removal which is simply accomplished by acid or base induced hydrolysis giving only un-reactive siloxane as by-product. It is also used extensively for the derivatization of hydroxy compounds to increase their volatility for gas chromatography and mass spectrometry [2]. Phosphorus pentoxide is a white, flammable, dangerous, corrosive to metal and extremely deliquescent compound [3]. P_2O_5 supported on SiO_2 as an inexpensive, heterogeneous stable, free flowing, and white powder was prepared. It has the advantage of being easily removed from the organic product by filtration and also this reagent is improved storage stability in moisture in comparison to P_2O_5.

A variety of hydroxy functional groups was protected as their corresponding trimethylsilyl ethers using HMDS in the presence of P_2O_5/Al_2O_3. The catalyst activates the HMDS and accelerates the reaction under mild reaction conditions at room temperature to afford the corresponding silylated products in excellent yields. The experimental conditions are very simple and the isolation of products also very easy. The highly catalytic nature of P_2O_5/Al_2O_3 and its wide applicability should make this protocol an attractive alternative over existing methods.

A wide range of structurally diverse and functionalized alcohols, phenols and naphthols underwent silylation by this procedure to provide the corresponding TMS ethers in excellent isolated yields, whereas amines and thiol remained unaffected under the reaction conditions (Scheme).

$$\text{ROH} + \text{HMDS} \xrightarrow[\text{room temperature}]{P_2O_5/Al_2O_3\text{(100 mg)}} \text{ROSiMe}_3 + \text{NH}_3$$

Solvent-Free

R=Primary, Secondary, Tertiary Alkyl, Aryl

Scheme

References:

[1] Greene, T.W. Wuts, P.G. M. Protective Groups in Organic Synthesis, third ed., Wiley, New York, 1999.
[2] Kocienski, P.J. in: Enders, R. Noyori, R. Trost, B.M. (Eds.), Protective Groups, Thieme, Stuttgart, 1994.
[3] Corbridge, D. E. C.; Phosphorus: An Outline of its Chemistry, Biochemistry, and Technology 5th Edition Elsevier: Amsterdam., Netherlands, 1978.

One pot and facial route to synthesis of new derivatives of penicillin

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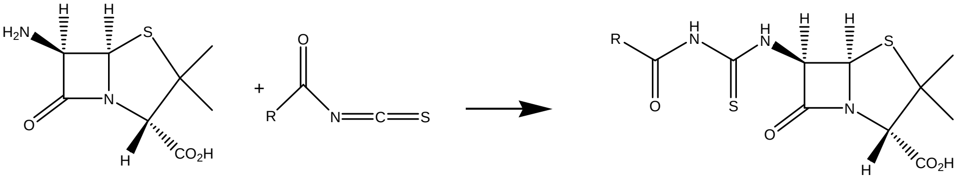
B-Lactam antibiotics such as penicillin and cephalosporins are the most commonly prescribed antibacterial agents. Synthesis of new derivatives of penicillin and drug investigation of them is very important. A larg number of penicillin derivatives have been synthesized and properties are investigated [1, 2, 3].

Herein, we wish to report one pot and facial route to synthesis of new derivatives of penicillin. Thus, compound 1 was allowed to react with isothiocyanate derivatives in reflex condition after 30 min to produce 3 in high yields. The structure of products has been assigned by spectroscopic data.
It is seem, that this compounds have pharmacologically and biologically activities.



References:

[1] Salton, M.R.J. and Shockman, G.D. eds & Lactam Antibiotics, Academic Press, London , **1981.**

[2] Lee, M.; Hesek, D.; Suvorov, M.; Lee, W.; Vakulenko, S.; Mobashery, S. *J. Am. Chem*. Soc**. 2003**, *125*, 16322.

[3] Aman Bhalla, Sachin Madan, Paloth Venugopalany and Shamsher S. Bari Tetrahedron **2006**, *62*, 5054.

Ab initio study of structural properties and carbonyl electrophilicity for acyl chlorides

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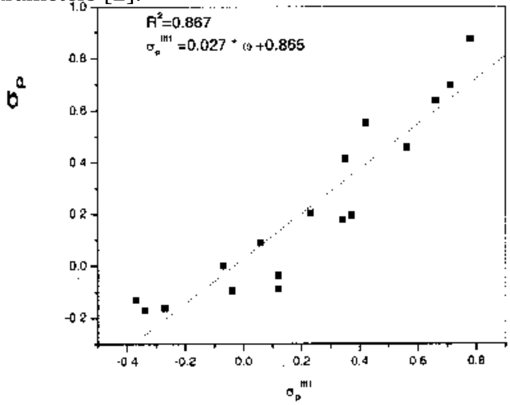
For more investigation on acyl chlorides reactions we studied different possible structures for R-CO-Cl (R=H, CH_3, CH_3CH_2, *n*-C_3H_7, *iso*-pro, *n*-C_4H_9 , *t*-Bu, *sec*-Bu, *iso*-Bu, *n*-C_5H_{11}, $CH_3CH(CH_3)CH(CH_3)$, $CH_3C(CH_3)_2CH_2$, $C_2H_5C(CH_3)_2$, *n*-C_3F_7)and Ar-CO-Cl (Ar=C_6H_5, *o*-Me(C_6H_4), *p*-Me(C_6H_4), *o,p*-Me_2(C_6H_3), di-*o*-Me_2(C_6H_3), *m*-Me(C_6H_4), *o*-NH_2(C_6H_4), *p*-NH_2(C_6H_4), *o,p*-$(NH_2)_2$(C_6H_3), di-*o*-$(NH_2)_2$(C_6H_3), *o*-HO-(C_6H_4), *p*-HO-(C_6H_4), *o,p*-$(HO)_2$-(C_6H_3), di-*o*-$(HO)_2$-(C_6H_3), *o*-NO_2-(C_6H_4), *p*-NO_2-(C_6H_4), *o,p*-$(NO_2)_2$-(C_6H_3), di-*o*-$(NO_2)_2$-(C_6H_3), *m*-NO_2-(C_6H_4), *o*-CHO-(C_6H_4), *p*-CHO-(C_6H_4), *o,p*-$(CHO)_2$-(C_6H_3), di-*o*-$(CHO)_2$- (C_6H_3)) geometries of the molecules are optimized using Gaussian 03 employing HF method with 6-31G* basis set [1]. Three structure were obtained carbonylic (1), singlet carbine (2) and triplet carbine (3). Carbonylic structure is the most stable. The calculated vibrational frequencies for all the molecules ensured that the geometries corresponding to the minimum energy are achieved. To study the chemical reactivity, experimental σ_P values and electronic electrophilicity index ω have compared and a statistical procedure has been developed to obtain correlation coefficient between these parameters [2].

(1) R-CO-Cl, (2) R-C-O-Cl (singlet)

(3) R-C-O-Cl (triplet)



References:

[1] Hyper chem., Release 7.0 for Windows, Molecular Modeling System: Hyper Cube, 2002, http://w.w.w.**hyper**.com

[2] *J. Chem. Sci., 117,* 1, **2005**, 61.

Diastereoselective Synthesis of β-Phosphonato Unsaturated Thioimidates

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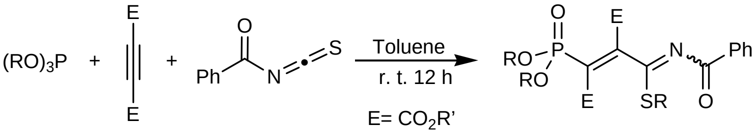
Thioimidates, especially unsaturated thioimidates are important building blocks in organic synthesis for the synthesis of heterocyclic compounds. Stereoselective synthesis of γ-lactams by iodine-induced lactamization of γ,δ-unsaturated thioimidates has been reported by Takahata and co-workers. Coupling reaction of a cyclic thioimidate with oxazolones is a key step in the synthesis of carzinophilin, which is an antitumor and natural antibiotic. Rearrangement of thiomethylimidate cyclopropane to a pyrrolothiomethylimidate intermediate was reported in the synthesis of dihydropyrroles. Synthesis of amidrazones using an engineered papain nitrile hydratase and cysteine protease-like structures by trapping thioimidate also shows their importance. Macrocyclic ligands containing the thioimidate group also exhibited good affinity towards metal ions, the complexes of which are known to act as a catalyst for RNA cleavage. Recently, glycosyl thioimidates are being used in glycol conjugates and oligosaccharide synthesis. [1-4]

We became interested in the application of benzenecarbonyl isothiocyanate for the synthesis of title compounds. Our new synthetic method, which has not been previously reported to our knowledge, is illustrated. Reaction between trialkyl phosphites **1**, dialkyl acetylenedicarboxylates **2**, and benzenecarbonyl isothiocyanate proceeds in toluene at room temperature to produce β-phosphonato unsaturated thioimidates **3** in 70–75% yields (Table 1).



1 **2** **3**

The data obtained from elemental analyses, IR, ^{1}H, ^{13}C and ^{31}P NMR, and mass spectra confirmed the molecular structure of products.

References:

[1] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104*, 199.
[2] Roger, R.; Neilson, D. G. *Chem. Rev.* **1961**, *61*, 179.
[3] Parlato, M.; Kamat, M.; Wang, H.; Stine, K. J.; Demchenko, A. V. *J. Org. Chem.* **2008**, *73*, 1716.
[4] Alizadeh, A.; Zohreh, N. *Synthesis* **2009**, 2737. and references 1-8 sited there.

Reaction between arylated amino acids and cyclohexyl isocyanide in alcohols:a simple route for alkylation of amino acids

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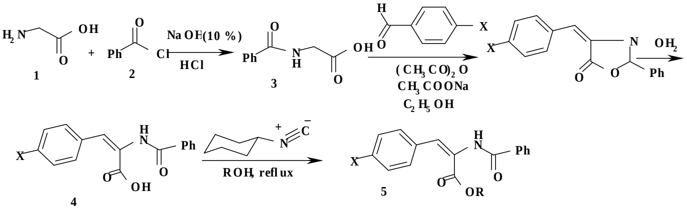
The addition reaction of different compounds to isocyanides has been of particular interest since many years ago. Isocyanides have been reported to react with two equivalent of carboxylic acids to afford the corresponding carboxylic formamide and carboxylic anhydride.[1] Recently it has been reported that the reaction of isocyanides with sulfonic acids lead to the corresponding sulfonamides.[2] Similar reaction was also reported between isocyanides and carboxylic acids in methanol as solvent to yield the corresponding carboxamides.[3] At first glycine(1) was reacted with benzoyl chloride(2) to afford N-benzoyl glycin(3) which then reacted with aromatic aldehydes to form aryl methylidinamino acids(4).The reaction of N-benzoyl-2-arylmethylidine glycin with isocyanides was carried out in different alcohols of solvent as shown in scheme**1**, these reaction affored a simple route for alkylation of these amino acid derivatives(5) under neutral condition.



5	X	R	%Yield*
a	H	CH_3	92
b	Cl	$(CH_3)_2CH$	90
c	NO_2	C_2H_5	91
d	Cl	CH_3	92
e	NO_2	CH_3	89

* Isolated yields

Scheme 1

References:

[1] Ugi, I. *Isonitrile Chemistry*. Academic Press, New York, Chapter 4, 65.
[2] Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.,* **2007**, *48*, 2185.
[3] Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.,* **2007**, *48*, 6137.

Synthesis and characterization of trimethoxyvinylsilane (TMVS)-modified styrene- acrylate emulsion copolymers and investigation of its paint properties for exterior application

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Aqueous emulsions used as binders in solvent- free paint formulations have to cope with the challenge to guarantee an excellent film formation and appearance as well as good mechanical properties . One strategy to fulfill these contradictory requirements is the employment of silicon monomer in resins synthesized by emulsion polymerization.a silicon styrene acrylic resin was synthesized by emulsion polymerization using ethyl methacrylate(EMA), butylacrylate(BA), methacrylic acid (MAA) , styrene and trimethoxyvinylsilane (TMVS) monomers at 90 □C in the presence of potassiumpersulphate (KPS) as initiator. Alkylphenol ethersulphate and Arkupal N-300 were used as anionic and non-ionic emulsifiers, respectively. The resulting copolymers were characterized by using Fourier Transform Infrared Spectroscopy (FTIR) and Minimum film formation temperature (MFFT) with total solid of 52% .a paint was prepared according to a commercial exterior paint formulation and its properties such as water vapor transmition, wet scrub resistance, water resistance, alkali resistance, gloss, uv resistance and adhesion has been investigated and compared with a commercial exterior paint. Paint properties showed that good improvement in paint properties can be obtained via entering of silicon monomer into the styrene acrylic structure.

References:

[1] H.J.Naghash; A. R. Momeni. *Turk J Chem*. **2007**, *31*, 257.
[2] H.J.Naghash; S. Mallakpour. *Progress in Organic Coatings*. **2006**, *55*, 375.
[3] R.S.Tigli; V.Erren. *Progress in Organic Coatings.* **2004**, *52*, 144.
[4] H.Peng; G.F.Huang. *Gongneng Gaofenzixuebao*. **2000**, *13*, 173.

Impact of SAP nano-composites on rheological properties and setting behavior of Portland cement composites (PCC)

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A superabsorbent polymer, SAP, is a polymeric material which is able to absorb a significant amount of liquid from the surroundings and to retain the liquid within its structure without dissolving [1].

SAPs have already a widespread use as a high-tech material e.g. for contact lenses, breast implants, fire fighting, drug delivery, baby diapers and as soil conditioners [2].

A relatively new application of SAP has been tried for internal curing of concrete, to further the existing methods such as using lightweight aggregates. The goal is providing water from within the body of the concrete to reduce self-desiccation and shrinkage, especially in high performance concrete. However, some problems are associated to this technique including difficulties in controlling consistency and a reduction in strength and elastic modulus [3,4].

In the present work, we have synthesized a variety of nano-composite SAP and studied the effect of their chemical functionality and ionicity and type of nano-fillers on consistency and flow properties as well as setting time characteristics of fresh cement paste .

The results can be used to design more efficient superabsorbent polymers for the exclusive purpose of production of water entrained concrete.

References:

[1] Buchholz FL, Graham AT (eds) (1998) Modern superabsorbent polymer technology. WILEY-VCH, New York.
[2] Zohuriaan-Mehr M.J. , Kabiri K. (2008) Superabsorbent Polymer Materials: A Review. Iranian Polymer Journal 17 (6): 451.
[3] Jensen OM, Hansen PF (2001) Water-entrained cement-based materials – I. Principle and theoretical background. Cem Concr Res 31(4):647.
[4] Jensen OM, Hansen PF (2002) Water-entrained cement-based materials – II. Implementation and experimental results. Cem Concr Res 32(6):973.

Simple three-component method for the synthesis of spiroindenopyridopyrimidine-indolines

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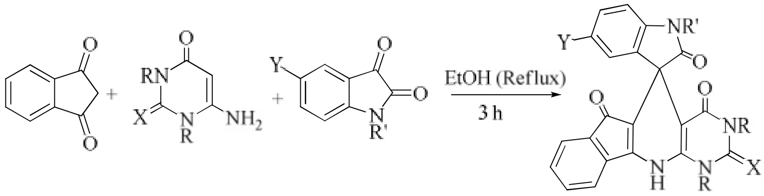
Pyrimidopyrimidines are annulated uraciles that have attracted considerable interest in recent years. Their derivatives have been known to display a wide range of pharmacological activities [1]. Multicomponent reactions of amino uracile, various CH-acids and aldehydes have recently attracted the interest of the synthetic community because the formation of different analogues of pyrimidopyrimidines can be expected [2]. Similarly, heterocycles containing indenone moiety are important class of heterocyclic compounds since many of this heterocyclic system exhibit biological and pharmaceutical activity Although several isatin-based multicomponent reactions have been reported by our reasearch group [3] or other groups [4] to the synthesis of spirooxindoles containing heterocycles, but reaction of amino uracil, isatin and CH-acid have not been reported yet.

Herein, for first time we report an efficient synthesis of spirooxindoles annulated indenopyridopyrimidine **4** based on a one-pot and three-component reaction of 1,3-indandione **1**, amino uracils **2** and isatins **3**.



1 **2** **3** **4**

References:

[1] (a) Sanghhvi, Y. S.; Larson, S. B.; Matsumoto, S. S.; Nord, L. D.; Smee, D. F.; Willis, R. C.; Avery, T. H.; Robins, R. K.; Revankar, G. R. *J. Med. Chem.* **1989**, *32*, 629.

[2] (a) Tu, S.; Zhang, J.; Zhu, X.; Xu, J.; Zhang, Y.; Wang, Q.; Jia, R.; Jiang, B.; Zhang, J. *Bioorg. Med. Chem. Lett*. **2006**, *16*, 3578.

[3] (a) Ahadi, S.; Ghahremanzadeh, R.; Mirzaei, P.; Bazgir, A. *Tetrahedron* **2009**, *65*, 9316; (b) Jadidi, K.; Ghahremanzadeh, R.; Bazgir, A. *J. Comb. Chem.* **2009**, *11*, 341; (c) Ghahremanzadeh, R.; Sayyafi, M.; Ahadi, S.; Bazgir, A. *J. Comb. Chem.* **2009**, *11*, 393.

[4] (a) Zhu, S.-L.; Ji, S.-J.; Zhang, Y. *Tetrahedron* **2007**, *63*, 9365.

Ionic liquid 3-methyl-1-sulfonic acid imidazolium chloride ([Msim]Cl): A new and highly efficient catalyst for the synthesis of benzimidazole at room temperature

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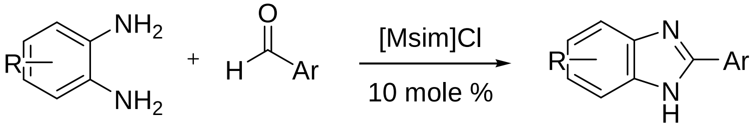
Benzimidazoles are very useful intermediate/subunits for the development of molecules of pharmaceutical or biological interest. Substituted benzimidazole derivatives have found applications in diverse therapeutic areas including antihypertensives, antivirals, antifungals, anticancers and antihistaminics to name just a few.[1]

More recently, we have synthesized ionic liquid 3-methyl-1-sulfonic acid imidazolium chloride ([Msim]Cl) as a new Brønsted acidic catalyst. we have successfully applied this new acidic catalyst for the efficient and rapid preparation of *N*-sulfonyl imines[2] and bis(indolyl)methanes.[3] To develop the applications of this new catalyst in organic synthesis, herein, we report a new and highly efficient method for the synthesis of various Benzimidazole derivatives from phenylenediamines and aldehydes (Scheme 1).



References:

[1] S. Lin, L. Yang, *Tetrahedron Lett*. 46 (**2005**) 4315.
[2] M.A. Zolfigol, A. Khazaei, A.R. Moosavi-Zare, A. Zare, *J. Iran. Chem. Soc.* in press.
[3] M.A. Zolfigol, A. Khazaei, A.R. Moosavi-Zare, A. Zare, *Org. Prep. Proced. Int.* 42 (**2010**) 95.

$BF_3.SiO_2$: An efficient and reusable catalyst for one-pot synthesis of photochromic naphthopyrans

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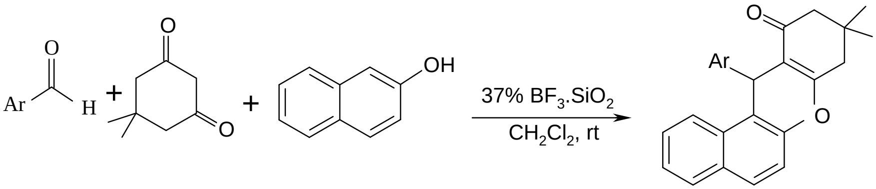
Naphtho[2,1-b]pyrans, also known as 1H-benzo[f]chromenes, are well known for their photochromic properties [1]. This property is the result of a facile electrocyclic pyran ring opening to yield a mixture of yellow or purple-colorless pyran ring upon removal of the source of irradiation: 1 leading to their importance in photochromic lenses which darken upon exposure to sunlight [2]. Furthermore, naphthopyrans are prevalent in numerous natural products with significant biological and medicinal properties [3].



Solid supported reagents have improved activity and selectivity than individual reagents. Because the surface area of the reagent is increased manifold [4]. In this work we report a mild procedure for the synthesis of different naphthopyrans by solid phase acidic catalyst with improved yields.

References:

[1] Nakatsuji, S. *Chem. Soc. Rev***. 2004**, *33*, 348.
[2] Van Gemert, B. *Mol. Cryst. Liq. Cryst*. **2000,** *344*, 57.
[3] Visentin, S.; Rolando, B.; Di Stilo, A.; Fruttero, R.; Novara, M.; Carrbone, E.; Roussel, C.; Vanthuyne, N.; Gasco, A. *J. Med. Chem*. **2004**, *47*, 2688.
[4] Corma, A.; Garcia, H. *Adv. Synth. Catal*. **2006**, *348*, 1391.

Ionic liquid promoted synthesis of Dihydropyrimidine-2-ones

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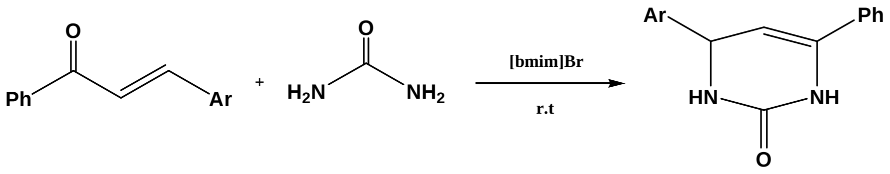
In the past decade, Ionic Liquids (ILs) have been received substantial attention in organic synthesis because of their environmentally benign nature, high polarity, and good thermal stability. Often shorter reaction times, high yields, cleaner reaction products, and high selectivity's are obtained from ionic-liquid reaction media [1].

Ionic liquids have attracted increasing interest recently in the context of green organic synthesis. Although ionic liquids were initially introduced as alternative green reaction media because of their unique chemical and physical properties of no volatility, to non-inflammability, negligible vapor pressure, reusability and high thermal stability. Today they have marched far beyond this boundary, showing their significant role in controlling reactions as solvent or catalysts [2].

The present investigation describes the synthesis of pyrimidine-2-one derivatives under conventional and ionic liquids media. Application of ionic liquid shortened the reaction time of the generation of pyrimidines from 6 h under classical conditions to 40-50 min. Also the yields of products were improved 20–30% in compared with the thermal heating method [3].

In summary, we have described an optimized procedure for the preparation of pyrimidine-2-one derivatives under milder and cleaner conditions. The advantages of Ionic Liquids in chemical reactions such as shorter reaction time and higher yields and milder conditions could be of use in organic synthesis.



References:

[1] Zhao, D.; Wu, Min; Kou, Y.; Min, E. *Catal. Today*. **2002***, 74,* 157.
[2] Wasserscheid, P. Ionic Liquids in Synthesis. Wiley-VCH Verlag: Stuttgart, Germany. 2002.
[3] kidwai, M.; Misra, P. *Synth. Commun*. **1999**, *29*. 3237.

One-pot synthesis of substituted 4H-chromenes by three component reaction of alkyl isocyanides, dialkyl acetylenedicarboxylates and *N*-aryl-3-hydroxynaphthalene-2-carboxamide

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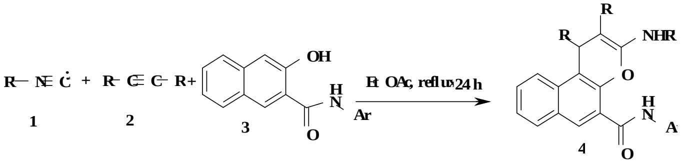
Chromenes often appears as an important component in both biologically active and natural compounds.Benzopyran fragment is widely performed in natural alkaloids, flavonoids, tocopherols and anthocyanins [1,2]. As part of our current studies on the development of new routs to heterocyclic systems [3,4].

Herein we have described a simple, and one-pot, three-component reaction between alkyl isocyanides, dialkyl acetylenedicarboxylates and *N*-aryl-3-hydroxynaphthalene-2-carboxamide for the preparation of substituted 4H-chromenes in good yields.



4	Ar	R	R'	Yield(%)
a	Ph	CO_2Me	Cyclohexyl	91
b	Ph	CO_2Me	t-Butyl	94
c	Ph	CO_2t-Bu	Cyclohexyl	89
d	2-Me-C_6H_4	CO_2Me	t-Butyl	90
e	2-Me-C_6H_4	CO_2Et	Cyclohexyl	91

The structures of 4a-e were determined on the basis of their elemental analyses, MS, ^1H, ^{13}NMR and IR spectroscopic data.

References:

[1] Polyakov, V. V. *Chem. Nat. Compd.* (Engl. Trans1.) **1999**, *1*, 21.
[2] Harbone, J. B. *The Flavonoids-Advances in Research, chapman & Hall,* London, 1988.
[3] Anary-Abbasinejad, M.; Anaraky-Ardakani, H.; Rastegari, F.; Hassanabadi, A. *J. Chem. Res.* **2007**, *10*, 602.
[4] Anary-Abbasinejad, M.; Hassanabadi, A. *J. Chem. Res.* **200**8, *2*, 95.

Molecular imprinted polymer: synthesis, sharacterization and applications as extractant for preconcentration and determination of Clonazepam

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Recently molecularly imprinting polymer has been used for purification and preconcentration of bioproducts[1, 2]. Molecular imprinted polymers (MIPs) were prepared from methacrylic acid and Allyl glycidil ether/ iminodiacetic acid as the functional monomer and N, N methylene- diacrylamid as the cross-linker in methanol solution using clonazepam as the template molecule and benzoyle proxide as the initiator. The polymer was by elemental analysis, IR and thermogravimetric analysis (TGA) and studied for preconcentration and determination of clonazepam using high performance liquid chromatography for drug monitoring. The effects of amount of the cross-linker, the ratio of template molecule and functional monomer, amount of solvent and amount of the radical initiator on the polymerization were examined. The polymerization also was performed in presence of Cu (II) which can coordinate the drug and retain it in polymer. Clearly, in the last polymerization manner, the polymer first was doped with Cu (II) then acted as a sorbent. The synthesized polymer was successfully applied for drug determination from tablet matrix.

References:

[1] N. M.Bergmann, N. A. peppas, recognition, *prog .poly.Sci*. **2008,** *33*, 271.

[2] M. Ulbricht, M. Belter, U. Langenhangen, F. Schneider, W. Weigel., Desalination, **2002,** *149*, 293.

$PdCl_2$-*N*-Heterocyclic carbene catalyzed Heck vinylation reactions of 2,6-diaryl-3,5-dibromo-4-pyrones

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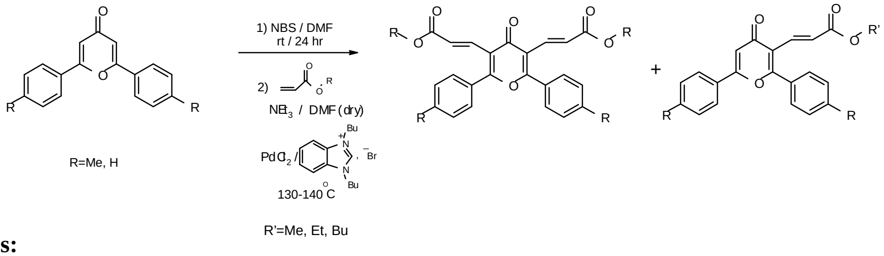
The Heck reaction is one of the most important carbon–carbon bond forming methodologies in organic synthesis [1]. The traditional Heck reaction usually proceeds using phosphine-based palladium catalysts in the presence of a suitable base. However, the use of phosphine ligands exhibits serious limitations for industrial applications [2]. Over the past 40 years, *N*-heterocyclic carbenes (NHC_S) have blossomed into a class of ligands that have proven to be useful for a broad range of transition metals. As strong, two-electron donors, they generally coordinate to metals in a fashion that is analogous to phosphines [3]. Furthermore the 4-pyrone unit is seen in a wide variety of biologically interesting natural products [4]. So Herein we report synthesis of new olefin derivatives of 4-pyrones by using *N,N*-dibutyl benzimidazolium bromide as a NHC-precurcor. In this direction 2,6-bis(4-methyl phenyl)-3,5-dibromo-4*H*-pyran-4-one and 3,5-dibromo-2,6-diphenyl-4*H*-pyran-4-one were prepared by reaction of corresponding pyrones with excess NBS in DMF and then treated with methyl, ethyl and butyl acrylate in the presence of triethyl amine (base), DMF (solvent), $PdCl_2$ (catalyst) and NHC-precurcor. Best results were obtained at 130-140 ºC for 18 hours. All symmetric and ussymmetric olefin products were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR data and CHNS analysis.



References:

[1] Cai, Y.; Lu, Y.; Liu, Y. *Catalysis Communications*. **2008**, 9, 1209.
[2] Antunes, O.A.C.; F. Mendes, J.; Duque Estrada, O. *Catalysis Communications*. **2008**, 9, 1734.
[3] Khramov, D.; Vu y, P. *Tetrahedron*. **2008**, 64, 6853.
[4] Kamino, T.; Kuramochib, K.; Kobayashia, S. *Tetrahedron Letters*. **2003**, 44, 7349.

Sulfuric acid ([3-(3-silicapropyl)sulfanyl]propyl)ester: As an efficient and recyclable solid acid catalyst for the three-component synthesis of α-amino nitriles

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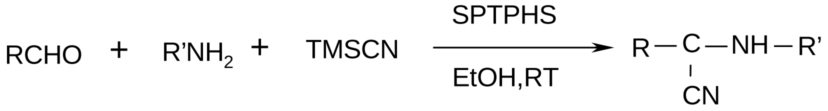
The addition of cyanide anion to imines (the Strecker reaction) [1] provides one of the most important and straightforward method for the synthesis of α-aminonitriles, which are useful intermediates for the synthesis of amino acids [2] and nitrogen containing heterocycles such as thiadiazoles and imidazoles, etc. [3] The classical Strecker reaction usually is carried out in aqueous solution and the work-up procedure is also tedious.

Herein, we introduced silica bonded sulfuric acid ([3-(propyl)sulfanyl]propyl]ester **(SPTPHS)** as a recyclable catalyst for the synthesis of α-amino nitriles. These syntheses were performed via a one-pot three-component condensation of aldehydes, amines, and trimethylsilyl cyanide under mild reaction conditions at room temperature.



$$\mathrm{RCHO} + \mathrm{R'NH_2} + \mathrm{TMSCN} \xrightarrow[\mathrm{EtOH,RT}]{\mathrm{SPTPHS}} \mathrm{R{-}\underset{\displaystyle CN}{\underset{|}{C}}{-}NH{-}R'}$$

R= Aliphatic, Aromatic R'=Primary, Secondary

References:

[1] Strecker, A. *Ann. Chem. Pharm.* **1850**, *27,* 75.
[2] Shafran, Y. M.; Bakulev,V. S.;. Mokrushin, V.S. *Russ. Chem. Rev.* **1989**, *58*, 148.
[3] March, J. *Advanced Organic Chemistry*, 4th ed., Wiley, New York. pp. 965, **1995**.

Efficient and new synthesis of benzimidazole derivatives by nano-silica supported boron trifluoride catalyst

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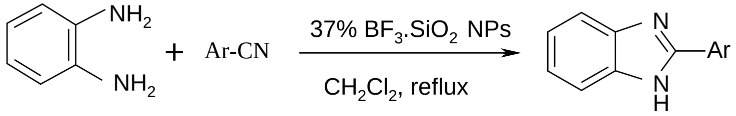
Benzimidazole derivatives exhibit important biological activities. They are potent inhibitors of TIE-2 and VEGFR-2 tyrosine kinase receptors, antitumor agents and gamma-aminobutyric acid agonists [1]. Substituted benzimidazole derivatives have found commercial applications in veterinarian medicine as anthelmintic agents and in diverse human therapeutic areas such as treatment of ulcers and as antihistaminics [2]. So it is worthwhile to introduce useful and efficient methods for their synthesis.



Solid supported reagents have improved activity and selectivity than individual reagents. Because the surface area of the reagent is increased manifold [3]. In summary, we have developed a new and high efficient, one-pot selective method for synthesis of 2-Aryl-benzimidazole derivatives in the presence of nano-silica supported boron trifluoride catalyst.

References:

[1] lFalco, J.; Pique, MGonzalez, m.; Buira, I.; Mendez, E.; Terencio, J.; Perez, C.; Princep, M.; Palomer, A.; Guglietta, A. *Eur. J. Med. Chem*. **2006**, *41*, 985.
[2] Zhu, Z.; Lippa, B.; Drach, J. C.; Townsend, L.B. *J. Med. Chem*, **2000**, *43*, 2430.
[3] Corma, A.; Garcia, H. *Adv. Synth. Catal*. **2006**, *348*, 1391.

Synthesis of four substituted imidazoles derivatives using magnetic nano particles Fe_3O_4 as a rusable catalyst under solvent free condition

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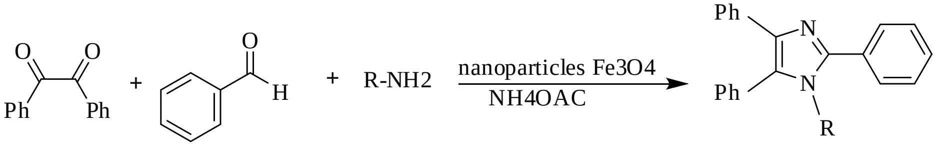
A simple and efficient method for the imidazol derivatives synthesis from the condensation benzil and ammonium acetate with different aromatic aldehydes in the presence of a catalytic amount of magnetic nanoparticles Fe_3O_4 is described The reason proposed for higher catalytic activity of nano-sized magnetic nanoparticles Fe_3O_4 is a combination effect of the small particle size and high-density surface defects. The practical and simple method led to excellent yields of the four substituted imidazoles derivatives under mild conditions and within short times.



References:

[1] Sushma Drabu, Nitin Kumar and Siddeswaran Munirjan, *Indian J. Heterocycl. Chem.* **2005**, 15, 195.

[2] Jag Mohan and Ashok Kumar, *Indian J. Heterocycl. Chem*. **2002**, 12, 41.

[3] Mary J M, Richard A H and Pamela C C, Lippincott's Illustrated Reviews; LippincottWilliams and Wilkins: London, 2000, 145.

Synthesis and characterization of new macrocyclic from the reaction of 2-hydroxybenzaldehyde, 1, 2-phenylendiamine and phthaldialdehyde

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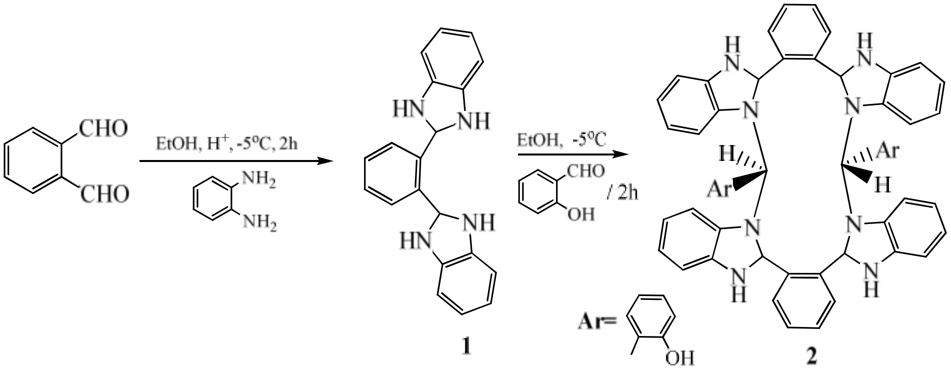
The synthesis of macrocyclic ring systems, such as crown ethers, cryptands, cyclophanes, porphyrins, and macrolides, is an important area in organic chemistry. There are several strategies for obtaining macrocycles, including cyclization, capping, and condensation uses thermal reactions and photochemical methods. Among them condensation reaction attention has been paid to the synthesis of macrocyclic compounds [1, 2, 3, 4].

In this paper, we describe synthesis of macrocyclic compounds using condensation reactions of 1, 2- phenylendiamine 2- Hydroxybenzaldehyde and Phthaldialdehyde in EtOH solvent at -5 °C. The mechanism of reaction was studied and separation intermediate of **1.** The structures of intermediate 1 and product **2** are proposed in accordance with the elemental analysis, ^{1}H and ^{13}C NMR, IR and mass spectral.



References:

[1] A.T. Colak., M. Tumer., S. Serin., *Trasition Metal Chemistry*. **2005,** *25*, 200
[2] E. Nataliya., M. D. Borisova., M. D. Reshetova., A. Yu. Ustynyuk., *Chem. Rev.* **2007**, *107*, 46
[3] T. T. Tidwell., *Angew. Chem. Int. Ed.***2008**, *47*, 1016.
[4] A. Kakanejadifard., A. Zabardasti and H., Koshki. *Journal of Coordination Chemistry*.**2009**, *62*, 3552

Modified montmorillonite as a catalyst for synthesis of bezimidazole and benzothiazole derivatives under heating and solvent free conditions

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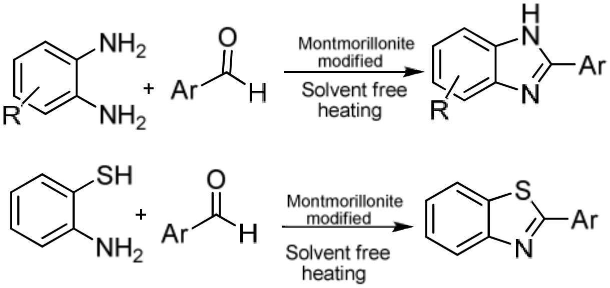
The benzimidazole and benzothiazole have been an important pharmacophore and privileged structure in medicinal chemistry, encompassing a diverse range of biological activities including anti-arrhythmic, antinuclear, anthelmintical, inotropic, anti-histamine, anti-fungal, anti-viral, and cytotoxicity displaying diverse range of biological activities [1]. Benzimidazoles exhibit significant activity as potential antitumor agents [2], antimicrobial agents [3], smooth muscle cell proliferation inhibitors [4], a treatment for intestinal cystitis [5], and in diverse area of chemistry [6]. Modified montmorillonite was prepared by acid activation and pillaring as a catalyst has shown to be excellent catalysts for organic reaction. Montmorillonite modified is an efficient environmental friendly catalyst for synthesis of bezimidazole and benzothiazole derivatives. The preparation was performed with an aldehyde, and 1, 2-phenylene diamine or O-aminothiophenole under solvent-free conditions.



References:

[1] D.A. Horton, G.T. Bourne, M.L. *Smythe, Chem. Rev*. **2003,** 103, 893e,
[2] W.A. Denny, G.W. Rewcastle, B.C. Baguley, *J. Med. Chem*. **1990,** 33, 814e819.
[3] T. Fonseca, B. Gigante, T.L. Gilchrist, *Tetrahedron.* **2001,** 57, 1793e.
[4] H.M. Elokdah, S.Y. Chai, T.L. Sulkowski, U.S. Patent 5, 763, 473, June 9, **1998**. *Chem. Abstr*. **1998,** 129, 58784g.
[5] S. Iyenger, M.A. Nuhlhauser, K.B. Thor, *U.S. Patent* **1996,** 13, 129. International PCT Patent 33,873, September 18, 1997. *Chem. Abstr*. **1997,** 127, 293221p.
[6] C. Stevenson, R. Davies, H. Jeremy, *Chem. Res. Toxicol*. **1999,** 12, 38e.

One-pot synthesis of dialkyl 2-alkylamino-5-oxo-4*H*, 5H-pyrano [3, 2-c] chromene-3, 4-dicarboxylates and alkyl benzoylaminoacids

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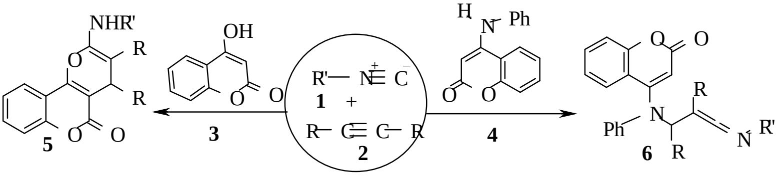
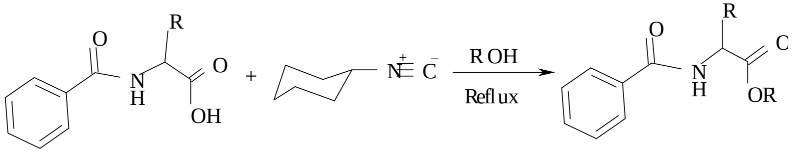
Isocyanides by virtue of their carbenic character, react readily with most common multiple bonds [1]. The reaction of isocyanides with carbon-carbon triple bonds tend to occur in a stepwise manner as is initiated by a zwitterionic intermediate whose ultimate fate appears to be dictated by the nature of the original triple-bonded substrate. These reactions are of interest for the synthesis of functionalized heterocyclic ring systems. The reaction between alkyl isocyanides and dialkyl acetylenedicarboxylates has been carried out in the presence of different electrophiles, in order to trap the zwitterionic intermediate [2].

Here we report the results of our studies on the reaction between alkyl isocyanides **1** dialkyl acetylenedicarboxylates **2** in the presence of 4-hydroxy coumarine **3** or 4-phenylamino coumarine **4** to produce dialkyl 2-alkylamino-5-oxo-4*H*,5*H*-pyrano[3,2-c]chromene-3,4-dicarboxylates**5** or functionalized keteneimins **6** in good yields.



Alkylation of alanine, phenylalanine, and glycine in the Ni(II) complexes of their Schiffs bases with S-2-N-(N'-benzylpropyl)aminobenzophenone followed by Chromatographic separation of the diastereomers has given optically pure S- and R- α-methyl- α-aminoacids [3]. Herein we report a rapid, simple, new and efficient one-pot of alkylation of benzoylaminoacids with alcohols in the presence of cyclohexyl isocyanide at reflux temperature.



References:

[1] Domling, A.;Ugi, I, *Angew Chem Int Ed* **2000**, *39*,3168.

[2] Yavari, I.; Djahaniani, H.; Nasiri, F. *Tetrahedron* **2003**, *59*, 9409.

[3] Belokon,Yu. N.; Chernoglazova, N. I.; Bakhmutov,V. I.; Garbalinskaya, N. S.; Belikov, V. M. *Russian Chem. Bulletin*, **1987**, 2595.

Ring opening of epoxides using polymer supported $ZrCl_4$ as catalyst

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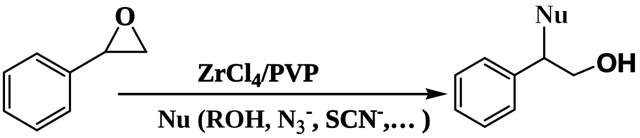
Polymer supported heterogeneous reagents and catalysts are becoming popular in organic transformations since they offer advantages such as easy work up, recyclability , greater selectivity, enhanced stability, easier handling, non-toxicity and low cost [1,2]. Since these reagents are easily isolated by simple filtration in most cases, they lend themselves well to lessen environmental pollution. Such polymer metal complexes (PMCs) work as heterogeneous green catalysts in several organic transformations such as oxidative reactions, hydrogenation reactions, hydrolysis, hydroformylation, hydrosilylation and polymerization initiation [1]. Polymer metal complexes are easily prepared from polymers having coordinating atoms such as polyvinylpyrrolidone [3].

Epoxide ring opening with nucleophiles is a very useful reaction since it offers a suitable route to the formation of C–C, C–N, C–O or C–S bonds. Epoxide ring opening reactions to give β- substituted alcohols with various nucleophiles is a useful tool in organic synthesis and these reactions are generally catalyzed by Lewis acids [1].

In this work, $ZrCl_4$/PVP was prepared from the reaction of $ZrCl_4$ with cross-linked polyvinylpyrrolidone. Then this polymeric complex was used as a catalyst for nucleophilic ring opening of epoxides with various nucleophiles such as ROH, N_3^- and SCN^-. Alcohols reacted with epoxides to form β-alkoxy alcohols in good to excellent yields at solvent-free conditions. Simple work-up, short reaction times and recycling of catalyst are advantages of this method.



References:

[1] Yarapathi, R. V.; Reddy, S. R.; Tammishetti, S. J. *React. Funct. Polym.* **2005**, *64*, 157.
[2] Wang, L.; Cai, C. *Monatsh.Chem.* **2009**, *140*, 541.
[3] Yarapathi, R. V.; Mekala, S.; Rao, B. V.; Tammishetti, S. J. *Catal. Com.* **2006**, *7*, 466.

Rapid and efficient aromatization of Hantzsch 1,4-dihydropyridines with urea-hydrogen peroxide catalyzed by manganese (III) tetra phenyl porphyrin

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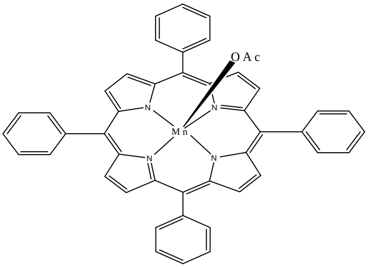
The aromatization of Hantzsch 1, 4-dihydropyridines (1,4-DHPs) is an important method for the preparation of pyridine derivatives. A number of methods and reagents have been reported recently in the literature for this purpose [1-2]. Some of these methods suffer from disadvantages such as the use of strong or toxic oxidants, the requirement of severe conditions or need excess of the oxidants. Other drawbacks are long reaction times, production of by products, the lower yields of products and/or the requirement of tedious work-up procedures.

Thus, in this study, Mn(TPP)OAc; **1**, has been prepared with pyrrol, benzaldehyde and $Mn(OAc)_2.4H_2O$ and characterized by Uv-Vis and IR spectra [3-4]. This complex catalyze the oxidation of Hantzsch 1,4-DHPs to the corresponding pyridine derivatives by urea-hydrogen peroxide UHP as an safe oxidant. The effect of the reaction conditions on the oxidations were studied by varying solvent, nature of additives (i.e. imidazoles) and amount of the catalyst and substrate. The catalytic behavior of the studied complexes was shown to be dependent on the conditions applied.



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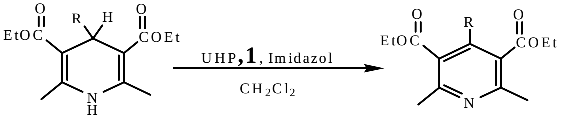

References:

[1] Nasr-Esfahani, M.; Moghadam, M.; Tangestaninejad, Sh.; Mirkhani, V.; Momeni, A. R. *Bioorg. Med. Chem. Lett.* **2006**, 14, 2720.
[2] Moghadam, M.; Nasr-Esfahani, M.; Tangestaninejad, Sh.; Mirkhani, V. *Bioorg. Med. Chem. Lett.* **2006**, 16, 2026 and references therein.
[3] Adler A D; Longo F R; Finarelli J D; Goldmacher J; Assour J; Korsakoff L. *J Org Chem*. **1967**, 32, 476.
[4] Adler A D; Longo F R; Kampas F; Kim J. *J Inorg Nucl Chem*. **1970**, 32, 2443.

Efficient tetrahydropyranylation of alcohols using catalytic amounts of polymer supported $AlCl_3$

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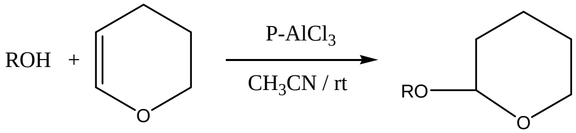
In recent years, great efforts in catalysis research have been devoted to the introduction and application of effective and safe heterogeneous catalysts. The use of polymer-supported catalysts in organic transformations has been receiving extra-ordinary attention, and the design of functionalized polymers carrying metal species has generated substantial interest [1]. Using those polymer supported species as polymeric reagents has many advantages over their monomeric counterparts such as easy separation of the supported species from reaction mixture, the possibility to use an excess of the reagent to force the reaction to completion, reusing of the supported reagent after regeneration, reduced toxicity of supported species compared with low molecular weight unsupported analogues, and increasing stability and selectivity [2].

On the other hand, tetrahydropyranylation is one of the most frequently used processes to protect hydroxyl groups due to the remarkable stability of tetrahydropyranyl ethers under a variety of conditions such as alkaline media, Grignard reagents, alkyl lithiums, metal hydrides, oxidative reagents and alkylating and acylating reagents [3].

Herein we report the preparation of poly [1,3-phenylene diamine-co-pyridine-2,5-dicarboxylic acid]-supported aluminum chloride as a new and efficient catalyst for tetrahydropyranylation of alcohols by reacting various alcohols with 3,4-dihydro-2H-pyran at room temperature in the presence of the polymeric catalyst. Simple work-up, high yields and regenerability of the catalyst are other advantages of this method.



References:

[1] Wang. L.; Cai, C. *Monatsh chem.* **2009,** *140,* 541.
[2] Tamami, B.; Parvanak Borujeni, K. *Iranian Polymer Journal* **2009**, *18,* 191.
[3] Tamami, B.; Parvanak Borujeni, K. *Tetrahedron Lett.* **2004**, *45,* 715.

One-pot synthesis through reaction of [5-(5-nitrotiophen-2-yl)-1,3,4-thiadiazol-2-amine] with acetylendicarboxylatesters in the presence t-butyl-isocyanid

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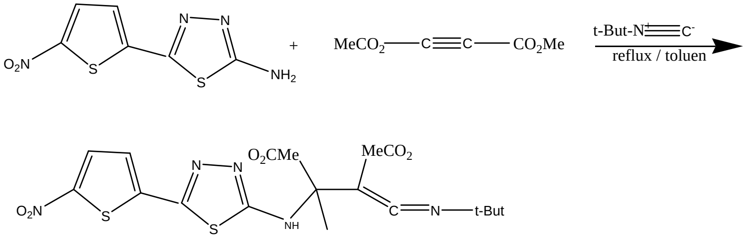
Varius 1,3,4-triazole derivatives have been reported to posses diverse types of biological properties such as antibacterial, antifungal, anti-inflammatory, antihypertensive, antiviral, antileishmanial and anti-migraine activities [1]. Isocyanide-based reactions have been known for about 80 years .With the first described in 1921 and named after its founder, passerine.Today most isocyanide-based multi-component reactions chemistry (IMCR) relates to the classical reactions of passerini and ugi [2].

Herein we report the reaction of [5-(5-Nitro thiophen-2-YL)-1,3,4-thiadiazole-2-Amine] with tert- butyl isocyanid and dimethyl ▯ cetylene dicarboxylat under condition reflux and solvent toluen.



References:
[1] Karabasanagouda, T.; Adhikari, A.V.; Suchethashetty, N.*Medicinal chemistry,* ,**2007**, *42*, 521.
[2] Ramazani, A.; Souldozi, A. *Arkivoc,* **2008,** *(xvi)* 235.

Substituent effects in the Diels–Alder reaction of para- substituted 2-phenylfuran with crotonolactone: A Hammett study via DFT

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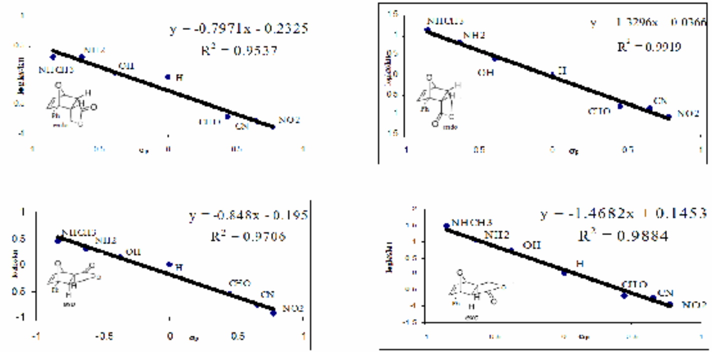
Cycloaddition reactions in general and the Diels–Alder (DA) reactions in particular have a special importance in organic synthesis. Indeed, the DA reactions offer a very efficient way to synthesize cycles from small fragments [1]. The reactivity of cycloaddition reactions can be altered significantly by varying the nature of substituent group on diene and/or dienophile [2]. In this research, the Hammett ρ values and regio(stereo)selectivity of the Diels–Alder reactions of para-substituted 2-phenylfuran where X= H, NO_2, CHO, CN, NH_2, OH and $NHCH_3$ with crotonolactone are obtained at the B3LYP/6-31G(d) using Gaussian 03. These reactions can take place along four reactive channels corresponding to the endo and exo approaches and in each in two regioisomeric pathways. Originally, Hammett study was based on ionizations of *m*- and *p*-XC_6H_4Y, where 'log $k_x/k_H=\rho\sigma$' was introduced as 'the Hammett equation'. In this equation k_H is the rate constant for X=H and k_X is the rate constant for the group X, ρ is a constant for a given reaction under a given set of conditions, and σ is a constant characteristic of the group X [3]. Regression plots of log k_X/k_H for cycloaddition reactions of para-substituted 2-phenylfuran against Hammett σ_p constants showed the expected linearity (following figure). Our results indicate that rate is increased by electron-releasing groups in the reaction.



Regression plots of log k_X/k_H for cycloaddition of para-substituted 2-phenylfuran against Hammett σ_p constants.

References:

[1] Mekelleche, S. M.; Benhabib, R., *Journal of Molecular Structure* (Theochem), **2004**, *709*, 31.
[2] Sharma, P.; Kumar, A.; Sahu, V., *J. Phys. Chem. A.*, **2010**, *114*, 1032.
[3] Maximiliano, S.; Yuji, T., *Journal of Molecular Structure* (Theochem), **2006**, *16*, 61.

Synthesis of functionalized pyrimidine-benzo[*g*]chromene derivatives

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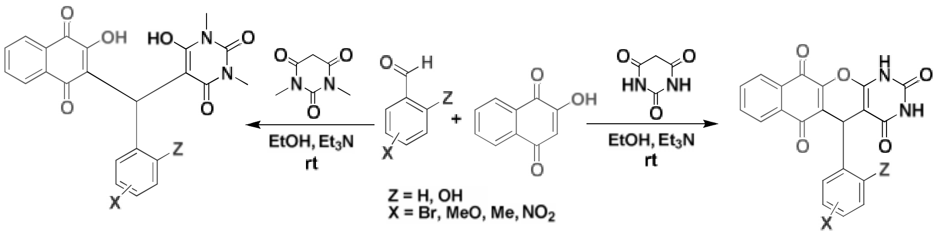
Naturally occurring pyrimidines show a broad spectrum of biological activities including anti cancer, anti-inflammatory, antimalarial, pesticides, and anti-HIV activities. Two classes of HIV inhibitors are nucleoside reverse transcriptase inhibitors (NRTIs) and non-nucleoside reverse transcriptase inhibitors (NNRTIs). To date, more than 30 different classes of NNRTIs have been reported; the core component of these compounds is pyrimidine moiety [1-3].

As a part of our continuing interest in the development of new synthetic methods in heterocyclic compounds [5-6], here in, we report new methods for the synthesis of pyrimidine-2,4-dione derivatives via reaction between an aldehyde, 2-hydroxynaphthalene-1,4-dione, and barbituric acid, or 1,3-dimethylbarbituric acid in the presence of a catalytic amount of triethylamine in EtOH at room temperature.

The procedure is very simple and clean. Products are separated from the reaction media with a simple filtration and no more purification is needed. Using EtOH as a green solvent increases the environment friendly aspects of the reaction.



References:

[1] Mitsuya, H.; Broder, S. *Nature* **1987**, *325*, 773.
[2] St. Clair, M. H.; Richards, C. A.; Spector, T.; Weinhold, K. J.; Miller, W. H.; Langlois, A. J.; Furman, P. A. *Antimicrob. Agents Chemother.* **1987**, *31*, 1972.
[3] Yarchoan, R.; Mitsuya, H.; Thomas, R. V.; Pluda, J. M.; Hartman, N. R.; Perno, C. F.; Marczyk, K. S.; Allain, J. P.; Johns, D. G.; Broder, S. *Science* **1989**, *245*, 412.
[4] Soria-Mercado, I. E.; Prieto-Davo, A.; Jensen, P. R.; Fenical, W. *J. Nat. Prod.* **2005**, *68*, 904.
[5] Shaabani, A.; Ghadari, R.; Sarvary, A.; Rezayan, A. H. *J. Org. Chem.* **2009**, *74*, 4372.
[6] Shaabani, A.; Ghadari, R.; Ghasemi, S.; Pedarpour, M.; Rezavan, A. H.; Sarvary, A.; Ng, S. W. *J. Comb. Chem.* **2009**, *11*, 956.

A facile method for the nitration of aromatic compounds under neutral conditions

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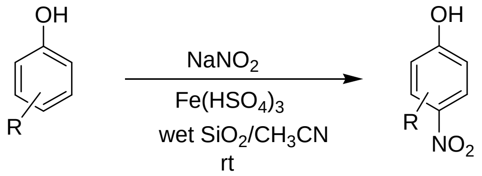
Nitration is one of the most important electrophilic aromatic substitution reactions in organic chemistry. The nitrated aromatic compounds are widely utilized as useful materials such as solvents,dyes, agrochemicals, pharmaceuticals, perfumes, plastics and explosives [1]. Nitration of phenolic compounds using nitrate salts such as $Bi(NO_3)_3.5H_2O$, $VO(NO_3)_3$, $Fe(NO_3)_3.9H_2O$, $(Me_4N)NO_3$, $Mg(NO_3)_2.6H_2O$ and $NaNO_3$ as the nitrating reagents has been reported [2,3]. Moreover, zeolites, a variety of other solid acids such as sulfuric acid on silica, clay-supported metal nitrates, metal exchanged clays and metal-modified montmorillonite have also been studied for nitration of aromatic compounds [4]. However, the majority of reported methods suffer from disadvantages such as low regioselectivity, overnitration, strongly acidic media, tedious workup, and safety problems. In this study, a new and efficient catalyst was introduced for the nitration of aromatic compounds like phenols into their corresponding nitrated compounds using $NaNO_2$ and wet SiO_2 at room temperature with appropriate yields.



References:

[1] Khder, A. S. Ahmed, A. I. *Appl. Catal. A: General*, **2009**, *354*, 153.
[2] Bigdeli, M. A. Heravi, M. M. Nemati, F. *Synth. Commun.*, **2007**, *37*, 2225.
[3] Heravi, M. M. Benmorad, T. Bakhtiari, K. Bamoharram, F. F. Oskooie, H. H. *Tetrahedron Lett.*, **2006**, *47*, 2507.
[4] Lalitha, A. Sivakumar, K. *Synth. Commun.*, **2008**, *38*, 1745.

DFT study of 1, 2-di substituted (amino, nitro, hydroxyl, thio, silyl) ethane and effects of hyperconjugation and …

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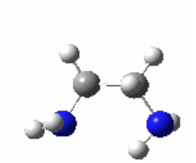
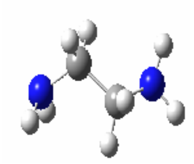
DFT calculation of 1,2-di haloethanes showed that for 1,2-di fluoro gauche conformer is favoured due to a C-H/C-F*hyperconjugation. But inothers trans form is favoured due to repulsion,hyperconjugation and electron delocalization [1].

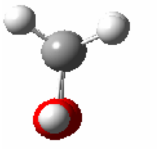
The intramolecular hydrogen bond is an important factor governing the conformational isomerism.In highly concentrated solution and neat liquid, intermolecular hydrogen. Bond takes place and favors the diaxial conformation in cyclic compounds [2].

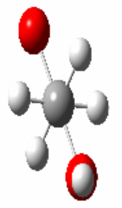
The gauche effect, a phenomenon responsible for the stability of structures having electronegative atoms in a gauche arrangement of an ethane fragment is an important factor to be considered in conformational analysis [3]. Recently, we reported the quantum chemical analysis of hydrazinoturns and the role of intramolecular hydrogen bond network in monomer of aza-β^3-peptide [4].

Now we study the effect of hyperconjugation,hydrogen bonding and steric effect on HF,DFT and MP2 calculation of 1,2-di amino ethane , 1-amino2-nitro ethane , 1,2-di hydroxyl ethane and 1,2-di thio ethane and 1,2-di silyl ethane.


MIN -NH2


MAX-NH2


MIN-OH


MAX-OH

References:

[1] R.souza, F.; P.freitas, M.; rittner, R. *J.Mol.Struc*. **2008**, 863, 137.
[2] J.duarte, C.; P.fretas, M. *J.Mol*.Struc **2009**, 930, 135.
[3] P.feritas, M.; rittner, R. *J.Mol.Struc*. **2007**, 807, 159.
[4] Dabbagh, H.A.; Rasti, E.; Le Grel, P.; Hocquet, A. *Tetrahedron*. **2010**, 66, 2322.

A new synthesis of Acylsilanes and Halovinylsilanes from α,β-epoxybis(silanes)

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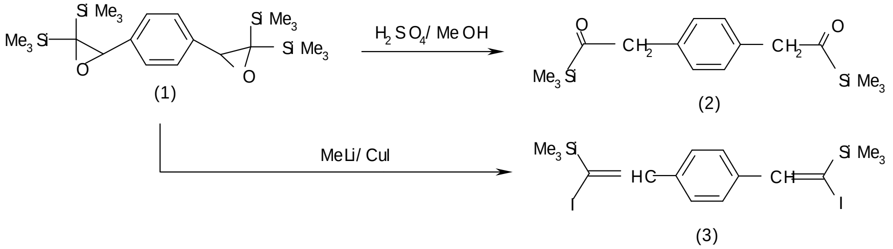
Epoxidation of vinylsilanes furnish α,β-epoxysilanes, a class of compounds of considerable interest to the organic chemists. The presence of trialkyle group provides regioselective control in the opening of epoxide by variety of nucleophiles. Epoxybis(silane) **1** was treated with H_2SO_4 (Conc.) in MeOH at room temperature and converted to the related acylsilane. This reaction may proceed by the protonation of the oxygen of epoxide, followed by a nucleophilic attack of MeOH on a trimethylsilyl group, inducing the trimethylsilylmethyl ether elimination, and generating the corresponding α-silyl enol. α-Silyl enol then converts to the related acylsilane **2**. The reaction of α,β-epoxysilanes with organocuprate reagents result in regiospecific opening of the epoxide ring to form β-hydroxyalkylsilanes. Surprisingly, in the reaction of epoxybis(silane) **1** with methylcopper reagent (MeLi/CuI 2:1), the iodovinylsilane **3** was the major product.



ZZ: EE= 98.3: 1.7%

References:

[1] Safa, K.D.; Paymard Samani, S.; Tofangdarzadeh, Sh.; Hassanpour, A. *J. Organomet. Chem.* **2008**, 693, 2004.

[2] Safa, K. D.; Hassanpour, A. and Tofangdarzadeh. Sh.; *J. Organomet. Chem.* **2008**. 693, 3622.

[3] Hreczycho, G.; Pawluc, P.; Marciniec, B.; *Synthesis* **2006**, 8, 1370.

[4] Hodgson, D.M.; Comina, P.J.; Drew, M.G.B.; *J. Chem. Soc., Perkin Trans. 1* **1997**, 2279.

Efficient synthesis of thiourazole derivatives via one pot tandem reaction

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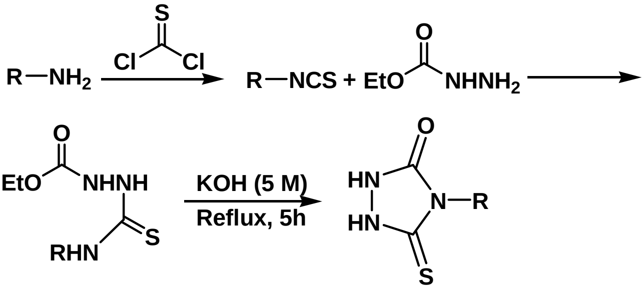
Combinatorial chemistry has emerged as an important component in the drug discovery program. Urazole derivatives are very interesting five-membered heterocyclic compounds, which at position 4 can provide a wide variety of aliphatic as well as aromatic constituents [1]. Urazoles were reported to possess herbicidal activity. A thiourazole compound, derived from its isourazole precursor after isomerization by glutathione Stransferase, also exhibited herbicidal activity [2].

In continuing of our studies in organic synthesis and synthetic methodologies [3-5], we decided to prepare a new series of thiourazoles. As depicted in Scheme 1, our approach involves the initial reaction of an amine with a thiophosgene to produce isothiocyanate. Then the resulting isothiocyanate reacted with ethyl carbazate, and the resultant intermediate is then refluxed to induce cyclization afford to thiourazole.



Scheme 1

References:

[1] Mallakpour, S. ; Rafiee, Z. *Synlett* **2007**, 1255.
[2] Shimizu, T.; Hashimoto, N.; Nakayama, I.; Nakao, T.; Mizutani, H.; Unai, T.; Yamaguchi, M.; Abe, H. *Plant Cell Physiol.* **1995**, *36*, 625.
[3] Ghorbani-Choghamarani, A.; Zeinivand, J. *J. Iran. Chem. Soc.* **2010**, *7*, 190.
[4] Ghorbani-Choghamarani, A.; Zolfigol, M. A.; Salehi, P.; Ghaemi, E.; Madrakian, E.; Nasr-Isfahanid, H.; Shahamirian, M. *Acta Chim. Slov.* **2008,** *55*, 644.
[5] Ghorbani-Choghamarani, A.; Zolfigol, M.A.; Ayazi-nasrabadi, R. *J. Braz. Chem. Soc.* **2010**, *21*, 33.

Amine synthesis with poly acids in preparation of fentanyl family

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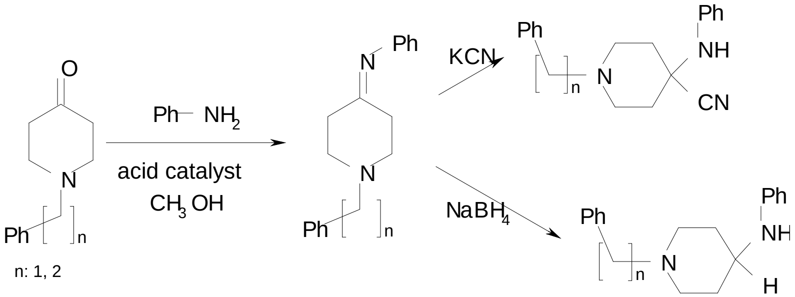
Fentanyl family are narcotic (opioid) pain medicines. fentanyl is currently the most widely used synthetic opioid in clinical practice, with several new improved delivery methods. In The preparation methods of them there is an amine intermediate. For amine synthesis, we convert Ketone to Imine (**step 1**) and then to Amine (**step 2**). **step 1** is promoted by varity of acids.

We carried out this reaction in presence of acidic catalysts such as PTSA[1] , Acetic acid [2] and poly acids: $H_3PW_{12}O_{40}$[3], $H_3PW_{12}O_{40}$ .SiO_2, Silica sulfuric acid (new methods).

Among them silica sulfuric acid has become an efficient catalyst for the clean and rapid reaction. In comprition with, this catalyst is industrial, frequently used and more available [4], [5].

Herein we report an efficient method for amine synthesis. ketone in methanol in the presence of acid forms Imine, then reaction with KCN and $NaBH_4$ produces amine in good yields and reaction duration.



References:

[1] Janssen, P.A.J. ; Van Daele, G.H.P. *US4179569*
[2] *Rubino, M.R. US2006/0100438*
[3] Heydari, A. ; Khaksar, S.; Akbari, J.; Esfandyari, M.; Pourayoubi، M.; Tajbakhshand M. *Tetrahedron lett.* **2007**, *48*, 1135.
[4] Salehi, P.; Zolfigol, M. A.; Shirini, F.; Baghbanzadeh, M. *Cur.Org.Chem.*, **2006**, 2171.
[5] Mojtahedi, M. M.; Abaee, M. S.; Abbasi, H. *J. Iran Chem.Soc.* **2006**, *3*, 93.

One pot synthesis of some new Amido and amino thioxanthone derivatives

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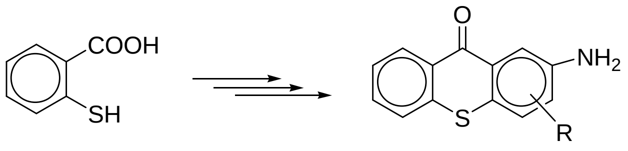
Thioxanthone and its derivatives are recognized as useful intermediates in the preparation of pharmaceuticals [1] and fine chemicals, which are useful as photoinitiators [2]. Thioxanthones are of particular interest as intermediates in the preparation of various drugs including: antitumor, antiparasitic, antifungal, antibacterial agents [1]. Photoinitiated polymerization finds industrial application in coatings for various materials, adhesives, printing inks, and photoresists [3].One method for the synthesis of the thioxanthone ring is a [6+0] cyclization of phenylthiobenzoic acids with concentrated sulfuric acid. Arur et al. prepared 2-nitrothioxanthone from 2-chloro-5-nitrobenzoic acid and thiophenol in two steps. 2-Aminothioxanthone prepared from 2-nitrothioxanthone is a starting material for the synthesis of 2-alkanamido and 2-benzamidothioxanthone [4] as a result 2-amidothioxanthones were prepared in four steps.

Herein we report the synthesis of some acetamido and amino thioxanthone derivatives in one step. The reaction of thiosalicylic acid (TSA) and Aniline derivatives in concentrated sulfuric acid affords a general and efficient pathway to prepare amido and amino thioxanthones.



R= OH, Me, OMe

References:

[1] (a) Hawking, F and Ross, W. F, *Brit. J. Pharm*. **1948**, *3,* 167. (b) Blair, D. M.; Hawking, F.; Meeser, C. V, and Ross, W. F. ibid, **1949**, *4,* 68. (c) Kikuth, W and Gonnert, R. *Ann. Trop. Med. Parasit*., **1949**, *42*, 256.

[2] Fouassier, J-P. and Lougnot, D-J. *J. Appl. Polym. Sci*. **1987,** *34,* 477.

[3] Aydin, M.; Arsu, N and Yagci, Y. *J. Marcromol. Commu*. **2003**, *24*, 718.

[4] Moon, J.-K.; Park, J.-W.; Lee, W.S.; Kang, Y.-J.; Chung, H.-A.; Shin, M.-S.; Yoon, Y.-J. and Park, K. H. *J. Heterocyclic Chem*. **1999**, *36, 793.*

Synthesis and characterization of novel poly (ether amide) imides in ionic liquids

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Amir Mohammad Gharekhani[c]

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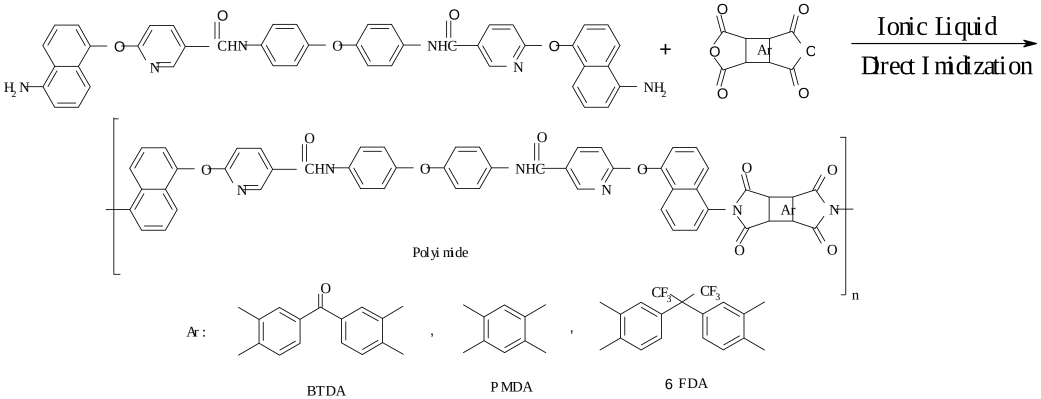
Applications of ionic liquids as green and polar media for different reactions have been reported. They are organic salts that are liquid at ambient temperatures. They are highly polar solvents that dissolve several organic and inorganic compounds and are non-volatile. Application of ILs as solvents for organic synthesis and polymerization facilities separation of the polymer, catalyst and also reduces the extent of side-reactions [1,2].

Here we wish to express the preparation of poly(ether imide)s from polycondensation of new diamine monomer with different dianhydrides using two different methods. A new diamine was prepared via reaction of 4,4'-oxyaniline (ODA) with 6-chloronicotinoyl chloride and subsequent reaction of this dichloro compound with 5-amino-1-naphthol. Thus the diamine was consisted of pyridine units, naphthalene moieties, ether groups, and amide structures. Polycondensation reactions of the prepared diamine with different types of dianhydrides using conventional and ionic liquid methods afforded different poly(ether imide)s with high thermal stability and improved solubility.



References:

[1] Vygodskii, Y. S.; Loziskaya, E. I.; Shaplov, A. S. *Macromol. Rapid Commun*. **2002**, *23*, 676.
[2] Yavari, I.; Kowsari, E. *Tetrahed. Lett.* **2007**, *48*, 3753.

A one-pot synthesis of functionalized 2,3-dihydrothiazoles from isothiocyanates, primary alkylamines and phenacyl bromides

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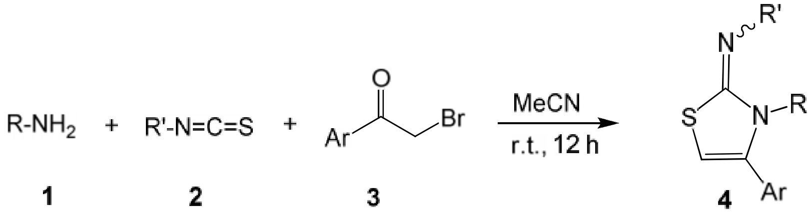
Thiazoles occupy a prominent position among heterocycles. In nature, the thiazolium ring is the chemically active center in the coenzyme derived from vitamin B_1 (thiamin). A large number of thiazoles obtained from microbial and marine origins exhibit important biological effects such as antitumor, antifungal, antibiotic, and antiviral activities [1]. Synthetic thiazoles have also been shown to exhibit a wide variety of biological activities [2], while others have found application as liquid crystals [3], and cosmetic sunscreens [4]. In view of the importance of thiazoles, several methods for their synthesis have been developed. The most widely used method is the Hantzsch synthesis [5–7] involving the reaction of *α*-halocarbonyl compounds with thioureas or thioamides.

We report an efficient procedure for direct synthesis of *N*-(4-aryl-3-alkylthiazol-2(3*H*)-ylidene)anilines and *N*-(4-aryl-3-alkylthiazol-2(3*H*)-ylidene)benzamides **4** from primary alkylamines **1**, isothiocyanates **2**, and α-bromoketones **3**, at r.t. This catalyst-free and one-pot synthetic method is facile; work up procedure is easy and gives pure target compounds.



References:

[1] Lewis, J. R. *Nat. Prod. Rep*., **1996**, *13*, 435.
[2] Metzger, J. V. *Thiazole and its Derivatives*; John Wiley & Sons: New York, **1979**.
[3] Kiryanov, A. A.; Sampson, P.; Seed, A. J. *J. Org. Chem*. **2002**, *66*, 7925.
[4] Bach, T.; Heuser, S. *Tetrahedron Lett*., **2000**, *41*, 1707.
[5] Hantzsch, A.; Weber, J. H. *Ber. Dtsch. Chem. Ges.* **1887,** *20*, 3118.
[6] Aguilar, E.; Meyers, A. I. *Tetrahedron Lett.* **1994**, *35*, 2473.
[7] Varma, R.S. *Pure Appl. Chem.* **2001**, *73*, 193.

Facile and convenient synthesis of 4,4' (arylmethylene) bis(1H-pyrazol-5-ols)catalyzed by $FeCl_3$

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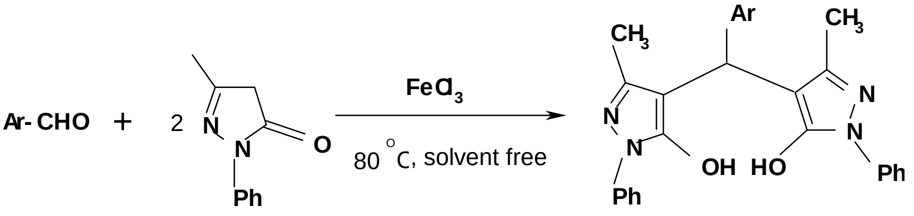
Corresponding Author E-mail:f. qassami@ gmail.com

Heterocylic compounds are considered as the most promising molecules for the design of new drugs [1].

Pyrazoles are an important class of bio-active drug targests in the pharmaceutical in dustry, as they are the core structure of numerous biologically active compounds [2]. Pyrazole derivatives are associated with wide spectrum of biological activities such as analgesic,anti pyretic and plant growt regulating [3].

Synthesis of 4,4' (arylmethylene) bis (1H-Pyrazol-5-ols) has been accomplished by tandem knoevenagel- Michael reaction of two equivalents of 3- methyl-1- phenyl- 2-pyrazoline-5-on with various aromatic aldehydes catalyzed by $Fecl_3$ in solvent free in shorter reaction time with 80-95% yelid [4].



References:

[1] Bocchetti, T. Gazz. *Chem. Ital.* **1961**, *91*, 866.
[2] Wang,W.; Wang, S.-X.; Qin,X.- Y.;Li. *J.- T. Synth.Commun*. **2005**, *35*, 1263.
[3] Desai Nc,Nayan Bhatt, Mukesh Kumar. *Indian J. Hetrocyclic Chem*. **2008**, *17*, 277.
[4] Niknam, K.; Saberi, D.; Sadegheyan, M.; Deris, A. *Tetrahedron lett.* **2010**, *51*, 692.

Facile and convenient synthesis of 4,4' (arylmethylene) bis(1H-pyrazol-5-ols) in the presence of silphox

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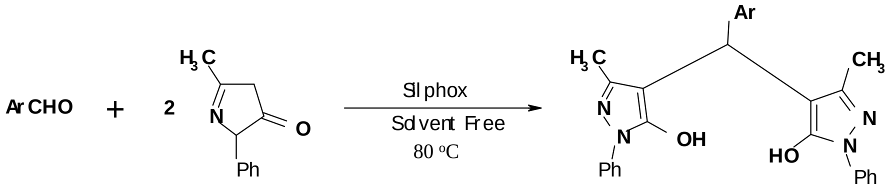
Heterocylic compounds are considered as the most promising molecules for the design of new drug. Pyrazoles are an important class of bio-active drug targests in the pharmaceutical in dustry, as they are the core structure of numerous biologically active compounds [1,2].Pyrazole derivatives are associated with wide spectrum of biological activities such as analgesic, anti- pyretic and plant growth regulating [3].

Synthesis of 4,4' (arylmethylene) bis (1H-Pyrazol-5-ols) has been accomplished by tandem knoevenagel- Michael reaction of two equivalents of 3- methyl-1- phenyl- 2-pyrazoline-5-on with various aromatic aldehydes catalyzed by silphox in solvent free with 75-95% yelid [4].



References:

[1] Stefan, S.L.; El-Behary, M.; Ramadan, A.A.; Mahaoud, *S.H. J. Chem. Res.*; *Miniprint*. **1992**, 1951.
[2] Bacchetti,T.; Gazz. *Chem. Ital*. **1961**, *91*, 866.
[3] Singh, D.;Singh, D. *J. Chem. Eng. Data*. **1984**, *29*,355-356
[4] Ahluwalia, V. k.; Sharma, P.; Goyal, B. *Indian J. Chem. Sect. B:org. chem. Incl. Med. Chem.* **1997,** *36*,1059.

Computational predictions and synthesis of molecular imprinted polymers with high selectivity for extraction of allopurinol

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*Corresponding Author E-mail: soheilaghassamipour@gmail.com

Molecular imprinted polymer (MIP) is a new kind of smart material, which has remarkable recognition properties for its template. The technology of molecular imprinting was put forward by Wulff and Sarhan in 1972 [1a] and has been developed quickly since 1993 when the MIP with the ophylline as template was reported by Mosbach and co-workers [1b]. Basically, MIPs are prepared by the polymerization of a suitable monomer and a cross-linker agent in the presence of a template molecule. After polymerization, the template is removed from the polymeric matrix leaving cavities complementary in size and shape to the template, and thus the resulting MIP is able to specifically rebind this molecule or related compounds from a complex mixture. Therefore, MIPs have been employed in those fields where a certain degree of selectivity is required such as catalysis [2a], solid-phase extraction [2b], sensors [2c] and chromatography [3,4].

Herein a computational approach was developed to screening functional monomers and polymerization solvents for rational design of High selective molecularly imprinted polymers (MIPs) for solid-phase extraction of allopurinol (ALP). Allopurinol is a drug used primarily to treat hyperuricemia (excess uric acid in blood plasma) and its complications, including chronic gout [5]. It was based on the comparison of the binding energy of the complexes between the template and functional monomers. The effect of the polymerization solvent was included using the polarizable continuum model. According to the theoretical calculation results, the MIP with allopurinol as template was prepared by precipitation polymerization method using acrylamide (AAM) as functional monomer and ethylene glycol dimethacrylate (EGDMA), as cross-linker in acetone. Having confirmed the results of computational method, three MIPs were synthesized with different functional monomers, i.e. acrylamide (AAM), methacrylic acid (MAA), and acrylonitrile (ACN), and then evaluated using Langmuir–Freundlich (LF) isotherm. The results of this study have indicated the possibility of using computer aided design for rational selection of functional monomers and solvents capable of extraction of allopurinol from biologic fluids.

References:

[1] (a) Wulff, G.; Sarhan, A. *Angew. Chem. Int. Ed. Engl.* **1972**, *11*, 341. (b) Vlatakis, G.; Andersson, L.I.; Muller, R.; Mosbach, K. *Nature*. 1993, *361*, 645.
[2] (a) Alexander, C.; Davidson, L.; Hayes, W. *Tetrahedron***, 2003**, *59*, 2025. (b) Masque, N.; Marce, R. M.; Borrull, Trends, F. *Anal. Chem*. 2001, *20*, 477. (c) Ye, L.; Haupt, K. *Anal. Bioanal. Chem.* **1887**, *378*, 1887.
[3] Sellergren, B. *J. Chromatogr. A*, **2001**, *906*, 227.
[4] Turiel, E.; Martin-Esteban, A. *Anal. Bioanal. Chem***. 2004**, *378*, 1876.
[5] Pacher P,; Nivorozhkin A,; Szabó C. *Pharmacol. Rev*. **2006**, 58 (1), 87.

Silica chloride: a reusable solid acid catalyst for the rapid synthesis of substituted benzimidazoles

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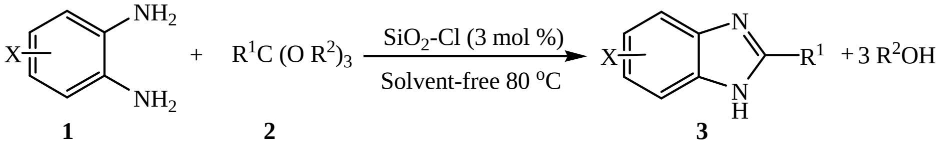
Among benz-fused azoles, benzimidazole and its derivatives as aromatic heterocyclic compounds are important class of bioactive molecules in the field of drugs and pharmaceuticals [1] because of their significant activity against several viruses in including HIV [2] and herpes (HSV-10) [3]. Due to their wide range of applications, these compounds have received a lot of attention to synthetic organic chemists and biologists in recent years.

In this synthetic procedure, benzimidazoles **3** can be synthesized efficiently and rapidly by treatmeant of 1,2-aryl diamines **1** with ortho esters **2** using silica chloride as a heterogeneous catalyst under solvent-free conditions. The present method has the advantages such as availability of starting materials, clean reaction without using organic solvents as media, simple work-up, reusability of the catalyst, cheapness, short reaction times and high yields of the products (Scheme).



R_1= H, Me,Et R_2= Me, Et

X= H, Cl, Me, NO_2

References:

[1] Valdez, J.; cedilla, R.; Herna'ndez-campos, A.; Ye'pez, L.; Herna'ndez-Luis, F.; Navarrete-va'zquez, G.; Tapia, A.; Corte's, R.; Hema'ndezc, M .; Castilloa, R. *Bioorg. med. Chem .Lett*. **2002**, *12*, 2221.

[2] (a) Porcari, A. R.; Devivar , R. V.; S.Kucera, L.; Drach, J. C.; Townsend, L. B. *J .Med . chem*. **1998**, *41*, 1252.; (b) Roth, M.; Morningstar, M. L.; Boyer, P. L.; Hughes, S. H.; Buckheit, R. W. *J. Med.Chem*. **1997**, *40,* 4199.

[3] Migawa, M. T.; Girardet, J.; Walker, J. A.; Koszalka , G. W.; Chamberlain, S. D.; Drach, J. C.; Townsend, L. B. *J. Med .Chem.* **1998**, 41, 1242.

Iron-catalyzed green and practical *N*-formylation of Amines under solvent free conditions

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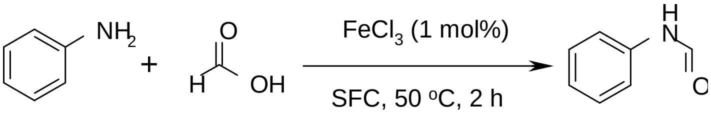
A lot of attention is currently being focused upon the replacement of volatile organic solvents by environmentally less hazardous ones or solvent free conditions. On the other hands, *N*-Formyl compounds have been widely used in organic synthesis as protecting group of amines, precursor for isocyanide preparation, an intermediate for mono methylated amines from primary amines, and catalyst for allylation or reduction. Thus a number of formylating methods have been reported.

An important part of our efforts towards an environmentally friendly green chemistry is aimed at reducing the use of organic solvents, in this paper, simple and practical N-formylation of primary and secondary, aromatic and aliphatic amines have been achieved in excellent yields by employing formic acid in the presence of very cheap and environmentally friendly iron catalyst under solvent free conditions.



References:

[1] Chen, F. M. F.; Benoiton, N. L. *Synthesis* **1979**, 709.
[2] Shekhar, A. C.; Kumar, A. R.; Sathaiah, G.; Paul, V. L.; Sridhar, M.; P. Rao, P. S. *Tetrahedron Lett.* **2009**, *50*, 7099.
[3] Das, B.; Krishnaiah, M.; Balasubramanyam, P.;Veeranjaneyulu, B.; Nandankumar, D. *Tetrahedron Lett.* **2008**, *49*, 2225.

A facile and efficient addition reaction of nitrogen-containing heterocyclic compounds with DMAD under neat conditions

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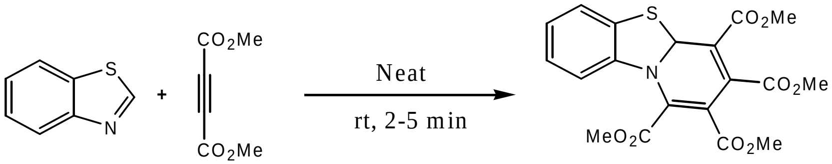
A simple and efficient method was developed for the reaction of dimethyl acetylenedicarboxylate (DMAD) with benzothiazole, isoquinoline, quinoline, 3-bromopyridine, pyridine and 5,6-dimethyl benzimidazole for the high yield synthesis of the related heterocyclic products (1-6) in very short reaction time under neat procedure. The reaction of isoquinoline, 3-bromopyridine and pyridine afforded to diastereomeric mixtures of products 2, 4 and 5 respectively. However, only one isomer of products 1, 3 and 6 were identified from the reaction of benzothiazole, quinoline and 5,6-dimethyl benzimidazole respectively. Benzotriazole afforded to product 7 under these conditions. For comparison, the reactions were examined in different reaction mediums and/or under microwave irradiation.



References:

[1] Acheson, R.M.; Plunkett, A.O. *J. Chem. Soc.* **1964**, 2676.
[2] Shaabani, A.; Rezayan, A.H.; Sarvary, A.; Khavasi, H.R. *Tetrahedron Lett.* **2008**, *49*, 1469.
[3] Adib, M.; Yavari, H.; Mollahosseini, M. *Tetrahedron Lett*. **2004**, *45*, 1803.

Computational predictions of enantioselectivity in asymmetric *N*-heterocyclic carbene-catalyzed intermolecular cross-benzoin condensations

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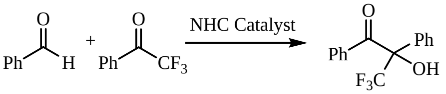
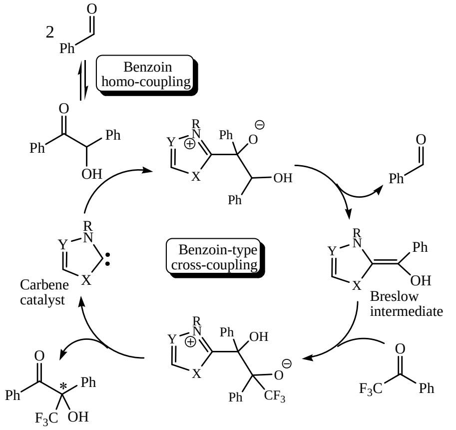
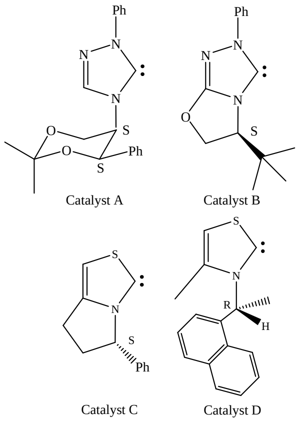
The formation of carbon–carbon bonds through reverse polarity, or umpolung, catalysis has provided an efficient, non-traditional route to many organic compounds. Recent developments in the field have extended reactions from the well known aldehyde coupling of the benzoin condensation, to coupling of ketones, alkenes and silyls [1]. In this work the catalytic asymmetric *N*-heterocyclic carbenes (NHC)-catalyzed intermolecular cross-benzoin condensations of benzaldehyde and trifluoroacetophenone are investigated Breslow mechanism [2], *via* computational methods.

We have studied four different known stereoselective benzoin condensations which involve the following four chairal catalysts, **A** to **D**. Transition-state geometries for stereoselective C–C bond formations are optimized at through B3LYP level of theory with 3–21G(d) basis set on all atoms with the Gaussian 98 [3]. The final transition-state energies are computed with single-point B3LYP/6-31G(d) calculations. Catalyst **A** is predicted to exert a higher enantioselectivity then **B**, **C**, and **D**.







References:
[1] Enders, D.; Niemeier, O.; Henseler, A. *Chem. Rev*. **2007**, *107*, 5606.
[2] Breslow, R. *J. Am. Chem. Soc.* **1958**, *80*, 3719.
[3] Frisch, M. J.; *et al*, Gaussian 98, Revision A.07, Gaussian, Inc., Wallingford CT, USA, 1998.

Superabsorbent hydrogel-silver nanocomposites based on sodium alginate and poly vinyl alcohol grafted with polyacrylamide

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In recent years there has been significant new interest in the development of metal nanosystems that have been considered as a novel class of materials for catalytic, electronic, and biomedical applications [1]. To stabilize and control the nanoparticles structures various surfactants, polymers, denderimers, biological templates, and biomacromolecules were used [2]. Hydrogels are networked structures of polymer chains cross-linked to each other. The swelling and shrinking properties exhibited by the hydrogel nanocomposites are currently being exploited in a number of applications including biosensors, drug delivery, and electronics [3]. Hydrogels have huge free space between the crosslinked networks in the swollen state that behaves as nano reactors for generating the nanoparticles [4].

In this work, a series of superabsorbent-silver nanocomposites based on sodium alginate and polyvinyl alcohol was synthesized via graft copolymerization of acrylamide (AAm) in aqueous medium using methylenebisacrylamide (MBA) as a crosslinking agent and ammonium persulfate (APS) as an initiator. The effects of reaction variables, such as MBA, AAm, and APS concentration as well as alginate/polyvinyl alcohol weight ratio on the water absorbency and the gel content of the superabsorbent were systematically optimized. Evidence of grafting was obtained by comparing the FT-IR and TG spectra of the initial substrates with that of the superabsorbent composite. Highly stable silver nanoparticles have been obtained with hydrogel networks as nanoreactors via in situ reduction of silver nitrate by using sodium borohydride as reducing agent. The formation of silver nanoparticles has been confirmed with scanning electron microscopy (SEM) and energy dispersive x-ray (EDX) analysis.

References:

[1] Thomas, V.; Yallapu, M. M.; Sreedhar, B.; Bajpai, S. K. *J. Colloid Interface Sci.* **2007**, *315*, 389.
[2] Vimala, K.; Samba Sivudu, k,; Murali Mohan, Y.; Sreedhar, B.; Mohana Raju, K. *Carbohydr.Polym.* **2009**, *75*, 463.
[3] Saravanan, P.; Padmanabha Raju, M.; Alam, S. Mater. Chem. Phys. **2007,** *103*, 278.
[4] Samba Sivudu, K.; Mallikarjuna Reddy, N.; Nagendra Prasad, M.; Mohana Raju, K.; Murali Mohan, Y.; Yadav, J.S.; Sabitha, G.; Shailaja. D. *J Mol Catal A: Chem,* **2008,** *295*, 10.

Palladium-Catalyzed direct cyanation of indoles through C-H bond activation

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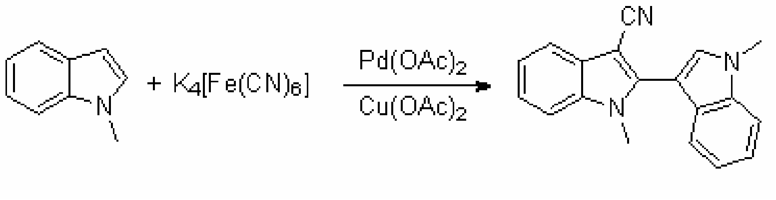
Aromatic nitriles are not only key components of numerous commercial compounds such as some natural products, pharmaceuticals, agrochemicals, pigments, and dyes, but also valuable in the installation of functional groups, such as aldehydes, ketones, amines, amidines, amide oximes, tetrazoles, oxazoles, thiazoles, oxazolidines, and carboxylic acid derivatives [1].

On the other hand, indoles and biindolyls are useful structural units that are frequently found in natural products, pharmaceuticals and functional materials. Transition-metal catalyzed selective and controllable C-H functionalization of indoles has been extensively studied in recent years [2].

As part of our current studies on the development of efficient methods for the preparation of heterocyclic compounds, herein, we report a palladium catalysis one-pot procedure for regioselective dimerization and cyanation of indoles through C-H bond activation. The reaction uses safe and nontoxic $K_4[Fe(CN)_6]$ as cyanating agent and selectively introduces a cyano group into the 3-position of biindolyls with high efficiency[3].



References:

[1] (a) Nagamura, S.; Kobayashi, E.; Gomi, K.; Saito, H. *Bioorg. Med. Chem.* **1996**, *4*, 1379. (b) Sundermeier, M.; Zapf, A.; Beller, M.; Sans, S. *Tetrahedron Lett.* **2001**, *42*, 6707. (c) Rappoport, Z. *The Chemistry of the Cyano Group*; Interscience Publishers: London, 1970.
[2] (a) Humphrey, G. R.; Kuethe, J. T. *Chem. Rev*. **2006**, *106*, 2875. (b) Bandini, M.; Eichholzer, A. *Angew. Chem., Int. Ed.* **2009**, *48*, 9608. (c) Yang, S. D.; Sun, C. L.; Fang, Z.; Li, B. J.; Li, Y. Z.; Shi, Z. J. *Angew. Chem., Int. Ed.* **2008**, *47*, 1473.
[3] (a) Schareina, T.; Zapf, A.; Beller, M. *Chem Commun.* **2004**, 1388. (b) DeBlase, C.; Leadbeater, N. E. *Tetrahedron* **2010**, *66*, 1098.

Ph_3P-Mediated synthesis of functionalized thioxo-1*H*-imidazoles and 2,5-dihydro-2-oxo-5,5-diaryl-1H-imidazols

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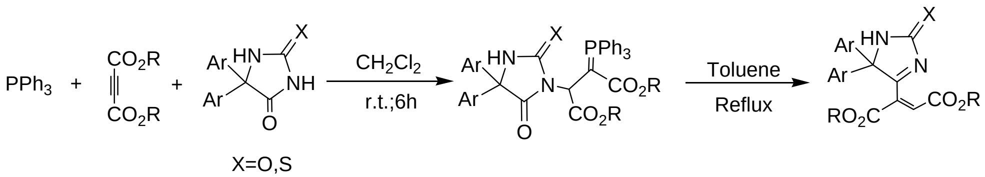
Thiohydantoins and their derivatives represent an important class of biologically active molecules having broad medicinal and agrochemical applications. Furthermore, many thiohydantoins are responsible for inhibition of fatty acid hydrolases, glycogen phosphorylases, amylases and serine proteases [1]. Phenytoin or 5,5-diphenylimidazolidine-2,4-dione is an anticonvulsant drug which can be useful in the treatment of epilepsy. The primary site of action appears to be the motor cortex, where spreading of the seizure activity is inhibited. Phenytoin is indicated for the control of grand mal and psychomotor seizures [2].

As part of our study on the development of new routes to heterocyclic and carbocyclic systems, we now report on the chemoselective synthesis of functionalized 2,5-dihydro-5,5-diaryl-2-thioxo-1*H*-imidazols. Thus, the reaction of thiohydantoins or hydantoins [3] and activated acetylenes in the presence of triphenylphosphine (Ph_3P) leads to phosphoranes, which undergo intramolecular Wittig reaction to produce dialkyl (E)-2-(2,5-dihydro-2-oxo-5,5-diaryl-1H-imidazol-4-yl)fumarate and dialkyl 2-(2,5-dihydro-2-oxo-5,5-diaryl-1H-imidazol-4-yl)fumarate in good yields.



References:
[1] Kumar, R.; Prem. S. C. M. *Tetrahedron Letters.* **2008**, 49, 5475.
[2] Safari, J.; Naeimi, H.; Ghanbari, M. M.; Sabzi-Fini, O. *Russ. J. Org. Chem.* **2009**, 45, 477.
[3] Yavari, I.; Zabarjad-Shiraz, N.; *Monats. Chem.* **2003**, 134, 445.

Synthesis and characterization of a new thermal stable poly (amide-imide) /cadmium hydroxide nanocomposite

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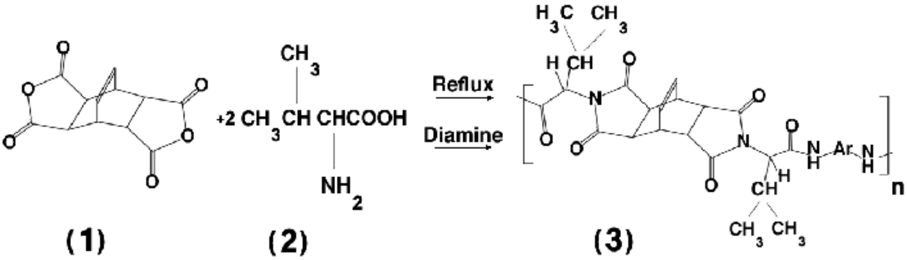
Poly(amide-imide)s are well known as a class of polymer with a good compromise between thermal stability and process capability [1]. The use of polymer composites has grown at a phenomenal rate since the 1960s, and these materials now have an impressive and diverse range of applications. Improving the fire retardant behavior of polymers is a major challenge for extending their use to most applications [2]. In this article, we describe synthesis and characterization of a new poly (amide-imide). Then the influence of inorganic phase on the thermal properties of PAI matrix was studied using thermogravimetry analysis.

N,N'-(Bicyclo[2,2,2]oct-7-ene-2,3,5,6-tetracarboxylic)-bis-L-valine diacid was synthesized by the condensation reaction of two equimolar of L-valine(2) with one equimolar of dianhydride (1) in acetic acid.

Poly (amide-imide) (3) was synthesized by solution polycondensation reaction of an equimolar mixture of monomer with aromatic diamine, as shown in Scheme. The structure of this polymer was confirmed by means of FT-IR spectroscopy and elemental analyses. Then cadmium hydroxide nanoparticles synthesised from hydrothermal recation [3] was added to PAI. The thermal stability of the PAI shifted towards higher temperature in the presence of the $Cd(OH)_2$ nanoparticles.



References:

[1] Ghosh, M. K.; Mittal, K. L. *Polyimides: fundamentals and applications*. **1996**, p, 49-70.
[2] Faghihi, K.; Shabanian, M.; Hajibeygi, M. *e-Polymers* **2009**, 142.
[3] Qu, P.; Yan, S.; Meng, H. *Solid State Science* **2010**, 12, 83.

The adsorption of the acetic acid on the graphite surface; DFT studies of chemical and physical adsorption

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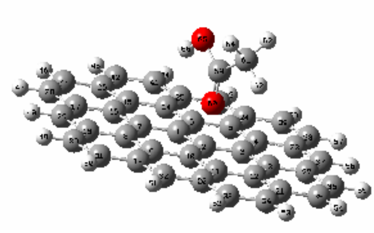
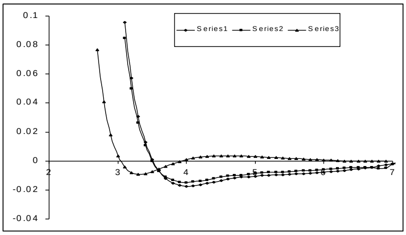
Experimental works on the interaction of acetic acid with graphite have been extensively studied in previous works [1-2]. Simulation works are scarce, and they have been carried out with semi-empirical and ab initio quantum chemical methods (with weaker basses set) [3]. Therefore we used higher accuracy method for our Computations to improve previous data.

Our Gaussian/ADF/B3LYP/6-31G calculations show that acetic acid interaction with graphite (closed-pack crystal structure) surface is mainly physical adsorption. Chemical adsorption can only appear when huge activation energy is provided. In order to observe chemical adsorption, acetic acid with spin multiplicity of the 3 and with an orientation to produce chemical bond is approached to the surface of the graphite and letting counter carbon atoms of the graphite to be flexible to change from sp^2 to sp^3 hybridizations. The same calculation with spin multiplicity of 1 is carried out to observe physical adsorption. Several orientations and approaches to the surface of graphite are performed. The effect inner layer of the graphite shows that the bond length C59 - C2 changes from mono-layer to di-layer from1.64332 to 1.63989 Ǻ.





References:

[1] Alessandra F. Freitas, Bruno B. França, Marisa F. Mendes, Gerson L.V. Coelho
[2] Anto´ nio Joa˜o Cruz, Joa˜o Pires, Ana P. Carvalho, and M. Brotas de Carvalho , *J. Chem. Eng. Data* **2004**, 49, 725.
[3] C. Mendoza, L.S. Rodrı´guez, F. Ruette, S. Schnell, *Surface Science* 602 (**2008**) 1053.

Synthesis and characterization of polyurethane/silica nanocomposites using tetrabutylammonium phthalimide-*N*-oxyl and tetraethylammonium 2-(carbamoyl)benzoate as efficient organocatalysts

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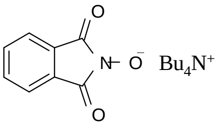
Polyurethane (PU) is one of the most versatile and useful engineering materials. By proper selection of reactants, the resulting PU can be used as rigid crystalline plastic, flexible elastomer, coatings, adhesives, leather, thermoplastic elastomers, and composites. They are prepared by polyaddition polymerization between polyisocyanates and polyols [1]. The Catalysis has been an important field for polyurethane chemistry and many improvements have been accomplished in recent years. The most important reaction between isocyanates is trimerization to form the isocyanurate ring. This heterocycle is thermally very stable and is used to enhance the physical properties of a wide variety of polyurethanes and other coating materials such as polyureas in commercial systems [2]. Polymeric blends of isocyanurates demonstrate increased thermal resistance, flame retardation, chemical resistance, and film-forming characteristics. Cyclotrimerization of isocyanates has been shown to be promoted by different catalytic systems. Furthermore, the sol–gel process is widely used for preparing silica-based organic–inorganic hybrid materials due to its mild reaction conditions and tunable structures of the hybrid materials [3].

We have recently introduced tetrabutylammonium phthalimide-*N*-oxyl (TBAPINO, **1**) [4] and tetraethylammonium 2-(carbamoyl)benzoate (TEACB, **2**) [5] as efficient and metal-free organocatalysts for cyanosilylation of carbonyl compounds and cyclotrimerization of isocyanates (**Figure 1**).



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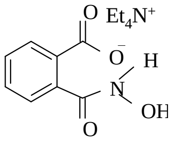

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Figure 1. The chemical structure of TBAPINO (**1**) and TEACB (**2**)

Furthermore, SiO_2 nanoparticles were prepared by a sol–gel process.Herein, we wish to report tetraethylammonium 2-(carbamoyl)benzoate as a new nucleophilic organocatalyst for preparation of the cross-linked PU/SiO_2 Nanocomposites. The PU/SiO_2 Nanocomposites were investigated by Fourier transform infrared spectra (FTIR), and atomic force microscopy (AFM).

References:

[1] Oprea,S.; Potolinca, O.*J. Mater Sci*. **2009**, *44*, 4181.
[2] Wegener, G.; Brandt, M.; Duda, L. *A: General*. **2001**, *221*, 303.
[3] Chen, C. Y.; Zhou, X. S. *J.Sol-Gel Sc. Technol* **2006**, *37*, 39.
[4] Dekamin, M. G.; Mokhtari, J.; Naimi-Jamal, M. R. *Catal. Commun*. **2009**, *10*, 582.
[5] Dekamin, M. G.; Sagheb-Asl, S. Naimi-Jamal, M. R. *Tetrahedron Lett*. **2009**, *50* ,4063.

Reductive methylation of primary and secondary amines and amino acids using $NaBH_4$ in 2, 2, 2- trifluoroethanol

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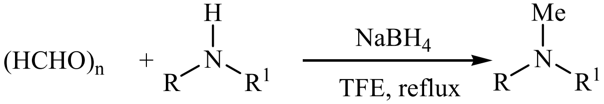
Tertiary amines are key structural elements in synthetic reagents and numerous biologically active natural products and pharmaceuticals like the clinically used antibiotic ciproflaxin which renders their synthesis an objective of high priority from the perspective of organic and medicinal chemistry [1]. *N,N*-dialkylated *α*-amino acids are very important compounds in biological chemistry [2] and they are ideal for the study of the effects that substituents and solvents have on the properties of *α*-amino acids.

In this work, we mainly studied the influence of TFE as a solvent in the reductive methylation reactions. In our initial experiments, in order to find the optimal reaction conditions, we have treated *N*-methyl aniline or phenylglycine (1 mmol) with paraformaldehyde (5 - 9 mmol) using $NaBH_4$ (2- 4mmol) in trifluoroethanol at reflux conditions. After completion of the reaction, products were formed in good to excellent yields. To test the generality of this reaction, a variety of primary and secondary aromatic and aliphatic amines and amino acids were reacted with paraformaldehyde under optimal reaction conditions and the corresponding secondary or tertiary amines and amino acids were obtained in good to excellent yields. One of the main advantages of this work is that, TFE can be recovered and reused in the subsequent reactions.



R, R^1= H, Aryl, Alkyl

Reference

[1] Menche, D.; Bohm, S.; Li, J.; Rudolph, S.; Zander, W. *Tetrahedron Letters* **2007**, *48*, 365.
[2] (a) White, A.; Handler, P.; Smith, E. L. *Principles of Biochemisrry*; McGraw Hill: New York, **1968**. (b) Bell, E. A. *FEBS. Lett.* **1976**, *64*, 29. (c) Mandava, N.; Anderson, J. D.; Dutky, S. R. *Photochemistry* **1974**, *13*, 2853.

A simple, clean and efficient three component synthesis of spirooxindoles with alum as a reusable catalyst

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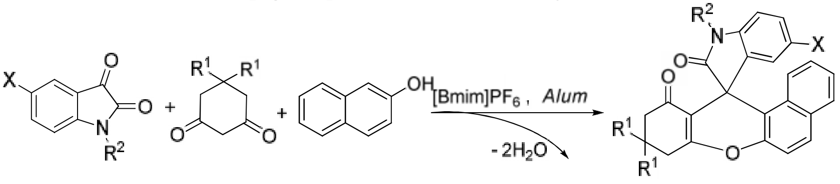
One-pot transformations, particularly multi-component reactions (MCRs) are of current interest to organic chemists. Since the first MCR reported in 1850 by Strecker, this methodology has emerged as an especially attractive synthetic strategy for rapid and efficient library generation due to the fact that the products are formed in a single step and diversity can be achieved simply by varying the reaction components. MCRs leading to interesting heterocyclic scaffolds are particularly useful for the creation of diverse chemical libraries of drug-like molecules for biological screening [1,2].

Ionic liquids (ILs) are a fascinating class of compounds with unique properties, which have recently attracted the attention of a wide number of researchers. Numerous works have been published in the last years reporting the possibility to perform several organic reactions and catalyzed processes in these media [3].

We have designed a three-component one-step synthesis of 9,10-dihydrospiro [benzo[a]xanthene-12,3'-indoline]-2',11(8H)-diones. For this, the use of $KAl(SO_4)_2.12H_2O$ (alum), which is relatively non-toxic and inexpensive, was at the centre of our study. In the course of our work on applications of $KAl(SO_4)_2.12H_2O$ in organic reactions, we have found that it is an effective promoter for the preparation of these compounds.

When a mixture of isatin, cyclohexane-1,3-dione and 2-naphtol in ionic liquid was stirred at 100 °C in the presence of a catalytic amount of alum, the reaction was completed in 30 min. Work-up gave products in excellent yields. (Scheme 1)



Schemes 1

References:

[1] Strecker, A. *Liebigs Ann. Chem*. **1850**, *75*, 27.
[2] Domling, A. *Curr. Opin. Chem. Biol*. **2002**, *6*, 306.
[3] Welton, T. Coord. *Chem Rew*. **2004**, *248*, 2459.

Zeolite encapsulated Heteropoly acid as an Efficient catalyst for sylilation of alcohols and phenols

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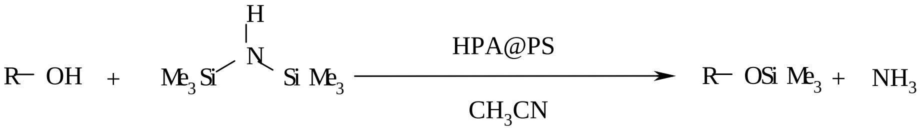
Functional group protection is the heart of multi-functional synthesis of target molecules. Protection of alcohols and phenols represents one of the most common steps. Protection of hydroxyl group as silyl ether is one of the most popular and widely used method. Many silylating agents have been used for the introduction of silyl group. The most common reagent for this purpose is 1,1,1,3,3,3-hexamethyldisilazane (HMDS) which is an inexpensive and commercially available reagent and gives ammonia as the sole by-product.

However, the low reactivity of HMDS is the main drawback of this reagent.Therefore, it is necessary to use a catalysts for activation of HMDS. In this study, a heteropoly acid encapsulated in zeolite has been used as an efficient catalyst for the silylation of hydroxyl groups. Different alcohols and phenols were silylated with HMDS in presense of this heterogeneous catalyst at room temperature with high yields (90-100%) and excellent selectivity. Substituted benzylic alcohols containing electron-donating and electron-withdrawing groups and also primary and secondary aliphatic alcohols were protected efficiently in short reaction times. The catalyst was recovered several times without loss of its catalytic activity.



$$R-OH + Me_3Si-N(H)-SiMe_3 \xrightarrow[CH_3CN]{HPA@PS} R-OSiMe_3 + NH_3$$

References:

[1] Wuts, P.G.M.; Greene, T.W., Green's Protective Groups in Organic Synthesis, 4thed., John Wiley & Sons, Hoboken, NJ, **2007**.

[2] Ghorbani-Vaghei, R.; Zolfigol, M.A.; Chegeny, M. Veisi, H., *Tetrahedron Lett*. **2006**, *47*, 4505.

[3] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, R. Shaibani, *J. Mol. Catal. A: Chem.*, **2004,** *219,* 73.

[4] M. Moghadam, S. Tangestaninejad, V. Mirkhani, R. Shaibani, *Tetrahedron* **2004,** *60,* 6105.

[5] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohammadpoor-Baltork, S.A. Taghavi, *J. Mol. Catal. A: Chem.* **2007,** *274,* 217.

Efficient method for the synthesis and characterization of novel Schiff bases and their complexes at room temperature conditions

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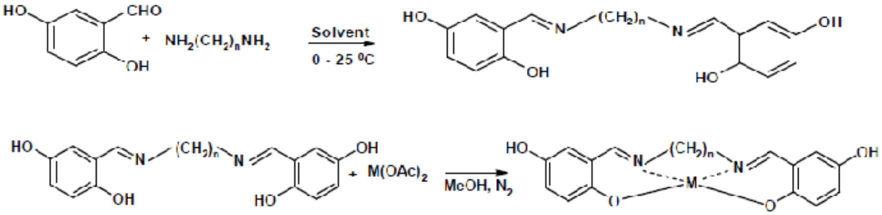
The condensation of primary amines with carbonyl compounds yields Schiff bases [1]. In the recent years, there has been considerable interest in the chemistry of transition metal complexes of Schiff bases [2]. This is due to the fact that Schiff bases offer opportunities for inducting substrate chirality, tuning the metal centered electronic factor, enhancing the solubility and stability of either homogeneous or heterogeneous catalysts [3, 4]. Schiff base complexes have been amongst the most widely studied coordination compounds in the past few years, since they are becoming increasingly important as biochemical, analytical and antimicrobial reagent [5]. The preparation of a new ligand was perhaps the most important step in the development of metal complexes which, exhibit unique properties and novel reactivity.

Schiff base ligands are easily synthesized and form complexes with almost all metal ions. Many Schiff base complexes show excellent catalytic activity in various reactions at high temperature and in the presence of moisture.

A considerable number of Schiff base complexes have potential biological interest, being used as biological models in understanding the structure of biomolecules and biological process [6].

In continuation of our research on the synthesis of Schiff bases and their complexes of metal ions, we have studied the preparation of complexes of these Schiff bases with transition metal ions under mild conditions. The corresponding complexes were characterized by spectroscopic and physical data.



References:

[1] Casellato, U.; Vigato, P.A. *Coord. Chem. Rev.* **1977**, *23*, 31.
[2] Murray, K.S. *Aust. J. Chem*. **1978**, *58*, 203.
[3] Opstal, T.; Verpoort, F. *Angew. Chem. Int. Ed.* **2003**, *42*, 2876.
[4] Tumer, M.; Koksal, H. *Trans. Met. Chem*. **1999**, *24*, 414.
[5] Kilic, A.; Tas, E.; Devereci, B. *Polyhedron*, **2007**, *26*, 4009.
[6] Chew, K. B.; Tarafder, M.T.H.; Crouse, K.A. *Polyhedron*, **2004**, *23*, 1385.

Fatty acid:A mild and efficient reusable catalyst for the one-pot synthesis of 1,2,4,5-tetrasubstituted imidazoles

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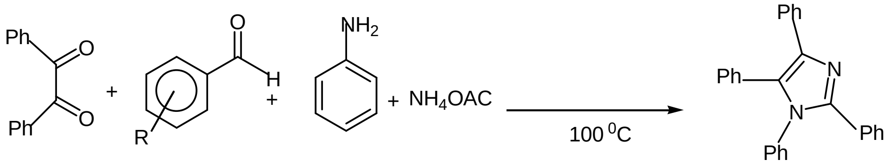
In the mainstream of current interest, multicomponent reactions permitted rapid access to combinatorial libraries of organic molecules for efficient lead structure identification and optimization in drug discovery [1]. One such reaction, which falls in this category was reported by Debus [2] in 1858, a reaction that pioneered a novel synthetic route to imidazole. Over the century, imidazoles have received significant attention due to their synthesis, reactions and biochemical properties. Imidazole derivatives have also been found to possess many pharmacological properties and are widely implicated in biochemical processes. The imidazole,being an active component in several drug molecules [3] (for eg. Losartan, Olmesartan, Eprosartan and Trifenagrel) and pesticides [4] has attracted attention in recent years.

The synthesis of 1,2,4,5-tetrasubstituted imidazoles are carried out by four-component condensation of a 1,2-diketone with an aldehyde, primary amine and ammonium acetate.

In continuation of our interest in methodology for the synthesis of tetrasubstituted imidazoles, herein we are pleased to report for the first time a novel, simple and efficient methodology for the synthesis of 1,2,4,5-tetrasubstituted imidazoles in good to excellent yields by four-component condensation of benzil or benzoin, aldehydes, amines and ammonium acetate using fatty acid as good catalytic media.



References:

[1] Weber, L.; Illgen, K.; Almstetter, M. *Synlett* .**1999**, 3, 366.
[2] Debus, H. .Liebigs *Ann. Chem.***1858**, 107, 199.
[3] Leister,C.; Wang,Y .; Zhao, Z.; Lindsley,C.V *Org. Lett*. **2004**,6, 1453.
[4] Maier,T.; Schmierer, H.; Bieringer, H.; Buerstell,H.; Sachse,B .*US Patent* 4820335 **1989.**

A greener rout for the one-pot synthesis of 1,2,4,5-tetrasubstituted imidazoles

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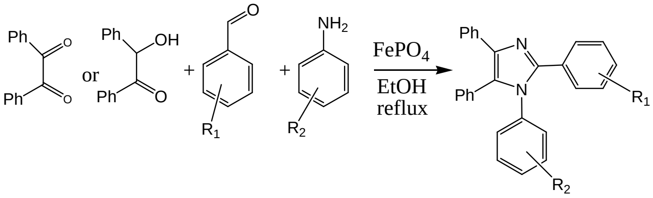
Imidazole derivatives are a very interesting class of heterocyclic compounds because they have many pharmacological properties and play important roles in biochemical processes [1, 2]. Many of the substituted imidazoles are known as inhibitors of P38 map kinase, fungicides and herbicides and therapeutic agents [3–5].

Herein, we have successfully developed an easy, green and efficient method to prepare a variety of tetrasubstituted imidazoles by four-component condensation of 1, 2-diketone/α-hydroxyketone aldehyde and primary amine in the presence of catalytic amount of $FePO_4$ refluxing ethanol (Scheme 1). The catalytic activity of $FePO_4$ is remarkable and the use of low cost, commercially available $FePO_4$ as catalyst for the synthesis of imidazoles in excellent yields is also significant under the aspect of environmentally benign processes.



Scheme 1

References:

[1] Lambardino, J.G.; Wiseman, E.H. *J. Med. Chem*. **1974**, *17*, 1182.
[2] Puratchikody, A.; Doble, M. *Bioorg. Med.Chem. Lett.* **2007**, *15*, 1083.
[3] Lee, J.C.; Laydon, J.T.; McDonnell, P.C.; Gallagher, T.F.; Kumar, S.; Green, D.; McNulty, D.; Blumenthal, M.; Heys, J.R.; Landvatter, S.W.; Strickler, J.E.; McLaughlin, M.M.; Siemens, I.R.; Fisher, S.M.; Livi, J.P.; White, J.R.; Adams, J.L.; Young, P.R. *Nature* **1994**, *372*,739.
[4] Maier, T.; Schmierer, R.; Bauer, K.; Bieringer, H.; Buerstell, H.; Sachse, B. *US Patent* **1989**,4820335.
[5] Heeres, J.; Backx, L.J.J.; Mostmans, J.H.; Cutsem, J.V. *J. Med. Chem.* **1979**, *22*, 1003.

Analysis and comparison of the chemical composition of the oils from individual aerial parts, gums and roots of Ferula gummosa

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Barijei is the famous name of the grassy plant from *Umbelliferae* family. The systematic name is *Ferula gummosa*, in Persian it is named to Bazard, Balinbo and Barijei [1], which is the permanent plant, monocarp with grayish- green leave, thick stem, yellow flowers and spread at an altitude of 1400-3200m from the sea [2].

Ferula gummosa is one of the most important plants in industrial and medicinal uses, so the gums of this plant exports to other countries as the important goods. In the folk medicine, this plant is used to improve cough, chronic bronchitis and as the anti hypertensive, there fore it can be offered to make the effective drugs by extracting of the compositions from the plant. This plant is also used to make invisible adhesive, dye, anti fungi and anti viruses [3]. Since there was dishonesty commercial composition of this plant in bazaar, as an example from Afghanistan, so we decided to collect individual aerial parts, gums (as two form pour and pile) and roots from the best natural growing in the highest altitude of Central Alborz.We obtained the oils by hydro distillation method (Clevenger type apparatus), and after drying over anhydrous $NaSO_4$, injected to GC/MS. In final, by comparing chromatograms of MS with our gathered library, the results showed terpenoids, aromatic compounds and cyclic hydrocarbons. Then we compared our results with others before published.

References:

[1] V. Mozaffarian, Farhang Names of Iranian Plants, Moaser Farhang, 5 Ed., 1386. K. Elizaii and H. Mahjoub. Identification of characterize of Barijei. Daftar Fanni Martaa 1386.
[2] A. Dehnavi. Study of compositions of the aerial parts of Barijei. Doctra thesis, Pharmacy College of Tehran University, 3845, 1376.

Synthesis of NMR Grade Deuterated Chloroform Using A New Catalyst for H/D Exchange

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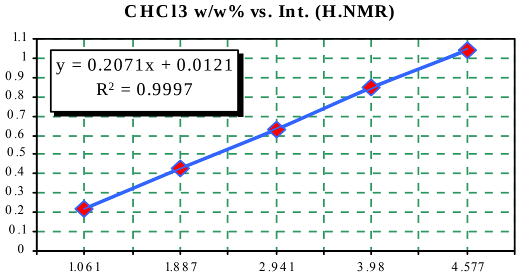
Deuterated chloroform is one of the most consumed and sometimes indispensable solvents for studies involving NMR spectroscopy and various synthesis methods have been reported [1-3].

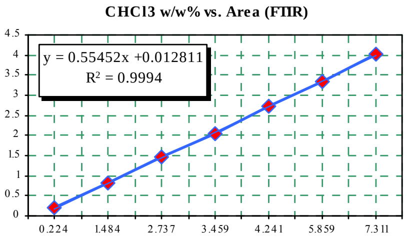
This work describes synthesis of NMR grade Chloroform-d by deuterium oxide as deuterium supply (from Arak Heavy Water Production Co.), sodium carbonate as base catalyst in trace amount at optimized temperature reaction, time reaction and system condition. The advantages of this method are trace impurities and fewer consumption of D_2O in comparison with other methods [4, 5] and to the best of our knowledge, such method has been not reported.

FTIR spectra of synthesized $CDCl_3$ didn't show any impurity in comparison with standard deuterated chloroform but NMR spectra showed two insignificant impurities. The impurities were distinguished by GC-MS analysis and in order to determination of these impurities; sample was analyzed by GC instrument. The impurities and their removing challenging are so important process.

Finally, the organic impurities were eliminated with fractional distillation that apparatus was assembled by special stainless steel packing.

Quantity of chloroform-d was certified by FTIR and NMR techniques and results were shown strong correlation between two analytical methods.





References:

[1] L. Pohl, W. Theysohn, R. Unger, United States Patent, 4026953, 1977.
[2] V. M. Molina, V. Montiel, M. Dominguez, A. Aldaz, *Electrochemistry Communications*, 5, **2003**, 246.
[3] T. Junk, W. J. Catallo, *Chemical society reviews*, **1997**, 26, 401-406.
[4] M. Nakahara, H. Enomoto, A. Kishita, K. Tsuda, T. Tennoh, E. Fujita, United States Patent, 5733984, 1998.
[5] H. J. Kock, Canadian Patent, 1085423.

Polymerization of carbazole under microwave irradiation

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Conducting polymers such as poly N-Methyl Pyrrole and polycarbazole have been widely investigated because of their unique properties such as electronic and optical properties, environmental stability and photoluminescence. They have also been used in the fabrication of many devices like field diodes, chemical sensors, biosensors and smart materials [1-2].

One of applications for microwave irradiation (MW) is in polymer synthesis. MW can be applied for radical polymerization, step-growth polymerization, ring-opening polymerization, polymer modification, and so on [3-4].

In this research work a new method for polymerization of carbazole using under microwave irradiation will be reported [5].

The effect of various parameters such as microwave power, oxidant, reaction times and solvent has been studied. In the above condition change in power of microwave irradiation can be cause the increasing of the degree of polymerization and_molecular weight of polymers.

The results indicate that the obtained polymer have not a considerable heat resistant and conductivity in compared with conventional heating and electric field process. However reactions under MW have the higher reaction rate and better yield within a shorter period of time. The structure of products was evaluated by IR, SEM and by thermogravimetry (TG) and differential thermal analysis (DTA) techniques.

References:

[1] Entezami A.; Hosseini S.H. *European Polymer Journal*, **1995**, 31 (7), 635.
[2] Sharma, A. L. Saxena, V. Annapoorni, S. Malhotra, B. D. *J. Appl. Polym. Sci.* **2001**, *81*, 1460.
[3] Bogdal, D. Penczek, P. Pielichowski, J. Prociak, A. *Adv. Polym. Sci.*, **2003,** *163*, 193.
[4] Huixia W. *Polymer Engineering and Science*. **2010**.
[5] Bogdal, D. Prociak, A. **2007**, Microwave-Enhanced Polymer Chmistery and Technology, 2121 State Avenue, Ames, Iowa 50014, USA, 3, 58.

PPA/SiO_2 an efficient heterogeneous catalyst for synthesis of coumarins via Pechmann condensation in solvent-free conditions

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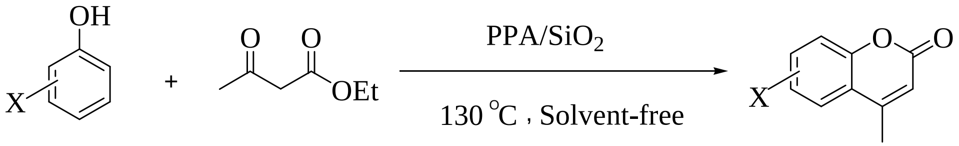
The synthesis of coumarins and their derivatives has attracted considerable attention from organic and medicinal chemists because they are widely used as additives in food, performs [1] , also act as intermediates for the synthesis of chromenes, coumarones and 2-acylresorsinols [2].

A Pechmann condensations is one of the most common procedures for the preparation of coumarins and its derivatives.this method involves the reactions between a phenol and β-keto ester in the presense of acidic catalyst. Several acid catalyst have been used in the von Pechmann reaction including such as H_2SO_4, HCl, $POCl_3$ [3].

Herein we report as the substituted phenols and ethyl acetoacetate undergo condensation in the presence of heterogeneous PPA/SiO_2 (Polyphosphoric acid adsorbed silica gel) catalyst under solvent-free conditions to produce the coumarins (scheme).



X=3-OH, 4-OH, 2,3-OH, 4-MeO, 2,3MeO, ...

scheme

PPA/SiO_2 was prepared by previously method [4].The experimental procedure is simple and involves mixing the phenol and ethyl acetoacetate in presence of PPA/SiO_2 under solvent free conditions and 130 °C temperature.A wide of substituted phenols underwent smooth reaction to give corresponding coumarins in excellent yield with good purity.

References:

[1] Kennedy, R.O.; Thornes, R.D. Coumarins: Biology, Applications and Mode of Action, John and Sons: Chichester. **1997.**

[2] Mitra, A.K.; De, A.; Karchaudhuri, N.; Misra, S.K.; Mulkopadhyay, A.K**.** *J. Indian Chem. Soc* . **1998**, *75*, 666.

[3] Sethna, S.; Phadke, R. *Org. React*. **1953**, *1*.

[4] Takido, T.; Kodomori, M. *Synlett*. **2004**, *13*, 2307.

Utilizing commercial bleaches in the presence of $NiCl_2$ for the catalytic Baeyer–Villiger oxidation of cyclic ketones

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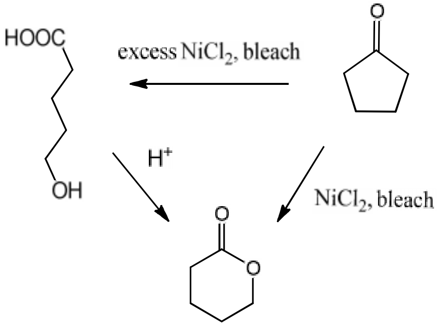
The Baeyer–Villiger (B–V) reaction has been widely employed in organic synthesis by virtue of the unique transformation. An oxygen atom can be inserted into a carbon–carbon single bond by an oxidant [1]. The Baeyer–Villiger reaction has become an immensely important reaction in organic chemistry because the lactones or esters are important industrial intermediates in the production of polymers, agrochemicals, pharmaceuticals and herbicides [2–4].

The efficient, green, facile, mild and straightforward conversion procedure for the oxidation of cyclic ketones to lactones at room temperature utilizing commercial bleaches in the presence of NiCl2 for the catalytic Baeyer–Villiger oxidation of cyclic ketones are reported with high yields (70-95%) and high purities in this seminar.

This reaction is chemoselective while the reaction preformed in the presence of excess catalyst. In this circumstance the glutaric acid is a sole product with almost 100% yield conversion.



References:

[1] Baeyer, A.; Villiger, V. *Ber. Dtsch. Chem. Ges.* **1899**, 32, 3625.
[2] Krow, G. C.; *Org. React*. **1993**, *43*, 251.
[3] Hassall,C. H. *Org. React*. **1957**, 9, 73.
[4] Bolm, C., Adv. Catal. Process. **1997**, 2, 43.

A simple procedure for synthesis of optically active 1,2-bis *s*-triazolothiadiazole derivatives containing L-amino acid moieties

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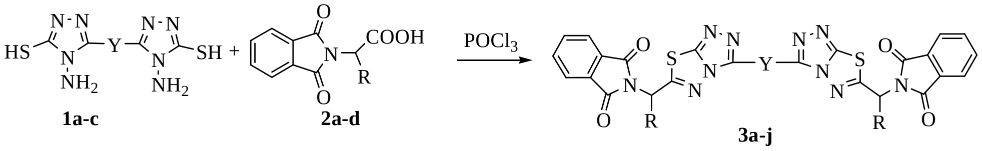
Bis heterocyclic compounds exhibit various biological activities [1]. Heterocycles bearing a triazole or 1,3,4-thiadiazole moiety are reported to show biological properties such as Antinociceptive.and antimycotic, activities [2].

Prompted by these observations, as part of our research program aimed at developing heterocycle derivatives containing 1,2,4-triazole and optically active compounds [3,4], we report the synthesis of some new 3,6-disubstituted 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles containing L-amino acid.

This paper describes a facile one step synthesis of bis triazolothiadiazole derivatives **3** via reaction between one mole of bis amino triazole with aliphatic acids. Compounds **1a–c** was converted to *s*-triazolothiadiazoles **3a–j** through one pot reaction by condensation with *N*-phthaloyl-L-amino acids **2a–d** in the presence of $POCl_3$ as outlined in Scheme.



References:

[1] Jayashankara, B.; Lokanatha K. M. *E-J. Chem.* **2008**, *5*, 309.
[2] Onkol, T.; Cakir, B.; Sahin, M. F. *Turk. J. Chem.* **2004**, 28, 461.
[3] Foroughifar, N.; Mobinikhaledi, A.; Ebrahimi, S.; Bodaghi Fard, M. A.; Moghanian, M. *J. Chin. Chem. Soc.* **2009**, *56*, 1043.
[4] Foroughifar, N.; Mobinikhaledi, A.; Khanpour, M.; Ebrahimi, S.; *Eur. J. Chem.* **2010**, *1*, 33.

Copper oxide nanoparticles as efficient nanocatalyst for the rapid and green synthesis of 3,4-dihydropyrano[c]chromenes

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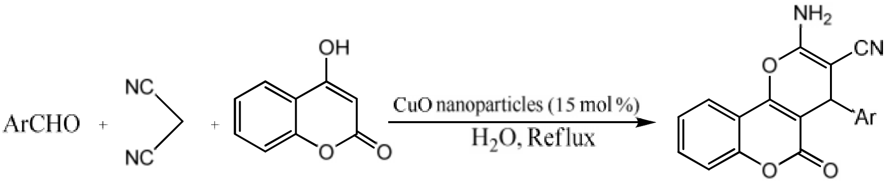
The application of copper oxide nanoparticles for organic reactions has attracted immense attention in recent years [1]. Because this class of catalysts appears as one of the most promising solutions toward efficient reactions under mild and environmentally benign conditions in the context of green chemistry [2, 3].

Therefore, we decided to use nanosized copper oxide as catalyst for preparation of 3,4-dihydropyrano[c]chromenes by three-component condensation of aromatic aldehydes, malononitrile and 4-hydroxycoumarin in water as reaction medium (Scheme 1).



Scheme 1.

Copper oxide nanoparticles were characterized by X-Ray diffraction (XRD), scanning electron microscopy (SEM), IR spectroscopy, thermal gravimetry analysis and differential thermal analysis (TGA/DTA).

In conclusion, we have reported an efficient procedure for the synthesis of 3,4-dihyropyrano[c]chromenes using CuO nanoparticles as a non-toxic and inexpensive heterogeneous nanocatalyst. The major advantage of this method is the ease of the work-up; i.e., clean reaction, high yields of products and very short reaction times, which make it a useful and attractive strategy for the synthesis of 3,4-dihyropyrano[c]chromenes.

References:

[1] Kantam, M. L.; Laha, S.; Yadav, J.; Bhargava, S. *Tetrahedron Lett.* **2008**, *49*, 3083.
[2] Astruc, D. *Inorg. Chem.* **2007**, *46*, 1884.
[3] Lu, F.; Ruiz, J. A.; Astruc, D. *Angew. Chem., Int. Ed.* **2005**, *44*, 7399.

A simple and improved regioselective brominations of aromatic compounds using *o*-xylylenebis (triphenylphosphonium) peroxodisulfate

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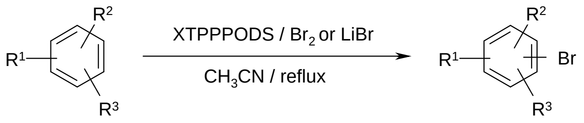
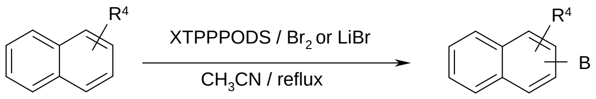
Direct bromination of wide range of aromatic compounds substituted with electron donating groups such as methoxy, hydroxy, or amino functionality have been achieved with high regioselectivity in the reaction with Br_2 in the presence of *o*-xylylenebis (triphenylphosphonium) Peroxodisulfate (OXPPPODS) under mild conditions in acetonitrile . The use of lithium bromide as a bromination reagent afforded high yields of monobromo compounds with complete regioselectivity under neutral and mild reaction conditions in acetonitrile at reflux temprature.



R^1, R^2, R^3 = H, OH, OMe, Cl, NO_2, CH_3, $N(CH_3)_2$, COOH



R^4 = OH, OMe

References:
[1] M. Y. Park, S. G. Yang, V. Jadhav, Y. H. Kim, *Tetrahedron Lett*. **2004,** *45,* 4887.
[2] H. Tajik, I. Mohammadpoor-Baltork, J. Albadi, *Synth. Commun.* **2007,** *37,* 323.
[3] Q. H. Chen, F. P. Wang, *Chin. Chem. Lett.* **2001,** *12,* 421.

Synthesis of nonlinear optical polymer

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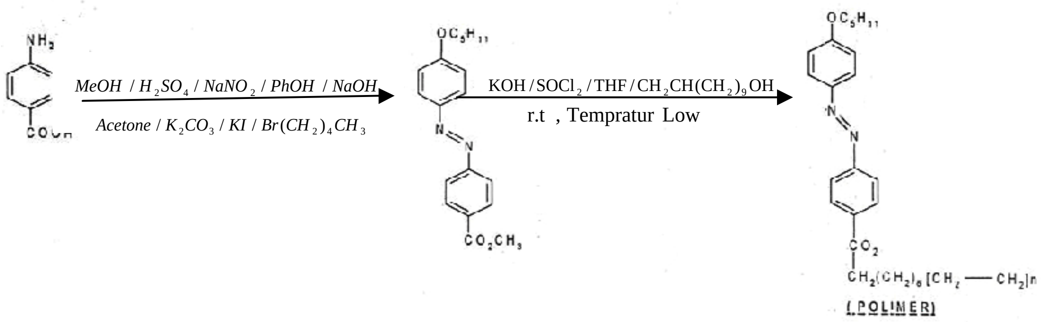
Azo aromatic compounds are highly colored & stable and are produced by very cheap raw materials. That's why they have been used for more than a century [1].
By Aromatic Amin (cold solution) type 1 (0-5^{0}C) reacting in Acid Aqueous (HCl or H_2SO_4) with sodium Nitrite, $ArN_2^+x^-$ salt is produced which are highly active compounds and serve as a medium in producing various kinds of aromatic structures [2].

Diazinium ions are weak electrophiles which react with highly reactive aromatic compounds such as phenols and produce Azo compounds, known as Azo coupling process [3].
Azo NLO polymere from 4- Amino Benzoic Acid found by reflux, distillation & centrifugation monomer is obtained by common salts & alcohole (CH_2=CH(CH_2)$_9$OH)

This polymer's being cheap is an advantage. Also NLO polymer has rapid reaction time & optical activity threshold which made it attractive & is used in electronic nose & telecommunication network & etc.



References:

[1] T.W. Solomons. **1996**, 130.

[2] Norman, L.; Allinger; Michael, P.; Cava; Donc. Dejongh. Carl, R.; Johnson. Norman, A.; ebel. Calvin, L.; *stevens.org. chem*. **1979**, 432.

[3] Cary. Francis, A.; sundberg, J.; *Advanced. Org. chem*. (partA). **2001**, 587.

Salicylaldehyde Schiff base complex grafted with poly vinyl amine/SBA-15 composite: preparation and application for oxidation of alcohols

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Organic–inorganic hybridizing materials, especially the composites consisting of nano-inorganic particles and polymer resin, have received considerable attention recently due to the resultant materials are supposed to have better mechanical and/or thermal properties [1].

On the other hand, a novel porous material, i. e. mesoporous molecular sieve has attracted a great deal of interests for its particular characteristics such as large internal surface area, uniform framework and easily controlled pore diameter. Thus some of their application including catalysts, sorbent, and separating materials are expected. Furthermore, several researchers published finding on the host–guest polymerization of organic molecules in such inorganic mesoporous materials [2]. Incorporation of metals and metal complexes in polymers occur by coordination interactions [3].

In this study, poly(acryl amide)/mesoporous SBA-15 (PAA/SBA-15) composite were prepared by in–situ polymerization within the nano-channels of SBA-15 and through the Hoffman reaction, poly(vinyl amine)/mesoporous SBA-15 (PVAm/SBA-15) were obtained. This composite developed by incorporation of salicylaldehyde Schiff base complex in poly(vinyl amine) and applied as an efficient heterogeneous catalyst for selective oxidation of alcohols in the presrnce of tert-butylhydro peroxide. The structural feature of composite was studied by FT-IR, XRD, SEM, TG and BET techniques.

Schiff base complexes of manganese(II), cobalt(II), chromium(II) were tested for their activity in the oxidation of alcohol to aldehyde. The reaction was catalyzed more successfully with Schiff base complexes of manganese(II) ions than other Schiff base complexes. The effect of mole ratio of salicylaldehyde, metal ion and amount of mesoporous molecular sieve for synthesis of catalyst was studied. Also, the effects of solvent, reaction temperature, amount of catalyst in the reaction were investigated. The reaction performed in the acetonitrile solvent and the product obtained in high yield (100 %) after a simple work-up.

References:

[1] Run, M.T.; Wu, S.Z.; Zhang, D.Y.; Wu, G. *Mater. Chem. Phys.* **2007**,*105,* 341.
[2] Li, X.F.; Guan, W.C.; Yan, H.B. Huang, L. *Mater. Chem. Phys.***2004**, *88,* 53.
[3] Kickelbick, Guido. *Prog. Polym. Sci.***2003**, *28*, 83.

Solvent-free one-pot synthesis of 2-aryl-1-arylmethyl-1*H*-1,3-benzimidazoles using MFR-H$^+$

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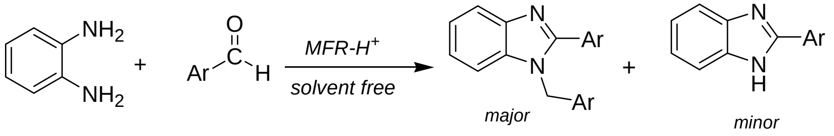
The benzimidazole nucleus is of significant important to medicinal chemistry [1]. The traditional synthesis of benzimidazoles involves the reaction between an *O*-phenylendiamine and carboxylic acids or their derivatives (nitriles, amide, orthoesters) under harsh dehydrating conditions [2]. Another method for the synthesis of these compounds is the reaction of *O*-phenylendiamine with aldehydes in the presence of acidic catalysts under various reaction conditions [3].

Solvent-free synthesis of organic molecules has merged with medicinal chemistry in the last few years as a powerful method for time-and labor-efficient generation of both lead discovery and lead optimization libraries [4].

In this work, we have applied one pot, efficient and simple procedure for the synthesis of 2-aryl-1-methyl-1*H*-1, 3-benzimidazole derivatives using protonated melamine formaldehyde resin (MFR-H$^+$) under solvent free conditions. The ease of products purification by simple filtration and crystallization and reusability of catalyst suggest a favorable prospect for the applicability of this process.



References:

[1] Zhu, Z.; Lippa, B.; Drach, J. C.; Townsend, L. b. *J. Med. Chem,* **2000,** *43*, 2430.
[2] Dudd, L. M.; Vanderdou, E.; Garcia-Verdugo, Licence, P.; Blake, A. J.; Wilson, C.; Poliakoff, M. *Green Chem***. 2003**, *5*, 187.
[3] Perumal, S.; Mariappan, S.; Selvaraj, S. *Arkivoc*, **2004**, *8,* 46.
[4] Ouyang, X.; Tamayo, N.; Kiselyov, A. S. *Tetrahedron*, **1999**, *55,* 2827.

Gold nanoparticles stabilized in periodic mesoporous organosilicas as efficient catalyst for aerobic oxidation of alcohols

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The selective oxidation of alcohols to carbonyl compounds is one of the most important process [1]. However, due to the stringent environmental standards and economical pressures, many attentions have been recently directed toward the use of transition-metal catalysts to achieve effective oxidation of alcohols with molecular oxygen as terminal oxidant [2], [3]. In view of the fact that the heterogeneous transition metal based catalysts have been shown acceptable results in the aerobic oxidation of alcohols, such as pd supported hydroxyapatite Pd (HAP) [4], Ru (HAP) [5], Pd-SBA-15 [6], Ru-Al_2O_3 [7], Au/CeO_2 [8], Au-Pd/TiO_2 [9], Au/$Ga_3Al_3O_9$ [10], Au-Pd/PVP [11], PI-Au [12], PI-Au-Pt [13], Si-BOX-Pd [14]. Among them, gold nanoparticles have paying attention considerable interest because of their extraordinarily high activity and selectivity [15].

Along this line, we prepared gold nanoparticles stabilized in a bifunctional periodic mesoporous organosilica, which was found to be an efficient catalyst system for the aerobic oxidation of various types of alcohols into their corresponding aldehydes and ketones.

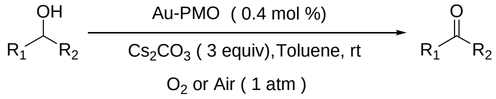

Figure 1. Reaction condition

This method is highly selective for oxidation of primary benzylic alcohols to their aldehydes and no over oxidation to the corresponding carboxylic acids were observed even after prolonged reaction times, a feature at least rarely observed with the previous heterogeneous gold catalysts.

This method was also applicable to the oxidation of secondary aromatic alcohols to afford the corresponding ketones in quantitive yields. Straight chain and cyclic secondary aliphatic alcohols were oxidized efficiently to afford the corresponding carbonyl compounds in high yields. It was also noted that the alcohols that contained heteroatoms could be oxidized in moderate yields. The catalyst was used for seven times and exhibited consisted catalytic activity for the aerobic oxidation of benzyl alcohol without further purification and/or reactivation.

References:

[1] M.Hudlicky, Oxidation in Organic Chemistry, ACS Monograph Series; American Chemical Scociety, Washington DC, 1990.
[2] J.-E.Bäckvall, *Modern Oxidation Methods*, Wiley-VCH, Weinheim, **2004.**
[3] Y. M. A.Yamada, T.Arakawa, H.Hocke, Y.Uozumi, *Angew. Chem. Int. Ed.* **2007**, *46*, 704.
[4] K. Mori, K.Yamaguchi, T.Hara, T.Mizugaki, K. Ebitani and K. Kaneda, *J. Am. Chem. Soc.* 2002, **124**, 11572.
[5] K. Yamaguchi, K. Mori, T. Mizugaki, K. Ebitani and K. Kaneda, *J. Am. Chem. Soc.* 2000, **122**, 7144.
[6] B. Karimi, S. Abedi, J. H. Clark and V. Budarin, *Angew. Chem. Int. Ed.* 2006, **45**, 4776.
[7] K. Yamaguchi and N. Mizuno, *Angew. Chem. Int. Ed.* 2002, **41**, 4538.
[8] A. Abad, P. Conception, A. Corma and H. García, *Angew. Chem. Int. Ed.* 2005, **44**, 4066.
[9] D. I. Enache, J. K. Edwards, P. London, B. Solsona-Espriu, A. F. Carley, A. A. Herzing, M. Watanabe, C. J. Kiely, D.W. Knight and G. J. Hutchings, *Science* 2006, **311**, 362.
[10] F. Z. Su, Y.M. Liu, L. C. Wang, Y. Cao, H. Y. He and K. N. Fan, *Angew. Chem. Int. Ed.* 2008, **47**, 334.
[11] W. Hou, N. A. Dehm and R. W. J. Scott, *J. Catal.* 2008, **253**, 22.
[12] H. Miyamura, R. Matsubara, Y. Miyazaki and S. Kobayashi, *Angew. Chem. Int. Ed.* **2007**, *46*, 4151.
[13] H. Miyamura, R. Matsubara, S. Kobayashi, *Chem. Commun.*, **2008**, 2031.
[14] L.-C. Wang, Y.-M. Liu, M. Chen, Y. Cao, H.-Y. He and K.-N. Fan, *J. Phys. Chem. C* **2008**, *112*, 6981.
[15] G. C. Bond, D. T. Thompson, *Catal. Rev. Eng.* **1999**, *41*, 319.

Chemical composition of the essential oil of Mentha Longifolia and a simple QSRR model for prediction of retention indices by multiple linear regression

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Herbs and spices are invaluable resources, useful in daily life as food additives, flavours, fragrances, pharmaceuticals, colours or directly in medicine. This use of plants has a long history all over the world, and over the centuries, humanity developed better methods for the extraction of essential oils from such materials. Essential oils are complex mixtures of volatile substances generally present at low concentrations. Before such substances can be analyzed, they have to be extracted from the matrix. The chemical composition of the essential oil extracted by hydrodistillation (HD), head-space solid phase microextraction (HS-SPME) and solvent-free microwave extraction (SFME) from the aerial parts of Mentha Longifolia were analyzed by employing GC-MS. The main components of this oil were piperitenone oxide (30.2%, 42.6%, 38.3%), piperitone epoxide (20.4%, 12.33%, 35.2%) and caryophyllene (5.9%, 4.3%, 0.7%) which isolated by HD, HS-SPME and SFME, respectively. Then quantitative structure-retention relationship (QSRR) study for prediction of retention indices of essential oil compounds were developed by application of the structural descriptors and multiple linear regression (MLR) method. A simple model with low standard errors and high correlation coefficients was selected. This model, with high statistical significance could be used adequately for the prediction and description of the retention indices of essential oil compounds.

Reference:

[1] Pollien, P., Ott, A., Flavour and Frag. J., 1998, 13, 413.
[2] Diaz-Maroto, C. M., Journal of chromatography A., 2002, 947, 23.
[3] Adams, R.P., Identification of essential oil componenets by gas chromatography / quadrupole mass spectrroscopy, 2004, Allured, USA.

DABCO catalyzed tandem reaction between 1,3-dicarbonyl compounds and dialkyl acetylenedicarboxylates

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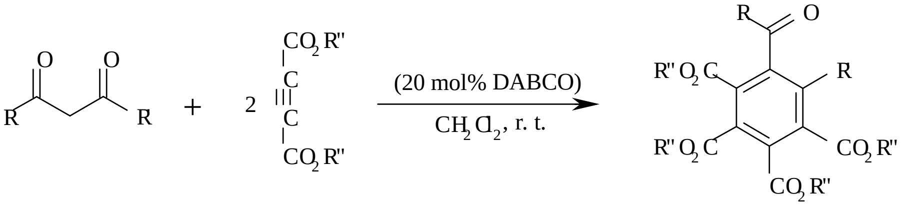
Benzene derivatives are uniquely important in organic chemistry and several strategies for the synthesis of functionalized benzenes were already developed [1]. Biaryles are also important as application in electronic device [2] and their biological activities [3]. Nair and co-workers have reported the reaction between *β*-ketoesters and dimethyl acetylenedicarboxylate in the presence of a catalytic amount of DMAP to produce polysubstituted benzene and biaryl derivatives [4]. We have previously reported the reaction between cyclic 1,3-diketones and dialkyl acetylenedicarboxylates in the presence of a catalytic amount of tertiary amines to produce chromene derivatives [5]. In this work we wish to report an efficient synthetic route to highly functionalized benzene and biaryl derivatives using acyclic 1,3 dicarbonyl compounds **1** and dialkyl acetylenedicarboxylates **2** in the presence of a catalytic amount of 1,4-diazabicyclo[2.2.2]octane (DABCO). The structures of products were deduced by ^{1}H, ^{13}C NMR, Mass, and IR spectroscopy.



1 **2** **3**

R, R': Me, Ph R'': Me, Et

References:

[1] Saito, S. ; Yamamoto, Y, *Chem. Rev*. **2000**, *100*, 2901.
[2] Roncali, J. *Chem. Rev*. **1992**, *92*, 711.
[3] Hassan, J. ; Sevignon, M. ; Gozzi, C. ; Schulz, E. ; Lemaire, M. *Chem Rev*. **2002**, *102*, 1359.
[4] Nair, V.; Vidya, N.; Biju, A. T.; Deepthi, A.; Abhilash, K. G.; Suresh, E. *Tetrahedron*, **2006**, *62*, 10136.
[5] Nasiri, F.; Pourdavaie, K.; Yosefdad, S.; Atashkar, B. *Mendeleev Comm*. **2007**, *17*, 352.

An efficient Synthesis of 1-Amino-1-Phenyl-2-(N-Piperidino methyl) Cyclohexane

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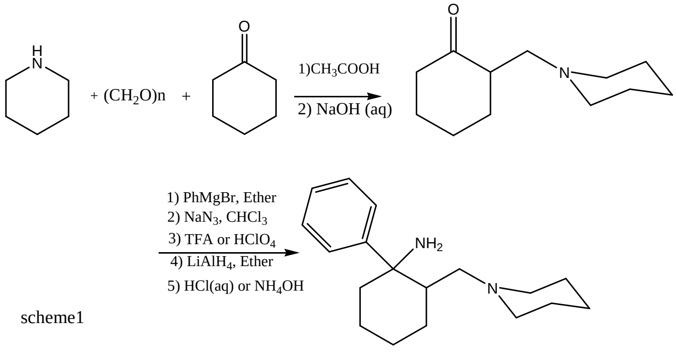
Primary and secondary amines are the most popular classes of building blocks. Amines are useful in a broad range of synthetic reactions and some of them are important in many pharmaceutical and agricultural products. Drugs that increase the levels of amine neurotransmitters are potential antidepressants. For example components with three cycles of piperidine have shown anti depression, antidimicilal and tranquiliser effects

It is not surprising that carbon-nitrogen bond formation reactions are found in most of the synthetic routes to date [1] Convenient strategies for selective synthesis of primary and secondary amines will thus have broad applicability in the synthesis field [2].

In this report we could prepare amine 5 with excellent yields. As shown in Scheme 1, for the synthesis of this component, According to the Manich reaction, β keto Amine 4 prepared from the cyclohexanone, piperidine and formaldehyde [3]. After that including five steps we could synthesis three cyclic amine of **5** quantitively. Structure of the amine **5** is assigned on the basis of IR, ^{1}H NMR, ^{13}C NMR and Mass spectral data.



scheme1

References:

[1] a) Berger, U. Medicinal Chemistry.Willey, **1981**, P.225. b) Booth, S.; Hermkens, P.H.H.; Ottenhdijm, H.C.J.; Rees, D.C. *Tetrahedron* **1998**, *54*, 15385

[2] Flick, K.; Frankus, E.;Arzneim, F.; Sikshi, S. A.; Hultin, P. G. *J. Org. Chem*. **2006**, *71*, 5888.

[3] a) Hedayatullae, M. *Tetrahedron Letters*, **1975**, 2455.b)Bover, J. H. *J. Org. Chem*, **1951**, *73*, 5865.

Preparation of carbonyl compound from Trimethylsilyl ether using oxone in mild condition

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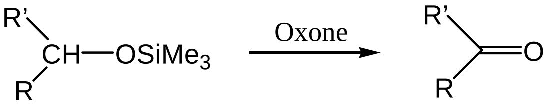
The oxidation of alcohols into corresponding aldehydes and ketones is a crucial reaction in organic chemistry, both with academic and industry relevance [1]. Aldehydes and ketones represent an important class of products and intermediates in the fine chemicals and specialities. The oxidation of trimethylsilyl ethers is an important transformation in organic synthesis, and several methods have been explored to accomplish such a conversion[2].Some of these methods involve the use of expensive reagents, long reaction times, low yields of the products and tedious work-up. Therefore, introduction of new methods and reagents for such functional group transformation is still in demand.

Recent reports have dealt with the use of a triple salt ($2KHSO_5 \cdot KHSO_4 \cdot K_2SO_4$), which is commercially available as Oxone®, This oxidation system has the following advantages. The reaction proceeds under mild conditions. Oxone® is an inorganic, water-soluble, commercially available, and inexpensive co-oxidant that has low toxicity [3].

In this paper we demonstrated the highly efficient oxidation of alcohols to their corresponding aldehydes and ketones under mild conditions at room temperature by Oxone® and with various aryl and alkyl group were converted to the corresponding carbonyl compound in excellent yields.



R : alkyl, aryl
R' : H,alkyl, aryl

References:
[1]. P.H. Yan, R.R. Wang, S. Wu, Z.Q. Lei, *Catal. Commun.* 9 (**2008**) 406.
[2]. Robert K. Boeckman, Jr. John R. Miller. *Org. Lett.*, Vol. 11, No. 20, (**2009)**
[3]. T.Yakura . M.Omoto. *Chem. Pharm. Bull.* 57(6) 643—645 (**2009**)

Three-component reaction between dialkyl acetylenedicarboxylates, 2-aminpyridiens and arylglyoxals in the presence of triphenylphosphine,: An efficient one-pot synthesis of highly functionalized pyrroles

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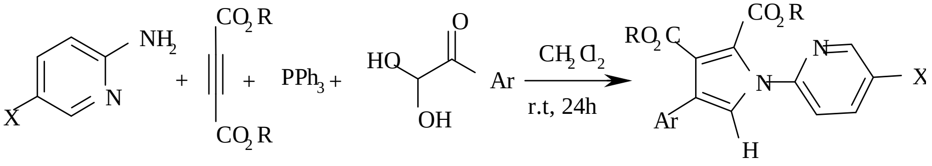
Simple nitrogen-containing heterocycles receive considerable attention in the literature as a consequence of their exciting biological properties and their role as pharmacophores of historical importance [1]. Of these heterocycles, the synthesis, reactions, and biological activities of pyrrole-containing molecules stand as an area of research in heteroaromatic chemistry, and this structural motif appears in a large number of pharmaceutical agents and natural products. Accordingly, many strategies have been developed for the preparation of pyrroles [2].

Three-component reaction between tripenylphosphine, dialkyl acetylenedicarboxylates (DAAD's) and organic acidic compounds is well known to produce phosphorus ylides. If the starting acidic compound posseses a carbonyl group in an appropriate position, these ylide intermediates may be converted to cyclic compounds by intramolecular Wittig reaction. This strategy has been recently utilized for the synthesis of a variety of heterocyclic and carbocylic compounds[3].

Here we report a three-component reaction between dialkyl acetylenedicarboxylates, 2-aminpyridiens and arylglyoxals promoted by triphenylphosphine, to produce functionalized pyrrole derivatives in high yields.



References:

[1] Yates, F. S. In Comprehensive heterocyclic chemistry, Boulton, A. J. and McKillop, A. Eds. (Pergamon, Oxford, **1984**), *2*, 511.
[2] Gilchrist, T. L. *J. Chem. Soc, Perkin Trans. 1*, **2001**, 2491.
[3] Mosslemin, M. H.; Yavari, I.; Anary-Abbasinejad, M.; Nateghi, M. R. *Synthesis* **2004**, *7*, 1029.

Tungstate sulfuric acid (TSA) and Molybdate sulfuric as heterogeneous acids for synthesis of pharmaceutical heterocyclic compounds

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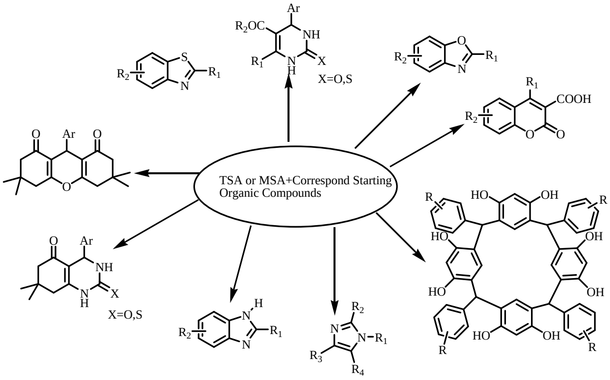
Heterocyclic organic compounds, pharmaceutical organic compounds, pharmaceutical heterocyclic compounds, organic compounds, heterocyclic compounds, heterocyclic products are widely used in pharmaceuticals and biotechnology industries. The generation of pharmaceutical heterocyclic compounds is an important process in modern synthetic organic chemistry. Numerous heterocycles compound with biological activity have been investigated, however many of them are not suitable for therapeutic use due to their toxic, carcinogenic and mutagenic properties. Nowadays, it is possible to make modifications of active chemical structures, in order to synthesize compounds with improved therapeutic activity and reduced toxicity [1].

In continuation of our recently studies [2] on the application of inorganic solid acid, herein we present tungstate sulfuric acid (TSA) and molybdate sulfuric acid as a new solid acids to catalytic synthesis of a variety of pharmaceutical heterocyclic compounds such as coumarin-3-carboxylic acids, 3,4-dihydropyrimidin-2(1H)-ones/thiones, benzimidazoles, benzoxazoles, benzothiazoles, 1,2,4,5-tetrasubtituted imidazoles, 1,8-Dioxo-octahydroxanthenes, 4-aryl-7,7-dimethyl-1,2,3,4,5,6,7,8-octahydroquinazoline-2-one/thione-5-one and calix [4] resorcinarene derivatives under heterogeneous and mild conditions in good to excellent yields (Scheme).



Scheme

References:

[1] Kostova, I. *Curr. Med. Chem. - Anti-Cancer Agents***, 2005,** 5**,** 29.
[2] (a) Karami B.; Montazerozohori, M.; Habibi, M.H.; Zolfigol, M. A. *Heterocyclic*
[3] *Commun.* **2005**, *11*, 513; (b) Karami B.; Montazerozohori, M.; Habibi, M.H.
[4] *Phosphorus, Sulphur, Silicon and related elements*, **2006**, *181*, 2825; (c) Karami, B.;
[5] Mallakpour, S.; Farahi, M. *Heteroatom Chem.*, **2008**, *19*, 389.

Effect of catalyst preparation parameters on the catalytic performance of Fe/Mn catalyst used in FTS

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The Fischer – Tropsch synthesis (FTS) offers the possibility of converting a mixture of hydrogen and carbon monoxide into the clean hydrocarbons [1,2]. Several metals, such as nickel, cobalt, ruthenium and iron, have been shown to be active for this reaction. However, only iron and cobalt based catalysts appear to be economically feasible on an industrial scale [3,4] .

In this research work, the effects of calcination temperature (400-900 °C) and calcination time (4-9 hours) on the catalytic performance of 50%Fe/50%Mn/5wt%Al_2O_3 catalyst was prepared using sol/gel technique were investigated for the FTS in a fixed-bed micro reactor. The result showed that the catalyst calcined at 600˚C has higher selectivity toward light olefins and lower selectivity to methane. So that this temperature was chosen as the optimum calcination temperature and the catalyst calcined at 600˚C for 7h has shown the better catalytic performance. Characterization of both precursor and calcined catalysts was carried out using Powder X-ray Diffraction (XRD), thermal analysis methods such as TGA and DSC and BET surface area measurements. It was observed that all of the different operating conditions influenced the structure, morphology and catalytic performance of the catalysts

References:

[1] Khodakov, A.Y. Catal. Today. 7 (**2008**) 5994.
[2] Rostrup-Nielsen, J.R., Catal. Rev. Sci. Eng. 46 (**2004**) 247.
[3] Khodakov, A.Y. Chu, w. Fongarland, P. Rev. **2007** ,107.
[4] Liu, Y. Teng, B.T. Guo, X.H. Chang, J. Tian, L. Hao, X. Wang, Y. Xiang, H.W. Xu, Y.Y. Li, Y.W. J. Mol. Catal. A: Chem, 272 (**2007**) 182-190.

Caro's acid-silica gel: promoted synthesis of 9-aryl-1,8-dioxooctahydroxanthane in aqueous media

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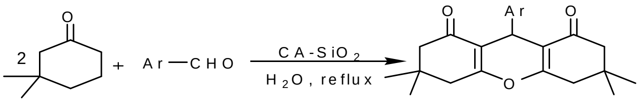
Water is an ideal solvent and reagent for biochemical transformations. In the past, use of water was not common as a solvent for synthetic organic chemistry due to the poor solubility and, in some cases, the instability of organic reagents in aqueous solutions. Now, it has been recognized that chemical reactions in mixed aqueous solutions or two-phase systems often give better results than in sole organic solvents and often the insolubility of the final products facilitates their isolation[1].

Xanthenes and benzoxanthenes are important classes of biologically active oxygen heterocycles possessing promising antibacterial, antiviral, and anti-inflammatory activities [2,3].

Herein we report an efficient method for synthesis of 9-aryl-1,8-dioxooctahydroxanthane of dimedone(2 mmol) and aldehyde (1mmol) under reflux in water in the presence of catalytic amount of Caro's acid-silica gel.

In conclusion, we have described a mild, convenient method for the preparation of 9-aryl-1,8-dioxo-octahydroxanthens using inexpensive, non-toxic, and easily available CA-SiO_2 heterogeneous catalyst.



Scheme1

References:

[1] Grieco, P. A. Organic Synthesis In water, Blackie Academic & Professional: Glasgow, 1998.

[2] Poupelin, J. P.; Saint-Ruf, G.; Foussard-Blanpin, O.; Narecisse, G.; Uchida-ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.***1973**, *13*, 67.

[3] Liu, J.; Diwu, Z.; Leung, W.-Y. *Bioorg. Med. Chem. Lett.* **2001**, *11*, 2903.

A simple synthesis of *N*-vinylpyrrole, *N*-vinylindole and *N*-vinylcarbazole derivatives

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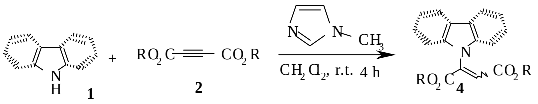
Vinylpyrroles and vinylindoles are common structural units in natural products, and are important organic skeletones that are frequently employed in the synthesis of alkaloids and other biologically important heterocycles.[1] In addition, vinylpyrroles have been extensivly studied in material science as vinyl monomers, molecular switches, photo- and electroconducting materials.[2] As a result, many efforts has been devoted to the development of new methodologies for efficient synthesis of vinylpyrroles and vinylindoles.[3] Herein we have described the reaction of pyrrole, indole and carbazole with dialkyl acetylenedicarboxylates catalyzed by N-methylimidazole provides a simple and efficient route for the synthesis of N-vinylpyrrole, N-vinylindole and N-vinylcarbazole derivatives in high yields.



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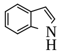
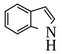
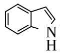
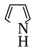
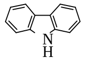
1		Me	95	95
2		Et	95	95
3		*t*-Bu	100	100
4		Me	95	95
5		Me	98	98

*Isolated Yields

References:

[1] A. Padwa, S. M. Lynch, J. M. Mejia-Oneto, H. Zhang, J. Org. Chem. **2005**, 70, 2206.
[2] Z. Yanshi, Tetrahedron Lett, **2006**, 62, 3917.
[3] A. B. Trofimov, E. Y. Zaitsev, A. M. Schmidt, A. I. Vasil'tsov, I. A. Mikhaleva, A. V. Ushakov, N. V. Vashchenko, Tetrahedron Lett., **2004**, **45**, 3789.

Cellulose sulfonic acid as an efficient solid acid catalyst in the ring opening of epoxides: preparation of azido alcohols and hydroxy thiocyanates

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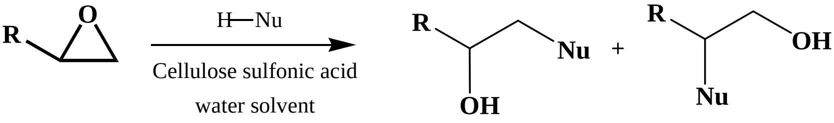
Epoxides are very important reagents in synthesis organic chemistry, because their cyclic system become easily created and destroyed. The other hand, this cyclic system was found in many industrial and biological active compounds [1].

Many reactions of epoxides were studied such as nucleophile addition to epoxides and formation of (1, 2) additional productions [2].

Ring opening of epoxides can do in basic, acidic and neutral conditions. It was defined that presence of acid easily makes ring opening of epoxides [3].

In this research, cellulose sulfonic acid has been prepared as a solid acid from reaction between cellulose and chlorosulfonic acid.This solid acid was easily supported on silica gel and used as an efficient catalyst in the ring opening of epoxides by N_3^-, SCN^-. The obtained results shown that this new catalyst is effective in the formation of β-azido alcohols and β-hydroxy thiocyanates. Reactions were done in short time with very good yields.



(1) (2)

References:

[1] Niknam, K. *J. Phosphorus, sulfur and silicon and related elements*. **2004**, *179*, 499.
[2] Smith, J.G. *J. Syn*. **1984**, *629*.
[3] Wohl, R.A. *J. Chimia*. **1974**, *28*, 1.

Thioester synthesis from alkyl halide mediated by polymer supported sodium acetate

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Thioesters are activated carboxylic acid derivatives which exhibit acylating properties similar to those of acid anhydride [1]. Thioesters show higher reactivity and selectivity toward nucleophiles than their oxygen analogues and they play important roles in biological systems such as acyl coenzyme A, and S-acetyl dihydrolipolic acid [2].

Until the mid-1980s, Thioesters were prepared by conventional methods, i.e. condensational of thiols with the parent carboxylic acids in the presence of an activating agent or substitution of acid chlorides or acid anhydrides with metal thiolates [3].

Although polymer-supported reagents especially anion exchange resins have been widely applied in organic synthesis, there is only a few report in the literature for the synthesis of organic thioesters based on polymeric reagents.

Now we wish to report an efficient and easy method for preparation of alkyl thioesters from alkyl halides by using a polymer supported thioaacetate anion under mild, nonaqueous and heterogeneous conditions in high yields (Scheme 1).

$$1)\quad [P_4\text{-}VP]\ 2\ \%\ DVB + Me\text{-}I \longrightarrow [P_4\text{-}VP]I$$

$$2)\quad [P_4\text{-}VP]I + NaSCOCH_3\,(aq) \longrightarrow NaI\,(aq) + [P_4\text{-}VP]SCOCH_3$$

$$3)\quad [P_4\text{-}VP]SCOCH_3 + R\text{-}X \xrightarrow{\text{Ethanol, rt}} RS\text{-}CO\text{-}CH_3 + [P_4\text{-}VP]X$$

$$4)\quad [P_4\text{-}VP]X + NaSCOCH_3(aq) \longrightarrow [P_4\text{-}VP]SCOCH_3 + NaX(aq)\ \text{(Regeneration)}$$

Scheme 1: Mechanism of the reaction and regeneration of polymeric reagent

References:

[1] Ogawa, A.; Sonoda, N. Comp Org Functional Group Transformation **1995**, 5, 231.
[2] Bruice, T. C.; Benkovic, S. J Bioorganic Mechanism; Benjumin Inc; New York and Amsterdam **1966**, 1, Chap. 3.
[3] Mukaiyama, J.; Araki, M.; Takei, H. *J Am Chem Soc*. **1973**, *95*, 4763.

Clean and efficient synthesis of azo dyes using polymer-supported sodium nitrite and a polymeric acid

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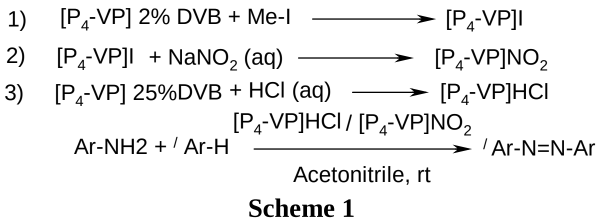
Azo compounds are very important in the field of dyes [1], azoic dye is the most important group of all synthetic dyes. Azo chromophores have a wide range of applications in the textile, leather, paper, and food, pharmaceutical and cosmetic industries.

There are many methods available for the synthesis of azo compounds. Direct synthesis of azo derivatives in good yields can be accomplished by the reduction of nitro aromatics with metal hydrides, zinc in strongly alkaline media, lead and triethylammonium formate, active-iron base reducing system, dicobalt octacarbonyl, etc [2,3]. These methods all suffer from either low yields, complex work-up procedures and undesired side reactions. In addition they may also require harsh conditions or can generate dangerous pollutants for the environment. Consequently, new methodologies with milder reaction conditions and simply work-up are welcomed.

A literature search shows a few reports covering the preparation of azo compounds based on polymeric acid or polymer-supported reagents under heterogeneous conditions. In continuing our studies on the development of application [P_4-VP] NO_2 in organic synthesis, the study of the diazotisation of primary aromatic amines in the presence of [P_4-VP] HCl and [P_4-VP] NO_2 is reported. Furthermore diazo components are prepared by coupling diazonium salt with an coupling component (Scheme1).



$$1)\quad [P_4\text{-VP}]\ 2\%\ DVB + Me\text{-}I \longrightarrow [P_4\text{-VP}]I$$

$$2)\quad [P_4\text{-VP}]I + NaNO_2\ (aq) \longrightarrow [P_4\text{-VP}]NO_2$$

$$3)\quad [P_4\text{-VP}]\ 25\%DVB + HCl\ (aq) \longrightarrow [P_4\text{-VP}]HCl$$

$$Ar\text{-}NH2 + {}^{/}Ar\text{-}H \xrightarrow[\text{Acetonitrile, rt}]{[P_4\text{-VP}]HCl\ /\ [P_4\text{-VP}]NO_2} {}^{/}Ar\text{-}N{=}N\text{-}Ar$$

Scheme 1

References:
[1] Waring, D. R.; Hallas, G. The Chemistry and Application of Dyes. New York: Plenum; **1990**.
[2] Kabalka, G. W.; Varma, R. S. Comprehensive Organic Synthesis. Trost, B. M.; Fleming, I. Eds; Pergamon Press: Oxford; **1991**; Vol 8; pp 363-380.
[3] Filimonov, V. D.; Trusova, M.; Postnikov, P.; Krasnckutskaya, E. A.; Lee, Y. M.; Hwang, H. Y.; Kim, H.; Chi, K. W. *Org Lett* **2008**, 10, 3961.

ZnO nanoparticles: an efficient nanocatalyst for one-pot synthesis of 1,2,4,5-tetra substituted imidazoles

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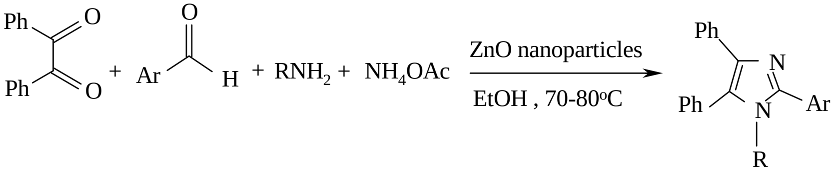
The tetrasubstituted imidazole core exists in many biological systems such as Losartan, Olmesartan and in some natural products and pharmacologically active compounds [1]. In a one-pot, four-component condensation of an aldehyde, an amine, benzil and ammonium acetate were used for the synthesis of 1,2,4,5-tetrasubstituted imidazoles. In the last few years, literature has highlighted the importance of nanosized materials in several scientific and technological areas, and many research councils have intensified investments in nanotechnology for the coming years [2]. Surface of metal oxides exhibit both Lewis acid and Lewis base character [3]. Nanomaterials is an exciting subject for both fundamental interests and their practical advanced applications.



ZnO nanoparticles as a reusable, non-toxic and inexpensive heterogeneous nanocatalyst.has a high efficiency of the imidazole synthesis. This simple methodology offers several advantages including a simple work-up, opportunities for scale-up and improved yields.

References:

[1] Wolkenberg, S.E.; Wisnoski, D.D.; Leister, W.H.; Wang, Y.; Zhao, Z.; Lindsley, C.W. *Org. Lett.* **2004**, *6*, 1453.
[2] Claus, P.; Bruckner, A.; Mohr, C.; Hofmeister, H. *J. Am. Chem. Soc.* **2000**, *122*, 11430.
[3] Tanabe, K. Solid Acids and Bases, Academic Press, New York, **1970**.

Synthesis and characterization of a new homo-bimetallic complex with tetradentate N_2O_2-Type Schiff base ligand

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Transition metal ions, such as Cr(VI) form complexes with Schiff bases having varied theoritical and practical applications some of them are capable of reversibly binding molecular oxygen (hemoglobin, etc.) [1,2]capacity of acting as catalysts in the study of oxygenation olefins, indols, phenols, etc.[3,5]

A new tetradentate N_2O_2-Type Schiff base 4-[4'-(3-hydroxy-1-ethyl-but-2-enylideneamino)-phenyl1-4-ylimino]-pent-2-en-ol was synthesized by the condensation of acetylacetone and 1,4-phenylenediamine in ETOH. The ligand and its complex of Cr(VI) have been synthesized by two different methods and their geometries were investigated by ^1H,^{13}C NMR, IR spectroscopy and elemental analysis.

References:

[1] Niederhoffer, E. C.; Timmons, J. H.; Martell, A. E., *Chem. Rev.* **1984,** *87*, 137.
[2] Chen, D.; Martell, A. E.; Sun, Y., *Inorg. Chem.* **1989,** *28*, 2647.
[3] Foster, S.; Rieker, A.; Maruyama, K.; Murata, K.; Nishinaga, A., *J. Org. Chem.* **1996,** *61*, 3320
[4] Maruyama, K.; Kasukawa, T.; Mashino, T.; Nishinaga, A., *J. Org. Chem.* **1996,** *61*, 3342.
[5] Bamhaud, T.; Prandi, J., *J. Chem. Soc. Chem. Commun.* **1996,** 1229.

Synthesis and characterization of novel thermally stable aromatic poly(amide-ester-imide)s based on the imide-triacid from trimellitic anhydride and L-aspartic acid and various aromatic diole

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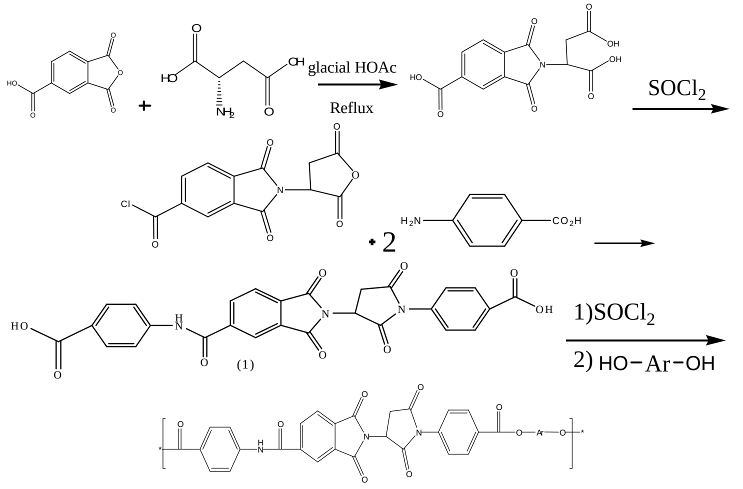
Polyesters are one the most important polymers that some of them use in polymer industries but changing the properties of polyesters has been investigated recently by changing their structure [1-4].Including amide and imide functional groups in the backbone of polyesters can improve thermal properties of these polymers [5].

In this project, a novel monomer was synthesis from a natural amino acid that is named L-aspartic acid and trimellitic anhydride according to following reaction after that, the synthetic diacid I was transformed to the corresponding diacyl chloride and then the interfacial polymerization applied to prepare poly(amide-ester-imide)s [6,7]. All polymers were characterized by FT-IR and ^{1}HNMR Spectroscopy and CHN analysis. The FT-IR Spectra of polymers showed a peak at around 2925 (C-H Stretching), two bands at 1721 and 1780 cm^{-1} corresponding to the cyclic imide groups and a band at 1715 corresponding to the ester carbonyl groups. These polymers are highly soluble in polar aprotic solvents and show good thermal stability.



References:

[1] Behniafar, H.; Banihashemi, A . *Eur. Polym. J.* **2004**, *1409*, 1415.
[2] Yganeh, H.; Tamami, B.; Ghazi, I. *Ir. Polym. J.* **2005**, *277*, 285.
[3] Mallakpour, Sh.; Habibi, S. *Eur. Polym. J*. **2003**, *1823*, 1829.
[4] Mallakpour, Sh.; Kolahdoozan, M. *Eur. Polym. J*. **2007**, *3344*, 3354.
[5] Mallakpour , Sh.; Rafiee, Z. *Polym. J.* **2007**, *1185, 1192*.
[6] Hajipour, A, R.; Zahmatkesh, S.; Zarei, A.;Khazdooz, L.; Rouho, A, E. *Eur. Polym. J.* **2005**, *2290, 2296*.
[7] Vasanthi, B, J.; Ravikumar, L. *Eur. Polym. J.* **2007**, *4325*, 4331.

An unexpected oxa-michael additon of ethoxy group to 1-benzylidenenaphthalen-2(1H)-one derivatives in the presence of 2,5-dihydroxycyclohexa-2,5-diene-1,4-dione

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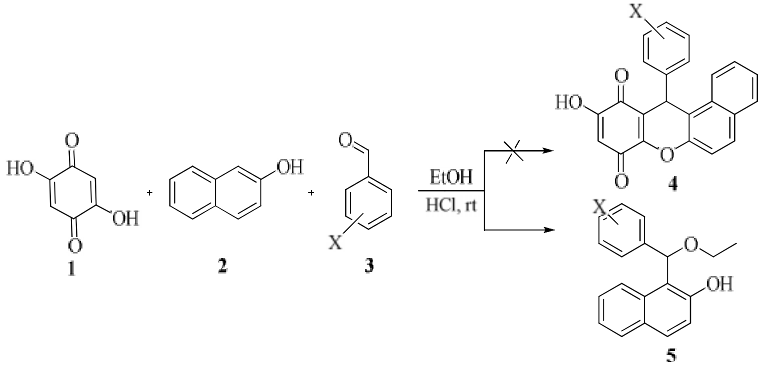
The oxa-Michael addition of oxygen nucleophiles to electrondeficient *α,β*-unsaturated ketones has been a significant challenge in organic synthesis, owing to the low reactivity coupled with the reversibility of the reaction [1-3].

As a part of our current studies on the multicomponent reactions (MCRs), and also chemistry of *CH*- acids [4] , we have investigated the possibility of trapping the heterodiene generated from the reaction beetwen naphthalen-2-ol **2** and aldehydes **3** with 2,5-dihydroxycyclohexa-2,5-diene-1,4-dione **1**. In the event we did not observe the expected MCR product **4**; instead the reaction afforded the corresponding 1-(ethoxy(phenyl)methyl)naphthalen-2-ol derivatives **5** (Scheme 1).



Scheme 1

References:

[1] Vanderwal, C. D.; Jacobsen, E. N. *J. Am. Chem. Soc* . **2004**, *126*, 14724.
[2] UndMn, H.; Ibrahem, I.; Zhao, G. L.; Eriksson, L.; CPrdova, A. *Chem. Eur . J.* **2007**, *13*, 574.
[3] Bernal, P.; Tamariz, J. *Tetrahedron Lett.* **2006**, *47*, 2905.
[4] a) Shaabani, A.; Rezayan, A. H.; Keshipour, S.; Sarvary, A.; Ng, W. S. *Org. Lett.* **2009**, *11*, 3342; b) Shaabani, A.; Soleimani, E.; Rezayan, A. H.; Sarvary, A.; Khavasi H. R. *Org. Lett.* **2008**, *10*, 2581; c) Shaabani, A.; Rezayan, A. H.; Sarvary, A.; Khavasi H. R. *Tetrahedron Lett.* **2008**, *49*, 1469; d) Shaabani, A.; Sarvary, A., Rezayan, A. H.; Keshipour, S. *Tetrahedron* **2009,** *65***,** 3492; e) Shaabani, A.; Sarvary, A.; Rezayan, A. H.; Keshipour, S.; Ghadari, R. *Tetrahedron* **2010**, *66*, 1911.

Study of three-component reaction between trialkyl phosphites, dialkyl acetylenedicarboxylates and 2,3-dihydroquinazolin-4(1H)-one derivatives

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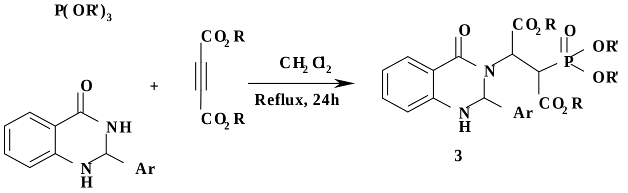
Organophosphonates have been used as substitutes for the corresponding esters and acids with high biological activity [1].There are some other recent reports on the reaction between phosphites and acetylenic esters in the presence of an acidic organic compound, all of them proceeding through a phosphite ylide intermediate [2]. In continuation of our works on the reaction between trivalent phosphorus nucleophiles and acetylenic esters in the presence of organic NH, OH, or CH-acids [3-5].Here we wish to report the results of our study on the reaction between dialkyl acetylendicarboxylates and trialkyl phosphites such as triethyl phosphite, tributyl phosphite or trimethyl phosphite in the presence of 2,3-dihydroquinazolin-4(1H)-ones.



3	R	Ar	R'	%Yield*
a	CH_3	C_6H_5	Me	90
b	C_2H_5	4-Cl C_6H_4	Me	92
c	*t*-Bu	4-Br C_6H_4	Et	89
d	CH_3	4- NO_2 C_6H_4	Bu	90

* Isolated yields

The structures of **3a-d** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:

[1] Kaboudin, B.; Nazari, R. *Tetrahedron Lett.* **2001**, *42*, 8211.
[2] Yavari, I.; Anary-Abbasinejad, M.; Hossaini, Z. *Org. Biomol. Chem.* **2003**, *3*, 560.
[3] Anary-Abbasinejad, M.; Hassanabadi, A. *J. Chem. Res.* **2007**, 475.
[4] Anary-Abbasinejad, M.; Hassanabadi, A.; Mazraeh-Seffid, M. *J. Chem. Res.* **2007**, 708.
[5] Anary-Abbasinejad, M.; Charkhati, K.; Hassanabadi, A. *J. Chem. Res.* **2009**, 319.

Synthesis and characterization of novel organo-soluble and thermally stable wholly aromatic polyesters containing triazine ring

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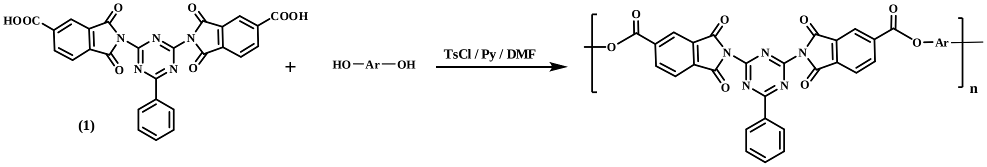
Polyesters (PE)s are one of the most versatile polymers. They contain widely different materials with large applications, which are produced by a variety of manufacturing techniques [1]. They have in common the polar ester group –CO–O– in the main chain, which brings about inter and intramolecular chain interactions that may reflect in some properties such as low solubility, mobility of the chain and melting characterizations. In addition, PEs often have limited heat and flame resistance. Several approaches have been proposed to develop structurally modified polymers having increased solubility, in order to improve their processability while maintaining a good thermal stability, based on the incorporation of flexible segments bearing ester, sulfone, imide, and ether moieties in the polymer backbone, without sacrificing heat resistance [2-4].

In this investigation, in order to improve the processability of the polyesters, new type of these polymers were synthesized based on diacid monomer containing triazine ring. 4-phenyl-2,6-bis(trimellitimid) 1,3,5-triazine (1) as a novel aromatic dicarboxilic acid containing triazine moiety and pendent group was synthesized by condensation of 2,6-diamino-4-phenyl-1,3,5-triazine with trimelitic anhydride in N,N-dimethylformamide (DMF). The structure of diacid **1** was confirmed using various spectroscopy methods. A series of novel PEs was prepared by the reaction of diacid monomer 1 with several aromatic diols via direct polyesterification with the tosyl chloride/pyridine/DMF system as a condensing agent (Scheme 1). The resulting novel poly(ester-imide)s were obtained in high yields and inherent viscosities. These polymers were characterized using FT-IR, ^{1}H-NMR, thermogravimetric techniques. The results show that triazine modified poly(ester-imide)s show high solubility and excellent thermal stability.



Scheme 1. Polyesterification of diacide 1 with various aromatic diols.

References:

[1] Mallakpour, S.; Kolahdoozan, M. *Eur. Polym. J.* **2007**, *43*, 3344.
[2] Liaw, D J.; Fan, C L.; Lin, C C.; Wang, K L. *J. Appl. Polym. Sci*. **2004**, *92*, 2486.
[3] Zhang, S.; Li, Y.; Yin, D.; Wang, X.; Zhao, X.; Shao, Y. *Eur. Polym. J.* **2005**,*41*,1097.
[4] Behniafar, H.; Khaje Mirzai, A.; Beit Saeed, A. *Polym. Int.* **2007,** *56*, 74.

Efficient Schiff bases synthesis of 2-amino benzimidazole catalyzed by metals nitrate

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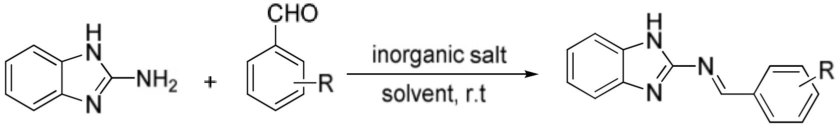
Compounds containing a benzimidazole moiety attached to a heterocyclic system are important chemical classes having a number of significant biological activities against several viruses such as HIV, herpes (HSV-1), influenza and Epstein-Barr [1-2].

Furthermore, Schiff bases derived from aromatic amines and aromatic aldehydes are of growing interest because of their applications in many fields including biological [3], inorganic [4] and analytical chemistry [5]. Synthesis of Schiff bases is often carried out by acid-catalyzed condensation reaction of primary amine and a carbonyl group in an organic solvent. This traditional synthetic method employs the harsh reaction conditions and the use of high boiling point volatile organic solvents, which forwarded by hard workup and extensive recrystalization. In view of the above-mentioned findings and due to continuation of our research for development of the simple and efficient methods for the synthesis of heterocyclic compounds [6], we are going to report the synthesis of Schiff bases, **3a-l** using metals nitrate as a homogeneous catalyst. Some of the major advantages of this environmentally benign procedure are high yields, use of available catalysts, easy workup and short reaction times.



1 **2** **3 (a-l)**

References:

[1] Tamm, I.; Sehgal, P. B. *Adv. Virus Res.* **1978**, *22*, 186.

[2] (a) Tamm, I. *Science* **1954**, *120*, 847. (b) Ottana, R.; Carotti, S.; Maccari, R.; Landini, I.; Chiricosta, G.; Cacigli, B.; Vigorita, G. M.; Mini, E. *Bioorg. Med. Chem. Lett.* **2005**, *15*, 3930.

[3] Hearn, J. M.; Cynamon, M. H. *J. Antimicrob. Chemother.* **2004**, *53*, 185.

[4] Türner, M.; Köksal, H.; Serin, S.; Patat, S. *Syn. Reac. Inorg. Met-org. Chem.* **1997**, *27*, 59.

[5] Salavati-Niasari, M. *J. Chemistry Lett.* **2005**, *34*, 1444.

[6] Mobinikhaledi, A.; Steel, P.J. *Syn. Reac. Inorg. Met-org. Chem.* **2009**, *39*, 189.

Acetyl chloride-promoted reaction of aromatic aldehydes and acetamide: an easy synthesis of symmetrical bisamides

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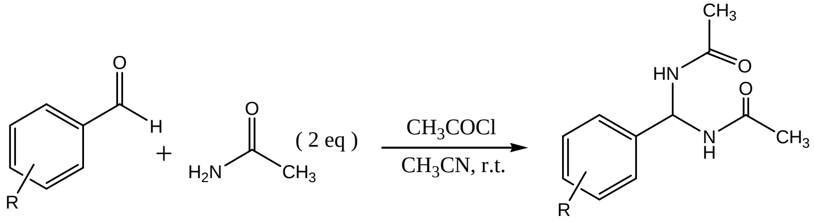
Bisamides are of considerable interest in the synthesis of peptidomimetic compounds [1]. Specifically, bisamides are key fragments for the introduction of *gem*-diaminoalkyl residues in retro-inverso pseudopeptide derivatives by treating the corresponding amide with iodobenzen bistrifluoroacetate [2, 3].

In the present study, we report a highly efficient method for the synthesis of symmetrical bisamides from aromatic aldehydes with acetamide using acetyl chloride at room temperature in excellent yields (Scheme 1).



Scheme 1

The structures of compounds were confirmed by their spectra (^{1}H NMR, ^{13}C NMR, and IR). For example, the ^{1}H NMR spectra of compounds exhibited a singlet around δ= 1.76-1.97 ppm for methyl groups protons, a triplet around δ= 6.46-6.64 ppm for methine group proton and a doublet around δ= 8.45-8.64 ppm for NH proton. In the IR spectra, the NH groups were observed around 3271-3283 cm^{-1} and the O=C-NH groups around 1662–1674 cm^{-1}.

In conclusion, we report here a simple one-pot reaction for the synthesis of symmetrical bisamide derivatives at room temperature. The present protocol offers several adventages including clean and simple reaction procedure, isolation of products by crystallization without employing purification methods like column chromatography, high yields and short reaction times.

References:

[1] Aleman, C.; Puiggali, J. *J. Org. Chem.* **1995**, *60*, 910.
[2] Nunami, K. I.; Yamazaki, T.; Goodman, M. *Biopolymers* **1991**, *31*, 1503.
[3] Pernak, J.; Mrowczynski, B.; Weglewski, J. *Synthesis* **1994**, 1415.

An efficient one-pot synthesis of tetrahydrobenzo[a]xanthene-11-one under solvent-free condition

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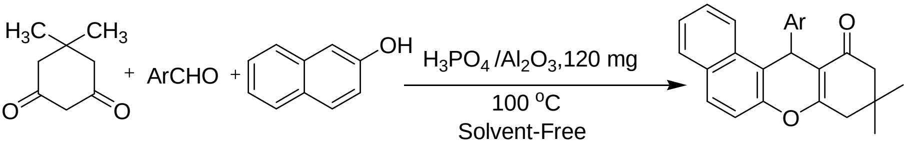
In the mainstream of current interest, multi-component processes have recently gained considerable economic and ecological interest as they address fundamental principles of synthetic efficiency and reaction design. Multi-component reactions (MCRs) have been proven to be a very elegant and rapid way to access complex structures in a single synthetic operation from simple building blocks and show high atom economy and high selectivity [1]. Xanthenes and benzoxanthenes are important biologically active heterocyclic compounds, which possess antiviral, anti-inflammatory and antibacterial activities. These are being utilized as antagonists for paralyzing action of zoxazolamineand in photodynamic therapy. Furthermore, these compounds can be used as dyes, in laser technologies and as pH sensitive fluorescent materials for visualization of biomoleculesm [2]. Herein, we are reporting the reaction of aldehydes, 2-naphthol and cyclic 1,3-dicarbonyl compounds for the formation of tetrahydrobenzo[a]xanthene-11- one derivatives in presence of catalytic amount of H_3PO_4/Al_2O_3 under solvent free conditions (Scheme). This catalyst not only makes the synthetic process clean, safe and inexpensive, but also affords the products in excellent yield.

Various 12-aryl/ alkyl-8,9,10,12-tetrahydrobenzo[a]xanthene-11-ones were synthesized by a one-pot, multi-component reaction of aldehydes, 2-naphthol and dimedone. The advantages of this method over other existing methods are reduced reaction times, higher yields, easy purification and economic viability of the catalyst.



Scheme

References:

[1] Zhu, J., Bienayme, H. Multicomponent Reactions;, Eds.; Wiley- VCH: Weinheim, Germany, 2005.

[2] (a) Sirkencioglu, O.; Talinli, N.; Akar, A. *J. Chem. Res.* **1995**, 502; (b) Ahmad, M.; King, T. A.; Ko, D.-K.; Cha, B. H.; Lee, J. J. Phys. D: *Appl. Phys*. **2002**, *35*, 1473; and references therein.

Al_2O_3-promoted synthesis of β-hydroxy sulfide under neutral solvent-free conditions

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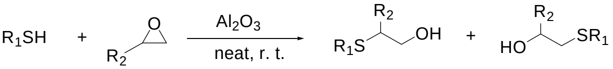
To minimize the amount of harmful organic solvents used in chemical processes, much attention has been devoted to the use of alternative reaction media. Besides the use of supercritical fluids, water, and ionic liquids, the possibility of performing chemical processes in the absence of solvent (solvent-free conditions) has been receiving more attention [1].

Thiolysis of 1,2-epoxides is a convenient, practical and widely employed strategy for the synthesis of β-Hydroxy sulfides, which constitute an important class of intermediates in organic chemistry and in particular in the field of pharmaceuticals [2]. It is also a versatile moiety for synthesizing allylic alcohols, benzoxathiepines, benzotiazepines, a-thioketones, and b-hydroxysulfoxides [3]. Thiolysis of epoxides has been extensively studied in organic solvents[4] and can be promoted by acids, a Lewis catalyst or metal salts[5], or bases (NaOH or Et_3N) in a protic solvent (i-PrOH or MeOH. Some groups [6] reported synthesis of these compounds in water under basic, natural and acidic conditions.



R_1, R_2 = alky and aryl

Herein, we have developed a simple and efficient procedure for preparation of β-Hydroxy sulfides. This solvent-free reaction is very useful both from economical and environmental points of view and also, offers some advantages over procedures reported earlier in that it avoids the use of hazardous organic solvents, toxic andexpensive reagents, as well as operational simplicity, high yields of products, and low costs. The reactions were highly regio- and stereoselective, and trans- β -hydroxy sulfides were produced in good to excellent yields under very mild conditions.

A series of thiols (both aromatic and aliphatic) were treated with various epoxides to afford the corresponding products. In all case of epoxides (unsymmetrical and symmetrical), the reactions were completely regioselective and proceeded via an SN_2 mechanism with an attack of the thiol at the less-hindered site. The only exception was in the case of styrene oxide, where mixtures of the two regioisomers were obtained.

References:

[1] (a) DeSimone, J. M. *Science* **2002**, *297*, 799; (b) Metzger, J. O. *Angew. Chem., Int. Ed.* **1998**, 37. 2975.
[2] Luly, J. R.; Yi, N.; Soderquist, J.; Stein, H.; Cohen, J.; Perun, T. J.; Plattner, J. J. *J. Med. Chem.*,**1987**, *30*, 1609.
[3] Movassagh, B.; Sobhani, S.; Kheirdoush, F.; Fadaei, Z. *Synth. Commun.*, **2003**, *33*, 3103 and references therein.
[4] (a) Yadav, J. S.; Reddy, B. V. S.; Baishya, G. *Chem. Lett.*, **2002**, 906; (b) Chandrasekhar, S.; Reddy, C. R.; Babu, B. N.; Chandrashekar, G. *Tetrahedron Lett.*, **2002**, *43*, 380.
[5] (a) Chini, M.; Crotti, P.; Giovani, E.; Macchia, F.; Pineschi, M. *Synlett*, **1992**, 303; (b) Vougiokas, A. E.; Kagan, H. B. *Tetrahedron Lett*., **1987**, *28*, 6065.
[6] (a) Movassagh, B.; Soleiman-Beigi, M. Synth. Commun. 2007, *37*, 3239; (b) Azizi, N.; Akbari, E.; Saidi, M. R. J. Iran. Chem. Soc., 2009, *6*, 165.

Cu/SiO$_2$-catalyzed one-pot synthesis of 12-aryl-8,9,10,12-tetrahydrobenzo[α]xanthen-11-ones under solvent-free conditions

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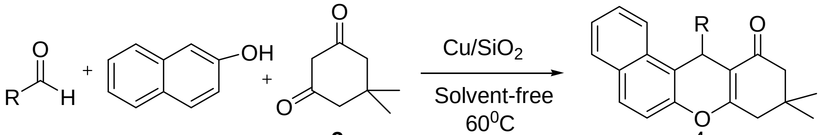
The development of multicomponent reactions (MCRs) designed to produce elaborate biologically active compounds has become an important area of research in organic, combinatorial, and medicinal chemistry. The MCR strategy offers significant advantage over conventional linear-type synthesis due to its flexible, convergent, and atom efficient nature.

Furthermore, the multicomponent reactions (MCRs) by virtue of their convergence, productivity, facile execution, and generally high yields of products, have attracted much attention from the vantage point of combinatorial chemistry.[1]

Xanthenes and their derivatives have been received special attention due to diverse array of biological activities such as anti-inflammatory, antibacterial and antiviral activities.[2,3]

Herein we report an efficient method for the synthesis tetrahydrobenzo[α]xanthen-11-ones in the presence of catalytic amount of Cu/SiO$_2$. Various aromatic, β-naphtol and dimedone were converted to the tetrahydrobenzo[α]xanthen-11-ones.

We have demonstrated the efficiency of Cu/SiO$_2$ composite as a new catalyst for the synthesis tetrahydrobenzo[α]xanthen-11-ones. The recovered solid catalyst can be reused at least for two times without a significant loss of activity.



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References:

[1] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104*, 199.
[2] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.
[3] Sikshi, S. A.; Hultin, P. G. *J. Org. Chem.* **2006**, *71*, 5888.

An efficient synthesis of bicyclo[3.3.1]nonane systems via tandem 1,3-dinucleophilic addition of 4-hydroxy-2-quinolinones to quinolinium salts

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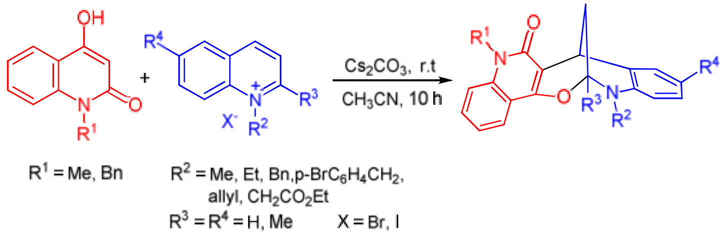
Quinolinones and annulated quinolinones are well-known for their remarkable biological activities. A broad number of fascinating pharmacological activities have been associated with quinolinones derivatives. The synthesis of such compounds has been the subject of several papers which demonstrate the high importance of this class of compounds.[1] Quinolinones have been investigated as antibacterials, antifungals, antivirals, anticonvulsants, analgesics, orally active antagonists, herbicides, cardiovasculars, memory enhancing and hypotensive agents.[2] Some quinolinone derivatives have been reported to show activity against wild-type HIV-1. In addition, they are useful intermediates for the preparation of alkaloid, non-peptide GnRH receptor antagonists and wide varieties of biologically active organic compound such as polycyclic condensed heterocycles, pyrano quinolines, piperazinyl carbomides, oxazino quinolines, isoxazolo quinolines.

Herein we report an efficient and novel method for the synthesis of newly bridgehead derivatives of quinolinones according to the following scheme. The reaction time is short and the procedure is easy and isolation is rapid.



References:

[1] (a) Hajdok, S.; Conrad, J.; Leutbecher, H.; Strobel, S.; Schleid, T.; Beifuss, U. *J. Org. Chem.* **2009**, *74*, 7230. (b) Razzaq, T.; Kappe, C. O. *Tetrahedron Lett.* **2007**, *48*, 2513. (c) Arya, K.; Agarwal, M. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 86. (d) Bernini, R.; Cacchi, S.; Salve, I. D.; Fabrizi, G. *Synlett* **2006**, 2947. (e) Dittmer. D. C.; Li, Q.; Avilov, D. V. *J. Org. Chem.* **2005**, *70*, 4682.

[2] (a) Mitscher, L. A.; *Chem. Rew*. **2005**, *105*, 559. (b) Afonso, A.; Weinstein, J.; Gentles, M. J. PCT Int. Appl. WO9203327, **1992**. (c) Hayashi, H.; Miwa, Y.; Miki, I.; Ichikawa, S.; Yoda, N.; Ishii, A.; Kono, M.; Suzuki, F. *J.*

Synthesis and characterization of new poly(hydrazide)s from 5-(2-(6-methyl pyridine-2-yl)-1,3-dioxoisoidoline-6-carboxamido) isophthalic acid as a novel monomer

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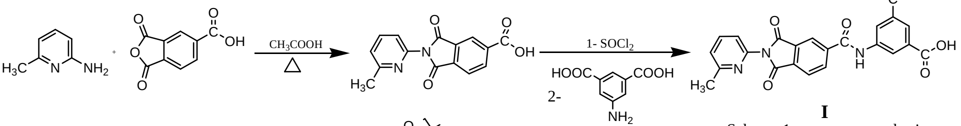
Polyhydrazides have been extensively studied since they enhance dyeability of synthetic fibers, improve elasticity over other polymer types, having fair absorption characteristics, can be cyclized to give polytriazoles and provide a synthetic base for the chelating polymers due to the ability of the hydrazide group (-CO-NH-NH-CO-) to make a complex with metal ions[1,2]. Meanwhile, wholly aromatic polymers exhibit high thermal stability. However, poor processability of these polymers is one of the disadvantages of them. To improve Processability of rigid chain polymers, a long and polar group is introduced to polymer molecules [3,4]. Recently, polymers, that bear pyridine moiety, have been synthesized. Pyridine rings help to enhance their thermal stability, solubility and adhesion to metal [5].

In this study, the above mentioned synthetic diacid (scheme 1), was transformed to the corresponding diacyl chloride, and then the interfacial polymerization applied to prepare eight new poly(dihydrazide)s (scheme 2). All polymers were characterized by UV, FT-IR and ^{1}HNMR Spectroscopy and CHN analysis. The FT-IR Spectra of polyhydrazides showed a peak at around 3422cm^{-1} (N-H Stretching), two bands at 1793 and 1727 cm^{-1} corresponding to the cyclic imide groups and a broad band at 1651 cm^{-1} corresponding to the hydrazide carbonyl groups. ^{1}HNMR spectra of these polymers also showed peaks at 10.70 and 10.90 ppm which confirm presence of amide and hydrazide protons. Inherent viscosity of poly(hydrazide)s are reasonable in the rang of 0.15 – 0.17 dl/g. These polymers are soluble in polar aprotic solvents and show good thermal stability.



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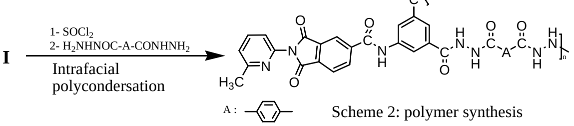
Scheme 1: monomer synthesis

I



Scheme 2: polymer synthesis

References:

[1] Hajipour, A.R.; Zahmatkesh, S.; Rouho, A. *High Performance Polym.* **2008**, 1.
[2] Aly, K.; Sarhan, A.W.; Emary, T. *Arabian J. Chem*. **2010**, *3*, 61.
[3] Ferrero, E.; Espeso, F.; Campa, G.; Abajo, J.; Lozano, A.E.; *J. Polym Sci. part A*, **2002**, *40*, 3711.
[4] Diakoumakos, C.D.; Mikroyannidis, *J.A.Eur.Polym.J*. **1995**, *31*, 761.
[5] Banihashemi, A.; Vakili, M. R. *e-polymer*. **2007**, *008,* 1.

Synthesis of novel polycyclic thiopyranocoumarin derivatives *via* domino Knoevenagel-hetero-Diels–Alder reaction in aqueous medium

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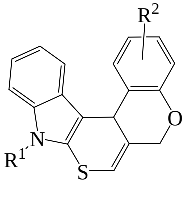
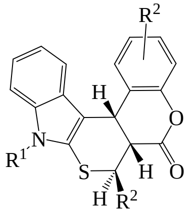
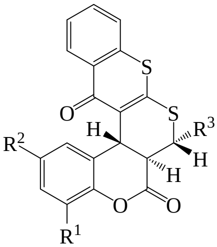
Intramolecular hetero-Diels–Alder reactions have widely been used in numerous reactions because of their economical and stereocontrolled nature [1]. These reactions allow the formation of two or more rings in one operation, thus avoiding sequential chemical transformations. Recently, domino reactions have been used as highly efficient processes for the improvement of reaction efficiency. Among these reactions, the domino Knoevenagel-hetero-Diels-Alder reaction is a very efficient process, especially in the field of heterocycles and natural products [2].

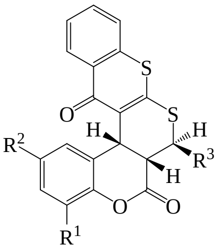
The 3,4-dihydrocoumarine system shows a wide range of biological activities such as aldose reductase inhibition, antiherpetic, protein kinases [3], and a moderate estrogenic activity. These wide range of biological applications have stimulated considerable interest in evolving newer synthetic methods for the construction of polycyclic of 3,4-dihydrocoumarine derivatives.

In the context of our general interest in the domino-Knoevenagel-hetero-Diels–Alder reaction and synthesis of sulfur-containing heterocycles, we herein report a new and highly efficient reaction for the preparation of polycyclic compounds, which consist of a thiochromone ring and a dihydrothiopyran ring annulated to a dihydrocoumarin ring [4].









References:

[1] Amos, D. T.; Renslo, A. R.; Danheiser, R. L. *J. Am. Chem. Soc.* **2003**, *125*, 4970.

[2] (a) Tietze, L. F.; Brasche, G.; Gericke, K. M. 'Domino Reactions in Organic Synthesis' Wiley- VCH, **2006**; (b) Tietze, L. F. *Chem. Rev.* **1996**, *96*, 115.

[3] Hsu, F. L.; Nonaka, G. I.; Nishioka, I. *Chem. Pharm. Bull. Tokyo* **1985**, *33*, 3142–3152.

[4] (a) Kiamehr, M.; Moghaddam, F. M. *Tetrahedron Lett.* **2009**, *50*, 6723; (b) Moghaddam, F. M.; Kiamehr, M.; Taheri, S.; Mirjafary Z. *Helv. Chim. Acta* **2010**, *93,* 964-973.

Kinetic investigation of the reactions between triphenylphosphine, dialkyl acetylenedicarboxilates and NH-acid such as Benzhydrazide by the UV spectrophotometry technique

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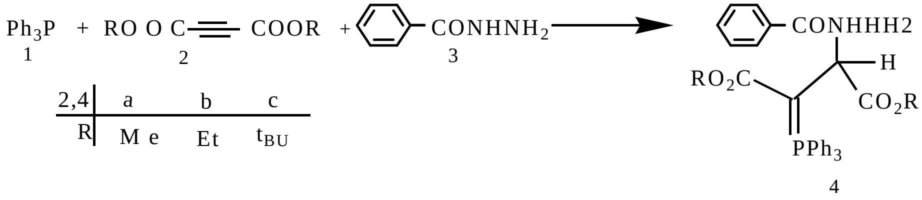
Development of simple synthetic routes for widely-used organic compounds from readily available reagents is one of the major tasks in organic chemistry [1]. Phosphorus ylides are reactive systems, which take part in many valuable reactions of the organic synthesis [2-3]. Stable crystalline phosphorus ylides were obtained in excellent yields from the 1:1:1 addition reaction between triphenylphosphine and dialkyl acetylenedicarboxylates, in the presence ofCH, SH and NH-acids [4, 5].

To determine the kinetic parameters of the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates and Benzhydrazide, they were monitored by UV spectrophotometery [6]. The second order fits were automatically drawn and the values of the second order rate constant (k_2) were calculated using standard equations within the program. At the temperature range studied the dependence of the second order rate constant (Ln k_2) on reciprocal temperature was in a good agreement with Arrhenius equation. This provided the relevant plots to calculate the activation energy of all reactions. Furthermore, useful information was obtained from studies of the effect of solvent, structure of reactants (different alkyl groups within the dialkyl acetylenedicarboxylates) and also concentration of reactants on the rate of reactions. Proposed mechanism was confirmed according to the obtained results and steady state approximation and first step (k_2) of reaction was recognized as a rate determining step on the basis of experimental data.



Refrences:

[1] Laszo, P.; Organic Reaction, Simplicity and Logic, Wiley, New York, 1995.
[2] Johnson, A.W.; Ylied Chemistry, Academic Press, London, 1966.
[3] Cadogan, J. I. G.; Organophosphorus Reagents in Organic Synthesis, Academic Press, New York, 1979.
[4] Yavari, I.; Adib, M.; Hojabri, L. *Tetrahedron*. **2002**, 58, 7213.
[5] Yavari, I.; Hossein Mosslemin, M. *Tetrahedron*. **1998**, 54, 9169.
[6]Habibi khorasani, S.M.; Maghsoodlou, M.T.; Ebrahimi, A.; Roohi, H.; Zakarianezhad, M. *Phosphorus, Sul S. M., fur and Silicon and Related Elements*, **2006**, 181, 1103-1115.

Synthesis of silver nanoparticles embedded in smart hydrogel networks containing antibiotics and study their antibacterial activity

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Silver has been in use since time immemorial in the form of metallic silver, silver nitrate, silver sulfadiazine for the treatment of burns, wounds and several bacterial infections. But due to the emergence of several antibiotics the use of these silver compounds has been declined remarkably. Nanotechnology is gaining tremendous impetus in the present century due to its capability of modulating metals into their nanosize, which drastically changes the chemical, physical and optical properties of metals. Metallic silver in the form of silver nanoparticles has made a remarkable comeback as a potential antimicrobial agent [1].

In this study the effects of silver nanoparticles prepared by reduction of silver nitrate using sodium borohydrate imbedded in semi interpenetrating hydrogel networks containing amoxyciline has been studied [2].

References:

[1] Mahendra, R.; Yadav, A.; Aniket, G. *J biotechadv*. **2009**, *27*, 76.
[2] Vimala, K. ; Samba Sivudu, K. ; Murali Mohan, Y. ; Sreedhar, B.; Mohana Raju, K. *Carbohydrate Polymers* **2009**, *75*, 463.

Kinetic and thermodynamic study of reaction of tautomerization of 5-methyl – 2, 4- dihydro- pyrazol-3-one

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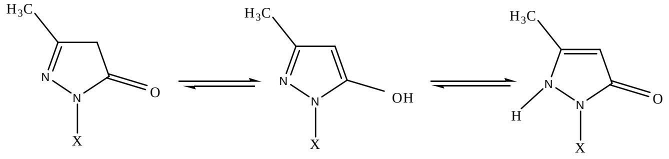
Heterocyclic compounds are considered as the most promising molecules for the design of new drugs [1]. Pyrazoles are an important class of bio-active drug targets in the pharmaceutical industry, as they are the core structure of numerous biologically active compounds [2].Pyrazole derivatives are associated with wide spectrum of biological activities such as analgesic, antipyretic, antimicrobial and plant growth regulating [3].
In this study kinetics and thermodynamics of the following reaction have investigated.



X =H

Theoretical methods have used to study all of the channels of this reaction. Ab initio calculations were carried out using the Gaussian 03 program. The geometries of all the stationary points were optimized at the MPWB1K [4], methods with 6-311++G** basis set. The potential energy surface for each possible pathway has been investigated by employing MPWB1K method. Harmonic vibrational frequencies were obtained at the MPWB1K/6-31++G** level in order to characterize stationary points as local minima or first-order saddle points and to obtain zero-point vibration energy corrections. The number of imaginary frequencies (0 or 1) indicates whether a minimum or a transition state has been located. Thermodynamics of these reactions has also studied with calculation of gibs energy for all channels. We have funded a lot of useful information about kinetics, mechanism and thermodynamics of these reactions, which will be presented in the conference.

References:

[1] Bacchetti, T.; Gazz. *Chem. Ital.***1961**, *91*, 866.
[2] McDonald, E.; jones, K.; Brough, P.A.; Drysdale, M. J.; Workman, P. *Curr. Top. Med. Chem.* ***2006****, 6* ,1193.
[3] Dhol P N ,Achary T E, Nayak A.*J Indian Chem Soc*. **1975**, *52*, 1196.
[4] Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A*. **2004**, *108*, 6908.

Synthesis and characteriza of conductive polypyrrole doped with PTSA under electric field

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Polipyrrole has drawn a lot of interests due to its high thermal and atmospheric stability in addition to high conductivity [1,2]. Intrinsic charge carriers in either bulk particles or their surfaces move locally under the applied electric field to generate a field-induced structure with polarized particles. Electric and magnetic field can influence the chemical reaction containing radicals [3] and induce orientation of most organic polymer molecules and biological macromolecules [4].

We synthesized polypyrrole in the presence of para-toluene-sulfonic acid (PTSA) as dopant at room temperature at different times [5,6]. So, we measured its mass and conductivity at the best time of polymerization. Then, we repeated this reaction under different electrical fields at the best time and measured the mass and conductivity, as well. In continue we carried chemically polymerization in best electric field at different times.

Then, produced polymers are characterized using FT-IR and UV-visible spectroscopies. The thermal properties of polymer were studied by thermo gravimetric (TGA) and differential scanning calorimetry (DSC). Scanning electron microscopy (SEM) images supported the formation of polymer and showed morphology feature and homogeneous structure on polymer. The experimental results show that the electric field has an orientation effect on polypyrrole chain and increase molecular weight and electrical conductivities. There exists the interaction between free radical initiator, high dielectric solvent (water) and cation radicals of aniline due to the electrostatic interaction. The longer polymerization time and the higher electric field can lead to degradation of polypyrrole film and decrease conductivity and molecular mass. The experimental results show that the electric field has an orientation effect on polypyrrole chain and increase molecular weight and electrical conductivities. Electrical conductivity of produced Polypyrrole has been studied by four-point probe method and produced 1.73×10^{-2} S/cm conductivity for it. The polymcrs can use in several industry applications.

References:

[1] Salmon, M.; Kanazawa , K.K.; Diaz , A.F.; Krounbi , M.; *J. Polym. Sci.Polym. Lett. Ed*. **1982**, *20* , 187.
[2] Chen , S.A.; Liao, C.S.; *Macromolecules.* **1993**, 26, 2810.
[3] Mac Diarmid , A. G.; *Angew. Chem. Inst. Ed*. **2001**, *40,* 2581.
[4] Zhao, X.; Mingzhu W.M.; *European Polymer Journal*, **2006**, *42*, 247.
[5] Kwan, S.J.; Hoosung, L.; Bongjin, M. *Synthetic Metals*. **2004**, *143*, 289.

Synthesis and capping of gold nanoparticles by the two amino acids L-tyrosine and L- argenine in aqueous solution with various pH values

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Nanoparticles have been increasingly used as carriers for binding proteins, enzymes, and other biologically active compounds. The interaction between the surface of nanoparticles and protein can easily disrupt the native conformation and, therefore, the protein function. This has implications for the biological impact of nanoparticles. [1]

The most common nanoparticles are metallic gold nanoparticles (GNP) prepared by the reduction of $HAuCl_4$ in the presence of a reducing agent. [2,3] In this work, we report a simple method and one-pot synthesis route to prepare chemically stable, well-dispersed, uniform sized amino acid-coated GNPs in aqueous solution. L-Arginine (a basic and very hydrophilic amino acid) and L-tyrosine (a neutral polar amino acid which because of the phenyl ring side chain is also hydrophobic in character) were acted both as a mild reductant and coating agent in the reaction.

The size of GNPs is controlled by adjusting the pH value of the reaction solution. The obtained particle sizes were varied in the range of 25-30 nm without loosing the uniformity in its size distribution by varying the concentration of the reducing agent, Fig. 1. The amino acid-coated gold nanoparticles were characterized by UV-Vis spectroscopy, Transmission electron microscopy (TEM), thermogravimetric analysis (TGA), and ^1H NMR spectroscopy.

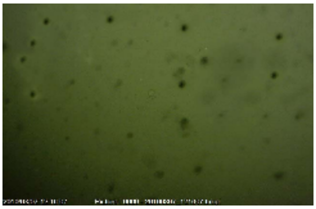

Fig 1. TEM image of the nanoparticles (<30nm)

References:

[1] Lynch, I.; Dawson, K.A. *Nanotoday* **2008**, *3*(1-2), 40.
[2] Zou, J.; Guo, Z.; Parkinson, J. A.; Chen, Y.; Sadler, P. J. Chem. Commun. 1999, 1359.
[3] Bhargava, S.K.; Booth, J. M.; Agrawal, S.; Coloe, P.; Kar, G. *Langmuir* **2005**, *21*(13), 5949.

Natural kaolin supported sulfuric acid as an efficient catalyst for selective hydrolysis of nitriles to amides

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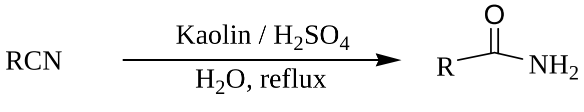
The Preparation of amides is an important transformation from both academic and industrial points of view. Amides not only constitute versatile building blocks in synthetic organic chemistry, but also exhibit a wide range of industrial applications and pharmacological interest [1]. Most of the known synthetic transformations leading to amides are based on the reaction between an activated carboxylic acid and an amine or ammonia. Nitriles are intrinsically more reactive than carboxylic acids and direct conversion of nitriles to primary amides are more interesting in organic synthesis. However, a base-catalyzed reaction leads to a carboxylate salt, because the second step of the hydrolysis is faster than the first one, and the reaction thus proceeds to the final hydration product rather than stopping at the amide stage. Although in strong acidic solutions it can be possible to obtain amides, it is then necessary to have careful control of the temperature and of the ratio of reagents in order to avoid the formation of polymers which is promoted by the exothermic character of the hydrolysis [2]. Several syntheses of primary amides from nitriles have been reported using $NaBO_3$/MW [3], $ZnCl_2$/MW [4], Co(III) complex, ruthenium complex/sealed tube, TMSCl, KOTMS, and nitrile hydratase. However, most of the reported methods have not been proven in general and practical in scope because of harsh condition or expensive catalyst. In this paper we introduced natural kaolin supported sulfuric acid as an efficient catalyst for the selective hydrolysis of nitriles to primary amides in aqueous conditions.



$$\mathrm{RCN} \xrightarrow[\mathrm{H_2O,\ reflux}]{\mathrm{Kaolin\ /\ H_2SO_4}} \mathrm{RC(O)NH_2}$$

References:

[1] Yamada, H.; Kobayashi, M. *Biosci. Biotechnol. Biochem.* **1996**, *60*, 1391.
[2] Edward, J. T.; Meacock, S. C. R. *J. Chem. Soc.* **1957,** 2000.
[3] Sharifi, A.; Mohsenzadeh, F.; Mojtahedi, M.M.; Saidi, M.R.; Balalaie, S. *Synth. Commun.* **2001**, *31*, 431.
[4] Manjula, K.; Pasha, M. A. *Synth. Commun.* **2007**, *37*, 1545.

Synthesis of some novel tetraimidazolium salts derived from diphenyland Dimethylglycolurils

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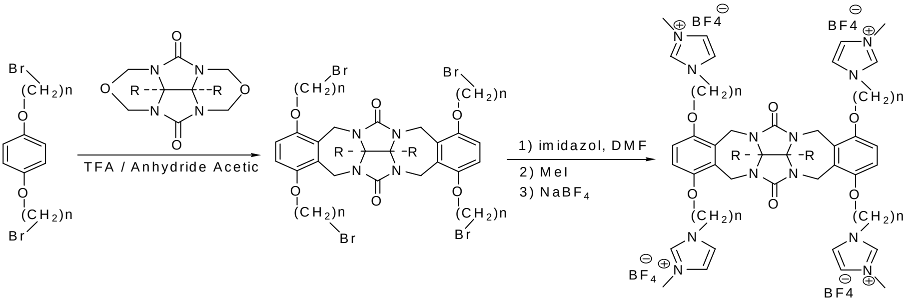
The design and synthesis of host molecules for the binding of neutral guest molecules continues to be an area of interest in supramolecular chemistry.[1] These "u-shaped" clips bind dihydroxy benzenes by means of hydrogen bonding between the hydroxyl groups of the guest and the urea carbonyl groups of the host and by π-π stacking interactions between the guest and the host side walls.[2,3] Also Molecular clips with a large variety of side walls have been synthesized, and the supramolecular chemistry of these clips has been extensively studied.[4]

In this study, several new tetra-imidazolium salts have been synthesized based on diphenylglycoluril and dimethylglycoluril moieties. These salts were readily obtained from the reaction of the corresponding tetrabromo derivatives with imidazole and subsequently methylated by methyliodide and exchanged the iodide anion by sodium tetrafluoroborate to give the tetraimidazolium salts. The results showed some of these salts have low melting points and consequently potential abilities to use as ionic liquids.



References:

[1] Lehn, J. M. *Comprehensive supramoleacular chemistry*, Elsevier science Ltd, Oxford, **1996**: Vol. *2*.
[2] Sijbesma, R. P.; Nolte, R. J. M. *Top. Curr. Chem.* **1995**, *179*, 25.
[3] Rowan, A. E.; Elemans, J. A. A. W.; Nolte, R. J. M. *Acc. Chem. Res.* **1999**, *32*, 995.
[4] Reek, J. N. H.; Priem, A. H.; Engelkamp, H.; Rowan, A. E.; Elemans, J. A. A. W., Nolte, R. J. M., *J. Am. Chem. Soc.* **1997**, *119*, 9956.

Synthesis of novel thiophen drivatives and investigation of electrochemical properties

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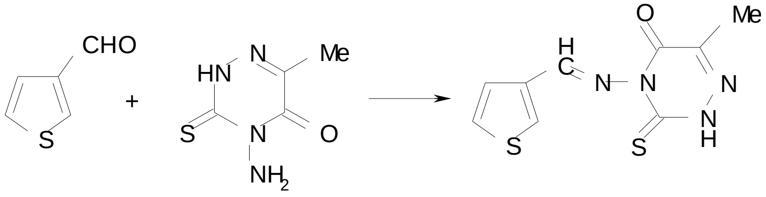
cyclic voltammetry is a simple and valuable way for the study of electrochemical behavior compounds were synthesised for the first one. With using this technique can obtain qualities and quantities information. cyclic voltammetry shows that oxidation/reduction process have done where in potential.in another way thiophen derivatives are suitable monomers for polythiophens among conducting polymers, polythiophene have been the most studied due to its stability to both moisture and oxygen[1-2]. Most conductive polythiophene films were prepared by electrochemical polymerization on noble metals (Pt, Au) in nonaqueous solvents [3-4].

The continue of this project consider an electropolymerization of thiophen in pulp carbon level and the effect of new functional groups in polymerization process and using of the application of new modified electrode for the measurment of some compounds. In this project the Synthesis and electrochemical behavior of new thiophen derivatives in pulp carbon level has been studied with cyclic voltammetrry.



Refrences:

[1] Garnier, F.; Tourillon, G.; Gazard, M.; Dubois, J.C., *J. Electroanal. Chem*. **1983,** *148*, 299.
[2] Wang, S.; Tanaka, K.; Yamabe T., *Synth. Met*. **1989,** *32* , 141.
[3] Sato, M.; Tanaka, S.; Kaerigma, K., *J. Chem. Commun*., **1985,** 713.
[4] Imanishi, K.; Yasuda,Y.; Satoh, M.; Tsushima, R.; Aoki, S., *J. Electroanal. Chem.* **1988,** *242* , 203.

Novel protocol based on green chemistry for the synthesis of benzo[*b*]pyrane derivatives

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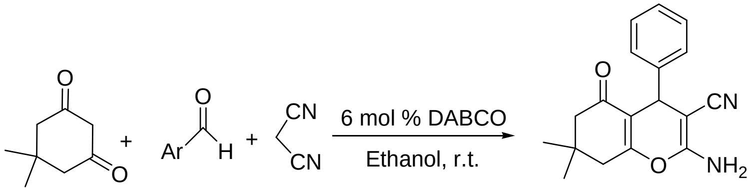
In recent years, 4*H*-benzo[b]pyran derivatives have attracted strong interest due to their useful biological and pharmacological properties [1]. Several methods have been reported for the synthesis of 4*H*-benzopyrans [2]. Most of them have some drawbacks such as low yields, difficult work-up and effluent pollution. Consequently, there is a need to develop an alternative method for the synthesis of tetrahydrobenzopyran derivatives under mild and environmentally friendly conditions.

In continuation of our researches on green chemistry protocols [3], herein we wish to report an efficient, one-pot multi-component reaction for the synthesis of various biologically important heterocyclic compounds *via* a one-pot three-component tandem Knoevengel-cyclocondensation reaction of 5,5-dimethylcyclohexane-1,3- dione, aromatic aldehydes and malononitrile in the presence of catalytic amounts of DABCO (6 mol%) as a catalyst in ethanol. In these conditions the reaction affords the title compounds in high to excellent yields in short reaction times at room temperature.



References:
[1] Bonsignore, L.; Loy, G.; Secci, D.; Calignano, A. *Eur. J. Med. Chem.* **1993**, *28*, 517.

[2] Zhou, J.F.; Tu, S.J.; Gao, Y.; Ji, M, *Chin. J. Org. Chem***. 2001**, 21 , 742–745.

[3] Hasaninejad, A.; Zare, A.; Zolfigol, M.A.; Shekouhy, M, *Synth .Commun.* **2009**, 39 , 569-579.

Synthesis and evaluation of two novel insect-repellent reactive dyes containing *N, N*-dimethyl-*m*- toluamide residue

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N, *N*-dimethyl-m- toluamide (DEET) is used as an insect-repellent chemical. This chemical is usually applied as an ingredient in skin ointments as well as finishing agent for fibre application [1]. In order to combine colouring and insect-repellent activity, two novel azo reactive dyes containing insect-repellent property were synthesized and evaluated. To do this, N, N-dimethyl-m-toluamide (DEET) was first nitrated at the para–position relative to amide functionality [2]. The nitrated product was reduced in the presence of C_2 H_5 OH, $SnCl_4$, HCl to amino group. The produced amine was then condensed with 2, 4, 6-trichloro-1, 3, 5-triazine (Cyanuric chloride) as a reactive group in below 5 °C. The resultant chemical was finally condensed with an amino group present in 6-amino-1-hydroxy naphthalene-3-sulfonic acid (J-acid) to produce 7-(3-chloro-5-(4-(diethylcarbamoyl)-2-methylphenylamino)phenylamino)-4-hydroxynaphthalene-2-sulfonic acid which is used as coupling component of an azo dye. In order to synthesis azo dye sulfanilic acid [1, 3] was diazotized using HCl and $NaNO_2$. The obtained diazonium salt was then coupled to the coupling component to produce insect-repellent reactive dyes. The dyes were then filtered off, purified. All the reactions were monitored step by step using TLC in order to completion. All the intermediates and the dyes were characterized by ^{1}H-NMR, FTIR and UV-VIS spectrophotometer. The spectral data are strongly confirming that the synthesis was successful.

References:

[1] Mokhtari, J.; Philips, D.; Taylor, J.*J. Dyes and Pigments*, **2004**, 63, 51.
[2] Liu, S.; Ma, J.; Zhao, D.*J. Dyes and Pigment*, **2007**, 75, 255.
[3] Kasting, G.; Bhatt, V.; Speaker, T.*J. Toxicology in Vitor*, **2008**, 22, 548.

Cesium carbonate in [omim][BF_4] ionic liquid: a green and recoverable medium for efficient room-temperature synthesis of various benzoxazinones in one pot

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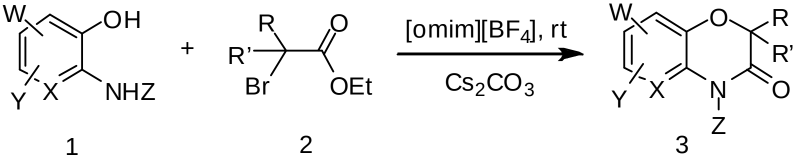
In line with recent environmental mandates to minimize the use of toxic solvents or replace them with safer alternatives, ionic liquids (ILs) have emerged as a new class of stable, non-volatile, and inert media for various organic transformations. Extensive research is carried out in recent years on benzoxazinone scaffold (i.e., 3) since they are important in synthetic and medicinal organic chemistry and contribute to the structure of many biologically active synthetic and natural compounds [1].

In the majority of the available methods, condensation of o-aminophenols or o-nitrophenols with substituted carbonyl compounds or their synthetic equivalents have served as the main pathway for the synthesis of benzoxazinones. Nevertheless, these methods either high temperature treatment is required, more than one step reaction is involved, external stimulant like microwave irradiation is used, or only limited range of substrates is employed.

In continuation of our investigations on heterocyclic chemistry [2], we would like to report a methodology where various o-aminophenols (1) undergo one-pot annulation with several 2-bromoalkanoates (2) at room temperature (1-Methyl-3-octyl-imidazolium tetrafluoroborate) using Cs_2CO_3. The conditions are noticeably mild and the IL medium is efficiently recycled into the subsequent reactions.



Reference:

[1] Ilaš, J.; Anderluh, P. Š.; Dolenc, M. S.; Kikelj, D. *Tetrahedron*. **2005**, *61*, 7325.
[2] Sharifi, A.; Barazandeh, M.; Abaee, M. S.; Mirzaei, M. *Tetrahedron, Lett.* **2010**, *51*, 1852.

Aromatization of 1,3,5-trisubstituted 4,5-dihydro-1H-pyrazoles by in-situ generation of NO^+ from 2,4,6-trichloro-1,3,5-triazine and sodium nitrite

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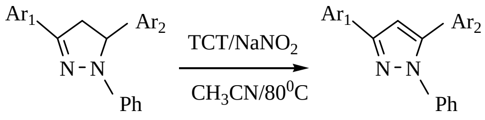
Pyrazoles and pyrazolines are important five-membered heterocyclic compounds, with a long history of applications in the pharmaceutical and agrochemical industries due to their herbicidal, fungicidal, insecticidal, analgesic, antipyretic, antitumor, antidiabetic, antidepressant, antibacterial and anti-inflammatory properties [1-2].

There have been many attempts to develop alternative methods for pyrazoles synthesis. The most important methodology toward synthesis of pyrazoles is oxidative aromatization of 1,3,5-trisubstituted-2-pyrazoline [3] to their corresponding pyrazole. Therefore, oxidative aromatization of pyrazolines with oxidizing reagents should provide an efficient method for the preparation of pyrazole derivatives [4-6].

Herein, we report a simple, versatile and cost-effective protocol for the aromatization of 1,3,5-trisubstituted-2-pyrazolines to the corresponding pyrazoles by in situ generation of NO^+ from 2,4,6-trichloro-1,3,5-triazine and sodium nitrite under thermal condition with moderate to good yields.



1a-m **2a-m**

References:

[1] Ahn, J. H.; Kim, H. M.; Jungs, S. H.; Kang, S. K.; Kim, K. R.; Rhee, S. D.; Yang, S. D.; Cheon, H. G.; Kim, S. S. *Bioorg. Med. Chem. Lett.* **2004,** *14*, 4461.
[2] Deng, L.; Tao, W.; Lv, J.; Wang, W. *J. Heterocycl. Chem.* **2009,** *46,* 640.
[3] Maleki, B.; Azarifar, D.; M. K.; Moghadam, S. F.; Hojati, M.; Gholizadeh, H. Salehabadi, *J. Serb. Chem. Soc.* **2009,** *74,* 1299.
[4] Kumar, A.; Maurya, A. R.; Sharma, S. *Bioorg. Med. Chem. Lett.* **2009,** *19,* 4432.
[5] Wentao, W.; Rui, L.; Qiang, L.; Longmin, W. *Chin. J. Org. Chem.* **2009,** *2,* 283
[6] Azarifar, D.; Zolfigol, M. A.; Maleki, B.*Synthesis* **2004**, *11,* 1744.

Synthesis, characterization and properties of geminal *N,N* -dimethyl aminopyridinium ionic liquids

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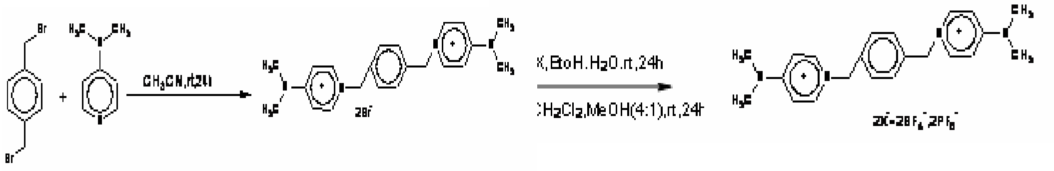
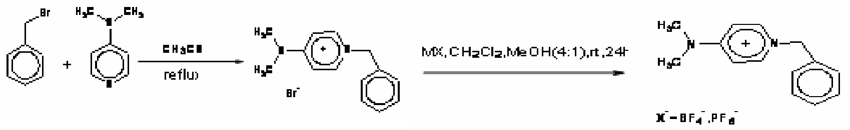
Geminal dicationic liquids have been shown to possess superior physical properties in terms of thermal stability and volatility compared to traditional ionic liquids (ILs) [1]. Consequently, they have been proposed as novel high-temperature lubricants [2], solvents in high-temperature reactions, and ultrastable separation phasesand have potential in extractions similar to monocationic liquids and mass spectrometry[3] where ordinary ILs fail.

Herein, a novel geminal N,N-dimethyl aminopyridinium ionic liquid with a rigid spacer, 1,1 ′- (1,4 –phenylene bis methylene) bis (N,N-dimethyl amino-pyridinium) dibromide was synthesized, with high yield of 92 %, and N-phenylen methylene 4- (N,N-dimethyl aminno) pyridinium bromide, was also synthesized, with yield of 96%.

Then the geminal dication and its monocationic analogue were exchanged with BF_4^- and PF_6^- of anions, and as a result, variation anion on some physicochemical properties of this compounds were investigated. FT-IR,^{1}HNMR,^{19}FNMR were applied to identify the molecular structure of two compounds in present each of anion.





References

[1] Anderson, J. L.; Ding, R.; Ellern, A.; Armstrong, D. W. *J. Am. Chem.Soc.* **2005**, 127, 593–604.

[2] Jin, C.-M.; Ye, C.; Phillips, B. S.; Zabinski, J. S.; Liu, X.; Liu, W.;Shreeve, J. M. *J. Mater. Chem.* **2006**, 16, 1529–1535.

[3] Han, X.; Armstrong, D. W. *Org. Lett.* **2005**, 7, 4205–4208.

One-pot, multi component reaction of triphenylphosphine, acetylenic esters and 1,3- Diimino isoindoline

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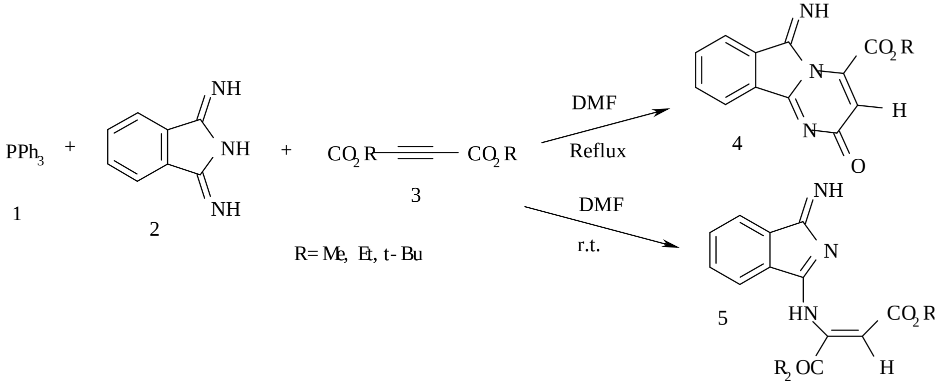
Six-membered nitrogen heterocyclic compounds occupy an important position in natural product chemistry, featuring in plant life, most notably as the flavonoids, and in the marine environment where they form a part of the wide range of macrocyclic molecules [1].

In recent years there has been increasing interest in the synthesis of organophosphorus compounds, those bearing a carbon atom bound directly to a phosphorus atom [2-4]. This interest has resulted from the recognition of the value of such compounds for a variety of industrial and chemical synthesic uses.

In this spirit we examined the triphenylphosphine (1) based multi component reaction of 1,3-diiminoisoindoline (2) with symmetric Acetylenic esters (3). The reactions proceeded in room temperature and refluxing DMF and afforded (4, 5) in good yields. The structure of products was deduced from ^{1}H NMR, ^{13}C NMR, Mass and IR spectral data.



References:

[1] Norcross, R. D.; Paterson, I. *Chem. Rev.* **1995**, *95*, 2041.
[2] Kolodiazhnyi, O. I. *Russ. Chem. Rev.* **1997**, *66*, 225.
[3] Bestmarm, H. J.; Vostrowsky, O. *Top. Curr. Chem.* **1983**, *109*, 85.
[4] Yavari, I.; Maghsoodlou, M. T. *Tetrahedron Lett.* **1998**, *39*, 4579.

Deoxygenation of sulfoxide with silica bromide

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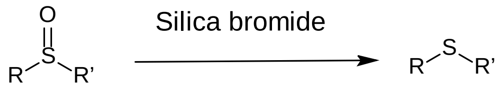
Deoxygenation of sulfoxide to sulfide is an important synthetic transformation in organic chemistry. Many reagent and methodologies [1-3] are developed for the deoxygenation of sulfoxides. One of the reported reagents for deoxygenation of sulfoxides is iodotrimethylsilane [4]. Its handling does not need special precaution and work up of reaction mixture is not time consuming. This reagent is however, expensive.

In this work, we wish to report synthesis and an application for silica bromide. We investigated the reaction of sulfoxides with silica bromide. The present method is mild and effective, using an inexpensive reagent, and thus offering significant advantages.

Silica bromide is obtained from reaction of silica gel and phosphorus tribromide. The resulting yellowish powder is sensitive to moisture and must be kept in a dessicator. Sulfoxides are converted to sulfides by reaction with silica bromide in dichloromethane at room temperature in excellent yields. Deoxygenation of both alkyl and aryl sulfoxides tales place very smoothly without any side product formation.



R, R' = Alkyl, Aryl

References:

[1] Madesclaire, M. *Tetrahedron* **1988**, *44*, 6537.

[2] Olah, G. A.; Narang, S. C.; Gupta, B. G. B.; Malhotra, R. *J. Org. Synthesis* **1976**, 61.

[3] Olah, G. A.; Husain A.; Singh, B. P.; Mehrotra, A. K. *J. Org. Chem*. **1983**, *48*, 3667.

[4] Olah, G. A.; Gupta B. G. B.; Narang S. C. *Synthesis*, **1977**, 583.

A cost effective synthesis of *1,8*-dioxo-decahydroacridines in water using AL(NO_3)$_3$ catalyst

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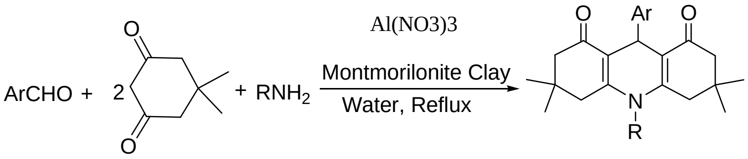
Acridine derivatives have proved to be valuable as drugs for the treatment of cardiovascular disorders, and constitute an important class of calcium channel. In the field of antitomour DNA-binding agents, the class of acridine derivatives plays an important role both in terms of number of compounds and their anticancer activities.

4-Aryl-1,4-dihydropyridines (1,4-DHPs) have proved to be valuable as drugs for the treatment of cardiovascular disorders, and constitute an important class of calcium channel blockers [1]. With a 1,4-DHP parent nucleus, 1,8-dioxo-decahydroacridines have been shown to have very high lasing efficiencies and used as photoinitiators [2]. Many acridinediones have been synthesized by the reactions of aldehydes with 2 equiv. of 1,3-cyclohexanedione or 5,5-dimethyl-1,3-cyclohexanedione and appropriate amines via various methods [3]. Most of the reported methods for the synthesis of acridine derivatives suffer from one or more disadvantages like: poor yields, difficult work-up, effluent pollution and/or need of special equipments.

Herein we would like to report an efficient synthesis of acridine derivatives from the reaction of dimedone (2 eq.), arylaldehyde (1 eq.) and amine (1 eq.) in water in the presence of catalytic ammounts of aluminium nitrat [Al(No_3)$_3$].

This method provides several advantages such as simple work-up, environmental friendliness and shorter reaction time along with high yields. The reactions examined with various structurally diverse aromatic aldehydes in the temperatour 80 and catalyst 25% and H_2O solvent., the reactions proceeded efficiently and the desired products were obtained in good to high yields.



References:

[1] Janis, R.A.; Triggle, D.J. *J. Med. Chem.* 1983, *26*, 775.
[2] Tu, S.; Miao, C.; Gao, Y.; Fang, F.; Zhuang, Q.; Feng, Y.; Shi, D. *Synlett* 2004, 255.
[3] Wang, G.W.; Miao, C.B. *Green Chem.* 2006, *8,* 1080.
[4] Kawabata, T.; Fujisaki, N.; Shishido, T.; Nomura, K.; Sano, T.; Takehira, K. *J. Mol. Catal. A: Chem.,* 2006, *253*, 279.

An efficient and simple route for the synthesis of *N*-(2-Pyridyl)-4-ethoxy-5-oxo-2,5-dihydro-1*H*-pyrolle-2,3-dicarboxylates.

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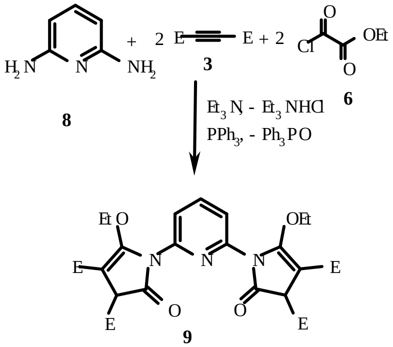
Three-component reaction of 2-aminopyridines, dialkyl acetylenedicarboxylates, triphenylphosphine and ethyl chlorooxoacetate in the presence of triethylamine provides a sufficient rout for the synthesis of dialkyl *N*-(2-pyridyl)-4-ethoxy-5-oxo-2,5-dihydro-1*H*-pyrolle-2,3-dicarboxylates in good yields.

General procedure for preparation of compounds **7a-h**: To a magnetically stirred solution of PPh_3 (2 mmol) and aminopyridine derivative (1 mmol) in CH_2Cl_2 (10 mL) was added dropwise a mixture of DAAD (2 mmol) in CH_2Cl_2 (3 mL) at room temperature over 2 min. The reaction mixture was then stirred for one more min. triethylamine (2 mmol) and ethyl chlorooxoacetate (2 mmol) was added and the reaction mixture was stirred for more 24 h. Solvent was evaporated and the residue was purified by column chromatography on SiO_2 using EtOAC-hexane (1:4) mixture as eluent.



3 , 9	E	%Yield of **9**
a	CO_2t-Bu	65
b	CO_2 Me	70

References:
[1] Yavari, I.; Ahmadian-Razlighi, L. *Phosphorus, Sulfur, and Silicon*, **2006**, 181, 771.
[2] Yavari, I.; Bayat, M. *Synthetic Commun.*, **2002**, 32, 2527.
[3] Anary-Abbasinejad, M.; Charkhati, K; Anaraki-Ardakani, H. *Synlett*, **2009**, In press.

Synthesis of amidoalkyl naphthols, diarylbenzoxanthenes and tetrahydrobenzo[a]xanthene-11-one in the presence of efficient catalysts

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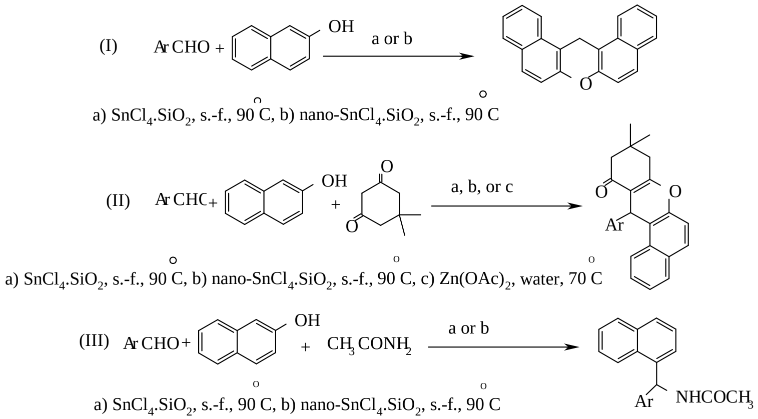
$TiCl_4$ as a dense, colourless distillable liquid is a strong Lewis acid that exothermically forming adducts with even weak bases such as THF and explosively with water, releasing HCl [1]. Neat $SnCl_4$ is difficult to handle due to its moisture sensitivity. Silica supported $TiCl_4$ ($TiCl_4.SiO_2$) is less hygroscopic, more stable and reactive than neat $TiCl_4$.

One pot multicomponent reactions (MCR's) increase the efficiency of the reaction and decrease the number of laboratory operations along with quantities of solvent and chemicals used. They also reduce the reaction time considerably and facilitate the yield of products than the normal multiple step methods [2].

We report herein, the synthesis of diarylbenzoxanthenes (I) and tetrahydrobenzo[a]xanthene-11-one (II) and amidoalkyl naphthols (III) in the presence of nano-$TiCl_4.SiO_2$ in solvent free condition at 90°C. Meanwhile, tetrahydrobenzo[a]xanthene-11-one (II) were synthesized in the presence of $Zn(OAc)_2$ in water at 70°C.



The advantages of these methods are reduced reaction times, higher yields, mild reaction condition and easy purification.

References:

[1] Hans, G.; Völz et al. "Pigments, Inorganic" in Ullmann's Encyclopedia of Industrial Chemistry, Wiley- VCH, Weinheim, 2006.
[2] Domling, A.; Ugi, I. *Angew. Chem. Intl. Ed.* **2000**, *39*, 3168.

Synthesis, characterization and antimicrobial activity studies of sulfonamides and dithiocarbamate complexes nanoparticles

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[b] *Member of Young Researchers Club, Islamic Azad University, Takestan, Iran .*
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The importance of sulfonamides and dithiocarbamate possess many types of biological activities, and representatives of this class of pharmacological agents are widely used in clinic as antibacterial, hypoglycemic, diuretic, anti-hypertensive, antifungal, antiviral and antitumour [1-3]. The dithiocarbamate ligands have also proven to be excellent compounds due to their extensive applications as fungicides, pesticides, vulcanization accelerators and in their use in motor fuels, and as high pressure lubricants [4]. Nanoparticles of sulfonamide are prepared by the reaction of a benzenesulfonyl chloride with ammonia or an amine in solvent (Scheme 1). Nanoparticles of dithiocarbamate complexes prepared by condensation of acetophenone or 4-Methylacetophenone with 1,6-hexamethylenediamine in methanol followed by reduction of the Schiff base with $NaBH_4$ in methanol. One-pot synthesis from this amine, carbon disulfide, triethylamine and $CoCl_2.6H_2O$ gave colorless precipitates. The ultrasonic treatment applied for preparation nanoparticles. The antibacterial activity of nanoparticles derivatives tested against microorganism and compared with non-nano conditions. The resulting dithiocarbamate macrocyclic nano complexes and sulfonamides nanoparticles were characterized by X-ray diffraction (XRD), infrared spectroscopy (IR) and transmission electron microscopy (TEM).

$$C_6H_5SO_2Cl + R - NH_2 \xrightarrow{r.t} C_6H_5SO_2NHR$$
$$R : alkyl\ , aryl$$

Scheme 1.

References:

[1] Abbate, F.; Casini, A.; Owa, T.; Scozzafava, A.; Supuran,. C. *Bioorganic & Medicinal Chemistry Letters*. **2004**, *4*, 217.
[2] Supuran, C.; Casini, A.; Scozzafava , A.. *Medicinal Research Reviews.* **2003**, *23*, 535.
[3] Mishra, A.K.; Kaushik N.K.;. *Spectrochimica Acta Part A.* **2008**, *69*, 842.
[4] Nishat, N.; Haq, M. M.; Siddiqi. K. S *Synthesis and Reactivity in Inorgranic, Metal-Organic and Nano-Metal Chemistry*. **2003**, *33*, 566.

Ultrasonic-assisted one-pot synthesis of pyrazolo[1,2-a][1,2,4]triazole-1,3-diones

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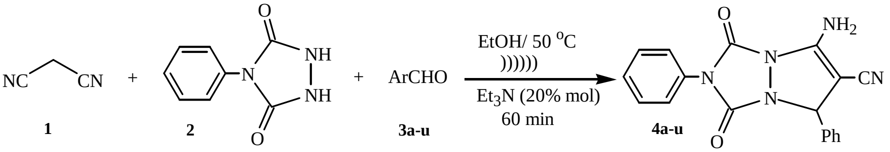
With regard to the previous reports on three-component reactions for the synthesis of fused-ring heterocycles including pyrazole-fused heterocycles [1-5], we were encouraged to preliminary examine polycondensation reaction of a mixture of malononitrile **1**, 4-phenylurazole **2**, and benzaldehyde **3a** in ethanol using a catalytic amount of triethylamine as an inexpensive and readily available catalyst under ultrasonic irradiation conditions.

In this reaction, pyrazolo[1,2-a][1,2,4]triazole-1,3-dione **4a** was afforded in 93% yield after 45 min irradiation at 50 °C. To achieve suitable reaction conditions, i.e., lower reaction times and temperature for the synthesis of 1*H*-pyrazolo[1,2-a][1,2,4]triazole-1,3-diones **4**, various solvents and reaction conditions were investigated in the reaction of malononitrile **1**, 4-phenylurazole **2**, and benzaldehyde **3a** as a model reaction.

When the reaction was carried out in the absence of the catalyst, no detectable amount of respective product was formed and the starting materials remained almost intact. To show the role of ultrasound, the reaction was investigated without ultrasonic irradiation at the same temperature (50 °C) in various solvents. In all cases it was observed that the use of ultrasound leads to the faster reaction and higher yields.



Scheme 1.

References:

[1] Ghahremanzadeh, R.; Imani Shakibaei, G.; Bazgir, A.; *Synlett*. **2008,** *8,* 1129.
[2] Temouri, M.B.; *Tetrahedron.* **2006**, *62,* 10849.
[3] Shaterian, H.R.; Hosseinian, A.; Ghashang, M.; *Arkivoc*. **2009**, *2*, 59.
[4] Shaterian, H.R.; Ghashang, M.; Feyzi, M.; *Appl. Catal. A Gen*. **2008**, *345*, 128.
[5] Al-Assar, F.; Zelenin, K.N.; Lesiovskaya, E.E.; Bezhan, I.P.; Chakchir, B.A.; *Pharm. Chem. J.* **2002**, *36*, 598.

Synthesis and characterization of UV-curable polydimethylsiloxane urethane dimethacrylate

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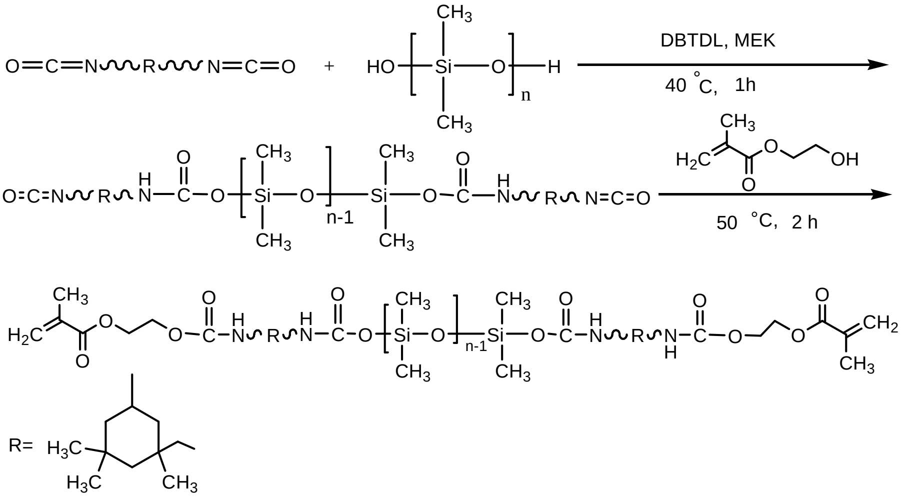
The UV-curable polydimethylsiloxane urethane dimethacrylates are linear unsaturated polydimethylsiloxane which two monomers of hydroxyethyl methacrylate (HEMA) were connected to two hydroxyl groups of polydimethylsiloxane by urethane bonds. These were synthesized in two steps. In the first step, polydimethylsiloxane diisocyanate was prepared by reaction of linear polydimethylsiloxane having hydroxyl terminal groups and isophorone diisocyanate (IPDI) in presence of methyl ethyl ketone (MEK) as solvent and dibutyld tin dilaurate (DBTDL) as catalyst. Then, unsaturated polydimethylsiloxane was prepared by reaction polydimethylsiloxane diisocyanate and hydroxyethyl methacrylate (HEMA). The UV-curable polydimethylsiloxane urethane dimethacrylates have been characterized with ^{1}H-NMR, FT-IR and GPC.



References:

[1] Chambon P.; Cloutet E.; Cramail H.; Tassaing T.; Besnard M. *Polymer*. **2005**, *46*, 1057.
[2] Madhavan K. ; Reddy B. *Journal of Membrane Science*. **2009**, *342*, 291.

One-pot synthesis of new 4-asetamide-2-amino-4H-chromenes in EtOH under ultra sonic condition

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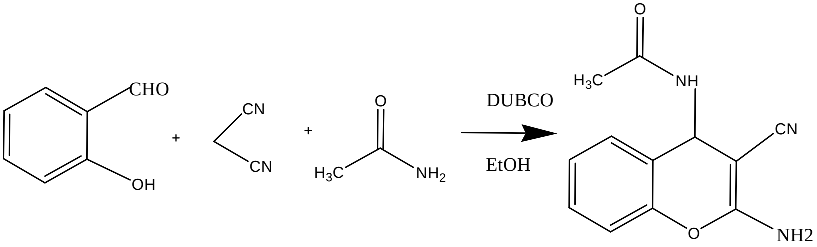
Corresponding Author E-mail: azarifar@basu.ac.ir

2-Aminochromoenes are widely employed as pigments, cosmetics,agrochemicals and represent an important class of chemidcal entities being the main constituents of many natural products[1].Due to the unique pharmacological properties of 2-Aminochromoenes, the development of synthetic methods enabling facile access to this hetrocycle is desirable .Muiticoponent reaction are special types of synthetically useful organic reaction in which three or more different starting materials react to a final product in a one-pot procedure. MCRs are powerful tools in modern drug discovery process and allow the fast , automated and high-throughput generation of organic compound[2]. According to current synthetic requirements effective and environmentally benign multicomponent procedures are particularly wecome. As part of our current studies on the design of new routs for the preparation of biologically active hetrocyclic compounds[3] , we herein wish to report our investigation of a new multicomponent reaction involving Aryllaldehyde, malononitrile and Asetamide and DUBCO in EtOH.



References:

[1] Hafez, E. A.; Elagameny, A. G. A. *Hetrocycles*, **1987**, *26*, 903.
[2] Domling, A. *Curr. Opin. Chem .Biol.* **2000**, *4*, 318.
[3] Shanthi, G; Subbulakshmi, G.; *Tetrahedron*, **2007**, *63*, 2057.

Substituent group effect on the performance of the benzodiazepine derivative drugs; A computational approach

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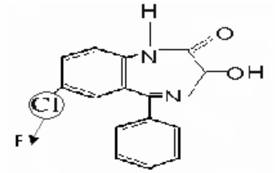
A benzodiazepine is a psychoactive drug whose core chemical structure is the fusion of a benzene ring and a diazepine ring[1]. Benzodiazepines enhance the effect of the neurotransmitter gamma-aminobutyric acid (GABA). GABA controls the excitability of neurons by binding to the $GABA_A$ receptor. The $GABA_A$ receptor is a protein complex located in the synapses of neurons [2].

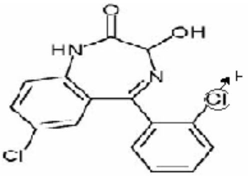
All $GABA_A$ receptors contain an ion channel that conducts chloride ions across neuronal cell membranes and two binding sites for the neurotransmitter gamma-aminobutyric acid (GABA). Benzodiazepines bind at the interface of the α and γ subunits on the $GABA_A$ receptor. Binding also requires that alpha subunits contain a histidine amino acid residue [3].

In this work, we have studied influence of substituent groups effects on the electronic and structural properties of the two benzodiazepine derivative drugs using the DFT-B3LYP method and 6-311G* basis set by Gaussian 03 program package. The results show that the presences of the substituent groups in the molecular skeleton of these drugs have not considerable effects on the geometry parameters; however, the overall atomic charges analysis shows that the side benzene rings electric charges are decreased considerably in both substitutions cases, therefore the electronic properties changed significantly.

According to the obtained results, it is possible to combine both electron donating and electron withdrawing groups in the molecular skeleton to designing new derivative of benzodiazepine drugs with the new and better performance effects.



Oxazepam



Lorazepam

References:

[1] Pallmann, T; Jonasb, U;Wagner, M; Thevisd, M; Kaeferstein, H; Rothschild, M. A; Bender, K. *European Journal of Pharmaceutical Sciences,* **2010,** *39,* 233.
[2] Whiting, P. J. *Drug Discov. Today,* **2003**, *8*, 445.
[3] Tietz, E. I.; Huang, X.; Chen, S.; Ferencak,W. F. *Neuroscience* **1999**, 91, 327.

p-Toluene sulfunic acid catalysed solvent free synthesis of furan derivatives

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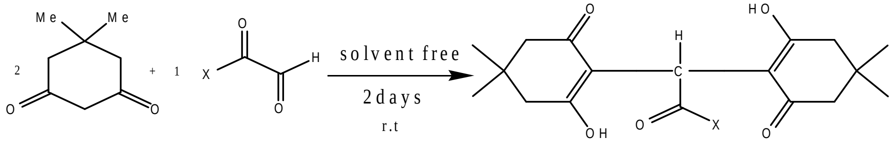
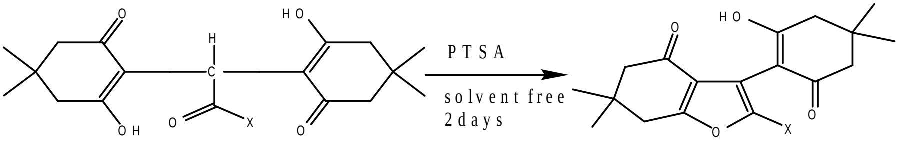
Polysubstituted furans play an important role in organic chemistry not only due to their presence as key structural units in many natural products and in important pharmaceuticals, but they can also be employed in synthetic chemistry as building blocks. For this reason the synthesis of Polysubstituted furans continues to attract the interest of many synthetic chemists. P-toluene sulfonic acid has gained interesting attraction in recent years due to economic and environmental consideration. this catalyst is generally inexpensive and easily available. They can conveniently be handled and removed from the reaction mixture, thus making the experimental procedure simple and eco-friendly. Herein we wish to repot a simple and efficient method for the synthesis of dihydro-3-(2-hydroxy -4,4-dimethy1-6-oxocyclohex-1-enyl)-6,6 dimethylbnzofuran-4(5h)-one by using of P-toluene sulfonic acid as a catalyst under solvent free conditiond . This reaction is cyclization of compound 3 that was obtained firstly by the reaction of a CH-acid such as dimedon with glyoxal in water as solvent and catalyst at room temperature. The experimental procedure in two steps is very simple and the products are in excellent yields.



Scheme 1

X = H, Ph, CH3, 3-Floro-Ph



Scheme 2

References:
[1] Lipshutz, B.H. *Chem.. Rev*. **1986**, 86, 795.
[2] Nakanishi, K. *Natural Products Chemistry*; Kodansha: Tokyo, **1974**.
[3] Daqs, B.; Thirupathi, P.; Mahender, I.; Reddy, K. R.; Ravikanth, B.; Nagarapu, L. *Catal. Commun*. **2007**, 8, 535.

HMDI-βCD as a new solid-liquid phase-transfer catalyst for facile conversion of benzyl halides to thiocyanates in water

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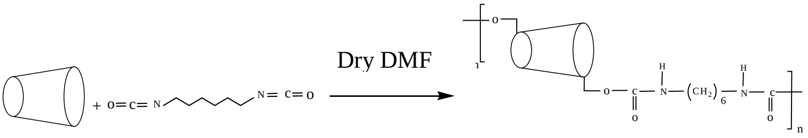
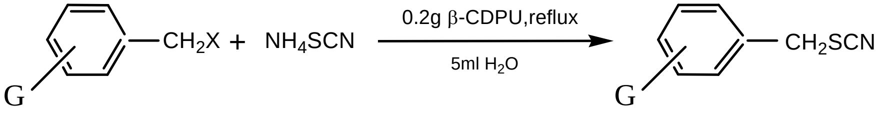
Cyclodextrins are ring-shaped molecules containing an apolar cavity with a diameter 4–8 Å wide and approximately 8 Å deep. Because of the hydrophilic nature of the surface, the materials are dissolved in water. However, hydrophobic groups on the inner surface of the nanoporous molecules attract hydrophobic organics that bind noncovalently to the apolar cavity[1].Recently, polycyclodextrins have been developed as binders for energetic materials and as sorbants for biological materials, and exhibit potential for development as sorbant materials for water filtration[2].

In this study, cyclodextrin polyurethane polymer was prepared (scheme1) and used as the phase transfer catalyst for efficient conversion of benzyl halides to the corresponding benzyl thiocyanates in water. (scheme2) The reaction performed under reflux condition and gave the products in excellent yields. Furthermore, the catalyst could be recycled by facile separation without any loss of activity.



(scheme1)



(scheme2)

Reference:
[1] Szejtli, *J. Chem. Rev*.**1998**, *98*, 1743.
[2] Li, D. Q., Ma, M., *Chemtech*., **1999,** *35*, 31.

Functionalized MCM-41 base-catalyzed one-pot synthesis of 2-amino-3-cyano-4-aryl-7,7-dimethyl-5-oxo-4*H*-5,6,7,8-tetrahydrobenzo[*b*]pyran

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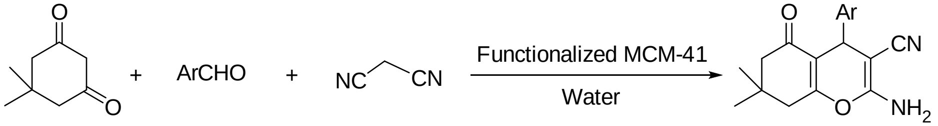
The 4*H*-benzo[*b*]pyran group and their derivatives have attracted strong interest due to their useful biological and pharmacological properties, such as anti-coagulant, spasmolytic, diuretic, anticancer, anti-anaphylactin. Furthermore, these compounds can be employed as pigment, photoactive materials, potential biodegradable agrochemicals and utilized as important regulators for potassium cation channel [1]. The importance of these compounds has led many workers to synthesize them with using new methods [2]. However, some methods suffer from drawbacks like some longer reaction times, unsatisfactory yields, harsh reaction conditions, and use of a large quantity of organic solvent.

In continuation of our investigations in the synthesis of 1,4-dihydropyridines (DHPs) and dihydropyrimidines (DHPMs) [3], herein we describe an efficient and convenient synthesis of 2-amino-3-cyano-4-aryl-7,7-dimethyl-5-oxo-4*H*-5,6,7,8-tetrahydrobenzo[*b*]-pyran using functiona-lized MCM-41 base catalyst. In this work we introduce a three-component reaction of aldehyde, malononitril, and dimedone in water in the presence of a catalytic amount of functionalized MCM-41 under mild conditions. 2-amino-4*H*-benzo[b]pyran derivatives are obtained in good to excellent yields by proceeding through a simple, mild, and efficient procedure utilizing functionalized MCM-41 base as catalyst in aqueous media.



References:

[1] a) Sun, H. B.; Hua, W.Y.; Chen, L.; Peng, S. X.; Wang, T.; Liu, G. Q. *Chem. J. Chin. Univ.* 1997, 18, 730; b) Andreani, L. L.; Lapi, E. *Bool. Chim. Farm.* **1960**, *99*, 583; c) Hafez, E. A.; Elnagdi, M. H.; Elagemey, A. G. A.; El-Taweel, F. M. A. A. *Heterocycles* **1987**, *26*, 903.

[2] a) Jin, T. S.; Wang, A. Q.; Wang, X.; Zhang, J. S.; Li, T. S. *Synlett* **2004**, 871; b) Gao, S.; Tsai, C. H.; Tseng, C.; Yao, C. F. *Tetrahedron* **2008**, *64*, 9143; c) Cella, R.; Stefani, H. A. *Tetrahedron* **2009**, *65*, 2619.

[3] a) Mirza-Aghayan, M., Moradi, A.; Bolourtchian, M.; Boukherroub, R. *Synth. Commun.* **2010**, *40*, 8; b) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. *J. Iran. Chem. Soc.* **2010**, *7*, 269; c) Mirza-Aghayan, M.; Khoshkameh Langrodi, M.; Rahimifard, M.; Boukherroub, R. *Appl. Organometal. Chem.* **2009**, *23*, 267.

Study of the level of energy in electro cycle opening Loop reaction of (Z)-3,4-dichlorohexa-1,3,5-triene and Dewar Benzene structure by using quantum Mechanic method of DFT by NBO Analysis

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Quantum mechanic calculation in theory of the level B3LYP/6-311+G**and HF/6-311+G** is done for surveying level of energy in opening Loop reaction of Benzene dewar and it's result is reported Result show that this reaction is .In below table Completely receiving heat and process of changing Isomer is along with one direction rotating that this Rotating is done for decreasing level of energy This rearrangement .Making constant structure Is along with replacing π electrons breaking One σ bond and forming constant structure of Benzene and activation energy for this structure Amount of energy .Is equal to 161.380075 KCal/mol Level in different reaction has been reported in Analysis result NBO show that Below table Rank of bonding after doing opening loop Mechanism Benzene dewar and forming the same Benzene is equal to 1.3.(Fig1)

Too Quantum mechanic calculation has done in theory of the level B3LYP/6-311+G**and HF/6-311+G**and results has been reported in below result show that this reaction is endothermic. Completely and by doing electrocycle reaction One circle structure of cyclohexa dine with That existing loop due to . two CL orines is formed Replacing π electron and finally forming one New σ bond, activation energy for this reaction Analysis of NBO Is equal to 63.9505800 KCal/mol Confirm this result.(Fig2)

Fig1:

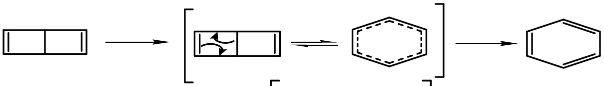
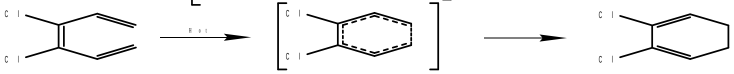


Fig2:



The calculations of quantum mechanics in theory level by using UHF/6-311+G** theory method operated on the structure of (Z)-3,4-dichlorohexa-1,3,5-triene. In order to this, firstly the structure of initial matter and product matter designed by using Chem Office 2008 software, and initial optimization operated by using Winmopac version 2.0 software and AM1 method .The transition mode of structure simulate by using keyword SADDLE and then transition state GAUSSIAN 03W package program and keyword QST2 implemented on a pentum-PC computer with a 730 MHz processor , used for finalization[2]. Eventually, the final optimization and calculation of energy levels operated in theory of the levels B3LYP/6-311+G** and HF/6-311+G**. Also NBO-version 03 program used for calculations of natural bond orbital (NBO).

Reference:

[1] John Mc Murry,*Organic chemistry*,5th.ed, **2000.**

[2] M. j. Frisch et al. *GAUSSIAN 03*, Revision C. 01, Gaussian Inc., Wallingford. CT, **2004.**

Aspartic acid catalyzed chemoselective trimethylsilylation of hydroxyl groups under mild and heterogeneous conditions

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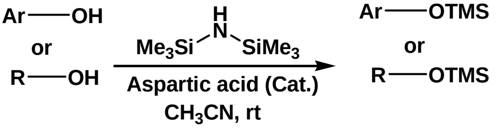
Trimethylsilylation is largely used to protect alcohols and phenols, especially in the chemistry of steroids, sugars and natural product synthesis. Silylation of alcohols is an important process not only as a protecting method of alcohols, but also for synthesis of functional organosilicon compounds [1]. Generally, silyl ethers could be synthesized by reaction of alcohols and phenols using a silylating agent such as hexamethyldisilazane, hydrosilanes, disilanes, alkylsilanes, allylsilanes, trimethylsilyl azide, and *etc* [2-3]; in the presence of a suitable catalyst.

In continuation of our studies on the application of new reagents and catalysts in organic functional group transformations [4-5], herein we disclose a new, efficient and mild procedure for the trimethylsilyl protection of a wide range of alcohols and phenols using 1,1,1,3,3,3-hexamethyldisilazane (HMDS) in the presence of catalytic amounts of aspartic acid under mild and heterogeneous conditions in acetonitrile at room temperature (Scheme 1).



Scheme 1

In summary herein we report a new catalytic method for the efficient trimethylsilylation of alcohol and phenol derivatives under metal-free, mild and heterogeneous conditions.

References:

[1] Shirakawa, E.; Hironaka, K.; Otsuka, H.; Hayashi, T. *Chem. Commun.* **2006**, 3927.
[2] Bffis, A.; Castello, E.; Zecca, M.; Basato, M. *Tetrahedron* **2001**, *79*, 10391.
[3] Shibata, T.; Kanda, K.; Ueno, Y.; Fujiwara, R. *Bull. Chem. Soc. Jpn.* **2006**, *79*, 1146.
[4] Ghorbani-Choghamarani, A.; Nikoorazm, M.; Goudarziafshar, H.; Tahmasbi, B. *Bull. Korean Chem. Soc.* **2009**, *30*, 1388.
[5] Zolfigol, M.A.; Amani, K.; Ghorbani-Choghamarani, A.; Hajjami, M.; Ayazi-Nasrabadi, R.; Jafari, S. *Catal. Commun.* **2008**, *9*, 1739.

Highly efficient heterogenous catalyst for synthesis coumarine dyes using HZSM5 zeolite

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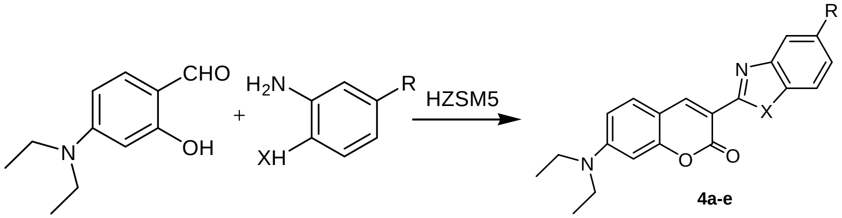
Nowadays, known activity, selectivity and reusability of acid zeolites with the advantage of being solid catalytic eco-friendly materials is leaded them to variety of transformations [1]. Coumarin derivatives with intense fluorescence have found extensive commercial use in a broad range of applications. Synthesis of laser dyes, fluorescent whiteners and organic nonlinear optical materials are some example of their importance in the field of industry. 7-Aminocoumarins, among coumarin dyes, are widely used as blue laser dyes as well as florescence probes in many chemical and physicochemical studies. An alternative one-pot synthesis of coumarin dyes through 10-12 h reflux in n-pentanol was also reported [2]. Along the lines of our investigation on efficient synthesis of coumarin dyes and to evaluate efficiency of green solid acids catalysts such as HZSM-5 zeolite current study reports efficient one pot three component syntheses of coumarin dyes in organic solvent, aquas media (H_2O) and under solvent free conditions.



4a-e

Compound	X	R
4a	O	Cl
4b	O	CH_3
4c	O	H
4d	O	SO_3Et
4e	NH	NH_2

References:

[1] Heravi, M. M.; Alimadadi Jani, B.; Derikvand, F. ; Bamoharram, H.; Oskooie, A. *Catalysis Communications* **2008**, *10* , 272–275.
[2] Ye, F. F.; Gao, J. R.; Sheng, W. J.; Jia, J. H.; *Dyes and Pigments* **2008**, *77*, 556-558.

Highly regioselective conversion of epoxides to *vicinal*-halohydrins using elemental iodine and bromine catalyzed by *meso*-tetraarylporphyrins

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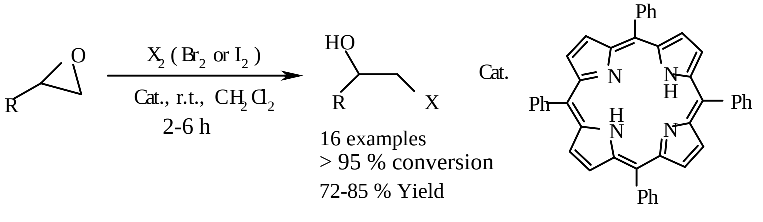
The vicinal halohyrins are very useful synthetic intermediates and have found wide applications in organic transformations and in the synthesis of marine natural products [1]. Although they are conveniently obtained by the addition of hypohalite–water to olefins [2-3], no regiospecific addition was observed. However, these procedures are associated with the disadvantages of intolerance to acid-sensitive moieties and byproduct formation [4]. Among these reagents lithium halides in combination with various Lewis acids are reported to be more convenient and efficient [5], However, the presence of strong Lewis acid and protic acid in these LiX combined reagent systems often leads to low yields of halohydrins.

We would like to describe herein that on treatment with elemental halogen in the presence of catalytic amounts of Meso-tetraarylporphyrins at room temperature a series of epoxide derivatives with a high regioselectivity converted into the corresponding halohydrins resulting from an attack of halogen atoms at the less substituted carbon atom. This method occurs under neutral and mild conditions with high yields in various aprotic solvents, even when sensitive functional groups are present. The regiochemical mode of epoxide cleavage by elemental iodine or bromine in the presence of catalyst can be viewed as occurring via nucleophilic attack by a halide ion (X_3^-) on the less sterically hindered epoxide carbon atom.



References:

[1] Bartlett, P. A.; Morrison, J. D. Asymmetric Synthesis, vol. 3, Academic Press, New York, 1984. p. 411.
[2] Smith, J. G.; Fieser, M. Fieser and Fieser's Reagent for Organic Synthesis; John Wiley and Sons: New York, 1990; Vols 1-12.
[3] Donahoe, H. B.; Vanderwerf, C. A. *Org. Synth*. Coll. IV **1963**, 157.
[4] Stewart, C. A.; Vanderwerf, C. A. *J. Am. Chem. Soc*. **1954**, *76*, 1259.
[5] Yadav, J. S.; Reddy, B. V. S.; Reddy, Ch. S.; Rajasekhar, K. *Chem. Lett*. **2004**, *33*, 476.

Silica supported $AgNO_3$ as an effective and reusable catalyst a for synthesis of Bis(indolyl)Methane's at room temperature

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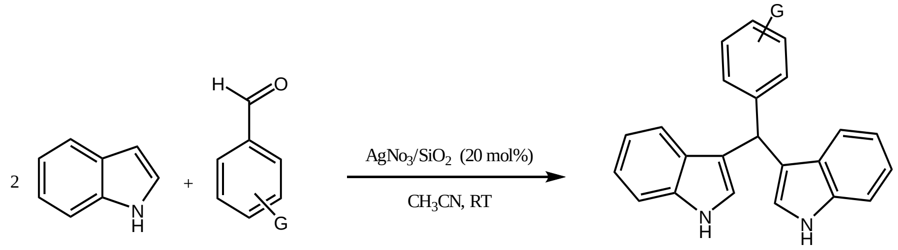
A simple, efficient and cost-effective method for the synthesis of Bis(indolyl) Methane's by a cyclo condensation of indol and aromatic aldehydes in the presence of Silica Supported $AgNo_3$ as an effective and reusable catalyst in actonitril at room temperature was reported [1]. The remarkable features of this new procedure are high conversions, shorter reaction times, cleaner reaction profiles, high yields of pure products and simple experimental and work-up procedures [2,3].



G: H, CN, NO_2, Me, Cl, OMe

References:

[1] B. P. Bandgar, K. A. Shaikh, *Tetrahedron Lett*. **2003**, *44*, 1959.
[2] (a) Maiti, A.-K.; Bhattacharyya, P. *J. Chem. Res*. **1997**,424. (b) Chakrabarty,M.; Ghosh, N.; Basak, R.; Harigaya,Y. *Synth. Commun*. **2004**, *34*, 421.
[3] (a) M. Uchida, H.-M. Kim, T. Kokubo, T. Nakamura, in: H.Ohgushi, G. W. Hastings, T. Yoshikawa (Eds.), *Bioceramics,*vol. 12, World Scientific, Singapore, **1999**, 149. (b) M. Kiyono, *Properties of Titanium Oxide and Its ApplicationTechnology*, **1993**, 55; (c) T. Kasuga, *Thin SolidFilms* **2006**, *496*, 141.

Three-component reaction of trimethylphosphit, benzaldehyde, and glycine : An efficient one-pot synthesis of phosphonato esters.

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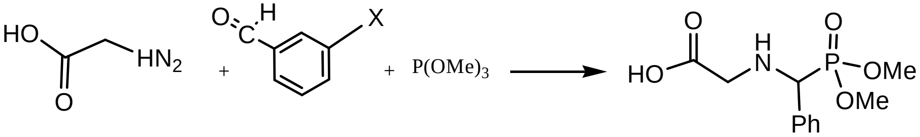
In recent years, there has been an increasing interestin the synthesis of organophosphorus compound.This interest has resulted from the recognition of the value of such compounds in a wide range of industrial,biological, and chemical synthetic aspects.

In this study phosphonato esters were obtained in excellent yields from the 1:1:1addition reaction between benzaldehyde **2**, glycine **1** in the presence of thrimethylphosphite **3** leads to posphonato esters. These reactions proceeded smoothly at ambient temperature and are completed within 24 h in high yield. TLC and 1H NMR spectra of the crude products clearly indicated formation of phosphonate esters **4** (see Scheme 1).The essential structures of the products **4a–c** were deduced from elemental analysis, IR, ^{1}H, ^{13}C, ^{31}P NMR, and mass spectra.



(Scheme 1)

Entry	Product	X	Yield %
A	4a	H	87%
B	4b	OMe	90%
C	4c	NO_2	93%
D	4d	Cl	92%

References:

[1] Maghsoodlou , M. T.; Rostami Charati, F.; Habibi Khorassani, S. M.; Ghasemzadeh, Makha, M. *Chem Res* **2008**, 55.
[2] Rostami Charati, F; Maghsoodlou , M. T; Habibi Khorassani, S. M; Makha, M. *Tetrahedron Lett.* **2008,** *49*, 343.

Synthesis of polyamides from 2,3-bis(4-bromophenyl)quinoxaline and different diamides in the presence of a copper(I) catalyst

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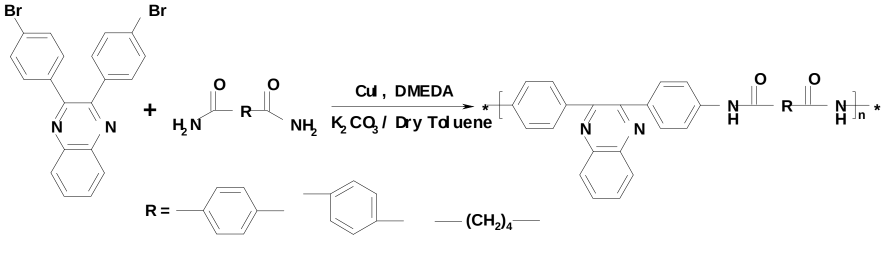
In the last few decades, thermally stable polymers have received extensive interest because of the increasing demands for high-temperature polymers as replacements for metals or ceramics in the automotive, aerospace, and microelectronics industries [1]. In recent years, there have been many reports focused on the deliberate use of ligands to facilitate the copper-catalyzed aryl amidation reaction [2,3].

2,3-bis(4-bromophenyl)quinoxaline was synthesized by condensation reaction from 4,4-dibromobenzil and O-phenylenediamine.This was reacted with benzamide for the preparation of a model compound and with terephthalamide, isophthalamide,and adipamide for the preparation of new polyamides in the presence of a mixture of 10 mol% CuI and 20 mol% N,N'-dimethylethylenediamine as a catalyst and K_2CO_3 as a base. The monomer and the model compound were characterized with FT-IR, NMR, and elemental analysis. The prepared polyamides were also characterized with FT-IR, NMR, DSC,TGA,solubility and viscosity measurements. The obtained polyamides possessed excellent solubility in common organic solvents, and they exhibited inherent viscosities in the range of 0.65-0.72 dL/g. According to the differential scanning calorimetry analysis, the glass-transition temperatures of the polyamides were in the range of 198-276°C. Thermogravimetric analysis indicated that a 10% weight loss of the polyamides occurred in the temperature range of 343-413 °C under a nitrogen atmosphere.



References:

[1] Cassidy P.E. *Thermally Stable Polymers*, New York, Marcel Dekker, **1980**.

[2] Ghaemy, M.; Barghamadi, M. *J. Appl. Polym. Sci*. **2009**, *111*, 1588.

[3] Wolter, M.; Nordmann, G.; Job, G. E.; Buchwald, S. L. *Org. Lett*. **2002**, 4, 973.

Synthesis and characterization of complexes of Cu (II) and Fe (III)

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The guanidine functionality is found widely in natural products, pharmaceutically active compounds. Many natural metabolites found in a variety of organisms contain guanidine. Argenine as Arg is an amino acid with the chemical formula $C_6H_{14}N_4O_2$. The mixed ligand complexes of Fe^{3+} ion with guanidinium and amino acid argenine were prepared. Cysteine had the chemical formula $HO_2CCH(NH_2)CH_2SH$ [1-2]. It is a non-essential amino acid, which means that it is biosynthesized in humans.The mixed ligand complexes of Cu^{2+} ion with oxalate and amino acid cysteine were prepared The structures of complexes were characterized by elemental analysis(C,H,N), electroconductivty (EC), IR and UV/Vis spectroscopy. The IR spectra were shown the coordination of both ligands guanidinium and amino acid argenine with Fe (III) and oxalate and amino acid cysteine with Cu (III). The electronic spectra data for the complexes were in accordance with an octahedral structure around the metal ions. The guanidinium acts a mono dentate ligand and argentine and cysteine act as bidentate ligand.

$$Fe^{3+} + 4G + \text{Amino-} \longrightarrow [Fe\,(G)_4(\text{Amino})]^{2+}$$

$$Cu^{2+} + 2\,Ox^{2-} + \text{cysteine} \longrightarrow [Cu\,(\text{cysteine})\,(ox)_2]^{3}-$$

G = Guanidiuium, Amino= argenine, Ox= Oxalate

References:

[1] K. M. Dokken, J. G. Parson, J. McClure, J. L. Gradea, Inorganica chimica Acta, 362 (**2009**) 395-401.
[2] Martines. L, Farias, R. F, Airoldi. C, thermochemica Acta 395 **(2003)** 21-26.

Synthesis and structural study of perfluorinated bis pyridyl compound

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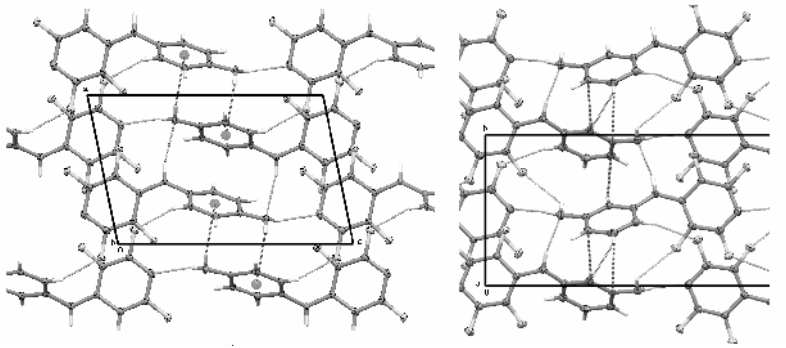
Highly fluorinated organic molecules do form a group of compounds distinctively different from their hydrocarbon counterparts [1,2]. Due to their high electronegativity fluorine atoms are able to alter the physico-chemical properties of molecules drastically. Fluorine is less polarizable and heavier than hydrogen, leading to more tightly packed denser materials. At the same time attractive interactions between fluoro moieties are weaker than in hydrocarbons, which cause the compounds to have lower surface energies and boiling points as liquids as well as weaker intermolecular interactions in the solid state. These and other related properties of perfluorinated compounds makes them a distinct class of compounds set apart from both polar as well as classical unpolar materials, and most highly fluorintated materials do not readily mix with their hydrocarbon counterparts, which opened the way to the development of fluorous biphase chemistry, providing a complementary approach to other known biphase systems for stoichiometric and catalytic chemical transformations [3].

Herein we would like to report synthesis of some fluorinated bis-pyridyl compounds and investigation of their structures by X-ray crystallography analysis. Our study indicated that the structures of compounds show the importance of stacking interaction between aromatic rings in the crystal packing of compounds containing fluorinated heterocycles.



References:

[1] Krafft, M. P.; Riess, J. G. *Chem. Rev.* **2009**, *109*,1714.
[2] Reichenbächer, K.; Süss, H. I.; Hulliger, J. *Chem. Soc. Rev.* **2005**, *34*, 22.
[3] Horvath, I. T. *Acc. Chem. Res*. **1998**, *31*, 641.

Synthesis, spectroscopic studies and DFT calculations of the proton, carbon chemical shift and FT-IR on functionalized benzo γ-lactone derivatives

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The spectroscopic studies and synthesis of functionalized benzo γ-lactone derivatives specific halogenated has been very considerable [1-2]. In this investigation we report the synthesis of these derivatives at one step reaction in high yields by ^{1}HNMR, ^{13}CNMR, FT-IR. The ^{1}H and ^{13}CNMR chemical shifts of the methyl 6-chloro-8-methyl-2-oxo-2-H-choromene-4-carboxylate, methyl 6-Bromo-8-methyl-2-oxo-2-H-choromene-4-carboxylate and methyl 6-Iodo-8-methyl-2-oxo-2-H-choromene-4-carboxylate was determined with the help of full spectral analysis. The geometry and electronic structure of the title compounds were investigated at both the ab initio Hartree-Fock, B3LYP and BPW91 levels with 6-31G(d,p) and 6-31++G(d,p) basis sets. The NMR data were calculated by mean of the GIAO Model. All Quantum-chemical calculations, including those of NMR data, were performed by ab initio level HF and DFT methods. Excellent agreement between the theoretical and experimental results was found for the HF and DFT method proton and carbon chemical shifts [3]. The parameters of molecular geometry and ^{1}H and ^{13}C chemical shift values of these compounds in the ground state have been calculated and compared with corresponding experimental result.

References:

[1] Yavari, I., Amiri, R.,Haghdadi, M., *Phosphorous, Sulfur and Silicon*., **2004**, *179*, 1.
[2] Yavari, I., Adib, M. andSayahi, M.H., *J. Chem. Soc. Perkin Trans.*, **2002**, *1*, 1517.
[3] Lii, J.-H.; Chen, K.-S.; Durkin, K. A.; Allinger, N. L. *J. Comput.Chem.* **2003**, *24*, 1473.

BF_3: As an efficient catalyst for synthesis of 2,4,6,8,10,12-hexabenzyl 2,4,6,8,10,12-hexaazaisowortzitane(HBIW)

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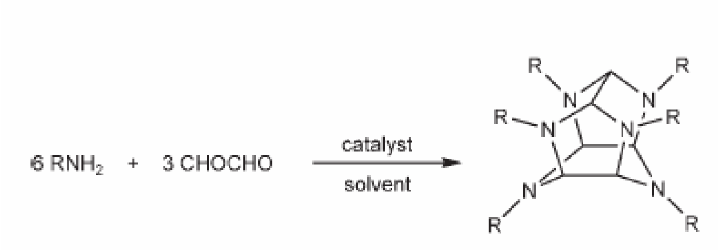
CL-20 is the most powerful explosive known [1, 2]. Almost in all methods of synthesis of CL-20 used from 2,4,6,8,10,12-hexabenzyl-2,4,6,8,10,12-hexaazaisowurtzitane (HBIW), that the acids as a catalyst have used for the synthesis. Optimization of synthesis of this material is research challenges in the field of energetic materials. The highest efficiency reported for the synthesis of HBIW in the solvent ethanol, is 58% that formic acid as a catalyst is used [3].

In this paper, the synthesis of 2, 4, 6, 8, 10, 12-hexabenzyl-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane (HBIW) in the presence of Lewis acid catalysts has been studied. The results showed that BF_3 catalyst, in addition to remove problems using acidic catalysts and also easy to wash from the product surface, will increase the efficiency of HBIW synthesis reaction about 20%. The structure and purity of the compounds were characterized by elemental analysis, HPLC, IR, ^{1}HNMR.



R= Benzyl

References:

[1] Sikder, A. K. Sikder, N. *Journal of Hazardous Materials* **2004**, *A112,* 1.
[2] Nair, U. R. Sivabalan, R. Gore, G. M. Geetha, M. Asthana, S.N. and Singh, H. *Combustion, Explosion, and Shock Waves,* **2005**, *41*, 121
[3] Herve, G. Jacob, G. and Gallo, R. *Chem. Eur. J.* **2006**, *12*, 3339.

Amination reaction of aryl halides using a new *N*-containing complex

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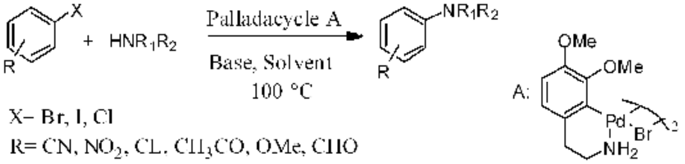
Aryl amines have wide application in the fine chemical industries [1], preparation of new ligands, artificial dyes, natural products, polymers, electronic materials and xerographic materials [2]. Therefore, in order to development of new methodologies that affectively can produce these compounds, a considerable amount of effort has been devoted in recent years [3]. These methods offer advantages over the classical methods. Recently, the use of transition metal catalysts in the synthesis of various kinds of organic molecules has experienced an exponential growth. The first application of organometal complexes in the formation of new C-N bonds was reported by Buchwald and Hartwig [4,5]. Although Buchwald applied P-containing electron-rich ligands in his work, but *N*-containing ligands are often preferred to them, because they are more accessible and recover easily.

Herein, because of importance of palladacycle systems as starting materials in organometallic chemistry and their application in the formation of C-C and C-heteroatom bond, we wish to report a new *N*-containing catalytic system and indicate its ability to catalyze amination reaction of aryl halides. Various types of secondary amines were undergoing amination reaction with different aryl halides. The yields of these reactions after work up were good under conventional heating.



References:

[1] a) Trost, B. M.; *Chem. Pharm. Bull.* **2002**, *50*, 1; b) Johannsen, M.; Jorgensen, K. A. *Chem. Rev.* **1998**, *98*, 1689; c) Trost, B. M.; Van Vranken, D. L.; Bingel, C. *J. Am Chem. Soc.* **1992**, *114*, 9327.
[2] Stanforth, S. P. *Tetrahedron* **1998**, *54*, 263.
[3] Yang, B. H.; Buchwald, S. L. *J. Organomett. Chem.* **1999**, *576*, 125.
[4] Wagaw, S.; Rennels R. A.; Buchwald, S. L. *J. Am. Chem. Soc.* **1997,** *119,* 8451.
[5] Driver, M. S.; Hartwig, J. F. *J. Am. Chem. Soc.* **1997**, *119*, 8232.

Synthesis and methodology for chiral high performance aromatic polyamides

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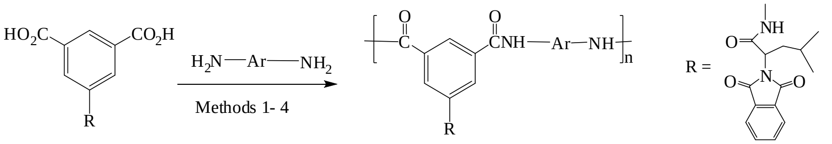
Wholly aromatic polyamides (**PA**)s represent a high performance class of polymers which commonly formed by the step-growth polymerization of diamines or diisocyanates with diacids. **PA**s have high thermal stability as well as outstanding mechanical properties [1]. Despite there exceptional properties, their use are encountered with some drawbacks caused by low organosolubility and high softening temperatures [2]. Introduction of chiral pendant groups can lead not only to the formation of optically activity **PA**s, but also to the polymers with processability enhancements. These advanced polymers can be applied as chiral stationary phases in HPLC techniques for resolution of racemic mixtures [3].

In this investigation a number of optically active aromatic **PA**s have been synthesized via several traditional and modern methodologies and some properties such as optical activity, solubility, thermal stability were studied. These **PA**s were synthesized by direct polymerization of a chiral diacid monomer and different aromatic diamines under microwave (MW) assisted and conventional heating technique in ionic liquid (IL) as well as in volatile *N*-methyl pyrrolidone (NMP). Four different methods were examined in order to optimize both condensation medium and reaction acceleration techniques as the two aspects of polymerization reactions. Through the first and the second methods, reactions were carried out in the presence of *N*-methyl pyrrolidone under oil bath or microwave heating conditions respectively and the last two methods were consist of the use of IL as polycondensation medium under two previously mentioned heating techniques. The results show that, the couple of IL and MW irradiation gave the best results. All of the above polymers were characterized by means of FT-IR spectroscopy and specific rotation methods and typical ones by ^{1}H-NMR, elemental and thermogravimetric analysis.



1: Triphenylphosphite / NMP / Py/$CaCl_2$ under Oil Bath Heating
2: Reagent 1 under MW Irradiation
3: Triphenylphosphite / IL under Oil Bath Heating
4: Reagent 3 under MW Irradiation

References:

[1] Mallakpour, S.; Kowsari, E. *Iranian Polym. J.* **2006**, *15*, 239.
[2] Abid, S.; Gharbi, R. E.; Gandidni, A. *Polymer* **2004**, *45*, 6469.
[3] Nakano, T. *J. Chromatogr. A* **2001**, *906*, 205.

An efficeint synthesis of 3-benzylthiazolo[3,2-a]pyrimidine-5,7-diones through palladium-catalyzed heteroannulation of acetylenic compounds

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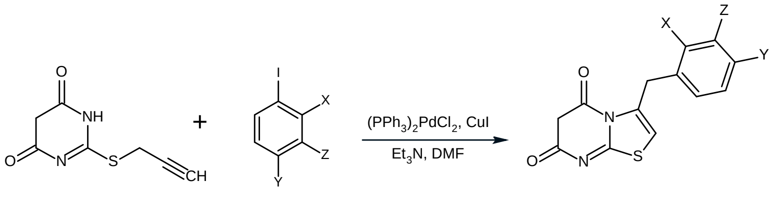
Many thiazolo[3,2-a]pyrimidines have been synthesized for evaluation of their biological activities [1].

Palladium-catalyzed annulation strategies have been successfully utilized for the synthesis of heterocyclic compounds [2]. In connection with our research program directed toward the application of palladium catalyst in organic synthesis [3], we became interested in developing an efficeint synthesis of substituted thiazolopyrimidines.

Herein we wish to report that when 2-(prop-2-ynylsulfanyl)pyrimidine-4,6-dione **1** is treated with various aryl iodides **2** in DMF and triethylamine in the presence of bis(triphenylphosphine)palladium chloride and copper(I) iodide, 3-benzylthiazolo[3,2-a]pyrimidine-5,7-diones **3** are obtained in good yields. This means that carbometalation, anion capture, cyclization, and aromatization have occurred in a one-pot reaction.



1 **2** **3**

X : H, NO_2, Cl
Y : H, NO_2, Cl, CO_2Et
Z : H, NO_2

References:

[1] Ashok, M.; Holla, B. S.; Kumari, N. S. ,*Eur. J. Med. Chem.*, **2007,** *42*, 380.
[2] Kirsch, G.; Hesse, S.; Comel, A. *Current Organic Synthesis, 2004, 1, 47-63*
[3] Heravi, M. M.; Kivanlooa, A.; Rahimizadeh, A.; Bakavoli, M.; Ghassemzadeh. M. *J. Heterocyclic Chem.*, **2007,** *44*, 1.

A comparative study in synthesis of α,α′-bis (substituted-benzylidene) cycloalkanones

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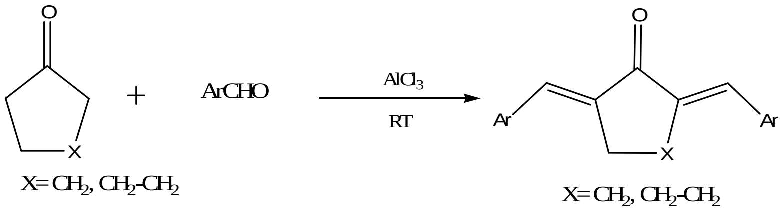
As we have already reported [1] the α,α′-bis (substituted-benzylidene) cycloalkanones are very important materials used commonly as precursors of potentially bioactive pyrimidine derivatives, organic materials for nonlinear optical applications, cytotoxic analogs, liquid crystalline polymers, perfumes, and pharmaceutical applications especially as HIV-1 integrase inhibitors. Many of these methods suffer however from side reactions giving the corresponding products in low yields [2].

In above mentioned paper we have introduced a new green condition for aldole condensation of cyclopentanone and cyclohexanoles with different aromatic aldehydes with both electron releasing and electron withdrawing groups followed by a dehydration to give corresponding α,α′-bis (substituted-benzylidene) cycloalkanones in good to excellent yields.

In present study we have investigated our new conditions for some other acyclic ketones. Our results show that the rate of reaction for cyclopentanone is rather than cyclohexanone. These results show clearly a direct relation between the rate of the reaction and the acidity of α protons of starting keton.



References:

[1] A. Amoozadeh, S. Rahmani and F. Nemati, *S. Afr. J. Chem. In Press.*

[2] M. S. Abaee, M. M. Mojtahedi, V. Hamidi, A. W. Mesbah, W. Massa, *Synthesis* **2008**, 2122; M. S. Abaee, M. M. Mojtahedi, R. Sharifi, M. M. Zahedi, *J. heterocycl. Chem.* **2007**, *44*, 497; M. S. Abaee, M. M. Mojtahedi, M. M. Zahedi, R. Sharifi, H. Khavasi, *Synthesis* **2007**, 3339.

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۲۱ تا ۲۳ مهرماه ۱۳۸۹
بابلسر ـ دانشگاه مازندران
دانشکده شیمی

Silica sulfuric acid as an efficient and recyclable catalyst for one-pot synthesis of benzo[*b*]furan derivatives

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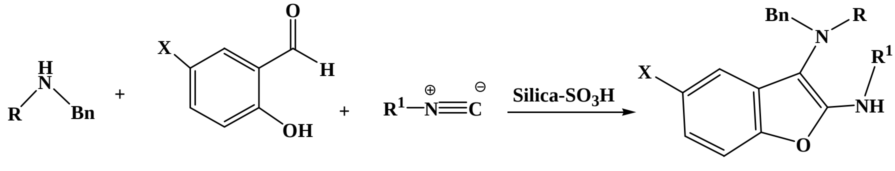
One of the most important objectives now is to adapt classical processes so that pollution effects are kept to a minimum, with both a reduction in energy and consumption of raw materials. In this respect, heterogeneous systems are promising, and a new approach has been undertaken using solid acids chemistry. Solid acid catalysts play a prominent role in organic synthesis under heterogeneous conditions. silica sulfuric acid as an excellent silica-based solid acid which could proceed all acid catalyzed reactions [1]. Multi-component reactions (MCRs) have attracted significant attention in combinatorial chemistry. Of pivotal importance in this area are the isocyanide-based MCRs such as the versatile Ugi and Passerini reactions [2]. The ability of isonitriles to undergo facile addition with a nucleophile and an electrophile under mild conditions makes them useful reactants for the development of novel MCRs. As part of our ongoing program to develop efficient and robust methods for the preparation of organic compounds [3,4], we wish to report a simple, one-pot, three-component reaction between isocyanides, secondary amines and an electron-poor 2-hydroxybenzaldehyde derivative in the presence of silica sulfuric acid at ambient temperature, leading to benzo[*b*]furan derivatives. In the absence of silica sulfuric acid, the yields were only *ca*. 20% at room temperature after 24 hours and in each case several by-products were observed. The structures of the products were deduced from their IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry. In summary, we have found a new and efficient method for the synthesis of benzo[*b*]furan derivatives. We believe the reported method offers a simple and efficient route for the preparation of the benzo[*b*]furan derivatives. Its ease of work-up and the acceptable yields make it a useful method.



Reference

[1] Niknam, K.; Karami, B.; Zolfigol, M. A. *Catal. Commun.* **2007**, *8*, 1427.
[2] Domling, A. *Chem. Rev*. **2006**, *106*, 17.
[3] Ramazani, A.; Rezaei, A. *Org Lett*. **2010**, *12*, 2852.
[4] Ramazani, A.; Mahyari, T. M.; Rouhani, M.; Rezaei, A. *Tetrahedron Lett.* **2009**, *50*, 5625.

Synthesis of pyridine-3,5-dicarbonitrile derivatives from reaction reaction of malononitrile with benzylidenebarbituric acid

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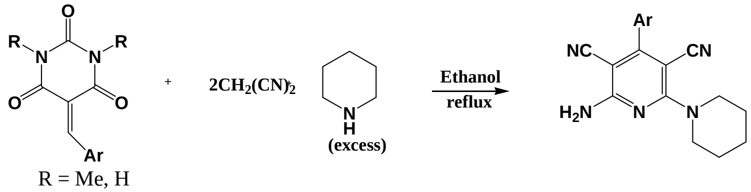
Polysubstituted pyridines represent molecular frameworks that serve as platforms for developing pharmaceutical agents for numerous applications. They have a vast range of potential biological activity such as the prevention or treatment of arthritis, colorectal cancer [1], electrical materials [2] and modulate androgen receptor function [3].

Thus pyridine derivatives have become increasingly important and hence numerous synthetic methods of pyridine rings have been reviewed [4,5]. Herein we have investigated the reaction of malononitrile with benzylidenebarbituric acid and 1,3-dimethyl barbituric acid aiming toward preparation of polysubstituted pyridines. We observed that barbituric acid structure act as leaving group in this reaction and pyridine-3,5-dicarbonitrile derivatives was obtained in good yields.



Refrences:

[1] Anderson, D. R.; Stehle, N. W.; Kolodziej, S. A.; Reinhard, E. J. WO Patent 2004055015, **2004**.

[2] Kambara, T.; Koshida, K.; Sato, N.; Kuwajima, I.; Kubota, K.; Yamamoto, T. *Chem. Lett.* **1992**, 21, 583.

[3] Nirschl, A. A.; Hamann, L. G. US Patent Appl. Publ. US2005182105 A1 20050818, **2005**.

[4] Newkome, G. R.; Paudler, W. W. Contemporary Heterocyclic Chemistry; Wiley: New York, **1982**.

[5] Brody, F.; Rudy, P. R. In Pyridine and Its Derivatives; Klingsberg, E., Ed.; Interscience: New York, **1960**; Vol. 14; Part 1; Chapter 2.

Study on physical properties of phenol compound

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Computational chemistry methods have been introduced that allow analysis of reaction mechanisms and prediction of the reactivity in synthetic chemistry. Therefore, computational chemistry is used to predict the reactivates of a wide variety of phenolic compounds [1].

QM methods have been successfully applied to the derivation of substituent effects of certain chemical groups in substituted phenols [2]. Ab initio methods (MP2) and density function methods (B3LYP) were used to study the effects of substitution of phenols [3]. Several kind of atomic charge of the carbons on the aromatic ring of phenol were calculated using semi-empirical and ab initio method using (RHF/3-21G), (RHF/6-31G), (RHF/6-31+G) and (B3LYP/6-311+G(2d,p) levels. There are only a few theoretical studies addressing substituent effects on phenol, especially those concerning ortho-substitution. The semi-empirical (AM1) level calculation performs well in terms of its geometrical description of phenol as indicated by the close agreement with the experimental bond lengths and angles. Physical properties of phenol compound such as steric energy, charge of oxygen, ionization potential, dipole moment, LUMO and bond length have been calculated. Approach: All molecular geometries were minimized by quantum mechanic especially at (AM1) method was used to investigate the effect of a variety of substituents on the phenol (H, o-Cl, p-Cl, m-Cl, o-CH_3, m-CH_3, p-CH_3, o-NH_2, m-NH_2, o-NO_2, m-NO_2, p-NO_2, 2,4-di-NO_2). Global descriptor such as electronic chemical potential (m), hardness (h), the maximum electronic charge and global electrophilicity index (w) were determined and used to predict the (pKa) values. The theoretical results found were in good agreement with experimental values. The predictive pKa calculated values by AM1 method gave excellent results with experimental values. The correlation between the predicted values especially global electrophilicity index showed excellent qualitative agreement with the experimental pKa (R2 = 0.95). The present research was to calculate the physical properties of phenol derivatives. Then, the calculated values were compared, quite favorably with experimental values of these properties. In future, we can predict any substituent of set of a phenol compound and compare its value with the experimental.

References:

[1] Astarola-Aierbe, G., J.M. Echeverria, J.L. Egiburu, M. Ormaetxea and L. Mondragon, *Polymer* **1998,** *39*, 3147.
[2] Zhang, H.Y., Y.M. Sun and X.L. Wang, Electronic effects on O-H proton dissociation energies of phenolic cation radicals: A DFT study. *J. Org. Chem.*, **2002,** 67, 2709.
[3] Krygowski, M.K. and B.T. Stepien, *Sigmaand Pi-electron delocalization: Focus on substituent effects. Chem. Rev.* **2005**, *105*, 3482.

Epoxidized liquid polysulfide polymer prepared from heavy end waste

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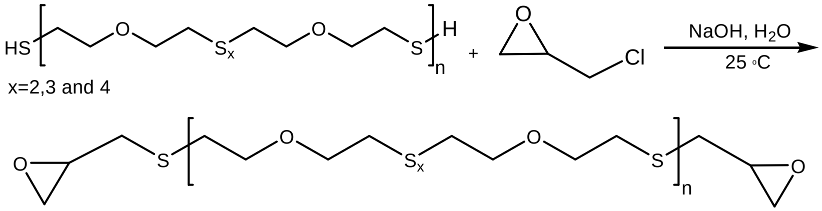
Polysulfide resin has thiol groups at its terminals, this resin does not have low-temperature and fast-curing properties. Polysulfide resin can be epoxidized or modified by epoxy resin to improve its chemical and mechanical properties. Epoxidized polysulfide polymer is hybrid polymers which combine the unique properties of polysulfide (softness) with those of epoxies (hardness) [1-3].

Thiols end groups in liquid polysulfides polymer are highly reactive and can be used as starting materials for other polyfunctional macromolecules. In this work polymerization of liquid polysulfide polymer (LPSP) and LPSP prepared from heavy end waste were studied in presence of epichlorohydrine (ECH) as a chlorine-containing derivative epoxy group and alkali condition at room temperature. The prepared polymers were characterized by ^{1}H-NMR, FT-IR, GPC and mechanical properties were compared.



References:

[1] G. B. Lowe, *Inter. J. Adhesion and Adhesive*, **1997**, *17*, 345.
[2] A. Wilford, T.C.P. Lee, T.J. Kemp, *Inter. J. Adhesion and Adhesives*, **1992**, *12*, 171.
[3] Terence J. Kemp, Andrea Wilford, Oliver W. Howarth, Timothy C.P. Lee, *Polymer*, **1992**, *33*, 1860.

DFT Study of cation-heteroatom interaction and its effects on enhancement of acidity of 2′ -deoxythymidine nucleoside

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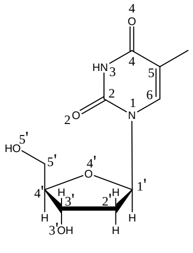
It is well known that Lewis acids play important role as catalysts and include the alkali-metal cations and divalent ions such as Mg^{2+}, Ca^{2+}, Zn^{2+}, and so on.[1] The catalytic activity of metal ions originates in the formation of a donor-acceptor complex between the cation and the reactant, which must act as a Lewis base[2] for instance, in many synthetic reactions, Lewis acids are used to enhance the enolization of an aldehyde or ketone as well as to enhance the electrophilicity of the carbonyl carbon.[3]

Nowadays, there is no doubt about the importance of investigation of nucleosides, as nucleic acid constituents.[1] The canonical 2'-deoxyribonucleosides are basic building units of DNA macromolecules.[2] They are composed of a cyclic, furanoside-type sugar (ß-D-2'-doxyribose) which is substituted at C1' by one of four different heterocycles (thymine, cytosine, guanine and adenine) attached by a ß- glycosyl C1'-N linkage. Acid and base properties of nucleobases and nucleosides are important for the formation of hydrogen bonding between DNA strands. The cations can interact with heteroatoms which are applied in the hydrogen bonding between DNA strands. This cation-heteroatom complex can increase the acidity of OH and NH groups in nucleosides and change the strength of hydrogen bonding. Then, In this work , we study the interaction of 2′ -deoxythymidine nucleoside with some of the mono and divalent cations (Li^+, Na^+ , K^+, Cu^+, Mg^{2+}, Ca^{2+} and Zn^{2+}), and determine the value of acidity enhancement for OH and NH groups in 2′ -deoxythymidine nucleoside in the presence of these cations. All of the calculations are done using Spartan software. Geometry optimization, frequency calculation are done using B3LYP/6-311++G(d,p) method.

The structure of 2′ -deoxythymidine nucleoside



References:

[1] Pena, D. A. ; Uphade, B. S. ; Reddy, E. P. ; Smirniotis, P. G. ; *J. Phys. Chem. B*. **2004**, *108,* 9927.
[2] Kennedy, J. W. J. ; Hall, D. G. ; *J. Am. Chem. Soc*. **2002**, *124*, 11586.
[3] Fattahi. A. R. ; Tavasoli, E. ; *J. Phys. Org. Chem*. **2008**, *21*, 112.

Solvents effects over coat and optimization of physical properties of Automobile Clear Coat

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This project has presented a formulation of automobile coat by using an Iranian resin through common industrial solvents and according to their roles, so that the final properties of optimized coat were already being formed by means of Catalyst and equalization factors .Polyurethane Acrylic Resin often forms a link on three-part HDI which can be followed by an appropriate production. The reason could be mentioned for the said product is faster combination of clear automobile coat. Some of the solvents prevent Isosianat and Polyurethane resin to be combined. It should be stated that, factors such as temperature and air pollution can be quite effective in forming coat and its transparency. This research would also be helpful in furnishing some of the problems accrued during the process of producing Two-part Coat such as inappropriate solvent in forming clear Coats so that the production process will be simplified for researchers and students thereafter. Main properties: Solvents effects over coat and optimization of physical properties of Automobile Clear Coat.

Conclusion: According to the studies and interpretations a coat has been produced with the the best formula: In order to make a proper and transparent/ clear coat, we should choose appropriate solvents and proper additives and this formula, in contrast to previous ones, has been optimized for its transparency The increase of drying time2- The increase of coat viscosity3.

References:

[1] R.lm. Winke Iried, ET.at, Organic Synthesis, VOL. 12 (1987) PP. 230-235.
[2] G. McAuliffe, Optimising the Adhesion of UV Coating, Paint Polymer Colour Journal 1(1995), P 24, 26, 37.
[3] Sayyed Mahmood Kasiriha, Additive Substances of Color.
[4] Mohammad-Ali Mazandarani, The Technology of Color and Resin
[5] Dr. Ardeshir Kamkar, The Solvents

Pectin-based biodegradable hydrogels with potential biomedical applications

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Crosslinked hydrophilic polymers can form hydrogels that are able to absorb and retain hundreds of times their weight of water and are known as superabsorbents [1]. The properties of these hydrogels have attracted the attention of many researchers and technologists and have found wide-spread applications in many fields, such as drug delivery systems. This work deals with the development of new biodegradable hydrogels developed by the polymerization of AN, and some formulations with MBA as crosslinker, in the presence of the Pectin.The Pectin-poly(Acrylonitrile) hydrogel exhibited a pH-responsive swelling-deswelling behavior at pH's 2 and 8 (Fig1)., This on-off switching behavior provides the hydrogel with the potential to control delivery of bioactive agents.

Also The swelling kinetics of the hydrogels with various particle sizes was preliminary investigated as well [3]. In addition, swelling measurements of the synthesized hydrogels in various chloride salt solutions was measured (Fig 2) The swelling of the hydrogel showed a second order kinetics of swelling in water.Release profiles of Asparin, from the hydrogels were studied under both simulated gastric and intestinal pH conditions.

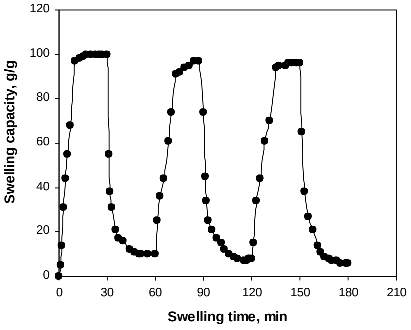

Figure 1. On-off switching behavior as reversible pulsatile PC-poly swelling (pH 8.0) and deswelling (pH 2.0) superabsorbent in of the Pectin-poly(Acrylonitrile) hydrogel. various concentrations.

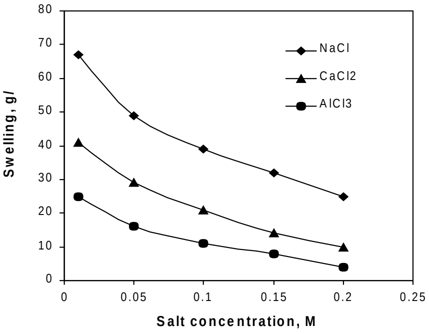

Figure 2. Swelling capacity variation of the (sodium acrylate-co-acrylamide) saline solutions with

References:
[1] H. Lynda, E. W. Marshall. Chromate ion adsorption by agricultural by-products modified with dimethyloldihydroxyethylene urea and choline chloride. *Water Res.* 2005, 39, 2869.
[2] X. Bourges, P. Weiss, G. Daculsi, G. Legeay. Synthesis and general properties of silatedhydroxypropyl methylcellulose in prospect of biomedical use. *Adv. Collo. Interf. Sci.* 2002, 99, 215.
[3] H. Lynda, E. W. Marshall. Chromate ion adsorption by agricultural by-products modified with dimethyloldihydroxyethylene urea and choline chloride. *Water Res.* 2005, 39, 2869.

Synthesis of 3-(5-Bromofuran-2-yl) isoxazole-5-carboxylic acid as a new compound

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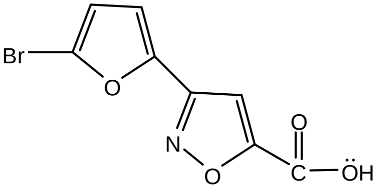
Isoxazole derivatives are an important class of heterocyclic compounds and their chemical properties have been studied over the years. They can be converted into several important synthetic units such as b-hydroxy ketones, γ-amino alcohols, α,β-unsaturated oxime, and β-hydroxy nitriles Isoxazole derivatives have long been targeted in synthetic investigation for their known biological activities and pharmacological properties such as hypoglycemic, analgesic, anti-inflammatory, and anti-bacterial activity [1], they are valuable as building blocks in organic synthesis [2], in present research four two of isoxazole and an oxim compound have been synthesized. At the first furan-2-carboldehyde changed into furan-2-carbaldehyde oxime (1) by hydroxylamine hydrochloride in ethanol and water at 0 °C, the compound 1 changed to nitrile oxide and [2+3] cycloaddition happened by using propagyle alcohole, as a result 3-(furan-2-yl) isoxozaole-5-carboxilic acid (2) was prepared, At the rest of the research 3-(5-Bromofuran-2-yl) isoxazole-5-carboxylic acid (3) was prepared by reaction of Br_2 and compound 2, The structure of compounds were confirmed by FT-IR and ^{1}H NMR spectroscopies.



Reference

[1] Ken Ichi Itoh, Akira Heriuchi, **2003**, *Formation of isoxazole derivatives via nitrile oxide using ammonium cerium nitrate (CAN): a novel one-pot synthesis of 3-acetyl- and 3-benzoylisoxazole derivatives,* Tetrahedron, Vol. 60, pp. 1671-1681.

[2] Sofia M., Hugh D., Burrows, Nunes C., Melo T., **2009**, *On the photophysical behaviour of 4-halo-5-phenyl-oxazoles and isoxazoles: A correction and observations on the photoinduced isomerisation and degradation of methyl 4-halo-5-phenyl-isoxazole-3-carboxylates*, Chem, Phys, lett, vol. 474, pp. 84-87.

Theoretical studies of aromaticity criterion and ligand fluxionality in $[M^*(\eta\ 1\text{-}Cp)\ (\eta 5\text{-}Cp)(L)]^n$, $[M(\eta 1\text{-}Cp)\ (L')]$

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In the present study, Density Function Theory (DFT) was used to investigate the mechanistic factors affecting cp ligand fluxionally in a series of complexes: [M*(η1-Cp) (η5-Cp)(L)]n(M*=Mn, Re, n=-1; M*= Fe, Ru, Os, n=0; M*=Co, Ir, n=+1) and [M(η1-Cp) $(CH_3)_3$] (M=C, Si, Ge`, Sn); [M(η1-Cp)$(CH_3)_2$](M=B, Ge, As, Sb) including different metals and different ligands. Remarkable agreement was achieved with the experiment [1-2] for the barrier heights of the 1,5-shift for complexes of transition metals such as [Fe(η1-Cp)(η5-Cp)$(CO)_2$] [3-5].The barriers have been properly rationalized in terms of hyperconjugation metal- cp bond strength and steric effects. The results reveal that hyperconjugation depends on the metal element and its charge. A detailed theoretical explanation of the factors involved in all of these 1,5 -shifts are also provided.

References:

[1] Hanse,M.L.; Mary nick, D.S.U.J.*Am.Chem.Soc*.**1988,** *110*, 2358.
[2] Romao,C.C.;Vieiros,L.F.*Organomatalics*.**2007,** *26*, 1777.
[3] Cotton,F.A.;Yogupski,G.*J.Am.Chem.Soc*.**1976,** *89*, 6136.
[4] Cotton,F.A.;Legzdins,P.*J.Am.Chem.Soc*.**1968,** *90*, 6232.
[5] Calderon,J.L.; Cotton,F.A.;Legzdins,P. *J.Am.Chem.Soc*.**1967,** *89*, 6136.

H_5IO_6 and $CrCl_3.6H_2O$: as effective, clean and inexpensive catalysts for the synthesis of 4,4'-(arylmethylene)-bis-(1*H*-pyrazol-5-ols)

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Sayed Mohammad Ghaem Ahmadi, [a] Farid Ruhandeh[a]

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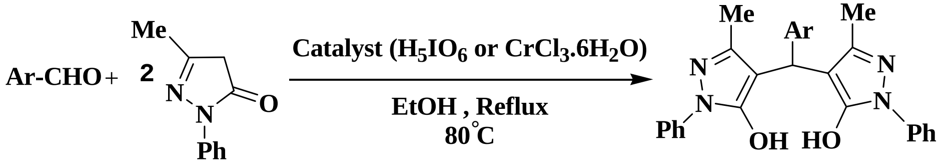
Pyrazoles are an important class of bio-active drug targets in the pharmaceutical industry, as they are the core structure of numerous biologically active compounds. For example, they exhibit anti-anxiety, antipyretic, analgesic and anti-inflammatory properties. 4,4'-(arylmethylene)-bis-(1*H*-pyrazol-5-ols) have antiviral activity against peste des petits ruminant virus (PPRV) [1].

The conventional chemical approach to 4,4'-(arylmethylene)-bis-(3-methyl-1-phenyl-pyrazol-5-ols) involves the successive Knoevenagel synthesis of the corresponding arylidenepyrazolones and its base-promoted Michael reaction and also one-pot tandem Knoevenagel-Michael reaction of arylaldehydes with two equivalents of 5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one performed under a variety of reaction conditions [2 , 3].

H_5IO_6 and $CrCl_3.6H_2O$ are employed as effective, clean and inexpensive catalysts for the condensation reaction of aromatic aldehydes with 3-methyl-1-phenyl-5-pyrazolone. This condensation reaction was performed in ethanol at refluxing conditions giving 4,4'-(arylmethylene)-bis-(1*H*-pyrazol-5-ols) in 75–95 % yields.



References :

[1] Sujatha, K.; Shanthi, G.; Selvam,N. P.; Manoharan, S.; Perumal, P. T.; Rajendran, M.*Bioorg.Med. Chem. Lett.* **2009**, *19*, 4501.
[2] Hamama , W. S. *Synth . Commun.* **2001**, *31*, 1335.
[3] Li, X.-L.; Wang, Y.-M.; Tian, B.; Matsuura, T.; Meng, J.-B. *J. Heterocycl. Chem.* **1998**, *35*, 129.

Tetramethylguanidine (*TMG*) as a selective and highly efficient catalyst for conjugate addition of cyanide to *α,β*-unsaturated enones

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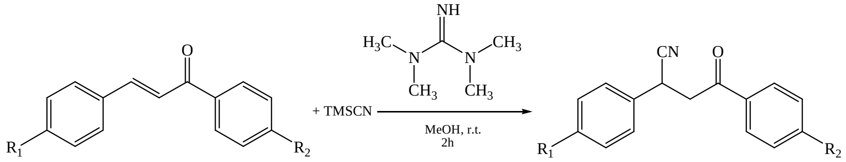
β-keto nitriles are important intermediates in organic synthesis due to their applications in the bioactive compounds and usually prepared from conjougate hydrocyanation of α,β-unsaturated carbonyl compounds [1]. The Michael addition is one of the most frequently used reactions in β-keto nitriles synthesis. First of all there is the problem of competition between 1, 4-addition and 1, 2-addition reactions [2]. There are a few useful methods for hydrocyanation using various cyanation reagents such as hydrogen cyanide, organoaluminum cyanide and acetone cyanohyrdine, which can generate cyanide ion [3]. In most cases excess amount of cyanide source is used and in some cases the protocols involves the use of harsh reaction conditions and work-up leading to the generation of large amount of waste. We herein reported the simple and selective process for the preparation of β-keto nitriles. The reaction generally involves the addition of *TMSCN* **2** to the chalcone derivatives **1** at the present of tetramethylguanidine (TMG) as a catalyst to form β-keto nitriles **3**. The procedure is a very mild, selective and efficient and the substrates are easily available (Scheme 1).



1 **2** **3**

R_1= H, Me, OMe Cl, Br
R_2= H, OMe, Cl, Br, Ph

References:

[1] (a) Davey, W.; Tivey, D. J. *J. Chem. Soc.* **1958**, 1230. (b) Lapworth, A.; Wechsler, E. *J. Chem. Soc.* **1910**, 97, 38.
[2] Iida, H.; Moromizato, T.; Hamanda, H.; Matsumoto, K. *Tetrahedron Letters*, **2007**, 48, 2037.
[3] Betts, B. E.; Davey, W. *J. Chem. Soc.* **1958**, 4193.

A simple and convenient method for deoxygenation of sulfoxides to thioethers using triphenylphosphine and catalytic amounts of molecular iodine

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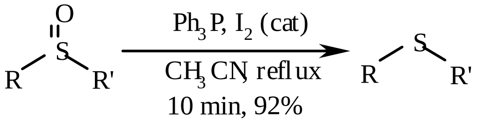
Reduction of sulfoxides to the corresponding sulfides is an important organic [1] and biological reaction [2] and has found wide applications in various synthetic transformations. Trivalent phosphorus compounds, either with electron-withdrawing or electron-donating groups are effective for the deoxygenation of sulfoxides [3]. A number of phosphorus containing reagent systems such as PPh_3/CCl_4 [4], 1,3,2-benzodioxaphospholes [5], $P(OEt)_3/I_2/NaI$ [6] and $P(NMe_2)_3/I_2/NaI$ [7] … have been reported for this transformation.

Trying to develop other applications for triphenylphosphine, through the generation of positively charged phosphorus atom, we succeeded to reduce sulfoxides to thioethers in the presence of triphenylphosphine and iodine in dry refluxing CH_3CN. At first, dibenzyl sulfoxide was chosen as a model compound and converted to its corresponding thioether by Ph_3P/I_2 system. Quantitative conversion of dibenzyl sulfoxide to dibenzyl sulfide was achieved in the presence of 0.3 molar equivalents of iodine within 10 minutes (Scheme 1).

We were able to develop a new catalytic method for the reduction of sulfoxides with molecular iodine as a catalyst. dialkyl sulfoxides, alkyl aryl sulfoxides, and diaryl sulfoxides were reduced to their corresponding sulfides with this method. High yields, short reaction times (10-15 min) and availability of the reagents could be considered as advantages of the present method.



Scheme 1

References:

[1] (a) Madesclaire, M. *Tetrahedron* **1988**, *44*, 6537. (b) Drabowicz, J.; Numata, T.; Oae, S. *Org. Prep. Proced. Int.* **1977**, *9*, 63.
[2] Black, S.; Harte, E. M.; Hudson, B.; Wartofsky, L. *J. Biol. Chem.*, **1960**, *235*, 2910.
[3] Amonoo-Neizer, E. H.; Ray, S. K.; Shaw, R. A.; Smith, B. C. *J. Chem. Soc.*, **1965**, 4296.
[4] Castrillón, J. P. A.; Szmant, H. H. *J. Org. Chem.*, **1965**, *30*, 1338.
[5] (a) Dreux, M.; Leroux, Y.; Savignac, P. *Synthesis* **1974**, 506.
[6] Singh, S. P.; Saxena, R. K. *Synth. Commun.*, **1987**, *17*, 575.
[7] Olah, G. A.; Gupta, B. G. B.; Narang, S. C. *J. Org. Chem.*, **1978**, *43*, 4503.

Chemoselective oxidation of sulfides into sulfoxides by poly(4-vinylpyridinium tribromide) as recoverable oxidizing agent

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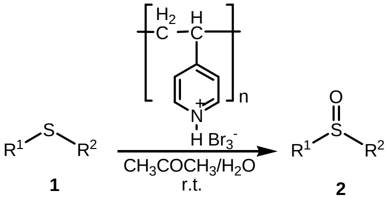
In the last few years, supported reagents on the organic polymers have become increasingly used in organic functional group transformations [1], mainly because the reactions are carried out under mild conditions. Sulfoxides are important synthetic intermediates for the construction of various chemically and biologically active molecules including drugs, flavors and germicides. Sulfoxides are also valuable in C-C bond-forming and molecular rearrangements [2]. In the last decade a lot of reagents and oxidants have been applied for the oxidation of sulfides [3-4] but some of these methods suffer from some drawbacks such as overoxidation to sulfone, tedious work up of products and no recoverability of the reagents.

In order to complete our studies about application of polymeric supported reagents [5] and heterogeneous media [6] in organic reactions, we interested to introduce a new oxidizing polymer for the chemoselective preparation of sulfoxides from sulfides. Consequently, we have presented chemoselective oxidation of a variety of aliphatic and aromatic sulfides **1** to the corresponding sulfoxides **2** by poly(4-vinylpyridinium tribromide) in acetone/water (5:1) as solvent at room temperature (Scheme 1).



Scheme 1

References:

[1] Chari, M.A.; Syamasundar, K.; *Catal Commun.* **2005**, *6*, 67.
[2] Carreno, M.C.; Hernandez-Torres, G.; Urbano, A.; Colobert, F. *Eur. J. Org. Chem.* **2008**, 2035.
[3] Karimi, B.; Zareyee, D. *J. Iran. Chem. Soc.* **2008**, *5*, S103.
[4] Supale, A.R.; Gokavi, G.S. *Catal. Lett.* **2008**, *124*, 284.
[5] Ghorbani-Choghamarani, A.; Chenani, Z.; Mallakpour, S. *Synth. Commun.* **2009**, *39*, 4264.
[6] Zolfigol, M.A.; Amani, K.; Ghorbani-Choghamarani, A.; Hajjami, M.; Ayazi-Nasrabadi, R.; Jafari, S. *Catal. Commun.* **2008**, *9*, 1739.

Facile one-pot three component synthesis of novel hexahydro-2-quinolinecarboxylic in solvent-free conditions

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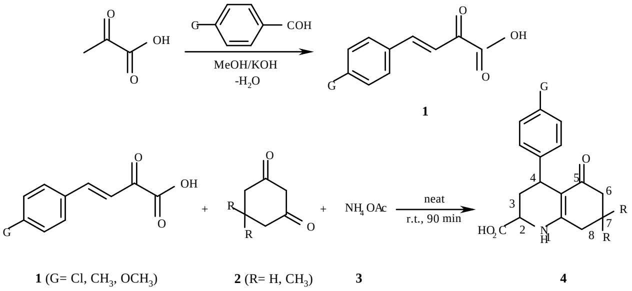
Heterocyclic containing nitrogen atom in their skeleton, are abundant in nature and exhibit various important chemical and biological activities. Among them quinolines are of interest because they constitute an important class of natural and non-natural products, many of which have different biological activities such as antimalarial, antibacterial, antimicrobial, and antistaphylococcal and also an important class of antibiotics posses 4-quinolone framework in their structure, in addition, they can be used as useful drugs for the treatment of Alzheimer's disease [1a-f].



Herein, we would like to report a very simple, efficient and clean synthetic route to 5-oxo-4-phenyl-1,4,5,6,7,8-hexahydro-2-quinolinecarboxylic acid derivatives **4** *via* three-component reaction of arylidenepyruvic acids, 1,3-cyclohexandiones and ammonium acetate in neat conditions.

References:

[1] a) Abdolmohammadi, S.; Balalaie, S. *Tetrahedron Lett*. **2007**, *48,* 3299. b) Zhang, M. Q.; Haemers, A.; Berghe, D. V.; Pattyn, S. R.; Bollaert, W. *J. Heterocycl Chem*., **1991**, *28,* 685. c) Roy, K.; Srivastava, R. P.; Tekwani, B. L.; Pandey, V. C.; Bhaduri, A. P. *Bioorg. Med. Chem. Lett*., **1996**, *6,* 121. d) Reuman, M.; Daum, S. J.; Singh, B.; Wentland, M. P.; Perni, B.; Pennock, P.; Carabates, P. M.; Gruett, M. D.; Saindane. M. T.; Droff, P. H.; Coughlin, S. A.; Sedlock, D. M.; Rake, J. B.; Lesher, G. Y. *J. Med. Chem*., **1995**, *38*: 2531. e) Bogialli, S.; D'Ascenzo, G.; Corcia, A. D.; Lagana, A.; Nicolardi, S. *Food Chemistry*, **2008**, *108*, 354. f) Suh, W. H.; Suslick, K. S.; Suh, Y.H. *Curr. Med. Chem. Central Nervous System Agents*, **2005**, *5,* 259.

Investigation the effect of ethylene glycol/ionic liquid ratio as reaction solvent on the formation of L-phenyl alanine anhydride from L-phenyl alanine

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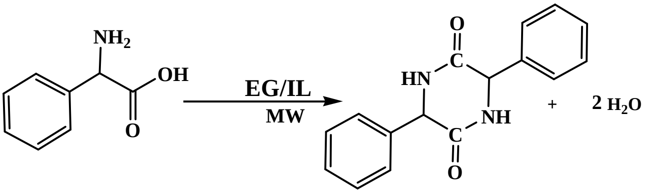
Diketopiperazines are the smallest cyclic peptides known, which are commonly biosynthesized from amino acids by different organisms, and are considered to be secondary functional metabolites or side products of terminal peptide cleavage. Cyclic dipeptides are extensively obtained by extraction from natural sources, and may also be easily synthesized [1]. The application of microwave energy to organic compounds for conducting synthetic reactions at highly accelerated rates is an emerging technique [2]. Ionic liquids (ILs) are a subclass of molten salts, which have a melting point below 100 C. ILs are known already for more than 90 years, however, only recently newly found members of this class showed promising applications in electrochemistry, analytics, technology, and engineering fluids. Many ILs are already liquid at room temperature, some even freeze only at temperatures as low as − 90 °C. Due to their salt like structure they usually exhibit a negligible vapor pressure up to very high temperatures for which they are often advertised to be suitable for “green chemistry”[3].

In this work we studied synthesis of L-phenyl alanine anhydride from corresponding amino acide in different ratio of ethylene glycol/ionic liquid as solvent under microwave irradiation. Higher yields obtained with cleaner and faster in present of IL rather than pure ethylene glycol condition. In this study, advantages of both of the IL and microwave irradiation have been utilized.



L-phenyl alanine **L-phenyl alanine anhydride**

References:

[1] Delaforge M; Bouill’e G; Jaouen, M; Jankowski,CK; Lamouroux, C; Bensoussan, C; *Peptides* **2001**, 22 (4), 557.
[2] Dommert, F; Schmidt, J; Krekeler, Ch; Zhao,Y.Y; Berger, R; Delle Site,L; Holm, Ch, *journal of molecular liquids*, **2010**, 1522.
[3] Santagada, V; Fiorino, F; Perissutti, E; Severino,B; Terracciano,S; Cirinob, G; Caliendoa, G, *Tetrahedron Lett. Pergamon,* **2003**, 44, 1148.

Synthesis and characterization of aliphatic poly(thioester)s via direct polycondensation of 3-mercaptopropionic acid

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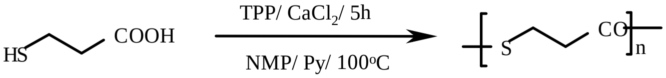
Recently, synthesis of polythioesters containing thioester linkages in their backbone have been the subject of much attention [1-2]. Few studies, on sulfur-containing aliphatic polythioesters have been reported, probably due to difficult synthesis, high cost, and lower stability [3]. In this report, Polythioester (2) was prepared from direct polycondensation reaction of 3-mercaptopropionic acid (1) with itself that carried out in a medium consisting of TPP (as activating agent), NMP, pyridine and Calcium chloride. The resulting polythioester (2) having inherent viscosity 0.45 dl.g $^{-1}$ was obtained in high yield. Polythioester (2) was fully characterized by IR and ^{1}H-NMR spectroscopy.



(1) (2)

References:

[1] Iwata, S.; Toshima, K.; Matsumura, S. Macromol. *Rapid Commun.***2003**, *24*, 467.
[2] Komura, K.; Itsuno, S. Macromol. *Chem. Phys.* **2002**, *203*, 931.
[3] Sanda, F.; Jirakanjana, D.; Hitomi, M.; Endo, T. *Journal of Polymer Science:part A: Polym Chem.* **2000**, *38*, 4057.

P_2O_5/SiO_2 as a highly efficient catalyst for dithioacetalization of carbonyl compounds and O-Silylation of hydroxyl compounds

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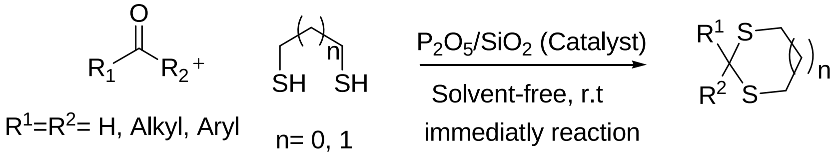
The development of mild and efficient methods for the protection of functional groups continues to be an important tool in the synthetic chemistry of poly-functional molecules in multi-steps synthesis [1]. In continuation of our research on new applications of heterogeneous catalysts in organic synthesis [2], in this research, we wish to report a mild and highly efficient procedure for the dithioacetalization of carbonyl compounds using trace amount of P_2O_5/SiO_2. Structurally diverse aldehydes undergo protection reaction with 1,2-ethanedithiol and 1, 3-propanedithiol in the presence of P_2O_5/SiO_2 (30% w/w) at room temperature to give the corresponding dithioacetals in good to excellent yields. The rate of reactions was found to be very fast and in all cases dithioacetal formation was completed immediately. Remarkably, cyclic aliphatic ketones can also be protected as thioketals in good yields under mention conditions.



In addition, O-silylation of hydroxyl compounds was studied. A variety of hydroxy functional groups was protected as their corresponding trimethylsilyl ethers using HMDS in the presence of P_2O_5/SiO_2. The catalyst activates the HMDS and accelerates the reaction under mild reaction conditions at room temperature to afford the corresponding silylated products in excellent yields. The experimental conditions are very simple and the isolation of products also very easy. The highly catalytic nature of P_2O_5/SiO_2 and its wide applicability should make this protocol an attractive alternative over existing methods.

$$\mathrm{ROH} + \mathrm{HMDS} \xrightarrow[\mathrm{T=100^{o}C}]{P_2O_5/SiO_2\ (80\ \mathrm{mg})} \mathrm{ROSiMe_3} + \mathrm{NH_3}$$

Solvent-Free

R=Primary, Secondary. Tertiary Alkyl, Aryl and Oxime

References:

[1] Green, T.W. Wuts, P.G.M. In Protective Groups in Organic Synthesis, third Ed., John Wiley and Sons, New York, **1999**.
[2] Shaterian, H. R.; Hosseinian, A.; Ghashang, M. *Synth. Commun.* **2008**, *38*, 4097.

Carbon-based solid acid: Green, efficient and reusable catalyst for one-pot synthesis of 2,4,6-triarylpyridines (Kröhnke pyridines)

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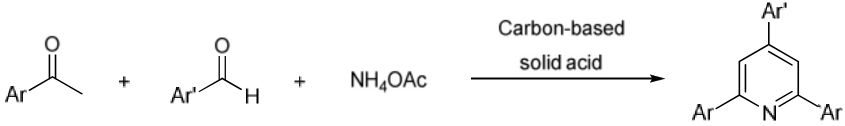
2,4,6-Triarylpyridines (Kröhnke pyridines) are structurally related to symmetrical triaryl-thiopyrylium, -selenopyrylium and -telluropyrylium photosensitizers, which have been recommended for photodynamic cell-specific cancer therapy [1]. These compounds have already been synthesized through the reaction of *N*-phenacylpyridinium salts with α,β-unsaturated ketones in the presence of ammonium acetate [2]. More recently, several new improved methods and procedures for preparation of 2,4,6-triarylpyridines have been reported such as reaction of α-ketoketene dithioacetals with methyl ketones in the presence of NH_4OAc, reaction of *N*-phosphinylethanimines with aldehydes, solvent-free reaction between acetophenones, benzaldehydes, and NH_4OAc in the presence of various catalysts such as Preyssler type heteropolyacid, $HClO_4$-SiO_2, and I_2, and the one-pot reaction of acetophenones, benzaldehydes and NH_4OAc without catalyst under microwave irradiation [3-6]. To the best of our knowledge, there are no examples of the use of carbon-based solid acid as catalyst for the synthesis of 2,4,6-triarylpyridines.

Thus, herein we would like to report an efficient procedure for the preparation of 2,4,6-triarylpyridines through a one-pot three-component reaction including acetophenones, aryl aldehydes, and NH_4OAc in the presence of carbon-based solid acid as catalyst. The catalyst can be reused after a simple work-up. Other advantages of these protocols are high yields, relatively short reaction times and easy work-up.



References:

[1] Leonard, K. A.; Nelen, M. I.; Simard, T. P.; et. al. *J. Med. Chem.*, **1999**, *42*, 3953.
[2] Kröhnke, F.; Zecher, W. *Angew Chem. Int. Ed.*, **1962**, *1*, 626.
[3] Potts, K. T.; Cipullo, M. J.; Ralli, P.; Theodoridis, G. *J. Am. Chem. Soc.*, **1981**, *103*, 3584.
[4] Kobayashi, T.; Kakiuchi, H.; Kato, H. *Bull. Chem. Soc. Jpn.*, **1991**, *64*, 392.
[5] Adib, M.; Tahermansouri, H.; Koloogani, SA.; et. al. *Tetrahedron Lett.*, **2006**, *47*, 5957.
[6] Heravi, M. M.; Bakhtiari, Kh.; et. al. *Catal. Commun.*, **2007**, *8*, 1991.

Synthesis of Schiff bases derivatives using diaminomaleonitrile and reduction of them with $NaBH_4$

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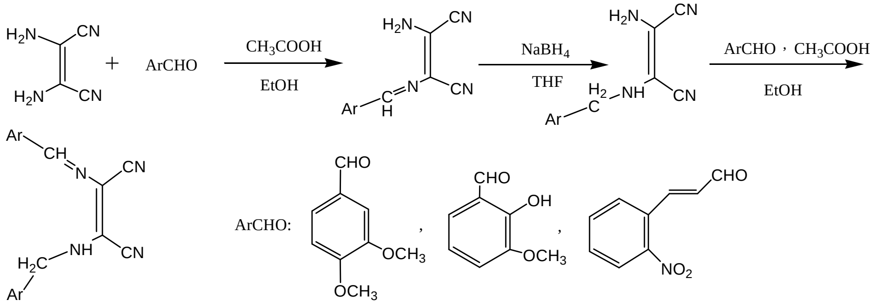
An imine is a functional group or chemical compound containing a carbon–nitrogen double bond [1]. Due to their diverse reactivity, imines are common substrates in a wide variety of transformations. An imine can be synthesized by the nucleophilic addition of an amine to a ketone or aldehyde giving a hemiaminal -C(OH)(NHR)- followed by an elimination of water to yield the imine. However, the equilibrium in this reaction usually lies in favor of the free carbonyl compound and amine, so that azeotrope distillation or use of a dehydrating agent such as molecular sieves is required to push the reaction in favor of imine formation [2,3]. In this work we synthesized three Schiff bases using diaminomaleonitrile with different aldehydes under reflux condition in the presence catalytic amount of acetic acid in ethanol as solvent. Reaction progress controlled with TLC. TLC confirms the purity of compounds. The mixture cooled to room temperature and filtered. The residue washed with boiling ethanol. The desired compounds were identified by melting point, IR, ^{1}H NMR.



References:

[1] Anthony, G.; Barrett, M.;. Hoffman, B, M.; Scott Beall, L.; Neelakandha , S, M.; Andrew J, P, White.; Williams, D, J.; *J. Org. Chem.* **1998,** *63,* 5806.
[2] Iqbal, A.; Moloney, M, G.; Siddiqui, H, L.; Thompson, A, L. *Tetrahedron Letters.* **2009**, *50,* 4523.
[3] House, H, O.; Menlo Park, B. *In Modern Synthetic Reactions*. **1972**, 359.

Synthesis of 4-aryl-3,4-dihydropyrano[4,3-b]pyran-2,5-diones under catalysis of ionic liquid

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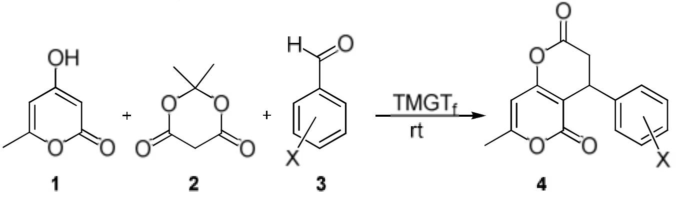
Multicomponent reactions (MCRs) have attracted the attention of synthetic organic chemists for building highly functionalized organic molecules and pharmacologically important heterocyclic compounds [1].

Pyran and its derivatives are the key building blocks of many natural products, [2] and constitute the core of valuable compounds exhibiting a broad spectrum of biological activities [3]. Certain pyran included motifs are often found as recurring themes in a variety of natural and biologicaly releavant products. Arisugacins, davallialactone, clavilactone, pyripyropenes, philigridrins and territrems are special classes of natural and secondary metabolite molecules being characterized by the presence of pyrano[4,3-b]pyran-5*H*-one nucleus in their structures.

In this view and in line with our interest in the synthesis of pyranopyranone compounds and also in performing reactions with the aid of ionic liquids, [4-5] herein we report an efficient one-pot synthesis of 4-Aryl-3,4-dihydro-7-methyl pyrano[4,3-b]pyran-2,5-diones in the mildly basic ionic liquid N,N,N,N-tetramethylguanidinium triflate (TMGTf).

The present approach beside affording some novel pyranopyrone compounds bears the advantages; requiring no metal catalysts or additional solvent and proceeding with appropriate rate respect to the methods that gave similar skeletone.



X=4-OMe / 2-Cl / 3-Cl / 3-Br / 4-Me / 4-NO_2 / (Thiophene-2-carboxaldehyde)

References:

[1] Domling, A.; Ugi, I. *Angew. Chem., Int. Ed.* **2000**, *39*, 3168.
[2] Tietze, L. F. *Angew. Chem., Int. Ed. Engl.*, **1983**, *22*, 828.
[3] Xu, Z. –Q.; Pupek, K.; Suling, W. J.; Enache, L.; Flavin, M. T. *Bioorg. Med. Chem.* **2006,** *14*, 4610.
[4] Rad-Moghadam, K.; Sharifi-Kiasaraie, M. *Tetrahedron.* **2009**, *65*, 8816.
[5] Rad-Moghadam, K.; Mohseni, M. *Monatsh. Chem.* **2004**, *135*, 817.

Determination of total phenolic and flavonoid compounds content of various *Hyssopus Officinalis* extracts

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The interest in natural antioxidants has increased considerably in recent years because many antioxidants exhibit beneficial biological effects, including antibacterial, antiviral, antiallergic, antithrombotic and because they are linked to lower incidence of cardiovascular disease and certain types of cancer disease [1].

Recently, the ability of phenolic substances including flavonoids and phenolic acids to act as antioxidants has been extensively investigated [2].

Hyssop, *Hyssopus officinalis* (Lamiaceae) is one of the most important pharmaceutical herbs [3]. Thus, present study was undertaken to evaluate the *in vitro* antioxidant effect of leaf, stem and flower extracts of *Hyssopus Officinalis*. In this investigation various parts of this plant were successively extracted with ethyl acetate, acetone, methanol and ethanol using a soxhlet extractor for 8 h each. The content of total phenolic compounds and flavonoids were measured in the plant extracts. The data obtained in the in vitro models clearly establish the antioxidant potency of all extracts.

Refrences:

[1] Nilsson, J.; Pillai, D.; Onning, G.; Persson, C.; Nilsson, A.; Akesson, B. *Molecular Nutrition and Food Research*, **2005**, *49*, 239.
[2] Rice-Evans, C.; Miller, N. J. *Methods in enzymology*; **1994**, *234*, 279.
[3] Kazazi, H.; Rezaei, K.; Ghotb-Sharif, S. J.; Emam-Djomeh, Z.; Yamini, Y. *Food Chem.* **2007,** *105*, 805.

Conjugate addition of indoles to electron-deficient olefins catalyzed by PEG-SO_3H under mild conditions

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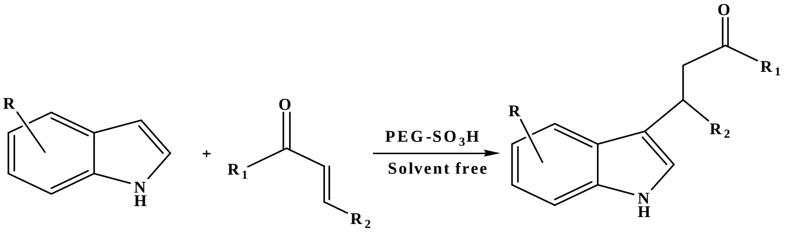
Over the past few years a variety of methods has been reported for the preparation of 3-substituted indoles. Addition reactions of indoles to electrondeficient olefins have received much interest because a number of their derivatives occur in nature and possess a variety of biological activities [1]. Since the 3- position of indole is the preferred site for electrophilic substitution reactions, 3-alkyl indoles are versatile intermediates for the synthesis of a wide range of indole derivatives [2]. A simple and direct method for the synthesis of 3-alkylated indoles involves the conjugate addition of indoles to α,β unsaturated compounds in the presence of either protic or Lewis acids. However, the acid-catalyzed conjugate addition of indoles requires careful control of acidity to prevent side reactions such as dimerisation or polymerization [3].

In continuation of our work on the development of useful synthetic methodologies we recently observed that poly(ethylene glycol)-bound Sulfonic acid (PEG-SO_3H) catalyzes the conjugate addition of indoles to electron-deficient olefins to form the corresponding Michael adducts under mild conditions. Initial research was focused on the reaction of indole with chalcone, and different solvents and different amounts of the catalyst were tested to find the optimized conditions.



References:

[1] Srivastava, N.; Banik, B. K. *J. Org. Chem*. **2003,** *68*, 2109.
[2] Bandini, M.; Melloni, A.; Tommi, S.; Umani-Ronchi, A. *Synlett* **2005**, 1199.
[3] Faulkner, D. J. *Nat. Prod. Rep.* **2002**, *19*, 1.

New application of silica chloride as catalyst in acetylation of aromatic active compounds using acetic anhydride

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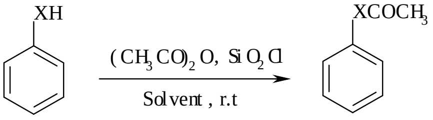
In recent years, the use of reagents and catalysts on solid supports has received significant attention. Silica gel is one of the extensively used surface material supports for different chemical transformations in organic chemistry [1]. One such modified silica chloride (SiO_2-Cl), which has been reported to be an efficient reagent for the synthesis of many organic compounds [2]. The efficiency of silica chloride, under operationally simple conditions, has prompted us to explore the possibility of this catalyst for the acetylation of aromatic active compounds [3].

Herein, we report a rapid, efficient, economic, environmentally benign and easy to scale-up method for the acetylation of aromatic active compounds using acetic anhydride in the presence of silica chloride in room temperature. This particular catalyst can be prepared very easily and found infrequent application in synthetic organic chemistry. The method developed has allowed us to obtain quantitative yields of the required products in reduced reaction times. One of the advantages of this method is that even hindered substrates can be acetylated in high yields under mild reaction conditions.



X: O, S, NH

References:

[1] Salehi, P.; Zolfigol, M. A.; Shirini, F.; Baghbanzadeh, M. *Current Organic Chemistry*, **2006,** *10,* 2171.
[2] Kamitori, Y.; Hojo, M.; Masuda, R.; Kimura, T.; Yoshida, T. *J. Org. Chem.* **1986,** *51,* 1427.
[3] Sathe, M.; Gupta, A. K.; Kaushik, M. P. *Tetrahedron Letters.* **2006,** *47,* 3107.

Preparation a novel and ecofreindly solid liquid phase transfer catalyst and its application in the ring opening of epoxide by acetate anion in water

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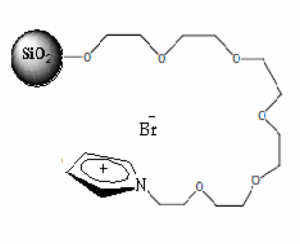
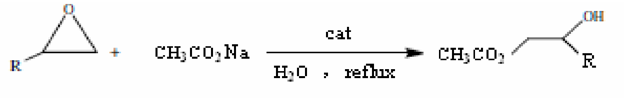
Epoxides are important intermediates in organic synthesis not only as building blocks, but also as synthetic intermediates. The synthetic importance of epoxides stems in large part from their facile and stereospecific nucleophilic ring opening with nucleophiles to furnish valuable 1,2-difunctional compounds. One of the important nucleophile can be used for opening of epoxides is acetate anion that produced a valuable class of difunctional organic compounds, β-acetoxy alcohols.

We now wish to describe here, a new method for preparation of silica gel immobilized polyethylene glycol imidazolium bromide as ecofriendly phase transfer catalysts (scheme1). The catalytic ability of this catalyst in the ring-opening of epoxides by sodium acetate in water was also studied (scheme 2).



Scheme 1



Scheme 2

This procedure provides an easy, eco friendly and efficient access to highly regioselective synthesis of acetoxy alcohols from the epoxides in water.

Reference:

[1] Ren-Hua Fan, Xue-Long Hou, *Tetrahedron Lett.* **2003**, *44,* 4411.

Ab Initio conformational analysis of P,P-dichloro and P,P-difluoro-1,4-diphosphorinane

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The substituents play an important role in the conformational path observed in many conformational equilibrium [1-3]. Herein, we wish to report a detailed ab initio study of the pyramidal phosphorus atom inversion of P,P-dichloro1,4-diphosphorinane(**1**) and P,P-difluoro 1,4-diphosphorinane(**2**) and ring inversion of (**1**) by using *ab initio* molecular orbital theory at the HF/6-31G, 6-31G*, 6-311G and MP2/6-31G ,6-31G*, 6-311G levels. We calculated the $\Delta G^{\ddagger}c$ for ring inversion(**1**) at the HF/6-311G level for chair(ax-ax) → half-chair, chair(eq-eq) → half-chair and chair(ax-eq) → half-chair to be 40.6, 44.6 and 41.5 kJ mol^{-1}, respectively.

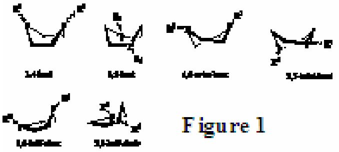

Figure 1

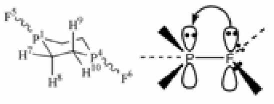

Figure 2

One interesting feature of (**1**) not present in cyclohexane are two, six, two and two possible forms of the twist-boat, boat, half-chair, and sofa structures. This arises from the fact that the two phosphorus atoms can occupy two different positions.(for example see **Figure 1**) For atom inversion, the diaxial conformer predominated over the diequatorial and axial-equatorial (**1**) (12.47 to 9.88 KJ.mol^{-1}) and (**2**) (12.47 to 21.72 KJ.mol^{-1}), this is a remarkably axial-axial preference. As is observed, in diaxial (**2**), the axial hydrogens in 3,5-syn-axial positions for lower energy conformer(diaxial) had a more positive charge distribution when compared with the other conformer(diequatorial) according to **Table 1**. This observation has led to a definitive assignment of the attractive nonbonded interactions.

Table 1. distribution of charge on atoms in P,P-difluoro-1,4-diphosphorinane

Atoms	P1	C2	C3	P4	F5	F6	H7	H8	H9	H10
ax-ax	1.03	-0.70	-0.70	1.03	-0.61	-0.61	0.23	0.25	0.23	0.25
eq-eq	1.05	-0.71	-0.71	1.05	-0.60	-0.60	0.24	0.24	0.24	0.24
ax-eq	1.05	-0.73	-0.68	1.03	-0.61	-0.60	0.25	0.23	0.25	0.27

The higher half-barrier had the withdrawal-substituted groups, a conclusion that no reported earlier. One might expect the inversion barrier in (**2**) to be higher than that for (**1**) because the assumed smaller **F-P-C** (96.5°) against **Cl-P-C** (98.5°) exocyclic bond angle in (**2**) should stabilize the ground-state pyramid. An important result is that the interaction of the lone pair on phosphorus with adjacent lone pairs on fluorine atoms may play a decisive role in determining the value of half-barrier at phosphorus inversion (**Figure 2**).

References:

[1] Brooks, P. J.; Gallagher, M. J.; Sarroff, A.; *Phosphorus, Sulfur, and Silicon*, **1989**, 44, 235.
[2] Jadidi, K.;Ghaffari Khaligh, N.; *15th Iranian Seminar of Organic Chemistry*, **2008**, 7.
[3] Jadidi, K.;Ghaffari Khaligh, N.; *16th Iranian Seminar of Organic Chemistry*, **2009**, 467.

Microwave-assisted clean synthesis of poly(ether-urethane-urea)s derived from L–leucine anhydride

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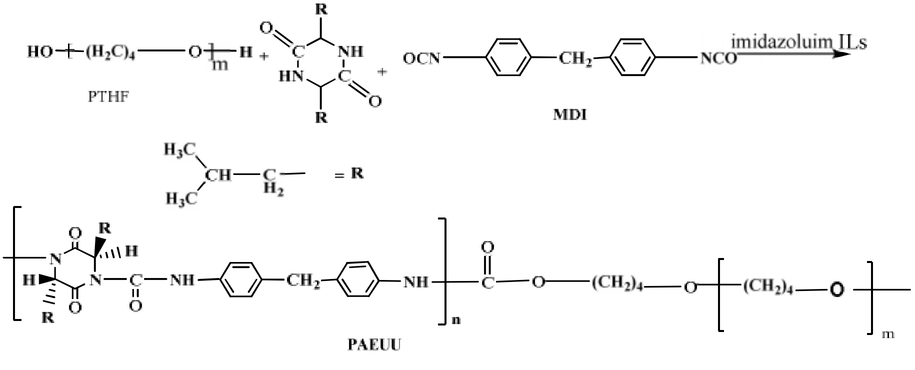
Ionic liquids (ILs) are subject to an enormous research effort due to their unique properties, such as non-volatility, high solution and reactivity ability, etc. For the first time ILs have been used as a solvent for preparing polymers via direct polycondensation. The influence of IL's nature and reaction parameters upon the polymer formulation has been investigated. Various polyamides, polyamide imides , and polyhydrazides have been obtained in quantitative yield and high molecular weight [1,2].

In this work a new class of poly(ether-urethane-urea)s (PEUUs) based on an α-amino acid anhydride was synthesized via direct reaction of 4,4'-methylene-bis(4-phenylisocyanate), L-leucine anhydride and polytetrahydrofuran as polyether soft segment. For the first time the direct polymerization reaction of an isocyanate with NH and OH groups was performed in imidazoluim ILs under microwave irradiation. The resulting polymers have inherent viscosities in the range of 0.02–.16 dL/g. These polymers are optically active, crystalline and thermally stable. Decomposition temperatures for 5% weight loss (T5) occurred above 300 °C by TGA. Some structural characterization and physical properties of these new PEUUs are reported.



References:

[1] Lozinskaya, E.I. ; Shaplov, A.S. ; Vygodskii, Ya.S. *Eur. Polym. J.* **2004**, 40, 2065.
[2] Mallakpour, S.; Rafiee, Z. *Eur. Polym. J.* **2007**, 43, 5017.

[HSO_3-PIM][CF_3SO_3]: A mild, reusable and highly efficient catalyst for the synthesis of 14- substituted- 14*H*- dibenzo [*a.j*] xanthenes under solvent-free conditions

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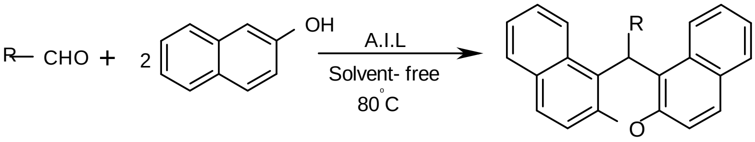
The synthesis of xanthens, especially benzoxanthenes has attracted great interest in recent years due to their wide range of biological and pharmaceutical properties such as antiviral, antibacterial and anti-inflammatory as well as sensitizers in photodynamic therapy [1].

In view of great importance of benzoxanthenes, various methods have been reported for their construction. A mong them, the reaction of aldehydes with β- naphthol is the most convenient method that catalized by homogeneous and heterogeneous acidic catalysts [2, 3].

In view of green chemistry, we was employed a novel Bronsted-acidic Task-spesific ionic liquid, (propyl- 3- sulfonic) imidazolium trifluoromethane sulfonate [HSO_3-PIM] [CF_3SO_3] as catalyst for synthesis of β-naphthol with aliphatic or aromatic aldehydes. The novel synthetic method offers the advantages of high yields, short reaction times, simplicity and easy work up compared to the conventional method of syntheses. The catalyst could be recycled and reused at least eight times without noticeably decreased in its activity.



R = aryl or alkyl
A.I.L = [HSO_3-PIM][CF_3SO_3]

References:

[1] Chibale, K.; Visser, M.; Schalkwyk, D. V.; Smith, P. J.; Saravanamuthu, A.; Fairlamb, A. H.; *Tetrahedron*. **2003**, *59*, 2289.
[2] Nandi, G. C.; Samai, S.; Kumar, R.; Singh, M. S.; *Tetrahedron*. **2009**, *65*, 7129.
[3] Kumar, R.; Nandi, G. C.; Kumar Verna, R.; Singh. M. S.; *Tetrahedron Letters.* **2010**, *51*, 442.

Dynamic NMR investigation of Clozapine

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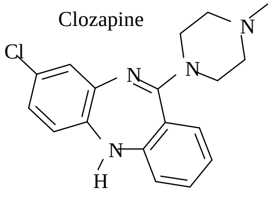
Nuclear magnetic resonance spectroscopy is one of the most commonly used spectroscopic tools for studying dynamic processes [1]. These dynamic processes can include conformational changes and chemical changes [2]. Rotation about single and double bond, valence and Keto-Enol tautomerism, intermolecular proton exchange, inversion about nitrogen and phosphorous, and conformational changes in ring compounds are of processes which have been studied by Dynamic NMR [3].

Herein we report the results for investigation of Clozapine (8-Chloro-11-(4-methyl-piperazin-1-yl)-5H-dibenzo[b,e][1,4]-diazepine) by NMR spectroscopy at various temperatures. Clozapine is an antipsychotic medication used in the treatment of schizophrenia [4]. Our studies showed that there was a barrier for rotation about C-N single bond between piperazine and seven membered rings. At low temperatures, piperazine ring lost its ability to rotate around C-N bond.

Arrhenius and Eyring plot diagrams were obtained using experimental data and comprised to the obtained results from Gaussian03 software with B3LYP/6-311 basis set. $\Delta G^{\ddagger}$=19.866, Ea=4.589 and $\Delta G^{\ddagger}$=18.352, Ea=4.883 kcal mol^{-1} were the results for activation energy obtained by experiment and theory, respectively.

Clozapine



References:

[1] Gutowsky, S.; Holm, H. *J. Chem. Phys.* **1956**, *25*, 1228.
[2] Monlien, F. J.; Helm, L. *Inorg. Chim. Acta*. **2002**, *331*, 257.
[3] Oki, M. *Application of Dynamic NMR Spectroscopy to Organic Chemistry,* VCH, **1985**.
[4] Myung A. L.; Karuna J.; Herbert Y. M. *Schizophrenia Research* **1999**, *37,* 1.

Synthesis of block copoly(methyl methacrylate–styrene) by RAFT/MADIX polymerization

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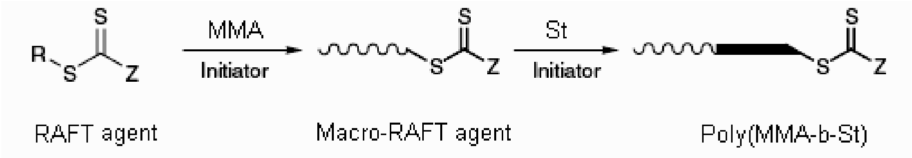
Block copolymers are of main scientific interest due to their phase separation and solution aggregation behavior [1]. To obtain significant phase separation, the combined polymer segments need to have different properties. The synthesis of block copolymers via Reversible Addition-Fragmentation chain Transfer (RAFT) polymerization has drawn significant attention due to the range of potential applications of these structures. Block copolymers are most commonly obtained via chain extension of a macro-RAFT agent. Most polymer chains generated during the RAFT process carry a thiocarbonylthio end group, which now acts as a so-called macro-RAFT agent. RAFT polymerization is recognized as one of the most versatile methods for block copolymer synthesis. This allows an easy entry to the synthesis of A-B diblock copolymer by the simple addition of a second monomer [2]. Xanthates (MADIX agents) are an important class of RAFT agents. When xanthates are used, the terminology MADIX (macromolecular design via the interchange of xanthates) is used to describe the process [3].

Here, the new RAFT agent was synthesized starting from reactions of ethanol, carbon disulfide and 4-nitro benzyl bromide. The polymerization of methyl methacrylate was done using this agent and at the next step a block copoly(methyl methacrylate-styrene) was obtained via addition of styrene monomer to this end-reactive polymer. All of the compounds were characterized by FTIR, H^1NMR, TGA and GPC analysis.



References:

[1] Thomas, E. L.; Anderson, D. M.; Henkee, C. S.; Hoffman, D. *Nature* **1988**, *334*, 598.

[2] Chong, B. Y. K.; Le, T. P. T.; Moad, G.; Rizzardo, E.; Thang, S. H. *Macromolecules* **1999**, *32*, 2071.

[3] Charmot, D.; Corpart, P.; Adam, H.; Zard, S. Z.; Biadatti, T.; Bouhadir, G. *Macromol. Symp.* **2000**, *150*, 23.

Polyphosphoric acid adsorbed silica gel as an efficient and chemoselective reagent for the preparation of acylals

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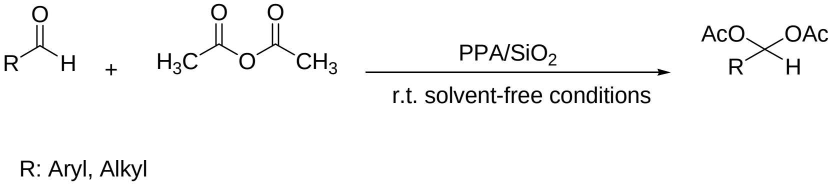
Acylals (geminal diesters) are frequently used as protecting groups for aldehydes because they are stable to both neutral and basic media as well as under acidic conditions [1]. Generally, acylals are prepared by treating aldehydes with acetic anhydride in the presence of protonic acids, Lewis acids, heteropoly acids or clays [2]. Noting recent reports on the use of PPA/SiO_2 [3] for various organic transformations, we now report that PPA/SiO_2 is an efficient catalyst for the chemoselective conversion of aromatic aldehydes to a variety of acylals (Scheme).



Scheme

The experimental procedure for the synthesis of the acylals is simple and involves mixing the aldehyde (1 mmol) and acetic anhydride (4 mmol) in presence of PPA/SiO_2 (0.1 gr) under solvent-free conditions at rt. In a control experiment, we observed that the reaction does not take place in the absence of PPA/SiO_2. A wide variety of aromatic and aliphatic aldehydes underwent smooth reaction to give the corresponding acylal in good to excellent yield. Ketones proved completely resistant to acylal synthesis with acetic anhydride and no diacetate formed under the same reaction conditions.

References:

[1] Greene, T. W.; Wuts, P. G. M.; Protective *groups in organic synthesis.* 3rd Ed., Wiley & Sons, New York, 1**999**.
[2] Rishi, K.; Tiwari, P.; Ranjan P.; Anup M.; Misra, K. *J. Mol. Catal. A: Chem.* **2006**, *247* ,27.
[3] Shaterian, H. R.; Hosseinian, A.; Ghashang, M. *Synth. Commun.* **2008**, *38*, 3375.

Phosphoric acid supported on alumina as a highly effective catalyst for Biginelli reaction

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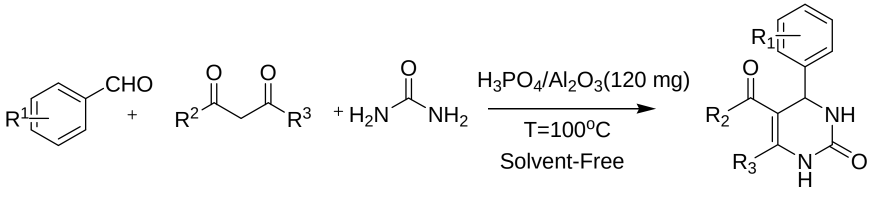
Biginelli products have attracted considerable attention since they exhibit potent antibacterial activity against staphylococcus aureus, escherichia coli, pseudomonas aeruginosa1 and calcium antagonist activity [1, 2, 3].

In continuation of our research work of developing methods in various organic transformations, we have developed a methodology for the synthesis of Biginelli products using H_3PO_4/Al_2O_3, which makes mild reaction under thermal and solvent-free conditions.

After optimization of conditions, the generality of this method was examined by the reaction of several substituted aldehydes, 1,3-dicarbonyl compounds, and urea/thiourea using H_3PO_4/Al_2O_3 as a catalyst under thermal conditions (Scheme). We have carried out the similar reaction with various aromatic aldehydes containing electron donating or electron withdrawing functional groups at different positions but it did not show any remarkable differences in the yields of product and reaction time. Also, it was observed that the reaction of aromatic aldehydes with urea and 1,3-dicarbonyl compounds is very fast as compared to thiourea.



Scheme

References:

[1] Kappe, C. O. *Acc. Chem. Res.*, **2000,** 33, 879.
[2] Kappe, C. O. *Tetrahedron* **1993**, *49*, 6937.
[3] Kappe, C. O. Eur. *J. Med. Chem*. **2000**, *35*, 1043.

Ultrasound-assisted synthesis of isoxazoline derivatives

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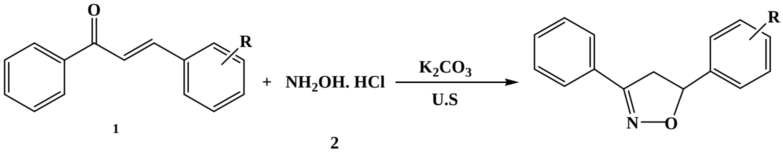
Ultrasound effects on organic reactions are attributed to cavitations, a physical process that create, enlarge, and implode gaseous and vaporous cavities in an irradiated liquid. Cavitations induces very high local temperatures and pressure inside the bubbles (cavities), leading to a turbulent flow in the liquid and enhanced mass transfer. Ultrasonic Irradiation in some organic reactions proceeds with facile reactions to provide high yields within a very short reaction time periods [1].

Heterocyclic compounds have so far been synthesized mainly due to the wide range of biological activities. Much attention has paid to the synthesis of heterocyclic compounds bearing nitrogen and oxygen containing ring system, like isoxazoline mainly due to their higher pharmacological activity.

In addition, isoxazoline derivatives have played a crucial role as intermediates in the organic synthesis of number of heterocyclic pharmacological active compounds.

The present investigation describes the synthesis of Isoxazoline derivatives under conventional and Ultrasonic Irradiation [2]. In these research chalcone derivatives **1** was reacted with hydroxylamine hydrochloride **2** in the presence of potassium carbonate in acetic acid to produce the isoxazolines **3**.

In the view of the interesting green chemistry for the synthesis organic compounds we could design optimized conditions for the preparation isoxazoline derivatives. These reactions were carried out under milder and cleaner conditions, shorter reaction times and so the yields of products were improved.



3a: R = H
3b: R = 2-CH_3
3c: R = 3- CH_3
3d: R = 4-CH_3
3e: R = 2-OCH_3
3f: R = 4-OCH_3
3g: R = 2,4-OCH_3
3h: R = $N(Me)_2$

References:

[1] Luche, J. L. Synthetic Organic Sonochemistry, Plenum Press, New York, **1999**, Chapter 2, pp. 55-56.
[2] Al- Issa, S. A. *J. K. A. U: Sci*, **2007**, *19*, 67.

Cyclization of 2-aminopyridine and 2-aminothiazole with Baylis-Hillman acetates of 2-carboxaldehyde-4-pyrones

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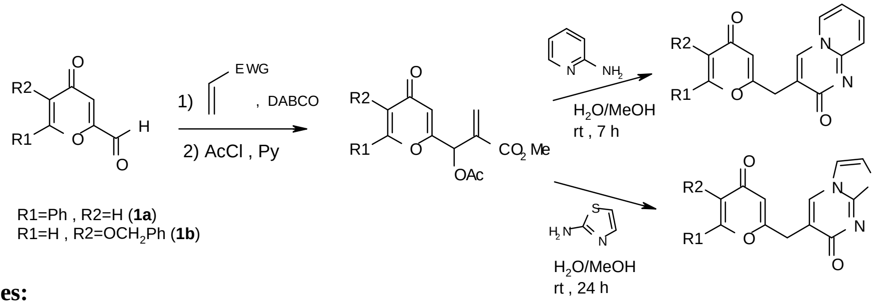
The fused pyrimidine derivatives are of interest not only for their rich and varied synthetic chemistry but also for their important medicinal and physiological properties [1]. The Baylis-Hillman reaction, a powerful tool for construction of a variety of cyclic and heterocyclic frameworks, has been used for the synthesis of various fused heterocyclic systems [2], such as fused pyrimidines [3,4]. Due to the biological and synthetic importance of a variety of heterocyclic derivatives of 4-pyrones [5], we herein report synthesis of fused pyrimidone derivatives of 4-pyrones from the acetates of Baylis-Hillman adducts. Baylis-Hillman coupling of methyl and ethyl acrylates and acrylonitrile with aldehydes **1a,b**, in the presence of a stoichiometric amount of DABCO (100 mol %) gave the Baylis-Hillman products**,** in short reaction times and excellent yields. The adducts obtained by the reaction of aldehydes **1a** and **1b** with methyl acrylate, were acetylated with acetyl chloride in the presence of pyridine in dichloromethane. Treatment of obtained acetates with 2-aminopyridine and 2-aminothiazole in MeOH-H_2O (1:1 v/v) at room temperature, gave the fused pyrimidone derivatives by simple work up in good yields.



References:

[1] Nair, V.; Chi, G.; Shu, Q.; Julander, J. *Bioorg. Med. Chem. Lett.*, **2009**, 19, 1425.
[2] Batra, S.; Singh, V. *Tetrahedron*, **2008**, 64, 4511.
[3] Nag, S.; Mishra, A.; Batra, S. *Tetrahedron*, **2008**, 64, 10162.
[4] Nag, S.; Madapa, S.; Batra, S. *Synthesis*, **2008**, 1, 101.
[5] South, M. S.; Ma, C. C.; Koeller, K. J. United States Patents, **2005**, 6, 916, 847 B2, *Chem. Abstr*, **2001**, 135, 303776e.

Zinc oxide nanoparticles: a clean and reusable nanocatalyst for the synthesis of octahydroquinazolinones via Biginelli reaction

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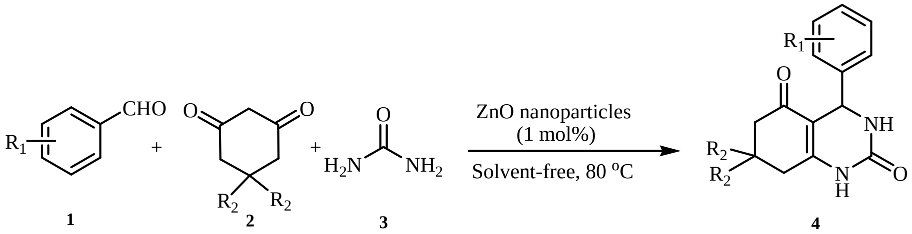
In recent years, heterocyclic compound synthesis has attracted much attention. Among heterocyclic compounds containing nitrogen atom, quinazoline derivatives are important because of their potential antibacterial activity against Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa [1] and also as a calcium antagonist [2]. Beside this, some of these compounds are identified as drugs used as diuretics, vasodilators and antihypertensive agents [3].

In this research, an efficient, simple and environmentally benign procedure for the preparation of octahydro quinazolinones was reported. This method entails the tree-components condensation of appropriate aromatic aldehydes **1**, 1,3-cyclohexanedione or dimedone **2** and urea **3** in the presence of catalytic amounts of ZnO nanoparticles under solvent-free conditions to afford octahydro quinazolinone derivatives **4**.

This method has emerged one of the most utilized reactions in organic synthesis because of its many appealing attributes. First, the starting material are either commercially available. Second, the catalyst is clean, recoverable and readily available. Third, comparing the other methods, yield of the products was very high and reactions time was very low. In addition, simple workup and use of the solvent-free conditions have made the method one of the most widely utilized catalytic reactions. General reaction scheme is presented below.



R_1= H, Cl, Br, NO_2, OCH_3, Me
R_2= H, Me

References:

[1] Kidwai, M.; Sexena, S.; Khan, M. K. R.; Thural, S. S. *Eur. J. Med. Chem.* **2005**, *40*, 816.
[2] Yarim, M.; Sarac, S.; Kilic, S. F.; Erol, K. *Farmaco.* **2003**, *58*, 17.
[3] Katritzky, A. R. *Comprehensive Heterocyclic Chemistry II* **1996**, *8*, 225.

Synthesis and characterization of new macrocyclic Schiff Base from the Reaction of synthesis and characterization of new Schiff Bases 2-(2-(2-(aryl)methyleneamino) (phenylthio)ethyl thio)-*N*-((aryl)methylene)benzeneamine

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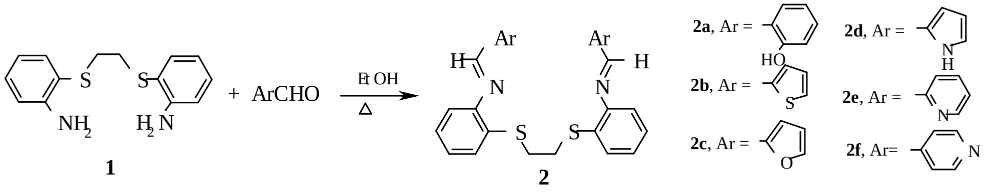
Schiff bases are an important class of ligands in coordination chemistry and find extensive applications in different fields.Schiff bases can be synthesized from an aromatic amine and a carbonyl compound by nucleophilic forming a hemiaminal, followed by a dehydration to generate an imine [1,2,3].

The purpose of these studies is to develop new Schiff base ligands .A series of Schiff bases four to six coordination sites $N_2S_2X_2$(X=O,N) 2-(2-(2-(aryl) methyleneamino)phenylthio) ethylthio)-N-((aryl)ethylene)benzene amine (**2c-f**) were prepared from the reaction of 1,2-di(2-aminophenylthio)ethane (**1**) with aromatic aldehydes. All compounds were characterized by means IR, mass, ^{1}H, ^{13}C NMR spectra, elemental analysis, and in the case of **2b** with X-ray diffraction**.** The X-ray crystal structure of **2b** showed that the resonance occurs between aromatic and thiophen rings, through C=N bond of the molecule.



References:

[1] N. E. Borisova, M. D. Reshetova, Y. A. Ustrynyuk, *Chem. Rev* **2007**, *107,* 46.
[2] A. G. Rajsekhar., C. P. Rao., P. Saarenketo., N. Nattinenb*, New J. Chem.* **2004,** *28,* 75.
[3] W.X. Zhang., C. Ma., *Trans. Met. Chem* **2001,** *26,* 38.

Synthesis of 1, 4-dihydropyridine derivatives with use of modified montmorillonite as an efficient catalyst

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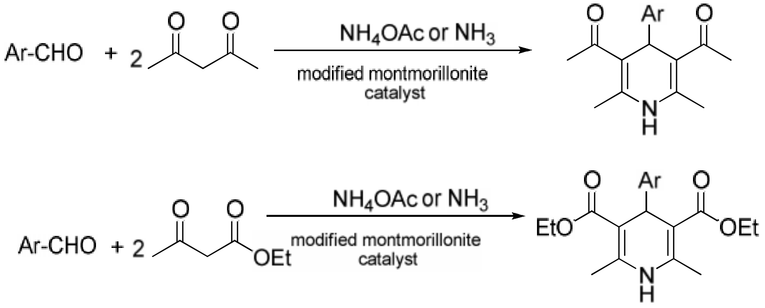
In recent years, considerable attention has been paid to the synthesis of 1, 4 dihydropyridines owing to their significant biological activity [1]. 1, 4-Dihydropyridine-containing drugs (1, 4-DHPs), such as nifedipine, nicardipine, amlodipine, felodipine and others have been found to be useful as calcium channel blockers [2-4]. In this study we synthesized a series of 1, 4-dihydropyridine derivatives with use of different aldehyds, ethylaceto acetate ammonium acetate or ammonia and modified montmorillonite as catalyst under heating and solvent free condition with excellent yield.



References:

[1] Sawada, Y.; Kayakiri, H.; Abe, Y.; Mizutani, T.; Inamura, N.; Asano, M.; Hatori, C.; Arsmori, I.; Oku, T.; Tanaka, H. J. *Med. Chem*. **2004**, 47, 2853.
[2] Janis, R. A.; Triggle, D. J. *J. Med. Chem*. **1983**, 26, 775.
[3] Bocker, R. H.; Guengerich, E. P. *J. Med. Chem*. **1986,** 29, 1596.
[4] Gordeev, M. F.; Patel, D. V.; Gordon, E. M. *J. Org. Chem*. **1996**, 61, 924.

Comparison of nucleophilicity of stable singlet carbenes in organic reactions

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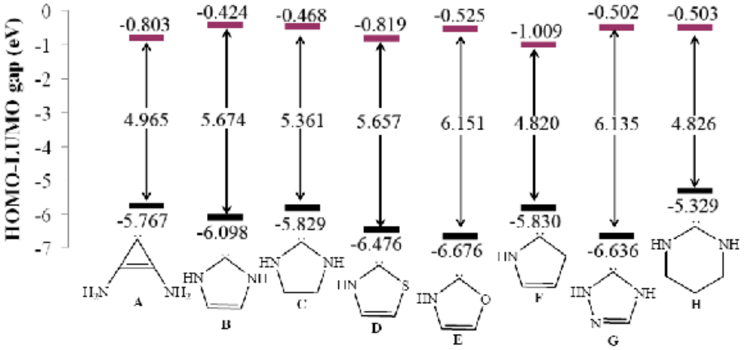
The exciting reports on the synthesis of stable singlet carbenes are a brilliant turning point in the organocatalyst reactions in which carbenes are probed as nucleophiles [1]. In this study B3LYP/AUG-cc-pVTZ//B3LYP/6-31+G* level of theory is employed to investigate the nucleophilicity and reactivity of the following eight carbenes (**A** - **H**).

The energy gaps between frontier molecular orbitals depicted in the Figure project a good rationale for the philicity of **A**-**H**. Nucleophilicity and electrophilicity of these carbenes are discussed using Domingo nucleophilicity index (N), which is calculated as $N = E_{\text{HOMO (Nu)}} - E_{\text{HOMO (TCE)}}$, where tetracyanoethylene is chosen as the reference. Also the global electrophilicity, ω, is calculated following the expression, $\omega = (\mu^2/2\eta)$, where μ is the chemical potential ($\mu \approx (E_{\text{HOMO}} - E_{\text{LUMO}})/2$) and η is the chemical hardness ($\eta = E_{\text{LUMO}} - E_{\text{HOMO}}$) [2]. Carbene **H** is predicted to exert a higher nucleophilicity then our other carbenes in organic reactions.



Singlet carbene	Nucleophilicity (N)	Electrophilicity (ω)
A	3.692	1.087
B	3.361	0.937
C	3.631	0.924
D	2.984	1.176
E	2.784	1.054
F	3.630	1.213
G	2.823	1.038
H	4.130	0.881

References:

[1] Enders, D.; Niemeier, O.; Henseler, A. *Chem. Rev*. **2007**, *107*, 5606.
[2] Domingo, L. R.; Chamorro, E.; Pérez, P. *J. Org. Chem.* **2008**, *73*, 4615.

Rout to greener catalytic aromatization of Hantzsch 1,4-dihydropyridines using catalytic amount of 18% Co/CeO_2-ZrO_2 nano fine particles as a novel and reusable catalyst

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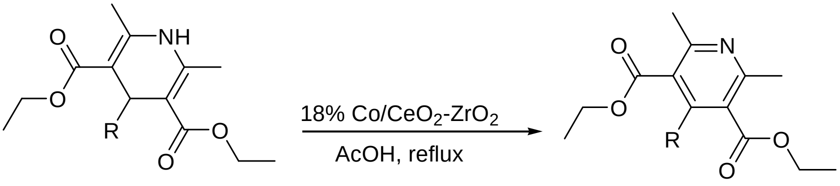
Recently preceding studies have suggested [1–7] that 1,4-DHP derivatives provide an antioxidant protective effect that may contribute to their pharmacological activities. This effect is not due to the Ca^{2+} antagonist effect, but is related to the reactivity of these compounds toward radical species [2]. The aromatization of 1, 4-DHPs is also one of the ubiquitous problems in organic chemistry, and several researchers have reported oxidation methods.

Herein, we interest to develope an efficient, mild and eco-friendly procedure for the oxidative aromatization of Hantzsch 1,4-dihydropyridines in the presence of a catalytic amount of 18% Co/CeO_2-ZrO_2 nano fine particles catalyst as reusable and green catalyst (Scheme 1).



Scheme 1

Reference:

[1] Aruoma, O.; Smith, C.; Cecchini, R.; Evans, P.; Halliwell,B. *Biol. Chem. Pharm.* **1991**, 42.
[2] Mason, R. P.; Mak, I. T.; Trumbore, N. W.; Mason, P. E. *Am. J. Cardiol*. **1999**, 84, 16L.
[3] Mak, I.; Boheme, P.; Wegliki, W. *Circ. Res*. **1992**, *70*, 1099.
[4] Van Amesterdam, F.; Roveri, A.; Maiprino, M.;Ratti, E.; Ursini, F. *Free Radical Biol. Med*. **1992**, *12*, 183.
[5] Toniolo, R.; Di Narda, F.; Bontempelli, G.; Ursini, F. *Bioelectro Chem*. **2000**, *51*, 193.
[6] Diaz-Araya; Nuneez-Vergara, L. j. *Gen. Pharmacol*. **1998**, *31*, 385.
[7] Eisner, U.; Kuthan, J. *Chem. Rev*. **1972**, *72*, 1.

A simple and efficient method for the preparation of β-enaminones and selective acetalization os aldehyde using catalic amount of polyphosphoric acid adsorbed silica gel (PPA/SiO$_2$)

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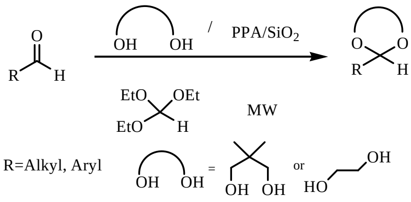
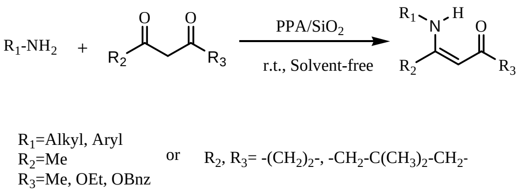
3-Aminoprop-2-en-1-one derivatives which are also known as β-enaminones are very useful components of natural products and versatile precursors for the preparation of pharmaceuticals [1]. Here we report an efficient solvent-free procedure for the preparation of β-enaminones using silica-supported polyphosphoric acid (PPA/SiO$_2$) as heterogeneous catalyst.

PPA/SiO$_2$ was prepared by previously reported method [2]. A number of β-enaminones were prepared in good to excellent yields. As a rule, primary aliphatic amines and benzylamines reacted with a broad range of structurally diverse 1,3-dicarbonyl compounds to afford the corresponding β-enaminones in high yields and in short time. The reaction was highly regioselective, and no by-products were detected.





Acetalization is a process that is widely used in organic synthesis to protect the carbonyl group [3]. Here we wish to introduce a simple, efficient and selective method for the acetalization of aldehydes using a catalytic amount of polyphosphoric acid adsorbed silica gel (PPA/SiO$_2$) in the presence of diole under solvent free conditions and microwave irradiation. A wide variety of aromatic aldehydes underwent smooth reaction to give the corresponding acetals in good to excellent yield. Ketones proved completely resistant to acetal synthesis under same reaction conditions.

References:

[1] Edafiogho, I.; Moore, M.; Alexander, K. *J .Pharm. Sic*. **1994**. *83*, 1155
[2] Takido, T.; Kodomori, M. *Synlett*. **2004**, *13*, 2307.
[3] Greene, T.w; Watts, P. *Protective Group in Organic Synthesis, seconded. Wiley, New York.* **1991**.

Selective and efficient oxidative deprotection of trimethylsilyl and tetrahydropyranyl ethers, ethylene acetals and ketals using *N*-benzyl *N,N*-dimethyl anilinium peroxodisulfate $[PhCH_2NMe_2Ph]_2S_2O_8$

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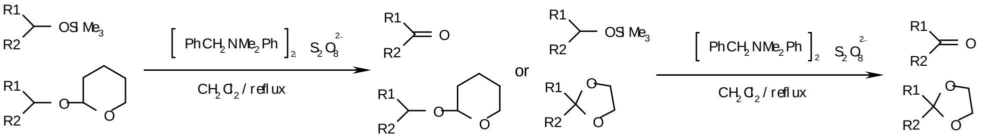
The protection of hydroxyl groups as their trimethylsilyl and tetrahydropyranyl ethers is an important reaction in organic chemistry [1]. Direct oxidation of these ethers to their corresponding carbonyl compounds under mild and aprotic conditions is also of synthetic value [2]. The carbonyl group is one of the most versatile functional groups in organic chemistry. The protection of carbonyl compounds as their ethylene acetals and ketals is important particularly, in multi-step natural product synthesis. Transformation of ethylene acetals and ketals to their parent carbonyl compounds under neutral, aprotic and nonaqueous conditions is of interest to synthetic organic chemists and several methods have been reported for this purpose [3].

In continuation of our research in this area, we now report *N*-benzyl *N,N*-dimethyl anilinium peroxodisulfate as an efficient reagent for the conversion of TMS and THP ethers, ethylene acetals and ketals to their corresponding carbonyl compounds.

We found that trimethylsilyl ethers are oxidized selectively in the presence of tetrahydropyranyl ethers, ethylene acetals and ketals. These selectivities are of value in organic synthesis.



References:

[1] Greene, T. W.; Wutz P. G. M.; *Protective Groups in Organic Synthesis*, 2nd ed., John Wiley, New York **1991**.

[2] Firouzabadi, H.; Mohammadpoor-Baltork, I. *Synth. Commun.* **1994**, *24*, 1065.

[3] Saravanan, P.; Chandrasekhar, M.; Anand, R.V.; Singh, V.K. *Tetrahedron Lett.* **1998**, *39*, 3091.

Head-space solid phase microextraction for chemical composition of the leaves and peel of Citrus Margarita and prediction of chromatographic retention index of essential oils based on molecular structure

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Head-space solid phase microextraction (HS-SPME) is a rapid, simple, inexpensive and solvent free technique for the extraction and preconcentration of volatile compounds. It is carried out by a fused silica fiber that is coated with different stationary phases and characterized by its high sensitivity to volatile organic compounds.

The essential oil of the leaves and peel of Citrus Margarita has been extracted by HS-SPME and analyzed by gas chromatography coupled to mass spectrometry (GC-MS). The principal constituents have been identified as γ-muurolene (8.3%), Elemene (7.9%) and ylangene (7.2%) in leaves and limonene (72.5%), myrcene (16.5%) and α-pinene (3.3%) in peel of Citrus Margarita, respectively. Then a simple, strong, descriptive and interpretable model, based on a quantitative structure-retention relationship (QSRR), is developed using step-wise multiple linear regression (SW-MLR) approach for prediction of the retention index (RI) of essential oil components. By molecular modeling and calculation of descriptors, five significant descriptors related to the retention index values of the essential oils, were identified. Then, the suitable set of the molecular descriptors was calculated and the important descriptors were selected with the aid of the step-wise multiple regression method. A model with low prediction error and good correlation coefficient was obtained. This model was used for the prediction of the RI values of some essential oil components which were not used in the modeling procedure.

Reference:

[1] Pollien, P., Ott, A., *Flavour and Frag. J.*, **1998**, 13, 413.
[2] Diaz-Maroto, C. M., *Journal of chromatography* A., **2002**, 947, 23.
[3] Adams, R.P., Identification of essential oil componenets by gas chromatography / quadrupole mass spectrroscopy, **2004**, Allured, USA.

Kinetics modelling of Fischer–Tropsch Synthesis over Fe/Mn/La_2O_3/Cs

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Fischer–Tropsch (FT) synthesis is one of the main methods of utilizing natural gas, and has gained significant industrial attention as an alternative to the use of limited crude oil resources [1]. FT synthesis always produces a wide range of light gases and distillates, including olefins, paraffins and oxygenated products [2]. Catalysts used for the FT process are generally based on iron or cobalt [3]. A brief literature review on the FT synthesis shows that the kinetics of the FT reaction has been the main focus of many researchers, and several kinetic models from different mechanisms have been proposed [4].

In this present, catalyst was prepared from precursor 50%Fe 50%Mn 0.2%Cs supported on 4.8%La_2O_3 using fusion method and was calcined at 600°C for 6hr. The kinetics of Fe/Mn/La_2O_3/Cs catalyst was studied in a Fixed-bed microreactor. Experimental conditions were varied as follows: reactor pressure of 1-15 bar, reactor temperatures of 573-603 K, H_2/CO feed ratio of 0.5-1.5, and constant space velocity of 4200 h^{-1}. The CO consumption rate was calculated by Poly Math software. Simulations using the optimal kinetic models derived showed good agreement both with experimental data and with some kinetic models from literature. On the basis of proposed reaction mechanisms, the kinetic expressions for paraffin and olfin formation are derived and Reactions rate constants for the iron- manganese oxide catalyst are reported.

References:

[1] Sharifnia, S ; Mortazavi, Y ; Khodadadi, A. *Fuel processing technology*. **2005**, 1253, 1264.
[2] Zaman, M ; Khodadi, A ; Mortazavi,Y. *Fuel processing technology*. **2009**, 1214, 1219.
[3] Mirzaei, A. A ; Habibpour, R ; Faizi, M ; Kashi, E. *Applied catalysis*. **2006**, 272, 283
[4] Ahon, V ; Lage, P ; Souza, C ; Mendes, F ; Schmal, M. *Natural gas chemistry*. **2006**, 307, 312.

p-TSA Catalyzed efficient synthesis of 5-unsubstituted-3,4-dihydropyrimidin-2(1H)-ones under solvent free conditions

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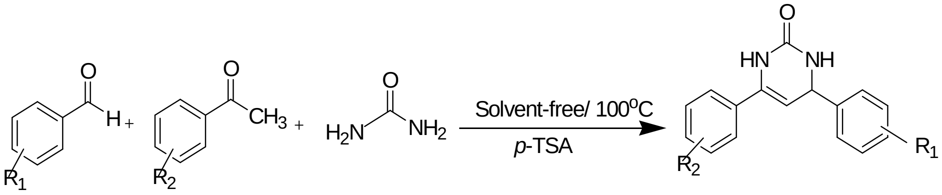
The development of Multicomponent reactions (MCRs) designed to produce elaborate biologically active compounds has become an important area of research in organic, combinatorial, and medicinal chemistry. The MCR strategy offers significant advantage over conventional linear-type synthesis due to its flexible, convergent, and atom efficient nature [1].

It is well known that 3,4-dihydropyrimidin-2(1H)-ones (DHPMs) and their derivatives exhibit a wide range of biological activities, pharmaceutical and therapeutic properties, such as antiviral, antitumor, antibacterial and anti- inflammatory activities[2,3].

In conclusion, we have reported herein *p*-TSA catalyzed for the synthesis of 5-unsubstituted-3,4-dihydropyrimidin-2(1H)-ones using under solvent free conditions. The advantages of the protocol are heterogeneous reaction conditions, shorter reaction times, and easy work up, inexpensive, ready availability of the catalyst make the procedure an attractive alternative to the existing methods for synthesis of 5-unsubstituted-3,4-dihydropyrimidin-2(1H)-ones.



References:

[1] Balme, G.; Bossharth, E.; Monteiro *Eur. J. Org. Chem.* **2003**, 4101.
[2] Kappe, C.O. *Eur. J. Med. Chem.* **2000,** *35*, 1043.
[3] Atwal, K.S.; Swanson, B.N.; Unger, S.E.; Floyd, D.M.; Moreland, S. *J. Med. Chem.* **1991**, *34*, 806.

Synthesis of *N*-substituted sulfonamides from amines mediated by polymer supported tosyl chloride

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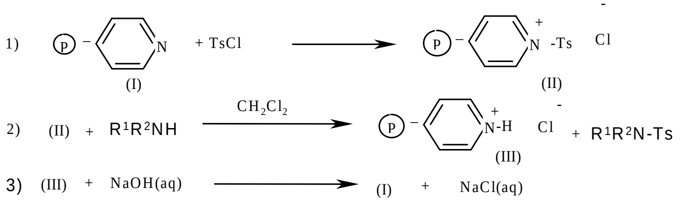
Sulfonamides have long been the subject of pharmaceutical interest as a result of their potent biological activities [1]. As a class; the sulfa drugs have a veritable history of application for the treatment of bacterial infection. Over 30 drugs containing this functionality are in clinical use, including, antibacterial, diuretics, anticonvulsants, anticancer, anti-inflammatory, antiviral agent, hypoglycemic, and HIV protease inhibitors [2].

Although many efforts have been made towards the development of novel sulfonamides, the conventional synthesis involves the nucleophilic attack by ammonia, or primary or secondary amines with sulfonyl chlorides in the presence of a base. However, these procedures involve the use of organic solvents, base and elevated temperatures, especially for less reactive aniline substrates. For sterically hindered primary amines withdrawing substituent, bis-sulfonylation is a common side reaction, which necessitates a further monodesulfonation step [3].

Although the applications of polymeric reagent in organic synthesis have been rapidly developed, reports are seldom seen in preparing sulfonamides by polymeric reagents in literature.

In continuing our studies on the development of application of cross linked poly (4-vinylpyridine) in organic synthesis, here we wish to report a simple, cheap and efficient method for synthesis of sulfonamides (Scheme 1).



(I) : Poly (4-vinylpyridine) cross-linked with 2% DVB, R^1 and R^2 = H, alkyl and aryl

Scheme 1

References:

[1] Harter, W. G.; Albert, H.; Brady, K.; Caprathe, B.; Dunbar, J.; Gilmore, J.; Hays, S.; Kostlan, C. R.; Lunney, B.; Walker, N. Bioorg *Med. Chem. Lett.* **2004**, *14*, 809.
[2] Kleemann, A.; Engel, J.; Kutscher, B.; Reichert, D Pharmaceutical Substances, Synthesis, Patents, Applications; Thieme: Stullgart, **1999**.
[3] Yasuhara, A.; Kameda, M.; Sakamoto, T. *Chem Pharm Bull*. **1999**, *47*, 809.

Synthesis and biological activity of some oxo- and thioxopyrimidines

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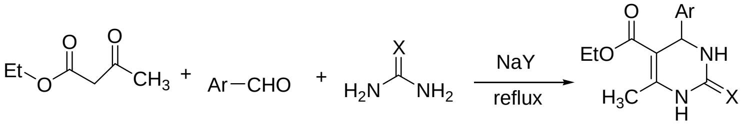
It is well known that a large number of 3,4-dihydropyrimidines, DHPMs, exhibit wide range of pharmacological activities such as antitumor [1], antiviral [2], anticancer [3], and antifungal [4] activities. Many pyrimidine derivatives with appropriate functional groups have emerged as antihypertensive agents [5].

Furthermore, there are numerous modified preparative methods for the synthesis of pyrimidines which known as Biginelli compounds [6]. Some of these methods need expensive reagent, toxic reagent or force reaction conditions.

In view of these points and continuation of our interest in the synthesis of pyrimidines [7], we wish to report the one-pot synthesis and biological activity of some pyrimidines **4(a-j)** which prepared in the presence of NaY zeolite as a friendly catalyst.



X = O, S **2** **3** **4 (a-j)**

References:

[1] Baraldi, P. G.; Pavani, M. G.; Nuez, M. D. C.; Brigidi, P.; Vitali, B.; Gambari, R.; Romagnoli, R.; *Bioorg. Med. Chem.* **2002**, *10*, 449.

[2] Nasr, M. N.; Gineinah, M. M. *Arch. Pharm.* **2002**, *335*, 289.

[3] Sondhi, S. M.; Johar, M.; Rajvanshi, S.; Dastidar, S. G.; Shukla, R.; Raghubir, R.; Lown, J. W. *Aust. J. Chem.* **2001**, *54*, 69.

[4] Mangalagiu, G.; Ungureanu, M.; Grosu, G.; Mangalagiu, I.; Petrovanu, M. *Annales Pharmaceutiques Francaises* **2001**, *59*, 139.

[5] Overman, L. E.; Rabinowitz, M. H.; Renhowe, P. A. *J. Am. Chem. Soc.* **1995**, *117*, 2657.

[6] Patil, A. D.; Kumar, N.; Kokke, W. C.; Bean, M.; Freyer, A. J.; De Brosse, C.; Mai S. *J. Org. Chem.* **1995**, *60*, 1182.

[7] Mobinikhaledi, A.; Foroughifar, N.; Fathinejad, H. *Phosphorus, Sulfur, Silicon Relat. Elem.***2004**, *179*, 2259.

Effect of calcinations conditions on the catalytic performance of impregnated Co-Ni-Al_2O_3 catalyst used in CO hydrogenation

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Fischer-Tropsch synthesis (FTS) has attracted increasing attention, since high quality diesel fuels without sulfur or aromatic compounds can be produced directly from synthesis gas derived from natural gas, coal, or biomass [1]. FTS also provides a means of converting coal and natural gas to petrochemicals and liquid transportation fuels. FTS involves a polymerization reaction beginning with an ethylene intermediate to produce a wide distribution of hydrocarbons ranging from methane to wax (C1-C60) [2, 3].

FTS hydrocarbon products are mostly n-paraffins or n-olefins. There is a considerable increase in the demand for light olefins such as ethylene, propylene and isobutylene because of the growing interest in their applications for the manufacture of highly desirable products such as polyethylene, polypropylene, methyl tertiary butyl ether (MTBE) and ethyl tertiary butyl ether (ETBE) [4].

A Co-Ni-Al2O3 catalyst was prepared using the incipient wetness impregnation method in order to study its catalytic activity and selectivity in the Fischer-Tropsch synthesis. The effect of calcinations temperature and time on the catalytic performance of 80%Co-20%Ni/90wt%Al_2O_3 catalyst was investigated. It was found that the optimum calcinations temperature is 550˚C and the optimum calcinations time is a 6h.

References:

[1] Luo, X. Li.; Asami, M. K. Catal. Today .**2004**, 89, 439.
[2] Adesina, A.A. Appl. Catal. A: Gen. **1996**, 138, 345.
[3] Dry, M.E. Appl. Catal. A: Gen. **1996**, 138, 319.
[4] Sethuraman, R.; Bakhshi, N.N.; Katikaneni, S.P.; Idem, R.O.Fuel Proc. Tech. **2001**, 73 197.

Synthesis of novel furo[3',2':5,6]pyrimido[2,1-c][1,2,4]triazines and furo[3,2-e][1,2,3,4]tetrazolo[1,5-a]pyrimidine

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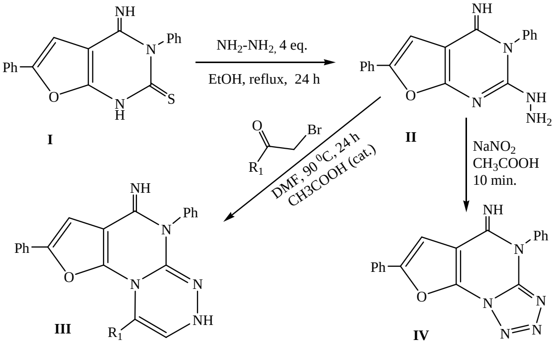
Furo[2,3-*d*]pyrimidines have received much attention due to their biological activities. Antifungal, antibacterial, antiviral, antifolate, antitumor, and anti-HCMV (human cytomegalovirus) activities have been described for these compounds [1]. Recently, some furopyrimidines were shown to be potent LCK (lymphocyte-specific kinase) [2], PI3K (phosphoinositide 3-kinase) [3], VEGFR2 (vascular endothelial growth factor receptor2) and EGFR (epidermal growth factor receptor) inhibitors [4]. Furthermore, a wide range of biological activities has been attributed to fused triazoles, triazines and tetrazoles [5].

In connection with our interest in the synthesis of polyheterocyclic systems, we now report here the utility of 4-imino-3,6-diphenyl-3,4-dihydrofuro[2,3-*d*]pyrimidine-2(1*H*)-thione **I** for the synthesis of some novel tricyclic fused furo[3',2':5,6]pyrimido [2,1-*c*][1,2,4]triazines **III** and furo[3,2-*e*][1,2,3,4]tetrazolo[1,5-*a*]pyrimidine **IV** from α-haloketones and nitrous acid respectively in high yields.



References:

[1] Robins, M. J.; Miranda, K.; Rajwanshi, V. K.; Peterson, M. A.; Andrei, G. *J. Med. Chem.* **2006**, *49*, 391.
[2] DiMauro, E. F.; Newcomb, J.; Nunes, J. J.; Bemis, J. E. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 2305.
[3] Hayakawa, M.; Kaizawa, H.; Moritomo, H.; Koizumi, T. *Bioorg. Med. Chem. Lett.* **2007**, *17*, 2438.
[4] Martin-Kohler, A.; Widmer, J.; Bold, G.; Meyer, T.; Séquin, U. *Helv. Chem. Acta* **2004**, *87*, 956.
[5] Hozien, Z. A.; Abdel-Wahab, A. A.; Hassan, K. M.; Atta, F. M.; Ahmed, S. A. *Pharmazie,* **1997**, *52*, 753.

Fatty acid:A mild and efficient reusable catalyst for the one-pot synthesis 2,4,5Triaryl-1H-imidazoles

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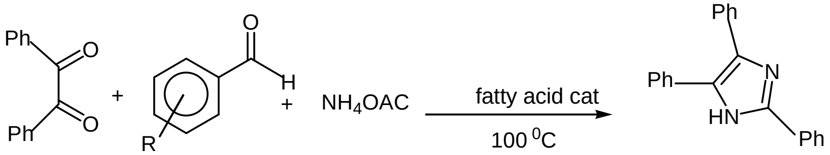
In the mainstream of current interest, multicomponent reactions permitted rapid access to combinatorial libraries of organic molecules for efficient lead structure identification and optimization in drug discovery.imidazole derivatives are very interstinng class of hetrocyclic compounds because they have very farmacological properties and play important roles in biochemical processes.

Many of substituted imidazoles are known as inhibitors of P38 map kinase[1], fubgicides and herbisides[2] and therapeutic agent[3]. some sunstituted triaryl imidazole are selective antagonists of glucagon reporter and inhibitors of IL-1 bio synthesise.

The synthesis of 2,4,5-trisubstituted imidazoles are carried out by condensation of a 1,2-diketone, with an aldehyde, and ammonium acetate.

In continuation of our interest in methodology for the synthesis of trisubstituted imidazoles, herein we are pleased to report for the first time a novel, simple and efficient methodology for the synthesis of 2,4,5-trisubstituted imidazoles in good to excellent yields by condensation of benzil or benzoin, aldehydes, and ammonium acetate using fatty acid as good catalytic media



References:

[1] Lee, J.C.; Laydon , J.T.; McDonnell, P.C.; Gallagher, T.F.; Kumar, S.; Green, D.; McNulty, D.; Blumenthal, N.; Heys. J.R.; Landvatter, S.W.; Strickler, J.E.; McLaughlin, M.M.; Siemens, I.R.; Fisher, S.M.; Livi, J.P.; White, J.R.; Adams, J.L.; Young P.R *Nature.* **1994**, *372*, 739.

[2] Maier, T.; Schmierer, R.; Bauer, K.; Bieringer, H.; Buerstell, H.; Sachse, B.; US Patent (1989) 4820335. *Chem Abstr.***1989** , *111*, 19494.

[3] Heeres, J.; Backx, L.J.J.; Mostmans, J.H.;Vancustem J. *J. Med. Chem.* **1979** ,*22*, 1003.

Synthesis of perydrotriazolotriazoles by 1,3-dipolar cycloaddition reaction (criss-cross cycloaddition) using ultrasonic irradiation and catalyzed by $TiCl_4$

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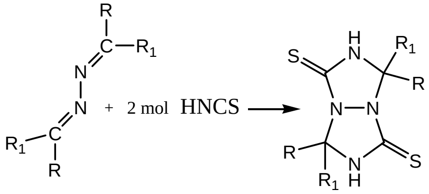
Ultrasonic- assisted organic synthesis (UAOS) as a green synthetic approach is a powerful technique that is being used more and more to accelerate organic reactions [1,2]. Criss-cross cycloaddition was described in 1917 as intermolecular reaction of benzaldazine with 2 equiv. of isothiocyanate affording a heterocyclic compound having two fused fivemembered ring [3]. 1,3-dipolar cycloaddition reactions are fundamental processes in organic chemistry, and their asymmetric version offers a powerful and reliable synthetic methodology to access five-membered heterocyclic rings in regio-and stereocontrolled fashion [4].

In order to expand the application of ultrasound in the synthesis of heterocyclic compound, we wish to report a general, efficient and eco-friendly method for the synthesis of perhydrotriazolotriazoles. The high yield transformations were carried out without any significant amounts of undesirable side products. Based on the results of this study, it seems that the ultrasound irradiation improves the reaction times and yield. Furthermore, we report a facial and efficient method for the synthesis perhydrotriazolotriazoles catalyzed by TiCl4. In an initial study, for examination of the catalytic activity of different catalysts such as BF_3, VCl_3, WCl_6, $AlCl_3$, $ZrCl_4$, $SbCl_3$, Al_2O_3-P_2O_5 and $TiCl_4$. In the course of this study we found that $TiCl_4$ was the most effective catalyst in term of yield of the perhydrotriazolotriazoles (98%) while other catalysts formed the product with the yields of 46-88%. In the absence of catalyst, the yield of the product was found to be very low.



References:

[1] Xu, H.; Liao, W.-M. ; Li, H.-F. *Ultrason. Sonochem.* **2007**, *14,* 779.
[2] Guzen, K. P.; Guarezemini, A. S.; Orfao, A. T. G.; Cella, C. M. P.; *Tetrahedron Lett.* **2007**, *48*, 1845.
[3] Bailey, J. R.; Moor, N. H. *J. Am. Chem. Soc.* **1917**, *39*, 279.
[4] Najera, C.; Sansano, J. M. Curr. *Org. Chem.* **2003**, *7*, 1105.

The catalytic effect of Mn(pbt)Cl_2 in oxidation of benzoin

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Benzoin is a classic precorcer for synthesis of benzil. Benzil is as an α-diketone, which is widely used as building block in the synthesis of hetero- and homo-cyclic compounds and multi-denthate ligands [1,2]. The oxidation of benzoin to benzil is the final step in the synthesis of α -diketons from corresponding aldehydes [3]. Though the reaction proceeds easily, but it is limited by utilization of strong oxidizing agents and alkaline media which are leading to oxidative cleavage reaction and benzil benzilic acid rearrangement [4], respectively. Aerobic oxidation provides an environmentally benign procedure which selectively converts benzoin to benzil. However, the aerobic oxidation is a slow procedure requiring to utilization of sufficient catalytic systems [5].

In this work, we have investigated the oxidation of benzoin by catalitic effect of Mn(pbt)Cl_2, where pbt is 2-(2-pyridy)bezothiazol. The catalyst was prepared from treatment of a methanolic solution of pbt with an equines solution of $MnCl_2$. the variations of main affecting parameter, including the amount of catalyst, the oxidant, temperature and the reaction time, were investigated.

The best results were obtained using H_2O_2 as oxidant 6% Mn(pbt)Cl_2 as catalyst in acetic acid at 80 °C.

References:

[1] Ogata, Y.; Kawasaki, A.; Sugiura, F. *J. Org. Chem.* **1969**, *34*, 3981.
[2] Jones, L. A.; Hancock, C. K.; Seligman, R. B. *J. Org. Chem.* **1961**, *26*, *228*-232.
[3] Estager, J.; Leveque, J-M.; Turgis, R.; Draye, M. *Tetrehedron Lett*. **2007**, *48*, 755.
[4] Marjani, k,; Asgarian, J and Mousavi, M. *J. Chem*. Res, **2007,** 548–551.
[5] Schultz, A,; Giannis, A, *Synthesis*, **2006,** DOI: 10.1055/s-2005924764.

Preparation of *α*-aminonitriles using $Al(H_2PO_4)_3$ as catalysts in solvent-free conditions

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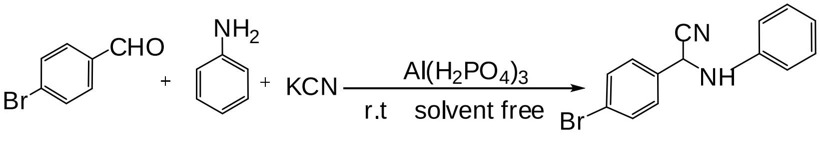
α-Aminonitriles are very important intermediate, particularly in the preparation of α-aminoacids nitrogen containing heterocycles, and other biologically active molecules. There are many reported protocols in the literature for the preparation of α-aminonitriles, among them the classical Strecker reaction represents one of the simplest and most economical method for this purpose through a nucleophilic addition of cyanide anion to imines [1].

Recently, modified method using one-pot procedure via a three-component condensation of aldehyde, amine and trimethylsilyl cyanide catalyzed by Lewis acids (or protic acids) in conventional organic solvents has been reported [2], In some cases, the protocols involve the use of strong and expensive Lewis acids, harsh conditions and tedious aqueous work-up leading to the generation of large amounts of toxic metal-containing waste. Hence, there is further scope to explore milder, safer and more efficient protocols for this reaction. In recent years, the use of solid acids as heterogeneous catalysts has received significant interest in different areas of organic synthesis [3], Heterogeneous solid acids are advantageous over conventional homogeneous acid catalysts as they can be easily recovered from the reaction mixture by simple filtration and can be reused after activation or without activation, thereby making the process economically more viable.

In this work, The reaction of various aldehydes and amines with KCN was performed in short reaction times with excellent yields of α-aminonitriles in the presence of $Al(H_2PO_4)_3$ under solvent-free conditions at room temperature. Both aromatic and aliphatic aldehydes afforded excellent yields whereas ketones did not give any satisfactory results, various types of structurally diverse aromalic aldehydes with either electron-withdrawing or electron-donating groups were converted to the corresponding α-aminonitriles in good to excellent yields.



References:

[1] Karimi, B.; Safari, A. A. *J. Org. Chem*. **2008**, 693, 2967–2970.
[2] Li, Z. J.; Sun, V. J.; Wei, P.; Shi, Y. H.; Ouyang, P. K. *Synlett.* **2007**, *803.*
[3] Wang, B.; Gu, Y.; Luo, C.; Yang, T.; Yang, L. *J. Tet. Lett*. **2004**, 45, 3369.

Synthesis and study of clathrate behavior of pyridinyl ferrocenyl methanols

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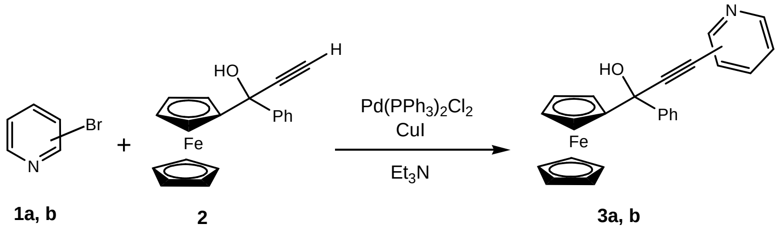
Organic molecules with a bulky and rigid structure including coordinating group can act as host compounds to incorporate other molecules as guest compounds [1]. Such Compounds containing hydroxyl group aggregate to some degree through the formation of a hydrogen bond network because of sterically crowded hydroxyl groups [2]. Earlier investigations have shown that 9-aryl-substituted fluoren-9-ols and related bridged triarylmehanols are efficient inclusion compounds [3]. In this study the synthesis of compounds **3a,b** from 2- and 3-bromopyridines(**1a,b**) and **2** is reported and their clathrate behavior were studied.



From the reaction of benzoyl ferrocene and trimethylsililacetylen, 3-(trimethylsilyl)-1-ferrocenyl-1-phenyl prop-2-yn-1-ol was formed, which in subsequent reaction with K_2CO_3 in MeOH and THF gave compound (**2**). Treatment of compound **2** with bromopyridines (**1a,b**) under Sonogashira reaction conditions afforded 1-ferrocenyl-1-phenyl -3-pyridinyl prop-2-yn-1-ol (**3a,b**). To investigate the clathrate behavior of compounds **3a,b,** we have crystallized these compounds with different solvents and determined the host: guest stiochiometric ratios by ^{1}H NMR.

References:

[1] Toda, F. *Top. Currr,* **1987***, 140,* 43.
[2] Skobridis, K.; Theodorou, V.; Seichter, W.; Weber, E. *Crystal Growth & Design,* **2010***, 10,* 862.
[3] Weber, E.; Meinhold, D.; Haase, R.; Seichter, W.; Rheinwald, G. *Supramolecul. Chem,* **2005***, 17,* 303.

The synthesis of and nuclear magnetic resonance studies on bimetallic molybdenum(VI) complex containing bridging 1,4 –phenylenediamine ligand

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There has been a great interest in the synthesis of homo-dinuclear metal complexes for their relevance as models for interesting magnetic properties [1,2], and also as active sites of biomolecules [3]. Complexes composed of transition metals like molybdenum and bidentate ligand such as 1, 10-phenanthroline have been shown to be useful photophysical and chemical probes of DNA and have found its importance in various biochemical and biomedical applications [4].

MoO_2 $(acac)_2$ {acac = acetyleacetonato} reacted with 1, 10-phenanlhrotine (L) and p-phenylenediamine (μ-N-N) ligands to form homo-dinuclear metal complex of type $[(MoO_2L)_2$ (μ-N-N)]. The structure of complex have been proposed on the basis of elemental analysis, IR, NMR and UV-Vis studies.

References:

[1] J. G. Duguid, V. A. Bloomfield, J. M. Benevides, G. J Thomas, *Biophys. J.* **1995,** *69*, 2623.

[2] E. V. Hanckl, S. V. kornilova, L. E. kapinos, V. V. Andrushchenko, V. L. Galkin, D. N. Grigoriev, *J. Mol. struct.* **1997**, 2, 229.

[3] D. R. McMillin, K. M. McNett, *Chem. Rev*. **1998,** *98*, 1201.

[4] K. E. Erkkila, D. T. Odom, J. K. Barton, *chem. Rev.* **1999,** *99*, 2777.

An efficient synthesis of 2*H*-benzo[*b*]xanthene-triones and dodecahydrochromeno[2,3-*b*]xanthene-1,6,8,13-tetraone derivatives catalyzed by L-proline in aqueous media

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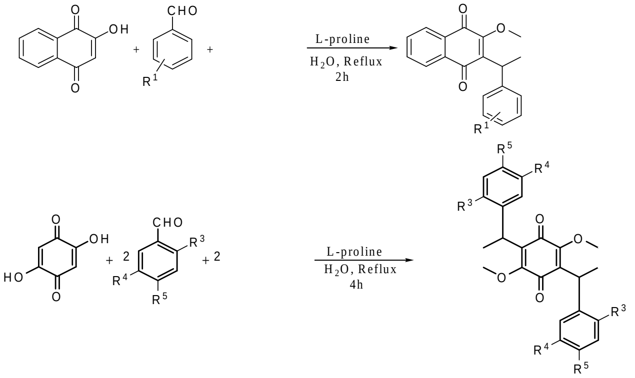
The quinone moiety is involved in wide variety of biochemical processes including electron transport and oxidative phosphorylation.[1] Various biological properties including enzyme inhibition, antibacterial, antifungal, and anticancer activities have been reported for quinones and quinone derivatives.[2–5] The antitumor activity of the quinone moiety has been studied thoroughly, and it is known that they act as topoisomerase inhibitors via DNA intercalation.[6,7]

In this work, we wish to report an efficient method for synthesis of 2*H*-benzo[*b*]xanthene-trione and dodecahydrochromeno[2,3-*b*]xanthene-1,6,8,13-tetraone derivatives *via* addition and subsequently cyclization of 2-hydroxynaphthalene-1,4-dione, 5,5-dimethylcyclohexane-1,3-dione, aldehydes, 5,5-dimethylcyclohexane-1,3-dione or cyclohexane-1,3-dione in the presence of a catalytic amount of L-proline in refluxing water in good to excellent yields.



References:

[1] Pratt, Y. T.; Drake, N. L. *J. Am. Chem. Soc*. **1960**, *8*, 1155.
[2] Skibo, E. B.; Islam, I.; Hileman, M. J.; Schulz, W. G. *J. Med. Chem*. **1994**, *37*, 78.
[3] Ryu, C. K.; Choi, K. U.; Shim, J. Y.; You, H. J.; Choi, I. H.; Chae, M. *J. Bioorg. Med. Chem*. **2003**, *11*, 4003.
[4] Ryu, C. K.; Kang, H. Y.; Yi, Y. J.; Shin, K. H.; Lee, B. H. *Bioorg. Med. Chem. Lett*. **2000**, *10*, 1589.
[5] Lin, A. J.; Cosby, L. P.; Sartorelli, A. C. *Cancer Chemother. Rep*. **1974**, *4*, 23.
[6] Denny, W. A.; Bagulet, B. C. *In Molecular Aspects of Anticancer Drug-DNA Interactions*, 2nd ed.; Waring, M. J., Neidle, S., Eds.; Macmillan: London, **1994**; 270.
[7] Pommier, Y.; Capranoco, G.; Orr, A.; Kohn, K. W. *Nucleic Acid Res*. **1991**, *19*, 5973.

Dimethyl methylphosphonate (DMMP) interacting with SWCNTs: *first-principles* study

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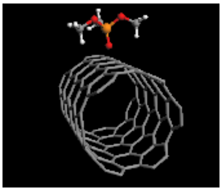
The uses of chemical warfare agents (CWAs) are significant as they can be readily synthesized by simple chemical reactions and often have an extremely high toxicity. Unfortunately, these chemicals were used on a large scale during the 1st World War [1]. Unfortunately, they act by first binding with, and then irreversibly inhibiting acetyl cholinesterase (AChE) and producing a toxic accumulation of acetylcholine (ACh), causing nausea, diarrhea, inability to perform simple mental tasks, and respiratory effects which include bronchoconstriction, excess secretion in airways [2].

It is imperative to have an early warning system consisting of readily deployable sensors for these lethal agents. Usually this is achieved by means of surface acoustic wave (SAW) sensors, conducting polymer arrays, vector machines, and color change paper sensors [3]. The need for higher specificity and sensitivity has led to the application of element specific detectors such as carbon nanotubes that were first used for organic vapour sensing as chemiresistors, where resistance changes in nanotubes were monitored continuously with time upon exposure to vapours [4].

Using *first-principles* simulations based on density functional theory (DFT) method for structural optimization and total energy calculations, we have investigated the interaction between the nerve agent dimethyl methylphosphonate DMMP and typical zigzag (semiconducting) and armchair (metallic) SWCNTs. Several possible configurations were selected for a DMMP molecule approaching the substrate of the carbon nanotubes, via its expected active sites. The calculated results showed that the DMMP affinity for the metallic nanotube is stronger than for metallic one. The adsorption energy values and bond distances obtained from the *ab initio* calculations are typical for the physisorption. The study of the electronic structure indicated that no significant hybridization between the respective orbitals of the two entities takes place, thus the unveiling the small interaction obtained quantitatively in terms of binding energies.



References:

[1] Somani S. M., Chemical Warfare Agents; Academic Press: London, **1992**.
[2] Munro N. B., Talmage S. S., Griffin G. D., Waters L. C., Watson A. P., King J. F., Hauschild V., *Environ. Health Perspect.* **1999,** *107*, 933.
[3] Cattanach K., Kulkarni R. D., Kozlov M. and Manohar S. K., *Nanotechnology* **2006**, *17*, 4123.
[4] Wang, F. *et al.*, *J.Am.Chem.Soc.*, **2008,** *130*, 5392.

Studies on the synthesis of new derivatives of pyridones using bio-supported solid acid catalyst

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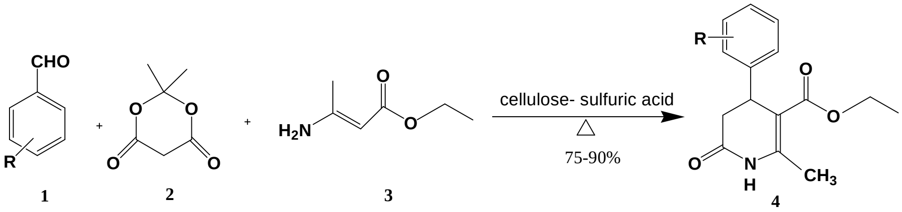
In recent years, an increasing interest has been focused on the synthesis of 1,4-dihydropyridine derivatives owing to their significant biological activities [1]. In particular, dihydropyridine drugs such as nifedipine, nicardipine, amlodipine and others are effective cardiovascularagents for the treatment of hypertension [2].

On the other hand solid acid catalysts for the synthesis of fine chemicals have attracted considerable attention from both environmental and economical points. The solid acid generally has high turn over numbers and can be easily separated from reaction mixture [3].

In continuation of our ongoing interest in the synthesis and use of *N*-heterocyclic compounds in organic synthesis [4], we have developed for the first time an efficient method for the synthesis of dihydropyridine derivatives namely dihydropyridones, via a one-pot three-component reaction of aldehyds (**1**), meldrum acid (**2**) and ethyl 3-amino crotonate (**3**) in the presence of premade and reusable cellulose-sulfuric acid as a bio-supported and heterogeneous catalyst. In this protocol the pyridone derivatives were obtained in high yields (75-90%) and reasonable reaction times (2-3 h).



References:

[1] Shan, R.; Velazquez, C.; Knaus, E. E. *J. Med. Chem.* **2004**, *47*, 254.
[2] Buhler, F. R.; Kiowski, W. *J. Hypertens.* **1987**, *S3,* 5.
[3] Shaabani, A.; Rahmati, A.; Badri, Z. *Catal. Commun*. **2008**, *9*, 13.
[4] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K. *Molecules* **2009**, *14*, 1468; Mamaghani, M.; Dastmard, S. *Ultrason. Sonochem.* **2009**, *16*, 445; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *Heterocycles* **2008**, *75*, 2825. Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N. O.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49*, 1450.

The synthesis of (Azo – $\mathrm{PAMAM_{(DIPA)}G_{2.5}}$)$_n$ polymer

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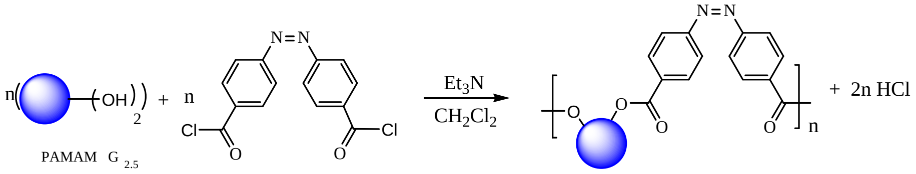
Dendrimers are macromolecules comprised of a series of branches extending outward from an inner core [1,2]. The word dendrimer originates from the Greek *dendron*, meaning “tree”. Ideally, they are perfectly monodisperse macromolecules with a regular and highly branched three-dimensional architecture. Dendrimers are usually produced in an iterative sequence of reaction steps, in which each additional iteration leads to a higher generation material [3-5]. Dendrimers possess three distinct parts, each of which can be modulated: a core, branching units, and branches [2]. In this research (Azo – $\mathrm{PAMAM_{(DIPA)}G_{2.5}}$)$_n$ Polymer was synthesized by tow monomers, which those were generation tow and half ($G_{2.5}$) of polyamidoamie (PAMAM) dendrimer with diisopropanolamine (DIPA) core and azobenzene's derivative respectively. It is shown in scheme (1) and characterized by FTIR, ^{1}HNMR, ^{13}CNMR, UV-Vis spectroscopies and CHNS elementary analysis.



Scheme 1: The Sythesis of (Azo – $\mathrm{PAMAM_{(DIPA)}G_{2.5}}$)$_n$ Polymer

References:

[1] Crespo, L., Sanclimens, G., et all. *Chem. Rev*. **2005,** *105*, 1663.
[2] Newkome, G. R.; Shreiner ,C. D. ; *Polymer* **2008**, *49*, 1-173.
[3] Massoudi. A.H, Vahedi. H, Louie.O and Sajjadiffar.S, *E-J. Chem* **2009**, *6*(3), 681.
[4] Massoudi, A. H., Maddahi, A., *Asian J Chem.*, **2008**, 20, *1*, 463.
[5] Louie, O., Massoudi , A.H., Vahedi, H., Sajjadifar, S.; *j. Polymer* ,**2009** ,*50*, 5605.

A convenient regioselective synthesis of new 2-imino-1,3-thiazolidin-4-ones

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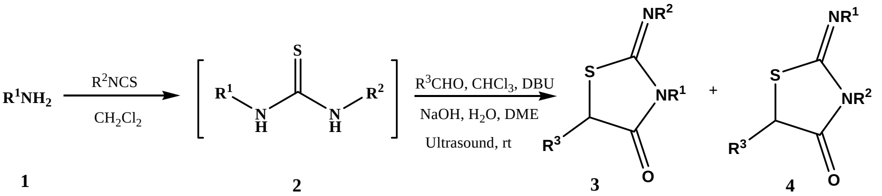
Thiazolidin-4-ones have been used as synthetic intermediates, and display diverse biological activities such as antiarthiritic, anti-bacterial, anti-viral, anti-convulsant, anti-inflammatory, anti-diabetic, and calcium antagonist [1]. This array of properties has resulted in a considerable number of reviews [2]. Interestingly, accounts of thiazolidinones are dominated by 4-thiazolidinones and in particular 2-iminothiazolidinones are prevalent [1]. There are many available methods for the synthesis of 2-imino-4-thiazolidinones [3]. However some of these methods use expensive starting materials, and suffer from multi-step synthesis, long reaction times, and low yields.

In continuation of our ongoing program aiming at the development of efficient methods for the synthesis of heterocycles with medicinal applications [4], we carried out a simple regioselective one-pot reaction for the synthesis of 2-iminothiazolidinones under ultrasonic irradiation (Scheme 1).

In this protocol a suitable amine and isocyanate reacted in CH_2Cl_2. Subsequent addition of aldehyde in a basic media (NaOH, DME) followed by application of ultrasound lead to the desired 2-iminothiazolidinones in 75-91% yields.



R^1 = H, C_2H_5, $C_6H_5CH_2$, CH_2=$CHCH_2$, cyclohexyl
R^2 = H, C_6H_5, 4-MeC_6H_4, thiazol-2-yl, C_2H_5 ; R^3 = H, C_6H_5, 4-MeC_6H_4

Scheme 1

References:

[1] Klika, K.D.; Janovec, L.; Imrich, J.; Suchar, G.; Kristian, P.; Sillanpaa, R.; Pihlaja, K. *Eur. J. Org. Chem.* **2002**, 1248; Kline, T.; Felise, H. B.; Barry, K. C.; Jackson, S. R.; Nguyen, H. V.; Miller, S. I. *J. Med. Chem.* **2008**, *51*, 7065.
[2] Singh, S. P.; Parmar, S.S.; Raman, K.; Stenberg, V. I. *Chem. Rev.* **1981**, *81*, 175.
[3] Sedlak, M.; Hanusek, J.; Machacek, V.; Hejtmankova, L. *J. Heterocycl. Chem.* **2002**, *39*, 1105.
[4] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K.; Kupaei Abiazi, M. *Mol. Divers.* **2009**, *13*, 389; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765.

Synthesis of some new xanthenes derivatives in the presence of acid catalyst

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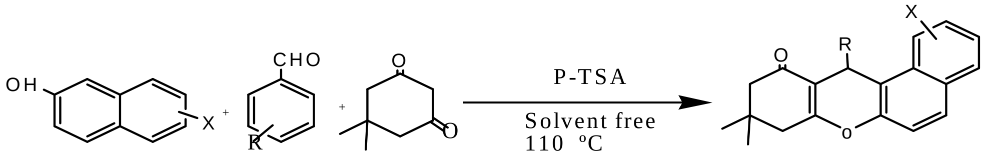
Xanthenes and benzoxanthenes have been used extensively as the rapeutic in medicinal chemistry[1].

Xanthene dyes are extracted naturally from soil and plants such as inigofera longeracemosa.

During the course of our recent studies directed toward the development of practical safe andenvironmentally friendly procedures for some transformations [2,4].

We have succeed in preparing the tetrahydrobenzo[α] xanthene-11-one derivatives, from condensation of aldehydes , dimedone, and β-naphthols in the presence of ρ-TSA , ammonium chloride in good yield.



X=H,OH,Br

R=H ,2-Cl ,4-OMe,...

References:

[1] Ion, R. M., Planner, wiktorowicz, K.; Frackowiak, D. *Acta Biochim.pol.* **1998**, 45, 833-845.
[2] Foroughifar, N.; Mobini khaledi, A; Moghanian, H. *Synlett*, **2008**, 821-826.
[3] Foroughifar, N; Mobini khaledi, A.; Moghanian, H. *S ynth. Commun*. **2009**, 39, 3668-3676.
[4] Foroughifar, N.; Mobini khaledi, A.; Moghanian, H. *Chem.L ett*. **2010**, 39, 180-181.

Rapid and facile synthesis of 2,5-diaryl-1,2,4-thiadiazoles *via* the reaction of thiobenzamides and *α*-bromobenzyl cyanide derivatives

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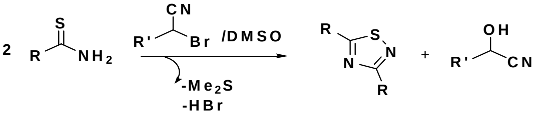
The synthesis of 1,2,4-thiadiazoles has attracted a great deal of interest through the years due to their biological activities. 1,2,4-Thiadiazole derivatives are widely found in bioorganic and medicinal chemistry with applications in drug discovery and development for treatment of human leukemia cell [1], such as Cathepsin B inhibitors [2], allosteric modulators [3], factor XIIIa inhibitors [4], non-ATP competitive glycogen synthase kinase 3β inhibitors [5], and dual 5-lipoxygenase and cyclooxygenase inhibitors [6]. Some of these show intense muscarinic [7] and cardiprotective activities [8]. The usefulness of 1,2,4-thiadiazole as pharmacophore in medicinal chemistry has attracted interest in the synthesis of this system. The main synthetic route to obtain symmetrical 3,5-dialkyl/diaryl-1,2,4-thiadiazole derivatives generally comprises an oxidation step of the thioamides following the cyclization to the corresponding thiadiazoles. Various oxidizing agents such as halogens [9], nitrous acid [10], hydrogen peroxide [11], thionyl chloride [12], a mixture of HCl-DMSO [13], and pyridinium salt-DMSO [14] have been employed for this procedure.

In the most synthetic methods of the 1,2,4-thiadiazoles, solvent, temperature, and the time play an important role in promoting the reaction courses. Performing the reaction at elevated temperatures and the long reaction times are important limitation factors for a good synthetic method. It was shown that in the reaction of α-bromo benzylcyanides and thiobenzamide derivatives in DMSO and in ordinary temperatures 1,2,4-thiadiazole derivatives were produced in good to excellent yields and in very short times (10-15 minutes). High yields, easy work-up, cheap starting materials, and short reaction times are the salient future of the presented method.



References:

[1] Romagnoli, R.; Baraldi, P. G.; Carrion, M. D.; CruzLopez, O.; Preti, D.; Aghazadeh Tabrizi, M.; Fruttarolo, F.; Heilmann, F.; Bermejo, J.; Estevez, F. *Bioorg. Med. Chem.Lett.* **20۰۷**, *17*, 2844.
[2] Leung-Toung, R.; Wodzinska, J.; Li, W.; Lowrie, J.; Kukreja, R.; Desilets, D.; Karimian, K.; Tam, T. F.; *Bioorg.Med Chem*. **2003**, *11*, 5529.
[3] Van Dem Nieuwendijk, A. M. C. H.; Pietra, D.; Heitman, L.; Goblyos, A.; IJzerman, A. P.; *J. Med. Chem*. **2004**, *47*, 663.
[4] Leung-Toung, R.; Tam, T. F.; Wodzinska, J. M.; Zhao, Y.; Lowrie, J.; Simpson, C. D.; Karimian, K.; Spino, M.; *J. Med.Chem*. **2005**, *48*, 2266.
[5] Martı´nez, A.; Alonso, M.; Castro, A.; Pe´rez, C.; Moreno, F. J.; *J. Med. Chem*. **2002**, *45*, 1292.
[6] Unangst, P. C.; Shrum, G. P.; Connor, D. T.; Dyer,R. D.; Schrier, D. J.; *J. Med. Chem*. **1992**, *35*, 3691.
[7] Macleod, A. M.; Baker, R.; Freedman, S. B.; Patel, S.; Merchant, K. J.; Roe, M.; Saunders, J.; *J. Med. Chem*. **1990**, *33*, 2052.
[8] Decking, U. K. M.; Hartmann, M.; Rose, H.; Bruckner, R.; Meil, J.; Schrader, J.; *Naunyn-Schmiedeberg's Arch. Pharmacol*. **1998**, *358*, 547.
[9] Hofmann, AQ. W.; Gabriel, S.; *Ber*. **1892**, *25*, 1578.
[10] Cronyn, M. W.; Nakagawa, T. W.; *J. Am. Chem. Soc*. **1952**, *74*, 3693.
[11] Cashman, J. R.; Hanzlik, R. P.; *J. Org. Chem*. **1982**, *47*, 4645.
[12] Castro, A.; Castano, T.; Encinas, A.; Porcal,W.; Gil, C.; *Bioorg. Med. Chem*. **2006**, *14*, 1644.
[13] Miotti, U.; *J. Chem. Soc., Perkin Trans*. **1991**, *2*, 617.
[14] Takikawa, Y.; Shimada, K.; Sato, K.; Sato, S.; *Bull.Chem. Soc. Jpn*. **1985**, *58*, 995.

Pd(II)/Silicadiphenyl phosphite(SDPP) as an efficient catalytic system for carbon monoxide-free aminocarbonylation of aryl halides (X = F, Cl, Br, I) with $POCl_3$ and DMF

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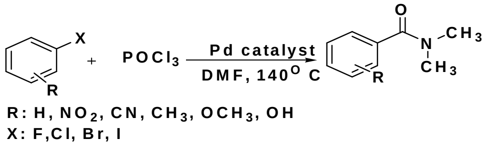
Transition metal-catalyzed carbonylation of aryl halides in the presence of nucleophiles is an efficient methodology for the preparation of aromatic carbonyl compounds such as carboxylic acids, esters, ketones and amides [1]. Among these compounds, amides are widely used in medicinal chemistry [2]. So, development of new synthetic methods for their synthesis is greatly attracted chemists. Some methods for aminocarbonylation of aryl halides using carbon monoxide and amine with various palladium based catalytic systems such as $PdBr_2(PPh_3)_2$/ $PdCl_2(PPh_3)_2$ [3], silica-supported bidentate arsine–palladium complex [4], $Pd(OAc)_2/PPh_3$ in ionic liquid [5] and $Pd(OAc)_2$/xantphos catalytic system [6] have been developed. However, these methods suffer from the difficulty in handling the toxic, gaseous carbon monoxide.

Herein we report an efficient method for aminocarbonylation of aryl iodides, bromides as well as for chlorides and fluorides carrying electron deficient, or electron releasing groups without the direct use of carbon monoxide. Aminocarbonylation is carried using $POCl_3$, N,N- Dimethylformamide (DMF) as both carbon monoxide and amine source and $Pd(OAc)_2$ catalyst in conjunction with silicadiphenyl phosphite (SDPP) as new phosphorylated silica and a heterogenous ligand (scheme).



Scheme

References:

[1] Tambade, P. J.; Patil , Y. P.; Bhanage, B. M. *Appl. Organometal. Chem.* **2009** , *23*, 235–240.

[2] a) Malawskai, B.; Kulig, K.; Gajda, J.; Szczeblewki, D.; Musaial, A.; Wickowski, K.; Maciag, D.; Stables, J. P. *ActaPoloniaePharm. Drug Res.* **2007**, *64*, 127; b) Malawska, B. *Curr. Top. Med. Chem.* **2005**, *5*, 69; c) Luszczki, J. J.; Swiader, M. J.; Swiader, K.; Paruszewski, R.; Turski, W. A.; Czuczwar, S. J. *Fund. Clin. Pharmacol.* **2008**, *22*, 69.

[3] Schoenberg, A.; Heck, R. F. *J. Org. Chem.* **1974**, *39*, 3327; d) Perry, R. J.; Wilson, B. D. *J. Org. Chem.* **1996**, *61*, 7482.

[4] Cai, M.; Huang, Y.; Hu, R.; Song, C. *J. Mol. Catal. A: Chem.* **2004**, *212*, 151.

[5] Skoda-Foldes, R.; Takacs, E.; Horvath, J.; Tuba, Z.; Kollar, L. *Green Chem.* **2003**, *5*, 643.

[6] Martinelli, J. R.; Watson, D. A.; Freckmann, D. M. M.; Barder, T. E.; Buchwald, S. L. *J. Org. Chem.* **2008**, *73*, 7102.

Heavy metal ion uptake of a polysaccharide-based hydrogel

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Hydrogels are three dimensional polymeric networks that can absorb water or other fluidic materials in a relatively short period of time and hold it even under pressure. Hydrogels made great attractions in the last decades because of their unique characteristics and broad applications in different industries. Such examples of hydrogel applications are; disposable infant diapers, agricultural and horticultural applications, dye and metal ion adsorption, biomedical applications and so on. Due to the biocompatibility, biodegradability and non-toxicity properties of the natural based hydrogels, researchers focused widely on their characteristics and swelling behavior in different conditions [1, 2].

Toxic metals pollution is a serious problem threatening plants and human health. Heavy metal ions such as Pb(II), Cd(II) and Hg(II) are toxic, non-biodegradable, carcinogen and can accumulate in living organisms. Therefore, one of the most important origin pollutants of water and waste water are these heavy metals. In order to remove heavy metal ions from various environments, the techniques such as precipitation, adsorption, ion exchange, reverse osmosis, electrochemical treatments, hyperfiltration, membrane separation, evaporation, coagulation, oxidation and biosorption processes are widely used [3].

In this paper, Cd(II) ion adsorption capacity of a carboxymethylcellulose-based hydrogel investigated in Cd(II) solutions with various concentrations, pHs and different adsorption times, by means of a flame atomic absorption spectrophotometer. The Cd (II) adsorption capacity of the hydrogel measured according to the standard diagram which plotted previously with known concentrations. In comparison to the other researches significant results obtained and the sample showed a well Cd (II) adsorption capacity.

References:

[1] Mark, H. F. *Encyclopedia of Polymer Science and Technology,* Vol. 2, Hydrogels, by Jay Friedrich Künzler, Bausch and Lomb Inc., John Wiley & Sons, Inc., **2004**, 691.
[2] Bagheri Marandi, G.; Hariri, S.; Mahdavinia, G. R. *Polym Int*, **2009**, *58*, 227.
[3] Ozay, O.; Ekici, S.; Baran, Y.; Aktas, N.; Sahiner, N. *Water Res*, **2009**, *43*, 4403.

Phytochemistry studies of dionysia revoluta boiss., subsp. revolute (primulaceae): components and antioxidant activity

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Dionysia revoluta boiss., subsp. revoluta is an endemic plant in Iran that is used for gastric disease prevention and also infectious wounds healing [1]. In this study, the plant samples were harvested from Sarikhani Mountain of Shiraz Province in April 2010. Initially, the shoots of sample plants was washed and dried to the shade. The aim of this work was to evaluate the chemical composition of Dionysia revoluta boiss., subsp. revoluta essential oils, isolated by hydro-distillation during 4 h using a Clevenger-type apparatus from the shoots including stems. The essential oils were kept in refrigerator until analysis. Biochemical component of essential oil was determined by GC-Mass analyzer. The results of GC-Mass showed that Dionysia revuluta have 22 biochemical compounds such as bisabolol, quinoline, and thymol. This essential oil has shown antioxidant activities.

Antioxidant activities of the samples were determined by two various testing systems namely DPPH, β-carotene/linoleic acid.

Scavenging capacity on DPPH radical: The free radical-scavenging activities of extract and oil were measured by using 2,2-diphenyl-1-picryl-hydrazyl (DPPH) with some modification. Three milliliters of various concentrations of the extract or the oil in ethanol was added to 1 ml of a 0.5 mM ethanol solution of DPPH. The mixture was strongly shaken and left to stand at room temperature for 60 min in the dark. Then, the absorbance was measured at 517 nm against a blank. The sample concentration providing 50% inhibition (IC_{50}) was calculated from the graph of inhibition percentage against sample concentration. Tests were carried out in triplicate. BHT was used as positive control.

β-Carotene linoleic acid assay was evaluated according to the reported method. Antioxidative capacities of the oil and the extract were compared with those of BHT and blank.

References:

[1] Magnus L. The genus Dionysia (Primulaceae), a synopsis and five new species. Wildenowia. **2007**, *37*: 37-61.

Directed efficient and rapid bromination of phenols and anilines with *N*-bromosaccharin using tungstophosphoric acid as a heterogeneous recyclable catalyst under solvent-free conditions

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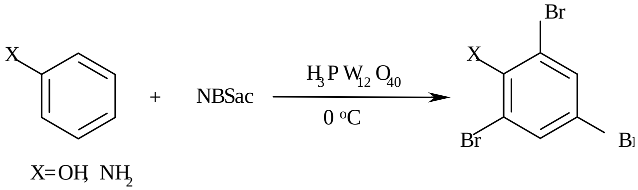
A consequence of the necessity to minimize the amount of toxic waste and by- products from chemical processes is a need for the development of new, more environmentally friendly synthetic methods in which fewer toxic substances are used [1]. Many organic solvents are ecologically harmful, and their use should therefore be minimized as far as possible or even avoided altogether.

Bromination of phenols and anilines belong to an important class of organic intermediates that are used as precursors of organometallic reagents in synthetic organic chemistry [2]. Brominating reagents such as *N*-bromosuccinimide [3] and pyridinium or tetraalkylammonium tribromides [4] make for easier handling and result in improved selectivity, but are unfortunately limited by their low atom efficiency and the need to remove the reagent's residue [5]. Although *N*-halosaccharins are more electrophilic than the structurally analogue NXS, they have found little attention in the synthetic organic chemistry [6]. Heteropolyacids (HPAs) are solid superacids that catalyze a variety of organic transformations [7].

Now, we wish to report efficient, operationally simple, and cost-effective procedure for the synthesis of tribromo phenol and aniline derivatives using NBSac in the presence of a catalytic amount of $H_3PW_{12}O_{40}$.



References

[1] Anastas, P. T.; Williamson, T. C. *in Green Chemistry, Designing Chemistry for the Environment.American Chemical Society*, Washington DC, **1996.**
[2] Larock, J. R. C. *Comprehensive Organic Transformations: A Guide to Functional Group Protection*; Wiley-VCH: New York, **1997**.
[3] Pravst, I.; Zupan , M.; Stavber, S. *Green Chem*, **2006**, *8*, 1001.
[4] Chiappe, C.; Leandri, E.; Pieraccini, D. *Chem Commun*, **2004**, *22*, 2536.
[5] Eissen, M.; Lenoir, D. *Chem Eur J*, **2008**, *14*, 9830.
[6] Dolenc, D.; *Synlett* **2000**, 544.
[7] Misono, M.; Okuhara, T. *Chem Technol.* **1993**, *11*, 23.

Spectral studies of the interaction of methylen blue and thionine with ct-DNA

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Binding properties of methylen blue (MB) and thionine (Th) in the presence of various concentration of calf thymus DNA (ct-DNA), has been investigated in 7.5 mM phosphate buffer, pH =7.2 and various ionic strengths by UV-vis absorption. The results show that both dyes does not have any affinity for aggregation due to increasing of salt concentration and exists as monomers even in homogeneous aqueous solutions of high ionic strengths (more than 2M NaCl). A spectral change of MB and Th with addition of DNA exhibited the hypochromism on the incremental addition DNA with varying degrees of bathochromic shift, indicating interaction of dye with DNA. The percentage hypochromicity of maximum band of two dyes upon binding to DNA was found over to be 35%. Red shift were 10 nm and 14nm for MB and Th, respectively. From above mentioned changes (large hypochromicity and moderate red shift), we considered the interaction MB and Th dyes with DNA were both outside groove-binding modes. The binding constant for the interaction of two dyes with DNA were determined by absorption spectrophotometric titrations at room temperature. The apparent binding constants of MB and Th were calculated to be 1.25×10^5 M^{-1} and 5.25×10^5 M^{-1} , respectively. Data indicated that affinity binding of Th is more than of MB.

References:

[1] Strahan, G. D.; Lu, D.; Tsuboi, M.; Nakamato, K. *J. Phys. Chem.***1992**, *96*, 6450.
[2] Mohammadi, S.; Perree Fauvet, M.; Gresh, N. ; Hillairet, K.; Taillandier, E. *Biochem.*, **1998,** *37*, 6165.
[3] Kang, J.; Wu, H.; Lu, X.; Wang, Y.; Zhou, L. *Spectrochim. Acta, Part A***., 2005,** *61*, 2041.
[4] Ghanadzadeh Gilani, A.; Tajalli, H.; Zakerhamidi, M. S. *J. Mol.r Liq.* **2008**, *143,* 81.

Polyvinyl sulfonic acid fixed on Clinoptilolite nanozeolite as an efficient polymeric catalyst in the protection of carbonyl group

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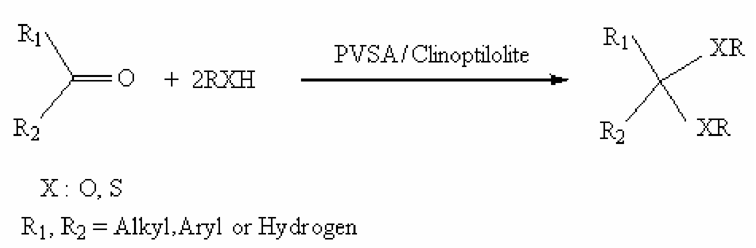
There are inherent drawbacks to the use of liquid acids as catalysts, such as formation of undesirable by-products, hazardous operating conditions, and large-volume waste streams. Therefore, there is now increasing interest in finding new alternative solid acid catalysts. Solid acid catalysts, which are reusable and readily separable from the reaction product, offer the opportunity to reduce the impact on the environment and increase profits [1]. The protection of carbonyl groups as acetals or dithioacetals is now commonly used as an important synthetic technique in the course of preparation of many organic compounds including multifunctional complex molecules [2].

In this project, a new polymeric solid acid, polyvinyl sulfonic acid, was easily prepared from the reaction of polyvinyl alcohol and Chlorosulfonic acid under solvent free condition and fixed on Clinoptilolite. The obtained solid acid was used as efficient solid acid in the protection of carbonyl groups as acetal, ketals and cyclic acetals and ketals and the products were obtained in high isolated yields and in short reaction times.



Reference:

[1] Tanabe, K.; Holderich, W. F. *Appl. Catal. A: Gen.* **1999**, *181*, 399.
[2] Kawabata, T.; Mizugaki, T.; Ebitani, K.; Kaneda, K. *J. Am. Chem. Soc.* **2003**, *125*, 10486.

Synthesis and characterization of new fluorinated aromatic poly(amide-imide)s derived from a new imide-containing aromatic dicarboxylic acid

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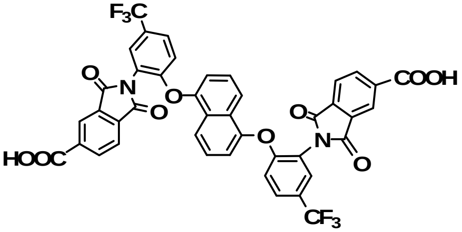
Wholly aromatic polyamides are characterized as highly thermally stable polymers with a favorable balance of physical and chemical properties. However, the rigidity of the backbone and strong hydrogen bonding result in high melting temperatures or glass-transition temperatures and limited solubility in most organic solvents. The properties make them generally intractable or difficult to process, thus restricting their applications in some fields (1).

To overcome these limitations, polymer-structure modification becomes necessary. Therefore, there is interest in diminishing the cohesive energy through lowering the interchain interactions as a way of improving the solubility (2). In addition to using meta substitution in the main chain phenylene residues, this can be achieved by reducing the hydrogen bond effectiveness through the introduction of bulky side groups to the main chain, by employing nonsymmetric monomers, or by introducing flexible linkages to the polymer backbone.

In this paper, we report the synthesis and characterization of a series of new poly(amide-imide)s bearing naphtalen groups based on a new diacid, 1,5-bis(trifluoromethyl-2-trimelitimido phenoxy)- naphtalen (**I**) using yamazaki's phosphorylation polyamidation.



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References:

[1] (a) Cassidy, P. E.; *Thermally Stable Polymers*; Marcel Dekker: New York, **1980**. (b) Yang, H. H. *Aromatic High-Strength Fibers*; Wiley: New York, **1989**.

[2] (a) Hsiao, S. H.; Li, C. T.; *Macromolecules* **1998**, *31*, 721. (b) Liou,G. S. *J. Polym. Sci., Part A: Polym. Chem.* **1998**, *36*, 1937.

Yttrium nitrate hexahydrate: a new and powerful transition metal catalyst for the one-pot synthesis of 2, 4, 5-trisubstituted imidazoles

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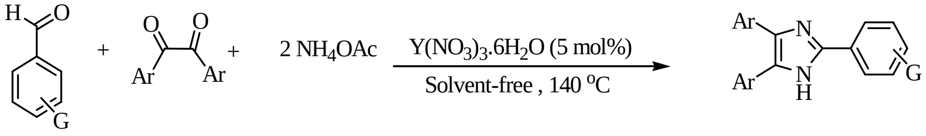
In recent years, lot of attention has been paid to synthesis of heterocyclic compounds. Imidazole and its derivatives are nitrogen heterocycles of great practical and theoretical interest which constitute useful intermediates in organic synthesis [1].

So far, numerous compounds with biological activity have been investigated. Many products, which contain the subunit of imidazole, exhibit useful and diverse biological activity such as analgesic, antibacterial and anti-inflammatory activities, etc. [2] or serve as HIV protease inhibitors [3]. They are also used in photography as photosensitive compound [4].

In this synthetic work paper, an eco-friendly and rapidly one-pot synthesis of 2,4,5-trisubstituted imidazoles based on tree-component condensation of aldehydes, ammonium acetate and aromatic 1,2 dicarbonyl compounds by the use of catalytic amounts of Yttrium nitrate hexahydrate in solvent-free conditions was described.



G= H, CH_3, NO_2, Cl, Br, OCH_3

Advantages of the present method include simple work-up, short reaction times, high yields of the products and avoiding from use of toxic organic solvents which made this technique a valid contribution to the existing methodologies.

References:

[1] G. W. H. Cheeseman, E. S. G. Werstiuk, *Adv. Heterocycl. Chem.*, **1978**, *22*, 367.
[2] Nagalkshmi, G. *E. J. Chem*. **2008**, *5*, 447.
[3] Wahyuningrum. D.; Achmad, S.; Syah, Y. M.; Bundjali. B.; Ariwahjoedi, B.; *Int. J. Electrochem. Sci*. **2008**, *3*, 154.
[4] satoru, I. *Chem Abstr*. **1989**, *111*, 214482.

The modification and characterization of maleic anhydride copolymers by carbazole groups

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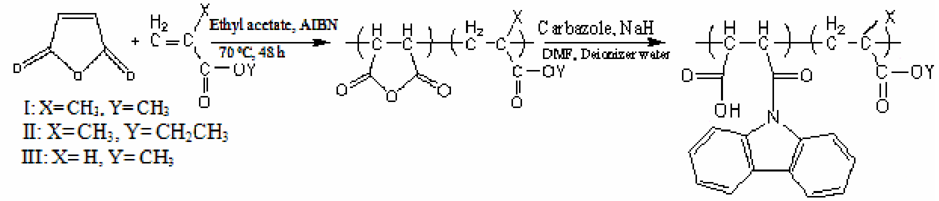
Chemical modification of polymer structures is an important route for modification of polymer properties such as mechanical, thermal and surface properties [1,2]. Maleic anhydride (MAN) is an excellent monomer which can provide reactive anhydride or carboxylic groups, with nucleophilic molecules. The anhydride moiety constitutes a nice handle to modify the polymer [3]. Carbazole (Cz), as a heterocyclic aromatic compound containing a dibenzopyrrole system, is the best-known chromophore that is often used to construct polymers with photoconducting, photorefractive and hole transporting properties [4].

Here in, the maleic anhydride (MAN) was copolymerized with methyl methacrylate (MMA), ethyl methacrylate (EMA) and methyl acrylate (MA) by free radical polymerization method at 70±1 ºC using α,ά-azobis(isobutyronitrile)(AIBN) as an initiator and the copolymers I, II, III collected respectively. Then, copolymers of maleic anhydride have been modified by incorporation of the carbazole groups through the ring opening reaction of anhydride groups in the presence of sodium hydride and preparation of sodium carbazole salt. Finally, the white polymers containing carbazole Substituents in the side chains were poured into an excess cold deionizer water. All the polymers containing carbazole groups showed a high glass transition temperature (190, 195, 163 ºC) respectively in comparation with copolymers I, II, III (92, 94, 36 ºC). The increase of glass transition temperature reflects the substantial increase in rigidity of new polymers bearing substituents in side chains.



The glass transition temperature (T_g) is an important intrinsic characteristic that influences the properties of a polymer and its potential applications. Further more, polymers with high glass transition temperatures are attractive for industrial polymer science because of strong economic rewards that may arise from their potential applications.

References:

[1] Babazadeh, M. Polymer Degradation and Stability. **2006**, 91, 3245.
[2] Safa, K. D.; Eram, H. A.; Nasirtabrizi, M. H. Iranian Polymer Journal. **2006**, 15, 249.
[3] Nieuwhof, R.; Koudijs, A.; Marcelis, A.; Sudholter, E. Macromolecules. **1999**, 32, 6499.
[4] Cho, Y. S.; Kim, S. W.; Ihn, C. S.; Lee, J. S. Polymer. **2001**, 54, 133.

Synthesis of hyperbranched polymers from tetracarboxylic acid and different diamines as a nanostructured material

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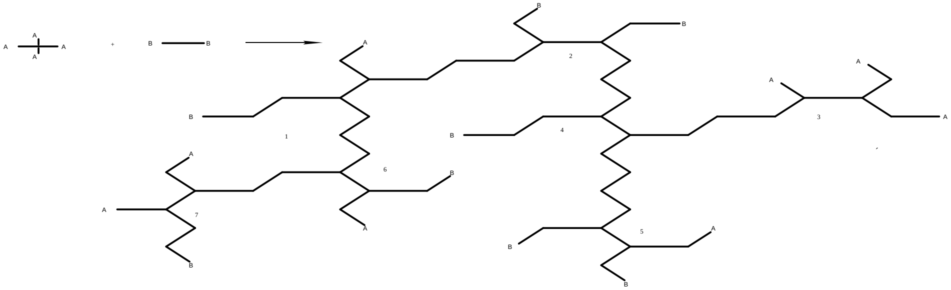
Over the 15 years, hyperbranched polymers have received much attention due to their unique chemical and physical properties as well as their potential application in coatings, additives, drug and gene delivery, macromolecular building blocks, nanotechnology, and superamolecular science [1-3]. The subject of this research is to describe the synthesis of hyperbranched poly(amide-imide)s in an $A_2A'_2 + B_2$ approach. A tetrafunctional monomer was designed and synthesized from L-cysteine in three-step reaction procedure.The characterization of the branched structure of the polymers was facilitated by the study of a model reaction of ethylenediaminetetraacetic acid (EDTA) with different diamines. The synthesis of all of the branched polymers was taking placed in direct polycondensation conditions using triphenylphosphite. Reaction parameters such as temperature, time, monomer concentration and stirring speed were such optimized to gel a soluble material. This was performed by controlling the reaction progress to gel point. The functional conversion of reaction up to the gel point was performed using titrimetric technique. Different conversions were obtained for different diamines to reach the gel point of polymerization. The chemical structure of the prepared monomer and polymers was confirmed by IR, NMR, CHN analysis and optical rotation measurements. Resulting branched polymers showed good solubility in various organic solvents and reduced solution viscosity compared to linear similar polymers. Scanning electron microscopy (SEM) showed nano-sized globular particles with a relatively uniform size distribution.



References:
[1] Scholl, M., Kadlecova, Z., Klok, H. A. *Prog. Polym. Sci.*, **2009**, 34.
[2] Yates, C. R., Hayes, W. *Eur. Polym. J.*, **2004**, 40, 1257.
[3] Inoue, K. *Prog. Polym. Sci.*, **2000**, 25, 453.

Metaborosulfric acid: A novel catalyst to synthesis of 2-arylbenzothiazoles

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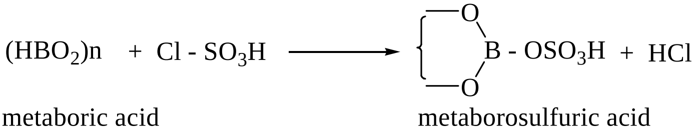
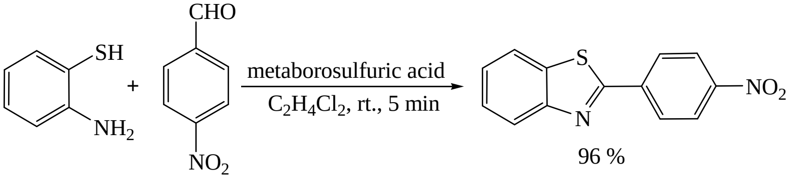
In the last two decades, many heterocyclic compounds from the benzothiazole series were synthesized and their biological and pharmacological activity investigated. They were studied extensively for their anti-allergic, anti-inflammatory, anti-tumor and analgesic activity [1-3].

There are many methods for the synthesis of 2-arylbenzothiazoles. The most common direct method is the condensation of 2-aminothiophenol with the substituted aromatic aldehydes, carboxylic acids or its derivatives [4].

We report here an efficient, convenient, and facile method for the condensation of 2-aminothiophenol with aldehydes to the corresponding 2-arylbenzothiazol derivatives using a catalytic amount of metaborosulfuric acid (MBSA) in dichloroethane at room temperature.





Reference:

[1] Ban, M.; Taguchi, H.; Katsushima, T.; Takahashi, M.; Shinoda, K.; Watanabe, A.; Tominaga, T. Bioorg. *Med. Chem.* **1998**, *6*, 1069.

[2] Chung, Y.; Shin, Y.-K.; Zhan, C.-G.; Lee, S.; Cho, H. *Arch. Pharm. Res.* **2004**, *27*,893.

[3] Baell, J. B.; Forsyth, S. A.; Gable, R. W.; Norton, R. S.; Mulder, R. J. *J. Comput. Aided. Mol. Des.* **2002**, *15*, 1119.

[4] a) Roe, A.; Tucker, W. P. J. Heterocycl. Chem. **1965**, *2*, 148. b) Spitulnik, M. J. *Synthesis* **1976**, 730. c) Ben-Alloum, A.; Bakkas, S.; Soufiaoui, M. *Tetrahedron Lett.* **1997**, *38*, 6395. d) Takagi, K. *Chem. Lett.* **1986**, 265. e) Bougrin, K.; Loupy, A.; Soufiaoui, M. *Tetrahedron* **1998**, *54*, 8055. f) Tale, R. H. *Org. Lett.*, **1998**, *4*, 1641.

Synthesis, characterization and development of high performance Siloxane -modified epoxy resin

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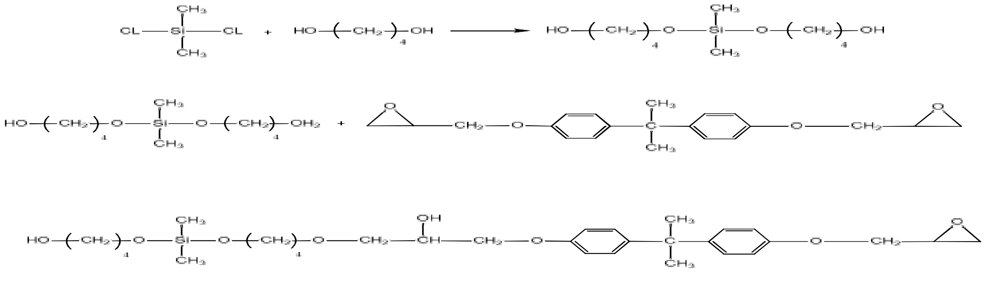
Silicone is considered to be one of the suitable modifiers for epoxy resins, owing to its superior thermal and thermo-oxidative stability, excellent moisture resistance, partial ionic nature, low surface energy, good flame retardancy and free rotation of chains about Si-O bonds, good hydrophobicity, compressivity and doping action [1]. However, silicones possess poor mechanical properties. The incorporation of silicone in epoxy resin results in the enhancement of physico-mechanical properties, thermal stability and anticorrosive characteristics, which include good processibility, flexibility, toughness, durability, UV, chemical and weather resistance along with thermo oxidative stability. The latter can be attributed to the high bond dissociation energy of Si-O unit bond i.e. 443.7 KJ/mol, compared to those of C- O bond (357.9 KJ/mol) .

Conventionally, the introduction of siloxane/silicone into polymers has been carried out through blending methods [2].

In this work, we synthesized a silicone containing diol by reaction of polybutylene glycol and dimethyl dichlorosilane in the presence of phosphoric acid and toluene at reflax temperature.

Then the obtained silicone containing diol was reacted with reacted with diglycidyl ether of bisphenol A (DGEBA) in the phosphoric acid and toluene at reflax temperature during 4h the resulted monomers was characterized by FTIR, HNMR,CNMR spectroscopies.



References:

[1] Lauter, U.; Kantor, S.W; Schmidt-Rohr, K.; MacKnight, W. *J. Macromol.* **1999**, *32* (10), 3426.

[2] Chojnowski, J.; Cypryk, M.; Fortuniak, W.; Scibiorek, M.; Rozga-Wijas, K. *J. Macromol.* **2003**,*36*, 3890.

Chemical modification of p-vinylbenzyl chloride polymers with benzyl alcohol

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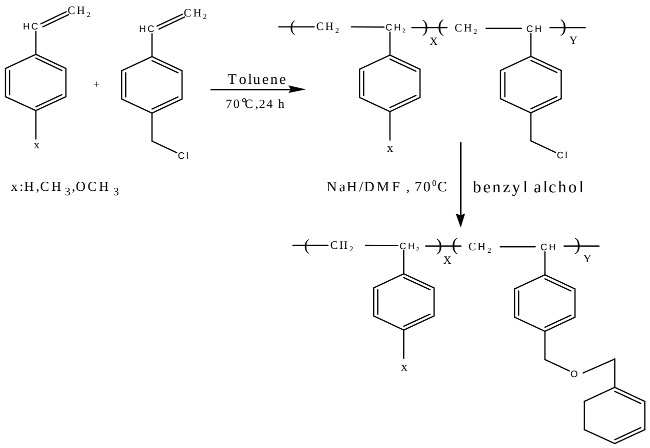
p-Chloromethyl styrene or p-vinylbenzyl chloride is a functional styrene with a reactive pendent benzyl group susceptible to nucleophilic substitution [1]. P-Chloromethyl styrene plays important role in various and numerous chemical transformations.

In this research, the p-vinylbenzyl chloride monomer was copolymerized with different styrenic monomers such as: styrene, methyl styrene and 4- methoxy styrene, in toluene at 70 ± 1˚C using α,α'-azobis(isobutyronitrile) (AIBN) as the radical polymerization initiator [2]. The benzyl alcohol substituents were attached to the obtained copolymers in N,N-dimthyl formamide (DMF) at 70 ± 1˚C for 48 h. In this reaction, all of the chlorine atoms are replaced with benzyl alcohol in chloromethyl styrene units. The polymers obtained in quantitative yields, were described by dynamic mechanical thermal analysis (DMTA), FT-IR and ^{1}H-NMR spectroscopic techniques [3].

The glass transition temperature value of obtained copolymers was found to increase with incorporation of benzyl alcohol groups in copolymer structures. Increasing of the glass transition temperature reflects the substantial increase in rigidity of new polymers bearing substituents in side chains [4].



References:

1. [1] Kamigaito, M.; Nakashima, J.; Satoh, K.; Sawamoto, M. *Macromolecules.* **2003**, *36*, 3540.
2. [2] Safa, K. D.; Eram, H. A.; Nasirtabrizi, M. H. *Iran. Polym. J.* **2006**, *15*, 249.
3. [3] Safa, K. D.; Nasirtabrizi, M. H. *Eur. Polym. J.* **2005**, *41*, 2310.
4. [4] Safa, K. D.; Babazadeh, M. A. *Eur. Polym. J.* **2004**, *40*, 1659.

Fe_3O_4 nanoparticles as a green and magnetically recoverable catalyst for synthesis of dihydropyrimidin-2(1H)-ones under solvent free conditions

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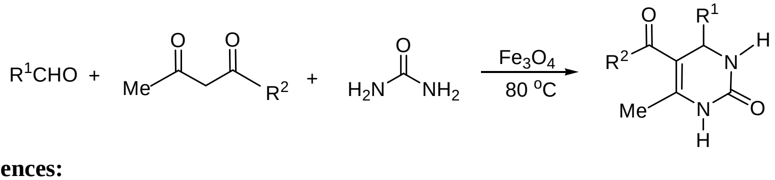
Dihydropyrimidinones derivatives have attracted considerable interest in recent years because of therapeutic and pharmacological properties such as calcium channel blockers, antihypertensive agents and α-1a-antagonist [1]. The classical biginelli reaction of an aldehyde, β-dicarbonyl and urea or thiourea requires strongly acidic conditions with relatively low yields. In order to improve the efficiency of biginelli reaction, a lot of catalysts have been used. Some of them are really fascinating from the synthetic chemist's points; however, some drawbacks still remain. Therefore many synthetic methods for the synthesis of this heterocyclic scaffold have been developed [2]. There are several disadvantages associated with the reported methodologies including unsatisfactory yields, long conversion times, difficult handling of reagents, toxic and inflammable organic solvents, and incompatibility with other functional groups in the molecules that limited these methods to small-scale synthesis. Thus, developments of facile and environmentally friendly synthetic methods for preparation of the dihydropyrimidinones are yet demanded.

Superparamagnetic Fe_3O_4 nanoparticles have attracted worldwide attention due to many biological and technological applications. These magnetic nanoparticles can be separated easily by external magnetic field. This strategy is simple, economical, environmentally friendly and promising for industrial applications.

In this work, we wish to report an efficient and convenient procedure for the synthesis of 3,4-dihydropyrimidin-2(1H)-ones from the aldehydes using Fe_3O_4 nanoparticles.



References:

[1] (a) Atwal, K. S.; Swanson, B. N.; Unger, S. E.; Floyd, D. M.; Moreland, S.; Hedberg, A.; O'Reilly, B. C. *J. Med. Chem.*, **1991**, *34*, 806; (b) Tanaka, K.; Toda, F. *Chem. Rev.* **2000**, *100*, 1025.

[2] (a) Khodaei, M. M.; Khosropour, A. R. Beygzadeh, M. *Synth. Commun.* **2004**, *34*, 1551; (b) Huang, Y.; Yang, F.; Zhu, C. *J. Am. Chem. Soc.* **2005**, *127*, 16386.

[3] (a) Nasr-Esfahani, M.; Karami, B.; Montazerozohori, M.; Abdi, K. *J. Heterocyclic Chem.*, **2008**, 45, 1183; (b) Nasr-Esfahani, M.; Khosropour, A. R. *Bull. Korean Chem. Soc.*, **2005**, *26*, 1331.

Synthesis of bis(dihydropyrimidinone)benzenes : evaluation of cytotoxic activities

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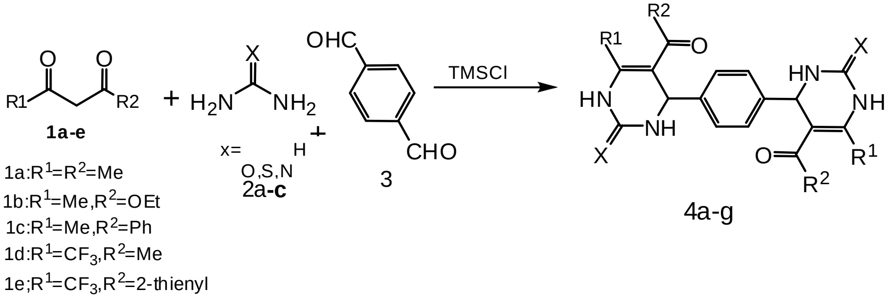
3,4-Dihydropyrimidinones (DHPMs) constitute a very important class of organic compounds due to their attractive pharmacological properties, including antiviral, antitumour, antibacterial activities. [1] They have emerged as integral backbones of several calcium channel blockers, antihypertensive agents, α-1a-antagonists, and neuropeptide Y (NPY) antagonists[2,3] . Moreover, several alkaloids containing the dihydropyrimidine core unit have been isolated from marine sources, which also exhibit interesting biological properties. We would like to introduce a facile procedure for the synthesis of bis(dihydropyrimidinone)benzenes via one-pot condensation of terephthalic aldehyde or isophthalic aldehyde with (thio)urea, guanidine and 1,3- dicarbonyl compounds .



Cell viability following exposure to synthetic compounds was estimated by using the MTT reduction assay [4] on human cell lines (SKOV-3, MCF7, Raji, LS-180 and HeLa cells). A structural analysis indicated that the key point was presence of sulfur instead of oxygen or nitrogen in C_2 position of pyrimidine ring. This implies that this position might play a role in cytotoxic effect of these compounds which can be a helpful hint for future designs.

References:

[1] Kappe, C. O.*Acc. Chem .Res.***2000**,*33*, 879.
[2] Kappe, CO. *Eur .J .Med .Chem.***2000** ,*35*,104.
[3] Rovnyak , G.C.; Kimball, S.D.; Beyer, B.; Cucinotta, G.; DiMarco, J.D.; Gougoutas , J.; Hedberg, A.; Malley, M.; McCarthy, J.P.; Zhang, R.*J. Med .Chem.***1995** ,*38*,119.
[4] Mehdipour, A.R.; Javidnia, K.; Hemmateenejad , B.; Amirghofran ,Z.; Miri, R. *Chem .Biol .Drug.Des.* **2007** ,*70*,337.

Morpholine catalyzed one-pot multi-component synthesis of compounds containing chromene core in water

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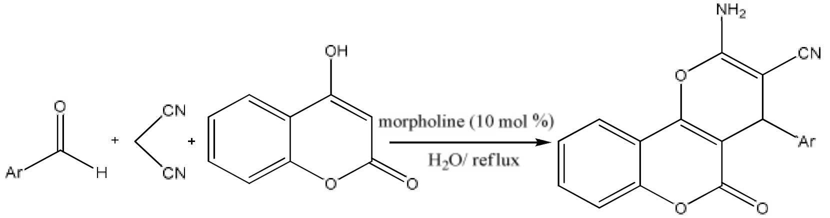
Green chemistry is a quickly developing new field that provides us a proactive path for the sustainable progress of future science and technologies. [1] Green chemistry uses highly efficient and environmental benign synthetic procedures to deliver life saving medicines, accelerating guide optimization processes in drug discovery, with reduced needless environmental impact.

Dihydropyrano[c]chromenes and their derivatives are of considerable interest as they possess a wide range of biological properties [2], such as spasmolytic, diuretic, anticoagulant, anti-cancer, and anti-anaphylactic activity [3].

Small organic molecules like morpholine, L-proline, and its derivatives are readily commercially available catalysts and have been used in various transformations with excellent yields [20]. More recently, morpholine, a cheap and facile weak base (pKb = 5.51), as the catalyst involving sequential aldol and Michael addition reactions of aromatic aldehydes with 2'-hydroxyacetophenone [4]. Our results demonstrate that morpholine is a very effective, environmentally friendly catalyst for the three component condensations of aldehyde 1, malononitrile 2 and 4-hydroxycoumarine 3 to form dihydropyrano[c]chromene derivatives in water under reflux in excellent yields.



References:

[1] Varma, R. S. *Green Chem*. **1999**, *1*, 43.
[2] Green, G. R.; Evans, J. M.; Vong, A. K. In Comprehensive Heterocyclic Chemistry II; Katritzky, A. R., Rees, C. W., Scriven, E. F. V., Eds.; Pergamon Press: Oxford, **1995**, *5*, 469.
[3] (a) Foye, W.O. Principi Di Chemico Farmaceutica; Piccin: Padova, Italy, **1991**; p 416. (b) Andreani, L. L.; Lapi, E. *Bull. Chim. Farm*. **1960**, *99*, 583.
[4] Shaker, R. M. *Pharmazie* **1996**, *51*, 148.

Study the effect of different alcohols and molar ratio in transesterification reaction with canola oil to produce biodiesel

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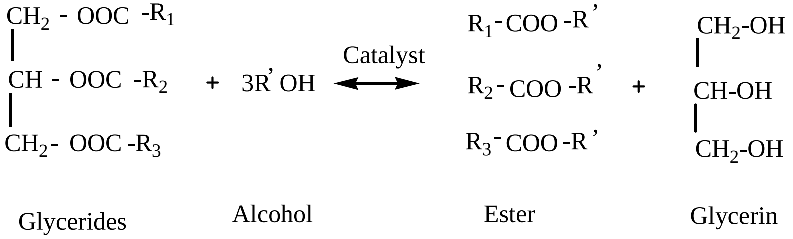
Fuels are inevitable for industrial development and growth of any country. The life span of fossil fuel resources has always been terrifying. Biodiesel, a renewable source of energy seems to be an ideal solution for global energy demands including India as well [1]. In the transesterification of different type of oils, triglycerides react with an alcohol, generally methanol or ethanol, to produce ester and glycerin. To make it possible, a catalyst is added to the reaction such as below: [2].



In this study biodiesel is produced by transesterification reaction using canola oil and KOH as a basic catalyst with different alcohol such as high pure methanol, ethanol, 1-propanol [3]. The properties of biodiesels has been accommodated with ASTM standards.

As tha results show the methanol was the most efficient reagent when the molar ratio of oil to methanol was 1:9, with comparing molar ratio of oil to 1-propanoland ethanol were 1:12.

References:

[1] Sharma, Y.C.; singh B.; Development of biodiesel: Current scenario. **2009**, 1646, 1651.
[2] Marchetti, J.M.; Miguel,V.U.; Errazu, A.F.; Possible methods for biodiesel production **2007**, 1300, 1311.
[3] Mangesh, G.; Kulkarni, A.K.; Dalai, N.N.; Bakhshi. Transesterification of canola oil in mixed methanol/ethanol system and use of esters as lubricity additive **2007**, 2027,2033

A new protocol for One-Pot Three-component synthesis of β-aminocarbonyl Compounds using Iron(III) phosphat as a green and heterogeneous catalyst.

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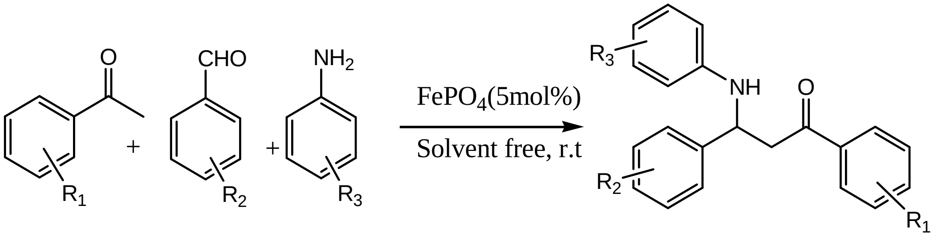
β-amino carbonyl compounds are important synthetic intermediates for various pharmaceuticals and natural products [1] and have found wide application in organic synthesis. Owing to the importance of β-amino carbonyl compounds, numerous methods for the synthesis of these compounds either by indirect-type or direct-type Mannich reactions have been reported over the years.

A Mannich-type reaction is a multicomponent reaction of a non-enolizable aldehyde, a primary or secondary amine, and an enolizable carbonyl compound to afford the corresponding β-amino carbonyl compound [2].

$FePO_4$ is a readily accessible, cheap, and highly effective catalyst. In this communication, herein, we interest to report a simple and effective methodology for one-pot, three-component, Mannich-type reactions of aromatic aldehydes, amines, and ketones in the presence of FePO4 as a green and reusable catalyst.



References:

[1] a) Davis, F. A.; Zhang,Y.; Anilkumar, G. *J. Org. Chem*. **2003**,*68*, 8061; b) Ev.ans, G. B.; Furneaux, R. H.; Tyler, P. C.; Schramm, V. L. *Org. Lett***. 2003**, *5*, 3639; c) Fujita, T.; Nagasawa, H.; Uto, Y.; Hashimoto, T.; Asakawa, Y.; Hori, H. *Org.Lett***. 2004**, *6*, 827; d) Joshi, N. S.; Whitaker, L. R.; Francis, M. B. J. *Am. Chem. Soc***.** **2004**, *126*, 15942; e) Ishi-maru, K.; Kojima, T. *Tetrahedron Lett*. **2003**, *44*, 5441.
[2] Mannich, C.; Krosche, W. *Arch. Pharm*. **1912**, *250*, 647.

Efficient synthesis of new derivatives of high functionalized imidazol

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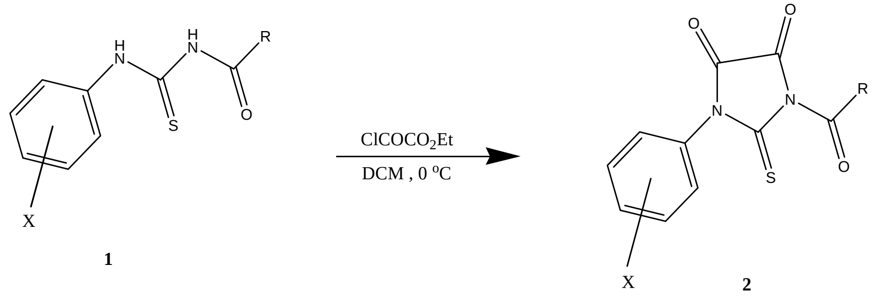
Imidazol and related compounds of this family are significant group of organic compounds which have attracted a great deal of attention in organic synthesis due to diverse biological activities such as bactericidal, fungicidal ant-inflammatory and hypertensive activities [1, 2].

During the course of our studies towards the development of new routes to the synthesis of heterocyclic compounds, we wish to report a facial and efficient route for synthesis of new derivatives of imidazol **2**, from the reaction of N-acyl-N-aryl thiourea **1** with chlorooxoethylacetate.

The structure of products was deduced by spectroscopic data.



X : Et , Me , Cl , Br , ...

R :Ph , P-Cl-Bz , ...

References:

[1] M.R. Grimmett, in: A.R. Katritzky, C.W. Ree (Eds), *Comprehensive Heterocyclic Chemistry,* Vol. 5, pergamon Press, London, **1984**, p. 374.

[2] M. Misono, *Chem. Commun*. (**2001**) 1141.

Synthesis of novel superabsorbent hydrogel based on alginate and its application in waste treatment

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Superabsorbent hydrogels are an important class of partially crosslinked polymeric materials that are able to absorb large quantities of fluid generally water and aqueous solutions in a short time and retain water under pressure [1, 2]. Superabsorbent hydrogels based on natural polymer such as polysaccharides or proteins have high biodegradability as compared to synthetic kinds. Hydrogels have been the focus of a number of investigations in recent years because of their considerable applications in many fields such as hygienic products, horticulture, drug-delivery systems, removing heavy metals from waste water, etc [3]. Removal of heavy metal ions and dyes by using polymers having different functional groups would be of great importance in environmental applications due to their high adsorption capacities. For this purpose, different polymeric adsorbents especially the hydrogels which have complexing ability with metal ions and dyes have been investigated.

In this study, graft copolymerization of acrylamide and itaconic acid onto alginate polysaccharide_was carried out in the presence of methylenebisacrylamide crosslinker and ammonium persulfate as an initiator. Equilibrium water absorbency in de-ionized water was 600(g/g). The removal of Cd^{2+} ion (with different concentrations) and methylene blue form aqueous solutions was performed and good results were obtained.

References:

[1] Lanthong, P.; Nuisin, R.; Kiatkamjornwong, S. *Carbohydrate Polymer*, **2006**, *104*, 199.
[2] Su, X.; Zhang, G.; Xu, K.; Wang, J.; Song, C.; Wang, P. *Polymer Bulletin*, **2008**, *60*, 69.
[3] Rodriguez, E.; Katime, I. *Journal of Applied Polymer Science*, **2003**, *90*, 530.

Reaction of 2,3-dichloro quinoxalin with benzotriazole

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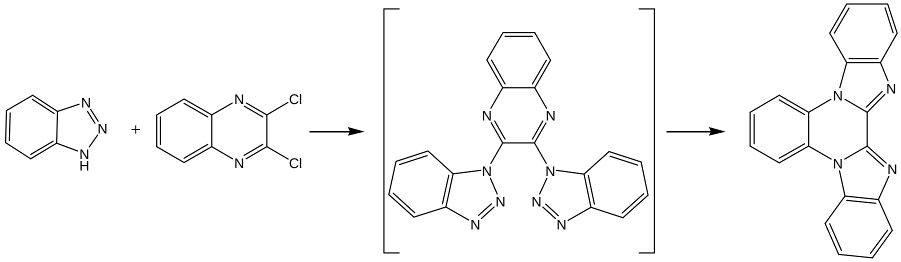
We have reported several rearrangements including losing CO_2 by heating derivatives of quinoxalin in presence of base under reflux conditions [1-4]. Heating 2 equivalent of benzotriazole [5] (**1**) with 2,3-dichloro quinoxalin (**2**) at 110-130 ºC gave hexacyclic heterocycle (**3**) by lose of nitrogen as shown below. The structure of (**3**) was confirmed by ^{1}H- NMR, ^{13}C-NMR, FT-IR and mass spectrometery.



1 **2** **3**

References:

[1] Molla Ebrahimlo, A. R.; Khalafy, J. *Arkivoc*. **2008**, *xiii*, 65.
[2] Molla Ebrahimlo, A. R.; Khalafy, J.; Prager, R. H. *Aust. J. Chem.* **2009**, *62*, 126.
[3] Khalafy, J.; Prager, R. H.; Smith, J. A. *J. Chem. Res (M)* **1999**, 518.
[4] Molla Ebrahimlo, A. R.; Khalafy, J.; Poursattar Marjani A.; Prager, R. H. *Arkivoc.* **2009**, *xii*, 17.
[5] Vogel, Textbook of practical organic chemist, Sthedition, Page 1163.

Eco-friendly protocl for fast and efficient reduction of carbonyl compounds with $NaBH_4$ in the presence of copolymer styrene alternative maleic acid

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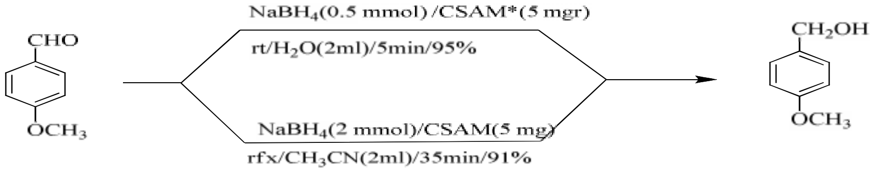
Reduction of aldehydes and ketones to alcohols is needed for many synthesis processes, and literature survey shows that many improvements have been reported for the reduction of carbonyl compounds [1,2]. Sodium borohydride is commonly used hydride transferring agent, which provides simple and convenient routes for the reduction of many organic compounds [3, 4]. This reagent usually reduces carbonyl compounds in protic and aprotic solvents such as EtOH, MeOH, CH_3CN, and THF. Therefore, these solvents creats ecological problems in the world.

On the other hand in recent years, the emphasis of science and technology has shifted more towards environmentally friendly and sustainable resources and processes [5].

This is comparative research that introduces a simple and convenient procedure for reduction a variety of carbonyl compounds with sodium borohydride in the presence of copolymer styrene alternative maleic acid in water as a green solvent. The obtained results show that this protocol is fast and eco- friendly method and is more efficient than when the reaction performs under aprotic condition in CH_3CN (Scheme).



CSAM* :Copolymer Styrene Alternative Maleic acid

It would better to mention that copolymer styrene alternative maleic acid is soluable in water so this solubility helps us to extract it easily from the reaction mixture.

Refrences:

[1] Nagendrappa, G. *Resonance* **2002**, 59.
[2] Varma, R. S., Nambooiri, V. V. *Pure Appl. Chem*. **2001**, *73*, 1309.
[3] Firouzabadi, H., Zeynizadeh, B. *Bull. Chem. Soc. Jpn*. **1996**, *69.*
[4] Hudlicky, M. *Reduction in Organic Chemistry*, Ellis Horwood, Chichester, **1984.**
[5] Rajender reddy, K., Rajgopal, K., Uma Maheswari, C., and Lakashmi Kantam, M. *New. J. Chem*. **2006**, *30*, 1549.

$ZrCl_4$/[bmim]BF_4 catalyzed condensation of salicylaldehydes and malononitrile: Single step synthesis of 3-cyanocoumarin derivatives

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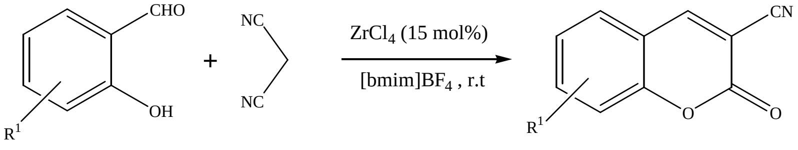
Coumarins and their derivatives are very important organic compounds. They are the structural unit of several natural products. Their applications range from pharmaceuticals, optical brighteners and laser dyes. Also, coumarins and functionalized coumarins have shown activity as antimicrobials and chemotherapeutics. Knoevenagel condensation is one of the most important methods for carbon-carbon double bond formation in synthetic chemistry. Generally, Knoevenagel reactions are carried out by the condensation of active methylene compounds with aldehydes with some organic bases as well as their salts as catalysts. Alternative protocols for Knoevenagel condensations catalyzed by Lewis acids and various heterogeneous solid bases have been reported in literature. We reported the synthesis of coumarin derivatives via Knoevenagel reaction of 2-hydroxybenzaldehyde derivatives with some active methylene compounds in aqueous media and also in ionic liquids. In this report, a versatile and efficient single step route to 3-cyanocoumarins via Knoevenagel condensation of salisylaldehdes and malononitrile using $ZrCl_4$ as the catalyst (15 mol%) in ionic liquid 1-(n-butyl)-3-methylimidazolium tetrafluoroborate, [bmim]BF_4, as reaction medium and catalyst is described. The novel procedure features single step, short reaction time, good yields and simple workup.



References

[1] Han, J. J.; Xu, Y. F.; Su, Y. P. *Catal. Commun.* **2008**, *9*, 2077.
[2] Valizadeh, H.; Heravi, M. M.; Amiri, M. *Mol. Divers.* **2009**, published online. (b) Valizadeh, H.; Amiri, M.; Gholipour. H. *J. Heterocycl. Chem.* **2009**, *46*, 108. (c) Valizadeh, H.; Shockravi, A. *Synth. Commun.*, **2009**, *39*, 4341. (d) Valizadeh, H.; Dinparast, L. *Heteroatom Chem.* **2009**, *20*, 177. (e) Valizadeh, H.; Shockravi, A. *Heteroatom Chem.* **2009**, *20*, 5, 284.

Protonated melamine formaldehyde resin (MFR-H^+) as an efficient and reusable catalyst for cross-aldol condensation of ketones with aromatic aldehydes under solvent-free conditions

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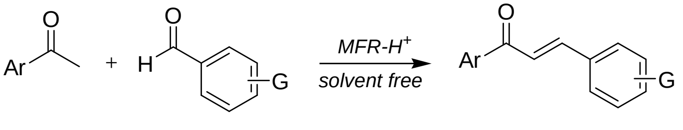
Chalcones (1,3-diaryl-2-propene-1-ones) are natural substances found in a number of planets or synthetically prepared [1]. They display many biological activities [2]. Several strategies for the synthesis of these systems based on the formation of carbon-carbon bond have been reported. Among them, the direct aldol condensation still occupies prominent position. In aldol condensation, the preparation of chalcones requires at least two-steps aldol formation and dehydration. The aldol reaction is usually preformed under acidic or basic medium and recently various modified methods for the synthesis of chalcones have been reported so far [3]. However, many of these methods suffered from many disadvantageous including harsh reaction condition, toxic reagents, strong acidic or basic conditions, prolonged reaction time, poor yields and low selectivity. Nonetheless of several modifications which had been already carried out to diminish these problems, but still there is a need to improve and establish an efficient method for above reaction.

Herein, we have described the synthesis of chalcone using MFR-H^+ as a catalyst under solvent-free condition. The main goal for the present studding is to develop an efficient protocol for aldol condensation of substituted aromatic aldehydes with ketones which is catalyzed by protonated melamine formaldehyde resin (MFR-H^+) to attain the corresponding chalcones (1,3-diaryl-2-propene-1-ones) in good to excellent yields and also in short reaction time without formation of side products.



G: NO_2, Me, Cl,...

References:

[1] Yadav, J. S.; Subba Reddy, B. V.; Nagaraju, A.; Sarma, J. A. R. P. *Synth. Commun.* **2002**, *32*, 893.
[2] Iranpoor, N.; Kazemi, F. *Tetrahedron* **1998**, *54*, 9475.
[3] Salehi, P.; Khodaei, M. M.; Zolfigol, M. A.; Keyvan, A. *Monatsh. Chem.* **2002**, *133*, 1291.

In situ-generated *N*-thiocyanatosuccinimide (NTS) as a highly efficient reagent for the conversion of epoxides into thiocyanaohydrine

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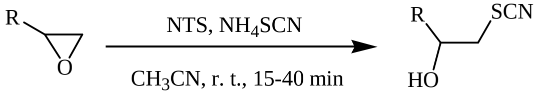
Epoxides or oxiranes are useful and important synthetic intermediates in organic synthesis [1]. The reaction of thiocyanate ion with epoxides has been extensively studied and is a suitable method for the preparation of thiocyanohydrines and thiranes depending on the reaction conditions [2]. In recent years, numerous combined reagents have been applied for the conversion of epoxides into thiocyanohydrines including phenol-containing macrocyclic diamides [3], poly-[*N*-(2-aminoethyl) acrylamido] trimethyl ammonium chloride [4], tetraphenylporphyrins (TPP) [5], 2-phenyl-2-(2-pyridyl)imidazolidine (PPI) [6] metalloporphyrins [7], 2,6-bis[2-(o-aminophenoxy)methyl]-4-bromo-1-methoxybenzene (BABMB) [8], [P(TPP)Cl_2]Cl [9], poly(ethylene glycol)-bound sulfonic acid (PEG-SO_3H) [10], $Al(HSO_4)_3$/silica gel [11]. However, the above mentioned methods suffer from one of a number of drawbacks such as using expensive catalysts, high temperature reaction conditions which are not only detrimental to certain functional groups, tedious work-up and use only for the specific oxiranes. These drawbacks encouraged us to report a new methodology using cost effective and easily available reagent and mild reaction conditions. Here, we report a new application of *N*-thiocyanatosuccinimide for the facile conversion of epoxides into thiocyanohydrine with NH_4SCN in acetonitrile at room temperature.



References:

[1] Corey, E. J.; Shibata, S.; Bakshi, R. K. *J. Org. Chem.* **1988**, *53*, 2861.
[2] a) Sander, M. *Chem. Rev.* **1966**, *66*, 297; (b) Jankowski, K.; Harvey, R. *Synthesis* **1972**, 627.
[3] Sharghi, H.; Nasseri, M. A.; Niknam, K. *J. Org. Chem.* **2001**, *66*, 7287.
[4] Tamami, B.; Mahdavi, H. *Tetrahedron Lett.* **2002**, *43*, 6225.
[5] Sharghi, H.; Nasseri, M. A.; Hasani-Nejad, A. *J. Mol. Catal. A* **2003**, *206*, 53.
[6] Sharghi, H.; Nasseri, M. A. *Phosphorus Sulfur Silicon* **2003**, *178*, 1353.
[7] Sharghi, H.; Hasani-Nejad, A.; Nasseri, M. A. *New. J. Chem.* **2004**, *28*, 946.
[8] Niknam, K.; *Phosphorus Sulfur Silicon* **2004**, *179*, 499.
[9] Sharghi, H.; Hasani-Nejad, A. *Phosphorus Sulfur Silicon* **2004**, *179*, 2297.
[10] (a) Kiasat, A. R.; Fallah-Mehrjardi, M. *Catalysis Commun.* **2008**, *9*, 1497; (b) Kiasat, A. R.; Fallah-Mehrjardi, M. *Synth. Commun.* **2008**, 38, 2995.
[11] Kiasat, A. R.; Mouradzadegun, A.; Elahi, S.; Fallah-Mehrjardi, M. *Chin. Chem. Lett.* **2010**, *21*, 146.

Silica sulfuric acid as a recyclable solid acid catalyst for efficient Fries rearrangement of phenolic esters or alkylation of phenols

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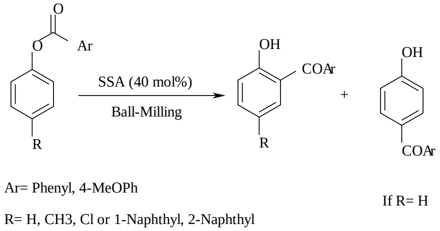
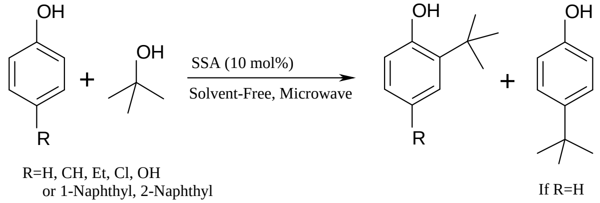
As found recently, silica sulfuric acid (SSA) has emerged as a powerful heterogeneous catalyst for various organic transformations, including synthesis of disulfides [1], phthalhydrazides [2]. Silica sulfuric acid is safe, environmentally benign with fewer disposals problems. On the other hand, the Fries rearrangement consists of the acid-catalyzed rearrangement of aryl esters into a mixture of *ortho*- and *para*-hydroxycarbonyl compounds [3]. We wish herein to report an efficient method for the Fries rearrangement using silica sulfuric acid as a recyclable solid acid catalyst under solvent-free conditions in a ball mill (Scheme 1).



Scheme 1**.** Fries rearrangement of aryl benzoates catalyzed by silica sulfuric acid (SSA).

Furthermore, in continuation of our interest on C-alkylation of phenols using alcohols in the presence of solid acids [4], we disclose a green methodology for C-alkylation of phenols by *tert*-butanol catalyzed by SSA as a powerful Bronsted and recyclable acidic catalyst under microwave conditions. The method is selective to afford corresponding C-alkylated products rather than O-alkylated ones (Scheme 2).



Scheme 2. C-alkylation of phenols with *t*-butanol catalyzed by silica sulfuric acid (SSA).

References:

[1] Zolfigol, M. A.; *Tetrahedron*. **2001**, *57*, 9509–9511.
[2] Shaterian, H. R.; Ghashang, M.; Feyzi, M.; *Appl Catal A*. **2008**, *345*, 128–133.
[3] Clark, J. H.; Dekamin, M. G.; Matloubi Moghaddam, F. *Green Chem.* **2002**, *4,* 366.
[4] Matloubi Moghaddam, F.; Akhlaghi, M.; Hojabri, L.; Dekamin, M.G. *Scientia Iranica Trans C: Chem. Chem. Eng.* **2010**, *16*, 81.

Reduction of aromatic nitro compounds in ionic liquids with Pd/C catalyst

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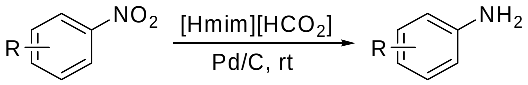
The reduction of nitro aromatic compounds to the corresponding amines is an important transformation since many aromatic amines exhibit biological activities and find a multitude of industrial applications and are intermediates for the synthesis of dyes, pharmaceuticals and agricultural chemicals [1].

A variety of methods for the reduction of nitro compounds is reported, among them catalytic hydrogenation and metal-mediated reduction are the most popular ones [2,3]. Also ionic liquids have drawn much attention to overcome many of environmental problems, due to their unique physicochemical properties profile, as they are nontoxic, nonvolatile, recyclable, nonflammable and chemically stable. Their purely ionic character makes them excellent solubilizers for a wide range of organic substrates [4].

In the present work, we report a mild, rapid and environmentally benign method for the reduction of nitro aromatics using the minimum (in comparison of other methods) amount of palladium on carbon as the catalyst and 1-methylimidazolium formate ([Hmim][HCO_2]) ionic liquid as the *in situ* hydrogen donor. Reductions were carried out in excellent yields at room temperature within 10-20 minutes.



R: CN, OH, Me, CH_2CN, NO_2

References:

[1] Khan, F. A.; Dash, J.; Sudheer, C.; Gupta, R.K. *Tetrahedron Lett.***2003**, *44*, 7783.
[2] Tafesh, A. M.; Weiguny, *J. Chem. Rev*. **1996**, *96*, 2035.
[3] Martin, E. L. *Org. Synth*. **1943**, *2*, 501.
[4] Seddon, K. R. *J. Chem. Technol. Biotechnol*. **1997**, *68*, 351.

Starch-sulfuric acid catalyzed synthesis of *N*-substituted decahydroacridine-1,8-diones

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Substituted acridines have been used as antimalarial for many years quite successfully and several of them have exhibited excellent results in chemotherapy of cancer [1]. These derivatives are frequently used in the industry, especially for the production of dyes. Beside these properties, analogues of acridine have also been shown to have very long lasting efficiencies and have interesting electrochemical behavior of heterocyclic compounds in the interaction with DNA [2,3].

In connection with our ongoing reseach in heterocycles synthesis [4], we report here an efficient method for the synthesis of *N*-substituted decahydroacridine-1,8-di-ones (Fig. 1) by the reaction of, dimedone, arylaldehydes and aniline derivatives in the presence of premade starch- sulfuric acid [5] as catalyst. This new catalytic method provided the desired products in high yields (75-87%) and reasonable reaction times.

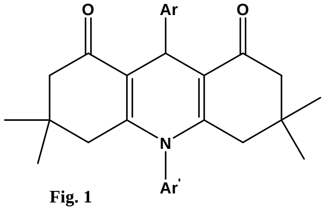

Fig. 1

The structures of all products were confirmed by spectroscopic methods (IR, ^{1}H NMR, ^{13}C NMR).

References:

[1] Girault, S.; Grellier, P.; Berecibar, A.; Maes, L.; Mouray, E.; Lemiere, P.; Debreu, M.; Davioud-Charvet, E.; Sergheraet, C. *J. Med. Chem.* **2000**, *43*, 2646.

[2] Cholody, W.; Horowska, B.; Paradziej- Lukowicz, J.; Martelli, S.; Konopa, J. *J. Med. Chem.* **1996**, *39*, 1028.

[3] Tilak, B. D.; Ayyangar, N. R. *Chem. Heterocycl. Compd.* **1973**, *9*, 579; Albert, A. *The Acridines*; Edward Arnold Publ., Ltd: London, 1966.

[4] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *Heterocycles* **2008**, *75*, 2825. Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N. O.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49*, 1450.

[5] Shaabani, A.; Rahmati, A.; Badri, Z. *Catal. Commun.* **2008**, *9*, 13.

Pereparation of benzimidazole derivatives in the presence of ionic liquid 3-methyl-1-sulfonic acid imidazolium chloride ([Msim]Cl) as a novel and highly efficient catalyst

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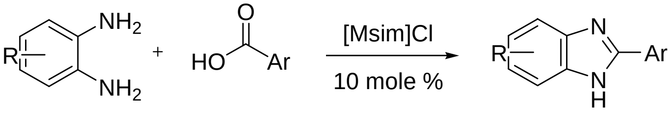
Benzo-fused heterocyclic systems such as benzimidazole due to a wide rang of biological properties and clinical applications are well-known.[1] These heterocyclic ring systems are present in numerous antiparasitic, fungicidal, anthelmintic and anti-inflammatory drugs.[1]

more recently, we have synthesized ionic liquid 3-methyl-1-sulfonic acid imidazolium chloride ([Msim]Cl) as a new Brønsted acidic catalyst. we have successfully applied this new acidic catalyst for the efficient and rapid preparation of *N*-sulfonyl imines[2] and bis(indolyl)methanes.[3]

To develop the applications of this new catalyst in organic synthesis, herein, we report an effiecent and simple method for preparation of various Benzimidazole derivatives from phenylenediamines and carboxylic acides.



Reference:

[1] A. R. Hasaninejad, K. Niknam, A. Zare, E. Farsimadan. M. Shekouhi, *Phosphorus, Sulfur, and Silicon*, **2009**, *184*, 147.
[2] M.A. Zolfigol, A. Khazaei, A.R. Moosavi-Zare, A. Zare, *J. Iran. Chem. Soc.* in press.
[3] M.A. Zolfigol, A. Khazaei, A.R. Moosavi-Zare, A. Zare, *Org. Prep. Proced. Int.* **2010**, *42,* 95.

Synthesis of novel optically active poly(amide-imide)/ZnO nanocomposites containing L-phenylalanine

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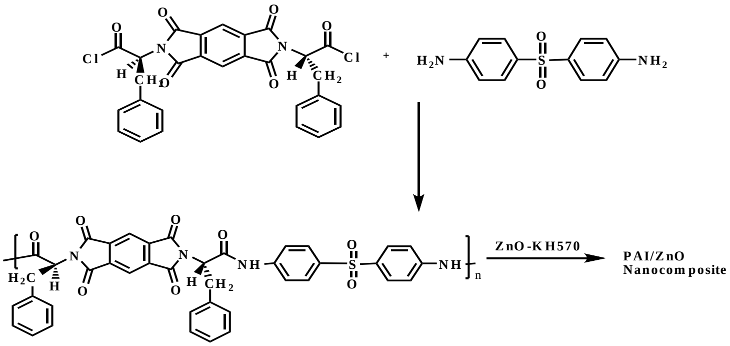
Metal or semiconductor nanoparticles dispersed in polymeric matrixes have been widely studied recently. These nanocomposites exhibit interesting properties and could be widely applied in the microelectronic and optoelectronic industries [1,2]. Zinc oxide (ZnO) is traditionally known as a wide band-gap (3.36 eV) semiconductor with an excitation binding energy (60 meV) larger than its thermal energy which ensures an efficient ultraviolet-blue emission (26 meV) at room temperature, thus yielding a wide range of potential applications in various devices such as UV lasers, solar cells, high sensitivity chemical gas or volatile organic compound sensors and DNA sequence sensors [3]. In this investigation, an optically active poly(amide-imide) (PAI) was prepared by the reaction of *N,N´*-(pyromellitoyl)-bis-L-phenylalanine diacid chloride with 4,4´-diaminodiphenyl sulfone and then it was used as host polymer to synthesize a series of novel PAI/ZnO nanocomposites with different ZnO contents. All of the obtained nanocomposites were characterized by means of fourier transformation infrared spectroscopy, thermogravimetric analysis, scanning electron microscope, X-ray diffraction and transmission electron microscopy techniques.



References:

[1] Chiang, P. C.; Whang, W. T. *Thin Solid Film* **2003**, *447*, 359.
[2] Chiang, P. C.; Whang, W. T. *Polymer* **2004**, *45*, 4465.
[3] Zhanhu, G.; Suying, W. *J. Mater. Chem.*, **2007**, *17*, 806.

Synthesis and characterization of nanoclay modified by quaternary phosphonium for preparation of nanocomposite polybutadiene

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Nanocomposites have attracted great interest both in industry and in science. The kind of nanocomposites exhibit improved properties compared to their micro or macro composites due to the fine phase dimensions and phase structure involved. In general, this kind of nanocomposites has superior mechanical properties, thermal stability, flame redundancy and gas barrier properties. Cis-1, 4- poly butadiene rubber (PBR) is widely used in the tire industry due to it is superior dynamic mechanical properties, abrasion, resistance, elasticity, and flex crack resistant. [1]. Nanoclay modification by quaternary phosphonium salts is one the ways of enhancing of physical property of nanocomposite [2]. In this work at first phosphonium quaternary salts were synthesized from reaction of triphenyl phosphine with n-butyl chloride and hexadocylchloride respectively then modified organonanoclays were prepared by ion exchange of sodium in natural nanoclay with octadecyl triphenylphosphnium and n-butyl triphenylphosphonium, change in structure were investigated using by x –ray diffraction (XRD) , differential scanning calorimetery (DSC) and IR. XRD showed that distance between layers of modified nanoclay was increased and therefore is suitable for preparation of nanocomposites and also DSC and IR confirmed existence of phosphorus in nanoclay. The effects of modified organoclay on mechanical properties, thermal stability and swelling behavior of PBR was investigated. When the organoclay was added to the PBR showed improvement in young's modulus, thermal stability and swelling behavior, which was attributed to the good barrier properties of organoclay layers [3].

Referances:

Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104*, 199

[1] Li, Qingshan, *Research advances in polymer/clay nano composites.Material Science and Technology* **2004** *12*,618-621.

[2] Seng, Chai; Zhong, Yi Zhang. *International Journal of Materials Engineering Innovation*. **2009, 12**, 1.

[3]Zheng Gu, Guojun Song, Weisheng Liu, Baojin Wang, Jin Li. *Preparation and properties of organo-montmorillonite/Cis-1,4-polybutadiene rubber nanocomposites by solution intercalation*.Applied Clay Science,**2009**,45,50-53. Li, Qingshan, Cong, Junying, Wang, *Qingrui, Research advances in polymer/clay nano composites*. Material Science and Technology , **2004**, 12, 618-621.J.h.;Koo. *Polymer Nanocomposites*. **2006**. McGraw-Hill Companies.Liao, Mingyi, Zhang, Weiqing, Shan, Wei,. *structure and properties of polybutadiene/montmorillonite nanocomposites prepared by in situ polymerization*. Journal of Applied Polymer Science, **2006**, 99,3615-3621.Liao, Mingyi, Zhang, Weiqing,Shan, Wei,. *Structure and properties of polybutadiene/montmorillonite nanocomposites prepared by in situ polymerization*. Journal of Applied Polymer Science, **2006**, 99, 3615-3621.

Photoisomerization study of 4-alkyl-2,4,6-triphenyl-4H-thiopyran trapped in a solid argon matrix

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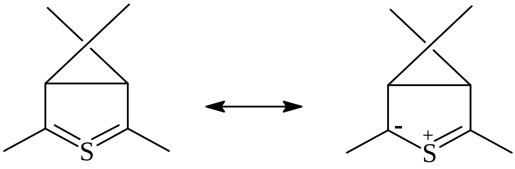
Recently increasing interest has been focused on reversible photochemical recording systems which are expected to replace magnetic recording devices. The reversible photocoloration and photoisomerization properties of 4H-thiopyran derivatives have been studied so extensively [1-3]. We first report on a novel photochromism phenomenon in sometetrasubstituted-4H-thiopyran in the solid state and the structures I and II were considered for 2,4,4,6-tetraaryl-4H-thiopyrans as colored species where no photochromic behavior could be observed for 4-alkyl-2,4,6-triphenyl-4H-thiopyrans [3].



I II

Subsequence semiemperical quantum chemical and kinetic study were also in agreement with this suggestion [4].Here, a novel photochromism observed in the 4-alkyl-2,4,6-triphenyl-4H-thiopyran in low temperature argon matrix have been investigated.

References:

[1] Pirelahi. H, Rahmani. H, Mouradzadegun. A, Fathi. A, Moujodi. A, *Phosphorus, sulfur and silicon.,* **1997**, *120, 404.*

[2] Sebek. P, Nespurek. S, Harbal. R, Adamec. M and Kuthan. J, *J. chem.. Soc., Perkin Trans.2,* **1992**, *1301*; Mori. Y and Maeda. K, *ibid*, **1991**, *2061*.

[3] Parchamazad. I, Pirelahi. H, and Shaikhebrahimi. S, *Proc.10th IUPAC Symp. On photochemistry, Interlanken, July* **1984**.

[4] Nespurek. S, Bohm. S and Kuthan. J, *Mol. Cryst. Liq. Cryst.,* **1994,** *246, 139.*

Synthesis, characterization and study of applied properties of polymers produced from thiophene derivatives

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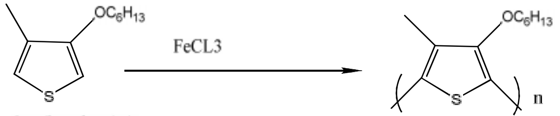
Polythiophene and its derivatives have attracted considerable attention because they are stable in the oxidized and neutral state. Relative ease of substitution at the 3-position of the thiophene ring has enabled the synthesis of a large number of derivatives, resulting in numerous polymers with different solubilities and stabilities [1-3].

Monomer 3-n-hexyloxy-4-methylthiophene(HOMT) isolated in pure form by the reaction of bromomethylthiophene with catalysts. Distillation of the crude material under vacuum was carried out for several times in order to reduce the presence of the alcohol which pur HOMT was isolated in liquid form. Polymer p-HOMT were obtained by chemical oxidation of the monomer 3-n-hexyloxy-4-methylthiophene(HOMT) using iron trichloroform, stirring at room temperature overnight.

Results obtained show that the interaction of p-HOMT with vapour of the solvents are quite reasonable with stable resistance of 600-800 ohms in most cases. Methoxythiophene (MOT) and (HOMT), monomers were electrochemically deposited($FeCL_3$)on polypyrrole, doped and characterized but shown high resistance and on heating the resistance measured has increased.



3-n-(hexyloxy)-4-methylthiophene

P-HOMT

References:

[1] Salo Gronowitz (univ. Uppsala, swed.).Arkiv kemi **1958**, *12*, 239; cf. C.A. *51*, 1935a.
[2] S.Gronowitz . Ark . kemi, **1954,** *7*, 361.
[3] Jen KY, Miller GG,Elsenbaumer RL. Highly conducting, soluble and environmentally stable poly (3-alkylthiophene).*J chem*. Soc, *chem. Commun.* **1986**, 1346.

One-pot synthesis of diphenylphosphine oxide derivatives

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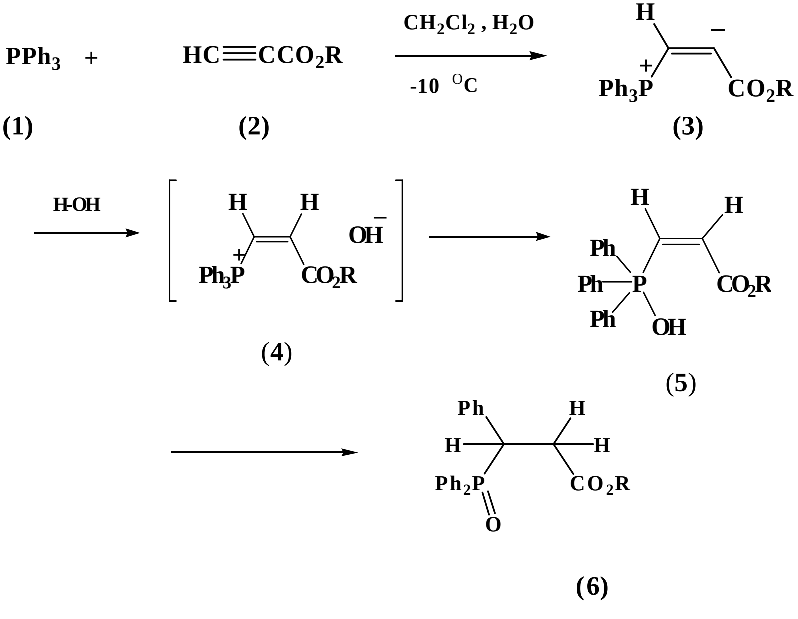
Protonation of the highly reactive 1:1 intermediates (3), produced in the reaction between triphenylphosphine (1) and alkyl acetylenecarboxylates (2) by water leads to vinyltriphenylphophonium salts (3), which undergo coupling reaction with conjugate base to produce corresponding pentavalent phosphorus intermediates (5). The pentavalent phosphorus intermediates (5) are unstable and rearange to stable diphenylphosphine oxide derivatives (6) under reaction conditions.



Reference:

[1] Ramazani, A.; Rezaei, A. *Org Lett* . **2010**, *12*, 2852.
[2] Ramazani, A.; Mahyari, T .M.; Rouhani, M.; Rezaei, A . *Tetrahedron Lett.* **2009**, *50,* 5625.

Studied of N-H proton exchange at Barbituric acid derivatives to using NMR

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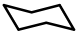
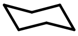
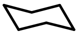
The phenomenon transfer of proton in chemical processes is undeniable importance.Proton exchanges catalysed by acids and bases are perhaps the most fundamental and widely studied chemical reactions.[1] Relaxation spectroscopy and dynamic NMR spectroscopy have been widely used to measure fast proton exchange reaction rates, in particular those involving oxygen and nitrogen acids and bases.

In this study, the rate of N-H proton transfer was studid between N,N-dimethil Barbituric acid derivatives,Dimedon, Meldrum acid polarized olefinic systems by NMR. In this assessment was used from change of signals resulting from coupling in spins 0f ^{15}N and ^{1}H of methain group adjacent nitrogen after addition potassium t-butoxide to the solution [2,3].

The rate constant of proton exchange in each isomer were obtained by fitting the ^{1}HNMR spectra to line shapes calculated on the simulated spectra using a computer program for an uncoupled two-site case [4,5].

The results are as follows:

Compound1	+	compound2	K(1)/K(2)
Meld-NH-Ph	+	Dimedon Ph – CH_2	8
Meld-NH-Ph	+	Dimethyl t-Bu	2
Dimethyl 	+	Dimethyl Ph – CH_2	2
Dimedon 	+	Dimedon Ph – CH_2	1.1
Dimedon 	+	Dimethyl Ph – CH_2	1.1

The results are ratienallyid by consideration of steric electronic and hydrogen bonding effects.

References:

[1] R. P Bell,” the proton in chemistry “, Methuen,London,(1959).
[2] I. Yavari, J. D. Roberts, J. Am. Chem. Soc. 100, 2517 (1978).
[3] I. Yavari and Hosain-Nia, Magn. Reson. Chem., 30, 413 (1992).
[4] I. Yavari and A. Shaabani and H. Sollemani, Magn. Reson. Chem, 34. 103 (1996).
[5] J. Sandstrom, Dynamic NMR Spectroscopy, Appendix. Academic press, London (1982).

Synthesis of 6-flouro-4-hydroxyquinoline-2-(1H)-one and their azo disperse dyes

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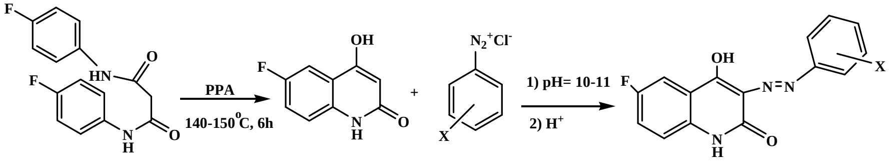
It is well known that azo pigments are used in several technical fields, e.g. printing inks, paints and the dyeing of artificial fabrics. The research on this class of dyes has made considerable progress in the last fifty decades. Especially heterocyclic azo dyes have attracted considerable interest and have played an important role in the development of the chemistry of dyes and dying process [1]. For example these classes of dyes have higher tinctorial strength and give brighter hues than those derived from aniline-based diazo components and also provide a pronounced bathochromic effect in comparison with the corresponding benzenoid compounds. The preparation of azo disperses dyes containing 4-hydroxyquinoline-2-(1H)-one as coupling component has been described in literature [2, 3].

In this study, 6-flouro-4-hydroxyquinoline-2-(1H)-one **2** were synthesized from corresponding dianilide**1**. This compound was coupled with some diazotized aromatic amines to give the corresponding azo disperse dyes. The structures of the quinolone derivative **2** and new azo dyes were confirmed by UV-vis, FT-IR, ^{1}H NMR and elemental analysis.



1 **2** **3-17**

(**3**):X= *p*-NO2
(**4**):X= *p*-CN
(**5**):X= *p*-COCH$_3$
(**6**):X= *p*-F
(**7**):X= *m*-NO$_2$
(**8**):X= *p*-Cl
(**9**):X= *p*-Br
(**10**):X= *m*-Cl
(**11**):X= *m*-CF$_3$
(**12**):X= *p*- I
(**13**):X= -H
(**14**):X= *m*-CH$_3$
(**15**):X= *p*-CH$_3$
(**16**):X= *p*-OCH$_3$
X= *p*-(**17**):NMe$_2$

References:

[1] I. Sener, F. Karci, N. Ertan, et al. *Dyes Pigments* 70 (**2006**) 143.
[2] M.R. Yazdanbakhsh, A. Ghanadzadeh, E. Moradi, *J. Mol. Liq.* 136 (**2007**) 165.
[3] Moradi-e-Rufchahi, E. *Chinese Chemical Letters* 21 (**2010**) 542.

A new method for synthesis of some novel macroacyclic schiff base ligands containing N_2S_2 donor set and their binuclear complexes

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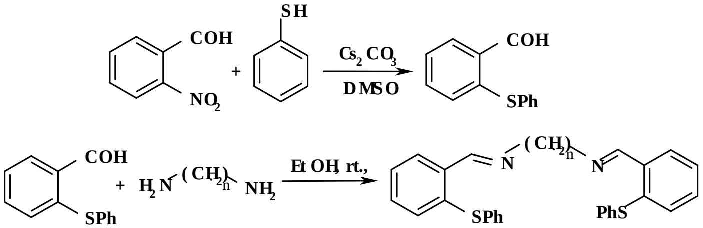
Schiff base ligands have significant importance in chemistry, especially in the development of schiff base complexes, because Schiff base ligands are potentially capable of forming stable complexes with metal ions [1] and have a variety of applications including catalytic, clinical and analytical [2]. Schiff bases that have solvent dependent Uv/Vis spectra (solvatochromicity) can be suitable NLO(Non linear optical active) materials [3]. With attention to the importance of these ligands, each year many literatures have been published from synthesis of these compounds through two component reactions to their application in different fields for various purposes. Nucleophilic aromatic substitution reactions (S_NAr reactions) of nitroarenes that have strong electron-withdrawing groups at the ortho or para positions are well-known processes [4].

Herein we report modifying an efficient method for S_NAr reactions [5] that an activated 2-nitrobenzaldehyde with aromatic thiols in the presence of cesium carbonate as a strong base converted to 2-phenylthiobenzaldehyde. First, we describe the successful synthesis of novel tetradentate ligands containing N_2S_2 donor set formed by the condensation reaction between this benzaldehyde derivative and various aliphatic and aromatic diamines. In continuation of our research, we studied the preparation of complexes of these Schiff bases with transition metal ions under mild conditions. The corresponding complexes were characterized by spectroscopic and physical data.



References:

[1] Johnson, C.P.; Atwood, J.L.; Steed, J.W.; Bauer, C.B.; Rogers, R.D. *Inorg. Chem*. **1996**, 35, 2602.
[2] a) Che, C. M.; ***Huang***, J. S. **Coord**. **Chem**. **Rev**. *2003*, ***242, 97***. b) Cozzi, P. G. *Chem. Soc. Rev*.**,** **2004**, 33, 410.
[3] Alemi, A.A.; Shaabani, B. *Acta. Chim. Slov*. **2000**, 47, 363.
[4] Penney, J. M. *Tetrahedron Lett*. **2004**, 45, 2667.
[5] Kondoh, A.; Yorimitsu, H.; Oshima, K.; *Tetrahedron*. **2006**, 62, 2357.

Application of silica-supported Pd nano catalyst and modified bentonit-supported Pd nanocatalyst in heck reaction

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The Heck reaction is among the most important and widely used reaction for the formation of carbon-carbon bonds, which allows the arylation, alkylation or vinylation of various alkenes through their reaction with aryl, vinyl, benzyl orallyl halides, acetates or triflates in the presence of palladium and a suitable base in a single step under mild conditions. In recent years, however, most studies have focused on the use of soluble Pd complexes with various types of ligands with the aim of increasing the effectiveness of the catalysts [1].

Palladium derivatives have been widely used in organic synthesis for formation of carbon-carbon and carbon-heteroatom bonds because of their versatility, compatibility with most functional groups and relative low toxicity [2].

Palladium is expensive. Very low Pd used in nano catalyst. So we senthesised our catalyst of silica-supported Pd nano catalyst and modified bentonit-supported Pd nano catalyst according to previous paper [3] and then used it in heck reaction.

References:

[1] Vivek Polshettiwar; Arpad Molnar. *Tetrahedron*. **2007**, *63*, 6949.
[2] Gong, J.; Liu, G.; Du, C.; Zhu, Y.; Wu, Y., *J. Organomet. Chem*. **2005**, *690*, 3963.
[3] Ghiaci, M.; Sadeghi, Z.; Sedaghat, M.E.; Karimi-Maleha, H.; Safaei-Ghomi, J.; Gil, A., *Applied Catalysis A: General*. **2010**, *381*, 121.

Synthesis of dicompartmental macro-acyclic ligands containing hexa- and tetradentate coordination sites

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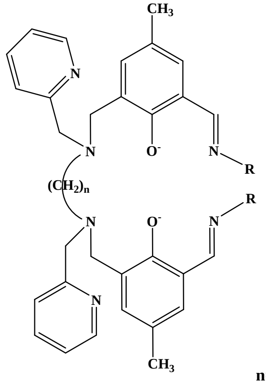
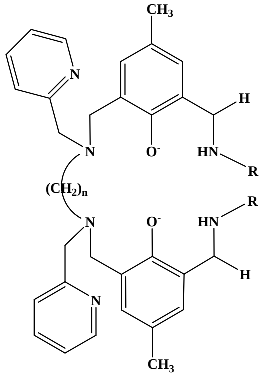
In recent years the design and synthesis of dinucleating macrocyclic and acyclic ligands and their corresponding dinuclear complexes have become a fascinating area of research, owing to their importance in basic and applied chemistry [1]. Such ligands can bind two metal ions in close proximity, have used as biomimetic studies of binuclear metalloenzymes and metalloproteins due to their interesting properties. Previously, we were reported synthesis of the ligands containing two different cyclic compartments: one includes 6-dentate (N_4O_2) and the other has a 5-dentate (N_3O_2) donor set [2, 3]. In this work, we describe the synthesis of dicompartmental (imines and amines) ligands presented below with stepwise procedure. The prepared compounds were characterized by NMR, IR spectroscopies.





n= 2, 3
R= CH_3, CH_3-CH_2

[a]

[b]

Reference

[1] E.Martell; Z. Wang, J. Reibenspies; *Inorg.Chem*.,**1997**,36,629-636.
[2] H.Golchoubian;W.L.Waltz;J.W.Quail; *Can.J.Chem.* **1999**, 37, *77*.
[3] H.Golchoubian;E. Baktash;R.Welter; *Inorg. Chem. Commun*.**2007**, 10, 1035.

Synthesis of new imine and amine containing organosilicon

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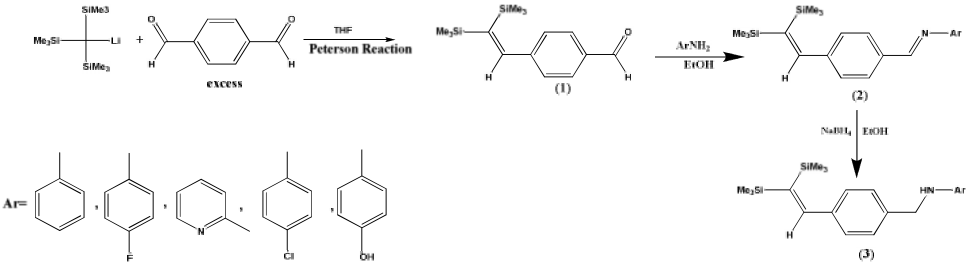
Vinylsilanes play an important and diverse role in organic chemistry. In particular, vinylsilanes have attracted considerable attention due to their versatility in both laboratory and industrial application [1-3]. The vinylsilane functionality is an extremely useful synthon as it can undergo a variety of synthetic transformations including oxidation, halogenation, and palladium-catalyzed cross coupling reactions [3-5]. The precursor $(Me_3Si)_3CH$, was prepared from the reaction between $CHCl_3$, Li and Me_3SiCl in THF. The organolithium reagent $(Me_3Si)_3CLi$, which was obtained by the treatment of $(Me_3Si)_3CH$ with MeLi under reflux in THF [6], reacts with excess terephthaldialdehyde in THF, the Peterson reaction readily takes place and gives the 4-(2,2-bis(trimethylsilyl)vinyl)benzaldehyde **(1)**. A series of novel imines (2) containing organosilicon groups was synthesized by treatment of new aldehyde **(1)** with various amines. Sodium borohydride reduced imines to corresponding secondary amines (3) containing organosilicon group in high to excellent isolate yields [7]. The new imines and amines have been characterized by elemental analysis, GC-MASS, FTIR, ^{1}H NMR and ^{13}C NMR.



References:

[1] Eaborn, C.; Hitchcock, P. B.; Kowaleska ,A.; Smith,J. D. *J. Organomet. Chem*. **1996**, *521*, 113.
[2] Safa ,K.D.; Babazadeh, M.. *J. Organomet. Chem*. **2005**, *690*, 79.
[3] Safa,K.D.; Hassanpour, A.; Nasirtabrizi, M.H.; Mossaie,U. *J. Organomet. Chem*. **2005**, *690*, 1606.
[4] Hawrelak,E. J.; Ladipo,F. T. *Organometallics*. **1999**, *18*, 1809.
[5] Safa, K. D.; Shahrivar, M.;Tofangdarzadeh, S.; Hassanpour,A. *Tetrahedron*. **2007**, *63*, 3189.
[6] Grobel,T.; Seebach,D. *Chem. Ber*. **1977**, *110* , 852.
[7] Cho,B.T.;Kang,S.K .*Tetrahedron* .**2005**,*61*, 5725.

One-pot green procedure for Biginelli reaction catalyzed TiO_2 nanoparticles

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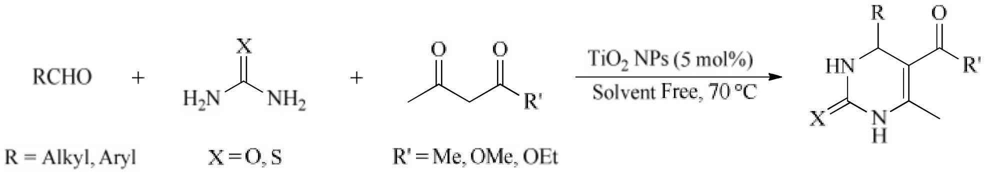
Nanotechnology is of growing importance in many branches of research because of the opportunity for miniaturization and the interesting properties associated with a small particle size [1]. In recent decades, nanostructured materials have attracted much attention for their novel electronic, magnetic, optical, chemical, and mechanical properties due to their unique characteristics which are different from bulk materials [2-4]. One of the interesting studies in this arena is that of transition metal oxide nanoparticles. Specifically titanium dioxide nanoparticles (TiO_2 NPs) have a great potential for being used as a catalyst for a variety of organic and inorganic reactions due to their high surface-to-volume ratio [5].

In this report, we wish to report an efficient and simple method for the synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones through three-component condensation of 1,3-dicarbonyl compounds, aldehydes and urea, using TiO_2 NPs as an inexpensive heterogeneous and recyclable catalyst under neutral and solvent-free-condition.



References:

[1] Rautio, J.; Perämäki, P.; Honkamo, J.; Jantunen, H. *Microchem. J.* **2009**, *91*, 272.
[2] Xia, Y. N.; Yang, P. D.; Sun, Y. G.; Wu, Y. Y.; Mayers, B.; Gates, B.; Yin, Y. D.; Kin, F.; Yan, H. Q.; *Adv. Mater.* **2003**, *15*, 353.
[3] Wang, Z. L.; Kong, X. Y.; Ding, Y.; Gao, P. X.; Hughes, W. L.; Yang, R.; Zhang, Y. *Adv. Funct. Mater.* **2004**, *14*, 943.
[4] Chae, W. S.; Shin, H. W.; Lee, E. S.; Shin, E. J.; Kim, Y. R. *J. Phys. Chem., B* **2005**, *109*, 6204.
[5] Narayanan, R.; El-Sayed, M. A. *J. Phys. Chem. B* **2005**, *109*, 12663.

Synthesis of bis oxo-thiazolidin compound by reaction of DMAD and DEAD with 1, 3-bis thiosemicarbazone derivatives

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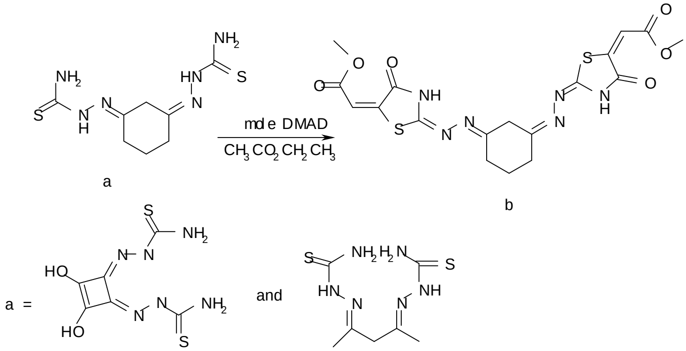
Thiazolin play very vital role in the manufacturing of various biologically active drug as analgesic [1], anti-inflammatory[2], anti-depressant [2], anti-cancer, antimicrobia, anti-diabetic [3]. Some of the thiazolin have shown a wide range of pharmaceutical properties [4]. Recently we have reported reaction of thiosemicarbazone derivatives with DMAD and DEAD [5].

Treatment of 1, 3 and 1, 2-dicarbonyl compounds with thiosemicarbazide afford the corresponding thiosemicarbazone derivatives.

In this work we synthesized [2-({3-[(5-Methoxycarbonylmethylene -4-oxo-thiazolidin-2-ylidene)-hydrazono]-cyclohexylidene}-hydrazono)-4-oxo-thiazolidin-5-ylidene]-acetic acid by reaction of 1,3-bisthiosemicarbazone derivatives of 1,3-bicarbonyl with DMAD and DEAD by two methods: a) in ethyl acetate as a solvent and ambient temperature b) A microwave-assisted synthesis under solvent-free conditions. The structure of the products were identified by ^{1}HNMR, ^{13}CNMR, IR spectroscopy and element analysis.



References

[1] Miriam, A.M.A.; Ricardo B, Maria T.G, Norman.B.D.Oscar.V. *Carbohydrate Research*. **2002**, *337*,1397.
[2] Hivayama, H.; Pang.k.S. *Drug Metab. Dispos*. **1990**, 18(5) 580.
[3] Benedit, D.; Daniel, V. *J. Med. Chem*. **1994,** *37*, 710.
[4] Viti, G.; Namnicine, R.; Ricci, R.; Pestelline, V.; Abeli, L.; Funo, M. *Eur. J. Med. Chem.* **1994**, *29*, 401.
[5] Darehkordi, A.; Saidi, K.; Islami, M.R. *Arkivoc*. **2007**, 180.

Preparation of novel bioactive poly(amide-imide)/TiO_2 nanocomposites

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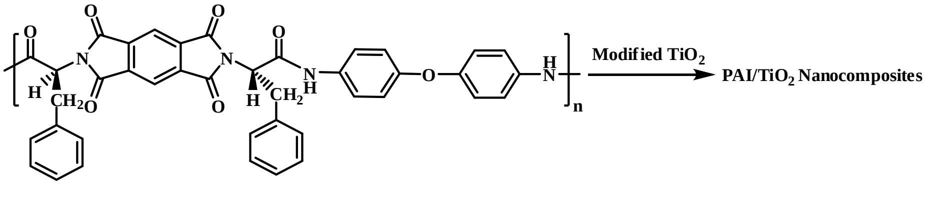
Poly(amide-imide)s (PAI)s are thermoplastic amorphous polymers that have exceptional mechanical, thermal, chemical resistant, excellent mechanical properties and hydrogen bonding interaction [1]. But they are glassy polymers which have usually low permeability to organic solvents and weak prefeasibility properties [2]. Therefore for improvement of this problem, PAIs must be modified. One method for modification of PAIs is introducing of pendent group.

Inorganic nanoparticles, such as TiO_2 are one of the most potential materials that has been widely used as a pigment and in sunscreens, paints, toothpaste, semiconductor and the focus of numerous studies in recent years due to its photo catalytic and superhydrophilicity effects [3, 4]. Herein we wish to describe the synthesis and characterization of metal oxide nanocomposites from the reaction of optically active PAI and modified TiO_2 nanoparticle. The chemical structure and morphology of the resulting nanocomposites were evaluated by fourier transformation infrared, UV-Vis spectroscopy, X-ray diffraction pattern, transmission and scanning electron microscopy as well as thermal gravimetric analysis.



References:
[1] Tsai, M.H.; Chang, C.J.; Chen, P.J; Ko, C.J. *Thin Solid Films.* **2008**, *516,* 5654.
[2] Jonquieres, A.; Clement, R.; Lochon, P. *Polym. J.* **2005**, *41,* **783**
[3] Chen, X.; Mao, S.S. *Chem. Rev.* **2007**, *107,* 2891.
[4] Rahimpour, A.; Madaeni, S.S.; Taheri, A.H.; Mansourpanah, Y. *J. Membrane Sci* .**2008**, *313,*158.

An efficient and regioselective iodination of aromatic compounds using DBU and I_2 in various reaction conditions

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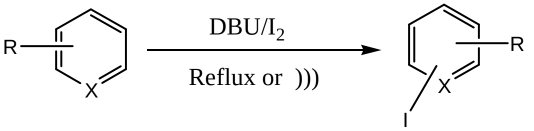
Aromatic iodo compounds are important intermediates for the synthesis of various pharmaceutical and bioactive compounds [1]. In recent years, iodination is carried out under harsh conditions in the presence of powerful oxidants such as nitrogen dioxide, diiodine pentoxide, Ag_2SO_4, HgO, $NaIO_4$, HIO_4, KIO_3, CrO_3, $KMnO_4$, Pb(ACO)2, NaOCl, ammonium hexanitrocerate, nitric acid, or liquid SO_3.[2]. Facile sonochemical route was demonstrated for reaction of aromatic compounds with iodine. Ultrasonic irradiation is the most valuable method for iodination of various compounds [3].

In this work, we would like to report iodination of various activated and inactivated aromatic compounds in ambient condition and under a dramatic acceleration condition using ultrasonic irradiation.

In continuation of our work on the development of useful synthetic methodologies [4], we have observed that iodine in the presence of a catalytic amount of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) is an effective reagent system for iodination of activated and inactivated aromatic compounds. DBU is a valuable reagent for various chemical transformations. Here, a series of activated and inactivated aromatic compounds have been iodinated using iodine–DBU at room temperature to form the corresponding iodo compounds .The I^+ electrophile generated in situ by the reaction of iodine and DBU.

Our research indicated that selected aromatic compounds were iodinated very simply under ultrasonic irradiation. Activated aromatic compounds such as aniline converted to corresponding iodinated compounds in very short reaction time (between 10-15 Min) and inactivated aromatic compounds such as quinoline gave iodo compounds in moderate reaction time.



R = NO_2, NH_2, Br, CH_3
X = C, N

References:

[1] Carril, M.; Corrae, A.; Bolm, C. *Angew. Chem., Int. Ed*. **2008**, *47*, 4862.
[2] Emmanuvel, L.; Shukla, R. K.; Sudalai, A.; Gurunath, S.; Sivaram, S. *Tetrahedron Lett*. **2006**, *47*, 4793.
[3] Kimura, T.; Fujita, M.; Sohmiya, H.; Ando, T. *Ultrasonics Sonochemistry*, **2002**, *9*, 205.
[4] Ranjbar-Karimi, R.; Hashemi-Uderji, S.; Mousavi, M. *J. Iranian Chem. Soc.* **2010**, Accepted for publication.

A rapid and efficient ultrasound-assisted synthesis of 5,5-diphenyl(thio)hydantoins

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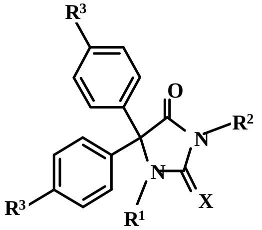
Hydantoins and thiohydantoins find important applications as medicinals (anticonvulsant drugs in the treatment of epilepsy) and as agrochemicals [1]. In recent years, considerable efforts has been devoted to the development of novel and more efficient methods for the preparation of (thio)hydantoin derivatives. Besides conventional multi-step methods, one-pot [2], solid-phase [3], microwave and ultrasound-assisted approaches [4,5] have been published. Nowadays, ultrasonic-assisted organic synthesis as a green synthetic approach is a powerful technique that is being used more and more to accelerate organic reactions [6]. The notable features of the ultrasound approach are inhanced reaction rates, formation of purer products in high yields, easier manipulation and considered a processing aid in terms of energy conservation and waste minimization which compared with traditional methods, this technique is more convenient talking green chemistry concepts into accounts [7-9]. In this work, we wish to report a rapid and highly efficient method for synthesis of 5,5-diphenylhydantoin and 5,5-diphenylthiohydantoin derivatives under ultrasound irradiation. This simple method affords the products at room temperature in short reaction time with high yield and purity.



X: O, S
R^1: H
R^2: H, CH_3
R^3: H, F, OCH_3

References:

[1] Lopez, A. C.; Trigo, C. G. The Chemistry of Hydantoins, *Advances in Heterocyclic Chemistry*, Katritzky A. R., Ed.; Academic Press: New York, **1985**, *38*, 177.
[2] Wilson, L. J.; Min, L.; Portlock, D. E. *Tetrahedron Lett.* **1998**, *39*, 5135.
[3] Belai, I. *Tetrahedron Lett.* **2003**, *44*, 7475.
[4] Safari, J.; Naeimi, H.; Ghanbari, M. M.; Sabzi Fini, O. *Russ. J. Org. Chem.* **2009**, *45*, 477.
[5] Safari, J.; Moshtael Arani, N.; Ramezan Isfahani, A. *Chin. J. Chem.* **2010**, *28*, 255.
[6] Xu, H.; Liao, W. M.; Li, H. F. *Ultrason. Sonochem.* **2007**, *14*, 779.
[7] Sinha, A. K.; Joshi, B. P.; Sharma, A.; Kumar, V.; Acharya, R. *Aust. J. Chem.* **2007**, *60*, 124.
[8] Sinha, A. K.; Sharma, A.; Joshi, B. P. *Tetrahedron* **2007**, *63*, 960.
[9] Kumar, V.; Sharma, A.; Sharma, M.; Sharma, U. K.; Sinha, A. K. *Tetrahedron* **2007**, *63*, 9718.

Silica-supported synthesis of mono-substituted porphyrins

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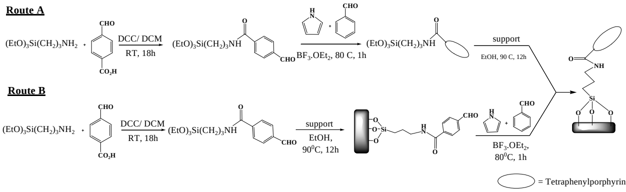
The synthesis of structurally complex porphyrins has seen tremendous progress in the last 30 years [1-2], and as such the synthesis of mono-substituted porphyrins can be achieved by utilizing many of the methods that have been developed [3]. However, the most common and direct methodology to synthesize these monosubstituted porphyrins is to condense a mixture of pyrrole, benzaldehyde, and the appropriately substituted benzaldehyde in a 4:3:1 ratio. This leads to the synthesis of the desired mono-substituted porphyrin along with a mixture of tetraphenylporphyrin, and di-, tri-, and tetrasubstituted compounds. We have modified the synthesis of mono-substituted porphyrins by using nanosilica support. SBA-15 support was synthesized according to the procedure described by Zhao *et al* [4] using Pluronic 123 as template. SEM micrograph of SBA-15 is shown in Fig 1. Two different strategies for preparation of these catalysts have been explored, mainly based on immobilisation of a functionalisated porphyrin (route A) or heterogenisation of an aromatic aldehyde and consecutive porphyrin formation (route B).



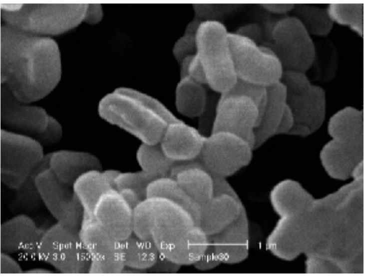


Fig 1. SEM micrograph of SBA-15

References:

[1] Porphyrins and Metalloporphyrins; Smith, K. M., Ed.; Elsevier Scientific: New York, **1975**.

[2] Lavallee, D. K. The Chemistry and Biochemistry of N-Substituted Porphyrins;VCH: New York, **1987**.

[3] Lindsey, J. S. In The Porphyrin Handbook; Kadish, K. M.; Smith, K. M.; Guilard, R.; Eds.;Academic Press: San Diego, CA, **2000**, pp 45–118.

[4] Zhao, D.; Huo, Q.; Feng, J.; Chmelka BF and Stucky GD. *J Am Chem Soc.***1998,** *120*60, 24–6036.

A novel and highly efficient one-pot synthesis of 2H-indazolo[2,1-b]phthalazine-triones via four-component reaction using $Ce(SO_4)_2.4H_2O$ as heterogeneous catalyst

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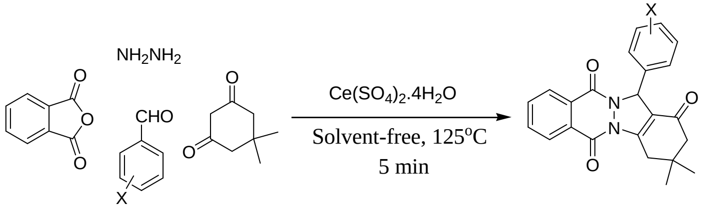
Nitrogen heterocycles containing phthalazine moiety are of special interest because they show some biological and pharmacological activities [1]. Therefore, a number of methods have been reported for the synthesis of phthalazine derivatives. The recent protocols usually employ three-component condensation. These protocols have their own limitations such as low yield use of acidic conditions, large amount of catalyst and tedious workup procedures. Thus, a search for new reagents and the development of new methods are still of practical importance. Due to the possible importance of these compounds in this study, we whish to report a new, efficient and environmentally benign protocols for the one-pot four-component synthesis of 2,2-dimethyl-13-phenyl-2,3-dihydro-1*H*-indazolo[2,1-*b*]phthalazine-4,6,11(13*H*)-trione by condensation of phthalicanhydride, hydrazinium hydroxide, aromatic aldehydes, and dimedone catalyzed by $Ce(SO_4)_2.4H_2O$ as ecofriendly catalyst with high catalytic activity and reusability at 125°C under solvent-free conditions. The reaction proceeded to completion within 5 min in 71-95% yield. All of obtained compounds were characterized by physical and spectroscopic data.

This methodology is of interest due to minimizing the cost operational hazards and environmental pollution, good to excellent yields, short reaction time, cost effective, simple work-up and reusability of catalyst. Also, to the best of our knowledge, this new procedure provides the first example of the efficient synthetic method for 2H-indazolo[2,1-b]phthalazine-1,6,11(13H)-trione by a four-component reaction.



References:

[1] Sayyafi, M.; Seyyedhamzeh, M.; Khavasi, H. R.; Bazgir, A. *Tetrahedron* **2008**, *64*, 2375
[2] Khurana, J. M.; Magoo, D. *Tetrahedron Lett*. **2009**, *50*, 7300.

Synthesis and characterization of Ni-poly(vinylpyrrolidone)-ZrO_2-TiO_2 nanocomposite as a highly efficient catalyst for the Suzuki-Miyaura reaction

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The importance of biaryl units as molecular components in pharmaceuticals, herbicides and natural products, as well as in engineering materials such as conducting polymers, molecular wires and liquid crystals, has attracted enormous interest [1]. The Suzuki–Miyaura (SM) reaction, based on the use of arylboronic acids or esters, is recognized as one of the most important synthetic methods for the construction of asymmetric biaryls as it represents an attractive alternative over methods that use organometallic species since the organoboranes used in the Suzuki reaction are air and moisture stable with relatively low toxicity [2,3]. Suzuki–Miyaura coupling reactions have been traditionally employed using homogeneous palladium catalysts in the presence of phosphine ligands. Such catalysts are not reusable and the resulting products are often contaminated by Pd metal and ligands [4]. Moreover, phosphine ligands are expensive, toxic; and in large-scale applications the phosphines may be more costly than the metal itself. In recent years there has been an increasing interest in developing greener processes. In this context, heterogeneous catalysis is emerging as an alternative to homogeneous processes since the catalysts can be recovered and reused. Catalyst recovery also decreases contamination of products with residual metal species. However, these catalysts have generally suffered from limited mass transfer, low specificity and selectivity in addition to leaching of the catalytic species from the surface of the support [5].

In the present work, for the first time, Ni-poly(vinylpyrrolidone)-ZrO_2-TiO_2 nanocomposite were prepared as a highly efficient heterogeneous catalyst by in situ polymerization method. It was characterized by XRD, FT-IR, BET, TGA, SEM and TEM techniques. This catalyst exhibits excellent catalytic activities for the Suzuki–Miyaura reaction. Over this catalyst, Suzuki–Miyaura cross-coupling reaction of aryl boronic esters with aryl bromides was successfully carried out in aqueous media at room temperature without the use of a ligand such as phosphine derivatives. Catalyst can be easily recycled after reaction and can be reused without significant loss of activity/selectivity performance. No by-product formation, high yields (85-98 %), short reaction times (10-50 min), mild reaction conditions, operational simplicity with reusability of the catalyst are the salient features of the present synthetic protocol. Presence of H_2O as a solvent, is also proposed as a ‘‘green method’’.

References:

[1] Paul, S.; Clark, J. H. *Green Chem.* **2003**, *5*, 635.
[2] Yin, L.; Liebscher, J. *Chem. Rev.* **2007**, *107*, 133.
[3] Phan, N. T. S.; Van Der Sluys, M.; Jones, C. W. *Adv. Synth. Catal.* **2006**, *348*, 609.
[4] Mubofu, E. B.; Clark, J. H.; Macquarrie, D. J. *Green Chem.* **2001**, *3*, 23.
[5] Yamada, Y. M. A.; Takeda, K.; Takahashi, H.; Ikegami, S. *Org. Lett.* **2002**, *4*, 3371.

A convenient method to synthesize *N,N'*-disubstituted formamidines

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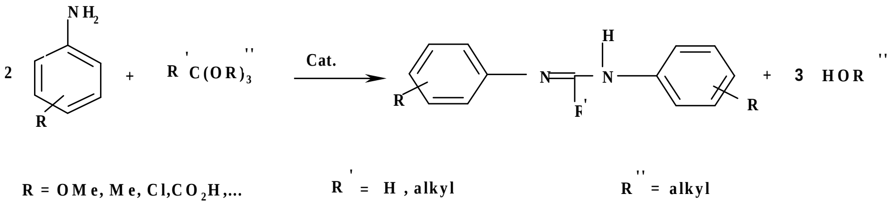
The synthesis of amidines has received much attention as a result of their biological properties [1] and applications in heterocyclic synthesis [2]. Formamidine, and their anion derivatives are common ligands frequently used in coordination chemistry, in which they were found binding to trasition metals with monodented, chelating or bridging modes [3]. Many of the synthetic methods for the preparation of amidines described in the literature [4], involve harsh reaction conditions, reagents that are difficult to handle, using hydrogen gas, fairly complicated isolation and the yields are usually low.

Among them the commercially available trialkyl orthoesters and different amines have become efficient reagents for the easy purification, clean and rapid introduction of the amidines which does not have the above mentioned drawbacks.

In this study for the synthesis of formamidines we threated trialkyl ortho esters with various aromatic primary amines in water as a green solvent in the presence of lewis acids such as: $AlCl_3$, in excellent yields, at 30-40°C. Best results are obtained with electron donating aromatic amins as substrates. Furthermore, in contrast to previous studies wich described imidate as intermediate the key advantage of our method is that amidines was the only product.



References:

[1] Som, P.; Werbovetz, K.; Stepnens, C.; Boykin, D. *Chem. Abstr.* **2004**, 139980.
Kitamura, S.; Fukushi, I.; Miyawaki, T.; Kawamura, M.; Terashita, E.; Naka, T.; *Chem. Pharm. Bull.* **2001**, *49*, 268.
[2] Alanine, A. I. D.; Fishwick, C. W. G. *Tetrahedron Lett.* **1989**, *30*, 4443.
[3] Arnold, D.I.; Cotton, F. A.; Maloney, D. J.; Murillo, C. A.; Matonic, J. H.; *Polyhedron* **1997**, *16*, 133.
[4] Partridge, M. W.; Short, W. F.; *J. Org. Chem*. **1947**, 390.
Porcheddu, A.; Giacomelli, G.; Piredda, I.; *J. Comb. Chem.* **2009**, *11*, 126.

An efficient one-pot synthesis of 2-amino spiro[oxindole-pyrimidines]

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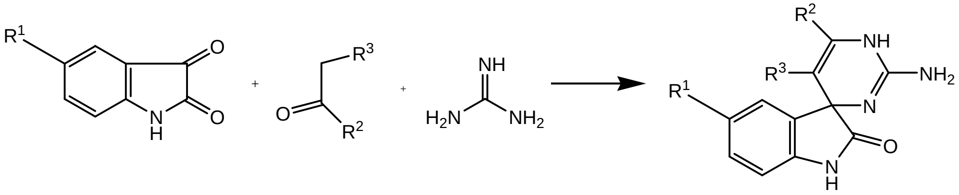
Dihidropyrimidine and oxindole are two important structural motifs constituting numerous natural products and pharmaceutically active compounds. Synthesis and high throughput screening of indoles have revealed that sharing of indole 3-carbon atom in the formation of spiro indoline derivatives highly enhances their biological activities [1-3]. Also, dihydropyrimidinones have attracted great attention of synthetic organic chemists due to their anti-hypertensive activities as well behaving as calcium channel blockers, α-1a-antagonists and neuropeptides-Y antagonists [4-6]. The Biginelli reaction is one of the well established multicomponent reactions (MCRs) which frequently was employed for synthesis of 3,4-dihydropyrimidine-2(1H)-ones (DHPMs).

Herein, we wish to report, for the first time, a simple approach to novel spiro[oxindole-pyrimidine]ones via a new Biginelli-like reaction consisting of a three-component cyclocondensation of acyclic carbonyl compounds, guanidine and isatin derivatives instead of aromatic aldehydes. This method has shown the ability to tolerate a reasonable variety of substituent in all three components; therefore we anticipate that it will be adopted in combinatorial chemistry to synthesize the related spiro oxindoles of potent biological importance for screening.



References:

[1] Da-Silva, J. F. M.; Garden, S. J.; Pinto, A. C. *J. Braz. Chem. Soc.*, **2001,** *12,* 273.
[2] Joshi, K. C.; Jain, R.; Sharma, K. *J. Indian Chem. Soc.*, **1998,** *115,* 202.
[3] Abdel-Rahman, A. H.; Keshk, E. M.; Hanna, M. A. *Bioorg. Med. Chem.*, **2004**, *12,* 2483.
[4] Zorkun, I. S.; Sarac, S.; Celebi, S.; Erol, K. *Bioorg. Med. Chem.*, **2006**, *14,* 8582.
[5] Kappe, C. O. *Eur. J. Med. Chem.*, **2000,** *35,* 1043.
[6] Kappe, C. O.; Fabian, W. M. F.; Semones, M. A. *Tetrahedron*, **1997,** *53,* 2803.

Theoretical studies on benzil-benzilic acid rearrangement

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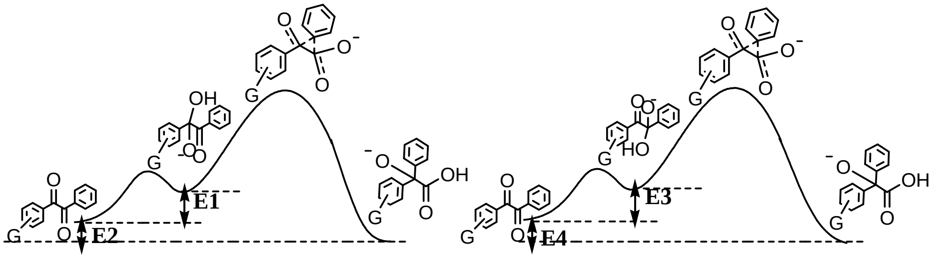
The Benzil-Benzilic acid rearrangement is the conversion of benzil to benzilic acid in the alkalic media.The reaction first reported by Justus Liebig in 1838 [1]. This type of rearrangement reaction has industrial importance in the production of phenytoin, an antiepileptic drug [2]. Although the benzilic acid rearrangement is a well-known foundamental organic reaction (consisting of only C, H and O atoms) and a classic reaction (since 1838), its mechanism has not been studied in detail [3]. So we desided to investigate the mechanism of benzil-benzilic acid rearrangement using theoretical study. The rearrangement of the series of benzil derivatives have been investigated. In the first stage the benzil molecule was optimized in the gas phase and solution. In addition by scaning of dihedral angle between carbonyl groups. The best conformation was found. Also a series of substituted benzyl molecules was investigated.



A METHOD **B METHOD**

References :

[1] Liebig, J. *Annalen der Chemie*. **1838**, 5, 1-35.

[2] Unverferth, K..; Rundfeldt, C. *Antiepileptics, in Ullmann's Encyclopedia of Industrial Chemistry.* Wiley, Hoboken, NJ. **2000**, http://www.mrw.interscience.wiley.com/ueic/articles/a03_013/frame. html.

[3] Yamabe, S.; Tsuchida, N.; Yamazaki, S. *J. Org. Chem.* **2006**, *71*, 1777-1783.

Feasibility study of cresol synthesis in sub- and supercritical water

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The use of supercritical fluids as a medium for chemical reactions has recently received a great deal of attention. The dramatic decrease in solvent viscosity, increase in substrate solubility and enhanced sensitivity of solvating properties of the supercritical fluid to temperature and pressure make them attractive as potential solvents.

Cresol is used as solvent for some chemicals, and as disinfectants, household cleaners, in photographic developers and etc. One of the classical synthesis method of cresol is alkaline fusion of sodium toluene sulfonate (STS). Herein we do above reaction in sub- and supercritical water medium.

Water in many respects shows unique properties that are well characterized at ordinary conditions , at states above it's critical point (T_c=647K P_c=250 bar) it shows remarkable properties. In many chemical applications supercritical water acts as a solvent or working fluid for many interesting reactions such as oxidation, hydrolysis, pyrolysis. By tuning temperature and pressure water becomes completely miscible with nonpolar compounds while polar and ionic compounds remain highly soluble as well.

Alkaline solutions of 1-5% STS (pH adjusted to 12 with KOH) was used, reaction was performed in the supercritical water reactor cell in temperature range of 200-350 ºc and pressure range of 200-250 bar. Analysis of samples was done by HPLC.

The results were compared with those which obtained by classical method.

References

[1] H. Weingartner, E. Frank *Angew. Chem. Ind. Ed.* **2005**, 44, 2672-2692
[2] F. Donald, *Ind. Eng. Chem.* **1953**, 45, 193-197.

Synthesis of molecular receptors based on p-sulfonylcalix[4]arenes derivates for recognition of amino acids

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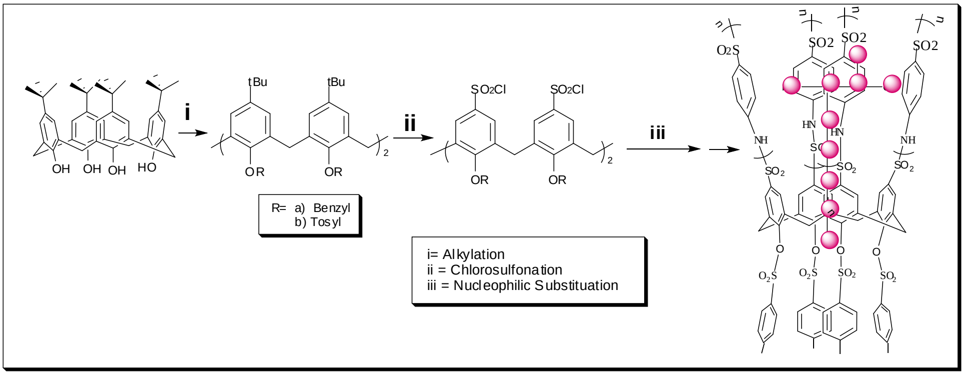
There is increasing interest in the biological and material science applications of calix[4]arenes derivatives.[1] The utility of the calixarenes is based on their capability of forming complexes, adducts and inclusion compounds with neutral or ionic organic and inorganic compounds.[2] Recently, chlorosulfonylated calix[4]arenes[3] and calix[6]arenes[4] have received much attention as a nautral anion receptors and metallo-enzyme active sites with a selectivity for special ion or enzyme. They are flexible enough to adjust the cavity dimension and able to form inclution compounds with ionic or neutral molecules such as amino acids.[5]

In this work, our strategy consists of the synthesis of the p-sulfonamidcalix[4]arenes derivatives with Ipso-Chlorosulfonylation and then reaction of this derivatives with p-Amino-benzenesulfonyl chloride to extension of conic cavities of calix[4]arenes.

Obtained receptord have been characterized by ^{1}HNMR, ^{13}CNMR, FTIR and MS. The complexation properties and host behavior of the p-sulfonamides calix[4]arene derivatives some amino acids and peptides have been studied.



Reference

[1] Gustche , C.D,;Muthukrishnan , *R.H Org.Chem*. **1978** ,43,4905.
[2] US Patent ;5,952,526,**1999.**
[3] Morzherin, Y. ; Verboom, W. ; Reinhoudt, D. N. *J. Org. Chem*. **1993**, 58, 7602.
[4] Coquiere, D. ; Cadeau, H. ;et al ; *J. Org. Chem*. **2006**, 71, 4059-4065.
[5] Mourer, M. ; Psychogios, N. ; et al. *J. Bioorganic & Medicinal Chemistry*. **2010**, 18, 36-45.

Synthesis and characterization of 4-methyl vinyl pyridinium hydroxide-SiO_2-Al_2O_3 by in situ polymerization and it's application as basic catalyst

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Solid base catalysts have many advantages over liquid bases. They are noncorrosive and environmentally benign, presenting fewer disposal problems, while allowing easier separation and recovery of the products, catalysts and the solvent. Furthermore, high activity and selectivity are often obtained only by solid base catalysts for various kinds of reaction. Recently, many solid base catalysts have been reported which is effective for a number of base-catalyzed reactions [1-3].

The organic–inorganic hybrid composites can be obtained by increasing the interfacial interactions between both components via the formation of hydrogen bonds or covalent bonds, in the processed mixing the corresponding polymers [4]. These materials with specific mechanical and thermal stability have numerous industrial applications.

In this work, Al_2O_3 is mixed with SiO_2 and 4-vinylpyridine by the sol-gel method, to make a composite which is used as a heterogeneous basic catalyst for Knoevenagel condensation reaction.

The physical and chemical properties of the composite catalyst were investigated by XRD, FT-IR, TG, BET and SEM techniques.

The catalytic performance of each material was determined for the Knoevenagel condensation reaction between carbonyl compound and malononitrile. The reaction performed in solvent-free conditions and the product obtained in high yield and purity after a simple work-up.

The effects of reaction temperature, the amount of catalyst, amount of support, solvent and the amount of benzoyl peroxide for the synthesis of composite, were investigated as well as recyclability of the heterogeneous composite. The composite catalyst used for this synthetically useful transformation showed considerable level of reusability besides very good activity.

References:

[1] Wang, H.; Wang, M.; Zhao, N.; Wei, W.; Sun, Y. *Catal. Lett*. **2005**, *105*, 253.
[2] Ai, M. *Appl. Catal. A: Gen.* **2005**, *288*, 211.
[3] Liu, X.; Wang, H.; He, Y.; Zhu, S. *Catal. Commun.* **2007**, *8*, 1107.
[4] Mammeri, F.; Bourhis. E. L.; Rozes. L.; Sanchez. C. *J. Mater. Chem.* **2005**, *15*, 3787.

One-pot synthesis of chromene derivatives

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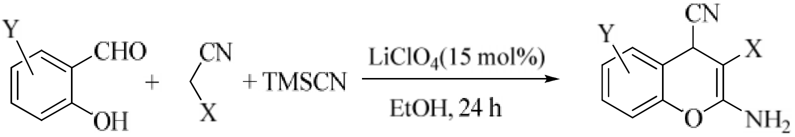
Chromenes constitute a major class of naturally occurring compounds, and interest in their chemistry continues unabated because of their usefulness as biologically active agents [1]. They widely exist in plants, including edible vegetables and fruits [2]. Synthetic analogues were developed over the years, some of them displaying remarkable effects as pharmaceuticals, including antifungal and antimicrobial activity [3]. 2-Aminochromenes are widely employed as pigments [4], cosmetics, agrochemicals [5] and represent an important class of chemical entities being the main constituents of many natural products.

Herein we have described a facile and three-component method for the synthesis of 2-amino-4-cyano-4*H*-chromenes by the reaction of salicylaldehydes, malononitrile or cyanoacetamide and TMSCN at room temperature.



References:

[1] Miao, H.; Yang, Z. *Org. Lett.* **2000**, *2*, 1765.
[2] Curini, M.; Cravotto, G.; Epifano, F.; Giannone, G. *Curr. Med. Chem.* **2006**, *13*, 199.
[3] Kraus, G. A.; Kim, I. *J. Org. Chem.* **2003**, *68*, 4517.
[4] Ellis, G. P. In: *the Chemistry of Heterocyclic Compounds. Chromenes, Chromanes, and Chromones*; Weissberger, A., Taylor, E. C., Eds.; John Wiley: New York, **1977**; Chapter II, pp 11–141.
[5] Hafez, E. A.; Elnagdi, M. H.; Elagamey, A. G. A.; El-Taweel, F. M. A. A. *Heterocycles* **1987**, *26*, 903.

A theoretical quest for boranorcaradienes with more stability than their corresponding borepins

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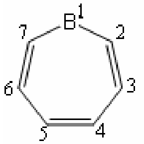
Typical borepins (***i***) appear ~ 40 kcal/mol more stable than their corresponding tautomeric boranorcaradienes (***ii***) [1-3]. To push the equilibrium in favor of the latter we have probed nineteen bimolecular tautomerization systems involving mono-, di-, and tri-aza substituted 6*H*-dibenzo[*c*,*e*]borepins as well as 1a,2,7b-tetrahydro-1*H*-indeceno[4,5-*b*]borirenes, at B3LYP/6-311+G** and MP2/6-31G*//MP2/6-311+G** levels. Among them two new boranorcaradienes are found which apear more stable than their respective borepins. They are namely: 1a,9b-dihydro-1*H*-borireno[2,3-*h*]pyridazino[4,3-*f*]cinnoline (**I**) and 1a,9b-dihydro-1*H*-borireno[2,3-*h*]pyrimido[5,4-*f*]quinazoline (**II**).



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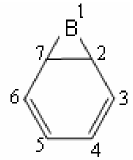

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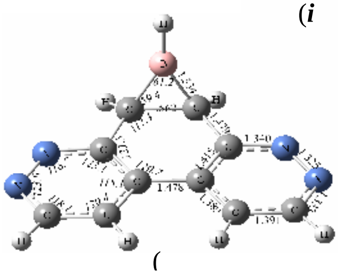

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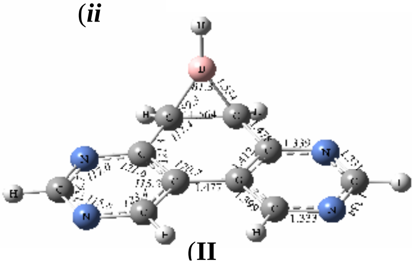

(**II**

References:

[1] Schulman, J.M.; Disch, R.L.; Sabio, M.L.; *J. Am. Chem. Soc.* **1984**, *106*, 7696.
[2] Schulman, J.M.; Disch, R.L.; Sabio, M.L.; *Tetrahedron. Lett.* **1983**, *24*, 1863.
[3] Schulman, J.M.; Disch, R.L.; *Organometallics.* **1989**, *8*, 733.

Preparation of pyridine derivatives of dacarbazine and evaluation of their antitumor activity

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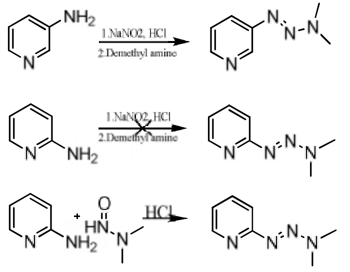
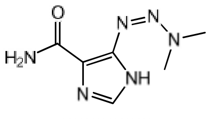
Dacarbazine is an antitumor drug to cure the malignant metastatic. Melanoma and Hodgkin's disease which has an Imidazole ring in its structure. Dacarbazine is a prodrug which is converted to an active form by undergoing demethylation with liver enzymes. The active form prevents the progress of disease via alkylation of DNA strand. On the basis of the mechanism of action of this drug, it is possible that the ring and carboxamide group do not have a key role in activity but the chain has a vital effect. On the other hand, Imidazole ring has a unique tautomerization which may participate in the mechanism of action of Dacarbazine and carboxamide group may determine the rich Cytosine pieces in DNA strand.[1]

In Order to investigate the role of Imidazole ring tautomerization in dacarbazine structure and the carboxamide group, two new derivatives of dacarbazine whit a pyridine ring instead of Imidazole ring synthesized using the reactions in the following scheme.[2,3]

The cytotoxicity effect of the compounds and dacarbazine on isolated hepatocytes were evaluated and compared with each other. Both Dacarbazine and compounds A and B resulted in reactive oxygen spices (ROS) formation up on their addition to the isolated rat hepatocytes. They also decreased mitochondrial membrane potential and lysosomal membrane rupture. Cytotoxicity were prevented by ROS scavengers and antioxidants. Glutathione depletion makes the hepatocytes resistant to the cytotoxic effect of Dacarbazine and compounds A and B by n-Bromoheptane. Cytoxicity is also prevented by CYP450 inhibitors and lysosomal inactivators and MPT blockers. Cytotoxicity are associated whit mitochondrial/ lysosomal damage caused by the reduced biological metabolites and ROS. The induced cytotoxicity could be increased by oxidative stress and crosstalk between mitochondrial and lysosomal damage.




Dacarbazine

Refrences:

[1] Daidone G. , Maggio B. , Raffa D. , et al. , *Farmaco* , 2004; 59 (5) : 413-417.

[2] Martin J. Wanner, Melle Koch, and Gerrit-Jan Koomen, J. Med. Chem. 2004, 47, 6875-6883

[3] David B. Kimball and Michael M. Haley, Angew. Chem. Int. Ed. 2002, 41, 3338- 3351.

Synthesis of different diamines and preparation of related polyamides and study the effect of pendant group on their physical properties

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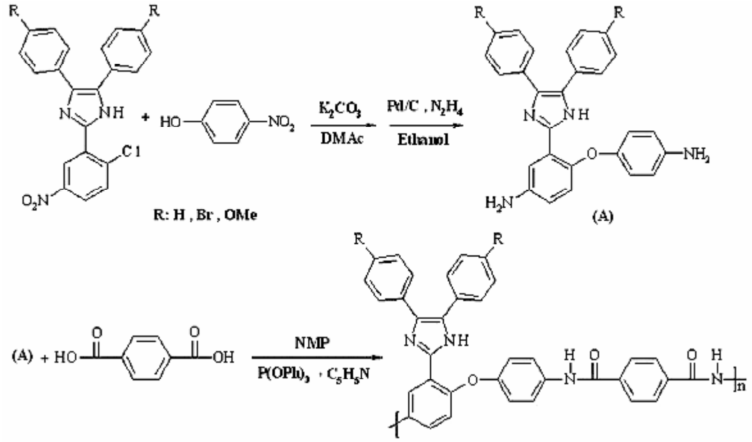
A series of new unsymmetrical diamines containing triaryl imidazole pendent group was successfully synthesized by the nucleophilic substitution reaction of 4-nitro phenol with 2-(2-chloro-5-nitrophenyl)-4, 5-diphenyl-1H-imidazole. A series of polyamides (PAs) were prepared from a diamine containing bulky imidazole with different substituents and terphthalic acid via phosphorylation polyamidation. These PAs are readily soluble in many organic solvents; their inherent viscosities were suitable and gave tough and flexible films by solution-casting. The PAs were characterized using FT-IR, ^{1}H NMR, UV–vis spectroscopy, fluorimetry and elemental analysis. Thermal properties of new PAs were evaluated by thermogravimetric analysis and differential scanning calorimetry [1, 2, 3].



References:

[1] Feng, K.; Hsub, F. L.; Van DerVeer, D.; Bota, K.; Xiu, R. *J. Photochem- Photobiol . A: Chem.* **2004**, *165*, 223.
[2] Ghaemy, M.; Alizadeh, R.; Behmadi, H. *Eur. Polym. J.* **2009**, *45* , 3108.
[3] Ghaemy, M.; Amini Nasab, S. M. *Reac. Funct. l Polym.* **2010**, *70*, 306.

Study of reaction between triethylphosphite and acetilenic esters in the presence NH- and SH- containing compounds

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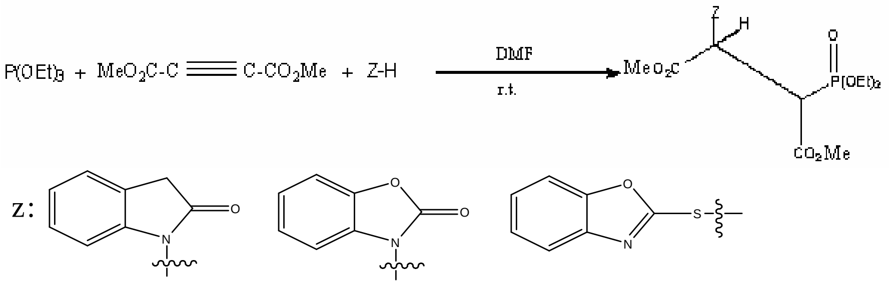
Organophosphorus compounds, those bearing a carbon atom directly bound to a phosphorus atom, are synthetic targets of interest, not least because of their value for a variety of industrial, biological, and chemical synthetic uses [1-3]. As a result, a large number of methods have appeared describing novel synthesis of organophosphorus compounds. There are many studies on the reaction between trivalent phosphorus and α,β-unsaturated carbonyl compounds in the presence of proton sources [4-6]. In this research, reaction between triethylphosphite with dimethylacetylenedicarboxylate (DMAD) in the presence of aromatic and heterocyclic compounds has been studied. The products are phosphonate esters. All known products were characterized by comparison of IR and NMR spectra with authentic samples and the new compounds were characterized by melting point, IR, NMR (^{1}H, ^{13}C and ^{31}P) spectroscopy.



References:

[1] D. E. C. Corbridge, Phosphorus. An Outline of Its Chemistry Biochemistry and Uses , 5th edn, Elsevier, Amsterdam, **1995**.
[2] R. Engle, Synthesis of Carbon-Phosphorus Bond, CRC Press, Boca Raton, FL, **1988**.
[3] I. Yavari, M. Anaary-Abbasinejad and Z. Hossaini, Org Biomol Chem **2003,** 1, 560.
[4] M. V. George, S. K. Khetan and R. K. Gupta, Adva. Heterocycl. Chem, **1976**, 19, 354.
[5] R. Burgada, Y. Leroux, M. Zabloka and Y. U. El Khoshnieh, Tetrahedron Letter, **1981**, 22, 3533
[6] M. T. Maghsoodlou, S. M. Habibi-Khorassani, M. K. Rofouei, S. R. Adhamdoust, Nassiri, M. Arkivoc **2006**, xii, 145.

Essential oils composition of flowers and leaves of *Salvia reuterana* Boiss. and antioxidant activity of the essential oils and methanol extracts of *Salvia sclarea* L. from Kashan area

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The genus *Salvia*, which belongs to the lamiaceae family, consists of about 700 to 900 species widespread throughout the world. In Iran, about 57 species are present, of which some are endemic [1]. *Salvia* (Lamiaceae) and their essential oil are used in food flavoring, pharmaceuticals and in perfumery [2].

The essential oils were obtained by hydrodistillation by Simultaneous Distillation Extraction (SDE) and were analyzed by GC/MS (The yields were 0.15% and 0.04% w/w). The flower oil consisted of 31 identified compounds representing 99.99% of the oil composition.The main compounds were Benzoic acid hexyl ester (16.96%), β-Gurjunene (7.51%), β-Eudesmol (6.86%) and Ishwarene (6.04%). On the other hand, Germacrene D (21.22%), Epi-Laurenene (9.53%), (8S),13-Cedrandiol (9.86%) and Bicyclogermacrene (8.18%) were the main components among the 26 constituents characterized in the leaf oil representing 99.98% of the total compounds detected. Antioxidant activity of the essential oils and methanol extracts of *Salvia sclarea* L. were determined by β- carotene linoleic acid. In this assay, the best inhibition belonged to the methanol extract of leaves of this plant with 47.58 ± 3.09 % Inhibition. Total phenolic content of the methanol extracts of flowers and leaves, as Gallic acid equivalents, were 116. 22 ± 2.11 and 106.72 ± 2.25 µg/mg.

References

[1] Lari Yazdi, H.; Goudarzi, M.; Yazdani, D.; Chehregai, A.K. *Journal of Medicinal Plants*. **2005**, *4*, 16, 15.
[2] Nejad Habibvash, F.; Rajamand M.A.; Heidari, R.; Hosseini Sarghein, S.; Heidari Ricani, M.; *Pakistan Journal of Biological Sciences*. **2007**, *10* (20): 3516.

Isocyanide-based three-component synthesis of highly substituted 3,4-dihydro-benzo[g]quinoxalin-2-amine derivatives

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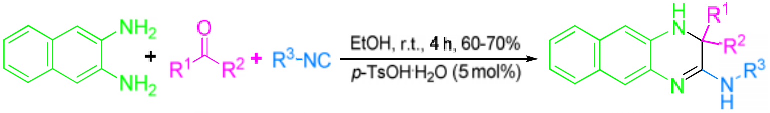
Quinoxalines and their derivatives are important class of benzoheterocycles [1] displaying a broad spectrum of biological activities [2], including antidiabetic [3] and antiviral effects, in particular against retroviruses such as HIV [4]. They also are inhibitors of aldose reductase [5,6], partial agonists of the γ-aminobutyric acid (GABA)/benzodiazepine receptor complex [7], and antagonists of the AMPA and angiotensin II receptors [8]. They have also found applications as dyes [9] and building blocks in the synthesis of organic semiconductors [10], and they also serve as useful rigid subunits in macrocyclic receptors for molecular recognition [11] and chemically controllable switches [12]. 3,4-Dihydroquinoxalines possess biological activity, for example, as inhibitors of cholesteryl ester transfer proteins[13].

In this work, a new approach isocyanide-based multicomponent reactions for synthesis of novel class of highly substituted 3,4-dihydro-benzo[*g*]quinoxalin-2-amine derivatives including spirocyclic compounds from three-component condensation reaction between naphthalene-2,3-diamine, diverse carbonyl compounds and isocyanides in the presence of a catalytic amount of *p*-toluenesulfonic acid in good to excellent yields at room temperature.



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References:

[1] Porter, A. E. In *Comprehensive Heterocyclic Chemistry*; Katritzky, A. R., Rees, C. W., Eds; **1984**; Vol. 3, part 2B, p 157.
[2] Seitz, L. E.; Suling, W. J.; Reynolds, R. C. *J. Med. Chem.* **2002**, *45*, 5604.
[3] Gupta, D.; Ghosh, N. N.; Chandra, R. *Bioorg. Med. Chem. Lett.* **2005**, *15*, 1019.
[4] Rösner, M.; Billhardt-Troughton, U.-M.; Kirsh, R.; Kleim, J.-P.; Meichsner, C.; Riess, G.; Winkler, I. U.S. Patent 5723461, **1998**. Sarges, R.; Lyga, J. W. *J. Heterocycl. Chem.* **1988**, *25*, 1475.
[5] Sarges, R.; Lyga, J. W. *J. Heterocycl. Chem.* **1988**, *25*, 1475.
[6] Bunin, B. A.; Ellman, J. A. *J. Am. Chem. Soc.* **1992**, *114*, 10997.
[7] Lee, L.; Murray, W. V.; Rivero, R. A. *J. Org. Chem.* **1997**, *62*, 3874.
[8] Morales, G. A.; Corbett, J. W.; DeGrado, W. F. *J. Org. Chem.* **1998**, *63*, 1172.
[9] Brock, E. D.; Lewis, D. M.; Yousaf, T. I.; Harper, H. H. (The Proctor and Gamble Company) WO 9951688, **1999**.
[10] Dailey, S.; Feast, J. W.; Peace, R. J.; Sage, I. C.; Till, S.; Wood, E. L. *J. Mater. Chem.* **2001**, *11*, 2238.
[11] Mizuno, T.; Wei, W.-H.; Eller, L. R.; Sessler, J. L. *J. Am. Chem. Soc*. **2002**, *124*, 1134.
[12] Crossley, J. C.; Johnston, L. A. *Chem. Commun*. **2002**, 1122.
[13] Jones, Z.; Groneberg, R.; Drew, M.; Eary, C. T. U.S. Patent 20050282812, **2005**.

PEG-SO_3H catalyzed coumarin synthesis via Pechmann condensation

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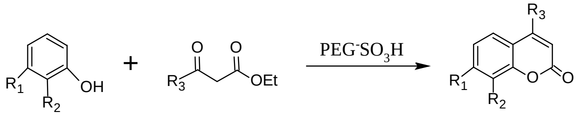
The synthesis of coumarins and their derivatives has attracted considerable attention from organic and medicinal chemists for their remarkable biological activities. This is why there is a great deal of interest in the development of efficient synthetic approaches to these heterocyclic ring systems [1]. Conventional routes for the synthesis of coumarins involve the Pechmann reaction –condensation of phenols and β-ketoester -in some cases reaction mixtures were allowed long time or were heated above temperature, tedious workup and low selectivity . Chromones may also be formed as By –products. For these reasons there have been some attempts to find alternative environmentally benign synthetic routes. Some organic acids and metallic Lewis acids are also examined for this purpose in the Pechmann condensation [2]. Although these methods are suitable for certain synthetic applications, many of these procedures are associated with disadvantages such as expensive or corrosive reagents and moreover organic solvent are harmful for ecosystem. So in this work we used PEG-SO3H as a green solvent and environment friendly media that can catalyze the Pechmann reaction. Solubility in water and recoverability are considerable in use of PEG-SO3H in Pechmann reaction. There for to a mixture of equimolar quantities of phenolic compound **1** and β-ketoester **2** was added solution of PEG in room temperature. The mixture of reaction was refluxed for 25-30 min. The reaction was monitored by TLC. After completion, the reaction mixture was poured into ice/H2O and the separated solid was filtered off. The product was crystallized from hot ethanol to afford the coumarin derivatives with high yield [3].



(1) (2)

R_1=OH,OME,OEt,OPh,H,Me R_3=Me,Et

R_2=OH,H

References:

[1] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62*, 6968.
[2] D. Li, F. Shi, S. Guo, Y. Deng, *Tetrahedron Lett.* **2005**, *47*,671.
[3] Kiasat, A.; Fallah Mehrjardi, M. *Catal. commun.* **2007**, *9*, 1497.

The synthesis of PAMAM-E_n.$NHCOCH_2CH_2COOH$ nano dendrimer and estimation of their carboxylic acid functional terminal groups

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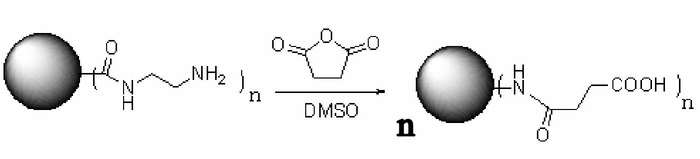
Dendrimers are repeatedly branched molecules, first described by a number of authors in the late 1970s and early 1980s[1]. A dendrimer is a uniform, spherical and nanostructure ranging from 10 to 200 angstroms in diameter [2]. There are two main methods of synthesis for dendrimers, the divergent and convergent methods [3]. In this research the synthesis of Poly (amidoamine) (PAMAM) by divergent method was carried out using ethylene diamine as a (EDA)-cored PAMAM dendrimer [4,5]. The EDA core is alkylated with methyl acrylate through Michael addition. This synthesis was resulted to the PAMAM dendrimer of Generation 1 and 2 with amine terminal groups. This is followed by reaction with succinic anhydride to generate PAMAM with ***carboxylic acid functional terminal groups.*** These components were characterized by FT-IR, ^{1}H-NMR, ^{13}C-NMR, AFM and Elementary Analysis (CHNO). Moreover the amount of carboxyl end groups was determined by Potentiometric Titration.



References:

[1] Fre´chet J.J., Tomalia D.A. Dendrimers and Other Dendritic Polymers, John Wiley & Sons, Ltd., New York, **2001**.
[2] Klajnert B, Bryszewska M. Dendrimers: properties and applications, Acta Biochimica Polonica, **2001**, 48 (1), 199–208.
[3] Shi X, Lesniak W, Mohammad T. Islam, Maria C. MuN iz, Lajos P. Balogh, James R. Baker Jr., Physicochem. Eng. Aspects. **2006**, 272, 139–150.
[4] Louie O., Massoudi A. H., Vahedi H., Sajjadifar S.; *j. Polymer* . **2009** ,50, 5605-5607.
[5] Massoudi A. H. , Vahedi H.**,** Louie O. ,Sajjadifar S. *E – Journal of Chemistry*. **2009,** 6(3)681- 684.

Synthesis of 1,4-dihydropyridine derivatives under solvent-free and grinding conditions

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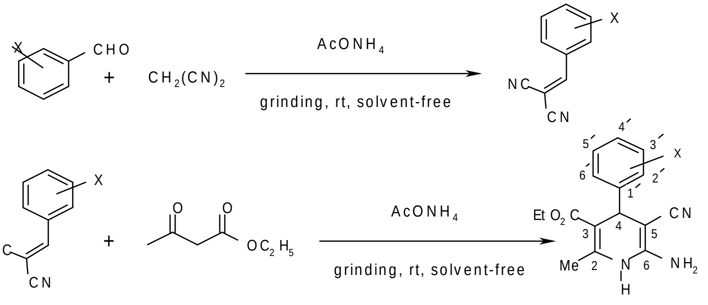
1,4-Dihydropyridines (1,4-DHPs) are important class of compounds in the field of drugs and pharmaceuticals [1]. Hantzsch 1,4-dihydropyridines (dialkyl 1,4-dihydro-2,6-dimethylpyridine-3,5-dicarboxylates) are widely used clinically as calcium channel blockers for the treatment of cardiovascular diseases, including hypertension and angina pectoris. In spite of the widely developed chemistry of the 1,4-DHPs, little is known about 1,4-DHPs bearing substituents other than hydrogen atoms or alkyl groups at C2 and C6. A survey of the current literature has shown that 6-amino substituted 1,4-DHPs (**I**) induced a remarkable neuroprotective affect against toxicity caused by [k^+]-elicited [Ca^{2+}] overload, meanwhile, prevent calcium overload and neuronal death [2].

In this work, we have developed a simple, efficient and environmentally friendly method for the synthesis of 6-amino substituted 1,4-DHPs (**2a-g**) at room temperature in solvent-free conditions. We used a one-pot, two stage synthesis of this specific group of 1,4-dihydropyridines via a Knovenagel condensation involving malononitrile and a subsequent Micheal addition/cyclisation (Scheme 1). The experimental simplicity, mildness of conversion, efficient yields, short reaction times, low cost, simple work-up and easy purification makes this procedure attractive to synthesize a variety of these derivatives.



2a-g

Scheme 1. synthesis of 6-amino-4-aryl-5-cyano-1,4- dihydropyridies.

References:

[1] (a) Reddy, G. M.; Shiradkar, M.; Chkravarthy, A. K. *Curr. Org. Chem.* **2007**, *11* (10), 847; (b) Goldmann, S.; Stoltefuss, J. *Angew. Chem. Int. Ed. Engl.* **1991**, *30*, 1559.

[2] (a) León, R.; de los Ríos, C.; Marco-Contelles, J.; López, M. G.; García, A. G.; Villarroya, M. *Eur. J. Med. Chem.* **2008**, *43*, 668; (b) Marco-Contelles, J.; León, R.; de los Ríos, C.; Guglietta, A.; Terencio, J.; López, M. G.; García, A. G.; Villarroya, M. *J. Med. Chem.* **2006**, *49(26)*, 7607.

Efficient and solvent-free synthesis of 1-amidoalkyl-2-naphthols using *N,N,N',N'*-tetrabromobenzene-1,3-disulfonamide

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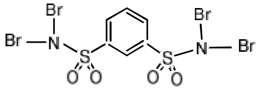
Multi-component reactions (MCRs) are powerful and useful synthetic tool to produce complex moleculs from simple precursors by a one-pot procedure [1]. Since they are performed without the need to isolate the any intermediate the process reduces the reaction time and saves both energy and raw materials [2]. Therefore, the design of novel MCR$_S$ has attracted great attention from research groups working in medicinal chemistry, drug discovery, and materials science [3].

Amidoalkyl naphthols are an important groups because, they have been found to possess useful biological activities. Thus, the synthesis of amidoalkyl naphthols is an important and useful task in organic chemistry.

Herein we report the application of *N,N,N',N'*-Tetrabromobenzene-1,3-disulfonamide [4], for the one-pot synthesis of 1-amidoalkyl-2-naphthol derivatives from various aromatic aldehydes, β-naphthol and urea under solvent-free conditions at room temperature with high yields.



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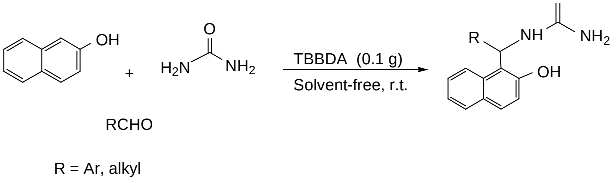

References:

[1] Rubin, Y.; Lin, S.; Knobler, C. B.; Antthjony, J.; Boldi, A. M.; Diederich, F. *J. Am. Chem. Soc*. **1991**, *113*, 6943.
[2] Chetia, A.; Saikia, C. J.; Lekhok, K. C.; Boruah, R. C. *Tetrahedron Lett*. **2004**, *45*, 2649.
[3] Shaterian, H. R.; Yarahmadi, H.; Ghashang, M. *Tetrahedron*. **2008**, *64*, 1263.
[4] Ghorbani-Vaghei, R.; Jalili, H. *Synthesis*. **2005**, 1099.

The synthesis of tetraaza-phenanthrene via base-catalysed rearrangement of 4,6-bis-(isoxazolinyl) pyrimidine

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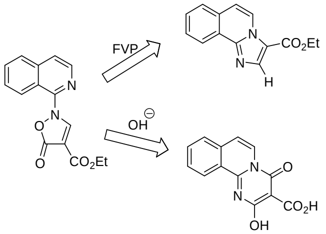
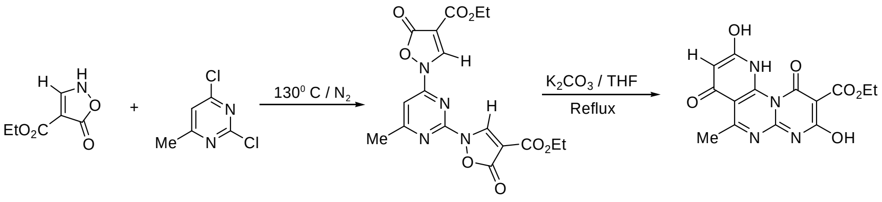
We have previously shown [1,2] that 2-isoxazolinyl azaheterocycles undergo rearrangement in the presence of bases, resulting in the annulation of a pyrimidine ring onto the azaheterocycle (Scheme1). By contrast, the use of triethylamine, photolysis or pyrolysis led to annelation of an imidazole ring onto the azaheterocycle (Scheme 1).



Scheme 1.

In this work, reaction of 2,4-Dichloro-6-methylpyrimidine **1** with two equivalents of the isoxazolones **2** gave the corresponding pyrimidine bis-adducts **3** and the reaction of bis adduct **3** with potassium carbonate in THF under reflux, gave the bis-annelated tetraazaphenanthrene **4** (Scheme 2).



2 **1** **3** **4**

Scheme 2.

References:

[1] Molla Ebrahimlo, A. R.; Khalafy, J. *Arkivoc* **2008**, (*xiii)*, 65.

[2] Molla Ebrahimlo, A. R.; Khalafy, J.; Prager, R. H. *Aust. J. Chem.* **2009**, *62*, 126.

[3] Khalafy, J.; Molla Ebrahimlo, A. R.; Eisavi, R.; Akbari Dilmaghani, K. *Arkivoc* **2005**, *xiv*,59.

[4] Khalafy, J.; Molla Ebrahimlo, A. R.; Akbari Dilmaghani, K. *J. Chin. Chem. Soc.* **2004**, *51*, 1347.

Preparation of *N*-[α-(β-Hydroxy-α-naphthyl)(benzyl)] *O*-Alkyl Carbamate Derivatives

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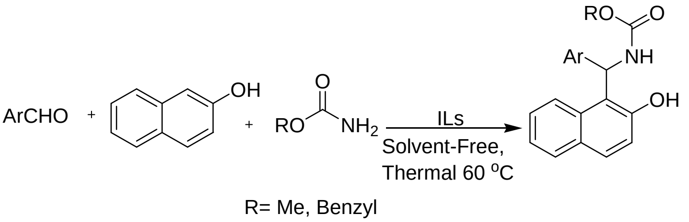
Room temperature ionic liquids have shown great promise as an attractive alternative to conventional organic solvents. They are non-volatile, recyclable, non-explosive, easily operable, and thermally robust [1].

Compounds bearing 1,3-amino-oxygenated functional groups are ubiquitous to a variety of biologically important natural products and potent drugs including a number of nucleoside antibiotics and HIV protease inhibitors, such as ritonavir and lipinavir [2].

In this research triphenyl(propyl-3-sulphonyl)phosphonium toluenesulfonate and (4-sulfobutyl)tris(4-sulfophenyl)phosphonium hydrogen sulfate as reusable catalytic amount of ionic liquids have been used for the preparation of a series of *N*-[α-(β-hydroxy-α-naphthyl)(benzyl)] *O*-alkyl carbamate under mild reaction conditions (Scheme 1).



ILs: (a) triphenyl(propyl-3-sulphonyl)phosphonium toluenesulfonate.; (b) (4-sulfobutyl)tris(4-sulfophenyl)phosphonium hydrogen sulfate

Scheme 1

References

[1] Welton, T. *Chem. Rev.* **1999**, *99*, 2071.
[2] Dingermann, T.; Steinhilber, D.; Folkers. G. In *Molecular Biology in Medicinal Chemistry*, Wiley-VCH, Weinheim, **2003.**

A novel polymeric catalyst for one-pot synthesis of 14- aryl-14H-dibenzo[a,j]xanthenes and 12-aryl -8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one

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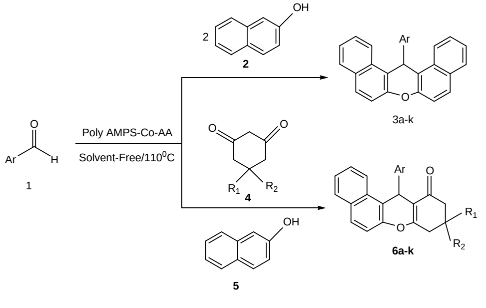
Polymer supported reagents have been in use since the 1946, and have been the subject of many review articles. Synthesis using these reagents is attractive and suitable for parallel synthesis because the reactions often proceed with high yields, and the workup involves simple filtration and evaporation of the solvent [1-2].

Xanthenes and benzoxanthene derivatives have received considerable interest from the pharmaceutical industry due to their wide range of interesting biological and therapeutic properties, such as antiviral, antibacterial, anti-inflammatory activities, as well as their use in photodynamic therapy [3-4]. The condensation of 2-naphthol with aromatic aldehydes in the presence of Crosslinked poly(AMPS-co-AA) under solvent-free media to afford the corresponding aryl-*14H*-dibenzo [*a.j*]xanthenes in excellent yields and short reaction times is described. The reaction work-up is very simple and the catalyst can be easily separated from the reaction mixture and reused several times in subsequent reactions. Also, this catalyst was used for synthesis of 12-aryl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one derivatives via a one-pot three-component reaction of aldehydes, 2-naphthol, and cyclic 1,3-dicarbonyl compounds [5].



References:

[1] Ley, S. V.; Baxendale, I. B.; Bream, R. N.; Jackson, P. S.; Leach, A. G.; Longbottom, D. A.; Nesi, M.; Scott, J. S.; Storer, R. I.; Taylor, S. J. *J. Chem. Soc. Perkin Trans. 1* **2000**, *23,* 3815.

[2] Kirschning, A.; Monenschein, H.; Wittenberg, R. *Angew. Chem. Int. Ed.* **2001**, *40,* 650.
Naya, A.; Ishikawa, M.; Matsuda, K.; Ohwaki, K.; Saeki, T.; Noguchi, K.; Ohtake, N. *Bioorg. Med. Chem.* **2003**, *11*, 875.

[3] Poupelin, J. P.; Saint-Ruf, G.; Foussard-Blanpin, O.; Narcisse, G.; Uchida-Ernouf, G.; Lacroix, R. *Eur. J. Med. Chem.* **1978**, *13,* 67.

[4] Ion, R. M. *Prog. Catal.* **1997**, *2,* 55.

[5] Zhang, Z. H.; Wang, H. J.; Ren, X. O.; Zhang, Y. Y. *Monatsh Chem.* **2009**, *140,* 1481.

Formation of highly functionalized thiophenes by reaction of tetramethylthiourea, acetylenic esters, and α-haloketones

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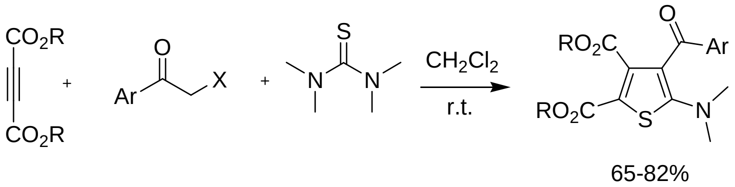
Thiophenes are an important class of heterocyclic compounds. A variety of molecules containing the thiophene ring system display biological activity and find application as pharmaceuticals [1], fragrance compounds [2], or pharmacophoric entities [3]. Substituted thiophenes can be prepared by proper functionalization of the thiophene ring. Recently, we described a synthesis of tetrasubstituted thiophens by reaction of tetramethylthiourea with acetylenic esters in the presence of ethyl bromopyruvate [4] at room temperature. This catalyst-free, one-pot synthetic method seems facile; the work-up procedure is easy and gives pure target compounds containing several potential centers for further modification.



References:

[1] Gronowitz, S. Ed. The Chemistry of Heterocyclic Compounds: Thiophene and Its Derivatives; *Wiley: New York*. **1991**, *44*.
[2] Bertram, H.J.; Emberger, R.; Güntert, M.; Sommer, H.; Werkhoff, P. *in Recent Developments in Flavor and Fragrance Chemistry*. (Weinheim), **1993**.
[3] Sperry, J.B.; Wright, D.L. *Curr Opin Drug Discovery Dev.* **2005**, *8*, 723.
[4] Yavari, I.; Hosseini, Z.; Seyfi, S.; Shirgahi-Talari , F. *Monatsh Chem.* **2008**, *139*, 1257.

Synthesis & characterization of segmented shape memory polyurethanes: Effect of soft segment length, hard segment & ionic group content on different properties

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Shape memory polymers (SMPs) are a class of smart materials, with the abilities to keep the deformed shape at the service temperature and revert back to the original shape by application of external stimuli, such as light, humidity, and heat or electrical and magnetic field [1]. The change in shape caused by heating is called thermally induced shape memory effect (SME). Among various SMPs, shape memory polyurethanes (SMPUs) are receiving much attention because of their excellent properties, such as wide shape recovery temperature range, high shape recovery rate, easy processing conditions, and possible biocompatibility [2].

In this study, we have synthesized different SMPUs including various soft segment lengths (SSL) & hard segment contents (HSC) based on 4,4’-diphenylmethane diisocyanate (MDI), 1,4-butanediol & Poly(ε-caprolactone) diol (Mw= 2000,3000,4000). In the next step, ionic groups were introduced into the material through application of dimethylol propionic acid (DMPA) as the second chain extender and ionic moiety, & triethylamine (TEA) as the neutralizing agent. The ionomer species augment the overall modulus of the polymer film via Columbic forces resulting from the increased cohesion among hard segments and micro-phase separation [3]. Characterization methods such as differential scanning calorimetry (DSC), infrared spectroscopy (IR), dynamic mechanical thermal analysis (DMTA) were carried out. Afterwards, cyclic tensile tests were done in order to investigate the shape memory properties of SMPUs.

It was found that the more the phase separation is in a system, the better the shape memory properties will be; On the other hand, it was found that a minimum hard segment content (HSC) was essential for the polyurethanes to show proper shape recovery. Also, fatigue of the SME is reduced with the incorporation of ionic moieties into hard segments. It was then evident that ionic moieties on hard segments can influence the SME significantly. Adjusting the interconnectivity among hard segments can be potentially used to control in particular the shape memory recovery ratio or alter the modulus of the rubbery state in SMPU.

References:

[1] I. Sedat Gunes, Feina Cao, Sadhan C. Jana*.; J.polymer*. **2008**, 49, 2223.
[2] Yong-Chan Chung.; Tae Keun Cho.; Byoung Chul Chun.; *J.Applied Polymer Science*. **2009**, 112.
[3] Yong Zhu.; Jinlian Hu.; Kwok-wing Yeung.; Ka-fai Choi.; Yeqiu Liu.; Haiming Liem.; *J.Applied Polymer Science*. **2007**, 103, 545.

Chemical modification of 4-chloromethyl styrene polymers with 9-anthracene carboxylic acid

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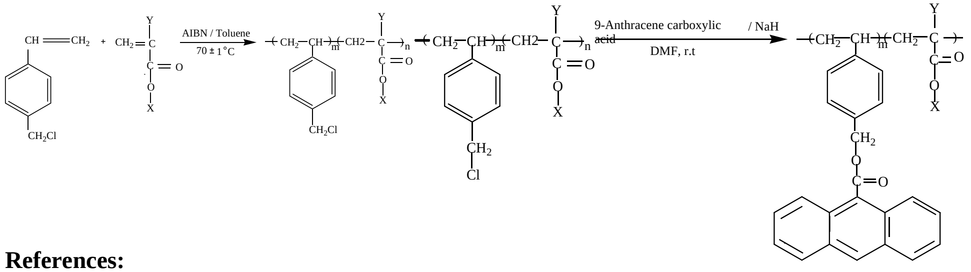
Vinyl benzyl chloride (VBC) or chloromethyl styrene (CMS) is probably one of the most important functional monomers. Poly VBC or related copolymers are able to react with various nucleophilic reagents, giving fairly good yields [1].

The chloromethylated polymers wich can also provide new products by means of nuclephilic reactions, is widely used in the many field such as ion exchange resins for the polymers support of catalysts [2]. In this work CMS or VBC was copolymerized with different monomers such as : Ethyl methacrylate (EMA) and Ethylacrylate (EA) by free radical polymerization method az 70+1ºC using (α-ά azobisisobutyronitrile) (AIBN) as an initiator and the copolymers collected. The copolymer composistion were obtained using related ^{1}HNMR spectra and the poly dispersity indices of the copolymers determined using gel permeation chromatography (GPC) [3].

The incorporation of 9-ACA groups took place frome the reaction between salt of 9-anthracene carboxylic acid compounds with chloromethyl groups, in the copolymers to yield the novel modified copolymers having esters substituents bound to aromatic rings via a methylene groups. The result polymers were characterized by FT-IR and ^{1}HNMR spectroscopic techniques. The glass transition tempretur (Tg) of all the copolymers was determined by dynamic termal analysis (DMTA) apparatus [4]. Study of (DMTA) curres for all copolymers indicated that glass transition temperature value of the groups [5]. Increases with incorporation of 9-ACA groups. The new polymer systems containing highly sterically hindered 9-ACA ligands can be used as separation membranes [6].



References:

[1] Montehard, J.; Jegat, C.; Camps, M. ; Macromol. *Chem. Phys*. **1999**, 135,174.
[2] Safa, K.; Nasirtabrizi, M.H.; Eram, A. *Iranian polymer Journal*. **2006**, 15(3), 249,257.
[3] Safa, K.; Nasirtabrizi, M.H.; Bahadori, A.; *Iranian polymer Journal*. **2008**, 17(1), 39, 41.
[4] Safa, K.;Nasirtabrizi,M.H.; *Polymer Bulltine*. **2006**, 57, 293-304.
[5] Safa, K.; Babazadeh, M.; *European polymer Journal*. **2004**, 40, 1659, 1669.
[6] Babazadeh, M.;Safa, K.; *E-polymer*. **2003**, 1618, 7229.

Synthesis *para* dimethyl vinyl siloxy benzoic acid monomer, and polymers

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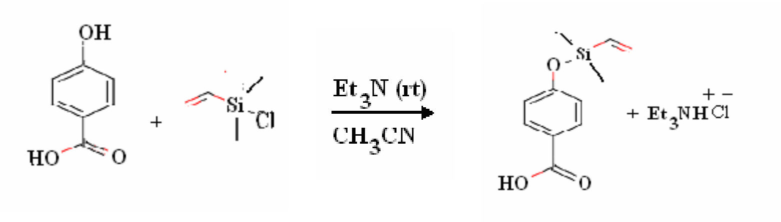
The main aim of this project is to prepare *P*ara dimethyl vinyl siloxy benzoic acid (PDMVSBA) monomer with the silicon agent dimethyl vinyl chloro silane and to synthesis sililized hydrogels with the aid of that monomer and to load different drugs upon these hydrogels and finally to verify their hydrolysis. By designer the hydrogelic systems, one can achieve a successful release of colonic drugs. with interning silicon groups in the hydrogelic constructs, new micromolocules are created which can be used as a separating memberance for both the liquids and the gasses. On the other hand, these hydrogels have a good compatibility with human body. And can be used as a matrixs in releasing drugs The organic silicon groups can be used the reformation of the mechanical and thermal properties of the polymer [1-2].

The reaction of the synthesis of 4-Hydroxybenzoic acid with Chlorodimethylvinylsilane in the presence of Et_3N and CH_3CN at rt produce *p*ara dimethylvinyl siloxy benzoic acid monomer [Schem1]. Then this monomer as a silylether polymerized with different monomers to prouduce network polymers and synthesized monomer were characterized by IR, H-NMR spectra



We showed that this monomer can be used as an ideal monomer in designing hydrogels instead of methacrylic acid monomer.

References:

[1] H.A.ALLCOCK,A.M.A.Ambrosio, *Biomaterias*. **1996**, 42, 195-202.

[2] A.Katchalsky, S.Lifson, H.Eisenberg, *J. polymer Technology*, **1990**, 6,7-75.

Ab initio investigations of structural and energetic properties of some synthesized heterocyclic compounds

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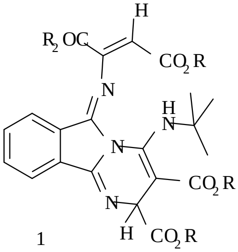
Recently, multi-component reactions have been receiving more and more attention because of their efficiency and diversity of products. Their utilities were fully realized in the process of drug discovery[7] and the total synthesis of complex natural products. Although a great number of such useful reactions have been reported, the development of a novel multi-component reaction is still important in the fields of medicinal and organic syntheses [1].

Molecular mechanics is a very fast method of determining the geometry, molecular energies, vibrational spectra, and enthalpies of formation of stable ground-state molecules. Because of its speed, it is widely used on large molecules such as those of biological or pharmaceutical importance that are currently beyond the reach of more computer-intensive molecular orbital methods [2].

We recently synthesized the heterocyclic compounds (**1, 2, 3, 4**) via multi-component reaction of 1,3-diimino isoindoline with acetylenic compounds in the presence of PPh3 or alkyl isocyanides. Herein, we report geometry optimizations of the synthesized compounds by ab initio HF and B3LYP [3] methods using 6–31G* basis set of the GAUSSIAN 98 system of programs [4].



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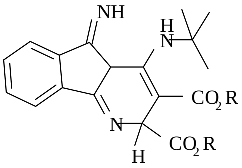

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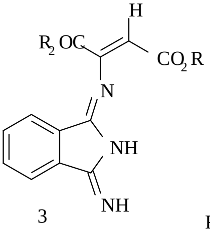

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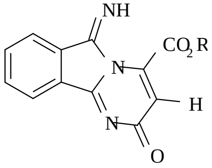

R= Me, Et, t-Bu 4

Refrences:

[1] Murai, K.; Nakatani, R.; Kita, Y.; Fujioka, H. *Tetrahedron* **2008.** *64,* 11034.
[2] Rogers, D. W. *Computational Chemistry Using the PC,* John Wiley & Sons, New Jersey, **2003**.
[3] Lee, C.; Yang, W.; Parr, R.G. *PhysicsReviewB* **1988,** *37,* 785.
[4] Becke, A.D. *Journal of Chemistry and Physics* **1993,** *98,* 5648.

Comparison of reducing power of different solvent extracts of Lotus (*Nelumbo nucifera*) seeds from north of Iran

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The addition of antioxidants in foods is required to preserve flavour and colour and to avoid vitamin destruction. Reports revealing that the most used synthetic antioxidants, such as butylated hydroxytoluene (BHT) and butylated hydroxyanisole (BHA), could be toxic and the higher manufacturing costs and the increasing regard to food additive safety, created a need for identifying alternative natural and safer sources of food antioxidants [1].

Lotus (*Nelumbo nucifera* Gaertn.), of the family Nymphaeaceae, is a perennial, rhizomatous and aquatic plant. Almost all parts of this plant are eaten as vegetable and also used in the indigenous system of medicine. Antioxidant activity of various parts of lotus is well established, e.g. leaf, stamens and rhizomes [2].

Reducing power is widely used in evaluating the antioxidant activity of polyphenols. The reducing property associated with the presence of reductones which exert antioxidant action by breaking the free radical chains via hydrogen atom donation. In this study, the reducing power of different solvent (water, methanol, aqueous methanol, acetone and ethyl acetate) extracts of lotus seeds was evaluated by ferric reducing antioxidant power (FRAP) assay according to the method of Oyaizu [3]. As standard reducing agents, ascorbic acid and gallic acid were used. The reducing power of all extracts was concentration dependent. The results from this study show that acetone is the best solvent for the extraction of antioxidant compounds from lotus seed.

Reference:

[1] Moure, A.; Cruz, J.M.; Franco, D.; Dominguez, J.M.; Sineiro, J.; Dominguez, H. ; Nunez, M.J. ; Parajo, J.C. *Food Chem. Rev.* **2001**, *72,* 145.
[2] Rai, S. ; Wahile, A. ; Mukherjee, K. ; Pada Saha, B. ; Mukherjee, P.K. *J. Ethnopharm.* **2006**, *104,* 322.
[3] Oyaizu, M. *Jpn. J. Nutr*. **1986** , *44,* 307.

A facile and expeditious three-component procedure for synthesis of spirooxindoles catalyzed by KF/Al_2O_3

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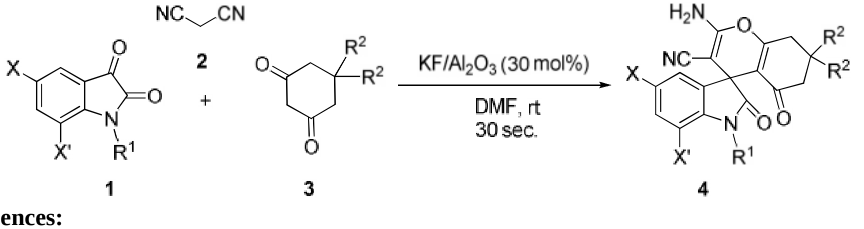
Isatin (1*H*-indole-2,3-dione) and its derivatives are synthetically versatile substrates that demonstrate a diverse array of pharmacological activities including cytotoxic and anticancer properties [1]. The heterocyclic spirooxindole ring is the core structure of many pharmaceutical and natural products [2]. Functionally substituted 4*H*-chromenes take a meaningful place among the oxygen containing heterocycles fused with spirooxindole ring system, some of them possess spasmolitic-, diuretic-, anticoagulant-, anticancer-, and antianaphylactic activities [3].

Over the past years, potassium fluoride loaded on alumina, KF/Al_2O_3, which was originally introduced by Ando et al. for alkylation reactions, has been commonly used as an efficient and versatile basic catalyst in organic reactions, such as elimination, addition, condensation, and the synthesis of heterocyclic compounds via multicomponent reactions [4].

Herein, we report a simple and efficient three-component approach for the synthesis of spiro[(2-amino-3-cyano-5-oxo-5,6,7,8-tetrahydro-*4H*-chromene)-4,3'-oxindoles] in the presence of KF/Al_2O_3 at ambient temperature. Further merits of this method include a short reaction times and the straightforwardness of the procedure, which make it an applicable and attractive process for the synthesis of these biological important compounds.



References:

[1] Vine, K. L.; Matesic, L.; Locke, J. M.; Ranson, M.; Skropeta, D. *Anti-cancer Agents Med. Chem*. **2009**, *9*, 397.

[2] Khafagy, M. M.; El-Wahas, A. H. F. A.; Eid, F. A.; El-Agrody, A. M. *Farmaco* **2002**, *57*, 715.

[3] Bonsignore, L.; Loy, G.; Secci, D.; Calignano, A. *Eur. J. Med. Chem*. **1993**, *28*, 517.

[4] Blass, B. E. *Tetrahedron* **2002**, *58*, 9301.

A calorimetric investigation for the bindings of mushroom tyrosinase to phenyl dithiocarbamate and *p*-phenylene-bis dithiocarbamate

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Mushroom Tyrosinase (MT) is a copper containing monooxygenase that catalyzes the hydroxylation of monophenols and the oxidation of *o*-dephenols to *o*-quinones, which is ubiquitously distributed in organisms and plays a pivotal role in melanin production [1]. Certain dithiocarbamate derivatives have been found to possess a wide range of biological activities, i.e., anti-bacterial, tuberculostatic, anti-diuretic, anti-hypertensive, etc. To see whether phenyl and *p*-phenylene-bis dithiocarbamates induced structural change of mushroom tyrosinase (at 27 and 37°C, in 10 mM phosphate buffer, pH=6.8) and how thermodynamical changes by ligand binding were occurred, the isothermal titration calorimetry (ITC) measurements were conducted. These studies suggest that there are two non cooperative binding sites for both ligands as inhibitors. We introduced a new equation for extended solvation theory to obtain useful information regarding the effect of ligands on thermal stability of mushroom tyrosinase [2-3].

$$q = q_{max} x'_B - \quad A \quad A \; A \quad B \; B \quad B \quad A \quad A \; A \quad B \; B \quad B' \; B \; \frac{[\text{Ligand}]_T}{[\text{Ligand}]_{max}}$$

L_A and L_B are the proportional contributions of the unbound and bound ligands to the enthalpies of dilution in with the exception of enzyme and can be calculated from the attained enthalpies of ligands in buffer [2-3]. The derived positive values of δ^θ_A and δ^θ_B for phenyl dithiocarbamate interaction, exhibit thermal stabilization of enzyme by inhibitor [3]. These results of $\delta^\theta_A > \delta^\theta_B$ at 27°C and $\delta^\theta_B > \delta^\theta_A$ at 37°C support that high phenyl dithiocarbamate concentration at 27°C and low phenyl dithiocarbamate concentration at 37°C cause more stabilization of MT. We can attribute the obtained negative values of δ^θ_A and δ^θ_B to destabilization of enzyme by *p*-phenylene-bis dithiocarbamate. Raising the concentration of ligand caused an increase in the amount of destabilization, at 27 and 37°C. The obtained enthalpies for these interactions from this method show a proper coincidence of reported heats of ITC and confirm the hypothesis of being endothermic of the first and being exothermic of the second bioreaction. We produced K_d and the induced positive thermodynamic parameters changes such as enthalpy and entropy, and the negative parameter change of the Gibbs free energy for phenyl dithiocarbamate interaction. We calculated the intrinsic equilibrium constant, the negative changes of molar enthalpy, the Gibbs free energy and the molar entropy for *p*-phenylene-bis dithiocarbamate interaction [2].

References:

[1] Yan Han, H.; Chang Zou, H.; Yeong Jeon, J.; Jing Wang, Y.; An Xu, W.; Mo Yang, J.; Doo Park, Y. *Biochimica et Biophysica Acta*. **2007**, *1774*, 822.

[2] Rezaei Behbehani, G.; Saboury, A. A; Divsalar, A. *Acta Biochim Biophys Sin.* **2008**, *40*, 964.

[3] Saeidfar, M.; Masouri-Torshizi, H.; Rezaei Behbehani, G.; Divsalar, A.; Saboury, A. A. *Bull. Korean Chem. Soc.* **2009**, *30*, 1951.

A Lewis acid-surfactant catalyst for stereoselective synthesis of β-amino ketones in water

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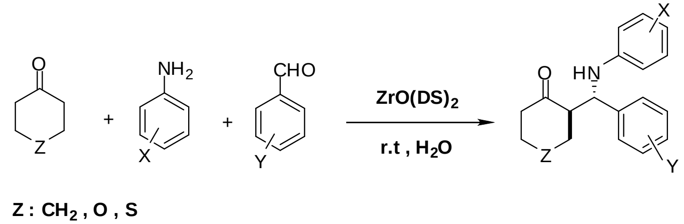
Mannich reaction [1] is a one of the most basic and important reactions to provide β-amino carbonyl derivatives, the moieties found in many natural products and used as versatile intermediates in organic synthesis [2].

Due to the effective catalysis of zirconium oxide chloride octahydrate in three-component mannich reaction of cyclic ketones with aromatic aldehyde and aromatic amines [3] and to get rid of organic solvents as the reaction medium, we use a combination of Lewis acid and asurfactant for catalysis of Mannich reaction in neat water without using any organic solvents. The combination is composed of ZrO^{2+} as a water-stable Lewis acidic cation and dodecyl sulfate as an anionic surfactant, easily prepared from $ZrOCl_2.8H_2O$ and SDS.

In this work, our trend to accomplish Mannich reaction in water with the aid of catalytic effect of a Lewis-acid led to high reactivity of the substrates with excellent anti selectivity for the products. In the workup procedure, the reaction medium was recycled and reused without any remarkable loss of efficiency. As a result of this work, a simple and useful method for Mannich reaction is developed. Also the commercial availability of the reagents is an advantage.



References:

[1] Li, H.; Zeng, H. Y.; Shao, H. W. *Tetrahedron Lett.* **2009**, *50*, 6858; Izumiseki, A.; Yoshida, K.; Yanagisawa, A. *Org. Lett.* **2009**, *11*, 5310.
[2] Dondoni, A.; Massi, A.; Sabbatini, S.; Bertolasi, V. *Tetrahedron Lett.* **2004**, *45*, 2381; Cardillo, G.; Tomasini, C. *Chem. Soc. Rev.* **1996**, 117.
[3] Eftekhari-Sis, B.; Abdollahifar, A.; Hashemi, M,; Zirak, M. *Eur. J. Org. Chem*. **2006**, 5152.

A convenient synthesis of 2-arylamino-2-imidazolines from aminoiminosulfonic acids.

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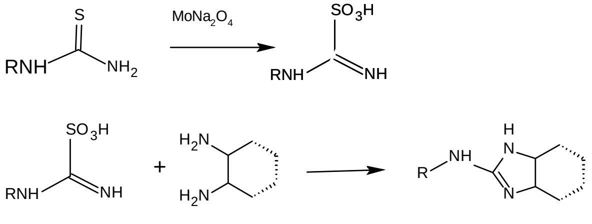
2-Arylamino-2-imidazolines have an interesting chemistry [1] and they are effective pharmacophores in medicinal chemistry. 2-Arylamino-2-imidazolines, in particular 2,6-dichlorophenylamino-2-imidazoline (clonidine) [2] have a pronounced, hypotensive action, which is coupled with sedative action.

The most widely employed commercial method for preparing 2-arylamino-2-imidazolines is the reaction of amines with S-alkylisothiouronium salts [3]. Further, most commercial processes utilize S-methylisothiouronium salts. The byproduct of this reaction is the noxious gas, methyl mercaptan; this foul smelling gas has a threshold of detection by humans of about 1 ppb. Other commercial alternative for the production of imidazolines are the reaction of amines with cyanamides, carbodiimdes, chloroformamidines, or dichloroisocyanides. Generally, these starting materials are corrosive, toxic, and / or moisture-sensitive.

Herein we report an efficient and green method for preparation of 2-arylamino-2-imidazolines and 2-aminoimidazolines by reaction of aminoiminosulfonic acids with ethylenediamines chemo selective in water or 2-propanol in excellent yields. Aminoiminosulfonic acids were prepared from oxidation reaction of thioures. Thioureas have been obtained from reaction of corresponding amines with benzoyl chloride and ammonium thiocyanate.



References:

[1] Saczewski, J.; Gdaniec, M. *J. Org. Chem.* **2003**, *68*, 4791.
[2] Bolme, E; Fuxe, F. *Eur. J. Pharmacol.* **1971**, *13*, 168.
[3] Braum, C. E. *J. Am. Chem. Soc.* **1933**, 55, 128.

Catalytic reduction of nitro benzimidazole to aminobenzimidazole compound by zinc-nickel alloy as catalyst

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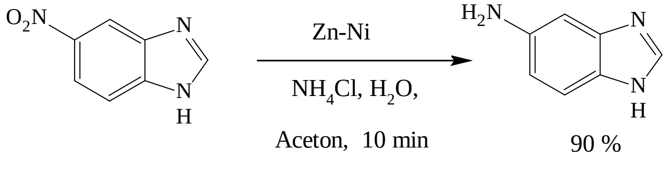
Benzimidazole compounds have important pharmaticial and biological applications. Aminobenzimidazole and hydroxyl aminobenzimidazole also can use in new drugs and industrials according to the recent studies. During the reduction of aromatic and heteroaromatic compounds, amines and hydroxylamine generate while nitro group react with reduction agent such as Zinc, Nickel, Palladium and etc throughout the charge transfer. In this process some detectable intermediates and some predictable are produced. In previous studies on reduction of Benzimidazole, Zinc powder and saturated solution of ammonium chloride were used. In the present study binary Zinc-Nickel alloy obtained from electrodeposition process in alkaline bath was used as a reduction agent. Various alloys containing different composition between 5 to 95 % of Zinc were used. Zinc-Nickel alloys include α, ß$_1$, ß$_2$, γ and δ structure witch γ structure is the major structure in this study. Reduction efficiency shows significant increase and reaction time is much lower compare to the pure zinc. Reduction efficiency is 90 % using Zn-Ni as catalyst while that is les than 75 % in the case of pure zinc. Fast kinetic and low reaction time (10 minutes) shows that Zn-Ni alloy could be a good alternative for common reduction agent such as Raney nickel and zinc powder.



References:
[1] Xuping Su, Nai-Yong Tang, and Jim M. Toguri, *Journal Of Phase Equilibria*, **2001**, Vol. 23 No.2
[2] George Penev Vassilev, Tomas Gomez-Acebo, and Jean-Claude Tedenac, *Journal Of Phase quilibria*, **2000**, Vol. 21 No.3
[3] Ung S., Falguieres A., Guy A., and Ferroud C., *Tetrahedron Lett*. **2005**, 46, 5913.
[4] Ambacheu K. D, Pleshakov V. G., Baatkh B. S., Zvolinskii V. P., Kharlamova M. D., Obynochnyi A. A., and Prostakov N. S., *Chemistry of Heterocyclic Compounds,* **2000**. Vol. 36, No. 4, 493.

A novel and one-pot synthesis of tetrahydronaphthodiazepine derivatives

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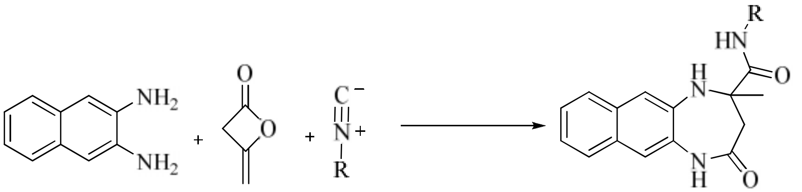
Heterocyclic compounds are highly ranked among pharmaceutically important natural and synthetic materials. The remarkable ability of heterocyclic nuclei to serve both as biomimetics and active pharmacophores has largely contributed to their unique value as traditional key elements of numerous drugs. Many members of the diazepine family are nowadays widely used as antianxiety, antidepressant, sedative, hypnotic, tranquilizing, anticonvulsant, antihistaminic, analgesic and anti-inflammatory agents [1,2].

In view of our current studies on isocyanide-based multicomponent reactions (IMCRs) of diamines [3] and diketene [4], herein, we wish to report an unknown IMCR which afford 4-oxo-2,3,4,5-tetrahydro-1*H*-naphtho[2,3-*b*][1,4]diazepine-2-carboxamide derivatives *via* a condensation reaction between naphthalene-2,3-diamine, diketene and an isocyanide.



References:

[1] Archer, G. A.; Sternbach, L. H. *Chem. Rev.* **1968**, *68*, 747.

[2] Hadac, E. M.; Dawson, E. S.; Darrow, J. W.; Sugg, E. E.; Lybrand, T. P.; Miller, L. J. *J. Med. Chem.* **2006**, *49*, 850.

[3] (a) Shaabani, A.; Maleki, A.; Moghimi-Rad, J. *J. Org. Chem.* **2007**, *72*, 6309. (b) Shaabani, A.; Maleki, A.; Mofakham, H.; Khavasi, H. R. *J. Comb. Chem.* **2008**, *10*, 323. (c) Shaabani, A.; Maleki, A.; Mofakham, H.; Moghimi-Rad, J. *J. Org. Chem.* **2008**, *73*, 3925. (d) Shaabani, A.; Maleki, A.; Mofakham, H. *J. Comb. Chem.***2008**, *10*, 595. (e) Shaabani, A.; Maleki, A.; hajishaabanha, F.; Mofakham, H.; Seyyedhamzeh, M.; Mahyari, M.; Ng, S.W. *J. Comb. Chem.* **2010**, *12*, 186.

[4] (a) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Rezazadeh, F.; Behnam, M. *J. Comb. Chem* **2009**, *11*, 375. (b) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Behnam, M.; Rezazadeh, F. *Tetrahedron Lett.* **2009**, *50*, 2911. (c) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Behnam, M. *Tetrahedron Lett.* **2009**, *50*, 6355. (d) Shaabani, A.; Seyyedhamzeh, M.; Maleki, A.; Hajishaabanha, F. *Tetrahedron* **2010**, *66*, 4040.

Synthesis of *β*-bromostyrenes from cinnamic acid derivatives using tribromides

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Vinyl bromide is a useful synthon in organic synthesis, especially in palladium and copper catalyzed coupling reactions [1]. It has been used to synthesize stilbenoids, pyridines, and N-alkenyloxazolidin-2-one. Moreover, vinyl bromide is a key agent for introducing styrene moieties in natural product synthesis [2].

The decarboxylation of organic carboxylic acids accompanied by a simultaneous replacement by a halogen under radical conditions is an extremely useful and selective reaction in organic chemistry for the synthesis of halogenated organic substances. The original method for oxidative halodecarboxylation, known as the Hunsdiecker reaction, is the reaction of a silver salt of a carboxylic acid with mainly bromine as the halogene [3].

β-bromostyrenes can be prepared from the corresponding cinnamic acid derivatives. There are some synthetic procedures for oxidative bromo-decarboxylation of cinnamic acids by which a bromine atom replaces the carboxylic substituent using NBS/iodosyl benzene [4], NBS/lithiumin acetate [5], NBS/tetrabutylammonium trifluoroacetate [6], and bis(collidine) halogen(I)hexafluorophosphate [7].

Herein we report an efficient method for synthesis of β-bromostyrenes from the corresponding cinnamic acids using imidazolium tribromides derivative. Treatment of cinnamic acid and its derivatives with tribromide in the presence of K_2CO_3 afforded the corresponding β-bromostyrenes in very good yields (70-90%). All the products were characterized by ^{1}HNMR spectra, melting point and comparison with authentic samples**.**

References:

[1] Meijere, A.; Diederich, F. *Metal-Catalyzed Cross-Coupling Reactions*. **2004**, Second Edition.
[2] Lu, J.; Tan, X.; Chen, C. *J. Am. Chem. Soc*. **2007**, *129*, 7768.
[3] Wilson, C. V. *Org. React*. **1957**, *9*, 332.
[4] Graven, A.; Jorgensen, K. A.; Dahl, S.; Stanczak, A. *J. Org. Chem*. **1994**, *59*, 3543.
[5] Chowdhury, S.; Roy, S. *J. Org. Chem*. **1997**, *62*, 199.
[6] Naskar, D.; Roy, S. *Tetrahedron Lett*. **2000**, *56*, 1369.
[7] Homsi, F.; Rousseau, G. *Tetrahedron Lett*. **1999**, *64*, 81.

Synthesis of α-amino phosphonates catalyzed with ZnO nanoparticles under solvent-free condition

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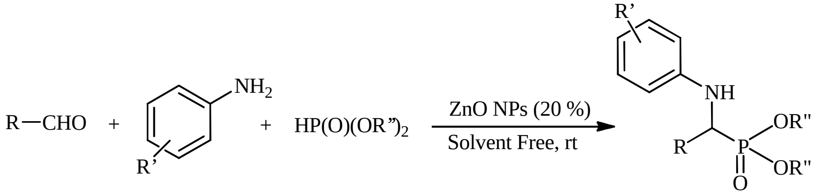
In the last few years, literature has highlighted the importance of nanosized materials in several scientific and technological areas, including the catalytic activity of metal oxide nanoparticles [1]. Zinc oxide nanoparticles (ZnO NPs) have been used in Dakin–West reaction [2], degradation of acid red B and rhodamine B [3], *etc*. On the other hand, α-amino phosphonates have attracted much interest as important biologically active compounds, and their synthesis has been a focus of considerable attention in the synthetic and medicinal chemistry [4,5]. They act as antibiotics, herbicides, inhibitors of the enzymes renin, EPSP synthase and HIV protease. In addition α-amino phosphonates have broad applications due to their antifungal and antibacterial activities. Various synthetic approaches have been reported for the synthesis of α-amino phosphonates, among which the most convenient are the Kabachnik–Fields synthesis and Pudovik reaction catalyzed by a base or an acid.

In this report, we disclose on construction of the ZnO NPs with a solid state reaction method and propose it as an efficient heterogeneous catalyst for the synthesis of α-amino phosphonates in the solvent free conditions, through three-component reaction of aldehydes, amines, and dialkyl phosphites.



References:

[1] Yamaguchi, A.; Uejo, F.; Yoda, T.; Uchida, T.; Tanamura, Y.; Teramae, N. *Nat. Mater*. **2004**, *3*. 337.

[2] Mirjafary, Z.; Saeidian, H.; Sadeghi, A.; Matloubi Moghaddam, F. *Catal. Commun.* **2008**, *9*, 299.

[3] Wang, J.; Jiang, Z.; Zhang, Z.; Xie, Y.; Wang, X.; Zhang, X. *Ultrason. Sonochem.* **2008**, *15*, 768.

[4] Birum, G. H. *J. Org. Chem.* **1974**, *39*, 209.

[5] Fields, S. C. *Tetrahedron* **1999**, *55*, 12237.

Synthesis of a novel conductive chiral-nano polymer; nano-poly [2-(*sec*-butyl) aniline]

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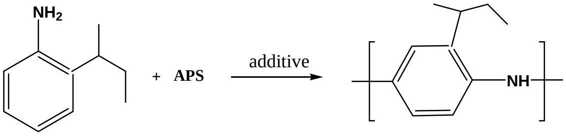
Conducting polymers have attracted great attention due to their potential application in variety of application such as light emitting diodes, chemical sensors, anti-corrosion coating, batteries and capacitors [1]. Polyaniline is unique among the family of conducting polymers because of its ease of syntheses, environmental stability and simple reversible acid-base doping-dedoping chemistry [2,3]. Microstructured and nanostructured conducting polymers have recently extensively studied due to their unique properties and promising applications in material science and nanodevices [4]. Substituted polyaniline have been investigated as a means of overcoming the limitation of polyaniline caused, primarily, by the difficulty in processing the polymer, which is largely insoluble in commonly used solvents [3]. Importance of chiral polymers is due to their applications in various areas [5]. In this research we use a chiral substituted polyaniline to impart these advantages.

Kaner and coworkers have shown that accelerating the rate of polymerization have a great impact on morphology of substituted polyanilines [6].

In the present research, we applied a chiral monomer, and chemical structures, conductivity and morphology of the obtained polymer were investigated. The polymerization of chiral substituted aniline (2-*sec*-butylaniline) was done successfully by rapid mixing method. The effect of additives on morphology and the concentration effect are investigated. The obtained polymers were characterized by FT-IR and UV-Vis techniques. The morphology of the resulting polymers was examined by scanning electron microscopy (SEM). Their conductivity is measured using four probe technique.



References:

[1] MacDiarmid, A.G. *Angew. Chem. Int. Ed.* **2001**, *40*, 2581.

[2] Huang, W.S.; Humphrey, B.D.; MacDiarmid, A.G. *J. Chem. Soc. Faraday Trans.* **1986**, *82*, 2385.

[3] Wallace, G.G.; Kane-Maguire, L.A.P.; Teasdale, P.R. *Conductive Electroactive Polymers: Intelligent Materials Systems*, CRC Press, 3th ed., Taylor & Francis Group, **2009**.

[4] Martin, C.R. *Science* **1994**, *266*, 1961.

[5] Pu, L. *Acta Polym.* **1997**, *48*, 116.

[6] Trane, H.D.; Kaner R.B. *Chem. Commun.* **2006**, 3915.

Highly efficient synthesis of [1,2,3]-triazoles using nano Cu(I) and Cu(II) supported on melamine-formaldehyde resin (MFR)

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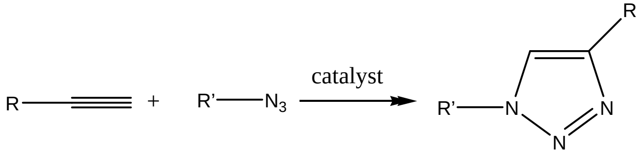
[1,2,3]-Triazoles are important five-membered nitrogen heterocycles involved in a wide range of industrial applications such as agrochemicals, corrosion inhibitors, dyes, optical brighteners as well as biologically active agents [1]. The well established approach has been utilized so far for the synthesis of the [1,2,3]-triazole ring system relies on the thermal 1,3-dipolar Huisgen cycloaddition between alkynes and azides [2]. However, this non-catalyzed process exhibits several disadvantages including: (1) the requirement for high temperature conditions with the potential for decomposition of labile products, (2) the synthesis of the desired [1,2,3]-triazoles generally in low yields, and (3) poor regioselectivity given that the non-catalyzed cycloaddition affords a mixture of 1,4- and 1,5-disubstituted triazoles unless the alkyne is substituted with an electron withdrawing group [3].

In this work, we developed a copper catalyst as a heterogeneous catalytic system for Huisgen cycloaddition that can have several advantages such as fast and simple isolation of the reaction products by filtration as well as recycleability and reuseability of the catalyst. We wish to test the fixation and activity of copper salts on melamine-formaldehyde resin. This well-known polymer can act as appropriate solid support for copper salts. Meanwhile, the impact of some important factors such as reaction time, base, and structurally diverse and kind of azides and alkynes on the efficiency of this method was studied.



R, R': Alkyl, Aryl
Catalyst: copper salts on melamine-formaldehyde resin

References:

[1] Dehne, H.; *Methoden de Organischen Chemie* (Houben-Weyl); Schumann, E.; Thieme:Stuttgart, **1994**, Vol. E 8d, PP 305-320.
[2] Sha.C. K.; Mohanakrishan A. K. *Synthetic Application of 1,3-Dipolar Cycloaddition Chemistry Toward Heterocycles and Natural Products*, Padwa, A.; Pearson,W. H. Eds.; Willey: New York, **2003**, PP 623-680.
[3] Orgueira, H. A.; Fokas, D.; Isome,Y.; Chan, P.; Baldino, C. M. *Tetrahedron lett.* **2005**, *46*, 2911.

Synthesis of bis(silyl)alkenes via imine precursors

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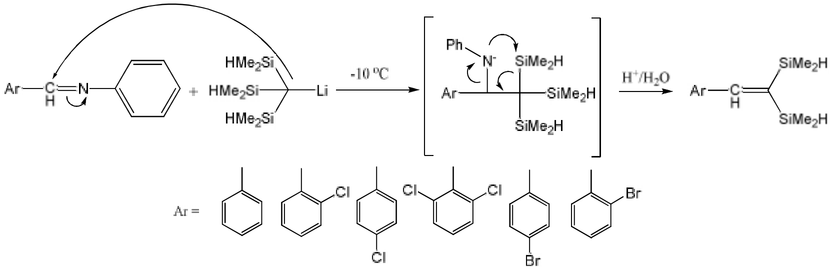
1,1-Dimetalated-1-alkenes constitute an important class of organometallic reagents which are currently widely used as potential intermediates in the organic and organometallic synthesis. Among the most, notable and commonly employed gemdiorganometallics, the 1,1-bis(silyl)-1-alkenes are of unique importance. Their use as precursors for the preparation of ketones as well as variety of important organosilicon intermediate such as acylsilanes, epoxysilanes, 1-halovinylsilanes, silylenolethers, (E)-alkeneylsilanes, silylenolacetates etc., stimulate interest in their synthetic availability [1-4]. The precursor $(HMe_2Si)_3CH$, which was made in 60 % yield from HMe_2SiCl, $CHBr_3$ and Mg in THF.$(HMe_2Si)_3CH$ was then metallated with lithiumdiisopropylamide (LDA) during 6 h and gave $(HMe_2Si)_3CLi$ [5]. $(HMe_2Si)_3CLi$ reacts with variety imine in THF, the Peterson-like reaction readily takes place and gives the corresponding 1,1-bis(silyl)-1-alkenes derivatives.



References:

[1] Eaborn, C. ; Hitchcock, P. B. ; Kowaleska, A. ; Smith J. D. *J. Organomet. Chem.* **1996**, 62, 113.
[2] Konodo, J.; Inoue, A.; Shinokubo, H.; Oshima, K. *Tetrahedron Lett.* **2002**, *43*, 2399.
[3] Marek, I. *Chem. Rev*. **2000,** *100*, 2887.
[4] Hodgson, D. M.; Comina, P. J. *J. Chem. Soc., Perkin Trnas*. 1 **1997**, 2279
[5] Eric, J.; Hawrelak, F.; Ladipo, T. *Organometallics* **1999**, *18*, 1804.

Synthesis of sodium thiopental

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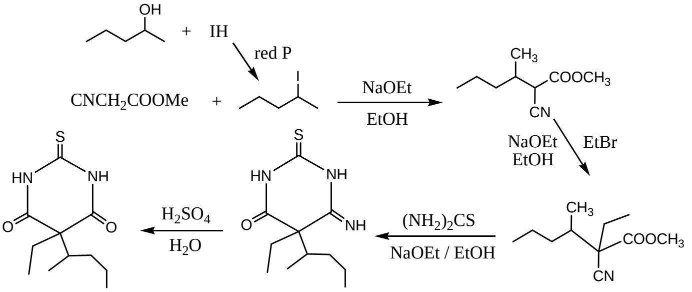
Barbiturates are a class of drugs that enhance the inhibitory action of the $GABA_A$ receptor in the brain and spinal cord and decrease neuronal activity. As an example, sodium thiopental, one of the common anesthetics, which is an ultra-short-acting barbiturate, has been used commonly in the induction phase of general anesthesia.
5-ethyl-5-(1-methylbutyl)-2-thiobarbituric acid sodium salt, known as sodium thiopental, has been synthesized in this work through a multi-step process starting from commercial materials and using known methods [1-4].

Methylcyanoacetate was reacted with 2-iodopentane (prepared from treatment of 2-pentanol with HI in presence of dried red phosphorus) in low temperature using sodium ethylate in ethanol as the basic catalyst resulting in synthesis of the first intermediate, methyl 2-cyano-3-methylhexanoate (1). Alkylation of (1) performed by refluxing with ethyl bromide in basic medium yielding methyl 2-cyano-2-ethyl-3-methylhexanoate (2).

The product (2) was then treated under reflux with thiourea in presence of sodium ethylate in ethanol to obtain the imino intermediate, ethyl (1-methylbutyl) iminothiobarbituric acid (3). The product (3) was then hydrolyzed with aqueous sulfuric acid resulting in production of thiopental (4), from which sodium thiopental was finally obtained by treating (4) with NaOH. ^{1}HNMR, ^{13}CNMR and UV spectra were utilized for characterization of the intermediates and the final product.



References:
[1] Volwiler, E.H.; Tabern D.L. US Pat. **1939**, No. 2153731.
[2] Abe, K.; et al, *J. Pharm. Soc. Japan,* **1955**, *75, 888.*
[3] Mcleish, M. J. *Anal. Profiles Drug Subst. Excipient,* ***1992****, 21, 535.*
[4] Balaban I.E. and Wilde B.E., Brit. Pat. No. 650354.

A new method for the preparation of vinylbis(silanes) via imines

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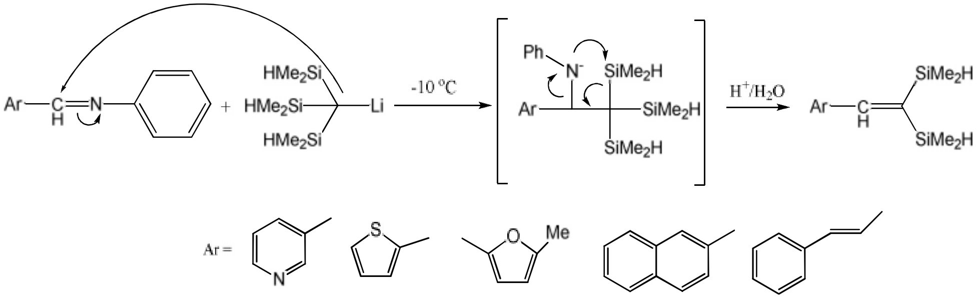
Vinylsilanes are useful organometallic reagent in organic synthesis because the C(sp^2)-Si bonds undergo numerous transformations [1]. Due to similar properties of vinylbis(silanes) to those of vinylsilanes, they have gained significant attention as potential synthons in the organic and organosilicon synthesis [2]. The potential use of the vinylbis(silanes) as precursors for the preparation of ketones and isoxazoline derivatives as well as a variety of important organosilicon reagents such as acylsilanes, epoxysilane, silanols, etc., has greatly stimulated their synthetic advancements. In contrast to vinylsilanes however, vinylbis(silanes) are a relatively unexplored class of materials [3]. $(HMe_2Si)_3CH$, has been conveniently prepared by the reaction of $CHBr_3$ and Mg with HMe_2SiCl in THF. The generation of $(HMe_2Si)_3CLi$ was easily accomplished by deprotonation of $(HMe_2Si)_3CH$ using LDA in THF [4]. The direct reaction of $(HMe_2Si)_3CLi$ with Variety imines containing heterocyclic groups led to corresponding vinylbis(silanes).



References:

[1] Mise, T.; Takaguchi, Y.; Wakatsuki, Y.; Takaguchi, Y. *Chem. Commun.* **1998**, *6*, 699.
[2] Safa, K. D.; Paymard Samani, S.; Tofangdarzadeh, Sh. *J. Organomet. Chem.* **2008**, *693*, 2004.
[3] Hodgson, D. M.; Comina, P. J.; Drew, M. G. B. *J. Chem. Soc., Perkin Trans. 1* **1997**, 2279.
[4] Hawrelak, E. J.; Ladipo, F. T.; Sata, D. *Organometallics* **1999**, *18*, 1804.

Synthesis and swelling studies of modified chitosan hydrogels containing alkyl sulfonate anionic pendant groups

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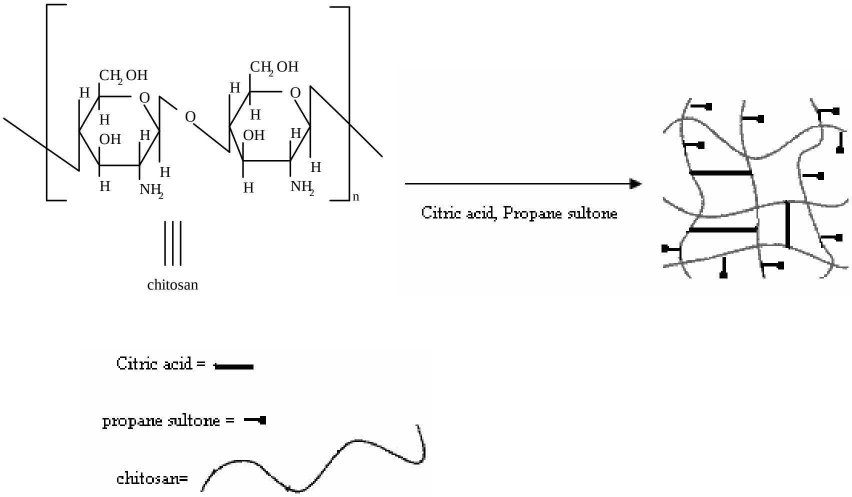
Chitosan (CS) is a natural polysaccharide,which has a linear β- (1-4)-linked glucosamine repeadly units. The primary amine groups render special properties that make CS very useful in pharmaceutical applications. Compared to many other natural polymers, chitosan has a positive charge and is mucoadhesive [1]. Therefore, it is used extensively in drug delivery applications [2–3]. But chitosan have low solubility in water, However, various chemical modifications of CS have been studied to alter its properties such as *N*-Trimethyl chitosan chloride (TMC) [4] and succinyl chitosan[5].

Herein we report the modification of CS with propane sultone and then crosslinking by citric acid in the presence of span 40 as a surfactant. The swelling studies were done at pH (3, 7.4, 9) and temperature (r.t, 37˚C, 60˚C) and the physical and mechanical properties were investigated by DSC, TGA, SEM.



References:
[1] Berscht, P. C.; Nies, B.; Liebendorfer, A.; Kreuter, J. *Biomaterials*. **1994**, *15*, 593– 600.
[2] Illum, L. *Pharm. Res*. **1998**, *15*, 1326– 1331.
[3] Dodane, V.; Vilivalam, V. D. *Pharm. Sci. Technol. Today*. **1998**, *1*, 246–253.
[4] Thanou, M.; Verhoef, J. C.; Marbach, P.; Junginger, H. E. *Pharm. Sci*. **2000**, *89*, 951– 957.
[5] Rekha, M. R.; Chandrap; Sharma. *Trends biomater. Artif. Organs.* **2008,** *21(2*), 107-115.

Synthesis and characterization of $MnFe_2O_4/Fe_3O_4$/Polyacrylic acid (PAA) nanocomposites with multi core-shell structure based on polythiophene

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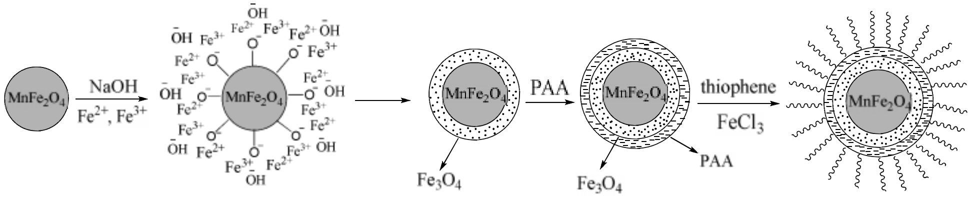
In recent years, magnetic nanoparticle and nanostructure studies have attracted considerable attentions. They combine a broad range of synthetic and investigative techniques from physics, chemistry and materials science [1,2]. The multi core-shell structure composites often exhibit improved physical and chemical properties over their single-component counterpart and hence are very useful in a broader rang of application [3]. When applied to the combination of three types of materials, the coating not only avoids the substitution in the core phase, but also interacts with the core phase to improve the magnetic properties of the composite.

In this work, first, $MnFe_2O_4/Fe_3O_4$/Polyacrylic acid (PAA) nanocomposites with multi core-shell structure were successfully synthesized with two-step co-precipitation method and one step masking shell method. Then we have tried to prepare composite based on polythiophene (PTh) with multi core-shell structure. A composite of polythiophene with $MnFe_2O_4/Fe_3O_4$/Polyacrylic acid (PAA) was prepared via chemical oxidative polymerization of thiophene monomer in presence of a dispersion of $MnFe_2O_4/Fe_3O_4$/PAA (powder) in $CHCl_3$ solvent using anhydrous $FeCl_3$ oxidant.

Then, morphological, crystalline, structural, electrical conductivity, magnetically and microwave absorption properties confirmed by transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), four-probe measurement, vibrating sample magnetometer (VSM) and vector network analyzer, respectively.



References:

[1] Sun, S. H.; Zeng, H. *J. Am. Chem. Soc.* **2002**, *124*, 8204.
[2] Fried, T.; Shemer, G.; Markovich, G. *Adv. Mater.* **2001**, *13*, 1158.
[3] Tamil Selvan, S.; Patra, P.K.; Ang, C.Y.; Ying, J.Y. Angew. Chem. Int. Ed. **2007**, *40,* 1.

One-pot three-component reaction of *tert*-butyl isocyanide and dialkyl acetylenedicarboxylates in presence of 2,4-thiazolidinedione

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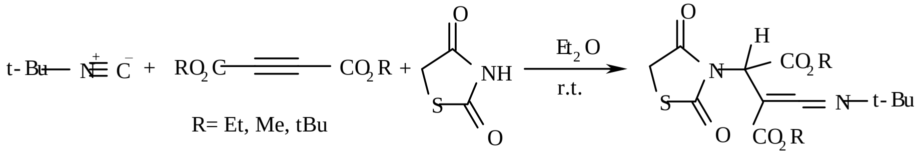
Thiazolidinedione (TZD) derivatives have been found to possess potent immunostimulatory properties as well as antiarthritic, antidiabetic and oncostatic activities [1]. In recent years, the treatment of type 2 diabetes has been revolutionized with the advent of thiazolidinediones (TZDs) class of molecules that ameliorate insulin resistance and normalize elevated blood glucose level, lipid, and insulin levels in rodent models of Type 2 diabetes and obesity [2]. Thiazolidinedione was synthesized according to the procedure from monochloroacetic acid and thiourea [3,4].

A multi-component reaction (MCR) is a chemical reaction where three or more compounds react to form a single product. Isocyanide based MCRs are most frequently exploited because the isocyanide is an extraordinary functional group [5]. We examined the *tert*-butyl isocyanide **1** based multi-component reaction of 2,4-thiazolidinedione **3** with dialkyl acetylenedicarboxylates **2**. The reactions proceeded in diethyl ether and afforded **4** in good yields. ^{1}H NMR, ^{13}C NMR, Mass and IR spectral studies confirmed the structure of product **4**.



1 **2** **3** **4**

References:

[1] Moretti, R. M.; Marelli, M. M.; Motta, M.; Limonta, P. *Int. J. Cancer* **2001**, *92,* 733.
[2] Saltiel, A. R.; Olefsky, J. M. *Diabetes* **1996**, *45*, 1661.
[3] Volhard, J. J. *J. Prakt. Chem.* **1874**, *9*, 217.
[4] Charles, K. B.; Frances, C. B. *J. Am. Chem. Soc*. **1956**, *78,* 6189.
[5] Armstrong, R.W.; Combs, A. P.; Tempest, P. A.; Brown, S. D.; Keating, T. A. *Acc. Chem. Res*. **1996**, *29,* 123.

Stabilization of dicyclopropylcarbene: toward stable heteroatom-free singlet dialkylcarbenes

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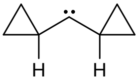
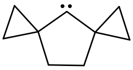
Ammann et al. reported the spectroscopic characterization of dicyclopropylcarbene, generated from the irradiation of dicyclopropyldiazirine in a matrix of N_2 at 6 K [1]. This achievement was the result of both theoretical and experimental interest on cyclopropylcarbene [2] which benefits from the stabilizing interaction of the occupied Walsh orbitals with the empty carbene *p* orbital ($W \rightarrow p$).

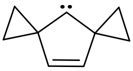
Herein we present the results of the first computational examination on the stabilization of dicyclopropylcarbene through cyclization and unsaturation. We probe the effects of substituents and hydrogen bonding on further stabilization of the most stable singlet carbenes. We hope this study helps to convert singlet dialkylcarbenes from illusive intermediates to more isolable species such as diaminocarbenes.



I



II



III

We found **III** as the most accessible carbene through appropriate substitution. Introducing hydroxy and amino substituents to the cyclopropyls creates stabilizing hydrogen bonding while electron-attracting groups on the double bond induce moderate aromaticity.

References:
[1] Ammann, J. R.; Subramanian, R.; Sheridan, R. S. *J. Am. Chem. Soc.* **1992**, *114,* 7592.
[2] Shevlin, P. B.; McKee, M. L. *J. Am. Chem. Soc.* **1989**, *111*, 519.

Stereoselective vinylation of 2,3-dihydroquinazolin-4(1H)-one derivatives mediated by vinyl triphenylphosphnium salts

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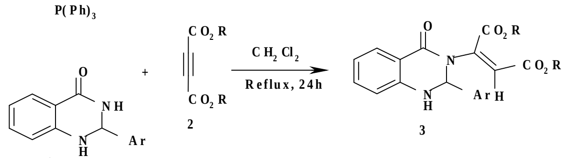
Organophosphorus compounds have been used in organic synthesis as useful reagents as well as ligands of a number of transition metal catalysts [1] and are synthesis targets of interest, not least because of their value for a variety of industrial, biological, and chemical synthetic uses. However, there are a few reactions in which organophosphorus(III) species work as catalysts [2-4].Reaction of acetylenic esters with triphenylphosphine in the presence of an organic compound possessing an acidic-hydrogen has been recently reported to produce phosphorus ylides [5]. Herein we have described Ph_3P promoted one-pot synthesis of dialkyl 2-(2-aryl)4- oxo-1,4-dihydro-2H-quinazolin3-yl) but-2-enedioates from a reaction of 2,3-dihydroquinazolin-4(1H)-ones and dialkyl acetylenedicarboxylates.



3	R	Ar	% Yield*
a	CH_3	C_6H_5	91
b	C_2H_5	4-Cl C_6H_4	89
c	*t*-Bu	4-Br C_6H_4	93
d	C_2H_5	4- OMe C_6H_4	90
e	CH_3	4- NO_2 C_6H_4	90
f	C_2H_5	4- CH_3 C_6H_4	92

* Isolated yields

The structures of **3a-f** were determined on the basis of their elemental analyses, MS, ^{1}H, ^{13}NMR and IR spectroscopic data.

References:

[1] Wilson, K.; Adams, D. J.; Rothenberg, G.; Clark, J.H. *J. Mol. Catal. A: Chem*. **2000**, *159,* 309.
[2] Yavari, I.; Ramazani, A. *Synth. Commun*. **1997**, *27* , 1449.
[3] Yavari, I.; Norouzi-Arasi, H. *Phosphorus Sulfur Silicon*, **2002**, *177*, 87.
[4] Yavari, I.; Souri, S.; Sirouspour, M.; Djahaniani, H.; Nasiri, F. *Synthesis,* **2005**, 1761.
[5] Yavari, I.; Karimi, E. *Phosphorus, Sulfur and Silicon Relat. Elem,* **2007,** *182*, 595.

Three-component reaction between triphenylphosphine, dimethyl acetylenedicarboxylate and aldehyde benzoylhydrazones: An efficient one-pot synthesis of stable phosphorus ylides

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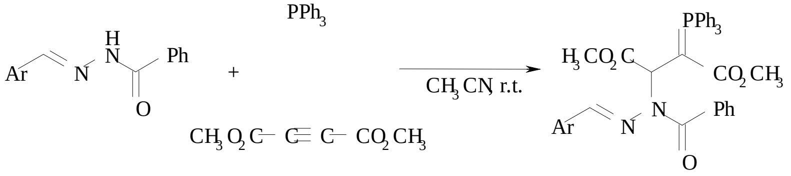
Phosphorus ylides are reactive systems, which take part in many reactions of value in organic synthesis [1]. Several methods have been developed for the preparation of phosphorus ylides. These ylides are usually prepared by treatment of an appropriate phosphonium salt with a base; the corresponding phosphonium salts are usually obtained from the phosphine and an alkyl halide [2]. Phosphonium salts are also prepared by Michael addition of phosphorus nucleophiles to activated olefins. Reaction of acetylenic esters with triphenylphosphine in the presence of an organic compound containing an acidic hydrogen has also been reported to produce phosphorus ylides.

In continuation of our works on the reaction between trivalent phosphorus nucleophiles and electron-deficient acetylenic compounds in the presence of organic N-H, O-H or C-H acids [3], we herein report an efficient synthetic route to stable phosphorus ylides using triphenylphosphine, dimethyl acetylenedicarboxylate and benzoylhydrazones.



References:

[1] Corbridge, D. E. C. Phosphorus: An Outline of the Chemistry, Biochemistry, and Uses, 5th ed.; Elsevier: Amsterdam, **1995**.

[2] Engel, R. Synthesis of Carbon-Phosphorus Bonds; CRC Press: Boca Raton, FL, **1988.**

[3] Yavari, I, Anary-Abbasinejad, M. *Org. Biomol. Chem.* **2003**, *3*, 560.

Synthesis of 1,3,5-trisubstituted pyrazoles in the presence of efficient catalysts

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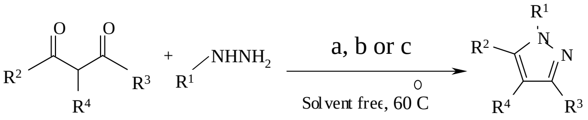
pyrazoles with a wide range of biological activities can be synthesized via 1,3-dipolar cycloadditions of diazo compounds [1], reaction of chalcones[2] and hydrazines, a four-component coupling of terminal alkynes, hydrazine, carbon monoxide, and aryl iodides [3], and the direct condensation of 1,3-diketones and hydrazines in the presence of an acidic catalyst [4]. The last one is the simplest and most straightforward procedure for the synthesis of pyrazoles.

$BF_3.SiO_2$ [5], nano-$BF_3.SiO_2$ or $Mg(HSO_4)_2$ [6] are bench-top catalysts which are reusable, readily available, eco-friendly, versatile, and efficient for promotion of many acid catalyzed organic transformations. These catalysts do not need special precautions for handling or storage, and they can be stored at an ambient temperature for months without losing their catalytic activity. In this report, we have investigated the synthesis of pyrazoles derivatives in the presence of $BF_3.SiO_2$, nano-$BF_3.SiO_2$ or $Mg(HSO_4)_2$ *via* condensation of 1,3-diketones and hydrazines in solvent free condition.



a) nano-37% $BF_3.SiO_2$, b) 37% $BF_3.SiO_2$, c) $Mg(HSO_4)_2$

In conclusion, the activity of nano- $BF_3.SiO_2$ is three times of $BF_3.SiO_2$ and ten times of $Mg(HSO_4)_2$. These catalysts were applied for preparation of pyrazoles in a simple and straightforward protocol. Short reaction time, high yields, scale-up, clean process, simplicity of operation, easy work-up, and green conditions are the advantages of these protocols.

References:

[1] Aggarwal, V. K.; Vicente, D. V.; Bonnert, R. V.; J. Org. Chem. **2003**, *68*, 5381.
[2] Bhat, B. A.; Puri, S. C.; Qurishi, M. A.; Dhar, K. L.; Qazi, G. N.; Synth. Commun. **2005**, *35*, 1135.
[3] Ahmed, M. S. M.; Kobayashi, K.; Mori, A.; Org. Lett. **2005**, *7*, 4487.
[4] Katritzky, A. R.; Handbook of Heterocyclic Chemistry; Pergamon; New York, 1985, p. 416.
[5] Mirjalili, B. F.; Bamoniri, A.; Akbari, A. Tetrahedron Lett. 2008, 49 , 6454.
[6] Shirini, F.; Zolfigol. M. A.; Mallakpour, B.; Mallakpour, S. E.; Hajipour, A. R. *Aust. J. Chem*. **2001**, *54*, 405.

An efficient and simple route for the synthesis of N-(2-pyridyl)-4-ethoxy-5-oxo-2,5-dihydro-1H-pyrolle-2,3-dicarboxylates

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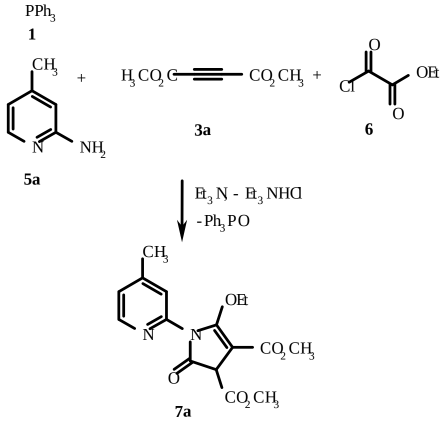
Three-component reaction of 2-aminopyridines, dialkyl acetylenedicarboxylates, triphenylphosphine and ethyl chlorooxoacetate in the presence of triethylamine provides a sufficient rout for the synthesis of dialkyl *N*-(2-pyridyl)-4-ethoxy-5-oxo-2,5-dihydro-1*H*-pyrolle-2,3-dicarboxylates in good yields.

In conclusion here we report the reaction between dialkyl acetylenedicarboxylates, aminopyridine derivatives and ethyl chlorooxoacetate promoted by triphenylphosphine and triethylamine, to produce functionalized 3-pyrollin-2-one derivatives in high yields. The present method carries the advantage that not only is the reaction performed under neutral conditions but also that the substances can be mixed without any activation or modification.



References:

[1] Anary-Abbasinejad, M.; Anaraki-Ardakani, H.; Dehghan A.; Hassanabadi, A.; Seyedmir, M. R. *J. Chem. Res*. **2007**, 574.

[2] Yavari, I.; Adib, M.; Hojabri, L. *Tetrahedron*. **2002**, 58, 7213.

[3] Anary-Abbasinejad, M.; Charkhati, K; Anaraki-Ardakani, H. *Synlett* **2009**, In press.

A simple and efficient approach to the synthesis of 7-benzylidene-3,3a,4,5,6,7-hexahydro-2,3-diphenyl-2*H*-indazole

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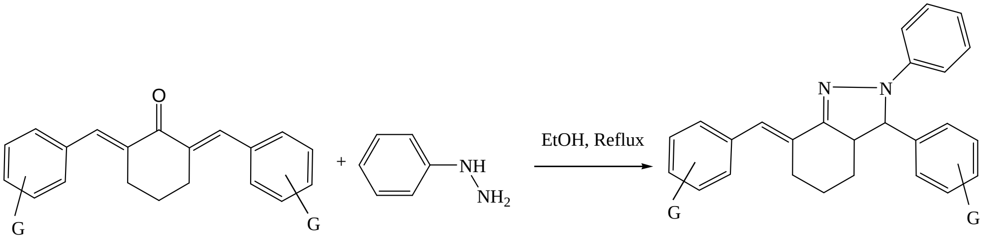
Condensation of nitrogen-containing binucleophilic agents with α,β-unsaturated ketones is one of the most suitable synthetic pathways to five-, six- and seven-membered partially hydrogenated heterocyclic compounds-potential pharmaceutically active analogs of natural compounds. High regioselectivity of the discussed reaction owing to the pronounced difference in electrophilic parameters of carbonyl and β-carbon reaction centers is the most important advantage of this reaction, which allows synthesizing several hardly accessible compounds [1].

Indazoline systems are known to be biologically active and agrochemical products. Tri substituted indazole represent a very important class of biologically active agents and focus of a significant amount of research interest. These compounds have found use as antitumor, antibacterial, antifungal, antiviral and insecticidal agents [2].

Herein we report an efficient method for synthesis of 7-benzylidene-3,3a,4,5,6,7-hexahydro-2,3-diphenyl-2*H*-indazole derivatives from α,ά-bis(substituted benzylidene)cycloalkanones in good yields.



References:

[1] Temple, C.; Coburn, W. C.; M. C. Thorpe, Montgomery, J.A. *J. Org. Chem.* **1965**, *30*, 2395.
[2] Sakya, S. M.; et al. *Bioorg. Med. Chem. Lett.* **2006,** *16*, 288 and references cited therein.

Three-component reaction of mercaptoethanol, triphenyl phosphite and acetylenic esters

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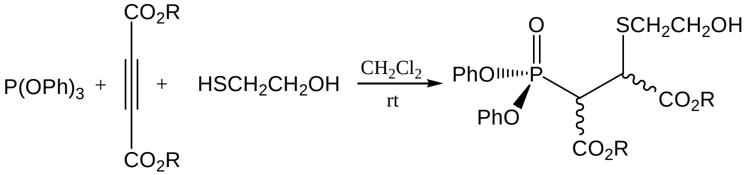
The rich chemistry that stems from the addition of nucleophiles to activated acetylenic compounds has evoked considerable interest. Trivalent phosphorous nucleophiles are known to form zwitterions with activated acetylene compounds such as dialkyl acetylenedicarboxylates [1-3]. Hence, it was of interest to investigate the reactivity of these zwitterions toward thiols such as mercaptoethanol for the synthesis of organophosphorous compounds.

As part of our current studies, we report the results of our studies involving the Three-component reaction of triphenyl phosphite **1** and dialkyl acetylenedicarboxylates **2** in the presence of mercaptoehanol, which constitute a synthesis of dialkyl 2-(diphenoxyphosphoryl)-3-[(2-hydroxy ethyl) sulfanyl] succinates **3**, as a mixture of two diastereoisomers (Scheme 1). The products were characterized based on their IR, Mass, ^{1}H-NMR, ^{13}C-NMR, and ^{31}P-NMR.



1 **2** **3**

Scheme 1

References:

[1] Winterfeldt, E. Schumann, Dillinger, D.H. *J. Chem. Ber*. **1994,** *2,* 1656.
[2] Dillinger,H.J. Fengler,G. Schumann, D. Winterfeldt,E. *Tetrahedron* **1994,** 2553 .
[3] Junjappa, H. Saxena, M. K. Ramaiah, D. Lohray, B. B. Rath, N. P. George, M. V. *J. Org. Chem.* **1994**, *63,* 9801.

Chemical composion and antibacterial activity of the essential oils from leaves and flowers of *Phlomis aucheri* Boiss. from Iran

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The genus *Phlomis* is comprised of about 100 species, 17 are described in the flora of Iran, among which 10 are endemic [1]. Chemical studies on some *Phlomis* species have resulted iridoids, triterpenes, phenyl propanoid glycosides and flavonoids. Previously we reported the essential oils of *P.persica*, *P. oliveri* and *P. pungens*.[2-3]. The major compounds of all three oils were germacrene D (38.2%, 26.4% and 24.5%) bicyclo germacrene (16.3 %, 12.7% and14.1%) and α- pinene(13.3%, 7.7% and 13.5%), respectively.The aim of our study is to identify the constituents and antibacterial activity of the essential oils of leaves and flowers of *P .aucheri*, endemic to Iran, growing wild at Eilam, Iran, in July 2009. The oils were obtained by hydrodistilation, using a Clevenger type apparatus and analyzed by GC and GC/MC.

Fifty five components representing 92.3% and fourty two constituents representing 90.1% were identified in the leaf and flower oils of *P. aucheri*, respectively.The major component of both oils was germacrene D(28.3% and 19.1%) , respectively and other notable components was β- caryophyllene (5.0% and 14.9%), bicyclo germacrene(8.9% and 7.6%)and γ- elemene(5.5% an7.9 %) ,respectively.In both oils sesquiterpenes (75.5% and 82.2 % predominated over monoterpenes(8.9% and 1.7%) respectively.

Antibacterial activity test was carried out on leaves and flowers of *Phlomis aucheri* essential oils using the growth in hibitory zone. The oils was active against Gram positive bacteria.

References:

[1] Mozaffarian, V, A Dictionary of Iranian Plant Names, Farhang Moaser Publishing, Tehran , Iran , **1996**, 406.
[2] Khalilzadeh , M.A.; Rustaiyan, A.; Masoudi ,S;Tajbakhsh ,M.J. Essent.Oil Res . **2005**,17,624.
[3] Masoudi, S; Rustaiyan, A.; Aberoomand Azar, P.; Larijani, K . J. Essent.Oil Res. **2006**,18,16.

New poly(amide-ester-imide)/ clay nanocomposite based on poly(ethylene glycol): synthesis, nanostructure and properties

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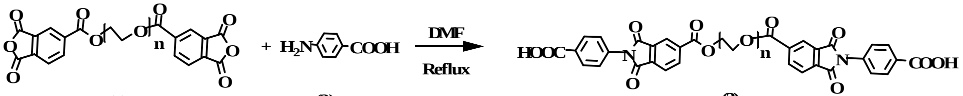
Poly (ethylene glycol) (PEG) is often introduced to the polymer's chain for its hydrophilicity, nontoxcity, biocompatibilituy and nonimmunogenicity [1, 2]. So, copolymers containing PEG as hydrophilic and soft segment have been widely studied. In addition copolymers such as poly(amide-imide)s containing PEG show high solubility [3]. But, polymers restrain PEG fragment do not show good mechanical and thermal properties. There has been extensive interest in the development of polymer-clay nanocomposite [4]. In this paper, the novel biodegradable poly(amide-ester-imide)s (**PAEI**)s with different molecular weight of PEG (M.W= 2000 and 6000) as hydrophilic and soft segment were prepared and intercalated into the gallery of modified montmorillonite (**MMT**). Poly(ethylene glycol)-bis-(N-trimellitylimido-4-phenyl carboxylic acid) **(3)** as a novel diacid monomer was synthesized via two step. The reaction of **PEG** with trimellitic anhydride yield poly(ethylene glycol)-bis-trimellitic anhydride (**1**). The reaction of dianhydride **1** with *p*-aminobenzoic acid (**2**) produces diacid monomer **3**. The direct polycondensation technique was used for the polyamidation of diacid with 4,4′-diaminodiphenylether using pyridine /2-methylpyrrolidone /triphenylphosphite /$CaCl_2$ as condensing agent. The intercalation of the resulting polymer chains between the silicates layer of modified **MMT** with different ratio were performed by ultrasonic technique. Thermogravimetric Analyses (**TGA**), Differential Scanning Calorimetry (**DSC**) and Dynamic Mechanical Thermal Analysis (**DMTA**) were used to study the thermal and mechanical behavior of the prepared nanocomposites. The morphological structures of the filled PAEIs were characterized by Scanning Electron Microscopy (**SEM**) and Transmission Electron Microscopy (**TEM**) techniques. It was also pointed out, by **DSC** analyses, that it exists a real competition between PEG 6000 and PEG 2000 for the intercalation into the interlayer spacing of the clay. The design of this polymer/clay nanocomposites were made to take advantages of PAEIs and clay in nanocomposite technology such as high solubility, high thermal efficiency and good mechanical properties.



(1) (2) (3)

References:

[1] Urry, D. W. *J. Protein Chem*. **1988**, 7, 81-114.
[2] Cappello, J.; Crissman, J. W. *Polymer Prepr*. **1990**, 31, 193-4.
[3] Zhang, Y.; Zhuo, R.X. *J. Biomaterials*. **2005**, 26, 6736-6742.
[4] Ranade, A.; Anne D′Souza, N.; Gnade, B. *J. Polym*. **2002**, 43, 3759-3766.

Preparation and characterization of nano particle Ag supported on clinoptilolite and photocatalytic effect for degradation of azo dye pollutant Acid Red 206 in water

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In this investigation photocatalytic degradation of effect azo dye Acid Red 206(AR206) in water was studied. nano Ag supported clinoptilolite prepared and then charactrited with, XRF, SEM and BET Method. The results show that nano-gA supported clinoptilolite are an active photocatalyst. The maximum effect of photodegradation was observed at 20 wt% nano Ag, 80%wt clinoptilolite. Optimal experimental conditions catalyst amount, PH, temprature and dye concentration have been determined. Based on the results a model was proposed for photodegradation of dyes using immobilized [nano Ag /cp].This model can be useful for the development of this technology for wastewater treatment applications. The higher photoactivity of nano Ag-clinoptilolite than clinoptilolite under uv irradiation can be ascribed the effect of silver deposits acting as electron traps on the Ag-clinoptilolite surface .

Reference:

[1] D.F.ollis, photocatalytic purification and treatment of water and Air,Elsever,Amsterdam,1993 .
[2] N.Serpone and E. perizzeti photocatalysis fundamentals and Aplications,wiley/Interscience,New York,1989 .
[3] M.A. FOX, K. E. Doan and M. T. Dulay, Res.Chem . Intermed.,20(1994) 711.
[4] K.J.Greem and R.Rudham,.J.Chem.Soc.,faraday trans.,89(1993)1867.

A novel synthesis of pyrimidins from an efficient one-pot reaction of cyclohexylisocyanide and dialkyl-acetylene dicarboxlate in the presence of urea

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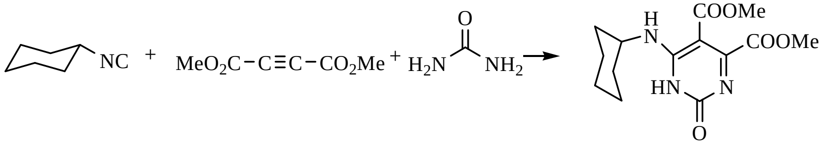
Pyrimidine is a heterocyclic aromatic organic compound similar to benzene and pyridine, containing two nitrogen atoms at positions 1 and 3 of the six-member ring [1]. Nitrogen-containing heterocyclic compounds are widespread in nature, and their applications to biologically active pharmaceuticals, and functional materials are becoming more and more important .the development of new efficient methods to synthesize N-heterocycles with structural diversity is one major interest of modern synthetic organic chemists [2].The rich chemistry that stems from the addition of nucleophiles interest isocyanides are known to form zwitterions with activated acetylene compounds such as dimethyletylenedicarboxylate(DMAD)[3].

In this work an efficient method for the synthesis of Dimethyl-6-(cyclohexylimino)-1,2-dihydro-2- oxopyrimidine-4,5-dicarboxylate analogues has been developed via one-pot reaction of cyclohexylisocyanide and dialkylacetylendicarboxylate in the presence of urea. The reaction provided Dimethyl-6-(cyclohexylimino)-1,2-dihydro-2-oxopyrimidine-4,5-dicarboxylate in moderate to good yield.The structures of these products were deduced from their elemental analyses and ^{1}H NMR, ^{13}C NMR and FTIR spectral data.



References:

[1] *Heterocyclic Chemistry* (3rd Edition) Thomas. L. Gilchrist ISBN 0-582-27843-0

[2] (a) padwa, A.; waterson, A. G. *curr. org. chem*. **2000**, *4*,175-203; (b) orru, R. V. A.; de greef, M. synthesis **2003**,1471-1499.

[3] Nair, V.; Rajesh, C., Vinod, A. U.; Bindu, S.; Sreekanth, A. R.; Mathen, J. S.; Balagopal, L. *ACC. Chem. Res*. **2003**, *36*, 899.

A novel multicomponent one-pot synthesis of azetidine-2,4-diones (Malonimides)

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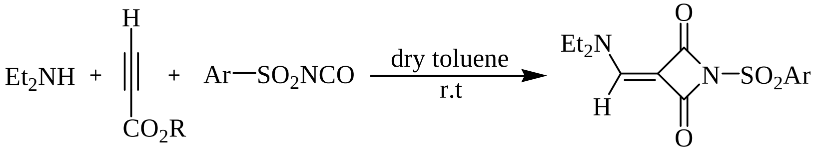
Azetidine-2,4-diones (malonimides) which are highly strained molecules have been shown to possess anti-inflammatory and sedative properties [1]. These compounds are employed as promoters in polymerizations.and their use not only permits low polymerization temperatures but gives rise to faster polymerization reactions than prior art procedures allow. Bachi and co-workers have reported that this category of compounds along with their 4-thioxo analogs can serve as useful intermediates for a variety *β*-lactam antibiotic [2,3].

In this research [4], we report a simple one-pot reaction between an enamines, derived from the addition of diethylamine to the alkyl propiolate, and an arylsulfonyl isocyanate leading to 3-[(diethylamino)methylene]-1-(arylsulfonyl)-2,4-azetidinedione derivatives. These malonimides show dynamic NMR behavior in solution because of restricted rotation around the C–N bond resulting from conjugation of the sidechain N-atom with the adjacent *α*,*β*-unsaturated carbonyl group.



The structure of products were determined on the basis of their IR, ^{1}H NMR, ^{13}C NMR and mass spectra.

References:

[1] Moore, J. A. In *Heterocyclic compounds with three and four membered rings*; part 2,Weissberger, A., Ed.: Wiley- Interscience: New York, **1964**, 951.
[2] (a) Bachi, M. D.; Goldberg, O.; Gross, A.; Vaya, J. *J. Org. Chem.* **1980**, *45*, 1477; (b) Chou, T. S.; Koppel, G. A.; Dorman, D. E.; Paschal, J. W. *J. Am. Chem. Soc.* **1976**, *98*, 7864.
[3] Brandt, A.; Bassignani, L.; Re, L. *Tetrahedron Lett.* **1976**, 3975.
[4] Alizadeh, A.; Rezvanian, A. *Synthesis* **2008**, *11*, 1747.

Facile entry to polycyclic indolylhydroquinoline skeletons *via* tandem *S*-alkylation and intramolecular *C*-alkylation

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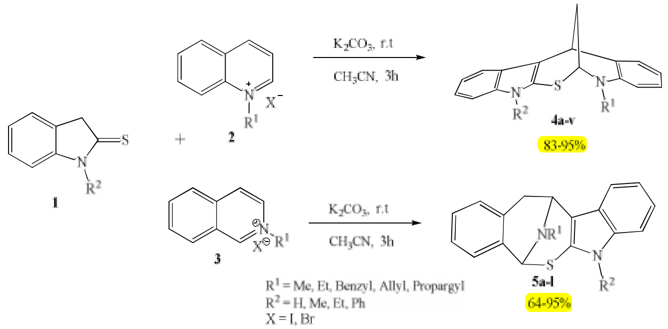
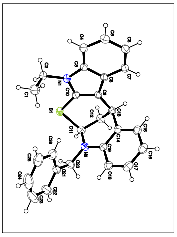
Great efforts have been made to discover new reactions to facilitate the construction of heterocycles contain indole. Recent challenges in organic synthesis include development of new methodologies that afford complex molecules from relatively simple starting materials via tandem reactions with fewer synthetic steps and mild reaction conditions leading to high yields [1]. Quinoline compounds are known to form salts with alkyl halides. The quinolinium salts can be reacted with a variety of bifunctional nucleophiles to give diverse compounds, which are useful precursors for the synthesis of biologically important heterocyclic compounds [2]. We wish to report an efficient, single step synthesis of hitherto unknown indole-annulated pentacyclic indolylhydroquinolines *via* tandem *S*-alkylation and intramolecular *C*-alkylation of indolin-2-thiones with *N*-alkylquinolinium salts in excellent yields (83-95%) is reported. This facile approach provides a powerful entry into polycyclic structures containing nitrogen and sulfur related to alkaloids. The structure of the product was determined by Röntgen crystal structure analysis.





References:

[1] Parenty, A. D. C.; Smith, L. V.; Pickering, A. L.; Long, D. L.; Cronin, L. *J. Org. Chem.* **2004**, *69*, 5934.
[2] Fakhfakh, M. A.; Franck, X.; Fournet, A.; Hocquemiller, R.; Figadere, B. *Tetrahedron Lett.* **2001,** *41*, 3847.

Ab initio study on the interaction between functionalized SWCNTs and methanol

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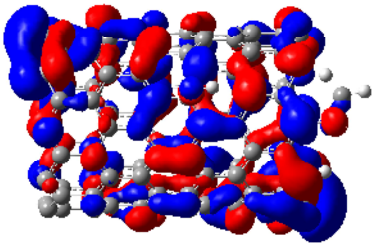
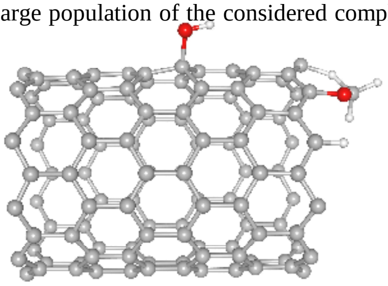
Methanol naturally is producing in the anaerobic metabolism of varieties of bacterial which can find ubiquitous in the environment and is an alternate fuel for internal combustion such as encouraging fuel cells based on methanol (MeOH) which are safe, renewable and easily storable [1]. The adsorption and decomposition of MeOH has been studied greatly on metal surfaces, alloys, and metal oxides [2, 3]. On the other hand, several study on methanol adsorption in carbon nanotubes have been done [4, 5] and the obtained results indicate that methanol does not adsorb onto SWCNTs at room temperature.

In the present work we study the interaction of a methanol molecule with the pristine SWCNTs with various diameters and chirality by using the density functional theory (DFT) calculations. We further considered the adsorption of methanol on the exterior surface as well as edge site of the functionalized SWCNTs. The obtained results indicate that the binding energy of methanol is significantly increased for adsorption on the sidewall of functionalized nanotubes. It was also found that the adsorption of methanol at the edge site of both functionalized and pristine SWCNT is remarkably different (chemisoption process) in comparison to the exterior sidewall of the tubes. Furthermore, the electronic structures and Mulliken charge population of the considered complexes at their ground state are analyzed.





References:

[1] Dicks, A.L. *J. Power Sources* **2006**, *156*, 128.
[2] Wachs, I.E. *Surf. Sci*. **2003**, *544*, 1.
[3] Henderson, M.A.; Otero-Tapia, Castro, S. *Faraday Discuss.* **1999**, *114*, 313.
[4] Burghaus, U.; Bye, D.; Cosert, K.; Goering, J.; Guerard, A.; Kadossov, E.; Lee, E.; Nadoyama, Y.; Richter, N.; Schaefer, E.; Smith, J.; Ulness, D.; Wymore, B. *Chem. Phys. Lett.* **2007**, *442*, 344.
[5] Ellison, M. D.; Morris, S. T.; Sender, M. R.; Brigham, J.; Padgett, N. E. *J. Phys. Chem. C* **2007**, *111*, 18127.

Heteropoly acid supported on SBA-15 and KIT-6 mesoporous silicas: Structural, characterization and catalytic application

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Ordered mesoporous materials have received attention owing to their potential applications in catalysis, adsorption, ion exchange and manufacture of advanced functional materials. Mesoporous siliceous materials such as MCM-41, MCM-48, SBA-15, SBA-1 and KIT-6 have been prepared by self-assembly methods using long-chain ionic and anionic surfactants as templates [1-3]. However to date, a limited number of mesoporous sieves with uniform pores, such as MCM-41, MCM-48 and SBA-15 have been studied as a host matrix of heteropoly acids (HPAs) [4]. In the present paper we focus our attention on the effects of the pore topology on the state of supported HPA species. SBA-15 silicas with a two-dimentional (2D) hexagonal arrangement of uniform cylindrical mesopores and KIT-6 silicas with an *Ia*3*d* symmetry and two interpenetrating branched networks of cylindrical pores are used as the supports. A conventional wet impregnation method, using HPA as a precursor, was applied for the introduction of heterpoly acid into the silica support.

$$\text{Support + HPA} \xrightarrow[\text{H}_2\text{O, r.t}]{\text{assembly}} \xrightarrow[\text{for 4 h at 110 }^{o}\text{C}]{\text{were dried}} \text{HPA/support}$$

Support = Al-KIT-6 or Al-SBA-15

References:

[1] Beck, J. S.; Vartuli, J. C.; Roth, W. J. *J. Am. Chem. Soc.* **1992**; *114*, 10834.
[2] Monnier, A.; Schuth, F.; Huo, Q.; *Science*, **1993**, *26*, 1299.
[3] Zhao, D.Y.; Feng, J. L.; Huo, Q. S. *Science*, **1998**, *279*, 548.
[4] Madhusudhan Rao, P.; Goldberg-Oppenheimer, P.; Kababya, S.; Vega, S.; Landau, M.V. *J. Mol. Catal. A: Chem.* **2007**, *275*, 214.

Three component synthesis of functionalized ketenimines from reaction of cyclohexyl isocyanid and dialkyl acetylenedicarboxylate in the presence of 2-quinolinol

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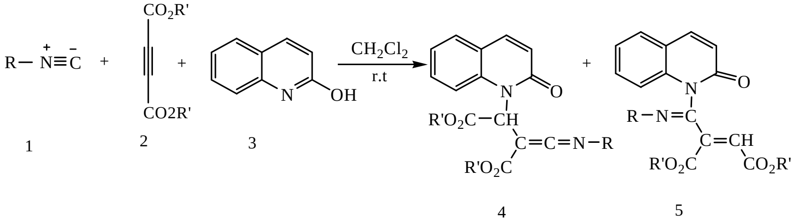
Ketenimines are important reactive intermediates that occur as transient compounds in many thermal and photochemical reactions[1]. Methods for the synthesis of ketenimines have been extensively reviewed. The addition of nucleophilic carbenes such as isocyanides to dialkyl acetylenedicarboxylates has been investigated in detail. The trapping of the 1:1 intermediate formed between dialkyl acetylenedicarboxylates and isocyanides with OH, NH, and CH acids has been widely studied[2]. In continuation of our interest in the application of isocyanides in multi-component reaction, MCR[3], we report here an efficient synthesis of ketenimine **4** from alkyl isocyanides **1** and dialkyl acetylenedicarboxylates **2** in the presence of strong NH-acid, such as quinolin-2-ol. In addition to ketenimine, minor amounts of 1-azadienes **5** are obtained (Scheme 1).



1	R
1a	CyHexyl

2	R'
2a	Me
2b	Et
2c	t-Bu

4,5	R	R'
4a,5a	CyHexyl	Me
4b,5b	CyHexyl	Et
4c,5c	CyHexyl	t-Bu

References:

[1] T. T. Tidwell, *Acc. Chem. Res.* **23** (1990) 273.
[2] I. Yavari, H. Zare, B. Mohtat, *Mol Divers*, **10** (2006) 24.
[3] I. Yavari, L. Moradi, F. Nasiri, H. Djahaniani, *Mendeleev Commun.* **15** (2006) 156.

Structural relationships and theoretical study of electron transfer kinetic of cephalosporin antibiotics and p-phenylenediamine derivatives with fullerenes in nanostructure of [R].C_n supramolecular complexes

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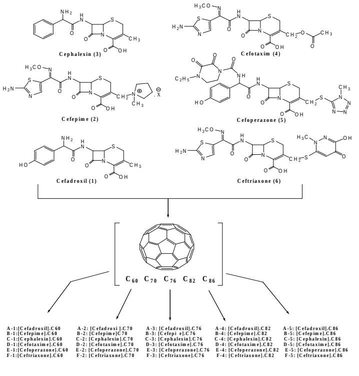
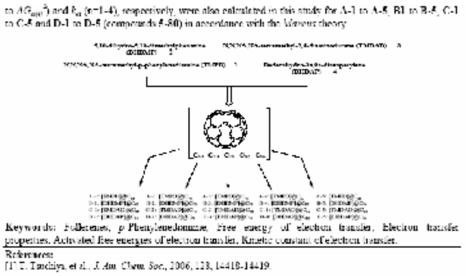
Various empty carbon fullerenes (C_n) with different carbon atoms have been obtained and investigated. The cephalosporin antibiotics and the derivatives have shown the important medicinal properties. Also the *p*-Phenylenediamine derivatives have shown the important electron transfer properties. Topological indices are purported to correlate chemical structures with various chemical and physical properties. They have been successfully used to construct effective and useful mathematical methods to establish clear relationships between structural data and the physical properties of these materials [1]. In this study, the number of carbon atoms in the fullerenes was used as an index to establish a relationship between the structures of selected cephalosporin antibiotics, **1-6** as well-known *β*-lactam antibiotics and *p*-Phenylenediamine, **1-4** with fullerenes C_n (n=60, 70, 76, 82 and 86)[2,3]. The calculations for the four reduction potentials ($^{Red.}E_1$ to $^{Red.}E_4$) of fullerenes C_n and four free-energies of electron transfer ($\Delta G_{et(1)}$ to $\Delta G_{et(4)}$) of supramolecular complexes were used to calculate the first to forth free activation energies of electron transfer and kinetic rate constants of the electron transfers $\Delta G_{et(1)}^{\#}$ to $\Delta G_{et(4)}^{\#}$ and $k_{et(\mathrm{n})}$ (n=1-4), in accordance with the *Marcus* theory.




to $\Delta G_{et(4)}^{\#}$) and k_{et} (n=1-4), respectively, were also calculated in this study for A-1 to A-5, B1 to B-5, C-1 to C-5 and D-1 to D-5 (compounds 5-80) in accordance with the *Marcus* theory

Keywords: Fullerenes, *p*-Phenylenediamine, Free energy of electron transfer, Electron transfer properties, Activated free energies of electron transfer, Kinetic constant of electron transfer.

References:
[1] T. Tsuchiya, et al., *J. Am. Chem. Soc.*, 2006, 128, 14418-14419.

References:

[1] El-Shaboury, S. R.; Saleh,; Mohamed, F. A.; Rageh, A. H. *Journal of Pharmaceutical and Biomedical Analysis* **2007**, *45, 1.*
[2] Taherpour, A. A. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **2008**, *16*, 196.
[3] Tsuchiya, T. et al., *J. Am. Chem. Soc.*, **2006**, *128*, 14418.

Mononitration of phenols with *in situ* generated NO_2^+ *via* combination of guanidinium nitrate and silica sulfuric acid (SiO_2-OSO_3H)

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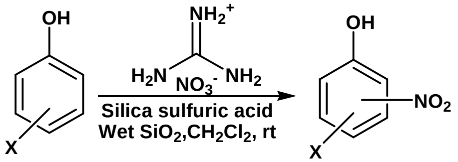
The replacement of current chemical processing techniques with more environmentally benign alternatives is an increasingly attractive subject. Nitration of organic substrates is a widely studied reaction of great industrial significance as many nitro-compounds are extensively utilized and act as intermediates for the manufacture of plastics, dyes, perfumes, drugs and pharmaceuticals [1]. Nitrophenols are very important organic intermediates and hence it is still interesting to develop regiospecific pollution-free nitrating procedures for phenolic compounds under mild conditions. Various nitrating reagents or reagent systems for the nitration of phenols have been emerged in the last decade [2-3], but many of these methods suffer from some drawbacks, including low selectivity, tedious work-up, toxicity, un-degradable reagents and catalyst and long reaction times. Therefore, we decided to overcome mentioned limitations by introducing of an environmentally friendly procedure for the preparation of nitrophenols.

A mixture of gunidinium nitrate, as non-metallic and green nitrate salt, and silica sulfuric acid might generate nitronium ion (NO_2^+), which is usable for the nitration of activated aromatic compounds. Consequently a wide variety of phenolic compounds were subjected for the nitration reaction using guanidinium nitrate and silica sulfuric acid in the presence of wet SiO_2 (50%, w/w) in dichloromethane (Scheme 1).



Scheme 1

In summary we have delineated an environmentally friendly and heterogeneous procedure for the preparation of substituted phenols. Furthermore, this method exhibits substrate versatility, mild reaction conditions, non-metallic conditions and easy and clean work-up of products.

References:

[1] Mallick, S.; Parida, K.M. *Catal. Commun.* **2007**, *8*, 1487.
[2] Lalitha, A.; Sivakumar, K. *Synth. Commun.* **2008**, *38*, 1745.
[3] Nandurkar, N.S.; Bhanushali, M.J.; Jagtap, S.R.; Bhanage, B.M. *Ultrason. Sonochem.* **2007**, *14*, 41.

Mononitration of phenols with *in situ* generated NO_2^+ *via* combination of guanidinium nitrate and silica sulfuric acid (SiO_2-OSO_3H)

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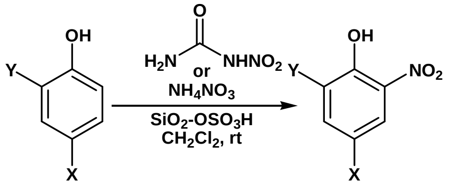
Nitration of aromatic compounds is one of the most fundamental and useful reactions for introducing the nitrogen atom directly into aromatic rings. Nitration of aromatic compounds is an industrially important reaction as the nitrated products are intermediates for fine chemicals and pharmaceuticals [1]. Usually, nitration of phenols are not region-selective and are the cause of environmental concerns regarding the disposal of large excesses of concentrated nitric acid and non-environmentally friendly metallic catalysts or reagents (such as WO_3-HNO_3, TiO_2-$[Ti_4H_{11}(PO_4)_9].nH_2O/HNO_3$, Yb-Mo-HKSF-$HNO_3$ and $ZnCl_2/HNO_3$), [2-3]. Therefore, designing systems, which is reducing the mentioned problems, is great of interest.

Recently we have examined a variety of heterogeneous systems, which are generating nitronioum ion (NO_2^+) that was used for different organic reactions [4-5]. In this light, we decided to disclose a new procedure for the nitration of substituted phenols by a mixture containing ammonium nitrate or nitro urea and silica sulfuric acid. Consequently, herein we decided to report a metal-free, green and heterogeneous procedure for the nitration of substituted phenolic compounds by ammonium nitrate and/or nitro urea and silica sulfuric acid under mild and heterogeneous conditions at room temperature (Scheme 1).



Y= H, *t*-Buthyl, OMe or Cl
X= H, Me, *iso*-Pr, *t*-Buthyl,OMe, OCH_2Ph, Ph, F, Cl, Br or OPh

Scheme 1

References:

[1] Anuradha, V.; Srinivas, P.V.; Aparna, P.; Rao, J.M. *Tetrahedron Lett.* **2006**, *47*, 4933.
[2] Bharadwaj, S.K.; Hussain, S.; Kar, M.; Chaudhuri, M.K. *Appl. Catal. A-Gen.* **2008**, *353*, 62.
[3] Yin, W.P.; Shi, M. *Arkivoc* **2009**, 6.
[4] Ghorbani-Choghamarani, A.; Goudarziafshar, H.; Nikoorazm, M.; Yousefi, S. *Can. J. Chem.* **2009**, *87*, 1144.
[5] Ghorbani-Choghamarani, A.; Hajjami, M.; Goudarziafshar, H.; Nikoorazm, M.; Mallakpour, S.; Sadeghizadeh, F.; Azadi, G. *Monatsh. Chem.* **2009**, *140*, 607.

12-Tungstophosphoric acid and wet SiO_2: Efficient and eco-friendly system for conversion of trimethylsilyl ethers to their corresponding alcohols

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Silyl protecting groups have played increasingly important roles in the synthesis of complicated molecules, especially biologically significant products [1]. Although there have been many new reports regarding the protection and deprotection of silyl groups, the removal of silyl groups under mild conditions with an easy work-up procedure is important [2].

Along this line, using heteropolyacids (HPAs), their salts and polyoxometalates (POMs) which are low in toxicity, highly stable towards humidity, recyclable and air stable have found more attention [3]. These compounds show very high catalytic activity for some acid-catalyzed reactions [4]. HPAs are usually solids that are insoluble in non-polar solvents but highly soluble in polar ones. The use of HPAs in non-polar solvents improves product selectivity and also provides easy separation of HPAs from the reaction mixture [5]. This allows it to be used as the catalyst for various phase reactions such as, preparation of silyl ethers [4], esterification of oleic acid [5], synthesis of xanthenedione derivatives [6], acylation of anisole [7], and etc.

In this work we hope to describe a simple procedure for conversion of trimethylsilyl ethers to their corresponding alcohols in the presence of 12-tungstophosphoric acid and wet SiO_2 as efficient and eco-friendly system in good to excellent yields under mild and heterogeneous conditions.

$$\text{ROTMS} \xrightarrow{H_3PW_{12}O_{40}\ /\ \text{wet SiO}_2} \text{ROH}$$

References:

[1] Banaszak, E.; Xu, L.W.; Bardeau, J.F.; Castanet, A.S.; Mortier, J. *Tetrahedron.* **2009**, *65*, 3961.
[2] Bamoniri, A.; Zolfigol, M.A.; Mohammadpoor-Baltork, I.; Mirjalili,B.F. *J. Iran. Chem. Soc.* **2006**, *3*, 85.
[3] Caliman, E.; Dias, J.A.; Dias, C.L.; Garcia, A.C.; Macedo, J. L.; Almeida, L. S. *Micropor. Mesopor. Mat.* **2010**,*132*, 103.
[4] Villabrille, P.; Romanelli, G.; Quaranta, N.; Vázquez, P. *Appl Catal B-Environ.* **2010**,*96*, 379.
[5] Oliveira, C. F.; Dezaneti, L.M.; Garcia, A.C.; Macedo, J. L.; Dias, J. A.; Dias, C.L.; Alvim, S.P. *Appl Catal A-Gen.* **2010**, *372*, 153.
[6] Karthikeyan, G.; Pandurangan, A. *J. Mol. Catal. A-Chem.* **2009**, *311*, 36.
[7] Parida, K.M.; Mallick, S.; Pradhan, G.C.; *J. Mol. Catal. A-Chem.* **2009**, *297*, 93.

Interaction of (E)-3-(3,4-dihydroxybenzylidene)-7-methoxychroman-4-one and(E)-3-(3,4-dihydroxybenzylidene)-7-propoxychroman-4-one with DNA

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Homoisoflavonoids (3-benzylidene-4-chromanones) are related to flavonoids and occur as natural products and exhibit biological activity. These compounds have been reported to possess antifungal, hypocholesterolemic, antimutagenic, and antiviral activities.[1]

A series of 3-benzylidene-7-alkoxychroman-4-one derivatives were synthesized and evaluated for their antioxidant activities.The antioxidant activity was assessed using three methods, namely, 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging, ferric reducing antioxidant power (FRAP), and thiobarbituric acid reactive substances (TBARS) assays.

3-Benzylidene-7-alkoxychroman-4-one derivatives bearing catecholic group on benzylidene moiety exhibited excellent antioxidant activity. [2]

this study was designed to examine the interactions of one of the most important kinds of antioxidants, called (E)-3-(3,4-dihydroxybenzylidene)-7-methoxychroman-4-one and (E)-3-(3,4-dihydroxybenzylidene)-7-propoxychroman-4-one (Fig.1) with calf thymus DNA in aqueous solution at physiological conditions, using constant DNA concentration (0.51mM)and various concentration of drug. UV-visible spectroscopic method have used to determine binding constant and the stability of DNA in (E)-3-(3,4-dihydroxybenzylidene)-7-methoxychroman-4-one and (E)-3-(3,4-dihydroxybenzylidene)-7-propoxychroman-4-one—DNA complexes in aqueous solution. spectroscopic evidence showed major binding of (E)-3-(3,4-dihydroxybenzylidene)-7-propoxychroman-4-one to DNA with overall binding constant of $K= 2.07\times10^{4}$ M^{-1} and weaker binding of (E)-3-(3,4- dihydroxybenzylidene)-7-methoxychroman-4-one to DNA with overall binding constant of $K= 5.1\times10^{3}$ M^{-1}(where K is the binding constant).

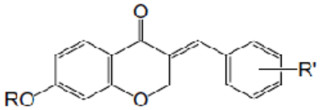

Fig 1. R: Me, n-Pr ; R‘: 3,4 -$(OH)_2$

References:

[1] Siddaiah, V.; Rao, C. V.; Venkateswarlu, S.; Krishnaraju, A. V.; Subbaraju, G. V. Bioorg. Med. Chem. 2006, 14, 2545.
[2] A. Foroumadi , A. Samzadeh-Kermani, S. Emami, G. Dehghan, M. Sorkhi, F. Arabsorkhi, M. Heidari, M. Abdollahi, A. Shafiee, Bioorg. Med. Chem. Lett. 17 (2007) 6764–6769.

A theoretical study: Borotropic and prototropic shifts on cyclopentadienyl ring.

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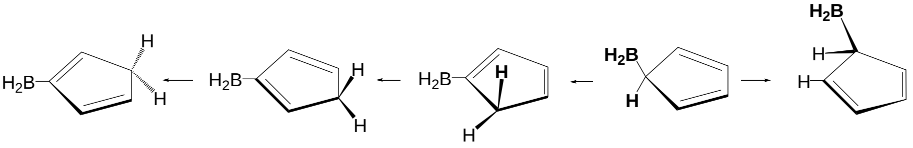
Structural and energetic behaviour of, borotropic and prototropic shifts of cyclopentadienyl(dihydro)borane was investigated using density functional theory (DFT) method. Experimental study of fluxional behavior of cyclopentadienyl(dihydro)borane(**1**) were performed by Gridnev and Meller [1].

In this work, we report the results of a theoretical investigation of the energetic and structural properties of four isomers of cyclopentadienyl(dihydro)borane which was performed by density functional theory using the GAUSSIAN 98 package of programs [2-4].

The energy barrier of Prototropic shift is higher than borotropic shifts. Consequently, the rate of sigmatropic migration of hydrogen atom is much slower than bor atom migration. These results indicate that the most stable isomers of compounds 1'–3' are the vinilic isomers (the BH_2 fragment in a vinilic position or compound 2). This behaviour is in good agreement with experimental data.



(3`) (3) (2) (1) (1`)

References:

[1] Gridnev, I. D.; Meller, A. *Main Group Metal Chem*. **1998**, *21*, 121.
[2] Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648.
[3] Lee, C.; Yang. W.; Parr, R. G. *Phys. Rev*. **1998**, *37*, 785.
[4] Seminario, J. M.; Politzer P. (eds.), *Modern Density Function Theory, A Tool for Chemistry,* Elsevier, Amsterdam, **1995**.

Dehydrogenation of 2-substituted imidazolines with sodium periodate catalyzed by Mn(TPP)Cl

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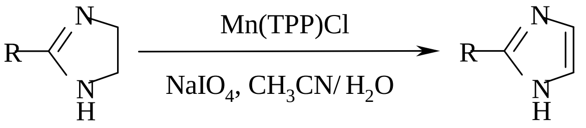
The development of efficient catalytic systems for oxidation reactions that mimic the action of cytochrome P-450 dependent monooxygenases has attracted much attention in recent years [1].Metalloporphyrins have been known as synthetic models for cytochrome P-450 and have been used as efficient and versatile catalysts in synthetic chemistry for the synthesis of several valuable compounds [2].

2-Imidazolines have been used as antihyperglycemic, antiinflammatory, antihypertensive and antihypercholesterolemic agents [3]. Furthermore, 2-imidazolines are widely used as convenient building blocks for the synthesis of biologically active molecules such as azapenams, (bis)dioxocyclams, diazapinones, and 2,3-diamino acids[4]. The oxidative dehydrogenation of imidazolines is a general ad reliable method of synthesizing 2-substituted imidazoles.

In this work, we report a new approach for dehydrogenation of 2-substituted imidazolines to their corresponding imidazoles with sodium periodate catalyzed by Mn(TPP)Cl. This catalytic system exhibits a high activity in 1:2 CH_3CN/H_2O mixtures.



References:

[1] Woggon, W. D. *Acc. Chem. Res.* **2005,** *38,* 127.
[2] James, G. B.; Molinaro, F. S.; Ibers, J. A.; Collman, J. P.; Brauman, J. I.; Rose, E.; Suslick, K. S. *J. Am. Chem. Soc.* **1980**, *102*, 3224.
[3] Li, H. Y.; Drummond, S.; DeLucca, I.; Boswell, G. A. *Tetrahedron* **1996**, *52*, 11153.
[4] Betschart, C.; Hegedus, L. S. *J. Am. Chem. Soc.* **1992**, *114*, 5010.

Synthesis and identification of new derivatives of tetrazoles based on barbituric acids

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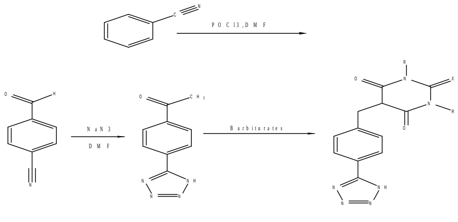
Since the 1980s, the growth of tetrazole chemistry has continued unabated due to its popular functionality with a wide range of applications [1]. Tetrazoles has been the subject of investigations during the last 20 years. In recent years tetrazoles have found a wide range of applications in coordination chemistry due to their role as mono- or bidentate ligands and strong networking ability .The nature of (1H)-tetrazole ($–CN_4H$) group is very similar to carboxylic acid (–COOH) group with respect to acidity (pKa ≈5) and solubility. Furthermore, it is more stable than carboxylicacid group. It has been widely used as a carboxylicacid pharmacophore in drug design [2]. Numerous tetrazole derivatives exhibit versatile biological activity due to the fact that the tetrazole ring is a metabolically stable replacement of carboxylic functionality [3]. Tetrazoles undergo various reactions such as alkylation and acylation, complex formation with metals, thermolysis, photolysis, and decomposition with formation of nitrenes, etc.

At first we synthesis cyanogen bromide and reaction with phenolic derivatives and phenyl cyanate derivatives (Aryl cyanate), including derivative 5– phenoxy tetrazole are obtained. Then reaction of derivatives phenyl cyanate with sodium azyde are resulted relevant tetrazole then with using of Vilsmeier reagent the corresponding composition para position can Formylation. This is formyled derived from 5– phenoxy tetrazole never has been synthesized. With knoevonagel condensation which in that active hydrogen compounds condense with aldehydes and ketones known as kneovonagel condensation. These aldol-like condensations usually are catalyzed with weak bases. Synthesized derivative from the tetrazole with Barbituric acids that have drug use compress.



References:

[1] Butler, R.N In: A.R Katritzky, C.W Rees and E.F.V Scriven, Editors. *Comprehensive Heterocyclic Chemistry*. **1996**, *4*, 897–904.

[2] Duncia**,** J.V.**;** Pierce**,** M.E.**;** Santella m**,** J.B. J. *J. Org. Chem*. **1991**, *56*, 2395–2400.

[3] Dabbagh A. H., Noroozi-Pesyan N., Bagheri A., Takemoto S. and Hayashi H. *Russian J. Org. Chem.* **2005**, *41*, 1055–1063.

New thiourea as coupling of derivatives thiotriazine and benzoylisothiocyanate

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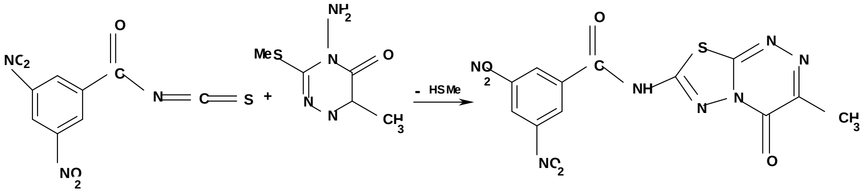
Reaction between two reactants produces product or products. These products can keep the physical and chemical properties of reactants or may be show completely different properties. Coupling an amine group of one compound and an isothiocyanate group of the other compound is the kind of these reactions. In this case, the obtained product is a thiourea derivative which its properties are comparable to the initial materials and find new properties. Various applications have been reported for benzoyl isothiocyanate such as anti bacterial and anti fungal. Presence of the other groups on its derivative can increase or decrease some properties.[1-3] Preservation of specific properties in reactants is one of the important aims in synthesis [1-3].

The reaction of coupling 3,5-dinitrobenzoylisothiocyanate with an amine group of thiotriazine derivative (4-amino-6-methyl-3-(methyl sulfanyl) 1,2,4- triazine-5(4H)-one (AMMSTO)) formed a new thiourea. In another reaction this thiotriazine derivative with benzoyl isothiocyanate lost hydrogen methanethiol or methyl hydrosulfide (HSMe) and was created the bond, the cycle and one benzamide compound. It is important existence of the withdrawing nitro groups are able to be effective on the formation of final product or can change predictive product.

This new compound of 3,5-dinitrobenzoylisothiocyanate and AMMSTO was characterized by IR, ^{1}HNMR, ^{13}CNMR and mass spectroscopies. Determination of structure of the new compound may be carried out by X-ray single crystal structure of the suitable crystals of the new compound. Research of biological activities this new compound is another aim of this synthesis.



References:

[1] Ramadas, K; Svinivasan, N. *Synth. Commun*. **1995**, *25*, 338.
[2] Bermejo, E.; Carballo, R.; Castineoras, A.; Dominguez, R.; Maichle-Mossmer, C.; Strahle, *J. Polyhedron* **1999**, *18*, 3695.
[3] Kaminsky, W. Goldberg, K.I. West, D.X. *J. Molecular Structure* **2002**, *605*, 9.

A convenient synthesis of 2, 4, 6-triarylpyridines under solvent-free conditions

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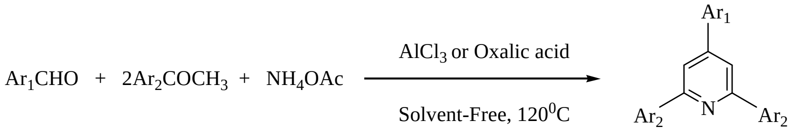
2,4,6-Triarylpyridines are prominent building blocks in supramolecular chemistry and are important because of the occurrence of their saturated and partially saturated derivatives inbiologically active compounds and natural products such as NAD nucleotides, pyridoxol (vitamin B_6), and pyridine alkaloids. Some examples are used as antimalarial, anticonvulsant, anesthetic, antioxidant, antibacterial, and antiparasitic properties .

More recently, one-pot syntheses of 2,4,6-triarylpyridines by three-components condensation of aromatic ketones, aldehydes, and ammonium acetate have been reported [1-6]. However, most of the established methods suffer from some disadvantages, such as multi-step procedures, costly catalysts, use of toxic reagents, acidic media and organic solvents. To avoid these drawbacks, development of more simple, inexpensive, green and efficient protocols are highly demanded.

We now report a simple and an efficient route for the synthesis of 2,4,6-triarylpyridines (**3**) using aromatic aldehydes **(1)**, ketones **(2)**, and ammonium acetate in the presence of $AlCl_3$ or Oxalic acid under solvent-free at 120^0C Scheme 1.



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References:

[1] Chubb, F. Hay, A. S.; Sandin, R.B.; *J. Am. Chem. Soc.* **1953**, 75, 6042.
[2] Heravi, M. M.; Bakhtiari, K.; Daroogheha, Z.; Bamoharram, F. F.; *Catal. Commun.* **2007**, *8,* 1991.
[3] Tu, S.; Li, T.; Shi, F.; Fang, F,; Zhu, S.; Wei, X.; Zong, Z.; *Chem. Lett.* **2005**, *35*, 732
[4] Nagarapu, L.; Peddiraju, A. R.; Apuri, S.; *Catal. Commun.* **2007**, *8,* 1973.
[5] Tu, S.; Jia, R.; Jiang, B.; Zhang, J.; Zhang, Y.; Yao, C.; Ji, S.; *Tetrahedron* **2007**, *63,* 381.
[6] Ren, Y. M.; Cai, C.; *Monatsh Chem*. **2009**, *140,* 49.

Solid acids as a novel catalytic system for synthesis of 1, 3, 5-triaryl-1,5-pentandiones

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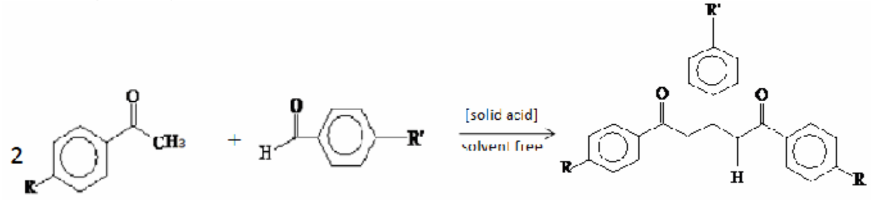
In view of green chemistry, the substitution of harmful liquid acids by reusable solid acids as catalysts in organic synthesis is the most promising application [1].

Recently, solid acids as environmentally friendly and economically viable catalyst are increasing continuously owing to their ease of handling, low cost, high catalytic activity, process simplicity and comparably easy work-up [2].

Although, 1,3,5-triaryl-1,5-pentandiones are used as the important precursors in synthesis, however the general methods used for synthesis of these compounds have some draw backs such as using harsh media and low yields.

Looking for cleaner alternatives to classical synthesis [3] and in developing green chemistry and also in pursuing our new interest, we report herein studies of some solid acids as efficient catalysts for synthesis of 1,3,5-triaryl-1,5-pentandiones from corresponding aldehydes and ketones.



References:

[1] K.Y. and Y. Lee Ko, Bull. *Korean Chem. Soc*. 25 (**2004**), p. 1929.
[2] F. Shirini, M.A. Zolfigol, P. Salehi, *Curr. Org. Chem*. 10 (**2006**) 2171.
[3] A. Mouradzadegun and N. Gheitasvand, *Phosphorus Sulfur Silicon* 180 (**2005**), p. 1385

Synthesis and characterization of cationic UV-curable polyurethane dispersion

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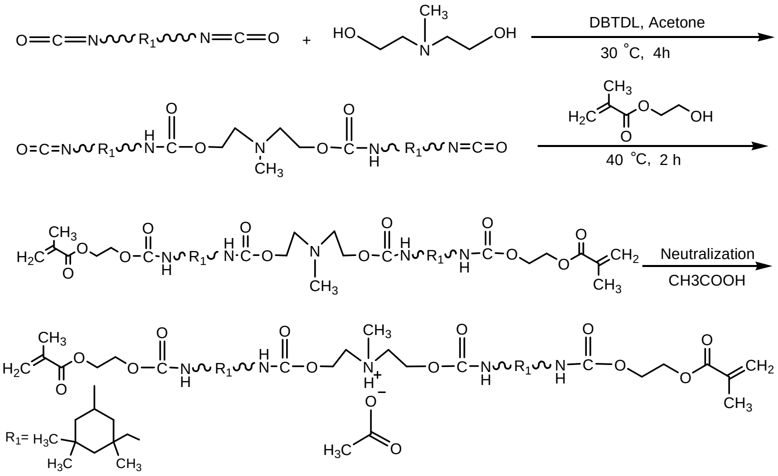
The cationic UV-curable polyurethane dispersions are unsaturated macromonomer with amine functional group that can disperse in water. These were synthesized in three steps. In the first step, macromonomer diisocyanate which has amine group was prepared by isophorone diisocyanate (IPDI), N-methyldiethanolamine in presence of acetone as solvent and dibutyldtin dilaurate (DBTDL) as catalyst. Then, unsaturated macromonomer was prepared by reaction of amine functionalized macromonomer diisocyanate and hydroxylethyl methacrylate (HEMA). Finally the last step involved neutralization and dispersion in water, where amine functional polyurethane was neutralized by the addition of acetic acid. The cationic UV-curable polyurethane dispersions have been characterized with ^{1}H-NMR, FT-IR and GPC.



References:
[1] Kim Y.; Kim H.; Yoo J Hong J. *Surface and Coatings Technology*. **2002**, *157*, 40.
[2] Yang Z.; Wicks D.; Yuan J.; Pu H.; Liu Y. *Polymer*. **2010**, *51*, 1572.
[3] Subramani S.; Cheong I.; Kim J. *European Polymer Journal*. **2004**, *40*, 2745.

Triphenylphosphine mediated reaction between 4-hydoxypyridine and dialkyl acetylenedicarboxylates

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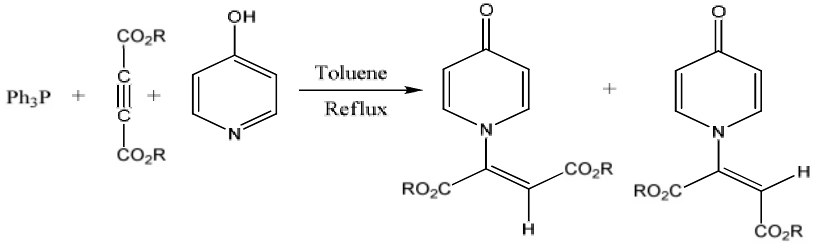
The addition reaction between electron-deficient acetylenic compounds and nitrogen-containing hetrocycles has been extensively investigated[1,2].We report herein that dialkyl acetylendicarboxylates undergo addition reaction with 4-hydroxypiridine in the presence of triphenylphosphine,yielding dialkyl 2-(4-oxopyridin-1(4H)-yl)fumarate and dialkyl 2-(4-oxopyridin-1(4H)-yl)maleate derivatives (**3,4**).The reaction of triphenylphosphine with acetylenic ester **1** in the presence of 4-hydroxypyridine **2** affords products **3,4** in good yields(Scheme 1).The structure of 3,4 were deduced IR, H NMR, C NMR spectra.The mass spectra of **3,4** are fairly similar and display molecular ion peaks.



1 **2** **3** **4**

R=Me,Et,*tert*-butyl

Scheme 1

The reaction of 4-hydroxypyridine with acetylenic esters in the presence of triphenylphosphine provides a simple one-pot entry into the synthesis of compounds of potential interest.This procedure has the advantages of high yields, mild reaction condition, and simple experimental and work-up condition.

Reference:

[1] Acheson, R. M.; Elmor, N. F. *Adv. in hetro. Chem*. **1978**, *23*, 263
[2] Yavari, I.; Alborzi, A. R.; Mohtat, B. *J. Chem. Res.* **2007**, 401

Synthesis,characterization, and theorrical study of a new optically active azo dye derived from binaphtol.

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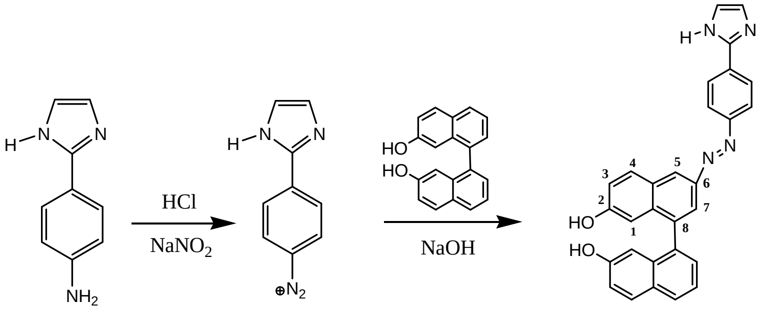
Azo dyes are compounds that contain azo groups linked to methine or aromatic sp2 hybridized C atoms [1]. The formation of diazotizing reagent starts with protonation of nitrous acid under strongly acidic conditions and azo coupling occurs at low tempreture in the presence of nucleophilic coupling components. BINOL and its derivatives have been extensively used to provide a chiral environment in asymmetric synthesis [2]. Recently synthesis of chiral azo dyes based on BINOL as an auxiliary have been investigated [3].



(R), (S), (R, S)

In the present study synthesis and characterization of a new optically active azo dye was reported. The coupling occurs at the position 6 in the BINOL molecule. We present a new azo reactive dye from racemic or optically active BINOL. This dye was characterized by UV–Vis, FTIR, mass, H-NMR, and C-NMR spectroscopic techniques. In addition theoretical studies on the structure and physical properties of titled compound achieved using density functional theory (DFT) using standard 6-31G(d) basis function.

References:

[1] Zollinger, H. Color chemistry, 3rd ed.; Helvetica Y. Chimica Acta: Switzerland, **2003**.
[2] Noyori, R. Asymmetric Catalysis in Organic ; Wiley: New York, NY, **1994**.
[3] Teimouri, A. ; Chermahini, A. N.; Emami, M. *Tetrahedron*. **2006**, *71*, 5888.

Synthesis of 1,2-bis(ethoxycarbonylmethyl)-4-phenyl-1,2,4-triazolidine-3,5-dione

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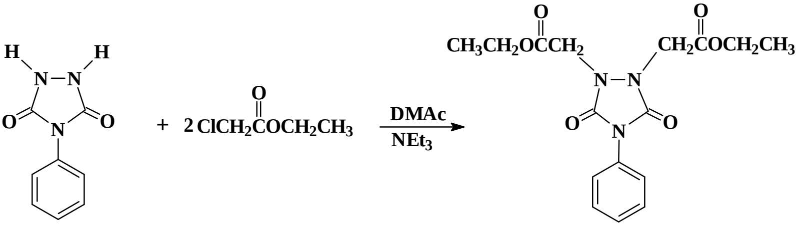
Five–membered heterocyclic compounds are important components of biologically active natural products and synthetic compounds of medicinal interest [1]. Among them, urazoles are an important class of drugs, which can provide a wide variety of aliphatic and aromatic substituents at position 4. Urazole derivatives have two N-H protons which are acidic. Thus they are used as monomers for the synthesis of new heterocyclic polymers [2, 3]. Anti-cancer property of some urazole derivatives has been improved in human and murine. Another biological property of urazoles is their hypolypidemic activity in blood, via lowering both the cholesterol level and triglyceride value [4]. Also urazoles are used as pesticides, herbicides, and insecticides. Manufacturing of thermoplastics, heat resistant coatings, and tire with high greapability and melamine resins are the other urazole applications [5, 6].

Because of low thermal stability of polyamides and polyureas derived from urazoles, we decided to prepare new monomer(s) based on 4-phenylurazoles, in which the nitrogen atom of the urazole is attached directly to the non-electrophilic group or atom, instead of carbonyl group in polyamide and polyureas synthesized by us. To achieve this goal, 4-phenylurazole was reacted with two moles of ethylchloroacetate in dimethylacetamide (DMAc) in the presence of triethylamine as scavenger. The resulting product, 1,2-bis(ethoxycarbonylmethyl)-4-phenyl-1,2,4-triazolidine-3,5-dione, was obtained in excellent yield, and identified by IR and ^{1}H-NMR methods. Various polymerization reactions of the target monomer are under investigation.



References:

[1] Zolfigol, M.A.; Shahamirian, M.; Safaiee, M.; Mallakpour, S.; *Tet. Lett.* **2005,** 5581.
[2] Mallakpour, S. E.; Rafiee,Z.; *European Polymer Journal*, **2007**, *43*, 1510.
[3] Mallakpour, S. E.; Nasr-Isfahani,H.; *Polymer Science, Ser. B*, **2001,** *43*, 1.
[4] Simlot, R.; Izydore, R. A.; Wong, O. T.; *J. Pharm. Sci.*, **1993,** *82*, 408.
[5] Bausch, M. J.; David B.; *Annu. Conf. Mater. Technol*, **1991,** *7th*, 41.
[6] Rottmaier, L.; Merten, R.; *Ger Offen.* **1982**, 3,106,944.

Synthesis of 2-aryl-1-arylmethyl-1*H*-benzimidazoles catalyzed by $Cu(PF_6)(CH_3CN)_4$, $Cr(Cl)_3$ or $Sr(NO)_3$

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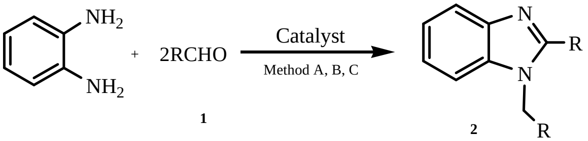
The benzimidazole nucleus is of significant importance to medicinal chemistry and many benzimidazole-containing compounds exhibit important biological activities such as selective neuropeptide YY1 receptor antagonism, and as 5-lipoxygenase inhibitors for use as novel antiallergic agents, factor Xa (FXa) inhibitors, poly (ADP-ribose) polymerase (PARP) inhibitors, and as human cytomegalovirus (HCMV) inhibitors.

The synthesis of benzimidazoles traditionally involves the condensation of *o*-phenylendiamine with aldehydes, and carboxylic acids or their derivatives (nitriles, amidates, orthoesters) under harsh dehydrating conditions. Benzimidazoles have also been prepared on solid-phase to provide a combinatorial approach.

Another approach reported to these compounds is the reaction of *o*-phenylenediamine with aldehydes in the presence of catalysts under various reaction conditions. [1-4]

Recently, a one-pot solvent-free synthesis of biologically active benzimidazole derivatives using a simple grinding method, [5] and also under the heterogeneous catalysis of Amberlite IR-120 has been reported.

We report here a series of 2-aryl-1-arylmethyl-1*H*-1, 3-benzimidazoles **2** were prepared in high to excellent yields by three methods (A, B, C).



Method A: $Cu(PF_6)(CH_3CN)_4$ (reflux (80 °C))
Method B: $Cr(Cl)_3$ (Microvawe Solvent-Free and r.t conditions)
Method C: Sr(NO)3 (Microvawe Solvent-Free and r.t conditions)

References:

[1] Perry, R. J.; Wilson, B. D.; *J. Org. Chem.* **1993**, 58**,** 7016.
[2] Anastasiou, D.; Campi, E. M.; Chaouk, H.; Jackson, W. R.; *Tetrahedron* **1992,** 48 , 7467.
[3] Perumal, S.; Mariappan, S.; Selvaraj, S.; *ARKIVOC,* **2004,** 8**,** 46.
[4] Thakuria, H.; Das, G.; *ARKIVOC* **2008**, 15**,** 321.
[5] Sharma, S. D.; Kowar, D.; *Synth. Commun*. **2009**, 39**,** 980.

K60 Silica as a reusable and low cost heterogeneous catalyst for Peptide synthesis

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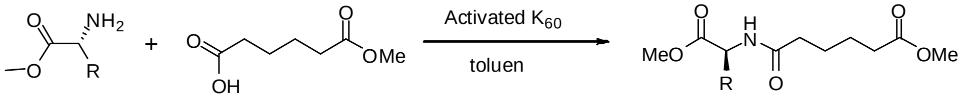
The amide bond plays a major role in the elaboration and composition of biological systems [1]. It is one of the most important linkages in organic chemistry and constitutes the key functional group in peptides, polymers and many natural products and pharmaceuticals. But their synthesis is still troublesome. The American Chemical Society Green Chemistry Institute Pharmaceutical Roundtable recently identified amide formation as one of the most utilized and problematic syntheses in the pharmaceutical industry and as such have been labeled as a high priority research area. [2].

In this work, we have developed a heterogeneous silica catalyst that can effectively catalyse amide synthesis from aminoacids derivatives and acids or other aminoacid derivatives, without production of toxic by-products according to the following reaction.



References

[1] Han, S.-Y.; and Kim Y.-A.; *Tetrahedron* **2004**, *602*, 447–2467.
[2] Yang, X.D.; Zeng, X.H.; Zhao, Y.H.; Wang, X.Q.; Pan, Z.Q., Li, L.; and Zhang, H.B.; *J. Comb. Chem.* **2010,** *12*, 307–310.

Potassium aluminum sulfate (alum): An efficient catalyst for the synthesis of pyrimido[4,5-*d*]pyrimidines

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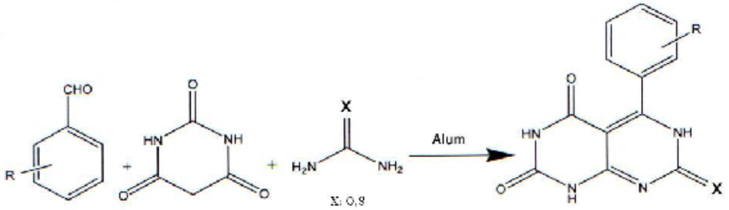
Derivatives of pyrimido pyrimidine are known to display a wide range of pharmacological activities. Numerous reports delineate the antitumour, antiviral, antioxidant, antifungal and heptatoprotective activities [1-3].

Also, Biginelli reactions are ranked as one of the most powerful tools for the facile synthesis of complex heterocyclic scaffolds for therapeutic and pharmacological properties. In recent decades, the scope of the original Biginelli reaction was extended by variation of the 1,3-dicarbonyl compound building blocks [4,5].

Herein, we wish to report for the first time an efficient, facile and solvent free procedure for the synthesis of pyrimido[4,5-*d*]pyrimidines by the reaction of aldehydes, barbituric acid and urea/thiourea in presence of catalytic amount of alum as catalyst. An advantage of this catalyst is that it is non-toxic, reuseable and inexpensive. Easy isolation of products, avoids problems connected with conventional solvent use, completely compatible with environment are other advantages of this procedure.



References

[1] Sanghhvi, Y. S.; Larson, S. B.; Matsumoto, S. S.; Nord, L. D.; Smee, D. F.; Willis, R. C.; Avery, T. H.; Robins, R. K.; Revankar, G. R. *J. Med. Chem*. **1989**, *32*, 629.
[2] Tenser, R. B.; Gaydos, A.; Hay, K. A. *Antimicrob. Agents Chemother*. **2001**, *45*, 3657.
[3] De la Cruz, J. P.; Carrasco, T.; Ortega, G.; Sanchez Dela Cuesta, F. *Lipids*. **1992**, *27*, 192.
[4] Stadler, A.; Kappe, C. O. *J. Chem. Soc. Perkin. Trans. 1* **2000,** 1363.
[5] Ranu, B. C.; Hajra, a. Jana, U. *J. Org. Chem.* **2000,** *65*, 6270.

Solvent-free Beckmann rearrangement of ketoximes over melamine-formaldehyde resin supported anhydrous ferric chloride

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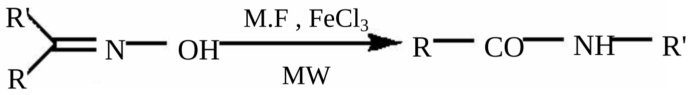
The Beckmann Rearrangement, a most important and useful transformation in synthetic chemistry [1], is generally effected starting from an oxime that is derived from the corresponding ketones [2]. Many reagents have been used in the Beckmann rearrangement of ketoximes in solution [3]. However most of them are strong Bronsted acids and cause serious problems on starting materials and products.

Here we present a convenient and efficient method for isomerization of ketoximes into the corresponding amides by the cheap and commercially available Melamine-formaldehyde resin supported anhydrous ferric chloride in the absence of solvent. Symmetrical oximes were converted to the corresponding amides in good yields. In the case of unsymmetrical oximes the reaction was stereoselective and one of the two amides produced mainly. The present procedure not only has the chemical, economical and environmental advantages of solvent-free reactions but also constitute a method for good yield Beckmann rearrangement of symmetrical and unsymmetrical ketoximes.



M.F: Melamine-formaldehyde resin
MW: Microwave

References:

[1] Craig, D.;*Comprehensive Organic Synthesis*, Pergamon Press, Oxford, **1991**, *Vol 7*, 689.
[2] Khodaei, M.M.; Meybodi, F.A.; Rezai, N.; Salehi, P.; *Synth. Commun*, **2001**, *31*, 2047.
[3] Luca, L. D.; Giacomelli, G.; Porcheddu, A.; *J. Org. Chem*. **2002**, *67*, 6272.

Trichloroisocyanuric acid as an efficient catalyt for the synthesis of 2-oxazolines and 2-imidazolines

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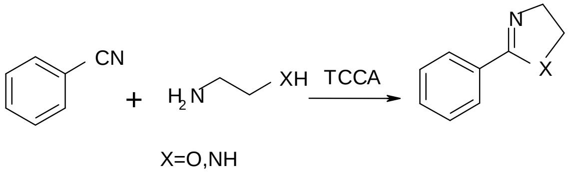
2-Oxazolines and 2-imidazolines are very important moieties due to their extensive applications in chemistry, biochemistry and pharmacology. These heterocycles are found in the structures of many biologically active natural products. They also exhibit several pharmaceutical activities such as antidiabetic, antihypertensive, antidepressive , anticancer , anti HIV-1 antitumor and antialzheimer activities [1].

There are several methods for the synthesis of 2-imidazolines and 2-oxazolines from carboxylic acids, esters, nitriles , orthoesters , hydroximoylchlorides, hydroxy amides , and mono or di-substituted (chlorodicyanovinyl) benzene. However, some of the methods which are reported, suffer from disadvantages such as long reaction times, low yields, difficulty in preparation of starting materials and tedious work-up, acidic conditions, use of complex reagents and toxic solvents[2].

Herein we wish to report an efficient catalytic procedure for the synthesis of 2-oxazolines and 2-imidazolines under solvent-free conditions. Different nitriles reacted with ethylenediamine or 2-aminoalcohole in the presence of catalytic amounts of TCCA to afford corresponding 2-oxazolines and 2-imidazolines in high yields. short reaction times, high yield of products, absence of solvent, mild reaction conditions and availability, stability, non-toxicity and cheapness of the catalyst are noteworthy advantages of the present work. Furthermore, mono- and bis-oxazolines and mono-imidazolines were generated from dinitriles by the current method.



References:

[1] Mohammadpoor-Baltork , I.; Moghadam, M.; Tangestaninejad, Sh.; Mirkhani, V.; Hojati, S.F. *Catal.Commun*. **2008**, *9*, 1153.

[2] Mirkhani, V.; Mohammadpoor-Baltork , I.; Moghadam, M.; Tangestaninejad, Sh.; Abdollahi-Alibeik, M.; Kargar, H. *Appl.Catal*. **2007**, *325*, 99.

Theoretical study of the tramadol and its derivatives properties

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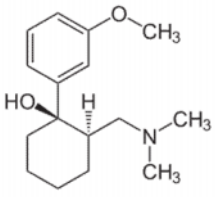
Tramadol ((1RS,2RS)-2-[(dimethylamino)methyl]- 1-(3-methoxyphenyl)cyclohexanol) is a centrally-acting analgesic, used for treating moderate to moderately severe pain. It is a synthetic stripped-down piperidine-analog of the phenanthrene alkaloid codeine and, as such, is an opioid and also a prodrug. The opioid agonistic effect of tramadol and its major metabolite(s) are almost exclusively mediated by the substances action at the μ-opioid receptor [1]. This characteristic distinguishes tramadol from many other substances (including morphine) of the opioid drug class, which generally do not possess tramadol's degree of subtype selectivity. However, the mechanism of action of tramadol remains unclear because its binding affinity for opioid receptors appears to be too low to account for the antinociceptive effect via this system, and the noradrenergic and serotonergic involvement is still not completely understood [2].

In this study, the effect of an electron-donating group and an electron-withdrawing group on the electronic and geometric properties of the tramadol is calculated by quantum mechanical, DFT-B3LYP method using 6-31++G** basis set. All computations were performed using Gaussian 03 package.



(1*R*,2*R*)-tramadol

The obtained results show that using both electron donating and electron withdrawing groups that located in four aromatic regions in benzene ring is one method for tailoring the electronic properties of the tramadol and its analogue molecules. Furthermore, it can conclude that new appropriate groups can be used to designing new molecules with new performance.

References:

[1] H. Sindrup, S.; Andersen, G.; Madsen, C.; Smitha, T.; Brùsenb, K.; S. Jensenc, T.; *Pain* **1999**, *83*, 85.

[2] Oliva, P.; Aurilio, C.; Massimo, F.; Grella, A.; Maione S.; Grella, E.; Scafuro, M.; Rossi, F,; Berrino, L.; *Eur. J. Pharm.* **2002**, *445*, 179.

Highly efficient synthesis of new heterocyclic systems: [2,5-bis-(4-chloro-phenyl)-[1,3]-dioxol-4-yl]-cyclohexyl-amine derivatives

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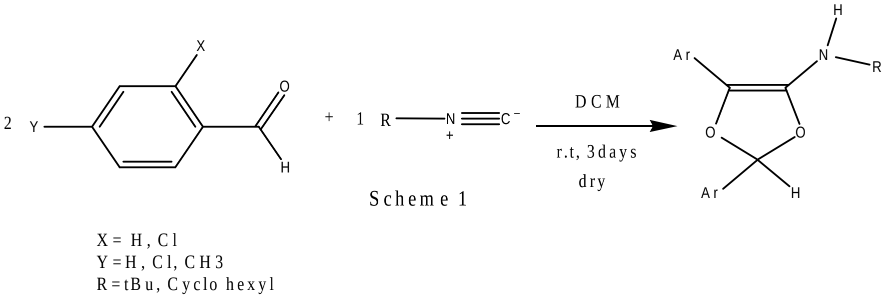
Dioxols are a branch of heterocyclic compounds having a diversity of biological effects such as exhibited antibacterial activity against Pseudomonous aeruginosa, and antifungal activity against Aspergillus fumigates [1]. To the best of our knowledge, there are no reports on the synthesis of these compounds using isocyanides in the literatures.

As part of our ongoing development of efficient protocols for the preparation of biologically active heterocycles from common intermediates using isocyanide-based reactions, [2] and electron deficient compounds, [3,4] we herein report an efficient one-pot reaction of alkyl isocyanides and aromatic aldehydes (1:2 ratio) in dry dichloromethane at room temperature, which afforded a heterocyclic system of [2,5-Bis-(4-chloro-phenyl)-[1,3]-dioxol-4-yl]-cyclohexyl-amine derivatives in high isolated yields in the absence of any catalyst (Scheme 1).

^{1}H and ^{13}C NMR spectrum of the crude products clearly indicated the formation of 1,3-dioxol **3**. Any product other than **3** could not be detected by NMR spectroscopy. The structures of the products **3** were deduced from their IR, Mass, ^{1}H and ^{13}C NMR spectrum.

The present method carries the advantages that, not only is the reaction performed under neutral conditions, but the substances can be mixed without any activation or modification. In addition to the reaction is simple, clean and high yield.



Scheme 1

Reference:

[1] Ishizuka, N.; Matsumura, K. I.; Kikuchi, J.; Nakai, H. *Bioorg. Med. Chem.* **2002**, *10,* 3965.
[2] Bayat, M.; Imanieh, H.;Abbasi, H. *Helv. Chim. Acta* **2010**, *93*, 757.
[3] Bayat, M.; Imanieh, H.; Zabarjad, N. S. *Monatsh. Chem* **2010**, *14*, 333.
[4] Bayat, M.; Imanieh, H. Hosseininejad, E. *Synth. Commun.* **2008**, *38*, 1532.

Synthesis and structure of dihydropyrroles and α,β-unsaturated dicarbonyl compounds

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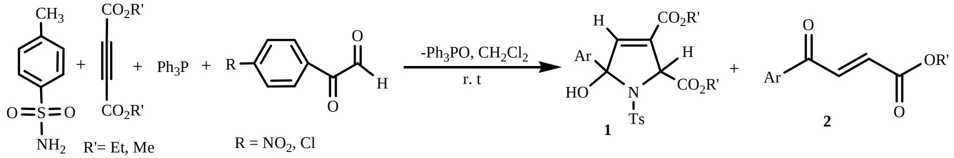
Recently, considerable attention has been paid to the multi-component reactions (MCRs) which led to the synthesis of heterocycles [1]. Accordingly, many procedures have been developed for the application of MCRs to providing nitrogen-containing heterocycles [2]. Of these reactions, the three-component condensation of phosphines, active acetylene and *NH* active stand as an area of research for synthesis of heterocyclic compounds [3]. Recently, we report the synthesis of functionalized pyrroles using this strategy. Due to the pharmacological activity of sulfonamides [4] and in continuation of our work, we decided to investigate the reaction of NH sulfonamides, triphenylphosphine and dialkyl diacetylenedicarbonylate (DMAD or DEAD).

Here in we report, reaction between sulfonamides, substituted phosphorous ylied and arylglyoxals to produce new 2,5-dihydropyrrols or *α*,*β*-unsaturated diketones based on the kind of substituents under neutral mild conditions.



Entry	R'	Ar	Yeild (%)
1	Me	4-$NO_2C_6H_4$	79
	Et	4-$NO_2C_6H_4$	80
2	Me	4-$NO_2C_6H_4$	80
	Et	4-ClC_6H_4	78

References:

[1] Mukhopadhyay, C.; Kumar, P. T.; Butcher, R. J.; *Tetrahedron Lett*. **2010**, *51*, 1797.
[2] Rahmati, A. *Tetrahedron Lett*. **2010**, *51*, 2967.
[3] Yavari, I.; Adib, M. *Tetrahedron*. **2001**, *57*, 5873.
[4] G. T. Brooks, in L. A. Dmiani (Eds.) *The Sulfur Containing Drugs and Related Organic Compounds,* Ellis Harwood, NewYork, **1998**, 1, 60.

Synthesis of bis(indolyl)methanes using trifluoroethanol as a homogeneous and recyclable medium

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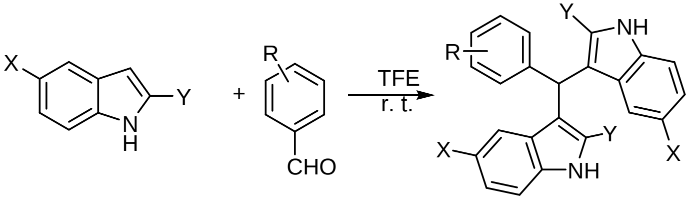
Indole and its myriad derivatives continue to capture the attention of synthetic organic chemists, and a large number of original indole ring syntheses and application of known methods to problems in indole chemistry have been repoted [1]. Development of bis(indolyl)alkane synthesis has been of considerable interest in organic synthesis because of their wide occurrence in various natural products possessing biological activity [2] and usefulness for drug design [3]. Bis(indolyl)methanes are most active cruciferous substances for promoting beneficial estrogen metabolism and inducing apoptosis in human cancer cells. Consequently, numerous methods have been reported for the synthesis of bis(indolyl)methanes [4]. Herein we report the results of our studies involving electrophilic substitution reactions of indoles with various aldehydes were carried out in trifluoroethanol as a homogeneous and recyclable medium at room temperature in the absence of any other catalyst to afford bis(indolyl)-methanes in good yields.



References:

[1] Gribble, G. W. *J. Chem. Soc., Perkin Trans.* **2000**, *1*, 1045.
[2] Bell, R.; Carmeli, S. *J. Nat. Prod.* **1994**, *57*, 1587.
[3] Sundberg, R. J. *The Chemistry of Indoles*, Academic, New York, **1996**.
[4] Chakrabarty, M.; Basak, R. *Heterocycles* **2001**, *55*, 2431.

Cation–π interactions: structures and absolute binding energies of alkali and alkaline earth cation-indole complexes

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The interaction of metal ions with the π surfaces of aromatic molecules, a central and traditional concern of organometallic chemistry, is receiving a good deal of new attention. Indole is an especially important model molecule for developing understanding of biologically interesting cation/π interactions, inasmuch as it is the side chain of tryptophan, and thus serves to model binding sites widely available on proteins [1]. Thus, improving the understanding of the cation/π interactions of indole is highly relevant to thinking about where and how strongly various types of metal ions will approach, interact with, and bind to exposed tryptophane sites [2].

In this work , we study the interaction of indole with alkali and alkaline earth cations (Li^+, Na^+ , K^+, Mg^{2+} and Ca^{2+}), and determine metal ion affinities (MIA in Kcal/mol) for it. The metal ion affinity is determined from the difference between the total energy of the indole…M^{n+} complex and the sum of the total energies of M^{n+} and indole [3]. All of the calculations are done using Spartan software. Geometry optimization, frequency calculation are done using B3LYP/6-311++G(d,p) method.

References:

[1] Dunbar, R. C.; *J. Phys. Chem. A.* **1998**, *102*, 8946.
[2] Srinivasa Rao, J. ; Zipse, H. ; Narahari Sastry, G. ; *J. Phys. Chem. B.* **2009**, *113*, 7225.
[3] Cheng, Y. ; Liu, L. ; Fu, Y. ; Li, X. S, ; Guo, Q. X. ; *J. Phys. Chem. A.* **2002**, *106*, 11215.

Synthesis of 3,5-bis(arylidene)-1-benzylpiperidin-4-ones as potential cytotoxic agents

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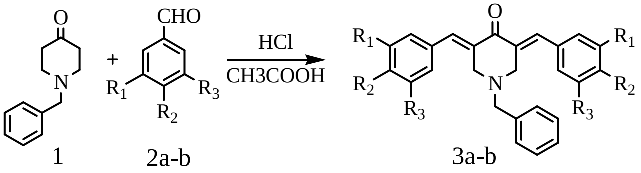
The incidents and mortality of breast cancer among woman worthwith have become one of the most important medical issues.several important drugs including Adriamycim (ADR), Vincristin (VCR) and Etopside (VP16) with different structures and mechanisms of anti-tumor activities fail to be effective due to drug resistance [1].

A number of α,β – unsaturated ketones display cytotoxic and anti cancer properties [2,3]. 3,5-bis(arylidene)-4-piperidones were prepared as candidate cytotoxic agents with a view to discrining those structure features which contributed to bioactivity. A claisen-schmidt condensation between 1-benzylpiperidin-4-one and the appropriate aryl aldehyde led to the formation of the 3,5-bis(arylidene)-4-piperidones [4].

Herein, we described the synthesis of 3,5-bis(arylidene)-4-piperidones as potential cytotoxic agents. The synthetic pathway is outlined as shown in the scheme.



1 2a-b 3a-b

R_1 = H, Br
R_2 = OH, OMe
R_3 = OMe

Referenece:

[1] Rasoul-Amini, S.; Khalaj, A.; Shafiee. *International Journal of Cancer Research 2,* **2006**, *2,* 102.
[2] Dimmock, J. R.; Elias, D. W.; Beazely, M. A. *Med. Chem.***1999**, *6*, 1125.
[3] Dimmock, J. R.; Kandepu, N. M.; Nazarali, A. J. *J. Med. Chem.***1999**, *42*, 1358.
[4] Dimmock, J. R.; Padmanilayam, M.P.; Puthucode, P.N. *J. Med.Chem.* **2001**, *44*, 586.

β-cyclodextrin based polyurethanes as a novel recoverable catalyst nucleophilic substitution reaction: preparation benzyl acetate

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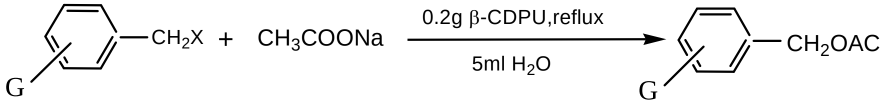
The removal of toxic contaminants from water remains a huge challenge for water supplying companies and municipalities. Liu et ai. Reported that CDs have a non-polar cavity which provides a micro-environment for the encapsulation of non-polar, low molecular weight compounds.They have been utilized extensively in chromatographic separations and purification methods[1].However, CDs are slightly soluble in water which limits their sole application for water treatment purposes,functionalisation and, in particular, polymerization of the parental CDs with suitable bi-functional linkers make them insoluble. β-cyclodextrin polyurethanes (β-CDPU) polymer was synthesized by the reaction of β-cyclodextrin with hexamethylene diisocyanate in dry dimethylformamide and widely tused as a sorbent for the solid phase extraction (SPE) of carcinogenic compounds from water[2]. since the study of organic reactions in water is special important and with regard to properties listed for β-CDPU use this polymer as a phase transfer catalyst in organic reactions were evaluated.

In this study it is proved that β-CDPU can be used as an efficient solid liquid phase transfer catalyst for nucleophilic substitutions reaction of benzyl halides with acetate ion in water to give benzyl acetates in excellent yield under mild reaction conditions. The polymeric catalyst easily recovered by simple filtration, shows no appreciable loss of activity when recycled several times.



Refrence:
[1] Bhaskar, M. ; Aruna, P.; Ganesh Jeevan, R. J.; Radhakrishan, G., *Analytica chimica Acta*. **2004,** *509*, 39.
[2] Schurig, V.; Nowotny, H. P., *Angew. Chem*. **1990**, *102*, 969.

Synthesis of acetaminophen by liquid phase Beckmann rearrangement of hydroxyacetophenone oxime over nano-ordered Zn-MCM-41

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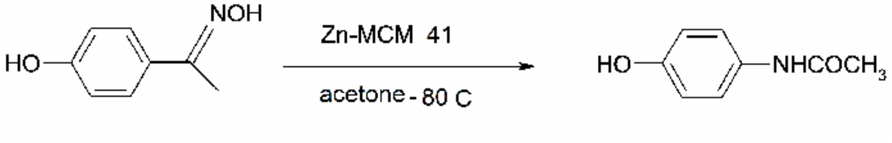
The rearrangement of ketoximes to amides or lactams in the presence of acid catalysts is a process commonly used for the preparation of acetaminophen (N-acetyl-*p*-aminophenol or). Acetaminophen is a valuable non-steroidal anti-inflammatory drug in widespread use for the treatment of pain and fever. Acetaminophen is a pharmaceutical for human consumption and the product has to be as pure as possible. Therefore, trace impurities from catalytic species or corrosion products are not allowed.

Preparation of acetaminophen involves a two-step process. The first step involves reacting 4-hydroxyacetophenone with hydroxylamine hydrochloride to obtain the corresponding ketoxime (4-hydroxyacetophenone oxime) followed by the Beckmann rearrangement in the presence of an acid catalyst, such as fuming sulfuric, hydrochloric, trifluoroacetic, methanesulfonic or *p*-toluenesulfonic acids, amberlyst, nafion, or thionyl chloride in liquid sulfur dioxide. The use of homogeneous acid catalysts requires tedious workup procedures and the necessary neutralization of the strong acidic media, produces undesired wastes.

Solid acid catalysts present clear advantages over the conventional homogeneous acid catalysts used commercially for the preparation of acetaminophen. In this work, acetaminophen was synthesized by an environmentally benign synthetic method over Zn-MCM-41. Zn-MCM-41 is very active and selective for the preparation of acetaminophen by Beckmann rearrangement, achieving good conversion of oximes in relatively short reaction time.



References:

[1] Silvestre-Albero, J.; Sepu´lveda-Escribano, A.; Rodrı´guez Reinoso, F. *Microporous and Mesoporous Materials*. **2008**, *113,* 362.

[2] Ghiaci , M.; Aghaei ,H.; Oroojeni ,M.; Aghabarari ,B.; Rives ,V.; Vicente ,M.A.; Sobrados , I.; Sanz,J. *Catalysis Communications* **2009**, *10,* 1486.

Synthesis of anti-corrosion inorganic-organic (Ca MoO_4 /polyaniline) nano capsules by green chemistry and study of its corrosion inhibition

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Current coating systems for corrosion protection consist largely of zinc/chromate primers and chromium conversion coatings. While these coatings have been proven to prevent corrosion, they continue to come under increased scrutiny from the Environmental Protection Agency (EPA). Some of the primary concerns of the EPA and the Navy are the dangers involved with the handling toxic materials, the leaching of these metals into marine environments, and the environmental and economic aspects of the safe disposal of these materials. Replacing hexavalent chromium and heavy metal additives in coatings will eliminate an environmental and health hazard resulting in annual cost savings of billions of dollars for military and commercial applications.

The majority of work done in the area of conducting polymers for corrosion inhibition has focused on polyaniline. These coatings are inexpensive and have been shown to work very well in acidic media. However, these coatings do not prevent corrosion or adhere to metal substrates in neutral and basic media such as seawater. Although, work is underway to improve the pH range of polyaniline corrosion inhibition. This polymer has been shown to inhibit corrosion as well as exhibit excellent adhesion to aluminum substrates in neutral and basic media. As this polymer and similar polymers continue to be shown to inhibit corrosion in a wide range of environments, they will likely replace hexavalent chromium and zinc in many systems.

Although these materials are interesting by themselves, composite materials made by “blending” conducting polymer with other organic or inorganic compounds2–6 have been prepared with the goal of improving, for example, the processibility or the mechanical resistance of the polymer. In addition, in some instances these composites may have unique properties which will be different from those of the individual components of the composite[1-4].

Herein we present synthesis of anti-corrosion inorganic-organic (Ca MoO4 /polyaniline) nano capsules by green chemistry and study of its corrosion inhibition.

This research has been done with cooperation of National Iranian South Oilfields Company.

References:

[1] (a) G. O. Ozin, Adv. Mater. **4**, 612 (1992); (b) E. Ruiz-Hitzky, Adv. Mater. **5**, 334 (1993).
[2] (a) C-G. Wu, D.C. DeGroot, H. O. Marcy, J. L. Schindler, C. R. Kannewurf, Y-J. Liu, W. Hirpo, and M. G. Kanatzidis, Chem. Mater. **8**, 1992 (1996); (b) L. Wang, J. Schindler, J. A. Thomas, C. R. Kannewurf, and M. G. Kanatzidis, Chem. Mater. **7**, 1753 (1995); (c) T. A. Kerr, H. Wu, and L. F. Nazar, Chem. Mater. **8**, 2005 (1996) and references therein.
[3] M. Wan, W. Shou, and J. Li, Synth. Met. **78**, 27 (1996).
[4] A. H. Gemeay, H. Nishiyama, S. Kuwabata, and H. Yoneyama, J. Electrochem. Soc. **142**, 4190 (1995) and references therein.

Preparation of novel thermally stable poly(ester-imide)s with improved solubility based on fluorene ring

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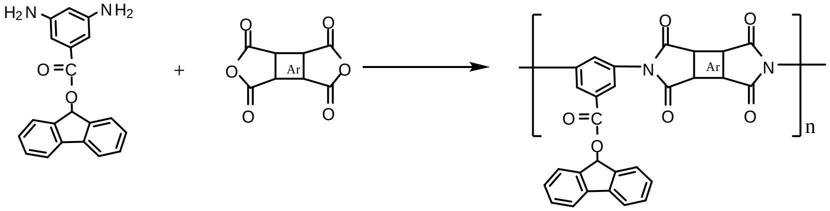
Thermally stable aromatic polyimides are polymers that exhibit favorable balance of physical and chemical properties and they are widely used in microelectronic and aerospace engineering [1]. Because of processing difficulties due to their high glass transition or melting temperature and poor solubility in most organic solvents, the technological and industrial applications of rigid polyimides are limited [2,3]. Preparation of modified polyimides with improved solubility and processability without sacrificing their thermal and physical properties was the main aim of this study. To extend the utility of these high performance polymers it has been a long desired goal to synthesize new diamines. Accordingly, the design and synthesis of new diamine with structural modifications were considered.

A novel ester diamine was synthesized via two successive reactions. Reaction of 9-hydroxy fluorene with 3,5- dinitrobenzoylchloride and subsequent reduction of nitro groups to amino groups. The new diamine was fully characterized and then was reacted with different dianhydrides for poly(ester-imide)s production.



The new polyimides were fully characterized and their properties were studied. These polymers showed nice balance of high thermal stability and improved solubility. Structural modifications including incorporation of fluorene bulky group, ester unit and meta-catenation were important modifications for preparation of these fully aromatic polyimides.

References:

[1] Kricheldorf, H.R.; Pakull, R. *Macromolecules.* **1998**, *21*, 551.
[2] Mehdipour-Ataei, S. ; Bahri-Laleh, N.; Amirshaghaghi, A. *Polym. Degrad. Stab*. **2006**, *91*, 2622.
[3] Jin, X.Z. ; Ishii, H. *J. Appl. Polym. Sci*. **2005**, *98*, 115.

A general and practical synthetic rout to 2-amino-4*H*-chromenes using NH_2-MCM-41 catalyst in water

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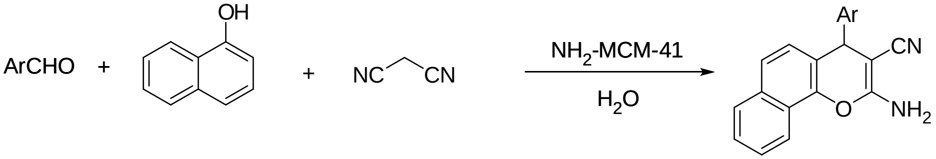
2-Amino-chromenes are widely employed as food additives, cosmetic agents and utilized as potential biodegradable agrochemicals [1]. Furthermore they are biologically active compounds with a wide spectrum of activities such as antimicrobial, mutagenicitical, antiviral, antiproliferative, antitumoral and central nervous system activities [2]. Thus the synthesis of 2-amino-4*H*-chromenes is of much importance to organic chemists [3].

In continuation of our investigations on the synthesis of 1,4-dihydropyridines (DHPs) and dihydropyrimidines (DHPMs) [4], herein we describe a simple and efficient method for the preparation of 2-Amino-4*H*-chromenes building blocks using functionalized NH_2-MCM-41 catalyst. In this work we introduce a new three-component condensation of aldehyde, malononitrile and an activated phenol in the presence of a catalytic amount of NH_2-MCM-41 catalyst in presence of water as a green solvent for synthesis of 2-amino-4-aryl-4*H*-benzo[*h*]chromene-3-carbonitrile derivatives. This efficient technique has the advantage to give 2-Amino-4*H*-chromenes using a base catalyst in good to high yields, to be completed in short reaction times and to offer a simple product isolation procedure.



References:

[1] Hafez, E. A.; Elnagdi, M. H.; Elagemey, A. G. A.; El-Taweel, F. M. A. A. *Heterocycles* **1987**, *26*, 903.
[2] Eiden, F.; Denk, F. *Arvh. Phrm. Weinheim Ger. (Arch. Pharm.)* **1991**, *324*, 353.
[3] Maggi, R.; Ballini, R.; Sartoria, G.; Sartorio, R. *Tetrahedron Lett*., **2004**, *45*, 2297.
[4] (a) Mirza-Aghayan, M., Moradi, A.; Bolourtchian, M.; Boukherroub, R. *Synth. Commun.* **2010**, *40*, 8; (b) Mirza-Aghayan, M.; Moradi, A.; Bolourtchian, M. *J. Iran. Chem. Soc.* **2010**, *7*, 269, (c) Mirza-Aghayan, M.; Khoshkameh Langrodi, M.; Rahimifard, M.; Boukherroub, R. *Appl. Organometal. Chem.* **2009**, *23*, 267.

A synthesis of phosphorylated dioxohexahydropyrimidines from N,N'-dimethylurea,activated acetylenes,and trialkyl phosphites

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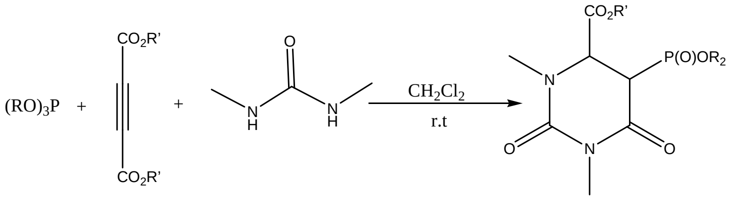
Multicomponent reactions, with three or more reactants combining in a one- pot procedure to give a single product, have become increasingly popular during the last decade[1].

Organophosphorus compounds, i.e., those bearing a carbon atom directly bound to a phosphorus atom , are synthetic targets of interest, not least due to their value for variety of industrial, biological, and chemical synthetic uses[2]. Organophosphonates have been used as substitutes of the corresponding esters and acides of relevant biological activity and as convenient probes for designing antibodies on the basis of trasition state models. As part of our current studies on the development of new routes to heterocyclic systems [3], we now report an efficient synthetic route to phosphorylated dioxohexahydropyrimidines.



References:

[1] Weber, L.; Multicomponent reaction and evolationary chemistry. *Drug discov Today* . **2002**, *7*, 143.
[2] Corbridg DEC Phosphorous. *An* outline of its chemistry biochemistry and uses5th edn, Elsevier, Amsterdam .**1995**.
[3] Yavari , I.; Hossaini, Z.; Sabbaghan , M.; Synthesis of functionalized 5-imino-2,5- dihydro-furans *Mol Divers.* **2006**, *10*, 479.

Reaction of vinylbenzylchloride copolymers with 9 anthracene carboxylic acid

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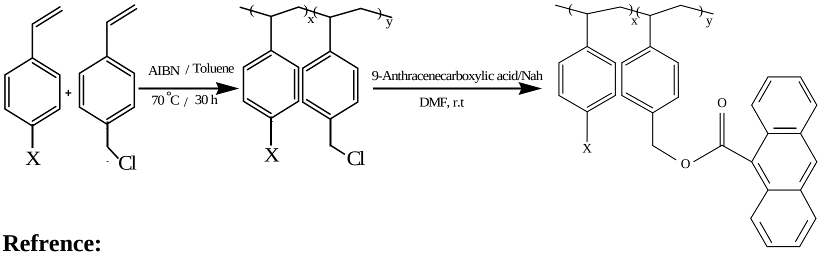
Vinylbenzylchlorid (VBC) can be easily polymerized with radical or cationic initiators [1]. Copolymerization reactions of VBC were performed with 4-methyl styrene and 4-methoxy styrene, in toluene at 70±1˚C using α,α′-azobis(isobutyronitrile) (AIBN) az the radical polymerization initiator and the copolymers I,II collected respectively in good yields. Polymers with chloromethyl group in the side chains are useful starting materials for the synthesis of various functional polymers [2].

The pendant chloromethyl group in the polymer can be modified readily by the substitution reactions with some nucleophilic reagents [3]. However, the employment of alkali metal salts of nucleophilic reagents is ordinary necessary for the reaction with pendant chloromethyl groups in the polymers [4].

The esterification reaction of polymers with salt of 9-anthracene carboxylic acid proceeded very smoothly to give the corresponding polymers with pendant ester residues. Characterizations of all the obtained polymers were performed with FT-IR and 1HNMR spectroscopic techniques. The glass transition temperature (Tg) of the copolymers (I,II) wasdetermined by dynamic mechanical thermal analysis (DMTA). The study of the DMTA curves for modified copolymers indicated that glass transition temperature values of the copolymers increase with incorporation of 9-anthracene carboxylate groups as side chains. The resulted copolymers are white solid and soluble in chloroform, dimethylsulphoxide and insoluble in nhexane, methanol, ethanol and water.



Refrence:
[1] D. Safa, K.; Eram, H.; Nasirtabrizi, M. H. *Iranian polymer Journal*. **2004**, 15(3), 249.
[2] Babazadeh, M. *International Journal of pharmaceutics*, **2006**, 316, 68.
[3] Shenhar, R.; Sanyal, A.; Rotello, M. *Macromolecules*, **2004**, 37, 92.
[4] D. Safa, K.; Nasirtabrizi, M. H. *polymer Bulletin*, **2006**, 57, 293.

A mild one-pot procedure for the conversion of aldehydes to methyl esters

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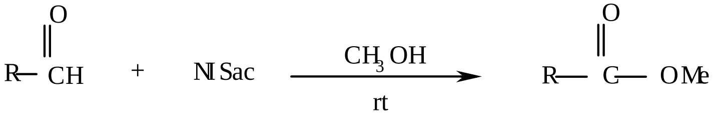
Esters are immensely important organic compounds due to their applications in a wide range of industrial products such as plasticizers, graphics, lubricants, flavours, perfumes and cosmetics [1]. The direct oxidative transformation of aldehydes to esters is an extremely useful and selective functional group interconversion in organic synthesis [2].

Although such functional group transformation of aldehydes to esters in the presence of alcohols has been reported, these methods usually require harsh conditions and are effective for a limited range of substrates. Several procedures involving oxone [3] and pyridinium hydrobromide perbromide[4] have been employed for the direct oxidative conversion of aldehydes to esters. This transformation generally involves an oxidative pathway and requires more than stoichiometric amount of oxidants and long reaction times. Also these reagents are unsatisfactory for aldehydes containing electronwithdrawing groups [5].

N-iodosaccharine has been used as an oxidant and halogenating agent which is simply prepared by halogenation of saccharin [6].

Herein we have reported simple, mild and efficient method for oxidative esterification of a variety of aldehydes with methanol in the presence of *N*-iodosaccharine in combination with K_2CO_3 at room temperature.



$$R-\overset{\overset{\displaystyle O}{\|}}{C}H + NISac \xrightarrow[rt]{CH_3OH} R-\overset{\overset{\displaystyle O}{\|}}{C}-OMe$$

R: alkyl, aryl

References:

[1] Sinha, A. K.; Sharma, A.; Swaroop, A.; Kumar, V. *Tetrahedron* **2007**, *63, 1000.*
[2] Karade, N. N.; Budhewar, V. H.; Katkar, A. N.; Tiwari, G. B. *Arkivoc* **2006**, *162.*
[3] Travis, B. R.; Sivakumar, M.; Hollist, G. O.; Borhan, B. *Org. Lett.* **2003**, *5, 1031*.
[4] Sayama, S.; Onami, T. *Synlett* **2004**, *2739.*
[5] Victor Paul Raj, I.; Sudalai, A.; *Tetrahedron Lett.* **2005**, *46, 8303.*
[6] Soraia, S.; Jaoquim, S.; Marco, D. *Synth. Commun.* **2003**, *33, 935.*

The effect of ultrasonic irradiation on the oxidation of 2-arylimidazolines with sodium periodate catalyzed by Mn(TPP)Cl supported on polystyrene

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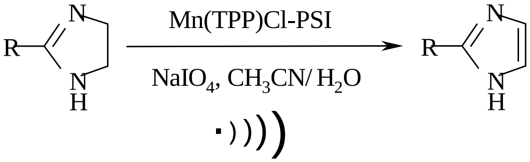
The chemical applications of ultrasound, ‘‘Sonochemistry’’, have become an exciting new field of research during the past decade. Ultrasound has increasingly been used in organic synthesis in recent years. A large number of organic reactions can be carried out in higher yields, shorter reaction times and milder conditions under ultrasonic irradiation [1]. Generally, ultrasonic waves were used to activate the catalyst [2].

2-Arylimidazolines can be easily prepared from nitriles and ethylenediamine [3]. Therefore, dehydrogenation of 2-imidazolines by an oxidizing agent should provide an efficient method for the preparation of imidazole derivatives [4].

In this work, the effect of ultrasonic irradiation on the oxidation of 2-arylimidazolines with sodium periodate by Mn(TPP)Cl supported on polystyrene-bound imidazole is reported. Mild reaction conditions, short reaction times and excellent yields are the main advantages of this method.



References:

[1] Li, J. T.; Li, X. L.;Li, T. S. *Ultrason.Sonchem*. **2006**, *13,* 200.
[2] Kun, I.; Török, B.; Felföldi, K.; Bartok, M. *Appl. Catal. A: Gen*. **2000**, *203*, 71.
[3] Mirkhani, V.; Moghadam, M.; Tangestaninejad, S.; Kargar, H. *Tetrahedron Lett.* **2006,** *47,* 2129.
[4] Mohammadpoor-Baltork, I.; Abdollahi-Alibeik, M.; Zolfigol, M. A. *Bioorg. Med. Chem. Lett.* **2004,** *14, 6079.*

A new synthesis of highly functionalized dialkyl 2-(4-hydroxyquinolin-3-yl)but-2-enedioate, alkyl 2-oxo-2H-pyrano[3,2-c] quinoline-4-carboxylate

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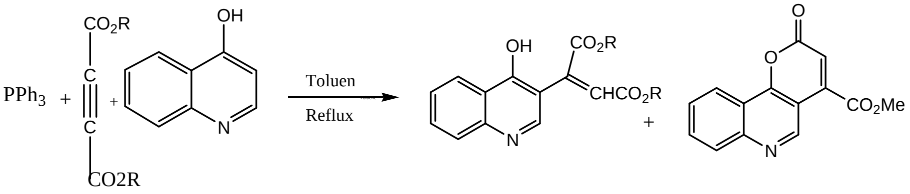
Coumarins fused with hetrocycles and aza-analogues of coumarins have received increasing attention due to their potential biological activities. In particular, those coumarins fused to pyridines have been reported to possess antiallergic, antidiabetic, and analgesic properties. In continuation of our current interest in the development of new routes to heterocyclic and carbocyclic systems we report herein that dialkyl acetylenedicarboxylates undergo addition reaction with 4-quinolinol in the presence of Ph_3P, yielding dialkyl 2-(4-hydroxyquinolin-3-yl)but-2-enedioate, and alkyl 2-oxo-2H-pyrano[3,2-c]quinoline-4-carboxylate. The structure of **3, 4** were deduced from IR, ^1H NMR, ^{13}C NMR spectra.



1 2 3 4

R= Me, Et, t-Bu

In conclusion, we have described a convenient route to aza coumarines, through nucleophilic addition to dialkyl acetylenedicarboxylate. These functionalised coumarines may be considered as potentially useful synthetic intermediates because they possess atoms with different oxidation states. The present method has the advantages that not only are the reaction performed under neutral conditions, but also the substances can be mixed without any modification. The simplicity of the present procedure makes it an interesting alternative to other approaches

References:

[1] (a) Murray, D. H; Mendez, j; brown, S. A. j. Wiley & Sons: New York, NY, **1982**.
[2] Yavari, I; Adib, M; Hojabri, L. *Tetrahedron*, **2001**, *57*, 7537.

Conversion of sugar cane waste to hydroxymethylfurfural as a fuel precursor (Liquid Alkanes)

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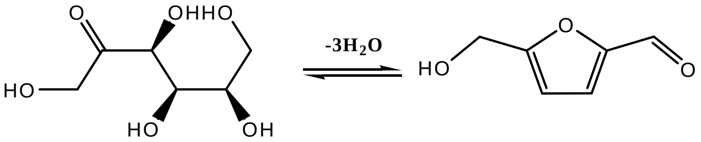
Furan derivatives obtained from renewable biomass resources, have the potential to serve as substitutes for the fossil fuels that are currently used in the production of plastics and fine chemicals. 5-hydroxymethyl-2-furaldehyde (HMF) is one of these derivatives which obtained from acid-catalyzed dehydration of carbohydrates and has a great potential as a biofuel [1]. HMF can subject to an aldol condensation followed by hydrogenation reaction to yield a composition of matter comprising alkanes [2].

Many methods have been done for achieving HMF in good yield [3].

In one embodiment the reaction is carried out in a small thick-walled glass tube which is filled with specific amounts of carbohydrate, different alcohols or ketons as an organic phase, H_2O as an aqueous phase and different organic or inorganic acids as a catalyst. The reactor is heated at 180 ^{0}C for 3min. and the reaction stopped by rapidly cooling the tube at -20 ^{0}C. The organic phase is separated and analysis for measuring the amount of HMF [4].

Herein we report a process for converting fructose of molasses and other carbohydrates from sugar cane bagasse to HMF using a biphasic reactor containing a reactive aqueous phase, methylisobutylketone (MIBK) as an organic phase and H_2SO_4 as a catalyst. Optimizing the production of HMF to get the best yield was investigated.



D-Fructose

5-hydroxymethyl-2-furaldehyde

References:

[1] Yuri Roman-leshkov, Juben N. Chheda, James A. Dumesic, *J. Science*, **2006**, *312*,1933.

[2] George w. Huber, Juben N. Chheda, Christopher J. Barrett, James A. Dumesic, *J. Science,* **2005**, *308,* 1446.

[3] X.Qi et al., *Ind.Eng.Chem.Res.*, **2008**,*47 (23), 9234-9239.*

[4] Dumesic et al. , U.S.Pat. No. :US 2008/0033188 A1, issued **Feb.7, 2008**.

Hexamethylenebis(*N*-methyl imidazolium dichloroiodate) as mild iodinating agent for anilines

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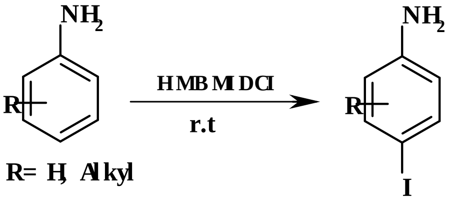
Aromatic iodides have long been used in organic synthesis as versatile intermediates that can be transformed to a variety of functional groups. Direct iodination of aromatic compounds is difficult due to the low electrophilicity of molecular iodine compared to the other halogens, and also due to the reducing effect of the hydrogen iodide produced [1].

Despite the great importance of aromatic iodinated compounds as precursors for organic transformation, there is still a great need for the discovery of a simple, inexpensive and nontoxic reagent for the introduction of iodine into an aromatic ring.

According to procedures reported in the literature that employed benzyltrimethyl [2] or benzyltriethylammonium dichloroiodates in both free [3] and polymer-supported form [4], Herein we report the preparation of a new reagent, Hexamethylenebis(*N*-methyl imidazolium dichloroiodate) (***HMBMIDCI***), which is a good iodinating agent for anilines at room temperature. (Scheme 1)



Scheme 1.

References:

[1] Stavber, S.; Jereb, M.; Zupan, M. *Synthesis*, **2008,** 1487.
[2] Kajigaeshi, S.; Kakinami, T.; Fujisaki, S.; Okamoto, T.; Yamasaki, H. *Bull. Chem. Soc. Jpn.* **1988,** *61*, 600.
[3] Custelceanu, R.; Vlassa, M.; Silberg, I. A. *Monatsh. Chem.* **1997,** *128*, 919.
[4] Mitra, S. S.; Sreekumar, K. *Eur. Polym. J.* **1998,** *34*, 561.

Synthesis of a new family of macrocycles by Claisen−Schmidt condensations

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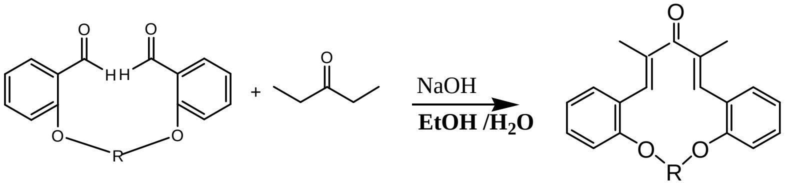
The reactions between a ketone and an aldehyde (crossed aldol condensation) or between two aldehydes also go by the name Claisen-Schmidt condensation[1,2].
Claisen-Schmidt condensations proceed under either acid or base catalysis, at moderate temperature, in high atom economy and with water as the sole byproduct. When the ratio of starting ketone to aldehyde is greater than 1:1 the orientation of double bonds generated is exclusively trans with respect to the aryl ring and the carbonyl group of the ketone[3].
Relative rates for potentially competing processes, including self-condensation of the ketone and Cannizzaro reactions of aryl aldehydes, are negligible.
We are prepared, dialdehydes by linking two salicylaldehyde molecules, with flexible linear tethers.

In the presence of base,Cyclization occurred through sequential Claisen-Schmidt condensations, at α position to the carbonyl group and macrocycles are obtaining low to moderate yields.
Crown ether can form metal cation complexes which are soluble in organic solvents and we are going to study this property on these new macrocycles in future.



R=2,3,4

References:

[1] Advanced organic Chemistry, Reactions, mechanisms and structure 3ed. Jerry March ISBN 0-471-85472-7.
[2] Amarajothi Dhakshinamoorthy, Mercedes Alvaro, Hermenegildo Garcia, *Advanced Synthesis & Catalysis,* **2010**, *352*, 711 .
[3] Christopher R. Strauss and et al,,*org. lett.* **2004**, *6*, 3257.

Solvent-free synthesis of disulfides via controlled oxidation of thiols by *o*-Xylylene triphenylphosphonium chlorochromate and *o*-Xylylene bis(triphenylphosphonium)dichromate salts.

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Organic reactions, carried out in dry media, have recently received careful attention with advantages such as replacement of volatile organic solvents from the reaction medium[1], avoidance of solvent waste, a simply work-up procedure and energy saving over against the solution reactions[2]. Oxidation of thiols to the corresponding disulfides is a characteristic functional group transformation, in which further oxidation(s) of the products to give disulfide S-oxides (thiolsulfinates), disulfide S-dioxides (thiolsulfonates), and sulfonic acids are possible, and consequently, considerable research has gone into controlling the initial oxidation [3].

Herein we report an efficient, environmentally friendly, clean and solvent less method for synthesis of disulfides with quantitative yield via controlled oxidation of thiols by o-xylylene triphenylphosphonium chlorochromate [Ph(CH2PPh3CrO3Cl)2, o-XTPPCC] and o-xylylene bis(triphenylphosphonium)dichromate [Ph(CH2PPh3)2Cr2O7, o-XBTPPDC] salts.

Various aliphatic, aromatic and benzylic thiols were converted to correspounding disulfides in excellent yields and short reaction times. The oxidation of thiols to disulfides without over-oxidation of disulfides, oxidation of the SH functional group in the presence of an OH group demonstrate the chemoselectivity of this method.

$$\mathrm{RSH}\xrightarrow[\textit{solvent free , r.t , ...}\ \langle\ 1.5\ min]{\mathrm{Ph(CH_2PPh_3CrO_3Cl)_2}}\mathrm{RS\text{-}SR}$$

R: alkyl, aryl

$$\mathrm{RSH}\xrightarrow[\textit{solvent free , r.t , ...}\ \langle\ 2\ min]{\mathrm{Ph(CH_2PPh_3)_2Cr_2O_7}}\mathrm{RS\text{-}SR}$$

R: alkyl, aryl

References:

[1] (a) Tundo, P.; Anastas, P.; Black, D. St C.; Breen, J.; Collins, T.; Memoli, S.; Miyamoto, J.; Polyakoff, M.; Tumas, W. *Pure Appl. Chem.* **2000**, *72*, 1207. (b) http://www.epa.gov/greenchemistry/pubs/principles.html, last accessed on July 7, **2009**.

[2] (a)Badri, R.; Mostoufi, A. *Phosphorus, Sulfur, and Silicon*. **2006,** *181*, 1513–1519. (b) Field, L.; Hoelzel, C. B.; Locke, J. M. *J. Am. Chem. Soc*. **1962**, *84*, 8410. (c) Firouzabadi, H.; Sharifi, A. *Synthesis*. **1992,** 999-1002. (d) Burgess, K. In Solid-Phase Organic Synthesis; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, **1999**. (e) Czarnik, A. W.; Solid-Phase Organic Syntheses; *Vol.1*, Wiley-VCH Verlag GmbH & Co.KGaA: Weinheim, **2001**. (f) Dörwald, F. Z.; Organic Synthesis on Solid Phase: Supports, Linkers, Reactions; 2nd ed., Wiley-VCH Verlag GmbH & Co. KGaA:

[3] Montazerozohori, M.; Joohari, S.; Karami, B.; Haghighat, N. *Molecules*. **2007**, *12*, 694-702.

Structural and energetic study of thermal cycloaddition reaction of 1,3-cycloheptadiene by using ab-initio an DFT methods

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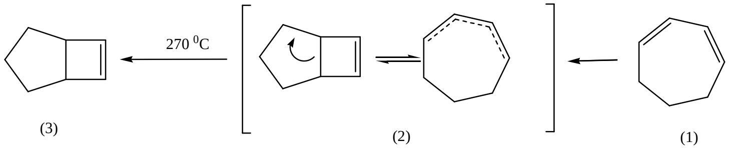
Pericyclic reactions are unimolecular processes which involve the exchange of π-bonds for ring-closing sigma-bonds. These reactions usually occur in thermal and photo conditions. The computational study of pericyclic reactions, an important general class of organic reactions, now provides information about the transition structures of these processes with chemical accuracy, as judged by comparisons with experimental data, such as activation energies [1].

In this work, we report the results of a theoretical investigation of the energetic and structural properties of intermolecular [2+2] cycloaddition of 1,3-cyclononadiene (**1**) for produce bicyclo[3.2.0]hept-6-ene (**3**) by using Ab initio and density functional theory calculations.



These calculations were carried out using HF/6-311+G** and B3LYP/6-311+G** levels of theory with the GAUSSIAN 03W package of programs[2].

Energy-minimum molecular geometries were located by minimizing energy; with respect to all geometrical coordinates without imposing any symmetrical constraints the structures of the molecular transition state geometries were located using the optimized geometries of the equilibrium molecular structures according to the Dewar et al. procedure (keyword SADDLE).These geometry structures were reoptimized by the QST2 subroutine at the HF/6-311+G** and B3LYP/6-311+G** levels. These results show that cyclization reaction in compound (**1**) is disrotatory and barrier height of the cyclization reaction are 29.37 and 41.12 kcal mol^{-1} in B3LYP/6-311+G** and HF/6-311+G** methods, respectively.

Reference:

[1] O. Wiest, D. C. Montiel and K. N. Houk,, *J. Phys. Chem. A*, 101 (45), pp 8378, **1997**
[2] M. j. Frisch et al. *GAUSSIAN 03,* Revision C. 01, Gaussian Inc., Wallingford. CT, **2004**.

Nucleophilicity and molecular structure of acyl lithiums: Ab initio calculations

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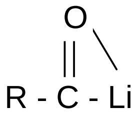
Acyl lithium derivatives represent exotic molecules. In contrast to the acyl cation or acylinium ion, which is a well-documented species, acyl lithium's are not discussed in depth in books on organic chemistry. The rich chemistry of acyl lithium is now available and further development of the chemistry of this quite reactive and unique species is very important [1].

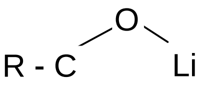
So we studied the structure and Nucleophilicity for some aliphatic acyl lithium's (RCOli :R=CH_3,C_2H_5,n-C_3H_7,iso-C_3H_7,n-C_4H_9,iso-C_4H_9,t-C_4H_9,n-C_5H_{11}) and Aromatic acyl lithium's (ArCOli: Ar=C_6H_5,CH_2-C_6H_4,o-CL-C_6H_4,o-No_2-C_6H_4,o-(CHO)-C_6H_4, o,p-$(CL)_2$-C_6H_3, o,p-$(No_2)_2$-C_6H_3, o,p-$(CHO)_2$-C_6H_3)We obtained three possible structures for all the compounds: cyclic (1)' singlet carbine (2) triplet carbine (3). Geometries of the molecules are optimized using Gaussian03 [2] employing HF and B3LYP methods with 6-311++g** basis set. The stability of these structures in all molecules are: cyclic > singlet > triplet .In order to investigate the effect of R and Ar groups on carbonyl nucleophilicity, we calculated charge on carbon (C=O) and sigma constants. In order to formulate substituent effects on nucleophilicity we correlate these with sigma constants. There are some extent good correlation between experimental sigma constants and calculated constants.

(1)



(2) R-C-O-Li (singlet)
R: alkyl, aryl

(3)



(triplet)

References:

[1] Modern carbonyl chemistry. Edited by Junzo Otera. Wiley VCH: **2000** .XIX, 613.

[2] M. J. Frisch.; G. W.; Trucks, H. B.; Schlegd, G. E.; Suseria, M. A.; Robb, J. R.; Cheese man, V. G.; Zakrzewski, J. A.; Montgomery Jr.; R. E.; Gill, B.; Johnso, W. L. Chen, M. W.; Wong, J.L.; Andres, M. Head-Gordon, E.S. Replogle , J. A.; Pople, Gaussian , Inc.; Pittsburgh, P.A.; **1998.**

Poly(4-vinylpyridinium tribromide) as new and efficient catalyst for chemoselective formylation of alcohols

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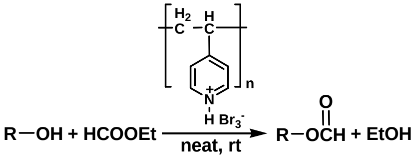
Formylation of the hydroxyl group is of great interest because of its importance in organic synthesis, which provides an efficient method for the protection of OH groups. A variety of literature methods has been reported for this transformation such as $HCOOH/SiO_2$, $(NH_4)_8[CeW_{10}O_{36}].20H_2O$/ethyl formate, sulfuric acid ([3-(3-silicapropyl)sulfanyl]propyl)ester/ethyl formate, [bmim]HSO_4/ethyl formate, and *etc* [1-3]. However most of these procedures suffer from one or more of the following drawbacks: harsh reaction conditions, long reaction times, low yields of products, heavy metal contamination and acidic media (which is not suitable for acid sensitive substrate and side reaction.

Therefore to improve above-mentioned limitations and in continuing of our experiments on the application of new reagents or reagent systems [4-5] for the organic functional group transformations we decided to use non-acidic catalyst and neutral conditions for the preparation of alkyl formate. In this light, a wide variety of alcohols were converted into corresponding alkyl formate using ethyl formate in the presence of catalytic amounts of poly(4-vinylpyridinium tribromide) at room temperature under solvent-free conditions (Scheme 1).



Scheme 1

In conclusion, herein we introduced poly(4-vinylpyridinium tribromide) as neutral catalyst for the conversion of alcohols into alkyl formates using ethyl formate.

References:

[1] Niknam, K.; Zolfigol, M.A.; Saberi, D.; Khonbazi, M. *Chin. J. Chem.* **2009**, *27*, 1548.
[2] Zolfigol, M.A.; Chehardoli, G.; Dehghanian, M.; Niknam, K.; Shirinid, F.; Khoramabadi-Zad, A. *J. Chin. Chem. Soc.* **2008**, *55*, 885.
[3] Shirini, F.; Marjani, K.; Nahzomi, H.T.; Zolfigol, M.A. *Phosphorus Sulfur Silicon* **2007**, *182*, 1245.
[4] Ghorbani-Choghamarani, A.; Zolfigol, M.A.; Azadbakht, T. *Phosphorous Sulfur Silicon* **2010**, *185*, 573.
[5] Ghorbani-Choghamarani, A.; Zeinivand, J. *J. Iran. Chem. Soc.* **2010**, *7*, 190.

Continuous syntheses of coumarine dyes by heteropoly acid catalysts

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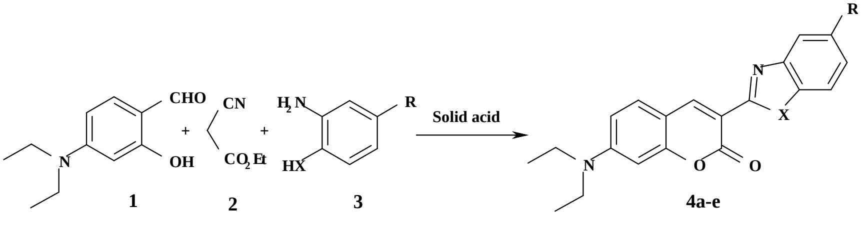
Heteropoly acids (HPAs) ($H_3PW_{12}O_{40}$, $H_4O_{40}SiW_{12}$) are more active catalyst than conventional inorganic and organic acids for various reactions in solution and solid HPAs have gained industrial importance due to easy work-up procedures and minimization of waste generation. They are noncorrosive and are environmentally benign, as they can be reused and recycled [1,2].The present methodology offers several advantages, such as high yields, short reaction times, mild reaction condition and a recyclable catalyst with a very easy work up. Concurrent formation of coumarin via green solid acids-mediated one-pot, three component synthesis was investigated. Furthermore, multi-component reactions (MCRs) are of increasing importance in organic synthesis. In a time when a premium is put on speed, MCR strategies with superior diversity and efficiency in the discovery process, offer significant advantages over conventional linear type syntheses . Coumarin derivatives with intense fluorescence have found extensive commercial use in a broad range of applications. Synthesis of laser dyes, fluorescent whiteners and organic nonlinear optical materials are some example of their importance in the field of industry.



Compound	X	R
4a	O	Cl
4b	O	CH_3
4c	O	H
4d	O	SO_3Et
4e	NH	NH_2

References:

[1] Chaskar, A.; Padalkar, V.; Phatangare, K; Patil, K.; Bodkhe, A.; Langi, B. Applied Catalysis A: General, **2009**, *359*, 84.

[2] Abdollahi-Alibeik, M.; Mohammadpoor-Baltork, I.; Zaghaghi, Z.; Youse, B. *Catalysis Communications*, **2008**, *9* , 2496.

Isotopic effect on tautomeric behaviour of 5-(2,6-disubstituted-aryloxy) tetrazoles

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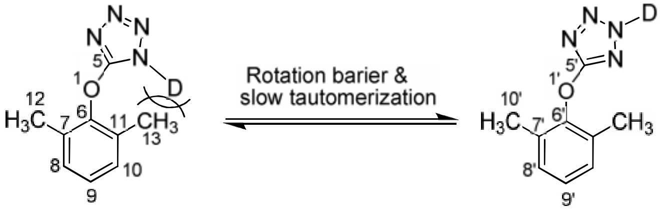
5-Substituted 1,2,3,4-tetrazoles are reported to possess antibacterial [1], antifungal [2], antiviral [3], analgesic [4], anti-inflammatory [5], antiulcer [6] and antihypertensive [7] activities.

In this work, our first aim was attempt to elucidate the predominant tautomeric forms of 5-aryloxy-tetrazole in DMSO that whether these compounds are exhibits in 5-aryloxy (1*H*)-tetrazole (**1A**) and/or 5-aryloxy (2*H*)-tetrazole (**1B**) forms in DMSO as a suitable solvent.

For instance, the ^{1}H and ^{13}C NMR spectra of 5-(2,6-dimethylphenoxy)-(1*H*)-tetrazole (**1b**) shows interesting phenomenon before and after adding D_2O. Before adding D_2O, the two methyl groups have nonequivalent chemical shift, approximately (at δ 2.09 ppm for two methyl groups and having a shoulder) while two methyl groups show two distinct singlets at δ 2.06 and 2.05 ppm after adding D_2O ($\Delta\delta = 0.01$ ppm).



1bA (a) **1bB**

References:

[1] Demarinis, R. M; Hoover, J. R. E.; Dunn, G. L.; Actor, P.; Uri, J. V.; Weisbach, J. A. *J. Antibiot.* **1975**, *28*, 463.

[2] Sangal, S. K.; Ashok Kumar, A. *J. Indian Chem. Soc.* **1986**, *63*, 351.

[3] Witkowski, J. K.; Robins, R. K.; Sidwell, R. W.; Simon, L. N. *J. Med. Chem.* **1972**, *15*, 1150.

[4] Mungnaini, A.; Friz, L.P.; Provinciali, E.; Rugarli, P.; Olivi, A.; Sanfilippo, E.; Almirante, L.; Murmann, N. *Bull. Chim. Farm.* **1966**, *105*, 596.

[5] Shukla, J. S.; Ahmed, J.; Saxena, S. *Indian Chem. Soc.* **1979**, *41*, 70.

[6] Shishoo, C. J.; Devani, M. B.; Karvekar, M. D.; Vilas, G. V.; Anantham, S.; Bhaati, V. S. *Ind. J. Chem.* **1982**, *21B*, 666.

[7] Uchida, M.; Komatsu, M.; Morita, S.; Kanbe, T.; Yamasaki, K.; Nakagawa, K. *Chem. Pharm. Bull.* **1989**, *37*, 958.

Synthesis and characterization of modified Merrifield polymer supported palladium nanoparticles as a novel polymer catalyst in Suzuki reaction

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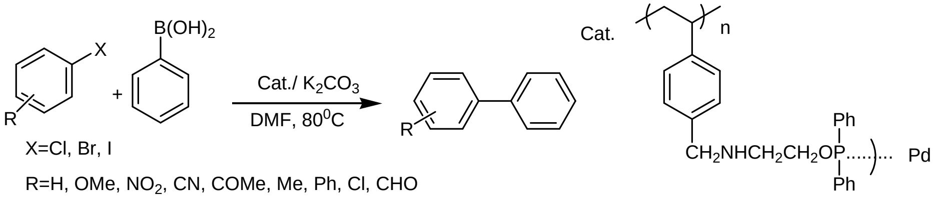
A polymeric catalyst or polymer-supported catalyst is a conventional catalytic species attached to a macromolecular backbone [1,2]. The use of polymer supported transition-metal nanoparticles in the catalysis of organic reactions provides a powerful means for the development of recyclable catalysts [3,4]. Herein, we report the synthesis of heterogeneous palladium catalyst containing phosphinite ligand based on modified Merrifield had been used successfully in C–C cross-coupling reactions. This catalyst can be applied in the Suzuki reaction which is one of the most powerful and versatile method for the generation of new biaryls. Transmission electron microscopy (TEM) shows that palladium particles were well-dispersed and of typical diameter of 10–30 nm. The X-ray powder diffraction (XRD) pattern of the Pd catalyst was consistent with the metallic Pd (0).



References:

[1] Sherrington, D. C.; Hodge, P. *Synthesis and Separation Using Functional Polymers*, John wiley and Sons, **1988**.
[2] Hodge, P.; Serrington, D. C. Eds., *Polymer-Supported Reactions in Organic Synthesis″,Wiley,London,* **1980**.
[3] *(a)* Bedford, R. B.; Singh, U. G.; Walton, R. I.; Williams, R. T.; Davis, S. A. *Chem. Mater*. **2005,** *17*, 701; (b) Zhang, Z.; Wang, Z. *J. Org. Chem*. **2006,** *717*, 485; (c) Choudary, B. M.; Madhi, S.; Chowdari, N. S.; Kantam, M. L.; Sreedhar, B. *J. Am. Chem. Soc*. **2002**, *124,* 14127.
[4] Tamami, B.; Ghasemi, S. *J. Mol. Catal. A: Chem*. **2010**, *322*, 98.

Silica-bonded *N,N,N*- tri sufamic acid (propyl diethylen tri amine) as a recyclable catalyst for chemoselective synthesis of 1,1-diacetates

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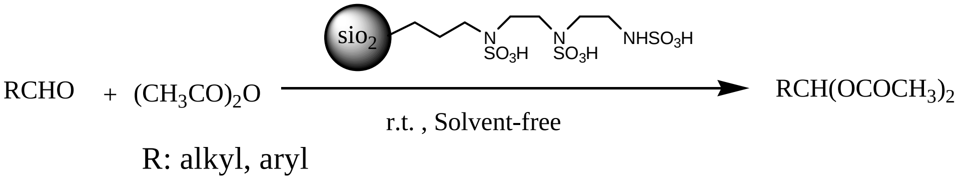
Selective protection and deprotection of carbonyl groups are essential steps in modern organic chemistry [1]. The protection of aldehyde as acetals, acylals, oxathioacetals or dithioacetals is common practice for manipulation of other functional groups during multi-step syntheses. Protection of aldehyde as acylals is often preferred due to their ease of preparation and their stability toward basic and neutral conditions [1,2]. In addition, the preparation of 1,1-diacetates from the corresponding aldehydes can be achieved very easily in the presence of ketones. Numerous methods for the preparation of 1,1-diacetates from aldehyde and acetic anhydride have been reported. However, the majority suffer from at least one of the following disadvantages; use of expensive reagent, tedious work up procedure, longer reaction time, harsh reaction conditions.

In this article we introduced a new catalyst for the prepatation of 1,1-diacetates, by the reaction of aldehyde, acetic anhydride in the presence of silica-bonded N,N,N- tri sufamic acid (propyl diethylen tri amine) as catalyst at room temperature in good to excellent yield (Scheme 1).



Scheme1

References:

[1] Greene, T. W.; Wuts, P. G. M. *Greene's Protective Groups in Organic Synthesis*, 4th ed.; Wiley: NewYork, **2007**.

[2] Kochhar, K. S.; Bal, B. S.; Deshpande, R. P.; Rajadyaksha, S. N.; Pinnich, H. W. *J. Org. Chem*. **1983**, *48*, 1765.

Molecular recognition by a novel sulfonamide derivative of calix[4]arenes

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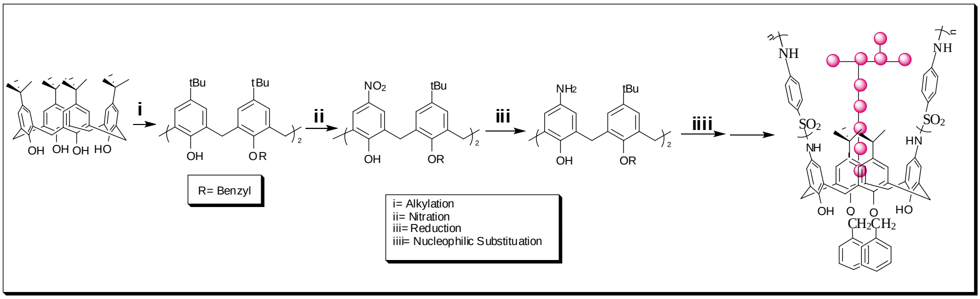
Molecular recognition is a major part of modern organic chemistry.Calixarenes are a versatile class of macrocyclic compounds which have attracted extensive interest due to their ability to from host_guest complexes [1,2]. At the upper rim functiolazed calixaren are key intermediates for construction of molecular receptors based calixarenes [3]. Upper rim functionalized compound can be obtained in a multi step procedure from suitably substituted precursors [4,5]. The synthesis and characterzation of a sulfunamide derivatives of calix[4]arenes has been described. In this work ,the synthesis of the p-aminocalix[4]arenes derivatives with ipso-nitration and then reaction of this derivatives with p-amino-benzenesulfonyl chloride have been carried out to extension of conic cavties of calix[4]aren .

Obtained receptors have been characterized by ^{1}HNMR, ^{13}CNMR, FTIR and MS. the complexation properties and host behavior of the p-sulfonamid calix[4]arenes derivatives some amino acids and peptides have been studied.



Refrences:

[1] Guoyuan L, Wei S, Xiaobin W, *Journal of Chemical Crystallography*, **2000**, Vol. 30,No. 3.

[2] Kumar sharma S, Varadarajan R, Chawla H.M, Hundal S.M, Hund G ,*Tetrahedon* **2004**, *60* , 1001.

[3] Kumar sharma S and Gutshe C.D, J.org.chem **1999**, *64*, 998.

[4] Rashidi P, taghvaei S, *molecules*. **2000**, *5*, 941.

[5] Grawarl YKA, Pancholi JP and Yas JM , *Journal of Scientific and Industrial research*. **2009,** 68, 745.

A detailed theoretical DFT study of the anticancer drug Mercaptopurine and compare by Adenine

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Mercaptopurine, a chemical analog of the purine adenine, inhibits the biosynthesis of adenine nucleotides by acting as an antimetabolite. In the body, 6-MP is converted to the corresponding ribonucleotide. 6-MP ribonucleotide is a potent inhibitor of the conversion of a compound called inosinic acid to adenine Without adenine, DNA cannot be synthesized.Computational chemistry methods, as a kind of extension of the experimental approach, have widely been applied in chemotherapy studies of DNA–drug binding. In order to control the DNA changes, these theoretical studies are used to predict appropriate structures of DNA–drugs. Molecular modeling is extensively used in the study of drug mechanisms, and has contributed to the design of several drugs [1]. DFT molecular modeling methods are a group of specific and reliable quantum mechanical calculations for computational studies [2–6].

In our current study, extensive quantum mechanical calculations of structure of Mercaptopurine and Adenine have been performed on a Pentium-4 based system using GAUSSIAN 03 program. At first, we have modeled the structures with Chem office package and then optimized at the DFT level of theory with B3LYP/ 6- 31G*basis set. After fully optimization of Mercaptopurine and Adenine structures, we have calculated optimization in different solvents at the level of B3LYP/ 6-31G* theory and then we have calculated NMR parameters and infrared (IR) intensities at the same as basis set. , and finally we calculate Natural Bond Oribital (NBO) parameters for two structures.

References:

[1] Huang, Y. Q. Jiang, H. L. Luo, M. X. Chen, K. X. Zhu, Y. C. Ji, R. Y. Cao, Y. *Acta Pharmacol*. Sin. **2000**, 21, 536.
[2] Riahi, S. Ganjali, M. R. Norouzi, P. *J. Theor. Comput. Chem.* **2008**, 7, 317.
[3] Riahi, S. Moghaddam, A. B. Ganjali, M. R. Norouzi, P. *J. Theor. Comput. Chem.* **2007**, 6 331.
[4] Riahi, S. Ganjali, M. R. Moghaddam, A. B. Norouzi, P. Hosseiny S. S. Davarani, Spectrochim. *Acta* **2008**, 70, 94.
[5] Riahi, S. Faridbod, F. Ganjali, M. R. *Sensor Lett*. **2009**, 7, 42.
[6] Riahi, S. Ganjali, M. R. Moghaddam, A. B. Norouzi, P. Niasari, M. *J. Mol. Struct.* (*THEOCHEM)* **2006**, 774, 107.

Ultrasound-promoted synthesis of dihydropyridines catalyzed by modified montmorillonite-K10

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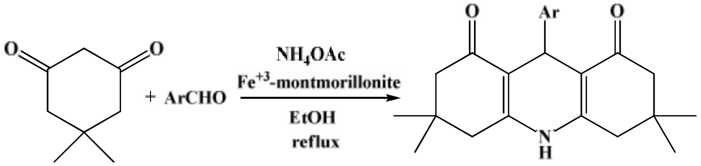
In recent years, an increasing interest has been focused on the synthesis of 1,4-dihydropyridyl compounds owing to their significant biological activity[1]. 4-aryl-1,4-dihydropyridines have been explored for their calcium channel activity and the heterocyclic rings are found in a variety of bioactive compounds such as vasodilator, bronchodilator, antiatherosclerotic, antitumor, antidiabetic, geroprotective and heptaprotective agents[2]. There are many methods to synthesize 1,4-dihydropyridines. The classical method involves the mixing of aldehyde with ethylacetoacetate and ammonia, in acetic acid or in refluxing alcohole[3]. Even though a number of modified methods under improved condition have been reported, which comprise the use of microwave, ionic liquid, at high temperature in refluxing solvent, TMSCl-NaI, metal triflates, I_2, and CAN[4].

Herein, we wish to report our preliminary results on the ultrasound synthesis of dihydropyridines catalyzed montmorrilonite-K10 from substituted benzaldehyde, dimedone and ammonium acetate.



Ar: $2\text{-}NO_2C_6H_4$, $3\text{-}NO_2C_6H_4$, $4\text{-}NO_2C_6H_4$, $2\text{-}ClC_6H_4$, $4\text{-}ClC_6H_4$, $3\text{-}BrC_6H_4$, $4\text{-}FC_6H_4$,...

References:

[1] Shan, R.; Velazquez, C.; Knaus, E. E. *J. Med. Chem*. **2004**, *47*, 254.
[2] Sausins, A.; Duburs, G.; *Heterocycles*,**1988**, *27*, 269.
[3] Love, B.; Sander, K. M. *J.Org.Chem*, **1965**, *30*, 1914.
[4] Ko, S.; Sastry, M. V. N, Lin, C, Yao, C. F. *Tetrahedron. Lett*. **2005**, *46*, 5771.

A convinient synthesis of a novel heterocyclic system: 7-aryl and 7-alkyl[1,2,4]triazino [4,3-b][1,2,4,5]tetrazines -6-one -3-thione.

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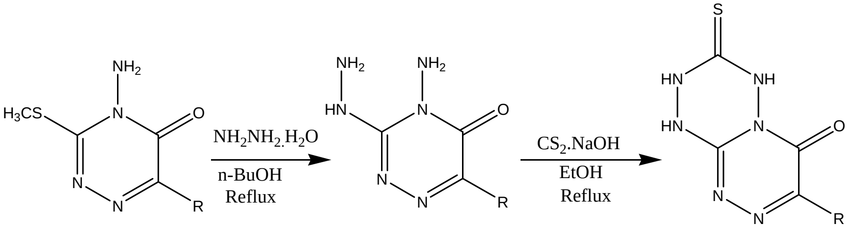
So far Iminophosphorane- mediated synthesis of [1,2,4]Triazino [4,3-b][1,2,4,5]Tetrazines derivatives has been reported by P.Molina et al.[1] Following our work on the preparation of fused triazines.[2,3,4], We now describe an easy method for the preparation of some drivatives of [1,2,4]Triazino [4,3-b] [1,2,4,5] Tetrazine as a novel system. 4-Amino -6-substituted -3-hydrazino[1,2,4]Triazin -5-one ,1(a,b),plays a centeral role for the following cyclocondesation reaction because of having two adjacent amino groups as nucleophile.Treatment of 4-Amino -6-substituted -3-methylthio[1,2,4]Triazin -5-one 1(a,b),with hydrazine hydrate in refluxing n-BuOH afforded 2(a,b) by displacement of hydrazine in the 3-position. Cyclocondensation of compounds 2(a,b) with carbon disulfide in the presence of sodiume hydroxide in refluxing Ethanol gave the corresponding 7-Aryl and 7-Alkyl[1,2,4]Triazino [4,3-b][1,2,4,5]Tetrazines -6-one -3-thione , 3(a,b).



1a) R = CH_3
b) R = Ph

2a) R = CH_3
b) R = Ph

3a) R = CH_3
b) R = Ph

References:

[1] Molina,P; Alajarin,M. and Vidal.; *J. Chem.Perkin Trans*.I,247-250 (1989).
[2] A. Nik Seresht et al 16th *Conference of Org. Chem*.,P.660 Zanjan uni.,Iran, 2009.
[3] A. Nik Seresht et al 15th *Conference of Org. Chem*.,P.219 Razi Uni.,Iran, 2008.
[4] Shawali A.S.,Elaghandour A.A.,El-Shikh S.M.,*J.Prakt.Chem*.342,1,96 ,(2008).

Synthesis of $[C_6H_{12}N_5O]_3[(PO_4)W_{12}O_{36}]{\cdot}5H_2O$, a novel hybrid compound and its characterization by X-Ray crystallography

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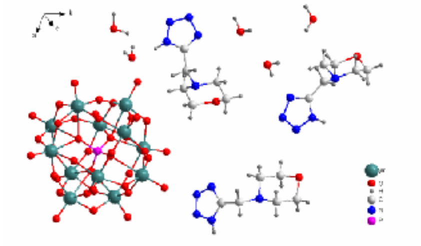
The contemporary interest in the chemistry of polyoxometalates (POMs) [1] not only stems from their applications in fields such as medicine [2], material science [3], and catalysis (homogeneous and heterogeneous) [4] but also stems from their intriguing variety of architectures and topologies. Thus, many numbers of heteropoly anions have been reported and some of them, especially Keggin type, were structurally and spectrally characterized [5]. The incorporation of organic moieties into inorganic oxide clusters provides a powerful method for structural modification and synthesis of novel inorganic-organic hybrid materials.

In thi research, a unique ionic hybrid material $[C_6H_{12}N_5O]_3[(PO_4)W_{12}O_{36}]{\cdot}5H_2O$ has been synthesized from the reaction of ((1*H*-tetrazole-5-yl)methyl)morpholine and α-$H_3[(PO_4)W_{12}O_{36}].21H_2O$ Scheme 1. It has successfully been characterized by elemental analysis, IR and ^1H NMR spectroscopies, TGA, and single-crystal X-ray diffraction method. The title compound is constructed from the three $[C_6H_{12}N_5O]^+$ cations and α-Keggin $[(PO_4)W_{12}O_{36}]^{3-}$ polyoxoanion.



Scheme 1

References:

[1] C. L. Hill, *Chem. Rev.* 98 (**1998**) 1.
[2] M. Michelon, M. Herve, G. Herve, *Biochim. Biophys. Acta* 916 (**1987**) 402.
[3] C.J. Gomez-Garcia, E. Coronado, L. Ouahab, *Angew. Chem. Int. Ed. Engl.* 240 (**1992**) 31.
[4] N. Seifi, M.H. Zahedi-Niaki, M.R. Barzegari, *J. Mol. Catal.* 260A (**2006**) 77.
[5] J. F. Liu, Y. G. Chen, L. Meng, *Polyhedron* 17 (**1998**) 1541.

Fe_3O_4 nanoparticles as an efficient catalyst for synthesis of benzimidazole derivatives

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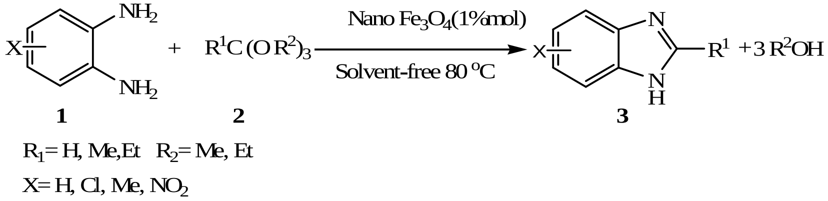
The benzimidazole moiety is found in various bioactive compounds having antiviral, antihypertension and anticancer properties [1].

A general method for the synthesis of Benzimidazole derivatives by reaction of o_ phenylendiamines with orth_ Oesters in presence of a catalytic amount of Fe_3O_4 nanoparticles under solvent-free conditions is reported. number of synthetic methods have been developed in recent years to uncovera variety new reagents for the synthesis of benzimidazole derivatives [2].

Recently, several methods have been introduced, where aldehydes, acid chloride, o-dinitrobenzene and 2-nitroanilines are used as starting materials for this synthesis.

However , the reported in this methods simple work-up , reusability of the catalyst short reaction times and high yields of the products easy handling and suitable temperature conditions solvent-free reaction [3]. (Scheme)



Refrences:

[1] (a) Gravatt , G . L; Baguley, B. C.; Wilson, W. R. Denny, W. A. *J .Med .Chem* .**1994**, 37, 4338;
(b) Kam, J. S.; Gatto, B.; Yu , C.; Liu, I.; Liu, L. F. ;Li Voie ,E .J . *J. Med. Chem* .**1996**, 39, 992;
(c) Horton, D. A.; Boyer, P .L.; Hughes, S. H.; Burne, G. T.; Smythe, M. L. *Chem. Rev*. **2003**, 103, 893.

[2] P.Tempest, V. Ma, S. Thomas, Z. Hua, M. G. Kelly, C. Hulme, *Tetrahedron Lett.* **2001,** 42, 4959.

[3] Majid M. Heravi; Samaheh Sadjadi; Hossein A .Oskooie; Rahim Hekmat Shoar ; Fatemeh F. Bamoharram, *Catal.Comun.* **2008**, 504.

Efficient, additive-free, and selective *N*-Boc protection of aromatic amines in the presence of aliphatic amines

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Protection and deprotection of organic functional groups play essential roles in accomplishing multi-step syntheses. Depending on the simplicity of the process, ease of operation and workup, yield of the desired product and its stability to the reaction conditions, and the overall expenses of the process, a suitable process will be chosen. On these grounds, diverse arrays of different methods are developed during the years for protection/deprotection of various functional groups [1,2].

A larg variety of protective groups have been formulated among which the commercially available di-tert butyl dicarbonate [$(BOC)_2O$] group is extensively used as an amino acid protecting group in organic synthesis, because this group is very stable to reaction conditions and is suitable for clean and rapid introduction [3].

Herein, we report an efficient and chemoselective protection of amines in the presence of no additive. Various aromatic, hetroaromatic, and hetrocyclic amines were converted to their N-t-Boc derivatives at room temperature and under solvent-free condition in good yields. Selective protection of aliphatic amines in the presence of aromatic or hetroaromatic amines was also achieved by this method.

$$R_2NH + (Boc)_2O \xrightarrow{R.T} R\text{-}NH(Boc) + C(CH_3)_3OH + CO_2$$

R= aryl

References

[1] Sadula, S.; Sanjit, K.; Srinivasa, R. P.; Achapudi, B. N. P. *Tetrahedron Lett.* **2008**, *49*, 2527.
[2] Dharita, J. U.; Alessandro, B.; Rachele, S.; Giancarlo, C. *Tetrahedron Lett.* **2007**, 48, 8318.
[3] Gan, W.; Chunju, L.; Jian, L.; Xueshun, J. *Tetrahedron Lett.* **2009**, 50, 1438.

$FeCl_2.4H_2O$ As an effective catalyst a for synthesis of bis(indolyl)methanes at room temperature

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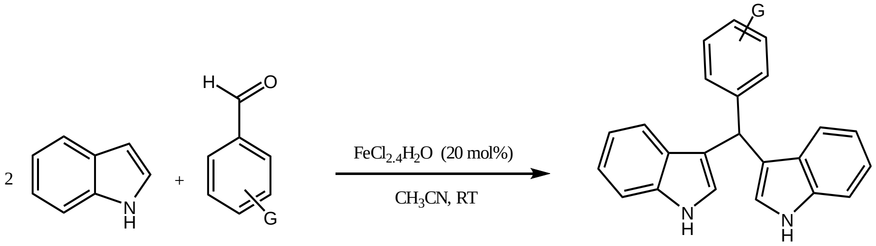
Bis (indolyl) methanes are most active cruciferous substances for promoting beneficial estrogen metabolism and inducing apoptosis in human cancer cells. $FeCl_2.4H_2O$ is found to be an efficient catalyst for the condensation reaction of indoles with aromatic aldehydes to afford the corresponding bis (indolyl) methanes in high yields in acetonitril solvent [1]. The remarkable features of this new procedure are high conversions, shorter reaction times, cleaner reaction profiles and simple experimental and work-up procedures [2,3].



G: H, CN, NO_2, Me, Cl, OMe

References:

[1] Chakrabarty, M.; Ghosh, N.; Basak, R.; Harigaya, Y. *Tetrahedron Lett.* **2002**, *43*, 4075.
[2] (a) Bandgar, B. P.; Shaikh, K. A. *Tetrahedron Lett*. **2003**, *44*, 1959. (b) Wang, Y.-Y.; Chen, C. *J. Chin. Chem. Soc*. **2007**, *54*, 1363.
[3] Reddy, A.V.; Ravinder, K.; Reddy, V. L. N.; VenkateshwerGoud, T.; Ravikanth, V.; Venkateswarlu, Y. *Synth. Commun.* **2003**, *33*, 3687.

Synthesis of phosphonate esters and stable phosphorus ylides from reaction between tri phosphite and dialkylacetylenedicarboxylate in the presence of N-H acid

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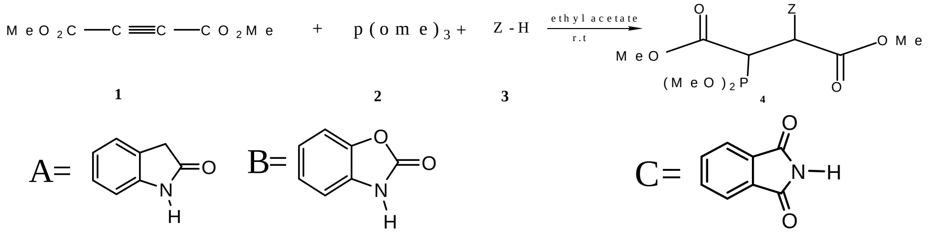
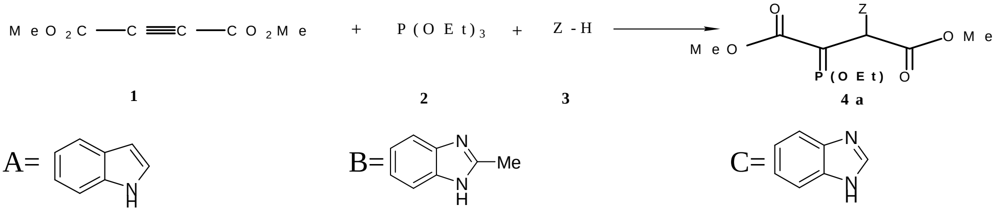
In recent years, there has been an increasing interestin the synthesis of organophosphorus compound.This interest has resulted from the recognition of the value of such compounds in a wide range of industrial,biological,and chemical synthetic uses.As a result, a large number of methods have appeared describing novel syntheses of organophosphorus compounds. In our previous work, triphenyl phosphine was employed as a phosphorus compound to generate stable phosphorus ylide and phosphonate esters. In continuation of our research work, triethyl phosphite (in spite of their high reactivity) was employed instead of triphenyl phosphine for generation of a new class of stable products.

In the current work, efficient stereoselective synthesis of phosphonate diesters and stable phosphorus ylides is reported from the reaction between trialkyl phosphite 2 and dialkylacetylenedicarboxylate **1** in the presence of NH-aromatic **3** within 24 h in high yield. TLC and ^{1}H NMR spectra of the crude products clearly indicated formation of phosphonate esters **4** and phosphorus ylide **4a** (see Scheme 1,2). The essential structures of the products **4a–e** were deduced from elemental analysis, IR, ^{1}H, ^{13}C, ^{31}P NMR, and mass spectra.





References:

[1] Maghsoodlou, M.T.; Shaterian, H. R.; Marandi, G.; Shahrakipoor, F.; Salehzadeh, J. *Arkivoc*, **2008** *13*, 218.
[2] Sheldrick, G. M. *Acta Cryst A* **2008**, *64*, 112.

Synthesis and characterization of oxidized polyethylene wax of Arak petrochemical complex

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Low molecular weight polyethylene (wax) was produced as a byproduct during of polyethylene production by slurry – phase processes in hexane [1, 2]. This compound is soluble in solvent and isolated in separation section. Wax is valuable and applicable in widespread industrial applications such as coating, lubricating, and etc. Oxidized polyethylene wax due to its polarity is used as lubricant for extrusion of PVC, polystyrene, polycarbonate, polymethylmethacrylate and other polar resins (pipes, sheets, profiles etc.) Now different grades of waxes are imported from foreign resources, therefore research and investigation on this byproduct is economically useful. Structural characterization of ARPC (Arak Petrochemical Complex) wax was carried out by chemical analysis and DSC, GPC techniques. Fractionation by molecular weight of wax was performed by solvent- nonsolvent method (heptane – ethanol). Also wax samples were oxidized at presence of air by benzoyl peroxide as catalyst at free solvent condition for production of oxidized wax. The effects of main parameters such as oxidation time, temperature and air flow rate on the acid number and IR spectrums were investigated. The results showed that under given reaction conditions, the acid numbers and intensity of CO band absorption (1700 cm^{-1}) were increased with temperature and reaction time.

References:

[1] Basell, *The Technology Manual of High Density Polyethylene Plant* **2008.**
[2] I. Krupa, *J. Polym*. **2003**, *42*, 7258.

Fatty acid: an efficient and reusable catalyst media for the 3,4-dihydropyrimidin-2(1H)-ones and their corresponding 2(1H) thione

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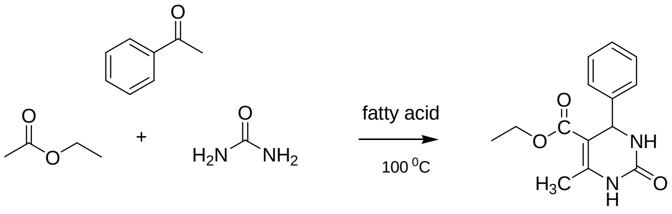
MCR strategies offer significant advantages over conventional linear-type synthesis. One such MCR that belongs in the latter category is the venerable Biginelli dihydropyrimidine synthesis [1].

The most simple and straightforward procedure for the synthesis of DHPMs was first reported by the Italian chemist Pietro Biginelli more than 100 years ago; it involves a three-component one-pot condensation of benzaldehyde, ethyl acetoacetate and urea under strongly acidic conditions[2]

In recent years several methods for the synthesis of DHPMs have been developed to improve and modify this reaction In continuation of our interest in methodology for the Biginelli reaction [3], herein we are pleased to report for the first time a novel, simple and efficient methodology for the synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones in good to excellent yields by the reaction of aldehydes, *β*-ketoesters and urea or thiourea using fatty acid as good catalytic media



Refrence:

[1] Kappe CO, *Acc Chem Res* , **2000**, 33: 879.
[2] Biginelli P, *Gazz Chim Ital*, **1893**, 23: 360.
[3] Hekmatshoar R**,** Heidari M, Heravi MM, Baghernejad B ,*Bulletin of the Chemical Society of Ethiopiaz*,**2009**, 23:141.

Engineering crystals by the strategy of molecular tectonics: Pinacolophanes as new tectons

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Molecular tectonics deals with the generation of molecular networks in the solid state. This approach is based on iterative molecular recognition processes using molecular building block called tectons. The majority of reported molecular networks are either based on hydrogen bonding or on coordination bonds.

Pinacolophane **1**, as shown its X-ray structure in fig 1, synthesized and characterized well and are potential tecton in crystal engineering.

The crystal packing of Pinacolophane **1** with cis configuration includes 16 molecules in which four asymmetric molecules are connected via strong hydrogen bonding (figure 1).

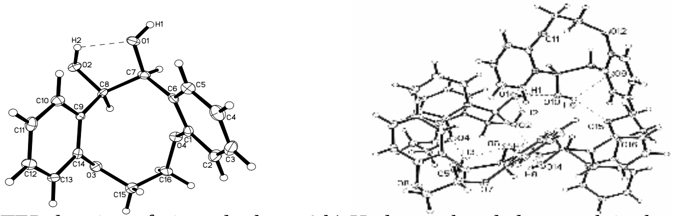

Figure1.a) ORTEP drawing of pinacolophane **1** b) Hydrogen bonded network in the solid state.

As shown in figure 2, two asymmetric molecules are in a back-to-back arrangement having one highly short intermolecular H-bond interaction (O1-H1…O2 = 2.00). However, two other asymmetric molecules are in a nearly face-to-face interaction without any intermolecular H-bond interaction. Moreover, both molecules have a short H-bond interaction with yellow one (O-H…O = 2.21 and 2.03, respectively) and also with green one (O-H…O = 1.92 and 2.36, respectively). Therefore, the molecules in crystal are arranged in designed shapes that result from the various intra- and intermolecular hydrogen bonding of the molecules (Figure 2).

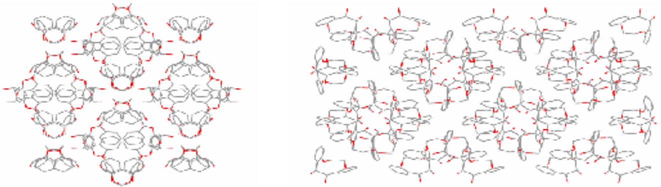

Figure 2. Crystal structure of pinacolophane **1** in the direction of the crystallographic along a axis (left) and c axis (right). Hydrogen atoms have been omitted for clarity.

References:

[1] Darabi, H. R.; Jadidi, K.; Mohebbi, A. R.; Faraji, L.; Aghapoor, K.; Shahbazian, S.; Azimzadeh Arani, M.; Nasseri, S. M. *Supramolecular Chem*. **2008**, *20*, 373.

Synthesis of a biodegradable polyamide from 2,3-bis(4-bromophenyl) quinoxaline and 2,5-dipiperazinedione in the presence of a copper (I) catalyst

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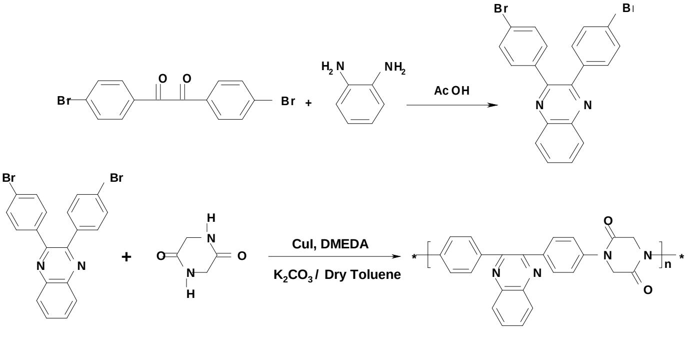
Aromatic polyamides are a class of high-temperature-resistance polymers with good chemical resistance and thermal stability, low flammability,and very good mechanical properties [1]. To date, catalysts based on several transition metals have been examined for the N-arylation of amides [2].

A novel polyamide has been successfully prepared through the reaction of 2,3-bis(4-bromophenyl)quinoxaline with 2,5-dipiperazinedione in the presence of a mixture of 10 mol% CuI and 20 mol% N,N'-dimethylethylenediamine as a catalyst and K_2CO_3 as a base.

2,3-bis(4-bromophenyl)quinoxaline was synthesized by condensation reaction from 4,4-dibromobenzil and O-phenylenediamine.The prepared polyamide was characterized with FT-IR, NMR,DSC,TGA,solubility and viscosity measurements.

The obtained polyamide exhibited inherent viscosity of 0.61 dL/g. According to the differential scanning calorimetry analysis analysis, the glass-transition temperatures of the polyamide was 280°C.Thermogravimetric analysis indicated that a 10% weight loss of the polyamide occurred in the temperature of 420°C under a nitrogen atmosphere.

Biodegradation study of this polyamide was also carried out in phosphate buffer solution containing Penicillin G Amidaz enzyme.



References:

[1] Yang, C. P.; Lin, J. H. *J Polym Sci Part A: Polym Chem.* **1996**, 34, 341.
[2] Ghaemy, M.; Barghamadi, M. *J. Appl. Polym. Sci*. **2008**, *110*, 1730.

Synthesis and characterization of mixed ligand complexes of Zn and Cu (II) - imidazol-oxalate

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Biological metal ions play key role in the structural organization and activation of certain enzymes, leading to the synthesis of specific proteins. The ternary complexes play an important role in biological processes. The complexes of Cu (II) were prepared. The mixed ligand complex involving oxalate and imidazole had been performed. The prepared complexes are characterized by IR and UV/Vis spectroscopic methods. The UV–Vis of oxalate complex had bonds at 228 and 295 nm. For ternary complex of Cu and oxalate and imidazole the absorption band appears at 225 and 269 nm. The elemental analysis and electro conductivity of complexes also were done. Based on elemental and spectra data, the complexes of binary and ternary of Cu had formula $Na_4\,[Cu\,(ox)_3]$ and $Na_2\,[Cu\,(imi)_2(ox)_2]$ respectively and the complexes of binary and ternary of Zn had formula $Na_2\,[Zn\,(imi)_2(ox)_2]$ and $Na_2\,[Zn_2\,(imi)_4(ox)_3]$ (imi = imidazol, ox= oxalat). At ternary complex of Cu, the octahedral structure was determined. The oxalate acts and bidentate ligand, and at $[Zn_2\,(imi)_4(ox)_3]$ oxalate acts as bridge ligand.

$$Cu^{2+} + 3\,Ox^{2-} \longrightarrow [Cu\,(ox)_3]^{4-}$$

$$Cu^{2+} + 2\,Ox^{2-} + 2\,imi \longrightarrow [Cu\,(imi)_2(ox)_2]^{2-}$$

$$Zn^{2+} + 2\,Ox^{2-} + 2\,imi \longrightarrow [Zn\,(imi)_2(ox)_2]^{2-}$$

$$Zn^{2+} + 3\,Ox^{2-} + 4\,imi \longrightarrow [Zn\,(imi)_4(ox)_3]^{2-}$$

(Ox= oxalate C_2O_4, imi = imidazol)

References:

[1] B. Kobely, J. Kiss, K.Hernadi, I. Palinkko, J of Molecular Structure 864-836 **(2007**) 345-348.
[2] Y. Xu, X. Song, L. Li, J Chem Crystallogr 37 **(2007**) 651- 654.
[3] A. S. Zidan, J of Thermal Analysis and Calorimetry, 68 **(2002)** 1045- 1059.

Synthesis of new macrocycles with nitrogen and oxygen bridges

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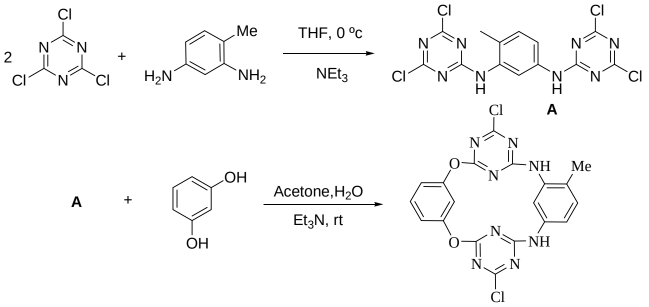
Macrocyclic chemistry is a great investigation arena and, for example, many Macrocyclic systems have been achieved since Pedersen`s earlier synthesis Of crown ether derivatives [1]. Macrocyclic compounds are now used for a diversity of usages [2] such as sensors, cryptands, imaging agents, catalysts and for ion analysis, affording more motivation for the development of this area. The amplification of drastic methodology for the synthesis of macrocyclic system with new molecular architectures, bearing heterocyclic planks within the loop sectors, is an arena of angoing ordinary interest and such macrocycle systems synthesized by performing reactions including nucleophilic attack at sp^2 and Sp^3 carbon sites that are exocyclic to heteroaromatic ring. perhalogenated heteroaromatic compounds, such as cyanuric chloride, are Multipurpose "bulding blocks" that combine with a number of acceptable difunctional Nucleophiles to obtain access to a diversity of macrocyclic.

Recently we described a general approach towards the synthesis some fluorinated Macrocycles by sequential nucleophilic aromatic substitution processes involving pentafluoropyridine and tetrafluoropyrimidine and various diamines as the structural components [3]

In this work, we would like to report synthesis of macrocycle from cyanuric chloride with bidentate nucleophiles in two steps.



References:

[1] Baldini, L.; Casnati, A.; Sansone, F.; Ungaro, R. *Chem. Soc. Rev.* **2007**, *36*, 254.

[2] Kim, J. S.; Quang, D. T. *Chem. Rev.* **2007**, *107*, 3780.

[3] Ranjbar-Karimi, R.; Sandford, G.; Yufit, D. S.; Howard, J. A. K. *J. Fluorine Chem.* **2008**, *129*, 307.

Copper-catalyzed coupling of amides with vinyl bromides in the presence of KF/Al_2O_3

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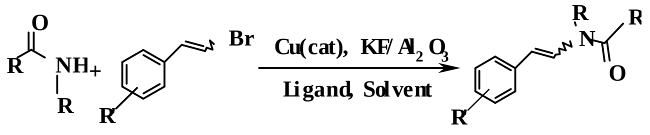
Enamides are important synthetic intermediates, as well as a structural component of many natural products [1]. Conventionally, protocols for their preparation include direct addition of amides to alkynes, acylation of imines, the Curtius rearrangement of α,β-unsaturated acyl azides, and the olefination of amides. Although these protocols provide access to enamides, they suffer from either low yield or lack of stereocontrol on the double bond geometry.

Transition metal-catalyzed C-N bond formation has been an area of intensive research during the past 20 years [2]. Most of the work has concentrated on the formation of aromatic C-N bonds, using palladium as catalyst [3]. More recently, this methodology was successfully extended to use copper as catalyst [4].

In this work, a general and efficient copper-catalyzed method for the amidation of vinyl bromides has been developed. This protocol uses a combination of copper iodide and KF/Al_2O_3. Yield of the reactions were good and all the products were characterized by ^{1}HNMR spectra, melting point and comparison with authentic samples.



R=H, Aryl, Alkyl
R′=H, OMe, Cl

Reference:

[1] Furstner, A.; Dierkes, T.; Thiel, O. R.; Blanda, G. *Chem Eur. J.* **2001**, *7*, 5286.
[2] Palomo, C.; Aizpurua, J. M.; Legido, M.; Picard, J. P.; Dunogues, J.; Constantieux, T. *Tetrahedron Lett*. **1992**, *33*, 3903.
[3] (a) Willis, M. C.; Brace, G. N. *Tetrahedron Lett*. **2002**, 43,9085. (b) Kozawa, Y.; Mori, M. *Tetrahedron Lett*. **2002**, 43, 111.
[4] Jiang, L.; Job, G. E.; Klapars , A.; Buchwald, S. L. *Org. Lett*.. **2003**, *5*,3667.

Synthesis and investigation of novel poly(ionic liquid)s with various anions

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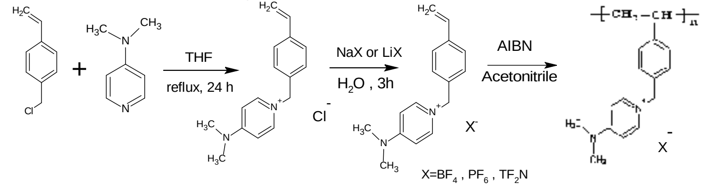
Ionic liquids are organic salts with a low melting point (_100 °C) that have been the focus of many investigations because of their chemical stability, low flammability, negligible vapor pressure, high ionic conductivity, and wide electrochemical window.[1]The interest of ionic liquids in polymer chemistry is very recent. Typical research has reported its use as green solvents for the synthesis of homopolymers [2] and block copolymers [3]. The polymer with IL inside chain may be a new class of polymer materials with exceptional properties such as thermal stability, mechanical properties, electrochemical activity and CO_2 absorption ability. This wide scope of applications offers good opportunities for the development of new kinds of ionic liquid-based polymers. Interestingly, functionalization of polymers having some of the characteristics of ionic liquids has been pursued as a way of developing high-performance polymer electrolytes [4,5] and gas separation membranes .

Herein we report the synthesis of new ionic liquid monomers such as *N*-(4vinyl benzyl) - 4 – (N,N-dimethylamino) pyridinium chloride , tetrafluoroborate ,hexafluorophosphate and bis (trifluoromethane)sulfonamide and their polymers. .In other word we synthesized new polystyrene with ionic liquid as side chain.Some of their properties such as the solubility and thermal stability of the obtained poly(ionic liquid)s are characterized and compared with poly(4-chloromethylstyrene). The anions strongly affected the properties of the polymers.



References:

[1] Rogers, R. D.; Seddon, K. R.; Volkov, S. In Green Industrial Applications of Ionic Liquids; Nato Science Series; Kluwer Academic: Boston, **2002**; pp1–545.
[2] Carmichael, A. J.; Haddleton, D. M.; Bon, S. A. F.; Seddon, K. R. *Chem Commun* **2000**, *1237*.
[3] Zhang, H.; Hong, K.; Mays, J. W. *Macromolecules* **2002**, *35*, 5738.
[4] Yoshizawa, M.; Ohno, H. *Electrochim Acta* **2001**, *46*, 1723.
[5] Yoshizawa, M.; Ogihura, W.; Ohno, H. *Polym Adv Technol* **2002**, *13*, 589.

Synthesis of polyhydroquinoline derivatives through the Hanthzsch four component using Iron (III) phosphate catalyst

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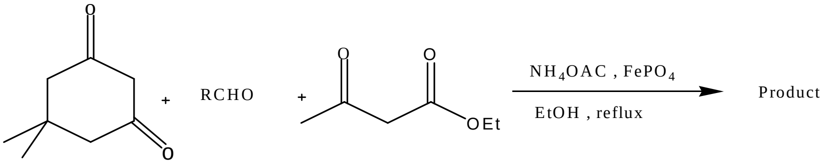
4-Substituted 1,4-dihydropyridine (DHPs) comprise a large family of medicinally important compounds. They can cure the disordered heart ratio as a chain- cutting agent of factor Ⅳ channel, possess the calcium channel agonist-antagonist modulation activities [1] and also behave as neuroprotectants, cerebral antiischaemic agents and chemosensitizers [2].

In this communication we wish to report the synthesis of polyhydroquinoline using dimedone with various aldehydes and ethyl acetoacetate and NH_4OAc in the presence of $FePO_4$ as a mild , green, efficient , reusable catalyst in ethanol under reflux condition (Scheme 1).



R: Aromatic, Aliphatic

Scheme 1

References:

[1] (a) U. Eisner, J. Kuthan, Chem. Rev. **1972** , 72, 1.
(b)M.Kawase,A.Shah,A.Gaveriya,N.Motohashi,H.Sakagami,A.Varga,J.Molnar,Bioorg. *J. Med. Chem.* **2002,** 10, 1051.
(c) R. Shan, C.Velaquez,E.E.Knaus, *J. Med. Chem.* **2004**, *47*, 254.
(d)Y.Sawada,H.Kayakiri,Y.Abe,T.Mizutani,N.Inamura,M.Asano,C.Hatori,I.Aramori,T.Oku, H.Tanake, *J.Med.Chem.* **2004**, *47*, 2853.
[2] (a) V. Klusa, Drugs Future**1995**, *20* , 135.
(b) R. Boer,V .Gekeler,Drugs Future **1995** , *20*, 499.

One-pot three component reaction of 4-hydroxy-1-methyl-2(1*H*)-quinolinone and acetylenic esters in the presence of PPh_3

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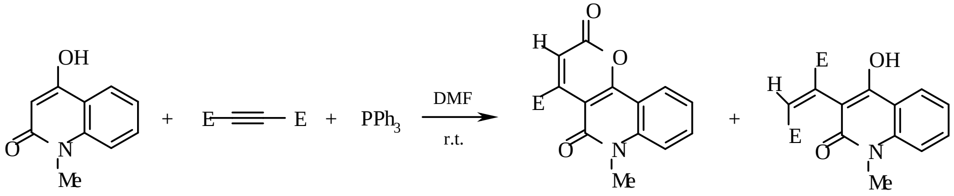
Pyranoquinoline derivatives constitute a large group of naturally occurring alkaloids [1]. These compounds are of current research interest because of their biological and medical properties [2]. In view of the importance of pyranoquinoline and its derivatives, several methods were developed for the synthesis of these heterocycles [3].

As a continuation of our research devoted to the development of new methods for preparation of heterocycles [4], we performed a one-pot three component reaction of 4-hydroxy-1-methyl-2(1*H*)-quinolinone **1** and dialkyl acetylenedicarboxylate **2** in the presence of triphenylphosphine which leads to alkyl 6-methyl-2,5-dioxo-5,6-dihydro-2*H*-pyrano[3,2-*c*]quinoline-4-carboxylate **3** and di(*tert*-butyl)(*E*)-2-(4-hydroxy-1-methyl-2-oxo-1,2-dihydro-3-quinolinyl)-2-butenedioate **4**.



1 **2** **3** **4**

	E	Yield (%)
3a	CO_2Me	60
3b	CO_2Et	66
4	$CO_2{}^tBu$	50

The Structures of **3** and **4** were deduced from their ^1H, ^{13}C NMR, IR and mass spectral data.

References:

[1] Michael, J. P. *Nat. Prod. Rep.* **1999**, *16*, 697.
[2] Yamada, N.; Kadowaki, S.; Takahashi, K.; Umezu, K. *Biochem. Pharmacol.* **1992**, *44*, 1211.
[3] Babu, G.; Perumal, P. T. *Tetrahedron Lett.* **1998**, *39*, 3225.
[4] Asghari, S.; Tajbakhsh, M.; Taghipour, V. *Tetrahedron lett.* **2008**, *49*, 1824.

Fast and eco-friendly reduction of carbonyl compounds with $NaBH_4$ in water

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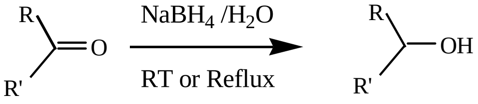
Solvents define a major part of the environmental performance of processes in chemical industry and also impact on cost, safety and health issues. The idea of green solvents expresses the goal to minimize the environmental impact resulting from the use of solvents in chemical production [1].

On the other hand, the use of a large amount of conventional volatile solvents required to conduct a chemical reaction creates ecological and economic concerns, therefore replacing a harmful and polluting organic solvent with a innocuous solvent, such as water, is an example of green chemistry[2]. Green chemistry is the name given to modifications implemented in chemical manufacturing processes which ensure a safer and cleaner environment. In this context, the use of water as a green solvent can be the best medium of choice to perform chemical reactions[3]. The reduction of carbonyl compounds to the corresponding alcohols in water is a fundamental functional transformation and it is one of the frequently used reactions in organic synthesis.

Reduction by hydrides, which at one time seemed impossible to carry out in water, are now a reality. Herein, we describe an efficient method for the reduction of varieties of carbonyl compounds such as aldehydes, ketones, conjugated aldehydes and ketones, α-diketones to their corresponding alcohols with $NaBH_4$ in water as a green solvent at room temperature or reflux conditions (Scheme I).



Reference:
[1] C. Capello, U.Fischer, K. Hungerbuhler. *Green Chem*. **2007**, *9*, 927.
[2] (a) Nagendrappa, G. *Resonance* **2002**, *59*. (b) Varma, R. S.; Namboodiri, V. V. *Pure Appl. Chem*. **2001**, *73*, 1309. (c) Varma, R. S. *Green Chem*. **1999**, *43*.
[3] (a) Grieco, P.A. *Organic Synthesis in Water*; Blackie Academic & Professional: New York, **1998**. (b) Adams, D. J.; Dyson, P. J.; Tavener, S. J. *Chemistry in Alternative Reaction Media*; Wiley: New York, **2003**.

Synthesis and characterization of waterborne polyurethane/clay nanocomposites

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In recent years, nanostructure hybrid organic-inorganic composites, based on organic polymer and inorganic clay minerals consisting of silicate layers whose thickness is 1 nm scale, have attracted the great interest of researchers. These composites exhibit improved performance properties because of their unique phase morphology by layer intercalation or exfoliation maximizes interfacial contact between the organic and inorganic phases and increases interfacial properties. Nanoparticles often strongly influence the properties of composites at very low-volume fractions. Waterborne polyurethane including coatings and adhesives has attracted great interest because it is no-toxic, non-flammable and friendly to environment [1].

These polymers exhibit weak water resistance and low adhesion in the moisture environment due to hydrophilic ioned bonds, ether groups, urethane groups as well as ester groups susceptible to hydrolysis. For better performance of water and solvent based polyurethane they are modified either by varying polyurethane microstructures or by dispersing inorganic fillers, especially by incorporating nanosized layered silicates within the polyurethane continuous matrix [2,3].

In our research, aqueous emulsion of polyurethane ionomers, based on PTMG as soft segment, isophorone diisocyanate (IPDI) as diisocyanate, dimethylol propionic acid as potential ionic center and chain extender, triethyl amine (TEA) as neutralizer were reinforced with organoclay (cloisite 30B) to obtain nanocomposites. The prepared samples were characterized with conventional techniques. The results show that thermal and tensile strength, modulus, hardness and contact angle are increased and water absorption is decreased. Also, X-ray and TEM studies showed that most of the nanoclays are partially exfoliated in the polymer matrix.

References:

[1] Irle, C., Bayona, M., Roschu, R., *Surf. Coat. Int., Part A* , **2005**, 88, 221.
[2] Sankaraiah, S., Jun-Younge, L., Jung Hyun K., In woo, Ch., *Compos. Sci. Technol.*, **2007**, 67, 1561.
[3] Xianghua, D., Fang, L., Yuanfang, L., Yong jun, Ch., Demin, J., *Prog. Org. Coat.*, **2007**, 60, 11.

Task-specific ionic liquid as catalyst for the efficient synthesis of (2-amino-3-cyano-4H-chromene-4-yl) phosphonic acid dialkyl esters derivatives

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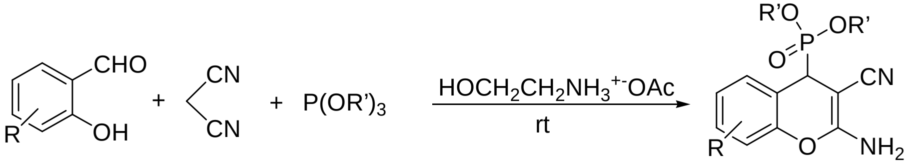
Phosphonates are fascinating and versatile compounds in organic synthesis. They have unique properties which expand their applications as enzyme inhibitors, metabolic probes, peptide mimetics, antibiotics, and pharmacological agents besides to their traditional roles as intermediates in organic synthesis [1].

Chromenes represent an important class of compounds being the main components of many natural occurring products and are widely employed as cosmetics, pigments, and potential biodegradable agrochemicals [2]. Fused chromenes are biologically active compounds with a wide spectrum of applications as antimicrobial, antiviral, mutagenicity, antiproliferative, sex pheromone, antitumor, and central nervous system agents [3].

Room-temperature ionic liquids (ILs) are composed of bulky organic cations and either an organic or inorganic anions. ILs has many unusual properties, such as extremely low vapor pressure, high thermal stability and chemical stability, excellent solvent ability for organic and inorganic compounds [4].

Herein, we wish to use a room temperature task-specific ionic liquid as an efficient catalyst for the synthesis of (2-amino-3-cyano-4H-chromene-4-yl) phosphonic acid dialkyl esters derivatives. Good to high yields, short reaction times, no by-product formation, simple operation are the advantageous of the present method for the preparation of these important scaffolds.



References:

[1] (a) Allen, M. C.; Fuhrer, W.; Tuck, B.; Wade, R.; Wood, J. M. *J. Med. Chem.* **1989**, *32*, 1652; (b) Patel, D. V.; Rielly-Gauvin, K.; Ryono, D. E. *Tetrahedron Lett.* **1990**, *31*, 5587.

[2] Hafez, E. A.; Elnagdi, M. H.; Elagemey, A. G. A. ; El-Taweel, F. M. A. A. *Heterocycles*. **1987**, *26*, 903.

[3] Khafagy, M. M.; El-Wahas, A. H. F. A.; Eid, F. A.; El-Agrody, A. M. *Farmaco*. **2002**, *57*, 715.

[4] Zhai, L.; Zhong, Q.; He, C.; Wang, J. *J. Hazard. Mater.* **2010**, *177*, 807.

Synthesis of some cyclooctane-based pyrazine-2,3-dicarbonitrile and derivatives

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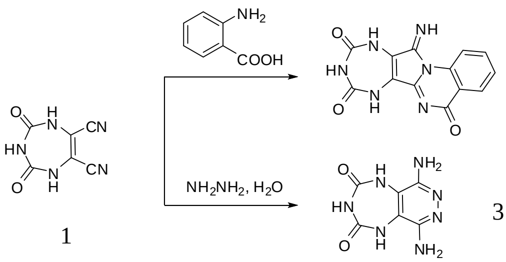
1,3,5-triazepine-2,4-dione 1 fromed from reaction of diaminomaleonitrile (DAMN) with chlorocarbonyl isocyanate and also related reactions on product 1 obtained 2,3 [1].



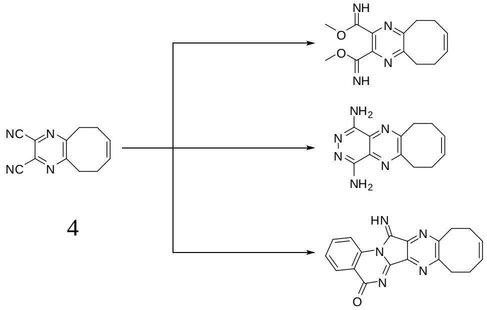
1

2

3

In this work, The product of condensation 1,2-diamine with alpha-ketole and 1,2-diketone is the same as for alpha-diketone product. As a result, once DAMN react with alpha-ketoles, forming pyrazine-2,3-dicarbonitrile derivatives.

The pyrazine-diimidate 5 was prepared by reaction of (Z)-5,6,9,10-tetrahydrocycloocta[b]pyrazine-2,3-dicarbonitrile 4 in solution that sodium methoxide in methanol [2,3]. When the reaction of compound 1 was treated with hydrazine hydrate was produced pyrazine-1,4-diamine 6. Consequently, the compound 4 was reacted with anthranalic acid in pyridine/triethylamine media was obtained 7.



4

5

6

7

References
[1] Abdel-Razik, H. H. *ARKIVOC* **2004** (i) 71.
[2] Kojima T. Nagasaki, F. *Journal of Heterocyclic chemistry*, **1980**, *17*, 455.
[3] Schaefer F. C. Peters, G. A. *Journal of organic chemistry*, **1960**, *26*, 412.

Sevoflurane synthesis modification and the bench scale preparation

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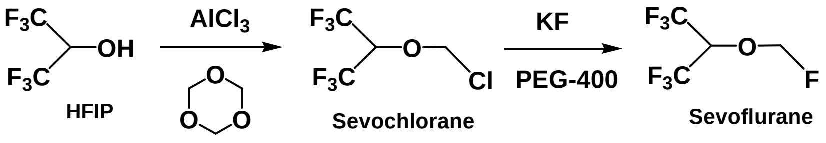
Sevoflurane, 1,1,1,3,3,3-hexafluoro-2-(fluoromethoxy)- propane, is one of the most widely used inhalation anesthetics. Major synthetic routes to Sevoflurane employ hexafluoroisopopyl alcohol (HFIP) as a starting material [1]. Sevoflurane is currently manufactured by a one-step reaction from HFIP and HF/H_2SO_4 and a three-step reaction. In the later process, HFIP is methylated followed by chlorination and Fluorine exchange reactions [2]. In addition, a two step method has been reported which can be run in a single vessel and affords pure Sevoflurane in high yield. The inventors of this method believe that this new process will be used in the future manufacture of Sevoflurane [3].

Among the disadvantages of this process is that large quantities of solvent and KF are used in the second step. The long reaction time of the first step (about 24 hour) is an additional disadvantage of the processes which incur additional costs. In this study, the reaction time of the first step was decreased to 4 hour by changing the ratio of the starting materials. The other advantage of this study is decreasing the amount of solvent and KF, in the second step, with no change on the yield and purity of the product. The reaction was monitored by^{19}FNMR spectroscopy and was scaled up in bench scale to afford 40-gr batches of 99.3% pure Sevoflurane. Both isolated Sevochlorane, as intermediate, and Sevoflurane were analyzed by ^{1}H, ^{13}C and ^{19}FNMR spectroscopy.



References:

[1] Longnecker, D. E.; Murphy, F. L. Introduction to Anesthesia; W. B. Saunders: Philadelphia, PA, **1992**.

[2] Max T. Baker, PhD; Anesth. Analg. **2007**, *104*, 1447.

[3] Kornpati Ramakrishna, Chris Behme, Ralph M. Schure, and Christopher Bieniarz; Org. Proc. Res. Dev., **2000**, *4 (6)*, 581.

An efficient and green approach for the synthesis of vinyl aryl ethers in the presence of guanidine hydrochloride

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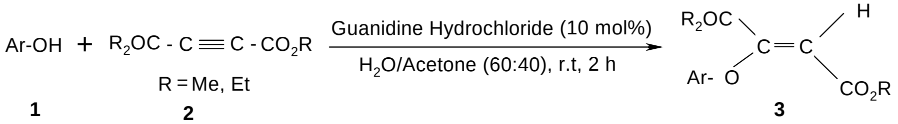
Vinyl ethers of alcohols and phenols are well established monomers, building blocks and auxiliaries in organic synthesis, steadily expanding their scope of applications [1]. This compounds are important raw materials as practical chemicals for the production of glutaraldehyde [2] as well as vinyl polymer materials [3] containing oxygen which are expected to degrade easily in nature. In the last decade, green chemistry has been recognized as a new approach in environmental protection [4]. Thus demands for substitutes for toxic and/or volatile molecular solvents are increasing.

In this paper we wish to report a stereoselective synthesis of dialkyl (Z)- aryloxy butenedioates **3** from the reaction of a wide range of functionalized phenols or naphtols **1** and dialkyl acetylenedicarboxylates **2** in water-acetone solution as green solvent using guanidine hydrochloride as a novel and effective catalyst. Guanidines can be categorized as organic superbases [5] owing to the resonance stabilization of their conjugated acids [6] and are therefore expected to catalyze various types of base-mediated organic reactions.



References:

[1] Tedeschi, R. J.; *Acetylene-based chemicals from coal and other natural resources*, Marcel Dekker. Wiley, New York. **1982**.
[2] Cope, A. C.; Dryden, H. L. J.; Howell. C. F. *Organic syntheses*; Wiley & Sons, New York, Collect. **1963**.
[3] Kojima, K.; Sawamoto, M.; Higashimura, T. *Macromolecules.* **1989**, *22*, 1552.
[4] Anastas, P. T.; Warner, J. C. *Green chemistry: theory and practice,* Oxford University Press. Oxford. **2000**.
[5] Kovacevic, B.; Maksic, Z. B. Organic Letters. **2001**, *3,* 1523.
[6] Yamamoto, Y.; Kojima, S. *The chemistry of amidines and imidates.*; Patai, S.; Rappoport, Z. Eds.; John Wiley & Sons Inc, New York. **1991**.

Synthesis and recognition of molecularly imprinted polymers for gastrodin based on surface modified silica nanoparticles

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Molecularly imprinted polymers (MIPs) were artificially synthesized material to imitate natural molecular recognition. MIPs are extensively applied in segregation analysis, biosensor, catalysis and other fields for its structure-effect predetermination, specific recognition and widely practicability[1-3]. A molecular imprinting material with high performance for recognizing Gastrodin (GAS) was prepared by adopting the novel surface molecular imprinting technique. Silica nanoparticles were first modified with 3-Methacryloxypropyltrimethoxysilane (KH-570) as a carrier material. Then GAS molecularly imprinted polymers based on the surface modified silica (GAS-SMIP) were prepared by polymerization with methacrylic acid as the functional monomer, ethylene glycol dimethacrylate as the crosslinker. The equilibrium adsorptive experiments indicated that GAS-SMIP had significantly higher adsorption capacity for GAS than its non-imprinted polymers. Scatchard analysis revealed that two classes of binding sites were formed in GAS-SMIP with dissociation constants of 1.019 and 7.278 μmol/mL, and the affinity binding sites of 17.82 and 83.11 μmol/g, respectively. The selectivity coefficient of GAS-SMIP for GAS in respect to competition species obtained was 3.455, which revealed GAS-SMIP had excellent selectivity and site accessibility for GAS. Kinetic binding study showed GAS-SMIP adsorbed quickly in the first 40 minutes, and reached saturation adsorption at 1 h.

References

[1] Puoci, F.; Cirillo, G.; Curcio, M. Analytica Chimica Acta 2007, 593, 164.
[2] Tamayo F. G., Turiel E., Martin-Esteban A., Journal of Chromatography A 2007, 1152, 32.
[3] Sadeghi, S.; Mofrad, A. A. Reactive and Functional Polymers 2007, 67, 966.

Composition and antibacterial activity of essential oil from leaves of *Thymus fedtschenkoi* Ronneger from Iran

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The genus *Thymus* , family Lamiacea , includes about 350 species worldwide and is distributed mainly in temperate Eurasia. In Iran 14 species are present, among which four are endemic [1]. *Thymus* species have also several folkloric uses,e.g.fresh and dried thyme leaves are used extensively for flavoring purposes.The chemical composition of the oils of various *Thymus* species has been extensively studied.Water distilled oil obtained from the aerial parts of *Th.kotschyanus, Th.pubescens* and *Th.carmanicus* have been the subject of our previous studies. The oil of all three species were rich in monoterpene phenols ,thymol(38.0%,37.9% and 40.8%) and carvacrol(14.2%,14.1% and 24.8%) [2]. The oil of *Th.caucasicus* was rich in thymol(34.2%),methyl chavicol(25.1%)and γ-terpinene(12.7%)[3]. The aim of our study is to identify and antibacterial activity of the constituents of the essential oil obtained by hydrodistillation from leaves of *Th.fedtschenkoi* growing wild at flowering stage in Miyaneh,Province of Azarbayejan,in July 2009,of Iran, and analyzed by GC and GC/MS.

Thirty-four compounds in the leaf oil of *Th.fedtschenkoi*, which represented about 100% of the total oil were identified.The oil of *Th.fedtschenkoi* consisted of ten monoterpene hydrocarbons (25.1%) , twelve oxygenated monoterpenes (60.8%) , eight sesquiterpene hydrocarbons (9.8%) , two oxygenated sesquiterpenes (1.9%) and two nonterpenoid compounds (2.1%) . The major components of this oil were thymol (28.1%) and p-cymene (10.0%) . Other notable constituents were borneol (6.5%) and 1,8-cineole (6.1%) . As can be seen from the above information in the leaf oil of *Th.fedtschenkoi* monoterpenes (85.9%) predominated over sesquiterpenes (11.7%) . Antibacterial activity was measured using the growth inhibitory zones. The Oil showed antibacterial activity against Gram-positive bacteria.

References:

[1] Mozaffarian, V. A Dictionary of Iranian Plant Names , Farhang Moaser Publishers , Tehran , Iran , **1996**,548.

[2] Rustaiyan, A.; Masoudi, S.; Monfared, A.; Kamalinejad, M.; Lajevardi, T.; Sedaghat, S.; Yari, M. Planta Med.**200**0,66,197.

[3] Masoudi S.; Aghajani , Z.; Rustaiyan, A.; Feizbakhsh,A.R.; Motavalizadeh, A.R. J.Essent. Oil Res.**2009.**21.5.

Synthesis of Formamidines Using Phenyl phosphonic acid as a Catalyst in Water

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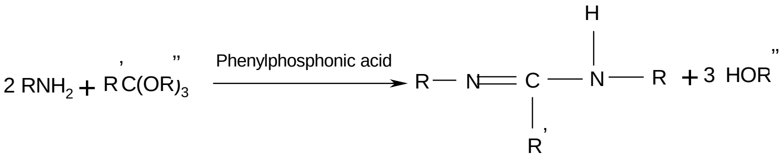
Formamidines are derivatives of the unstable imidic acid having a unique and fascinating spectrum of biological and pharmacological activity; therefore, they have been extensively studied in medicinal chemistry [1-2].

Formamidines, ArN=CHNHAr, and their anion derivatives are common ligands frequently used in coordination chemistry, in which they were found binding to transition metals with monodentate, chelating or bridging bonding modes [3]. The formation of formamidine would depend on the reaction condition and the catalyst used to catalyze the reaction [4].

Herein, we report a new method for synthesis of formamidines with amines and trialkylorthoester in water in the presence of catalytic amount of solid acid catalysts such as phenyl phosphonic acid. In this method a number of symmetrical formamjdines were synthesized in excellent yield.



$$2\,RNH_2 + R'C(OR'')_3 \xrightarrow{\text{Phenylphosphonic acid}} R-N{=}\underset{\underset{R'}{|}}{C}-\overset{\overset{H}{|}}{N}-R + 3\ HOR''$$

R=alkyl or aryl   R' = H , alkyl   R'' = alkyl

References:

[1] Diaz, D. D.; Finn, M. G. *Chem. Eur. J.* **2004**, *10*, 303–309.

[2] Leung, V. K. S.; Chan, T. Y. K.; Yeung, V. T. F. *J. Toxicol., Clin. Toxicol.* **1999**, *37*, 513–514.

[3] Cotton, F.A.; Daniels, L.M. ; Murillo, C.A. and ang, X. W. *Inorg. Chem*. **1997**, 36, 869.

[4] Roberts, R.M.; and Vogt, P.J. *J. Am. Chem.* Soc**. 1956**, 78, 4778.

Vinyltriphenylphosphonium salt mediated preparation of fully substituted furans and electron-poor imides from benzoic acid, tetramethylbutylisocyanide and acetylenic esters

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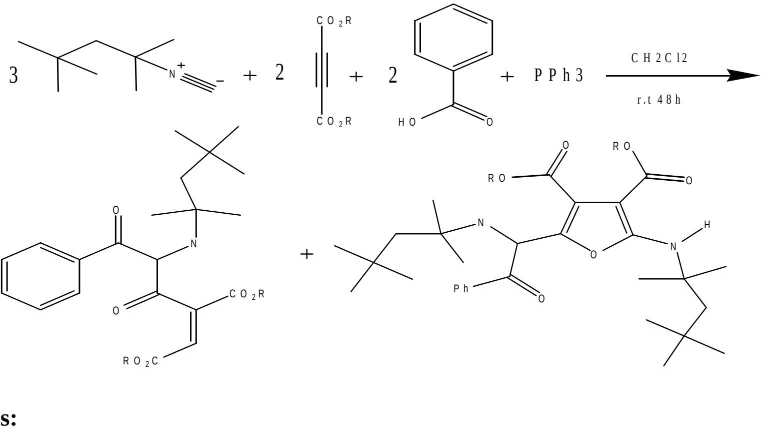
For several years acetylenic esters have attracted the attention of organic chemists and are reactive systems that can take part in many chemical syntheses [1,2], almost as a Michael acceptor in the organic reactions [1]. In recent years, we have established a one-pot method for the synthesis of stabilized ylides[1]. Protonation of the reactive intermediates produced in the reaction between triphenylphosphine and dialkyl acetylenedicarboxylates by benzoic acid leads to vinyltriphenylphosphonium salts, which undergo complex reactions with 1,1,3,3 tetramethylbutylisocyanide to produce corresponding densely functionalized furans and imides in fairly good yields in neutral conditions. The reaction proceeds smoothly and cleanly under reaction conditions and no side reactions were observed. The reactions were completed in 48 h. and densely functionalized furans observed as major products. In this reaction triphenylphosphine acts as a catalyst.



References:

[1] Ramazani, A.; Kazemizadeh, A. R.; Ahmadi, E.; Noshiranzadeh N.; Souldozi A. *Curr. Org. Chem*. **2008**, *12*, 59.
[2] Ramazani, A.; Kazemizadeh, A. R.; Ahmadi, E.; Ślepokura, K.; Lis, T. *Z. Naturforsch*., **2006**, *61b*, 1128.

Synthesis and characterization of linearly condensed pentathienoacene as a good building block in organic light emitting diodes (OLED)

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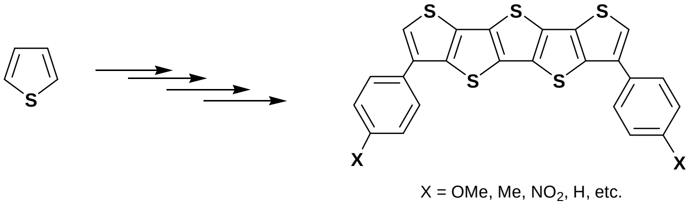
Organic semiconductors employed as active layers in fieldeffect transistors (FETs) are of great current interest because such FETs can potentially be fabricated at low cost, over large areas, and on flexible substrates [1]. Such facile fabrication approaches offer a significant advantage over silicon technology in numerous applications. Much progress on organic FETs has been made in various organic-based electronic circuits, such as displays [2], sensor [3], inverts, and logic elements [4]. We present the synthesis and characterization of a fused-ring compound, dithieno[2,3-d:2',3'-d']thieno[3,2-b:4,5-b']dithiophene derivatives (pentathienoacene, PTA) (Scheme 1).



Scheme 1.

References:

[1] Dimitrakopoulos, C. D.; Malenfant, P. R. L. *Adv. Mater.* **2002**, *14*, 99.
[2] Comiskey, B.; Albert, J. D.; Yoshizawa, H.; Jacobsen, J. *Nature* **1998**, *394*, 253.
[3] Crone, B.; Dodabalapur, A.; Lin, Y.-Y.; Filas, R. W.; Bao, Z.; LaDuca, A.; Sarpeshkar, R.; Katz, H. E.; Li, W. *Nature* **2000**, *403*, 521.
[4] Bartic, C.; Palan, B.; Campitelli, A.; Borghs, G. *Sens. Actuators, B,* **2002**, *83*, 115.

The effect of chloride ion on inhibition behaviour of 5-(4-methyl phenyl)-2H-tetrazole on carbon steel corrosion in sulfuric acid

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Corrosion prevention is of great importance in industrial application of materials [1]. Carbon steel has been widely employed as a construction material for pipe work in the oil and gas production, such as down hole tubular, flow lines and transmission pipelines. However, one of the major problems related to its use is its low corrosion resistance in these environments [2]. Organic compounds are usually used to protect metal against corrosion as inhibitors in acidic media. Azoles derivatives as heterocyclic compounds containing N and S atoms, like imidazoles[3] and tetrazoles[4], have attracted much attention because of the efficient inhibition abilities to the metal corrosion. Heteroatoms act as the active site for adsorption of organic molecules on metal surface [5].

In this research, inhibition of carbon steel corrosion in 0.5 M sulfuric acid was investigated within mixture of chloride ion and a tetrazole derivative namely, 5-(4-methyl phenyl)-2H-tetrazole. Weight loss method, scanning electron microscopy (SEM) and electrochemical techniques including potentiodynamic polarization and electrochemical impedance spectroscopy were employed in the present study. The results reveal that inhibition efficiency of studied tetrazole increases with increasing its concentration. Furthermore, the presence of 0.1 M chloride ion causes an increase in inhibition efficiency. According to the polarization plots the inhibition solution acts as a mixed type inhibitor. Different isotherms were evaluated on the adsorption of tetrazole and chloride ion on carbon steel surface and adsorption parameters, equilibrium constant (K_{ads}) and Gibbs free energy (ΔG_{ads}), were calculated. The results of experiments at different temperatures (25-45 °C) used to calculation of appearance activation energy and thermodynamic parameters of transition state.

References:

[1] Zhang, J., Liu, J., Yu, W., Yan, Y., You, L., Liu, L., *Corros. Sci.*, 2010, 52, 2059-2065.
[2] Ghareba, S., Omanovic, S., *Corro. Sci.*, 2010, 52, 2104-2113.
[3] Likhanova, N. V., Dominguez-Aguilar, M. A., Olivares-Xometl, O., Nava-Entzana, N., Hector Dorantes E., *Corros. Sci.*, 2010, 52, 2088-2097.
[4]Mihit, M., Laarej, K., Abou El Makarim, H., Bazzi, L., Salghi, R., Hammouti, B., *Arab. J. Chem.*, 2010, 3, 55-60.
[5] Ma H., Song, T., Sun, H., Li, X., *Thin Solid Films*, 2008, 516, 1020-1024.

Synthesis ,characterization and spectroscopic studies of N,N'-bis (salicylidene) 1,2 –phenylenediaminato dioxomolybdenum (VI)

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Molybdenum is an essential element in diverse biological systems, as the activities of various enzymes are based on the reactions of a molybdenum centre[1,2]. Related molybdenum compounds are also used to catalyse industrial processes including the isomerization of allyl alchols[3], oxo transfer reactions [4] and other properties.

An equimolar $MoO_2 (acac)_2$ { acac=acetylacetonato } reacted with an equimolar salphen (salphen = N ,N' – bis (salicylidene) 1 ,2 –phenylenediamine) tetradetate Schiff base ligand to form mononuclear, dioxomolybdenum (VI) Complex of type [MoO_2(salphen)]. Elemental analysis, magnetic measurements IR and NMR spectra as well as conductance measurements were used to confirm the structure which showing the geometry of the molybdenum ion to be octahedral.

References :

[1] R .Hill, Chem. Rev. 96 (1996) 2757.
[2] J. H. Enemark, J. J. A. Coon, J. J. Wang. R. H. Holm, Chem. Rev. 104 (2004) 1175.
[3] F. R. Froczek, R. L. Luck, G. Wang, Inorg. Chem. Commun. 5 (2002) 384.
[4] K. Most, J. HoBbach, D. Vidovic, J. Magull, N. C. Mosch-Zanet Ti, Adv. synth. Catal. 347 (2005) 463.

Synthesis, characterization and DNA-binding studies of two Mo (VI) aroylhydrazone complexes

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Schiff base complexes have attracted comprehensive attention in the development of new therapeutic agents and novel probes to define the structure of nucleic acid molecules [1]. Schiff bases are potential anticancer drugs and these compounds when administrated as their metal complexes, have more anticancer activity in comparison to the free ligand [2].

The remarkable biological activity of acid hydrazides, R–CO–NH–NH2, a class of Schiff base, and the dependence of the mode of chelation with transition metal ions in their corresponding aroylhydrazones, R–CO–NH–N=CH–R, have shown to be significant [3].

In this study we synthesized two aroylhydrazones as tridentate ligands. The resulted dioxomolybdenum complexes were isolated from 1:1 reaction mixture containing the Schiff base ligands and $MoO_2(acac)_2$.

The end products found to be $[MoO_2(L)(solv)]$(L=Schiff base ligand and solvent=MeOH). The characteristics of complexes molecular structure were addressed by spectroscopic techniques (IR, ^{1}H NMR, ^{13}C NMR, UV-Vis) and their ultimate molecular structures were determined by X-ray crystallography.

To address the biological effects, the interaction of the complexes with CT-DNA was investigated using UV-Vis, fluorescence and circular dichroism spectroscopies. The preliminary results indicated the possibility of binding of two complexes to DNA through an intercalative mode.

References:

[1] Qin, D.D.; Yang, Z.Y.; Wang, B.D. *Spectrochimica Acta A.* **2007**, *68*, 912.
[2] Majumder, A.; Rosair, G.M.; Mallick, A.; Chattopadhyay, N.; Mitra, S. *Polyhedron.* **2006**, *25,* 1753.
[3] Hosseini Monfared, H.; Sadighian, S.; Kamyabi, M.A.; Mayer, P. *J.Mo.l Catalysis A.* **2009**, *304,* 139.

Synthesis and characterization of a new phosphorus compound with formula $(C_6H_5)NH(CHC_6H_5)P(O)(OH)_2$

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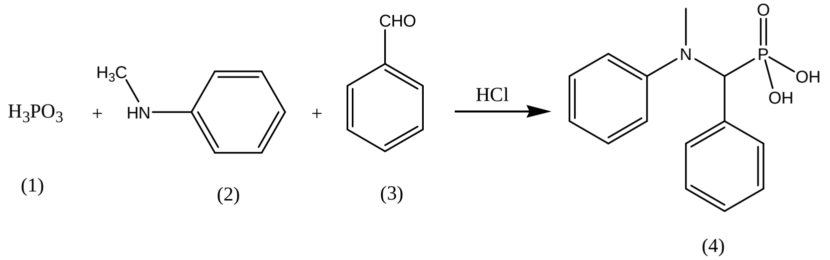
The synthesis of phosphorous compounds and their derivatives is a subject of considerable interest due to their crucial biological roles [1]. The major efforts were mainly focused on the biological area, where the species possessing the group under consideration play an important role as insecticides, pesticides and pharmacological agents, such as their urease inhibitor capacity. The synthesis and structures of some phosphorous compounds have been also reported [2-3]. In this work, a new ligand from phosphorous was synthesized and characterization by ^{1}H, ^{13}C, ^{31}P NMR and IR spectroscopies and elemental analyses. In this reaction, phosphoric acid (1) reacts with N-methyl aniline (2) and benzaldehyde (3) in the presence of hydrochloric acid to produce (methyl-phenyl-amino) phenyl- methyl- phosphonic acid (4), in fairly good yields.



References:

[1] Parang, K. *Bioorg. Med. Chem. Lett.*, **2002**, *12*, 1863.
[2] Iriarte, A.; Erben , M. *J. Mol. Struct.* **2008**, *886*, 66.
[3] Dueymes, C.; Pirat, C. *Tetrahedron Lett.* **2008**, *49*, 5300.

Palladium-catalyzed Heck reaction of 3, 4-dialkoxy iodobenzene with cycloalkenes

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The palladium-catalyzed arylation and vinylation of alkenes (Heck reaction) has become one of the most important and powerful transition-metal-catalyzed transformations in organic synthesis for generating new carbon-carbon bonds [1].

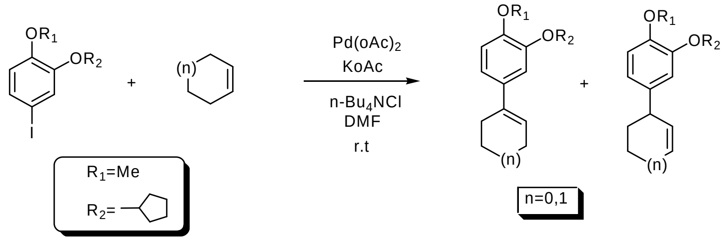
In addition, in most cases the Heck reaction of aryl halides and cycloalkenes proceeds extremely slowly, and thus only low yields of product are obtained [2]. But aryl iodides salts can be coupled with cycloalkenes more efficiently [3].

On the other hand, the influence of palladium catalysts and reaction conditions on the selectivity of Heck reaction of aryl iodide with cyclohexene has been investigated.

The purity of the synthesized compound was confirmed by chromatography. The structure of compound was characterized using IR, ^{1}HNMR and Mass spectra.

In this project an aryl iodide is coupled with cycloalkenes in the presence of Palladium acetate. (Scheme1)

Scheme 1



References:

[1] Beller, M.; Riermeier, T. H.; Stark, G. In *Transition Metals for Organic Synthesis*; Beller, M., Bolm, C., Eds.; VCH: Weinheim, Germany, **1998**; p 208.

[2] de Meijere, A.; Meyer, F. *Angew. Chem.* **1994**, *106*, 2473; *Angew. Chem., Int. Ed. Engl.* **1994**, *33*, 2379.

[3] Larock, R. C.; Baker, B. E. U.S. Patent 4 879 426, **1988**.

Efficient synthesis of dipeptides urea *via* four component Ugi reaction

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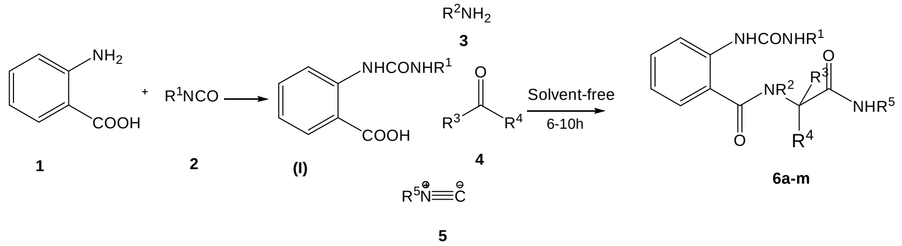
The synthesis of new biologically active molecules is important in the development of improved and innovative drugs. Finding a suitable route with fewer reaction steps for the synthesis of pharmaceutical scaffolds is very interesting. One of the best known these reactions is the Ugi four component coupling (4CC) reaction [1]. It has been well established that urea derivatives have got a significant place in modern medicinal chemistry. Urea derivatives have been reported in the literature as anticancer agent, anticonvulsant, and $CXCR_3$ antagonist [2, 3]. In this paper, carboxylic acids of urea functional group, which are produced by 2-amino benzoic acid and phenylisocyanate reaction, were selected for this work. We were interested in preparing a diverse set of polyfunctional dipeptides ureas using Ugi four-component condensation (Ugi-4CC) reaction conditions. Thus one-pot, five-component reactions of 2-amino benzoic acid (**1**), arylisocyanate **2,** primary amines **3**, oxo compound **4** and isocyanides **5** leading to the urea derivatives are described (Scheme1). We have established an efficient method for the synthesis of urea derivatives in high yields, *via* a one-pot, five-component reaction under mild and solvent-free conditions. The reaction scope is broad, permitting the use of four points of diversity in the starting materials. Due to the well-recognized utility of ureas, many libraries of compounds can be prepared using this method as structural scaffolds for further diversification.



References

[1] Dömling, A. In *Multicomponent Reactions*, Eds. Zhu, J.; Bienaymé, H. Wiley-VCH,Weinheim, **2005**, pp 76-95
[2] K.J. Hwang, K.H. Park, C.O. Lee, B.T. Kim, Arch. Pharm. Res. **2002**,25, 781-785.
[3] (a)J.A. Shimshoni, M. Bialer, B. Wlodarczyk, R.H. Finnell, B. Yagen, *J. Med. Chem.* **2007**, *50* , 6419-6427.(b) R.L. Knight, D. Meier, K. Oliver, J.W.G. Meissner, D.A. Owen, E.J. Thomas, N. Tremayne, S.C. Williams, Bioorg. *Med. Chem. Lett*. **2008**, *18*, 147-151.

A novel multi-component synthesis of pyrimidine and 1,4-dihydropyrimidine derivatives by Iron(III) phosphate as a catalyst

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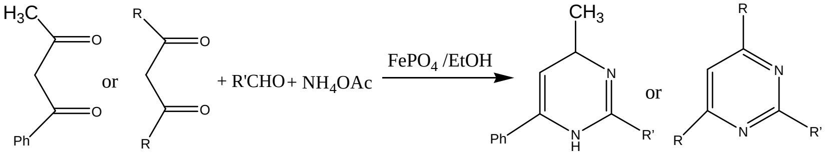
Azaheterocycles constitute a very important class of compounds. In particular, pyrimidines are of chemical and pharmacological interest. Compounds containing a pyrimidine ring system have been shown to possess antitumor, antibacterial, antifungal, anticonvulsant activities [1] Despite the important of dihydroazines for clarifying a wide range of theoretical, medicinal, which attracted attention because of their broad spectrum of biological action,such as aza-analogs of 4-aryl-1,4-dihydropyrimidines the chemistry of this group of compounds is still extremely spotty [2] 1,4-dihydropyrimidine containing saturated and unsaturated fragments are very convenient models for the study of such phenomena as the influence of substituents on the imine-enamine tautomeric equilibrium state [3] . owing to the unique of pyrimidine and 1,4-dihydropyrimidine derivaives, Modification of conventional strategies involving N-C-N fragment condensation with 1,3-dicarbonyl derivatives remains a common theme in current work . In this work we wish to reveal the preparation of 2,4,6-Trisubstituted pyrimidine via a simple , one-pot reaction from 1,3-diketone, aldehyde derivatives, ammonium acetate and using $FePo_4$ as a cost effective catalyst refluxingin in EtoH conditions in good to excellent yields. (Schem1)



R=alkyl,aryl

Scheme1

References:

[1] Agarwal, A.; Srivastava, k.; Puri, S.K.; Chauhan, P.M.S. *Bioorg.Med.Chem*. **2005**,13,4645.
[2] Weis, A.L.; Adu.*Heterocycl.chem.* **1995**,38,1.
[3] Desenko, SM.; Orlov, VD.; Shishkin, Ov.; Bozykin, KA.; Lindeman SV.; Stzuchkov, YuT(**1993**) Khimiya Geterotsk1 Soedin(Chemistry of Heterocyclic Compounds) 1539

Studies on the synthesis of new fused polycyclic 1,4-dihydropyridines

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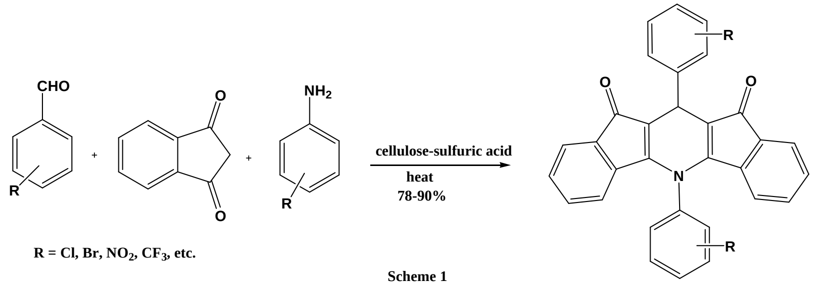
Five- and six-membered heterocyclic compounds are important constituents that often exist in biologically active natural products and synthetic compounds of medicinal interest. Among them, 1,4-dihydropyridines (1,4-DHPs) heterocyclic rings are a common feature of various bioactive compounds such as vasodilator, bronchodilator, anti-atherosclerotic, anti-cancer and anti-diabetic agents [1-2]. Additionally, 1,4-DHPs have several other medicinal applications which include neuroprotecting [3] and cerebral anti-ischemic properties for the treatment of alzheimer disease [4].

Classical method for the synthesis of these compounds is one-pot condensation of aldehyde with ethyl acetoacetate and ammonia in acetic acid or in refluxing alcohol. At present study as a result of our continued interest in the synthesis of biologically important products [5], new series of 1,4-dihydropyridines were prepared by a one-pot multi-component reaction of aldehydes, indenedione and aniline derivatives in the presence of cellulose-sulfuric acid as catalyst in high yields (78-90%) (Scheme 1). In this presentation various aspects of this novel protocol will be discussed.



Scheme 1

References:

[1] Sausins, A.; Duburs, G.; *Heterocycles* **1988,** *27*, 269.
[2] Godfraind, T.; Miller, R.; Wibo, M.; *Pharmacol. Rev*. **1986,** *38*, 321.
[3] Klusa, V.; *Drugs Fut.* **1995**, *20*, 135.
[4] Bretzel, R. G.; Bollen, C. C.; Maeser, E.; Federlin ,K.F.; *Drugs Fut.* **1992**, *17*, 465.
[5] Nikpassand, M.; Mamaghani, M.; Shirini, F.; Tabatabaeian, K. *Ultrason. Sonochem.* **2010**, *17*, 301; Nikpassand, M.; Mamaghani, M.; Tabatabaeian, K. *Molecules* **2009**, *14*, 1468; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *J. Heterocycl. Chem.* **2008**, *45*, 1765; Samimi, H. A.; Mamaghani, M.; Tabatabaeian, K. *Heterocycles* **2008**, *75*, 2825. Tabatabaeian, K.; Mamaghani, M.; Mahmoodi, N. O.; Khorshidi, A. *Tetrahedron Lett.* **2008**, *49*, 1450.

Highly efficient mannich reaction of aldehydes, secondary amines and naphthols catalyzed by nano-ordered B-MCM-41

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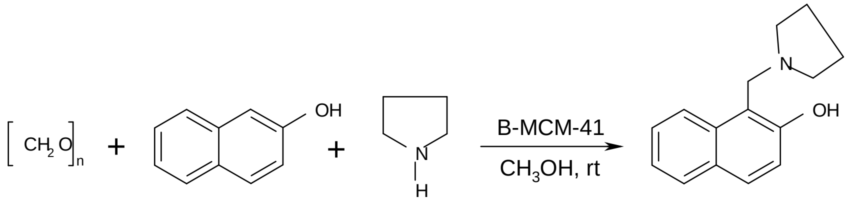
The Mannich reaction is one of the most important basic carbon–carbon bond-forming reactions in organic synthesis for preparation of different valuable synthetic intermediates such as β-amino carbonyl compounds and 1,2-amino alcohol. Lewis acids, Lewis bases, Bronsted acids, rare metal salts, and some organocatalsts have been investigated as the catalysts for this reaction over the past decades [1,2].

On the other hand, ordered mesoporous materials are very attractive as heterogeneous solid catalysts for fine chemicals synthesis. Mesoporous materials provide high surface areas which a high concentration of active sites often by incorporating metal ions into the siliceous framework is produced. Herein, we wish to report mesoporous boronsilicate (B-MCM-41) as an efficient nano-ordered solid acid catalyst for the three-component mannich reaction of aldehydes, secondary amines and naphthols at room temperature to afford the corresponding products in good to excellent yields [3].

In the initial experiments, different solvents were screened for Mannich reaction of paraformaldehyde, pyrrolidine and 2-naphthol at room temperature. Among the others, methanol was found to be the most efficient solvent for this reaction. The product can be separated easily from the reaction system.



References:

[1] Dong, F.; Kai, G.; Dai-zhen, Z.; Zu-liang, L. *Monatsh. Chem.* **2009**, *140*, 1325.
[2] Dong, F.; Jun, Z. Xin-Li; Zu-liang, L. *Catal. Lett.* **2007**, *116*, 76.
[3] Iwanami, K.; Seo, H.; Choi, J.c.; Sakakura, T.; Yasuda,H. *Tetrahedron Lett.* **2010**, 66, 1898.

Silica phosphoric acid: an eco-friendly solid acid for synthesis of some trisubstituted imidazoles under parafine bath condition

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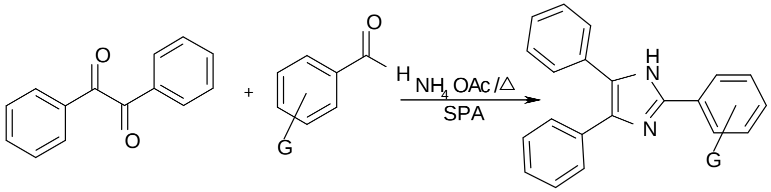
One important aspect of clean technology will be the use of environmentally friendly catalysis typically involving the use of solid acid catalyst that can be easily recovered when the reaction is complete. Employing such an approach results in minimal pollution and waste material production. The application of such catalysts for chemical manufacturing is likely to be increasingly important in the future [1].The toxicity and volatile nature of many organic solvents, particularly chlorinated hydrocarbons that are widely used in huge amounts for organic reactions have posed a serious threat to the environment[2] Thus, design of solvent -free catalytic reaction has received tremendous attention in recent times in the area of green synthesis [3].

Trisubstituted imidazoles are important class of compounds in the pharmaceutical industries and exhibit a wide range of biological activities [4].

In this report the synthesis and characterization of some trisubstituted imidazoles we prepared by condensation reaction of benzil and aldehyde derivatives *with amunium acetate* in the presence of silica phosphoric acid(SPA). ***The*** structure of products have been characterized by several spectroscopic techniques such as IR, UV, ^{1}H-NMR and ^{13}C-NMR.



References

[1] A.Shaabani,A. Rahmati, E. Farhangi, Z. Badri,*Catal. Commun*.,**2007**, 8, 1149-1152.
[2] W.M. Nelson, in: P.T. Anastas, T.C. Williamson (Eds.), "Green Chemistry", Oxford University Press, Oxford, **1998**.
[3] K. Tanaka, F. Toda, *Chem. Rev.* , **2000**, 100,1025; (b) G.W.V. Cave, C.L. Raston, J.L. Scott, *Chem. Commun*., **2001**, 2159-2160; (c) J.O. Metzger, *Angew. Chem., Int. Ed*., **1998,** 37,2975.
[4] J.G. Lombardino, E.H. Wiseman, *J. Med. Chem*., **1974,** 17, 1182.

Anhydrous $FePO_4$: a green and cost-effective catalyst for the one-pot three component synthesis of 2, 4, 5-trisubstituted imidazoles

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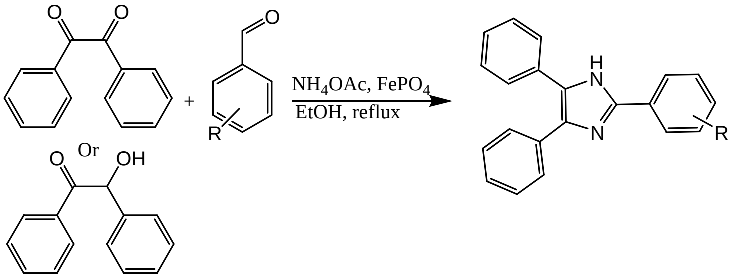
Imidazoles are the core structures of many biological systems [1], an active component in several drug molecules [2] and have received a lot of attention in recent years. Different substituted imidazoles show a broad range of biological activities such anti-allergic activity [3], and analgesic activity [4].

2,4,5-Trisubstituted imidazoles are synthesized by three-component cyclocondensation of 1,2-diketone or α-hydroxyketone with aldehyde derivatives, ammonium acetate [5, 6]. In this research we wish to report a simple highly versatile and efficient synthesis of 2, 4, 5-trisubstituted imidazoles is achieved by three-component cyclocondensation of benzyl and benzoin, aldehyde and ammonium acetate using $FePO_4$ as a catalyst refluxing ethanol (Scheme 1). The key advantages of this process are high yields, cost-effectiveness of catalyst, easy work-up, purification of products by non-chromatographic methods and developing of a new derivative of 2,4,5-trisubstituted imidazole.



Scheme 1

References:

[1] Laufer, S.A.; Zimmermann, W.; Ruff, K.J. *J. Med. Chem*. **2004**, *47*, 6311.
[2] Leister, C.; Wang. Y.; Zhao. Z.; Lindsley. CW. *Org. Lett.* **2004**, *6*, 1453.
[3] Black, J.W.; Durant, G.J.; Emmett, J.C.; Ganellin, C.R. *Nature.* **1974**, *248*, 65.
[4] Ucucu, U.; Karaburun, N.G.; Iskdag, I. Il *Farmaco.* **2001**,*56*, 285.
[5] De Laszlo, S. E.; Hacker, C.; Li, B.; Kim, D.; MacCoss, M.; Mantlo, N.; Pivnichny, J. V.; Colwell, L.; Koch, G. E.; Cascieri, M. A.; Hagmann, W. K. Bioorg. Med. Chem. Lett. **1999**, *9*, 641.
[6] Eyers, P. A.; Craxton, M.; Morrice N.; Cohen, P.; Goedert, M. (1998) Chem. Biol. **1998**, *5*, 321.

A convenient ionic liquid promoted one-pot synthesis of tetrahydrobenzopyran derivatives under ultrasonic condition

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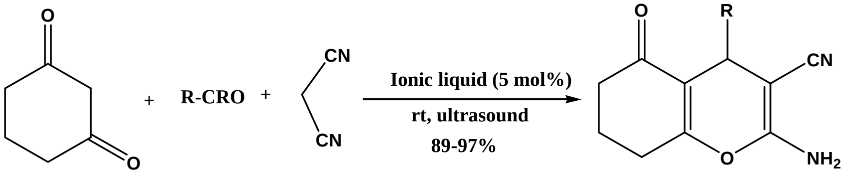
In recent years, 4*H*-benzopyran and its derivatives have attracted many interests due to their usful biological and pharmacological properties, such as anti-coagulant, spasmolytic , diuretic, anti-cancer and anti-anaphylactin activity. They have also been used as inhibitors of endoperoxide cyclooxygenase which prevents the conversion of unsaturated fatty acids to endoperoxides and therefore represent potent platelet aggregation inhibitors [1-3].

There are several reports on the synthesis of tetrahydrobenzopyrans [4] which some of them use hazardous materials and harsh reaction conditions. Herein we report an efficient one-pot three-component method for the synthesis of tetrrahydrobenzo[b]pyrans by condensation of aldehydes, cyclohexa-1,3-diones and malononitrile at room temperature in the presence of catalytic amount of basic ionic 1-butyl-2,3-dimethyl imidazolium hydroxide (5 mol%), under ultrasonic irradiations (Scheme 1). This method provides several advantages, such as simple work up procedure, high yields (89-97%) and short reaction times (5 min).



R = alkyl, aryl

Scheme 1

References:

[1] Bonsignore, L.; Loy, G..; Secci, D.; Calignano, A. *Eur. J. Med. Chem.* **1993**, *28*, 517.
[2] Bloxham, J.; Dell, C. P.; Smith, C. W. *Heterocycles* **1994**, *38*, 399.
[3] Nawwar,G. A. M.; Abdelrezek, F. M.; Swclam, R. H. *Arch. Pharm.* **1991** , 342, 875.
[4] Jiu, T.-S.; Wang, A.-Q.; Wang, X. ; Zhang, J.-S.; Li, T.-S. *Synlett* 2004, 871.
[5] Devi, I ; Bhuyan, P. J. *Tetrahedron Lett.* **2004**, *45*, 8625.

Synthesis and characterization of a novel diformyl drivative of pyridine and its Schiff base ligand

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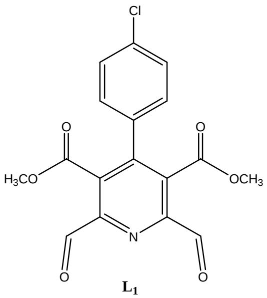
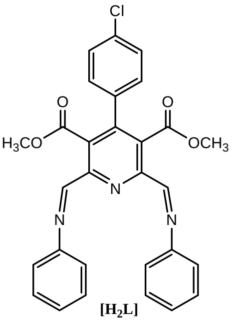
Schiff bases offer a versatile and flexible series of ligands capable to bind with transition, non-transition, lanthanide and actinid metal ions to give complexes with suitable properties for theoretical studies and/or practical applications [1].

A large number of Schiff bases and their metal complexes have been studied because of their interesting and important properties such as their ability to reversibly bind oxygen and their use in catalyses for: oxygenation and oxidation reactions of organic compounds, redox systems in biological processes, Aldol reactions, degradation of dyes through decomposition of hydrogen peroxide and other reagents, in textile industries, reduction of thionyl chloride and oxidation of DNA. Also, Schiff bases can be used in degradation of organic compounds and in radiopharmaceuticals [2].

In this work, first, we synthesized a novel di-aldehyde [dimethyl 4-(4-chlorophenyl)-2, 6-diformylpyridine-3,5 dicarboxylate] (**L_1**) by modified procedure [3-5]. Then this diformyl condensed with aniline, to produce a new Schiff base liand (H_2**L**). The L_1 and its Schiff base ligand were characterized by various spectroscopic methods.



L_1



[H_2L]

References:

[1] Shebl, M.; Spectrochimica Acta Part A. **2008**, 70, 850.
[2] Sancak, K.; Er, M.; Yildirim, M.; Degirmencioglu, I.; Transition Metal Chemistry. **2007**, 32, 16
[3] Ghorbani-Choghamarani*[a], A.; Zolfigol*[b], M.A.; Salehi[c], P.; Acta.chim.Slov. **2008**, 55, 644.
[4] Zolfigol*[a], M.A.; Shirini[b], F.; Ghorbani-Choghamarani[a], A.; Green Chemistry. **2002**, 4, 562.
[5] Chandler, C.J.; Deady, L.W.; Reiss, J.A.; J. Heterocycl Chem. **1981**, 18, 599.

Synthesis and spectral characterization of some new heterocyclic azo dyes derived from 4, 6-dihydroxy pyrimidine and 8-methyl -4-hydroxyl-2-quinolone

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Azo dyes are an important class of organic colorants which consist of at least a conjugated azo chromophore (–N=N–) and they are considered as the largest and most versatile class of dyes [1-2]. It has been known for many years that azo compounds are the most widely used class of dyes due to their versatile applications in various fields such as the dyeing of textile fiber, biological-medical studies and advanced applications in organic synthesis [3]. The research on this class of dyes has made considerable progress in the last fifty decades. Especially heterocyclic azo dyes have attracted considerable interest and have played an important role in the development of the chemistry of dyes and dying process. For example these classes of dyes have higher tinctorial strength and give brighter hues than those derived from aniline-based diazo components and also provide a pronounced bathochromic effect in comparison with the corresponding benzenoid compounds [4].

In this work, we synthesized some new azo dyes using 4, 6 – dihydroxy pyrimidine and 8-methyl -4-hydroxyl-2-quinolone as coupling components and diazotized heterocyclic and homocyclic aromatic amines. Spectroscopic data of these dyes were measured and evaluated in several polar and nonpolar solvents. The effects of substituents and pH on their absorption maxima, λ_{max}, were also examined.The structures were confirmed by IR spectra, UV-VIS spectra, ^{1}H-NMR, elemental analysis and mass spectroscopy.

References:

[1] Yazdanbakhsh. M.R.; Mohammadi A. *Journal of Molecular Liquids* **2009**, 148, 35.
[2] Wojciech. k, J. Wiak.; M.Magdalena.; K. Joanna.; S.Czaplin. *Dyes and Pigments* **2007**, 74, 9.
[3] Abildgaard. J.; Hansen. P. E; Josephsen. J.;. Hansen B. K. V. *Inorganica Chimica Acta* **2006,** 359, 4493.
[4] I. Sener.; F. Karci.; N. Ertan.; E. Kilic. *Dyes and Pigments* 2006,70, 143.

Synthesis of 1,8-dioxo-octahydroxanthenes in the peresent Al(NO3)$_3$ and Bi(NO$_3$)$_3$ catalysts under solvent-free conditions

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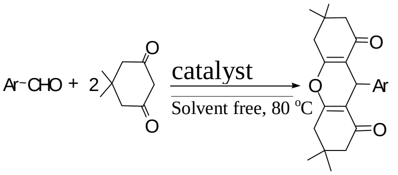
Xanthene derivatives occupy a prominent position in medicinal chemistry [1]; they have also been used as dyes, pH-sensitive fluorescent materials, and laser technology [2]. Many procedures describe the synthesis of xanthenes, including cyclodehydrations, trapping of benzynes by phenols, cyclocondensation between 2-hydroxyaromatic aldehydes and 2-tetralone, reaction of b-naphtol with aldehydes or acetals, and intramolecular phenyl carbonyl coupling reaction of benzaldehydes and acetophenones [3]. Even though there are many methods reported in the literature for the synthesis of xanthenes [4], we thought that there is scope for further innovation towards milder reaction conditions, short reaction time and better yields. Xanthenes are an important class of organic compounds that find use as dyes, fluorescent material for visualization of biomolecules and in laser technologies due to their useful spectroscopic properties.1 Xanthenes have also received significant attention from many pharmaceutical and organic chemists essentially because of the broad spectrum of their biological and pharmaceutical properties such as antiviral,2 antibacterial,3 anti-inflammatory activities4 as well as efficiency in photodynamic therapy5 and antagonist for the paralyzing action of zoxazolamine

.In order to find the best conditions for the synthesis of 1,8-dioxo-octahydroxanthenes the condensation of dimedone (2 mmol) with benzaldehyde (1mmol) was chosen as a model to provide compound ,and its behavior was examined in the presence of Al(NO$_3$)$_3$ and Bi(NO$_3$)$_3$ catalysts in several solvents; the solvent-free method is more efficient.

Catalysts: Bi(NO$_3$)$_3$, Al(NO$_3$)$_3$



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References

[1] Das, B.; Thirupathi, P.; Mahender, I.; Reddy, V.S.; Koteswara Rao, Y.; J. Mol. Catal. A: Chem. **2006**, *247*, 233.
[2] Hunter, R. C.; Beveridge, T. *J. Appl. Environ. Microibiol.* **2005**, *71*, 2501.
Jha, A.; Beal, J. *Tetrahedron Lett.* **2004**, *45*, 8999.
[3] Ion, R. M.; Frackowiak, D.; Planner, A.; Wiktorowicz, K. *Acta Biochim. Pol.* **1998**, *45*, 833.

Synthesis and characterization of silicone modified acrylic based polyurethane hybrid emulsion copolymers

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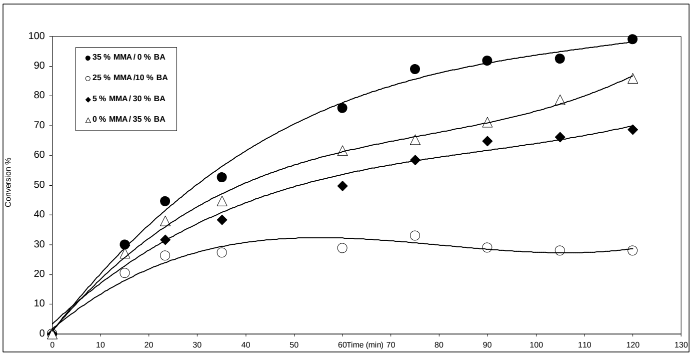
Hybrid polymer latexes polyurethane/Methylmethacrylat-Butylacrylate is prepared through miniemulsion polymerization of polyurethane solutions and triethoxyvinylsilane. The polyurethanes are prepared by condensation of isophorone diisocyanate on polypropylene glycol (M_n =1000) and butane diol as chain extender. The NCO chain ends being reacted with water (which act as a further chain extender producing some urea bonds). They are miniemulsified in a mixture of acrylete monomers by using potassium peroxodisulfate (KPS) as initiator. Films were obtained for different hybrid latexes of various compositions. Their mechanical properties have been compared with those of films from the basic components (polyurethane and acrylic latexes), as well as films from blends of these components. Some specific features of the surface of these films are also discussed from microscope images (SEM and OM) as well as from contact angle measurements.



References:

[1] Sartori, G.; Ballini, R.; Bigi, F.; Bosica, G.; Maggi, R.; Righi, P. *Chem. Rev.* **2004**, *104,* 199.
[2] Xiao, X.; Ngu, K.; Choa, C.; Patel, D. V. *J. Org. Chem.* **1997**, *62,* 6968.
[3] Sikshi, S. A.; Hultin, P. G. *J. Org. Chem.* **2006**, *71,* 5888.

The study of synthesis of 2-(7-methoxy-3,3-dimethylindolin-2-ylidene)malonaldehyde and its new pyrazole derivatives

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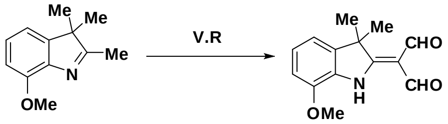
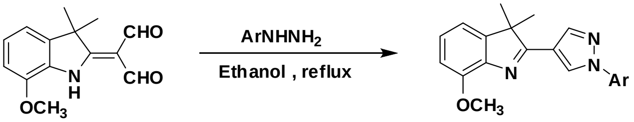
In 1959, Fritz [1] reported the N-formylation of the 3,3-disubstituted 3H-indole (indolenine) using the Vilsmeier reagent from DMF and $POCl_3$. Further reaction of N-formylated product with the Vilsmeier reagent and hydrolysis produced C-formylated product.

We expected 7-methoxy-2,3,3-trimethylindolenine (5) which was synthesized from the arylhydrazones of isopropyl methyl ketone by the fischer reaction to react with the Vilsmeier reagent to from N-formylated products, in line with the result described for Fritz 's indolenine. However, when (1) was subjected to the Vilsmeier conditions at 50 °C, followed by the usual alkaline hydrolysis, diformyl product (2) was obtained in quantitatively yields (scheme 1).



(1) (2)

On the other hand, Baradarani and Co. workers [2,3] reported the synthesis of pyrazole derivatives from reaction of diformyl derived from Indolenines with various aryl hydrazines and hydrazine. On this basis, we synthesized a number of pyrazole derivatives of diformyl (2) (scheme 2).



(2)

References:

[1] Fritz,H.Chem.Ber., **1959**,*92*,1809.
[2] A.Rashidi, A. Afghan, Mehdi.M Bradarani, and John A. Joule ; Heterocyclic Chem. **2009**,*46*,428-431.
[3] Madeleine Helliwell, A. Afghan, Foroogh Keshvari, Mehdi M. Baradarani and John A. Joule, Acta Cryst. Section E, **2010**, *E66*, o112-0122.

An improved procedure for the alkylation of imines in aqueous media using silver iodide as a heterogeneous catalyst

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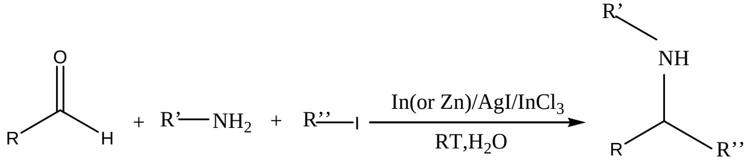
Organic reactions in aqueous media have attracted tremendous attention because of the many advantages that they offer. For example, organic reactions in aqueous media allow multistep synthesis to be carried out more efficiently without the need for protection–deprotection of the functional groups containing acidic protons. Furthermore, compounds containing water molecules or biomolecules can be used directly [1].

The Barbier–Grignard-type reaction is one of the most important reactions for carbon carbon bond formations in organic synthesis. Until recent decades, the Barbier–Grignard-type allylation benzylation, arylation, propargylation, and alkynylation reactions have been successfully developed in aqueous media using different metals [2].

In this study we have optimized the indium- or zinc-mediated allylation reactions of carbonyl compounds and imines in aqueous media [3].

In the presence of In or Zn/ AgI/InCl3, an efficient and practical method for the Barbier–Grignard-type alkylation reactions of simple imines using a one-pot condensation of various aldehydes, amines (including the aliphatic and chiral version), and secondary alkyl iodides has been developed. The reaction proceeded more efficiently in water than in organic solvents. Without the use of CuI, it mainly gave the imine self-reductive coupling product, which was not the alkylated product.



References:

[1] C-J Li, T-H Chan, J. Chem. Commun**. 2000**, *77*, 707.

[2] Z.-L. Shen, H.-L. Cheong, T.-P. Loh, *Chem. Eur. J.* **2008**, *14*, 1875–1880.

[3] Z.–L. Shen, Y.–L. Yeo, T.-P. Loh, *J. Org. Chem.* **2008**, *73*, 3922–3924.

Tandem aldol condensation and Diels-Alder reaction: one-pot reaction of isophorone with aldehydes and *N*-phenylmaliimide

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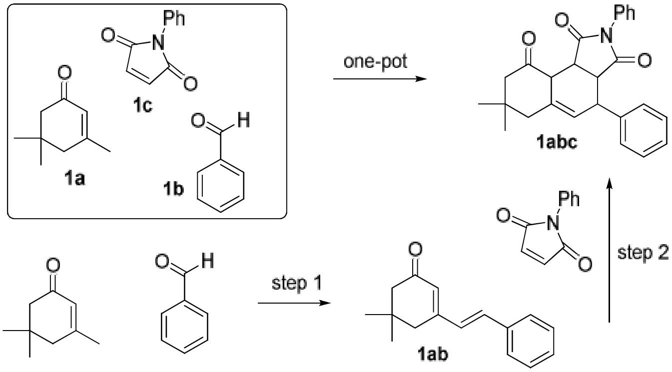
Recently, we reported a remarkably efficient procedure for the synthesis of novel styrylcyclohex-2-enones **1ab** at room temperature using a mild medium consisted of lithium perchlorate and *N*-(trimethylsilyl)diethylamine (NPM, **1c**) [1]. Several compounds of this class were synthesized conveniently and rapidly. These compounds were further investigated in our laboratory for their Diels-Alder activity.

In connection with our investigations on Diels–Alder reaction [2] and in regard with our previous work on the synthesis of styrylcyclohex-2-enone dienes, we now wish to report a novel Tandem sequence, in which **1a** and **1b** undergo an aldol condensation followed by an *in situ* Diels-Alder cycloaddition with **1c** to get access to **1abc** adducts in one-pot.



References:

[1] Mojtahedi, M. M., Abaee, M. S., Zahedi, M. M., Jalali, M. R., Mesbah, A. W., Yaghoubi, R., Forouzani, M. *Monatsh. Chem.* **2008**, *139*, 917.

[2] Ward, D. E., Abaee, M. S. *Org. Lett.* **2000**, *2*, 3937.

A general synthesis of new derivatives of pyrimido[4,5-e][1,2,4]triazolo[3,4-b] [1,3,4]thiadiazine

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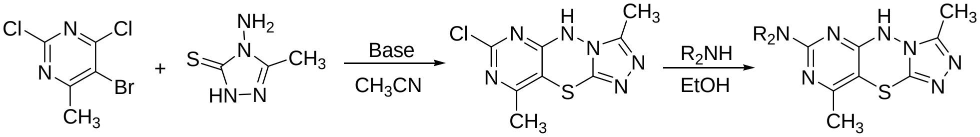
Some triazolothiadiazines have been reported to possess antibacterial and antifungal activity.[1] Therefore, it seems to be of interest to introduce a pyrimidine ring which has been fused to a triazolothiadiazine ring system. Some pyrimido[4,5-e][1,2,4]-triazolo[3,4-b][1,3,4]-thiadiazine-7,9-diones have been synthesized by the condensation of 3-alkyl-4-amino-5-mercapto-[1,2,4]-triazoles with 5-bromobarbituric acid.[2]

In continuation of our previous efforts on the synthesis of new derivatives of pyrimidine fused rings,[3] here, we report the synthesis of new derivatives, namely 7-chloro-3,9-dimethyl-5H-pyrimido[4,5-e][1,2,4]triazolo[3,4-b][1,3,4]thiadiazine **(3)** from the condensation of 5-bromo-2,4-dichloro-6-methylpyrimidine **(1)** with 4-amino-3-methyl-4,5-dihydro-1H-1,2,4-triazole-5-thione **(2)** in CH_3CN in alkaline conditions. Then, the resulting product was treated with various secondary amines to give the substituted chlorine atom products **4(a-e)** by amines in good to excellent yields.



(1) **(2)** **(3)** **4(a-e)**

References:

[1] Eweiss, N. F.; Bahajaj, A. A. *J. Heterocycl. Chem.*, **1987**, *24*, 1173.
[2] Gakhar, H. K.; Gill, J. K. *Monatsh. Chem.* **1985**, *116*, 633.
[3] Bakavoli, M.; Rahimizadeh, M.; Shiri, A.; Eshghi, H.; Nikpour, M. *Heterocycles*, **2008**, *75*, 1745.

A new Biginelli reaction procedure using active carbon sulfuric acid as catalyst for an efficient synthesis of 3,4-dihydropyrimidin-2(1*H*)-one

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Acid catalysts play a predominant role in organic synthesis and transformations.Many organic reactions such as alkylation, acylation, isomerization, nitration, esterification, and rearrangements like pinacol, Beckman, etc. are accomplished by acid catalysts. All these acid catalyzed reactions are mostly carried out by employing conventional mineral acids like H_2SO_4, HNO_3, and HF or Lewis acids such as $AlCl_3$ and BF_3. In view of environmental and economical reasons, there is an ongoing effort to replace the conventional catalysts with newer solid acids. This is mainly due to the distinct advantage of solid acid catalysts such as non-toxicity, non-corrosiveness, ease of handling, less expensive, and easy to recover and reuse.[1-3] In this direction, various solid acid systems were introduced which include hetropolyacids, ion exchange resigns (Amberlyst and Nafion-H), zeolites, and clays. Such materials are expensive and the acid activities are still much lower than that of sulfuric acid. These drawbacks have limited their practical utility .Herein, we report the synthesis of a carbon based solid acid with a high density of sulfonic acid groups (SO_3H) and discuss its performance as a novel strong and stable solid acid .Here, a new strategy is adopted for the development of new types of solid acid through the combined process of acid treatment, reduction and sulfurization reaction .The sulfonic groups are covalently bonded on the surface of the AC .This approach is simple and allows for the use of active carbon sulfuric acid strong, stable solvent soluble acid - as insoluble solid acid.

On the other hand, Dihydropyrimidinone derivatives have attracted considerable interest in recent years because these type of compounds exhibits attractive pharmacological profiles as calcium channel blockers, antihypertensive agents, alphala-antagonists and neuropeptide Y (NPY) antagonists.[4,5] In addition, several marine alkaloids containing the dihydropyrimidinone-5-carboxylate motifs also showed interesting biological properties. In the present work, the catalytic activity of the active carbon sulfuric acid was tested in the production of Dihydropyrimidinone derivatives.

References

[1] Corma, A.; Garcia, H. *Chem. Rev.* **2003,** *103*, 4307.
[2] Hamer, M. A.; Sun, Q. *Appl. Catal. A: Gen.* **2001,** *221*, 45.
[3] Okuhara, T. *Chem. Rev.* **2002,** *102*, 3641.
[4] Atwal, K. S.; Swanson, B. N.; Unger, S. E.; Floyd, D. M.; Moreland, S.; Hedberg, A.; O’Reilly, B. C. *J. Med. Chem.* **1991**, 34, 806.
[5] Snider, B. B.; Shi, Z. P. *J. Org. Chem.* **1993**, 58, 3828; and references cited therein.

Silica supported zinc oxide (zno/sio$_2$): a powerful and reusable catalyst for the synthesis of 14-alkyl or aryl-14 H- dibenzo[a,j] xanthenes

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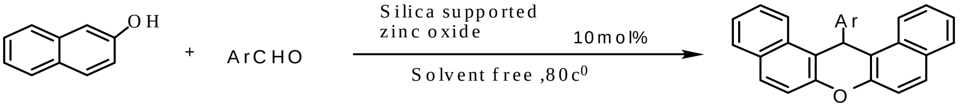
In recent years, Silica supported zinc oxide have attracted much attention [1]. The direct use of Silica supported zinc oxide without modification as recoverable catalysts for organic reactions is very rare [2]. Beside this, the use of the solid state in chemical transformation conveys enormous advantages in terms of separation and purification of materials.

In this research, a practical green chemistry procedure for synthesis of 14-alkyl or aryl-14 H- dibenzo[a,j] xanthenes based on Biginelli reaction between 2 naphtol and appropriate aromatic aldehydes using Silica supported zinc oxide (zno/sio2) as robust catalyst under solvent-free conditions was reported. Eco-friendly nature of the catalyst, simple work-up procedure and the high yields of products, short reaction times and avoid from using toxic organic solvents as media make this method a valid contribution to the existing methodologies.



References:
[1] S. Kantevari, R. Bantu, L. Nagarapu, J. Mol. Catal. A: Chem. 2007, 269, 53.
[2] Z. Zhang, Y. Lui, Catal. Commun. 2008, 9, 1715.
[3] K. Venkatesan, S.S.Pujari,R.J.Lahoti, K.V.Srinivasan,Ultrason. Sonochem. 2008, 15
[4] X. Fan, X. Hu, X. Zhang, J. Wang, Can. J. Chem. 2005, 83, 16-20.
[5] N. G, Kozlov and L. I. Basalaeva. Russian Journal of Chemistry (2005),75,617-621

Active carbon sulfuric acid as an efficient catalyst for the synthesis of quinoline derivatives

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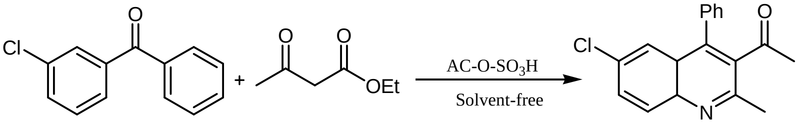
For many years, synthesis of quinoline has been of considerable interest in organic and medicinal chemistry since a large number of natural products and drugs contain these heterocyclic nucleuses. There are many reported methods for the synthesis of quinoline rings, the Friedlander procedure is still one of the most simple and straightforward methods for the synthesis of polyfunctional quinolines. Alternatively, this reaction was also investigated using different protic and Lewis acids such as Bi(OTf)$_3$, $ZnCl_2$, $FeCl_3$ and $Mg(ClO_4)_2$, AcOH under microwave irradiation, HCl, sodium fluoride, silvertungstophosphate, Y(OTf)$_3$, sulfamic acid, ionic liquid, $NaAuCl_4$, and PBBS and TBBDA [1-5]. However, most of the synthetic protocols reported so far suffer from high temperatures, prolonged reaction times, low yields and the use of hazardous and often expensive catalysts. Moreover, the synthesis of these heterocyclic compounds have been usually carried out in harmful solvents such as acetonitrile, THF, DMF, and DMSO, leading to difficult product isolation and recovery procedures, thus making these methods unsuitable for scale up in an environmentally benign and economical way considering the wide spread applications of the resultant compounds, we felt that a catalyst of choice should be one that is easily available and less costly, less toxic, and operable under environmentally friendly conditions so as to fulfill the 'triple bottom line' hilosophy of green chemistry. Thus to continue our investigation on developing new methodologies in organic chemistry, we interested in Active carbon sulfuric acid promoted synthesis of quinolines under solvent-free cunditions.



1 **2** **3**

References:

[1] Yadav, J. S.; Reddy, B. V. S.; Premalatha, K. *Synlett* **2004**, 963.
[2] McNaughton, B. R.; Miller, B. L. *Org. Lett*. **2003**, 5, 4257.
[3] Wu, J.; Zhang, L.; Diaoa, T. N. *Synlett* **2005**, 2653.
[4] Perzyna, A.; Houssin, R.; Barbry, D.; Hénichart, J. P. *Synlett* **2002**, 2077.
[5] Bailliez, V.; El Kaim, L.; Michaut, V. *Synth. Commun*. **2004**, *34*, 109.

Sulfamic acid as an eco-friendly catalyst for the synthesis of benzthiazols

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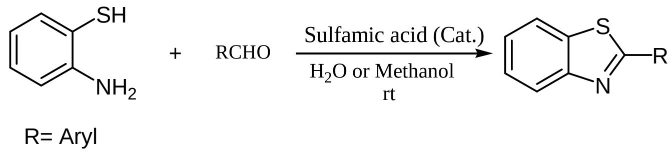
The benzothiazoyl-moiety is a structure element of compounds with potent and selective antitumor activity for example, 2-(4-aminophenyl)benzothiazoles exhibit nanomolar inhibitory activity against a range of human breast, ovarian, colon, and renal cell lines in vitro [1].

The most commonly used method for synthesis of benzothiazoles involves the condensation of *o*-aminothiophenols with substituted nitriles, carboxylic acids, acyl chlorides, or esters in the presence of a various catalysts [2]. Another route is based on oxidative cyclization of thiobenzanilides [3]. However, these methodologies suffer from one or more disadvantages, such as tedious workup, high temperature, prolonged reaction time, and toxic organic solvents such as DMF and DMSO.

Sulfamic acid (SA, H_2NSO_3H) is green and commercially available reagent. More important, its water resistance and incapability for formation of complexes make it an outstanding alternative to metal catalysts, in different areas of organic synthesis [4].

In continuation of our studies on environmentally benign chemical processes [5], herein we now report an efficient and environmentally benign synthesis of benzothiazoles from the reaction of aromatic aldehydes with *o*-aminothiophenol in the presence of catalytic amounts of SA in water or methanol at room temprature (Scheme 1).



Scheme 1

In summary, the significant advantages of this procedure are: a) using the eco-friendly, cost-effective and commercially available of catalyst b) mild reaction condition c) green aspects avoiding hazardous solvent, toxic catalyst and waste d) operational and experimental simplicity.

References:

[1] Bradshaw, T.D.; Wrigley, S.; Shi, D. F.; Schultz, R.J.; Paull, K.D. *Br. J. Cancer* **1998**, 77, 745.
[2] Chen, Y. X.; Qian, L.F.; Zhang, W.; Han, B. *Angew. Chem. Int. Ed.* **2008,** *47*, 9330.
[3] Inamoto, K.; Hasegawa, C.; Hiroya, K.; Doi, T. *Org. Lett.* **2008,** *10*, 5147.
[4] Heravi, M. M.; Baghernejad, B.; Oskooie, H. A. *Cur. Org. Chem.* **2009**, *13*, 1002.
[5] Rostami, A.; Akradi, J. *Tetrahedron Lett.* **2010**, *51*, 3501.

Highly efficient iodination of aromatic compounds with iodide catalyzed by iodic acid and periodic acid in water

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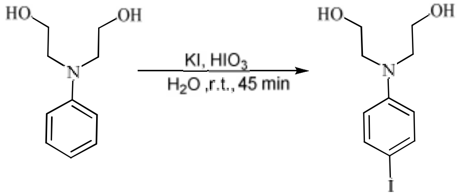
Molecular iodine is a versatile catalyst in organic synthesis, but it is highly corrosive, toxic and sublimable, making its use somewhat unattractive, also there are some environmental hazards with respect to its handling. In order to overcome these disadvantages with molecular iodine, an attempt to introduce molecular iodine in situ in the reaction mixture seems to be practically useful. During the last years, several new methods for in situ generation of bromine have been developed [1], but the numbers of protocols that are available to achieve molecular iodine in situ in the reaction mixture are limited [2-4]. In addition, most of these protocols suffer from disadvantages such as: complex and strong oxidizing agents, harsh reaction conditions and formation of significant amount of waste. Therefore the development of quick, inexpensive, widely applicable, and environmentally benign iodinating agents is still an active area of research. On the other hand, Replacement of expensive, toxic, flammable, not recyclable organic solvents with water is a challenge and in great demand from academia and chemical industries [5]. The use of water as the reaction medium has several benefits; water is a cheap and abundant, nontoxic, non-flammable and relatively green solvent. In this article a new environmentally friendly catalytic method is described for the efficient monoiodination of arenes using iodic acid as the oxidant. The method is based on using potasium iodide and iodic acid or iodide and periodic acid as an effective catalyst in water at room temperature or under reflux conditions.



References:

[1] Eissen, M.; Lenoir, D. *Chem. Eur. J.* **2008,** *14*, 9830.

[2] Bailey, A. D.; Cherney, S. M.; Anzalone, P. W.; Anderson, E. D.; Ernat, J. J.; Mohan, R. S. *Synlett* **2006**, 215.

[3] Firouzabadi, H.; Iranpoor, N.; Shiri, M. *Tetrahedron Lett.* **2003,** *44*, 8781.

[4] Krasnokutskaya, E. A.; Semenischeva, N. I.; Filimonov, V. D.; Knochel, P. *Synthtesis* **2007**, 81.

[5] Grieco, P. A. (Ed.), Organic Synthesis in Water, Blackie Academic and Professional, London, **1998**.

Syntheses of new derivatives of polyfunctionalized oxofuran via multicomponent reaction

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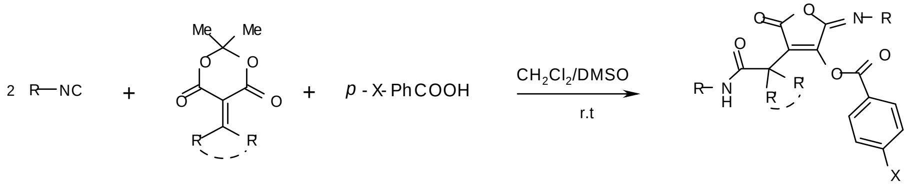
Multi-component reactions are one of the most important method in organic synthesis in which three or more starting materials reacts to give one complex product in good yields. Great efforts have been made to develope new multi-component reactions. Isocyanide-based multi-component reactions are very powerful condensation reaction in organic synthesis. Passerini and Ugi reactions are classical representation of this class [1]. As part of our current study [2] on the reaction between isocyanides , alkylidene substitited Meldrum's acid and RX-H acid, we have report a novel and interesting one-pot four-components reaction of isocyanides**1**(two molecules), alkylidene substitited Meldrum's acid **2** and carboxylic acid **3** leading to produce new derivatives of iminooxofuran **4**.The structure of products (**4a-j**) were deduced from their elemental analyses and their IR, ^{1}H NMR, ^{13}C NMR spectral data.



1 **2** **3** **4a-j**

References:

[1] Domling, A. *Chem. Rev.* **2006**, *106*, 17 and references sited herein.

[2] Habibi A., Mousavifar L. *Monatsh. Chem., 2007,* **138,** No. 6,603.

The Synthesis of (3-(3, 4-dimethoxyphenyl)isoxazol-5-yl-methyl acetate

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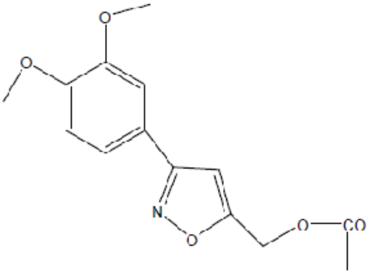
1, 3-Dipolar cycloaddition reaction are of the most important synthetic manipulations allowing the construction of five memberd heterocycles [1]. Isoxazole derivatives have been used as key intermediates in synthesis and have been investigated intensively for the last several years because of biological activities [2].

In this research work, some new compounds of isoxazole family were synthesized and characterized. First, 3, 4-methoxybenzaldehyde (**1**) was transformed to 3, 4- methoxybenzaldoxime (**2**) by using NH2OH in pyridine. The in situ generated nitril oxide from reaction between (**2)** and NaOCl, was reacted with propargyl alcohol to produce 3-(3, 4- methoxyphenyl)-5-hydroxymethyl isoxazole (**3**) in a cycloaddition procedure. Then, compound (**3**) reacted with CH3COOH and H2SO4 to produced (3-(3, 4-dimethoxyphenyl)isoxazol-5-yl-methyl acetate.

The structure of all the synthesized compounds was characterized and confirmed by FT-IR and NMR spectroscopy techniques.



References:
[1] Xu W. , Tang E. , Huang X. , 61, 2005. 501.
[2] Ruano J . , Fajardo C. , Martin R. , 61 2005 4363.

Synthesis of 2-(nitroaryl)-5-(4-substituted-1-piperazineyl)-1,3,4-thiadiazoles

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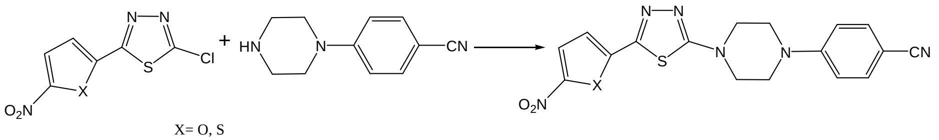
The antiparasitic property of 1,3,4-thiadiazoles has been well documented and their attachment with other heterocycles often ameliorated or diminished the bioresponses, depending upon the type of substituent and position of attachment [1]. Herein we report an efficient method for synthesis of a series of 2-[4-(5-(5-nitroaryl-2-yl)-1,3,4-thiadiazol-2-yl] piperazine-1-yl) benzo- nitriles and 4-[4-(5-(5-nitroaryl-2-yl)-1,3,4-thiadiazol-2-yl]piperazine-1-yl)benzonitriles. The required 2-chloro-5-(5-nitroaryl-2-yl)-1,3,4-thiadiazole was prepared according to the synthetic route suitable [2] and (piperazin-1-yl)benzonitriles were synthesized with new synthetic route.

The reaction of 2-chloro-5-(5-nitroaryl-2-yl)-1,3,4-thiadiazoles and (piperazin-1-yl)benzonitriles in refluxing ethylmethylketone gave derivatives of 2-(nitroaryl)-5-(4-substituted-1-piperazineyl)-1,3,4-thiadiazoles.



References:
[1] Rodrigues, R. F.; da Silva, E. F.; Echevarria, A´.; Fajardo- Bonin, R.; Amaral, V. F.; Leon, L. L.; Canto-Cavalheiro, M. M. *Eur. J. Med. Chem.* **2007**, *42,* 1039.
[2] Foroumadi, A.; Pournourmohammadi, S.; Soltani, F.; Asgharian-Rezaee, M.; Dabiri,S.; Kharazmi, A .; Shafiee, A. *Bioorg. Med. Chem. Lett.* **2005**, *15*, 1983.

Synthesis of some novel receptors as diamidic crown compounds

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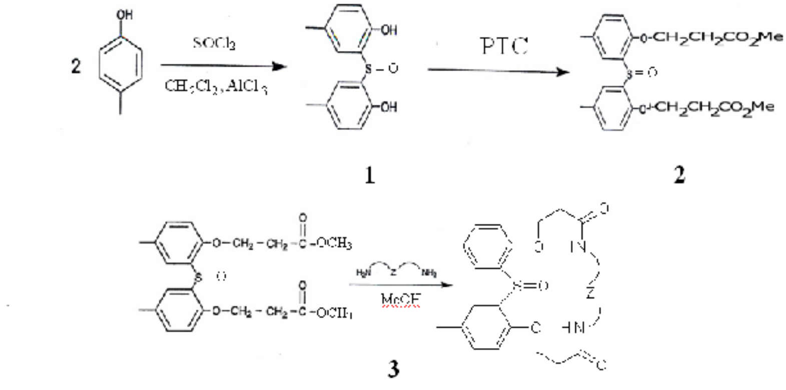
Macrocyclic diamides and corresponding aza crown compounds have gained a great deal of attention due to their wide applications in chemistry, biochemistry, nano technology, nuclear energy, medical, environmental, metal separation and transport, analysis, industrial uses, swiching , agriculture, catalysis, biophysics, ecology and they are selective ligands with high capability for heavy metals [1]. In our research work these compounds showed good antitumor activity and hight affinity for Ba^{+2}, Pb^{+2} in solution state [2]. They made important intermediate for preparation other ligands such lariat ether and bis crown ethers by reaction of amidic groups.

In this research work we wish to report the synthesis of some new Diamidic crown compounds as cationic and molecular receptors.

For this purpose first, primary the dibenzosulfoxide (1) was prepared by reaction of thionyle chloride with p-cresol in 50% yield.

Reaction of dibenzosulfoxide (1) with Methyl-3-Bromo propianat in the presence of PTC at room temperature efforded to dimethly ester (2) in 35% yield. In the next stage, macrocycle (3) was obtained by addition of suitable diamins with dimethyl ester (2) by amidation.



Z = $CH_2CH_2CH_2$, CH_2CH_2 , $CH_2CH_2NHCH_2CH_2$

References:

[1] Piatek. P.,Gryko.D. T., Szumna. A., Jurczak. J., 2004, Tetrahedron, 60, 5769-5776.
[2] Bradshaw, J.S.; Krakowiak, K.E.; Izatt. R.M., Tetrahedron, 1992, 48, 4475.

One pot synthesis of γ-iminolactones by three component reactions between alkyl isocyanides, acetylenic esters and benzyl phenyl ketone and its α-chloro derivative

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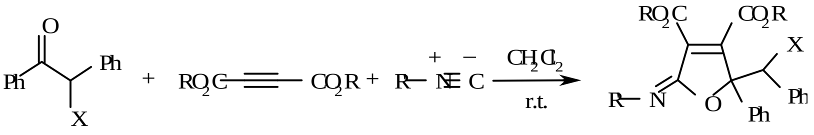
Isocyanide-based multicomponent reactions (IMCRs) now occupy an important position in synthetic organic chemistry, mainly in the synthesis of various heterocyclic systems like amino furans, iminopyrans and iminolactones from readily available starting materials [1,2]. The reaction of 1:1 zwitterionic species, generated *in situ* by the addition of isocyanide to dialkyl acetylenedicarboxylates can be trapped by a variety of electrophiles such as aldehydes, 1,3-diketones, isocyanates and proton donors for synthesis of heterocyclic compounds [3]. Recently, the reaction between isocyanides and acetylenic esters in the presence of some *α*-dicarbonyl compounds that leads to *γ*-iminolactones has been reported [4].

Here, we report the reactions of benzyl phenyl ketone and its *α*-chloro derivative **1** with dialkyl acetylenedicarboxylates **2** in the presence of alkyl isocyanides **3** which lead to *γ*-iminolactones **4**.



1 **2** **3** **4**

4	X	R	R'	% Yield
a	H	Me	^{t}Bu	60
b	H	Et	^{t}Bu	70
c	H	^{t}Bu	^{t}Bu	75
d	H	Me	cyclohexyl	60
e	H	Et	cyclohexyl	70
f	Cl	Me	^{t}Bu	85
g	Cl	Et	^{t}Bu	88
h	Cl	Me	cyclohexyl	75
i	Cl	Et	cyclohexyl	80

References:

[1] Dömling, A.; Ugi, I. *Angew. Chem. Int. Ed*. **2000**, *39*, 3168.
[2] Nair, V.; Viond, A. U.; Rajesh, C. *J. Org. Chem*. **2001**, *66*, 4427.
[3] Asghari, S. ; Qandalee, M. *Acta. Chim. Slov*. **2007**, *54*, 638.
[4] Yavari, I.; Hosseini, Z.; Sabbaghan, M. *Mol. Div*. **2006**, *10*, 479.

Preparation of ketene from acetic anhydride

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Ketene was prepared in the laboratory by the thermal decomposition of acetic anhydride in a flow system. This was done by passing of acetic anhydride vapors through a reaction vessel at 400ºC. A 500-cc round-bottomed flask was filled with acetic anhydride and connected by gas tight joints to the reaction vessel. The acetic anhydride was degassed by the freeze-thaw method, by using of liquid air as the freezing agent. Then the temperature of acetic anhydride was raised to 70–80ºC, in order to maintain a suitable vapor flow through the reaction vessel. The reaction vessel was made of Pyrex glass and packed with Pyrex tubes. The length of Pyrex tubes were approximately 60 centimeters. The reaction vessel was placed in a furnace. The temperature of furnace was maintained just below 400 ºC to give a high purity of ketene, without any side reactions taking place. As the acetic anhydride vapors enter to the reaction vessel, it decomposes to ketene and acetic acid.

$$CH_3 - CO - O - CO - CH_3 \longrightarrow CH_2 = CO \quad + \quad CH_3 - COOH$$

Produced gaseous ketene and acetic acid were left the reactor, and entered into the two traps. The two traps were kept at -78ºC using a solid carbon dioxide/acetone slush bath. The second trap was packed with glass beads. Produced acetic acid and unreacted acetic anhydride were trapped in first and second traps. Produced gaseous ketene was passed through the first and second traps, and was entered into the third trap which was kept at liquid air bath, and was collected in the third trap. A rotary oil pump was used to maintain a vacuum in the system. The collected ketene was degassed and distilled into a tube at liquid air temperature, -184 ºC. The first and last fractions in the trap were discarded. The pressure of ketene was kept low to avoid dimerization.

Preparation and spectroscopic characterization of a new dioxiomolybdenum (VI) complex of 1,8-naphthalenediamine

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As molybdenum is commonly available to biological systems, the coordination chemistry of Mo (VI) has produced considerable interest in view of its biochemical substance [1,2]. In particular, dioxomolybdenum (VI) complexes are studied as models for oxidized forms of molybdoenzymes, e.g. aldehyde and sulfite oxidases, which are supposed to contain cis_MoX_2 units (X= O, S) coordinated to sulfur, nitrogen and oxygen donor atoms of the protein structure [3].

Addition of 1,8-naphthalenediamine to the solution of $MoO_2(acac)_2$ {acac=acetylacetonato} in MeOH results in the formation of $[MoO_2(naph)_2]^{-2}$ complex. In this research we studied different aspects of this synthesis and the structure of the product was examined by ^{1}H , ^{13}C_NMR , IR spectroscopy.

References:

[1] D. Collison, C. D. Garner, J. A. Joule, Chem. Soc. Rev. (1996) 25.
[2] R. Hille, Chem. Rev. 96 (1996) 2757.
[3] G. C. Tucci, J. P. Donahve, R. H. Holm, Inorg. Chem. 37 (1998) 1602.

Sulfuriacid ([3-(3-silicapropyl)sulfanyl]propyl)ester:A new and recyclable catalyst for the silyation of hydroxyl groups) with hexamethyldisilazane(HMDS)

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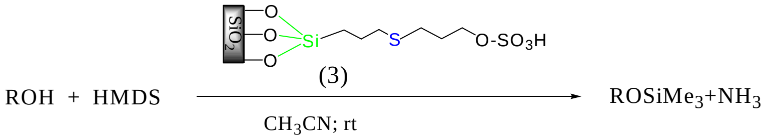
sulfuric acid([3-(3-silicapropyl)sulfanyl]propyl)ester(3) by the reaction of 3-(thio(propy-3-yl)silica)-propanol (2) and chlorosulfonic acid in chloroform.3-(thio(propy-3-yl)silica)-propanol was prepared by the rewas prepared by the reaction of 3-mercaptopropylsilica(MPS) with3-chloropropanol in refluxing toluene.[1] A good range of primary, secondary alcohols and phenolic hydroxyl groups were effectively converted into their corresponding trimethylsilyl ethers with hexamethyldisilazane(HMDS) in the presence of catalytic amounts of (3) under mild conditions at room temperature with short reaction times in good to excellent yields. [2] An excellent chemoselective silylation of hydroxyl groups in the presence of other functional groups were also observed. The heterogeneous catalyst was recycled for thirty runs upon the reaction of benzyl alcohol with HMDS without lossing its catalytic activity. The trimethylsilylation of hydroxyl groups is easily carried out at room temperature under mild conditions in the presence of (3) as a catalyst. [3]



R= primary, secondary alkyl, and aryl

References:

[1] Niknam, K.; saberi, D. *Applied catalysis A: General.*, **2009**, 366, 220-225.
[2] Niknam, K.; et al. *can.Chin. J.vol*. **2010**, 88, 164-171.
[3] (a) Niknam, K.; Zolfigol, M. A.; Khoramabadi-Zad, A.; Zare, R.; Shayegh, M. *Catal. Commun*. **2006**, 7 (7), 494. doi:10.1016/j.catcom. 2006. 01.004.; (b) Niknam, K.; Karimi, B.; Zolfigol, M. A. *Catal. Commun*. **2007**, 8 (9), 1427. doi:10.1016/j.catcom.2006.12.011.; (c) Niknam, K.; Saberi, Sefat, M. N. *Tetrahedron Lett*. **2009**, 50 (28), 4058. doi:10.1016/j.tetlet.2009.04.096.; (d) Niknam, K.; Saberi, D.; Mohagheghnejad, M. *Molecules*. **2009**, 14 (5), 1915. doi:10.3390/molecules 14051915. PMID: 19471211.

Synthesis of tetrahydrobenzo[a]xanthene-11-one and diazabenzo[a]anthracene-9,11-dione derivatives under eco-friendly conditions

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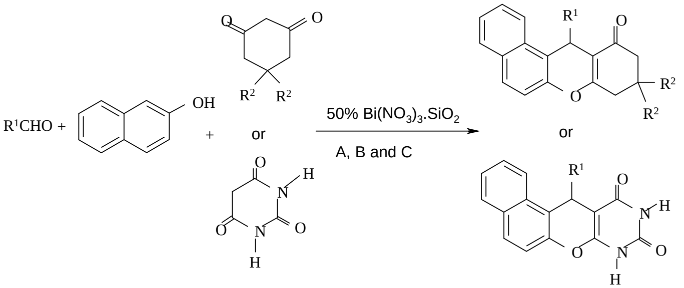
Xanthenes and benzoxanthenes are important biologically active heterocyclic compounds, which possess antiviral, anti-inflammatory, and antibacterial activities [1]. These are being utilized as antagonists for paralyzing action of zoxazolamine and in photodynamic therapy [2]. Furthermore, these compounds can be used as dyes [3], in laser technologies [4] and as pH sensitive fluorescent materials for visualization of biomolecules [5]. Herein, we are reporting the reaction of aldehydes, 2-naphthol and cyclic 1,3-dicarbonyl compounds for the formation of tetrahydrobenzo[a]xanthene-11-one and diazabenzo[a]anthracene-9,11-dione derivatives in presence of catalytic amount of 50% $Bi(NO_3)_3.5H_2O/SiO_2$ under solvent free (A), in water as solvent at 40 °C (B) and sonication in water (C) conditions.



In conclusion, we have developed three efficient and environmentally benign methodologies for the synthesis of 12-aryl/ alkyl-8,9,10,12-tetrahydrobenzo[a]xanthene-11-ones and 12-aryl-8,12-dihydro-7-oxa-8,10-diazabenzo[a]anthracene-9,11-diones by a one-pot, multi-component reaction. The advantages of these methods are reduced reaction times, higher yields, mild reaction condition, easy purification and economic viability of the catalyst.

References:

[1] Hideo, T.; Teruomi, J. (Sankyo Co.) Jpn. Patent 56005480, 1981.
[2] Ion, R. M.; Frackowiak, D.; Planner, A.; Wiktorowicz, K. *Acta Biochim. Pol.* **1998**, *45*, 833.
[3] Menchen, S. M.; Benson, S. C.; Lam, J. Y. L.; Zhen, W.; Sun, D.; Rosenblum, B. B.; Khan, S. H.; Taing, M. U.S. Patent 6,583,168, 2003.
[4] Ahmad, M.; King, T. A.; Ko, D.-K.; Cha, B. H.; Lee, J. *J. Phys. D: Appl. Phys.* **2002**, *35*, 1473.
[5] Knight, C. G.; Stephens, T. *Biochem. J.* **1989**, *258*, 683.

Synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones (thiones) in the presence of $SbCl_5.SiO_2$ in solvent free condition

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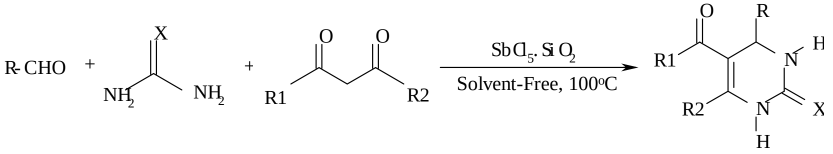
Dihydropyrimidines (thiones) are important compounds exhibiting broad spectra of pharmacological activities such as anti inflammatory, anti-microbial, 1a-adrenergic receptor antagonist and anti hypertensive. Antimony pentachloride is a reddish-yellow, oily liquid, which is strong hygroscopic material [1,2]. Neat $SbCl_5$ is an inexpensive, commercially available and selective acidic reagent which reacts with water to produce antimony pentoxide and hydrochloric acid. It is difficult to handle due to its moisture sensitivity. Silica supported antimony pentachloride ($SbCl_5.SiO_2$) is less hygroscopic, more stable and reactive than neat $SbCl_5$. We report, herein, the synthesis of different derivatives of 3,4-dihydropyrimidin-2(1*H*)-one and 3,4-dihydropyrimidin-2(1*H*)-thiones from one- pot condensation of aldehydes, ethylacetoacetate or 1,3-diketones and urea/ thiourea in the presence of $SbCl_5.SiO_2$ in solvent free condition at 100 °C (Scheme).



In conclusion, we have demonstrated a simple method for the synthesis of dihydropyrimidines (thiones) using $SbCl_5.SiO_2$ as a readily available and efficient catalyst. Short reaction times, high yields, scale-up, clean process, simple methodology, easy work-up, and green conditions are the advantages of this protocol.

References:

[1] Kappe, C. O. *Tetrahedron* **1993**, *49*, 6937.
[2] Grover, G. I.; Dzwonczyk, S.; McMullen, D. M.; Normadin, D. E.; Parham, C. S.; Sleph, P. G.; Moreland, S. *J. Cardiovasc. Pharmacol.* **1995**, *26,* 289.

Synthesis of aniline-sulfur crosslinked copolymer & studies of sensing properties for molecularly imprinted diazinon

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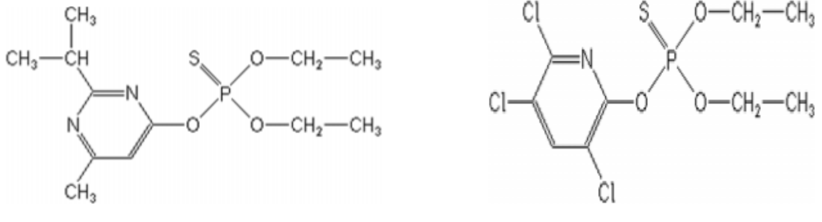
Conducting polymers (CP) have attracted considerable attention because of their electrical and optical properties and many potential applications such as energy storage, electromagnetic interference shielding, photoelectronic device, sensor and etc [1]. It was found that the manufacture of composites consisting of molecularly imprinted polymers (MIP) and conducting polymers results in obtaining materials that exhibit both predetermined selective molecular recognition and electrical conductivity [2]. This type of materials is of special interest for use in the field of sensor technology [3].

This paper has investigation the preparation of imprinted polymer using aniline-sulfur resin as a crosslinked, diazinin as a template and aniline as a monomer. MIP is synthesized by using the free radical polymerization technique. The MIP structure is characterized by FTIR and NMR. Also sensing properties of polymer studied in various qualifications (concentration, time, temperature) via measurement of conductance by using a four-point probe method. The selectivity in recognizing the print molecule by the imprinted surface was assessed by comparing the extent of uptake of other structurally resembling molecules namely chlorpyrifos. During a 6 month period, the sensitivity of the molecularly imprinted diazinon was found to remain constant, that considerable to comparison with non-imprinted polymer.



(a) (b)

Structure of a) diazinon b) chlorpyrifos

References:

[1] Hosseini, S. H.; Entezami, A. A., Polym. Adv. Technol. **2001**, 12, 482-493.
[2] Deora, B.; Chen, Z. D.; Nagaoka, T., Anal. Chem. **2000**, 72, 3989-3994.
[3] Shigi, H.; Kishmoto, M.; Yakabe, H.; Deore, B.; Nagaoka, T., Anal. Sci. **2002**, 18, 41-44.

Optimization of invironment condations onto Pictin- graft-AN

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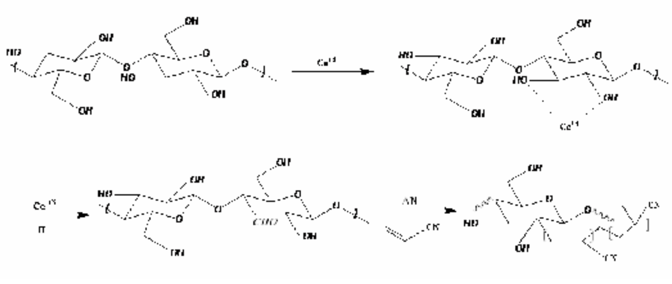
As the first part of a continued research on conversion of Pectin (PC) to useful biopolymer-based materials, large numbers of cyanide functional groups were introduced onto Pectin by grafting with polyacrylonitrile (PAN). A proposed mechanism for copolymer formation was suggested in the scheme1 and the structure of the product was established using FTIR spectroscopy[1].The graft copolymerization reactions were carried out under nitrogen atmosphere using ceric ammonium nitrate (CAN) as an initiator[2]. Evidence of grafting was obtained by comparing FTIR spectra of Pectin and the graft copolymer as well as solubility characteristics of the products. The synthetic conditions were systematically optimized through studying the effective factors including temperature and concentrations of initiator, acrylonitrile monomer, and PC. Finally, the PC-*g*-PAN copolymer was characterized thermally by using thermogravimetric analysis methods.



Scheme 1. A brief proposed mechanism for ceric-induced grafting of polyAN onto Pectin.

References:

[1] Jiang, Y.P.; Guo. X. *Carbohydr. Polym.* **2005**, *61*, 441.
[2] Opoku, G.; Qiu, X.; Doctor. V. *Carbohydr. Polym.* **2006**, *65*, 134.

Multi-wall carbon nanotubes supported manganese tetraphenylporphyrin: An efficient and highly reusable catalyst for epoxidation of alkenes with sodium periodate

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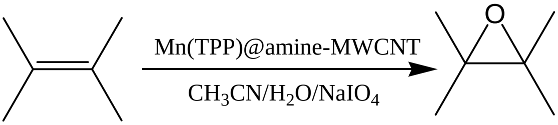
Epoxidation of alkenes is of academic and industrial interest, because epoxides are one of the most widely used intermediates in organic synthesis. Epoxides undergo ring-opening reactions with a variety of reagents to produce mono- or bi-functional organic products [1].

Metalloporphyrin species exist ubiquitously in nature and have found a broad spectrum of applications. Amongst, for example, the modeling of cytochrome P-450 for oxygenation of hydrocarbons has received much attention over decades. Therefore, great efforts have been made to develop new metalloporphyrin-based catalytic systems for the oxidation process, aiming at a higher degree of chemo- and stereoselectivities as well as efficiency under mild conditions [2-4].

Despite the high catalytic activity of homogeneous metalloporphyrins, these expensive catalysts are degraded or deactivated in the reaction media. One way to overcome these problems is to immobilize them on solid supports. Carbon nanotubes (CNTs) have attracted much attention in the synthesis, characterization, and other applications because of their unique structural, mechanical, thermal, optical and electronic properties. Since CNTs are insoluble in the most solvents, these materials can be used as catalysts support.

In the present work, highly efficient epoxidation of alkenes catalyzed by [Mn(TPP)Cl] supported on amine modified multi-wall carbon nanotubes, MWCNTs, is reported. The prepared catalyst was characterized by elemental analysis, scanning electron microscopy, FT-IR and diffuse reflectance UV-Vis spectroscopic methods. This new heterogenized catalyst, [Mn(TPP)Cl@amine-MWCNT], was used as highly efficient catalyst for epoxidation of alkenes with sodium periodate. This robust catalyst could be reused several times without loss of its catalytic activity.



References:

[1] Beller M.; Bolm C.; Transition Metals for Fine Chemicals and Organic Synthesis, vol. 2, Wiley-VCH, Weinheim, **1998**, 261.
[2] Feiters, M.C.; Rowan A.E.; Nalte R.J.M. *Chem. Soc. Rev.* **2000**, *29*, 375.
[3] Brule, E.; de Miguel, Y.R.; Hii, K.K.; *Tetrahedron* **2004**, *60*, 5913.
[4] Naik, R.; Joshi, P.; Umbarkar, S.; Deshpande, R.K.; *Catal. Commun.* **2005**, *6*, 125.

Efficient synthesis of isobenzofuran-1(3H)-ones

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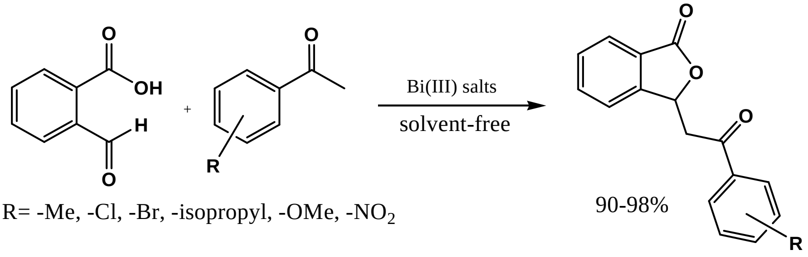
Isobenzofuran-1(3H)-ones constitute an important class of naturally occurring oxygen compounds, well known for their interesting biological and medicinal properties [1]. Their notable characteristics include anti-HIV, anti-tumor, anti-bacterial, anti-asthmatic and anti-convulsant [2]. They are also used as intermediates for the synthesis of iso-coumarins, anthracyclines and anthraquinones [3].

In view of their importance, several methods have been developed for the synthesis of isobenzofuran-1(3H)-ones. These methods involve the use of strong, harmful and corrosive acids and bases and high temperatures [4].

In this work, we report the synthesis of various derivatives of isobenzofuran-1(3H)-ones in the presence of Bi(Ш) salts under various conditions.

The experimental results show that using Bi(Ш) salts as catalysts, these compounds were obtained in excellent yields. These reactions were performed under solvent-free conditions. Therefore, this method can be considered as a green and environmentally benign procedure for the preparation of these heterocycles.



References:

[1] Sing, E.; Gupta, P. C. J. *Indian Chem. Soc*. **1973**, *50*, 676.
[2] Mor, S.; Dhavan, S. N.; Kapoor, M.; Kumar, D. *Tetrahedron* **2007**, *63*, 594.
[3] Kim, K. S.; Spatz, M. W.; Johnson, F. *Tetrahedron Lett*. **1979**, *20*, 331.
[4] Rendy, R.; Zhang, Y.; McElrea, A.; Gomez, A.; Klumpp, D. A. *J. Org. Chem*. **2004**, *69*, 2340.

One-pot synthesis of isobenzofuran-1(3H)-ones

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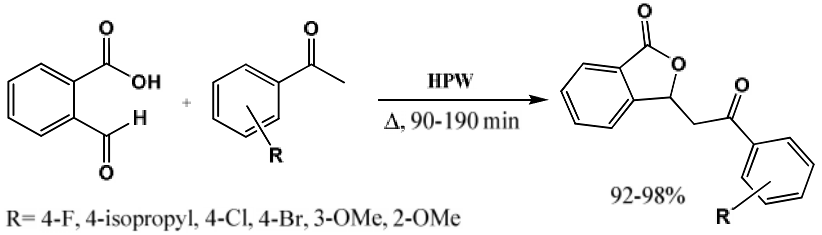
Substituted phthalides (isobenzofuran-1(3H)-ones) represent an important class of natural products that possess significant biological properties [1]. Their notable characteristics include anti-bacterial, anti-convulsant, anti-HIV, anti-asthmatic, anti-tumor and anti-platelet activities [2].

Due to the potential of phthalides, several methods have been developed for their synthesis [3]. These methods involve the use of strong, corrosive and harmful acids and bases, high temperatures and long reaction times [4]. Therefore, development of an efficient and environmentally-benign synthetic method for these compounds is still in demand.

Herein, we describe an efficient and expedient method for one-pot synthesis of substituted isobenzofuran-1(3H)-ones. Our new approach is based on the heteropoly acid catalyzed cyclization of phthalaldehydic acid with substituted acetophenone and it's derivatives. This catalytic system provides an efficient, environmentally-benign and selective procedure for the synthesis of isobenzofuran-1(3H)-ones.



References:

[1] Pahari, P.; Senapati, B.; Mal, D. *Tetrahedron Lett.* **2004**, *45*, 5109.
[2] Mal, D.; Pahari, P.; De, S. R. *Tetrahedron* **2007**, *63*, 11781.
[3] Bousquet, E. W.; Moran, M. D.; Harmon, J.; Johnson, A. L.; Summers, J. C. *J. Org. Chem.* **1975**, *40*, 2208.
[4] Rendy, R.; Zhang, Y.; McElrea, A.; Gomez, A.; Klumpp, D. A. *J. Org. Chem.* **2004**, *69*, 2340.

Ruthenium salophen supported on functionalized multi-wall carbon nanotubes: Efficient and highly reusable catalysts for epoxidation of alkenes with sodium periodate

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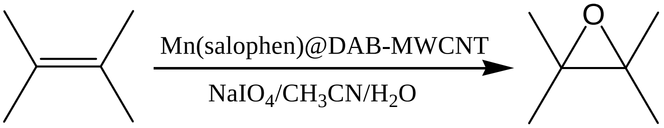
Cytochrome P-450 enzymes catalyze various reactions such as aliphatic and aromatic hydroxylation, olefin epoxidation and *N*-, *O*-, *S*-oxidation. As biomimetic models, transition metal Schiff base complexes have been found to be good catalysts in a variety of oxygenation reactions including epoxidation of olefins and the hydroxylation of alkanes [1]. In the last two decades, salen and salophen ligands bearing O and N donor atoms and their complexes have received much attention, mainly because of their extensive applications in the fields of synthesis and; catalysis. But, these homogeneous catalysts cannot be recovered from the reaction system and degraded in the reaction media and therefore contaminate the products. In comparison with the homogeneous catalysts, heterogeneous systems present many advantages such as easy separation and recovery of the catalyst from the reaction media, higher stability of the catalytic species and catalyst protection against destruction [2,3].

The preparation, characterization and investigation of catalytic activity of Ru(III) salophen supported on multi-wall carbon nanotubes modified with 1,4-phenylenediamine is reported. The catalyst, [Ru(salophen)Cl-DAB-MWCNT], was characterized by elemental analysis, scanning electron microscopy, FT-IR and diffuse reflectance UV–vis spectroscopic methods. This new heterogenized catalyst was used as an efficient catalyst for alkene epoxidation with sodium periodate in CH_3CN as solvent. This heterogeneous metal schiff base catalyst showed high stability and reusability in the epoxidation reactions without loss of its catalytic activity.



References:

[1] Bahramian, B.; Mirkhani, V.; Moghadam, M.; Tangestaninejad, S. *Appl. Catal. A: Gen.* **2006**, *301*, 169.

[2] Canalai L.; Sherrington, D.C. *Chem. Soc. Rev.* **1999**, *72*, 603.

[3] Mirkhani, V. ; Moghadam, M.; Tangestaninejad, S.; Bahramian, B. ;. Mallekpoor-Shalamzari, A. *Appl. Catal. A: Gen.* **2007**, *321*, 49.

Phytochemical investigation and cytotoxic activity of chemical constituents of wild *Satureja khuzistanica*

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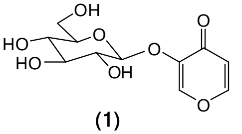
Medicinal and aromatic plants have been used for many centuries and are still popular in today’s alternative therapies. *Satureja khuzistanica* Jamzad (Marzeh Khuzistani in Persian, family of Lamiaceae) is an endemic plant that is widely distributed in the southern parts of Iran [1]. This plant has been used as analgesic and antiseptic among the inhabitants of southern parts of Iran. Infusion of aerial parts of this plant is credited in folk medicine to relieve toothache. In a previous work we investigated the chemical composition of dichloromethane extract of cultivated *S. khuzistanica* [2].

In this study, fractionation of the methanolic extract of the aerial parts of wild *S.khuzistanica* led to isolation of a hemiterpenoid glucoside named erigeroside (**1**), together with three other compounds; 5, 6, 4'-trihydroxy-7, 3'-dimethoxyflavone (**2**), ursolic acid and eriodictyol. Erigeroside has been reported previously in *Erigeron breviscapus* from compositae family [3], but this is the first report of it in Lamiaceae family. Generally, the chemistry of the genus *Satureja* has not been thoroughly studied. The natural occurrence of these compounds in *S. khuzistanica* can be conclusive for the chemotaxonomic characterization of this genus.

Among the isolated compounds, erigeroside and 5, 6, 4'-trihydroxy-7, 3'-dimethoxyflavone were tested for cytotoxicity on MCF7, WEHI164 and HepG2 cells. According to the results erigeroside was found to have inhibitory effect on MCF7 and 5, 6, 4'-trihydroxy-7, 3'-dimethoxyflavone on HepG2 cell lines.



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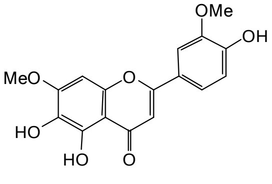

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References:

[1] Jamzad, Z. **1994**, *Iran J. Bot*. 6, 215.
[2] Matloubi Moghaddam, F.; Moridi Farimani, M.; Salahvarzi, S.; Amin, G. *Evid Based Complement Alternat Med* (eCAM) **2007**, 4, 95-98.
[3] Jianmin, Y.; Zhongwen, L.; Dezu, W., Handong, S. *Phytochemistry* **1994**, 36,717.

The electronic effects of halogens aryl ring on reductive elimination reactions in palladium(II) complexes with DFT studies

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Reductive elimination from Pd(II) complexes is usually introduced as the last step of the cross-coupling reactions [1,2,3,4,5]. In this regard, the reactions leading to formation of Aryl-Aryl bonds have attracted considerable interest. The studies showed that the ease of the reductive elimination from biarylpalladium complexes is controlled by the nature of the substituents on the aryl groups [6]. In general, the electron donating substituents facilitate the reductive elimination process while the electron withdrawing substituents retard it. Here we used the B3LYP method [7] to reveal how the electronic and steric properties of the substituents on the aryl ring affect the reductive elimination process. We will show that the electron withdrawing substituents such as F and CN increase the Pd-Ar bond strength causing such complexes to be reluctant towards reductive elimination [8]. Our calculations also predicted that the steric factors are able to exert some control over the rate of the Ar-Ar reductive elimination. The steric interactions are more dominant if the ortho-substituents are relatively bulky (groups such as CH_3 or CN and not F). The steric interactions raise the activation barrier, thus making the Ar-Ar elimination a difficult process

References:

[1] Tamao, K.; Sumitani, K.; Kumada, M. J. Am. Chem. Soc. **1972**, 94, 4374.
[2] Corriu, R. J. P; Masse, J. P.Chem. Commun.**1972**, 144
[3] (a) Milstein, D.; Stille, J. K. J. Am. Chem. Soc. **1978**, 100, 363. (b) Stille, J. K. Angew. Chem.,Int.Ed. Engl**. 1986**, 25, 508. (c) Espinet, P.; Echavarren, A. M. Angew. Chem., Int. Ed. **2004**, 43, 4704.
[4] Miyaura, N.; Suzuki, A. Chem. Rev. **1995**, 95, 2457.
[5] Hiyama T. in Metal-Catalyzed Cross- Coupling Reactions (Eds.: F. Diederich, P. J.Stang), Wiley VCH, Weinheim, **1998**, chap. 10.-
[6] Shekhar, S.; Hartwig, J. F. *J. Am. Chem. Soc.* **2004**, *126*, 13016
[7] M.J. Frisch et al., GAUSSIAN 03, Revision B.05, GAUSSIAN, Inc., Pittsburgh, PA**, 2003**.
[8] Holland, P. L.; Andersen, R. A.; Bergman, R. G. *Comment s Inorg.Chem.* 1999, *21*, 115.

Monomers of (*R*,S)-4-heptyl-2-(2’-hydroxy-binaphthyl)hydrogen phosphonate

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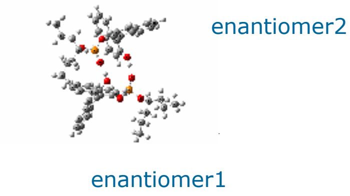
Two out of eight possible pairs of monomers units of (R,S)-4-heptyl-2-(2’-hydroxy-binaphthyl)hydrogen phosphonate are involved in the stereoselective formation of the dimmer BINOLS-PR:BINOLR-PS. The structure of dimmer is determined by x-ray crystallographic data, which reveal a centrosymmetric, 18- membered ring structure with Ci symmetry, consisting of two monomers strongly hydrogen- bonded between the oxygen of P=O units and hydroxyl hydrogen atoms. Mass spectrometric, melting point, and thermal decomposition point data, as well as NMR data, support the presence of strong, quasi-covalent hydrogen bonds. Computational analysis suggests that the Diastereoselectivity is controlled by molecularly constrained geometry of the monomers [1]In this study we investigated the conformational analysis of two enantiomers of BINOLS-PR(1) and BINOLR-PS(2).These enantiomers are involeved in the formation of dimer 3. PES could help predict which one of the conformer of the sixteen enantiomer participaite in the formation of the dimer 3.

All of the structures studied in this work were optimized by Hartree-Fock (HF) 6-311 basis set. Full geometry optimizations were performed and were successfully checked for imaginary frequencies. All calculations reported in the present study were carried out using the GAUSSIAN 03 software [15]. Potential energy scan (PES) studies of these compounds were performed in order to obtain the internal barrier to rotation at HF/6-311G level. The structural parameters were analyzed after optimization. We also compared conformers with energy minima and maxima obtained from the potential energy scan.

Dimer 3



References:

[1] Dabagh, H.A; et al. Can. J. Chem. **2007**, 85, **460.**

[2] Gaussian 03, Revision C.02, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S.

Synthesis and characterization of novel derivatives of 2, 9-disubstituted 1, 10- phenanthrolines as tetradentate ligands

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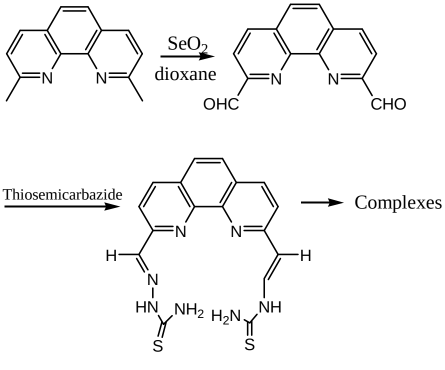
A large number of 1, 10-phenanthroline and their complexes are significant interest because of their biological activity including anticancer properties, and anti-carcinogenic properties [1]. 10-phenanthroline units, as an important building block, play an important role in development of the supramolecular chemistry with many novel supramolecular compounds including 1, 10-phenanthroline units [2,3]. The ligands are of interest because there are both `soft' and `hard' site in the ligands. Various and structurally different compounds containing transition metals have been shown to be active [4]. In this project we have synthesized a new seris of 2, 9-disubstituted-1, 10 phenanthrolines starting from 2, 9-diamino-1, 10- Phenanthrolines as tetradentate ligands. The ligands and complexes were characterized by FT-IR, ^{1}H NMR spectra.



References:

[1] Mansuri-Torshizi, H.; Mital, R.; Srivastava, T. S.; Parekh, H.; Chitnis, M. P. *J. Inorg. Biochem.* **1991**, *44*, 239.
[2] Dietrich-Buchecker, C. O.; Sauvage, J.-P. *Angew. Chem., Int. Ed. Engl.* **1989**, *28*, 189.
[3] Sallas, F.; Marsura, A.; Petot, V.; Pinte´ r, I.; Kova´ cs, J.; Jicisinszky, L. *Helv .Chim. Acta* **1998**, *81*, 632.
[4] Basile, L. A.; Barton, J. K. *J. Am. Chem. Soc.* **1987,** *109,* 7548.

Preparation and properties of new thermally stable poly(amide imide amide)s

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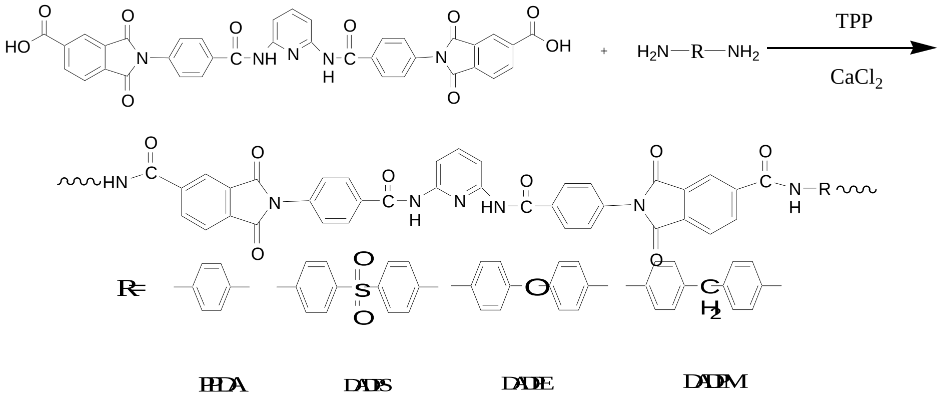
Polyimides and polyamides are two main categories of thermally stable polymers. Although polyimides have higher thermal stability than polyamides, they are generally insoluble and infusible in the imide form [1,2].Thermal resistance of polyamides is lower than that of polyimides, but polyamides have better solubility and processability than polyimides. Poly(amide imide)s were developed from high-performance polymers which inherit desirable characteristics from both polyamides and polyimides. They possess good thermal properties compared with polyamides, and better melt processability than polyimides [3].

In this study, 2,6-bis(4-aminobenzamido)pyridine was prepared via reaction of 2,6-diaminopyridine with two moles of 4-nitrobenzoyl chloride in the presence of propylene oxide. Reaction of this diamine with two moles of trimellitic anhydride afforded a diacid with preformed amide and imide structures. Poly(amide imide amide)s were prepared by polycondensation reactions of the diacid with different diamines in the presence of triphenyl phosphite. All the monomers and polymers were fully characterized and the physical properties of the polymers including solution viscosity, thermal stability, thermal behavior and solubility were studied. According to the obtained data the polymers showed suitable balance of properties including high thermal stability and improved solubility.



References:

[1] Ye, Y.S.; Yen, Y.C.; Chen, W.Y.; Cheng, C.C. *J. Polym. Sci. Part A: Polym. Chem.* **2008,** *46,* 6296.

[2] Mallakpour, S.; Kolahdoozan, M. *Iran. Polym. J.* **2008**, *17*, 531.

[3] Mehdipour-Ataei, S.; Arabi, H.; Bahri-Laleh, N. *Eur. Polym. J.* **2006,** *42*, 2343.

Theoretical study of electron reorganization energy in [5,5] armchair single-walled carbon nanotubes

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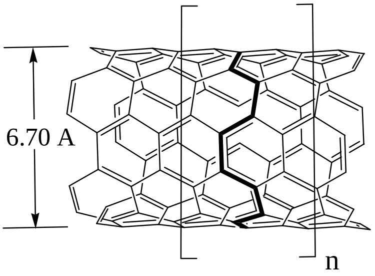
Electron transfer (ET) is one of the most important chemical processes in nature, playing plays a central role in many biological, physical and chemical (both organic and inorganic) systems. Solid state electronics depends on the control of the ET in semiconductors, and the new area of molecular electronics depends critically on the understanding and the control of the transfer of electrons in and between molecules and nanostructures. The reorganization energy is the energy it would take to force the reactants to have the same nuclear configuration as the products without permitting the electron transfer [1].

Nanotubes are cylindrical fullerenes that can be either single-walled (SWCNT) or multi-walled; the former attract more attention due to their unique electronic, optical and spectroscopic properties. One of the most recognizable types of carbon nanotubes is the (5,5) armchair single-walled carbon nanotube. The number of carbon atoms (n) of the SWCNTs is considered as one of the useful numerical and structural properties. In this study, the relationships between this index and electron reorganization energy (λ_e) in [5,5] armchair single-walled carbon nanotubes were presented and investigated [2].



n=20-190 **(1-18)**
n=200-300 **(19-29)**

References:

[1] R.A.Marcus. *Rev. Modern Physics* . **1993** , *65* , 599.
[2] A.A.Taherpour . *Chem Phys Lett* . **2009** , *469* , 135.

Structures, stabilities & conformational behavior of radicals & cations of Cytosine nucleosides: ion-molecule reactions of cation radicals in gas-phase

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Abstraction of hydrogen atom from DNA and RNA subunits leads to formation of a neutral radical [1]. This may occur from the direct effects of radiation or electron bombardment or by action of the radicals created during the radiolysis process in *vivo*. on the other hand, hydride ion abstraction of DNA subunits allowing prediction of the regioselectivity of potential damage to the sugar part of these molecules caused by carcinogenic agents of electrophilic agent. On the other hand, the radical cations of DNA constituents generated by the ionizing radiation initiate the alteration of the bases, which is one of the main types of cytotoxic DNA lesions [2]. This radical cation spices are known for their role in producing nucleic acid strand break, and it is important to identify the radical cation formation at particular atomic site in these molecules so that the major pathway for the nucleic acid damage may be trapped [3,4].

In the present work, we explore theoretically the energetic and structural properties of the possible radicals and cations formed from cytosine nucleosides. The structures and energies of forming radicals and cations in cytidine and deoxycytidine nucleosides at various sites of sugar part of these molecule have been studied by theoretically employing the B3LYP method using 6-311++G (d,p) basis sets. Moreover, geometries, adiabatic ionization energy, adiabatic electron affinity, charge distribution, molecular orbital analysis and proton-transfer process of cytosine and deoxycytidine cation radicals were investigated. The result of calculation revealed that cytosine radicals formed by deprotonation of cytosine cation radicals can exothermically abstract hydrogen atoms from thiol groups, phenol, and amino acid α-positions. These finding has several biological implications and may explain the possible degrees of damage to the DNA double strand.

References:

[1] Cleaver, J. E. *DNA Repair* **2002**, *1*, 977.
[2] A.-C. Colson, M.D. Sevilla, *J. Phys. Chem.* **1995**, 99, 3867
[3] E.O. Hole, W.H. Nelson, E. Sagstuen, D.M. Close, *Radiat. Res.* **1992**, *129*, 119.
[4] Gimisis, T.; Ialongo, G.; Chatgilialoglu, C. *Tetrahedron* **1998**, *54*, 573.

Preparation of magnetic and conduvtive graphite nanoflake composite by polypyrrole based on $MnFe_2O_4$ nanoparticles

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Polymer nanocomposites with conducting fillers have been the focus for many research groups in past few decades. Of all the conducting polymers we choose polypyrrole (PPy) as one of the components to produce nanocomposite materials, because of its good environmental stability to water and oxygen, facile synthesis and higher conductivity than many other conducting polymers [1]. Among the various conducting fillers, natural graphite, which possesses good electrical conductivity has been widely used [2]. Therefore graphite can be a good candidate in fabricating polymer conducting nanocomposites. We had use flake graphite to make expanded graphite and graphite nanosheets (NG).

In this study, nanocomposites of graphite nanosheets (NGs)/MnFe2O4 nanoparticles (NPs)/polypyrrole with trilayer core-shell structure, were prepared with both magnetic and conducting properties. First, The NGs were oxidized with KMno4 in the presence of surfactant, CTAB (Cetyltrimethylammonium bromide). The hydroxyl functionalized NGs were coated by MnFe2O4 nanoparticles. Then nanocomposites were surrounded with polypyrrole by in situ polymerization to make a trilayer core-shell structure..

The structure property, magnetic and conducting property composite were investigated by different experimental technique, including vibrating sample magnetometer (VSM), the standard four-point-probe method, transmission electron microscopy (TEM), scanning electron microscopy (SEM), and etc. The conductivity and magnetization measurements proved that the samples are conductive and have a superparamagnetic behavior. The TEM and SEM images reveal that NGs/MnFe2O4 NPs/PPY nanocomposites are core-shell structure.

Reference:

[1] Zunli, M.; Dandan, Z.; Hong, C.; Yinxia, S.; Ping, Z. European polymer Journal 43 (**2007**) 300-306.
[2] Zhao, Y.F.; Xiao, m.; Wang, X.C.Ge.; Meng, Y.Z. composites science and Technology 67 (**2007**)2528-2534.

An efficient one pot synthesis of quinolines derivatives under solvent free conditions

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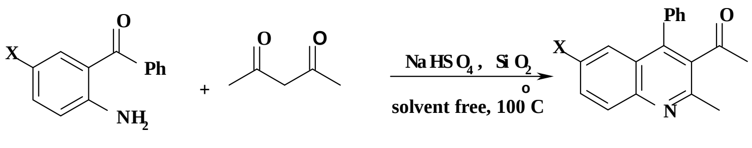
Quinolines and their derivatives have recently received great attention because of their wide range of therapeutic and biological properties [1]. They have emerged as antimalarial, antiasthmatic, anti-inflamatory, antibacterial, antihypertensive, and tyrosine kinase PDGF-RTK inhibiting agents [2]. Moreover, polyquinolines are found to undergo hierarchical selfassembly into a variety of nano- and meso-structures with enhanced electronic and photonic functions. The simple and straightforward method for the synthesis of polysubstituted quinolines was reported by Friedla¨nder in 1882 [3]. Friedla¨nder reactions are generally carried out either by refluxing an aqueous or alcoholic solution of reactants in the presence of base or by heating a mixture of the reactants at high temperatures ranging from150 to 220 ^{0}C in the absence of catalyst.

Here we report a simple and efficient method for the synthesis of quinolines and polycyclic quinolines using silica gel supported sodium hydrogen sulfate as reusable eco-friendly catalyst via Friedlander annulation under solvent- free conditions is described.

Thus, the reaction between 2-aminobenzophenone derivatives **1** with acetylacetone **2** to afford the Quinolines derivatives **3** in excellent yields.



1 **2** **3**

References:

[1] Roma, G.; Braccio, M.D.; Grossi, G.; Mattioli ,F.; Ghia, M. *J. Med. Chem .,* **2000,** 35, 1021.
[2] Kalluraya, B.; Sreenivasa, S. *Farmaco* **1998,** 53, 399.
[3] Friedla¨nder, P. *Chem. Ber.,* **1882,** 15, 2572.

Synthesis of novel asymmetric 1,4- dihydropyridines containing 4*H*-pyran-4-one derivatives

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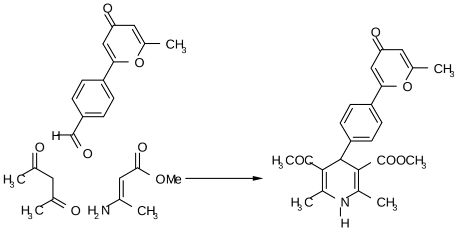
It is well known that 1,4-dihydropyridines (DHPs) exhibit a wide range of biological activities, acting as potent vasodilators, antihypertensives, branchodilators, antitumor and antidiabetic agents [1, 2]. DHPs are commercially used as calcium channel blockers for treatment of cardiovascular disease [3].

On the other hand, 4*H*-pyran-4-one derivatives constitute a useful class of heterocyclic compounds, which are widely distributed in a variety of natural and synthetic biologically active compounds [4]. Based on the above evidences revealing that both γ-pyrone derivatives and 1,4-dihydropyridine moieties turn to be pharmacophores with interesting effects, we have designed a synthetic strategy that implies including both moieties in the same molecule. Thus, we have synthesized new 1,4-dihydropyridine derivatives by introducing pyrone ring systems at the 4-position of the dihydropyridine nucleus.

1,4-Dihydropyridines are generally synthesized by the Hantzsch method [5], which involves cyclocondensation of an aldehyde, *β*-ketoester, and ammonia either in acetic acid or by refluxing in alcohols. The asymmetrical analogues were obtained by the modified Hantzsch reaction, using an aldehyde, *β*-ketoester and enaminone.



References:

[1] Bossert, F.; Vater, W. *Med. Res. Rev.* **1989**, 9, 291.
[2] Janis, R. A.; Triggle, D. J. *J. Med. Chem.* **1983**, 25: 775.
[3] Gaudio, A. C.; Korolkovas, A.; Takahata, Y. *J. Pharm. Sci.* **1994**, 83, 1110.
[4] Caturla, F.; Amat, M.; Reinoso, R. F.; Calaf, E. *Bioorg. Med. Chem. Lett.* **2006**, 16, 3605
[5] Hantzsch, A. *Justus Liebigs Ann. Chem.* **1882**, 215, 1.

1,3-Dibromo-5,5-dimethylhydantoin catalyzed synthesis of benzoxazoles, benzimidazoles and oxazolo[4,5-*b*]pyridines under solvent-free conditions

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Benzoxazole, benzimidazole and oxazolo[4,5-*b*]pyridine moieties have attracted special attention in chemistry and biochemistry. These heterocycles show various pharmaceutical properties such as antiviral, antibiotic, antibacterial, antifungal, anticancer, antitumor and anti-inflammatory activities[1].

A number of methods have been reported for the synthesis of these heterocycles which include condensation of carboxylic acids, orthoesters, acid chlorides, nitriles, amides, aldehydes and esters with o-substituted aminoaromatics, Beckmann rearrangement of o-acylphenol oximes and photocyclization of phenolic Schiff bases. However, some of these methods suffer from one or more of the following drawbacks such as strong acidic conditions, long reaction times, low yields of the products, tedious work-up, need to excess amounts of reagent and the use of toxic reagents, catalysts and/or solvents[2].

Herein we report reactions of orthoesters with o-substituted aminoaromatics and 2-amino-3-hydroxypyridine in the presence of catalytic amounts of the moisture stable and inexpensive 1,3-Dibromo-5,5-Dimethylhydantoin [DBDMH] under solvent-free conditions. The remarkable features of this new method are very short reaction times, high yield of products, absence of solvent and simple experimental and work-up procedure in combination with availability, stability, non-toxicity and cheapness of the catalyst.

References:

[1] Mohammadpoor-Baltorka, I.; Moghadama, M.; Tangestaninejada, S.; Mirkhania,V.; Zolfigol, M.A.; Hojati, S.F. *J. Iran. Chem .Soc.* **2008**, *5*, 65.

[2] Mohammadpoor-Baltork , I.; Khosropour, A.R.; Hojati, S.F. *Catal.Commun.* **2007**, *8*, 1865.

Studying of Michael reaction of acrylates and fumarates with barbituric acid and its derivatives in the presence of nanomordenite or without it under the green conditions

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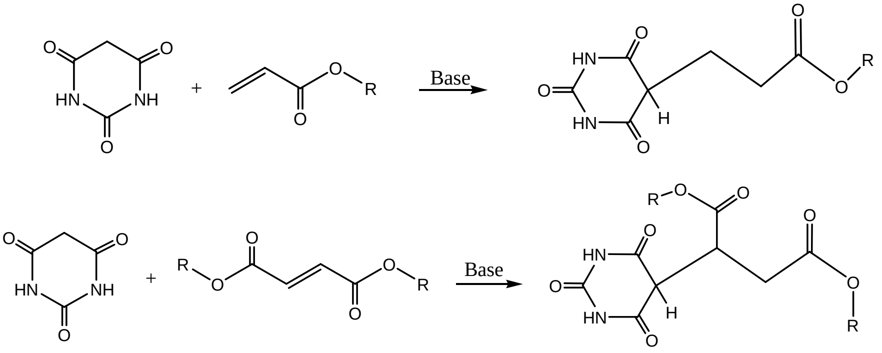
Barbitals are a group of organic compounds which exhibit biological properties [1] and most different derivatives of these compounds are synthesized by Michael reactions of barbituric acid and alkyl halides. In this project the preparation of some derivatives of these compounds by Michael addition of barbituric acid and corresponding acrylic and fumaric esters is investigated in the presence of nanomordenite [2].



References:

[3] Ding, F.; Pan, H.; Bigi, F.; Li, Z.; Liu, F.; Sun, F. *J. Lumin.* **2009**, *129*, 650.
[4] Mohamed, M. *J. Mol. Catal*. **2003**, *200* , 301.

Design and synthesis of new 2,3-diarylquinazolin-4 (1H)-one derivatives as cyclooxygenase-2 inhibitors

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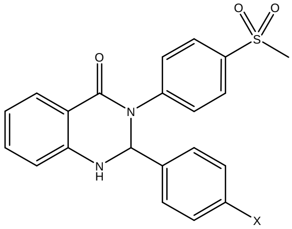
A new group of 2,3-diarylquinazolin-4-(1H)-one derivatives possessing a methylsulfonyl COX-2 pharmacophore at the *para* position of the N-3 phenyl ring were designed and synthesized as selective COX-2 inhibitors [1]. The binding interactions of designed compounds within the COX-2 binding site were investigated. Docking studies showed that the *p*-$MeSO_2$–phenyl moiety is oriented towards the COX-2 secondary pocket (Arg^{513}, Phe^{518} and Val^{523}). One of the *O*-atoms of *p*-$MeSO_2$ substituent forms a hydrogen binding interaction with amino group of Arg^{513} (distance<4 A^o) whereas the other *O*-atom is close to other hydrogen of this amino acid. The C=O of quinazolin-4-one ring is almost close to NH of Val^{349}. In addition, the phenyl moiety of the central ring is undergoing hydrophobic interactions with isopropyl group of Val^{349}. These results indicate that the designed compounds can bind to active site of COX-2 enzyme and show inhibitory activities.

The target molecules were synthesized by one-pot three-component cyclocondensation reaction using isatoic anhydride, 4-methylthioaniline and different aromatic aldehydes in the presence of a catalytic amount of alum in ethanol [2]. Oxidation of the cyclic products with H_2O_2 gave the desired compounds. The purity of all products was determined by thin layer chromatography using several solvent systems of different polarity. All compounds were pure and stable. The compounds were characterized by ^1H nuclear magnetic resonance, infrared, mass spectrometry and CHN analysis. The biological effects of synthesized compounds are under investigation.



References:

[1] Zarghi, A.; Zebardast, T.; Daraie, B.; Hedayati, M. Bioorg. Med. Chem. 2009, 17, 5369.
[2] Dabiri, M.; Salehi, P.; Otokesh, S.; Baghbanzadeh, M.; Kozehgary, G.; Mohammadi, A. A. Tetrahedron Lett. 2005, 46, 6123.

TBAH-Catalyzed one-pot synthesis of symmetrical trithiocarbonates from alkyl halides and carbon disulfide under neat aqueous conditions

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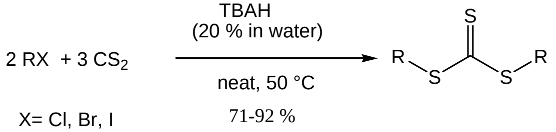
Trithiocarbonates constitute an important class of organic sulfur-containing compounds that have been used for various industrial, synthetic and medicinal applications [1]. Most of the convenient methods for the synthesis of symmetrical trithiocarbonates employ reactions of trithiocarbonate anion (CS_3^{2-}) with alkyl halides, or thiols with carbon disulfide (CS_2) and alkyl halides [2]. The trithiocarbonate anion has been prepared by two general routes: (1) Reaction of a metal sulfide with carbon disulfide [3], and (2) a one-pot preparation from carbon disulfide [4], catalyzed by a strong base (NaOH, KOH or NH_4OH) in the presence of either a phase-transfer catalyst, Cs_2CO_3, KF/Al_2O_3, Al_2O_3 or an anionexchange resin. Most of these methods have various disadvantages and limitations such as long reaction times, the use of highly toxic or malodorous chemicals, or suffer from low yields and the formation of unwanted side-products such as sulfide.

In recent decades, one of the main areas of progress in organic synthetic methodology has been the development of more environmentally friendly approaches that use ‘green’ conditions such as solvent-free,solid-phase, neat and aqueous conditions and require the use of fewer toxic substances[5].

Herein, we report a new, efficient and convenient one-pot synthesis of symmetrical dialkyl trithiocarbonates by the reaction of alkyl halides with carbon disulfide in the presence of an aqueous solution of tetra-*n*-butylammonium hydroxide (TBAH, 20% in H2O) at 50 °C.



A series of alkyl halids (benzyl, allyl, primary, secondary and tertiary halids) and aryl halids were examined. The procedure worked fine with benzyl, allyl and secondary as well as primary halids to give symmetrical ditrithiocarbonates.

In summary, we have developed a new, simple and efficient protocol for the one-pot synthesis of symmetrical dialkyl trithiocarbonates under aqueous, aerobic conditions.

This method offers significant and remarkable advantages over previously reported procedures in that it avoids the use of organic solvents, large excesses of carbon disulfide and toxic reagents such as thiophosgene. The approach is operationally simple, and gives high yields of products in short reaction times.

References:

[1] Gulea, M.; Masson, S. *Top. Curr. Chem.* **2004**, *250*, 257.
[2] Degani, I.; Fochi, R.; Gatti, A.; Regondi, V. *Synthesis* **1986**, 894.
[3] (a) Lee, A. W. M.; Chan, W. H.; Wong, H. C. *Synth.Commun.* **1988**, *18*, 1531; (b) Leung, M.-K.; Hsieh, D.-T.; Lee, K.-H.; Liou, J.-C. *J. Chem. Res.* **1995**, 478.
[4] Li, C. J.; Chang, T. H. *Organic Reactions in Aqueous Media*; Wiley: New York, **1997**.

A novel three-component reaction for the synthesis of alkyl nitrile derivatives *via* Michel-type addition reaction

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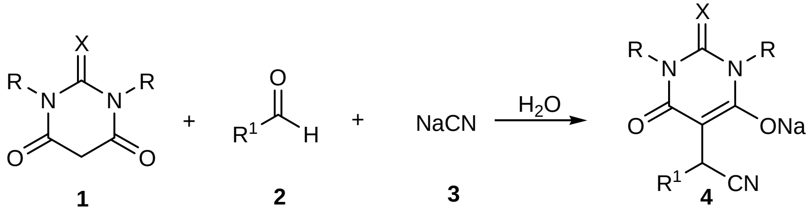
Alkyl nitriles[3] are useful intermediates in organic synthesis for the introduction of various functional groups as well as the construction of N-heterocycles. The preparation of nitriles by nucleophilic substitution of alkyl halides and sulfonates with inorganic cyanides are common and well known procedures. One of the best methods for the introduction of a cyanide group or β-Cyanocarbonyl involves the reaction of carbonyl compounds with cyanide via Michael addition.

As part of our continuing interest in the development of new synthetic methods in organic chemistry and our interest in multi-component reactions, herein we describe an efficient synthesis of nitriles **4** via the reaction of an barbituric acid with an aldehyde 2 and sodium cyanide 3 in high yields without using any catalyst at ambient temperature in water (Scheme 1).



References:

[1] Brase, S.; Gil, C.; Knepper, K.; Zimmermann, V. *Angew. Chem., Int. Ed.* **2005**, *44*, 5188.
[2] Serrano, J. L.; Sierra, T.; Gonzalez, Y.; Balm, C.; Weickhardi, K.; Magnus, A.; Moll, G. *J. Am. Chem. Soc*. **1995**, *117*, 8312.
[3] Soli, E. D.; Manoso, A. S.; Patterson, M. C.; Deshong, P. *J. Org. Chem*. **1999**, *64*, 3171.
[4] Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.* **2007**, *48*, 2185.
[5] Shaabani, A.; Soleimani, E.; Rezayan, A. H. *Tetrahedron Lett.* **2007**, *48*, 6137.

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Babolsar,Iran 13-15 October 2010

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دانشکده شیمی

Structural stability in a new polyazapolycyclic compound due to anomeric effects

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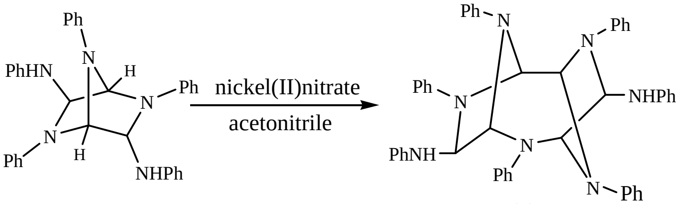
Catalytic synthesis of a pentaazatricyclo[5,2,1,1]undecane, a new polyazapolycyclic compound and a suitable precursor candidate for a new highly energetic compound, has been carried out in this work for the first time using nickel(II) nitrate as the catalytic agent.

N^3,N^6,2,5,7-Pentaphenyl-2,5,7-triazabicyclo-[2,2,1]heptane-3,6-diamine(1), a new compound produced in our previous work, was converted with good yield to N^4,N^8,3,6,9,10,11-Heptaphenyl-3,6,9,10,11-pentaazatricyclo[5,2,$1^{1,7}$,$1^{2,5}$]undecane-4,8-diamine(2) in acetonitrile using nickel(II) nitrate as catalyst.



(1) (2)

X-ray crystallographic analysis, used for structure determination of the product(II), demonstrated the existence of anomeric effects. This electronic interaction in N—C—N unites and its connotations for structural stability, reactivity and conformational behavior have been studied widely [1,2]. In the product(II), six unequal anomeric effects are distinguished in the N'—C—N'' fragments exhibited by the bond distances, N-atom pyramidality, and geometric parameters. Within the N'—C—N'' units, bond distances of N'—C are shorter than the C—N''. On the other hand, the pyramidality of N' (the sum of the three bond angles around N) are larger than that of N''. The angle at the bridging N-atom is 94.11(13)°. Although this bridge angle is comparable to those reported for azanorbornane and diazanorbornane [3], it still indicates the presence of ring strain.

References:

[1] Senderowitz, H.; Aped, P.; Fuchs, B. *Tetrahedron*, **1992**, *48*, 1131.
[2] Reed, A. E.; Schleyer, P. V. R. *Inorg. Chem*., **1988**, *27*, 3969.
[3] Davies, J. W.; Durrant, M. L.; Walker, M. P.; Malpass, J. R., *Tetrahedron*, **1992**, *48*, 4379.

Study of electronic interactions in a triazanorbornane skeleton

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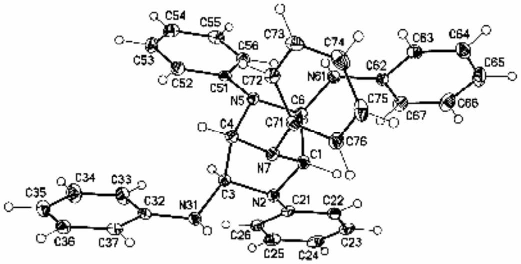
Polyazapolycyclics, constituted of saturated rings with multiple nitrogen atoms, are important precursors for synthesis of high density and highly energetic compounds [1,2].

N^3,N^6,2,5,7-pentaphenyl-2,5,7-triazabicyclo[2,2,1]heptane-3,6-diamine was synthesized for the first time in this work by catalytic reaction of 1,1',2,2'-tetrakis(phenylamino)ethane [3] with glyoxal in ethanol as solvent and in presence of excess glyoxal as catalyst and the product structure was fully established by X-ray structure determinations.

X-ray crystallographic analysis reveals the existence of some electronic interactions and four dissimilar anomeric effects manifested by the bond distances and nitrogen atom pyramidality on four N'—C—N'' fragments or $n_{N}\rightarrow\sigma^{*}_{C—N''}$ systems. Within the N'—C—N'' unit, the N'—C bond is shorter than the C—N'' bond. On the other hand, the pyramidality of N' (the sum of the three bond angles around N') is larger than that of N''. These geometric parameters are related to the anomeric effect, among them, the $n_{N5}\rightarrow\sigma^{*}_{C4—N7}$ system shows a distinguished anomeric interaction and the largest bond-length difference.



References:

[1] Nielsen, A. T.; Chafin, A. P., Christian; S. L., Moore; D. W., Nadler; M. P., Nissan; R. A.; Vanderah,

D. J. *Tetrahedron.* **1998**, *54*, 11793.

[2] Nielsen, A. T.; Moore, D. W.; Ogan, M. D.; Atkins, R. L. *J. Org. Chem.* **1979**, 44, 1678.

[3] Kliegman, J. M.; Barnes, R. K. *J. Org.Chem*. **1970**, *35*, 3140.

Characterization and comparison of tensile and fracture toughness properties of high performance epoxy nanocomposites

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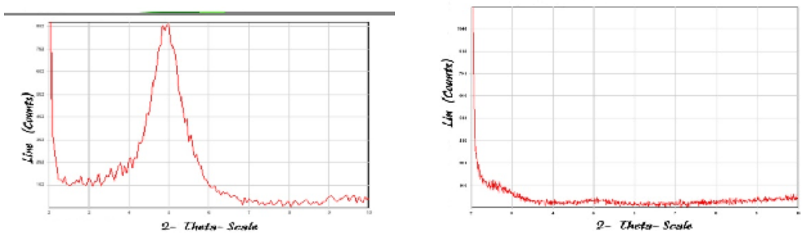
Zinc acrylate epoxy nanocomposites were prepared using an zinc acrylate epoxy resin, deglycidyl ether of bisphenolA, and cured with curing agent for TiO_2 and Clay nanofillers. The nanocomposites were processed by shear mixing at different clay concentrations. The shear force was controlled by changing the revolutions per minute on a mechanical mixer. The fracture toughness of the nanocomposites significantly increased with increasing nanofillers, suggesting a toughening effect from the nanoparticles.The mechanical properties of composites such as tensile strength and deflection at break are also investigated. Tensile strength and Young's modulus also increased with increasing TiO_2 and Clay loading. Scanning electron microscopy and wide angle X-ray diffraction were employed to reveal the morphology of zinc acrylate epoxy nanocomposites. Scanning electron microscopy observations of the zinc acrylate epoxy nanocomposites suggested that shear yielding of the matrix, voidind, and debonding of clay particles and zinc acrylate epoxy matrix are among the operative toughening mechanisms observed.



a b

XRD: (a) Cloisite 30B, (b) Zinc Acrylate epoxy nanocomposite

(a) Presents the WAXDs of Zinc Acrylate epoxy/clay nanocomposite as well as clay nanoparticles. (b) do not show any sharp crystalline diffraction peaks in this nanocomposie and we can find clay to dispersed in Zinc Acrylate epoxy matrix well.

References:

[1] Chow, F. H., *J. Mater. Sci***,** 2007, 42, 2690.
[2] Li, Sh., *J. Mater. Sci***, 2008**, 21, 2653.

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