In the name of God

It is our pride to host the acclaimed lectures, diligent researchers and students in the 27th Iranian Conference on Organic Chemistry in Faculty of Chemistry of Urmia University. Research and scientific investigations are directed towards solving the problems which are inter worn with human social life or expanding human knowledge borders, since today's science provides comfort and peace for human. Research is the main infrastructure of all future plans and programs.

We hope holding such events provides the ground of fresh and innovative ideas and exchange of diligent researcher's ideas of our country so that there are bases of accelerating scientific researches and more fruitful results and findings are obtained. Regarding the outstanding contribution of researches in this conference and submission of more than 490 papers in various branches of organic chemistry, there is possibility of holding this conference splendidly. It is worth mentioning that of 488 submitted papers, 2 papers are in public, 4 papers in keynote and 15 papers in specific presentation, respectively and all the rest in poster.

The executive committee considers it important to acknowledge the effort of Urmia University president, deputy of finance, deputy of vice chancellor for research and technology, deputy of human resource development and support, deputy of education, deputy of student assistant, University preservation office, dean of the faculty of chemistry, scientific and executive committees and everybody of Urmia University students in 27th ICOC executive committee.

With best wishes;

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بیست و هفتمین کنفرانس شیمی آلی ایران
۳۰ مرداد ماه الی ۱ شهریور ماه ۱۳۹۸
دانشگاه ارومیه

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برنامه برگزاری کارگاه ها:

ردیف	نام برگزار کننده	تاریخ	ساعت	مکان	عنوان کارگاه
۱	**دکتر محمود میرزایی**	**چهار شنبه ۱۳۹۸/۰۵/۳۰**	**۱۷–۱۸**	**کلاس ۱۰۳ دانشکده علوم**	**طراحی دارو به کمک کامپوتر**
۲	**خانم دکتر رادپو (شرکت مصباح انرژی)**	**چهار شنبه ۱۳۹۸/۰۵/۳۰**	**۱۷–۱۸**	**کلاس ۱۰۴ دانشکده علوم**	**ایزوتوپهای پایدار**
۳	**دکتر بهمن شریف‌زاده**	**چهار شنبه ۱۳۹۸/۰۵/۳۰**	**۱۷–۱۸**	**کلاس ۱۰۵ دانشکده علوم**	**آشنایی با روش‌های تجاری سازی دستاوردهای پژوهشی در قالب شرکت های دانش بنیان، مراکز رشد، استارت آپ ها و...**
۴	**پروفسور سعید بلالایی**	**پنج شنبه ۱۳۹۸/۰۵/۳۱**	**۱۷:۱۰–۱۸:۱۰**	**کلاس ۱۰۳ دانشکده علوم**	**معرفی امکان همکاری های پژوهشی در کشور آلمان برای دانشجویان و اساتید**
۵	**خانم دکتر شیوا کرمی**	**پنج شنبه ۱۳۹۸/۰۵/۳۱**	**۱۷:۱۰–۱۸:۱۰**	**کلاس ۱۰۴ دانشکده علوم**	**آشنایی با خاصیت مغناطیسی مواد و تفسیر نتایج بدست آمده از دستگاه** VSM
۶	**آقای میلان (کتابخانه مرکزی دانشگاه ارومیه)**	**چهار شنبه ۱۳۹۸/۰۵/۳۰**	**۱۷:۱۰–۱۸:۱۰**	**کلاس ۱۰۵ دانشکده علوم**	**آشنایی با پلاجیاریسم (بررسی سرقت ادبی مقالات**iThenticate **)**

Curing process of the binary epoxy resin systems with aromatic diamine hardener

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Keywords: Epoxy networks, Diglycidyl ether of bisphenol A, Diglycidyl ether of polyethylene glycol, 4,4′-Diaminodiphenyl sulfone.

Epoxy networks are one of the most important class of thermosetting materials for many engineering applications because of their high thermal and mechanical strength and good dielectric behavior.[1,2] Epoxy resins have normally poor crack resistance at room temperature, and are also highly brittle at cryogenic temperature, which makes them inappropriate for many cryogenic engineering applications.[3] Thus, it is necessary to improve the toughness and ductility of epoxy networks so that they can be suitable even at low temperatures.[4] In this approach, replacing rigid structures with more flexible backbones as well as utilization of epoxy/hardeners with higher molecular weights, consequently lower crosslink density can be considered. In this work, diglycidyl ether of polyethylene glycol (DGEPEG) was blended with diglycidyl ether of bisphenol A (DER-332) in various proportions and cured with 4,4′-diaminodiphenyl sulfone (DDS) hardener (Fig. 1). FT-IR and TGA techniques were used to characterize the samples obtained.

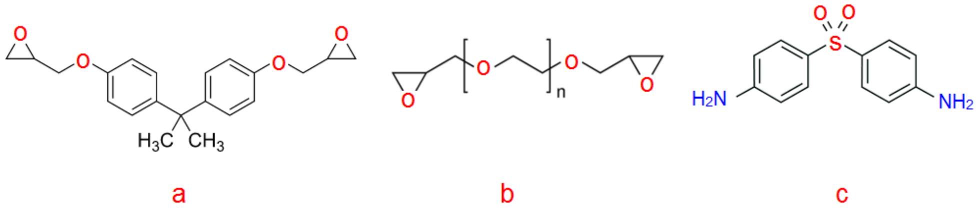

Fig. 1 Structures of DGEBA (a), DGEPEG (b) and DDS (c).

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Immobilization of chiral amino alcohol (S)-2-amino-4-methylpentan-1-ol on MCM-41 nanoporous silica and its applications in asymmetric allylic C-H bond oxidation of cycloalkenes

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Keywords: Chiral amino alcohol, Chiral heterogeneous catalysts, Chiral allylic ester, Allylic C-H bond oxidation.

There are several methods for the preparation of pure enantiomeric compounds which one of them is the use of chiral catalysts in asymmetric synthesis. For this purpose, we used a heterogeneous chiral catalyst because its separation and recycling is more convenient than homogeneous catalyst.[1, 2] The allylic oxidation of olefins using peresters in the presence of copper catalyst to give allylic esters is known as the Kharash-Sosnovsky reaction. This reaction has been the subject of great interest over the last decade and provides access to chiral allylic alcohols, which are key intermediates in natural product synthesis.[2] In this study, MCM-41 was prepared and modified by (3-chloropropyl) trimethoxy silane. Afterward, the chiral amino alcohol (*S*)-2-amino-4-methyl pentan-1-ol which is synthesized by reduction of corresponding chiral amino acid *L*-leucine, immobilized on Cl-MCM-41 mesoporous silica. The synthesized chiral heterogeneous ligand with copper salt was used in the asymmetric allylic C-H bond oxidation of cycloalkenes under different conditions. The chiral allylic esters were achieved in high yields and moderate enantioselectivities.[2 a,c]

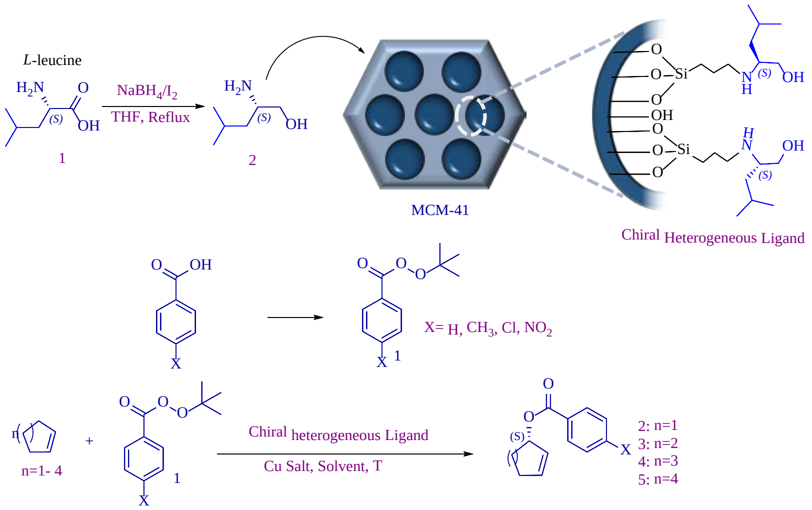

Fig. 1 Asymmetric allylic oxidation of cycloalkenes in the presence of chiral heterogeneous catalyst

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Immobilization of the amino acid (L)-valine and amino alcohol (L)-valinol on SBA-15 nanoporous silica and investigation of their potential in asymmetric allylic oxidation of alkenes

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Keywords: Amino acid, Amino alcohol, Chiral heterogeneous catalyst, Chiral allylic ester, SBA-15.

Immobilization of chiral ligands onto mesoporous silica such SBA-15, SBA-16, MCM-4, and MCM-41 for the preparation of chiral heterogeneous catalysts have attracted enormous interest in asymmetric synthesis[1, 2]. Chiral allylic esters that are one of the important intermediates in the pharmaceutical industry were prepared *via* asymmetric allylic C-H bond oxidation of cycloalkenes with perester in the presence of copper salt (Kharasch–Sosnovsky reaction) [3].

In this study, we prepared mesoporous silica SBA-15 and modified by 3-chloropropyl trimethoxy silane. Afterward, amino acid *L*-Valine and amino alcohol *L*-Valinol that is synthesized by reduction of corresponding amino acid *L*-Valine, immobilized on modified SBA-15. The synthesized heterogeneous chiral catalysts were characterized by using FT-IR, XRD, SEM, EDX, TGA and BET-BJH techniques. The copper complexes of these chiral heterogeneous catalysts were investigated in the asymmetric allylic C-H bond oxidation of cycloolefins. The chiral allylic esters were obtained in high yields and moderate enantioselectivities under the best condition [3] (Figure1).

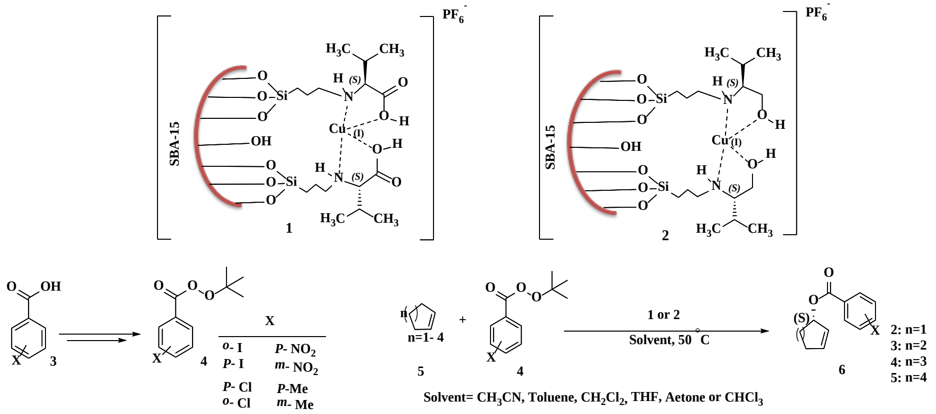

Fig. 1. The synthesis of chiral allylic esters in the presence of chiral heterogeneous catalysts.

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Enhancement of photocatalytic performance in two pillared metal–organic framework by solvent-assisted ligand exchange.

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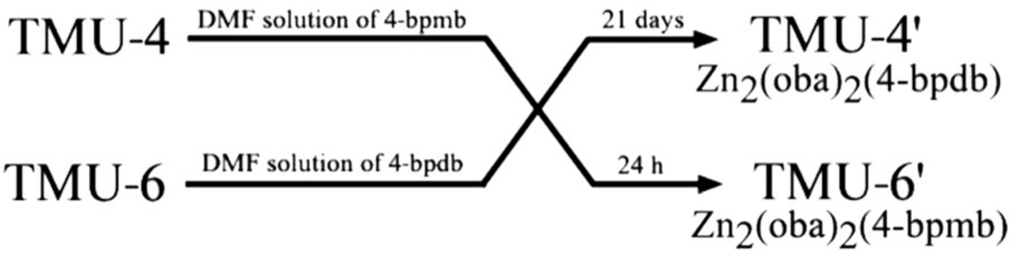
Keywords: Pillared metal−organic frameworks (MOF), Photocatalytic activity, Cr(VI) reduction, Solvent-assisted linker exchange (SALE).

As a class of newly developed porous solids, metal−organic frameworks (MOFs), constructed by metal ions or metal clusters and organic ligands through coordination bonds. Post-synthetic modifications (PSMs) provide alternative routes for functionalizing MOFs[1], and solvent-assisted linker exchange (SALE)[2] is one of the PSMs method with the ability of controlling catenation, accessing polymorphs with comparatively high energy, and producing MOFs with longer linkers, mixed linkers, and/or larger cages.[3] Herein, SALE was performed on two pillared MOF, $[Zn_2(oba)_2(4\text{-}bpdb)]_n \cdot (DMF)_2$ (TMU-4) and $[Zn(oba)(4\text{-}bpmb)_{0.5}]n \cdot (DMF)_{1.5}$ (TMU-6), for Cr(VI) reduction. An increase in the Brunauer– Emmett–Teller (BET) surface area along with defects in daughter SALE MOFs (TMU-4′ and TMU-6′) in comparison with the parent MOFs (TMU-4 and TMU-6) led to enhancement of their photocatalytic activity in the reduction of Cr(VI).



Scheme 1 Summary of the SALE reactions performed on TMU-4 and TMU-6.

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Synthesis of dipyrazolo-1,4-dihydropyridine in the presence of a novel deep eutectic system

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Keywords: Deep eutectic system, Dipyrazolo-1,4-dihydropyridine, Multicomponent reaction.

Dipyrazolopyridine are one of the most widely used organic compounds that have been used as high-Luminescent dyes, Nichrome diodes and anti-inflammaory, antiviral and antitumor druges. These compoundes have been synthesized from condensation of hydrazine, aldehyde, β-ketoester and ammonium acetate. Previously, p-TSA,[1] nano-ovalbumin,[2] nano-$CdZr_4(PO_4)_6$[3] and nano-$CuCr_2O_4$[4] have been used for promotion of this procedures.

Deep eutectic solvents (DES) are generally composed of two or three cheap and safe components which are capable of associating with each other, through hydrogen bond interactions, to form a eutectic mixture[5]. The resulting DES is characterized by a melting point lower than that of each individual component. From the view point of green chemistry, these DESs are even more attractive since some of them have been proven to be biodegradable and compatible with enzymes further increasing their interest. in this work, we have prepared a novel deep eutectic system from sodium acetate and triethanol amine (TEA) with low melting point and used it for synthesis of dipyrazolopyridine under microwave conditions (Fig. 1).

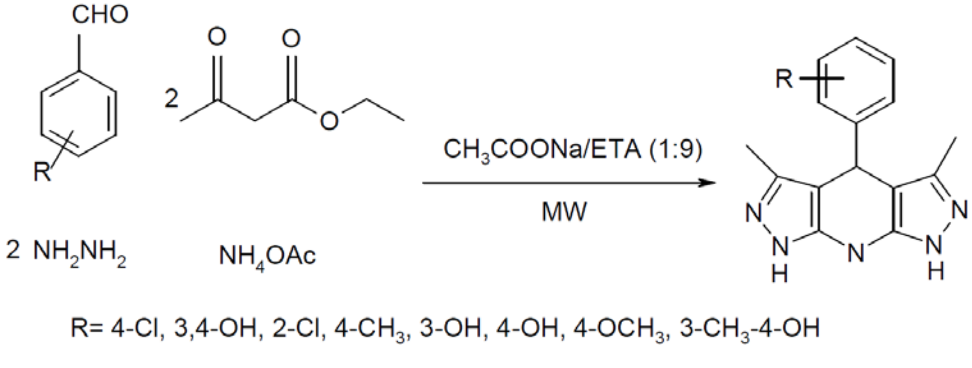

Fig. 1 Synthesis of dipyrazolo-1,4-dihydropyridine

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One-Pot Synthesis of 2,4,5-Trisubstituted Imidazoles by using Magnetic Cobalt Ferrite Nanocomposite Supported by Tungstic Acid as a Novel Catalyst

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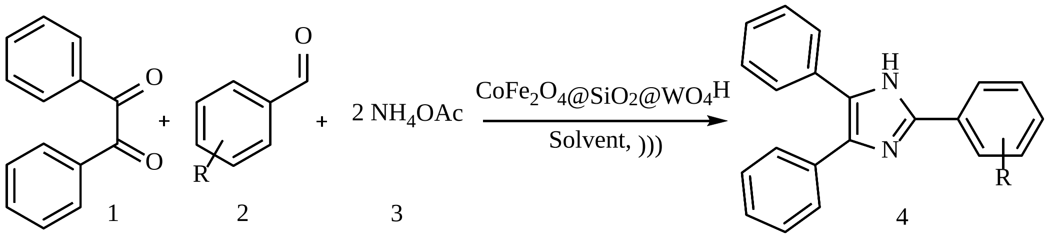
Keywords: Imidazole, One-Pot, Condensation reaction, Ultrasound irradiation.

Imidazole and its derivatives are an important group of five- membered nitrogen heterocyclic compounds, which usually play important roles for the synthesis of natural products and as therapeutic agents.[1-3] In particular, 2,4,5-trisubstituted imidazoles are biologically active and found in structures of anti-inflammatory,[4] anti-microbial,[5] analgesic,[6] etc. Herein, we report one-pot synthesis of 2,4,5-triaryl-1H-imidazoles (4) from the condensation reaction of 1,2-diketone (Benzyl, 1mmol)(1), Aldehydes (1mmol)(2) and Ammonium acetate (2mmol)(3) in the presence of solvent by using $CoFe_2O_4@SiO_2@WO_4H$ as a novel catalyst that provides required acidic conditions in addition of increasing the efficiency and reaction speed without the need of using harmful acidic catalysts under ultrasound irradiation at room temperature. The structure of synthesized derivatives was deduced from their FT-IR and ^1H NMR spectral data and checking melting point.



R= H, F, 4-Cl, 2-Cl, 2,4-Cl_2, 4-Br, 4-OH, 3-OH, 4-OCH_3, 2-NO_2, 3-NO_2, 4-NO_2

Fig. 1 Synthesis of 2,4,5-triaryl-1H-imidazoles in the presence of $CoFe_2O_4@SiO_2@WO_4H$ catalyst under ultrasound irradiation at room temperature.

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Synthesis of layered lipophilic graphene quantum dot over Fe@MgO catalyst

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Keywords: Graphene quantum dot (GQD), Lipophilic material, Layered material, Fe@MgO catalyst, Friction, Lubricant, Oil additive

Friction and wear are two reasons that cause energy losses in mechanical activities. Lubrication is the main subject for improving energy efficiency and mechanical durability. Regardless of the completion of each metal surface, it contains ridges, valleys, asperities, and depressions[1,2]. Graphene and GQDs Nano scrolls can efficiently reduce frictional loss in engines, turbines, and other machines. By the way, replacing traditional lubricants, GQDs could help the environment by replacing petroleum-based lubricants that must be disposed of biological disaster[3,4]. The design in GQD synthesis is based on the following considerations: well surface passivation of GQDs plays a key role in quantum dots fabrication. In our research, we chose citric acid as the carbon source due to its well-known low carbonization temperature (<200ºC), and used octyl amine as the capping and functionalizing reagent because of functionalized and passivation surface states with carboxyl groups having a good photo-induced electron transfer property.

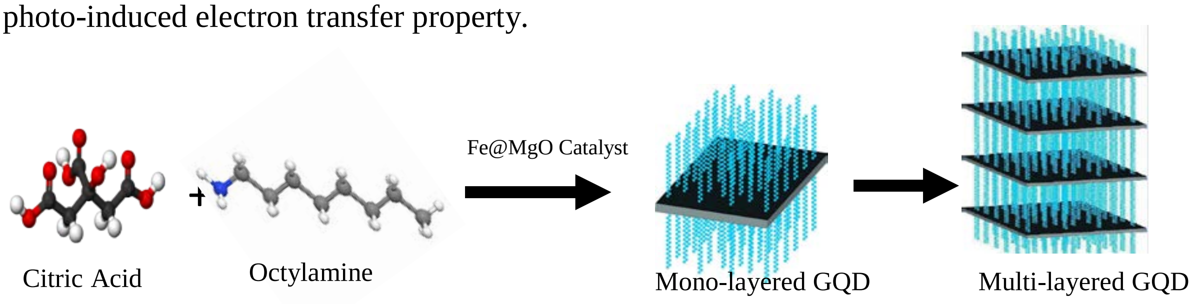

Fig. 1 Schematic synthesis of mono-layered and multi-layered GQD

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Graphene-based adsorbent synthesis and it's use in industrial wastewater treatment

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Keywords: Graphene Quantum Dot (GQD), Adsorbent, Polymer, Wastewater, Methylene blue

Graphene-based materials, including graphene and derivatives such as graphene oxide and graphene quantum dots, have considerable potential as key components in next-generation membrane technologies. Their tunable size, surface chemistry, and structure can be engineered for a spectrum of aqueous filtration purposes ranging from ultrafiltration to reverse osmosis[1]. Membrane-based separation technology has been introduced in dyes removal treatment and is well known for its advantages[2]. Previously various techniques such as nanofiltration, photodegradation, oxidation, biological treatment, adsorption, and liquid membrane separation have been developed for the degradation and removal of toxic dyes from contaminated water[3,4]. In this work, we have fabricated a GQD based polymer adsorbent. In a typical synthesis, GQD was synthesized through carbonization of citric acid and ammonia. The synthesized GQD was modified with methacrylic acid and (acrylamidomethyl)- cellulose acetate butyrate to form polymeric adsorbent. The different concentration of methylene blue solutions prepared and concentration of each solution before and after filtration was determined by UV spectrometer.

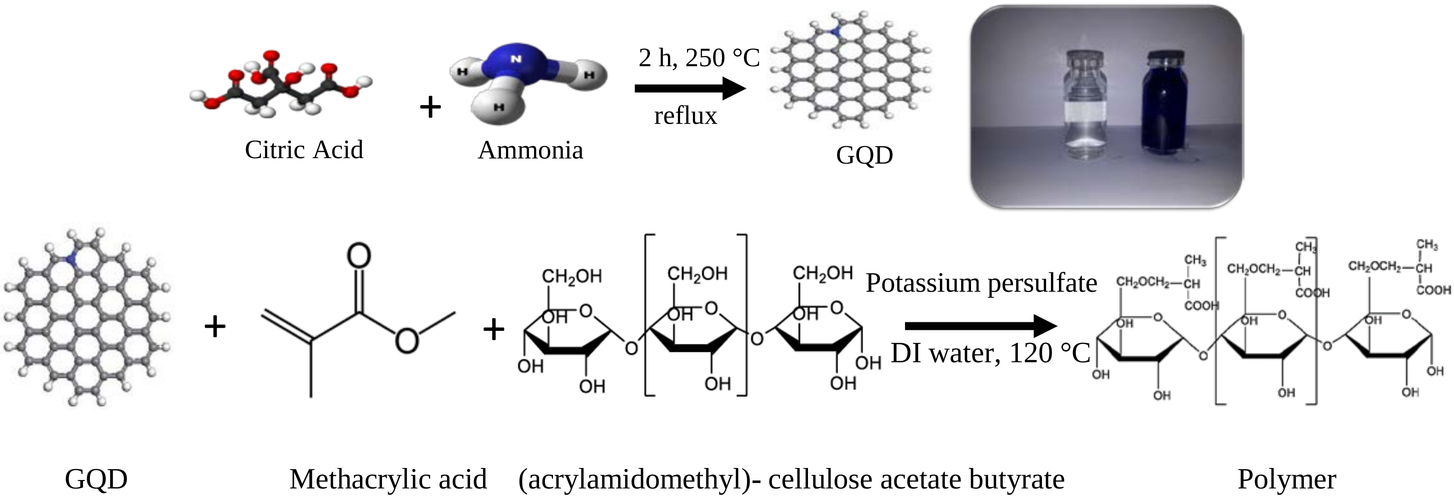

Fig. 1 Schematic synthesis of polymeric adsorbent and filtered methylene blue 100 ppm solution

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Immobilized tris(8-quinolinolato)iron onto the silica coated magnetite nanoparticle: sustainable development for the sulfide oxidaiton reaction

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Keywords: Magnetic nanoparticle, $Fe_3O_4@SiO_2$-FeQ_3, Sulfide oxidation.

The rapid progress of nanotechnology has enabled researchers to design and synthesis of uniform core-shell with magnetically responsive cores and functional shell at nano-scales [1]. Amon core-shell nanostuctures, $Fe_3O_4@SiO_2$ nanospheres have attracted considerable attention because of their unique geometry and espeical magnetic properties [2, 3]. Herien, we have reported a green, robust and eco-friendly procedure for the oxidation of aromatic organic sulfides to sulfones using H_2O_2 catalyzed by NH_2-coordinately immobilized tris(8-quinolinolato)iron onto the silica coated magnetite **Fig 1**. The catalytic activity $Fe_3O_4@SiO_2$-FeQ_3 for sulfides oxidation showed that this atom-economical protocol provided great conversion of various sulfones and allowed the sulfide function reaction conducting under the mild conditions thus to prevent the sulfide being over-oxidized to sulfoxides.

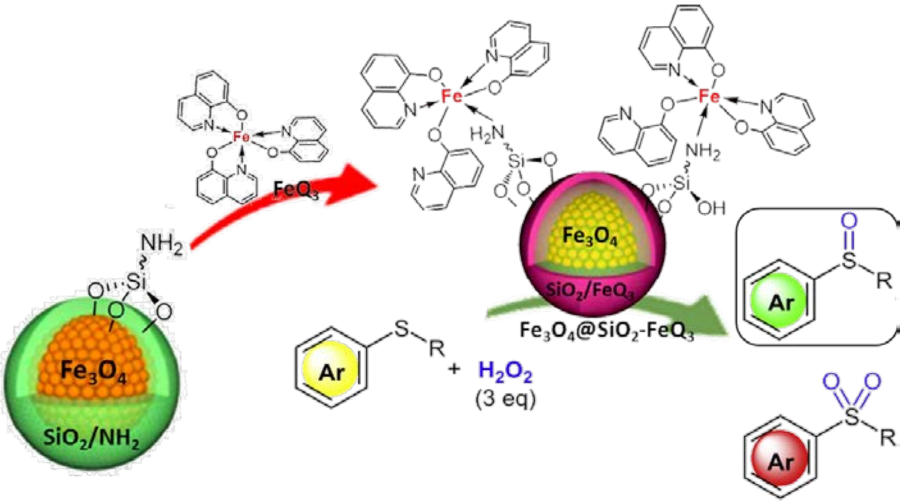

Fig. 1 Schematic illustration of $Fe_3O_4@SiO_2$-FeQ_3 for oxidation of sulfides.

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Design and Synthesis of novel urea-based oxadiazole derivatives as soluble epoxide hydrolase inhibitors

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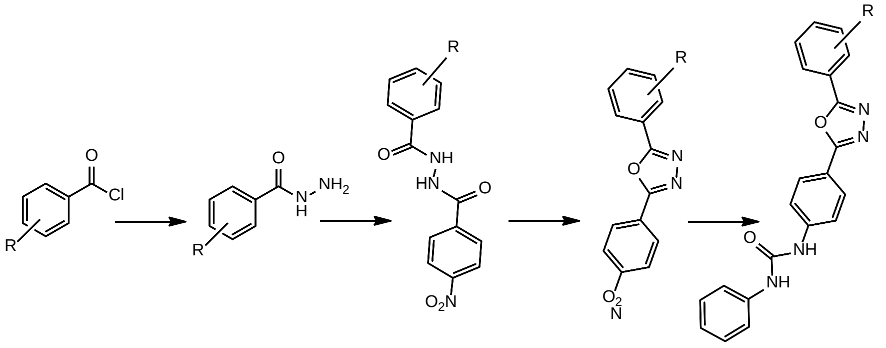
Keywords: Soluble epoxide hydrolase, synthesis, oxadiazole.

Soluble epoxide hydrolase is a member of the serine hydrolase family of enzymes that involved in the metabolism of endogenous mediator, epoxyeicosatrienoic acids, which is known as modulator of blood pressure and inflammation accumulate. Since the most potent sEH inhibitors reported in literature have limited pharmacokinetic profile, new scaffolds are needed for the therapeutic applications.[1] In this study, some oxadiazole derivative were designed and synthesized as soluble epoxide hydrolase inhibitors. N-benzoyl-4-nitrobenzohydrazide **2** was obtained via a reaction of benzoyl chloride and hydrazinium hydroxide followed by treatment with 4-nitrobenzoylchloride. A mixture of intermediate **2**, thionyl chloride and pyridine was refluxed to produce 2-(4-nitrophenyl)-5-phenyl-1,2,4-oxadiazole **3**. Finally finish products were achieved by reduction of the nitro group and reaction with various phenyl isocyanate analogs (Fig. 1).[3]



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

Fig. 1 schematic synthesis of compounds.

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Synthesis of coumarin (2*H*-chromen-2-ones) derivatives

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Keywords: Nanobiocatalysts, Phenols, Pechmann condensation, Coumarins

Enzymes are biological catalysts that are believed to be the cornerstones of life. The combined enzyme in nanoformats is called nanobiocatalyst. Nanofibers, hybrid nanoflowers, mesoporous/nanoporous carriers, carbon nanotubes, magnetic or non-magnetic nanoparticles, and nanocomposites as support carriers can be used for the immobilization of different enzymes to develop nanobiocatalysts with potential activity and stability characteristics.[1] Coumarin and its derivatives are important compounds due to their presence in naturally occurring aromatic products found in plants and cinnamon flavoured foods.[2] These compound have applications including antibacterial, anti-inflammatory, anti oxidant, anticoagulant, anticancer and anti-HIV.[3] Coumarins can be synthesized by various methods such as Perkin, Pechmann, Knoevenagel, Reformatsky and Witting reactions.[4] Here in, we initially synthesized $Fe_3O_4@SiO_2$ and then aminated, eventually, immobilized the trypsin onto it. We have demonstrated an efficient protocol for the synthesis of coumarin derivatives **3** via Pechmann condensation reactions of phenols **1** and β-ketoester **2** using as magnetically separable nanobiocatalyst as reusable catalyst in aqueous ethanol (Fig. 1). The purified products were characterized by spectral methods: FT-IR, ^{1}H-NMR, ^{13}C-NMR. The nanobiocatalyst was separated simply by using an external magnet, after completion of the reaction and recycled up to several times without loss of catalytic activity.

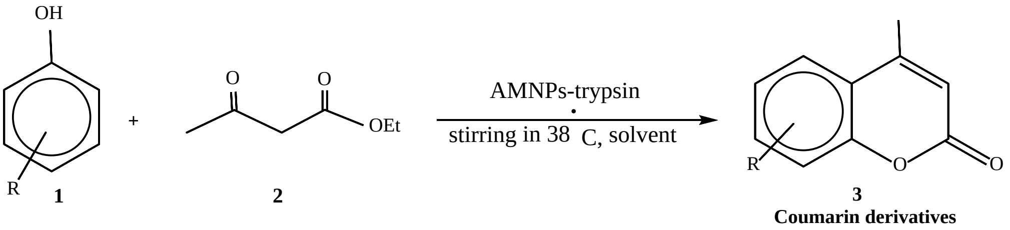

Fig. 1 The overall mechanism of the pechmann condensation in synthesis of coumarins

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Copper(II) Schiff Base Complex Immobilized on Core-shell $Fe_3O_4@SiO_2$ as a Magnetically Reusable and Highly Efficient Nanocatalyst for the Green Synthesis of 2-Amino-4*H*-chromene derivatives

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Keywords: Cu(II) Schiff-base complex, magnetic nanoparticles, 2-Amino-4H-chromene derivatives.

Fe_3O_4 based a new Cu(II) Schiff-base complex has been prepared by treating 1,3-Phenylenediamine with Salicylaldehyde in ethanol [1-4]. This catalyst has been characterized by TEM, SEM, XRD, FT-IR, TGA, XPS, VSM, ICP, EDX and successfully applied as a magnetically recyclable heterogeneous catalyst for the efficient one-pot, three-component synthesis of 2-Amino-4H-chromene derivatives. The catalyst can be recovered by magnetic separation and recycled several times without significant loss of catalytic activity.

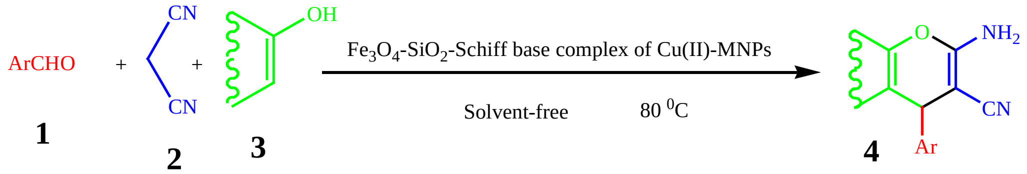

Fig 1. Fe_3O_4-SiO_2-Schiff base complex of Cu(II)-MNPs-Catalyzed synthesis of 2-amino-4H-chromene derivatives.

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Immobilized oxodiperoxo molybdenum complexes on the Cr-MOFs as promising and bifunctional catalyst for the selective thioether oxidation

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Keywords: Metal-organic framework, $MoO(O_2)_2$@En/MIL-100(Cr), Thioether oxidation.

Nanoporous metal-organic frameworks (MOFs) are self-assembled from organic linkers and inorganic connectors of metal ions/clusters, that they have interesting perspectives in the application of catalysis [1, 2]. MOFs are also the ideal platform for post-synthetic modification chemistry for improve catalytic activity [3]. Herein, we have demonstrated of MIL-100(Cr) as an efficient open metal site Cr-MOFs towards the direct grafting of ethylene diamine (En) ligand and then complexation of that with oxodiperoxo molybdenum complexes ($MoO(O_2)_2$.DMF) to achieve $MoO(O_2)_2$@En/MIL-100(Cr) **Fig 1**. The proposed nanocatalyst was then applied for H_2O_2 mediated selective thioether oxidation with excellent conversion.

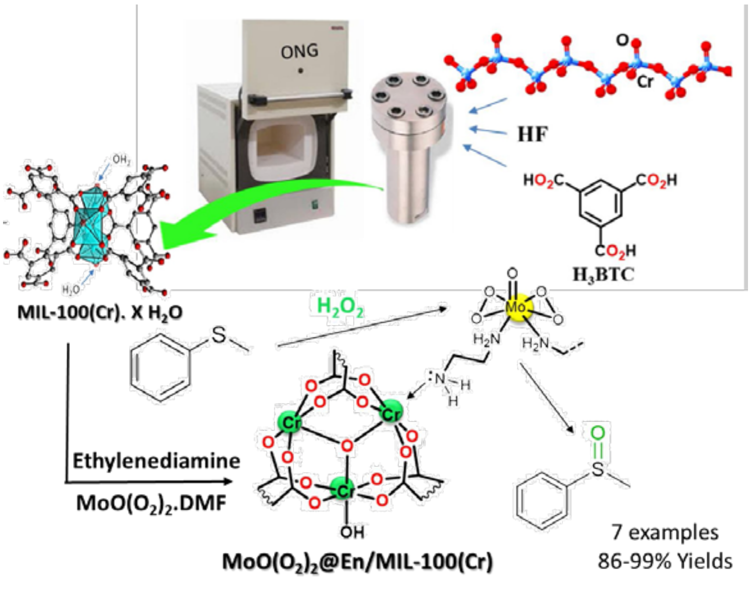

Fig. 1 Bifunctional $MoO(O_2)_2$@En/MIL-100(Cr) for selective oxidation of thioether.

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Linear diaminoplumbylenes in a theoretical focus (electronic & steric)

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Keywords: plumbylenes, NHTs, NHC, thermodynamic parameters, DFT.

Plumbylenes are the heaviest members of group 14 of divalent which appear to be more stable than carbenes [1]. This research to investigate the influence of diaminoplumbylenes structures and thermodynamic parameters on nucleophilicity. There series of diaminoplumbylenes including acyclic 1R_1-4R_2-diaminoplumbylenes ($\mathbf{A_{R1,R2}}$), are scrutinized at B3LYP/6-311++G** level of theory, for R_1 (or R_2) = adamantyl, NH_2, NMe_2,OMe,TMS phenyl, H, Et, Me, *i*-propyl, and *t*-butyl OH, SH, CN,CF_3, CO_2H, NO_2. Structural effects are made conspicuous by NH_2-substituents that make acyclic $\mathbf{A_{NH2,NH2}}$ the most nucleophilic among the scrutinized plumbylenes. The results indicate that acyclic diaminoplumbylenes ($\mathbf{A_{R1,R2}}$) is lowest *N*. In all scrutinized of $\mathbf{A_{R1,R2}}$ plumbylenes, the highest *N* is exhibited by $\mathbf{A_{R1,R2}}$ plumbylenes includes π-electron-donating of NH_2. Every abnormal diaminoplumbylenes turns out more nucleophile than its corresponding normal isomer. Specifically, to probe substituent effects on nucleophilicity of $\mathbf{A_{R1,R2}}$. We have examined thermodynamic parameters of our plumbylenes including: nucleophilicity (*N*), singlet-triplet energy gaps ($\Delta E_{S-T} = E_T - E_S$), band gap ($\Delta E_{HOMO-LUMO}$), bond angle and bond lengths (Fig. 1).

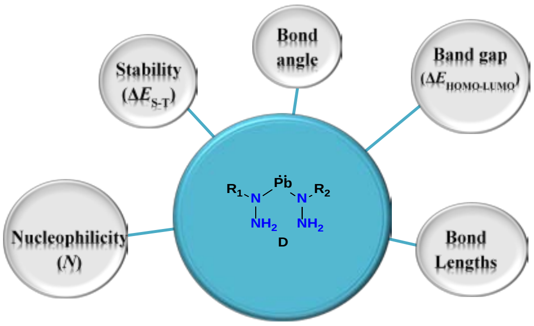

Fig. 1 A flow chart for scrutiny of acyclic diaminoplumbylenes ($\mathbf{A_{R1,R2}}$).

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Novel N-Heterocyclic Stannylenes (NHSns) using DFT

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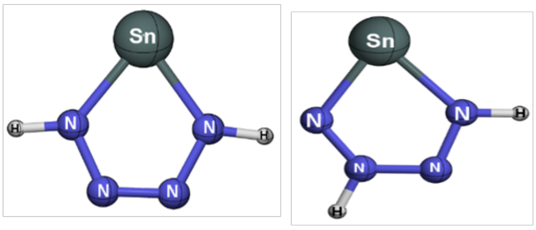
Keywords: Nucleophilicity, *N*-Heterocyclic, Stannylenes, DFT

Substitution effects are probed for novel *N*-heterocyclic stannylenes (NHSns), including 1,4-di(R)-tetrazole-5-stannylenes (1_R), and 1,3-di(R)-tetrazole-5-stannylenes (2_R), using B3LYP/6-311++G** level of theory. Nucleophilicity, multiplicity, and stability of 1_R and 2_R are calculated; with R = H, methyl, ethyl, *i*-propyl, *t*-butyl, Ph, OH, methoxy, NO_2, CN and CF_3. Asymmetric 2_H appears more nucleophilic ($N \sim 4$) than its corresponding symmetric 1_H isomer ($N \sim 3$), mostly due to the formers higher separation of charge. The N is more sensitive to electronic effects in 1_R stannylenes than those in the 2_R series. Electron donating R groups increase N with Hammett ρ constants of -3.3 and -2.7 for 1_R and 2_R, respectively. Stannylene 2_H is slightly more aromatic (NICS (1) = -10.31) than 1_H (NICS (1) = -10.25). Every 1_R is more stable than its corresponding 2_R isomer. Every 2_R is generally more nucleophilic and aromatic than its corresponding 1_R. In addition the former is less electrophilic with a larger band gap and narrower stannylene bond angle. Substituent effects are probed on N by devising proper isodesmic reactions. The trend for N is: $2_{t\text{-buthyl}} > 2_{iso\text{-propyl}} > 2_{\text{ethyl}} > 2_{\text{methyl}} > 2_{\text{ph}} > 2_{\text{OMeth}} > 1_{t\text{-buthyl}} > 2_{\text{OH}} > 2_{\text{H}} > 1_{\text{Ph}} > 1_{iso\text{-propyl}} > 1_{\text{OH}} > 1_{\text{ethyl}} > 1_{\text{methyl}} > 1_{\text{OMeth}} > 1_{\text{H}} > 2_{\text{CF3}} > 2_{\text{NO2}} > 2_{\text{CN}} > 1_{\text{CF3}} > 1_{\text{CN}} > 1_{\text{NO2}}$.



1_H 2_H

Fig 1. Scrutinized normal 1,4-dihydrotetrazastannole (1_H), and abnormal 1,3-dihydrotetrazastannole (2_H), at DFT.

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Biological profile of boronic acid multivalent functionalized MoS_2 nanosheets

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Keywords: Molybdenum disulfide, Boronic acid, Antibacterial, Antinematode and Wound healing.

Two-Dimensional MoS_2 has attracted high attention owing to its unique physicochemical properties as well as biocompatibility and biodegradability.[1-3] Surface functionalization of MoS_2 nanosheet through the incorporation of functional groups with the ability of attachments to the biological systems significantly improves its biological activity.[4, 5] In this work, boronic acid-functionalized 2D MoS_2 was synthesized and its covalent multivalent interactions at different biointerfaces including bacteria, nematode and diabetic wounds were investigated. The boronic acid-functionalized 2D MoS_2 (MoS_2-B) was synthesized by stepwise polymerization of glycidol and conjugation of boronic acid to the surface of MoS_2 sheets (Fig1). MoS_2-B showed strong interactions with the membrane of bacteria and body of nematode and destroyed both microorganisms in a short time. Due to the strong antibacterial and antinematode activity and its ability to make a thin-film on the surface of wounds, MoS_2-B was applied for the diabetic wound healing. Taking advantage of the straightforward synthesis, antibacterial and antinematode activities as well as healing the diabetic wounds, MoS_2-B is a promising candidate for a broad range of future biomedical applications.

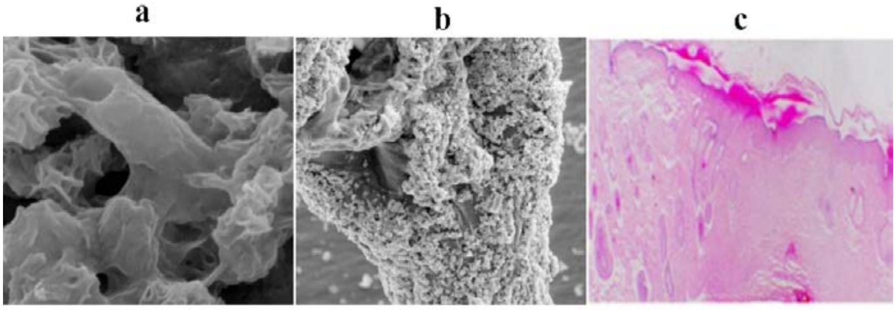

Fig. 1 FE-SEM image of a) *E.coli* bacteria and b) nematode incubated with MoS_2-B. Histological images of c) wound skin of rats after the treatment with MoS_2-B.

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Synthesis of acridinyl substituted amidoalkyl naphthols with pH-sensitive fluorescence activity

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Keywords: Multi-component reactions, Amidoalkyl naphthol, Acridine, Fluorescence.

Acridine and its derivatives are heterocyclic analogues of anthracene that central ring containing nitrogen instead of a carbon atom. Acridine and some of its derivatives have interesting photophysical properties, i.e., high fluorescence quantum yield and high molar absorption coefficients.[1-3] Synthesis of amidoalkyl naphthols is one of the most studied reactions because these compounds can be converted to useful and main biological building blocks, and their hydrolysis leads to 1-amino methyl-2-naphthols that show biological activities.[4]

Herein, we wish to report the synthesis of new acridinyl substituted amidoalkyl naphthols **4** from the multicomponent reaction of acridinyl benzamide **1**, 2-naphthol **2** and aromatic aldehydes **3** in the presence of *p*-toluene sulfonic acid as a catalyst (fig. 1). The structure of the synthesized compounds was determined on the basis of their spectroscopic data. These products have a strong fluorescence emission in pH = 7 while in acidic and basic pH the florescence emission of these compounds is quenched.

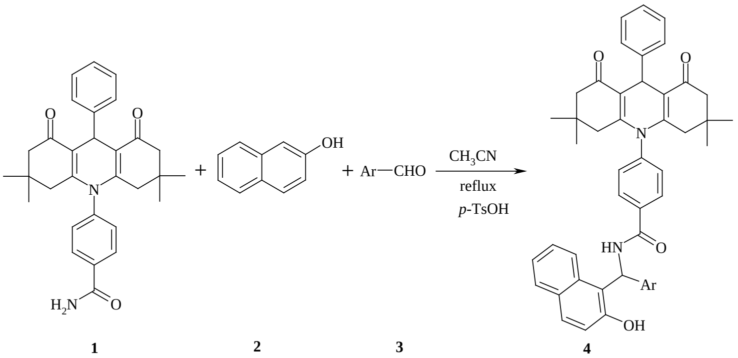

Fig. 1 Synthesis of new acridinyl substituted amidoalkyl naphthols

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The computational study of substituent influence on the anomeric effect, aromatization and hydride removal in 1, 4 DHPs

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Keywords: Computational study, Anomeric effect, Anomeric base oxidation, 1, 4 DHPs

Anomeric effect was introduced by stereoelectronical effect on carbohydrate chemistry almost 60 years ago. It caused preference of electronegative substituent in axial than equatorial position of pyranoid ring systems. Now anomeric effect is known as a basic issue in chemistry and has significant role in the field of organic transformations [1, 2]. For the first time the role of anomeric effect in oxidative aromatization of some heterocyclic molecules was investigated by our research groups and named "anomeric base oxidation (ABO)". Oxidation is happening by transfer of heteroatom lone pair electrons through resonance, then electrons interact with anti-bonding orbital of C-H bond and make hydride removal from the intermediate [3, 4]. In continuation of this research on ABO, was evaluated the substituent influence on cooperative vinylogous anomeric effect and aromatization in 1,4-DHPs (1,4-dihydropyridines). The characterization and energy of substituent effect on some of the 1,4-DHP derivatives were computed and found that the properties of substituent can play important role in anomeric effect and aromatization of these compounds.

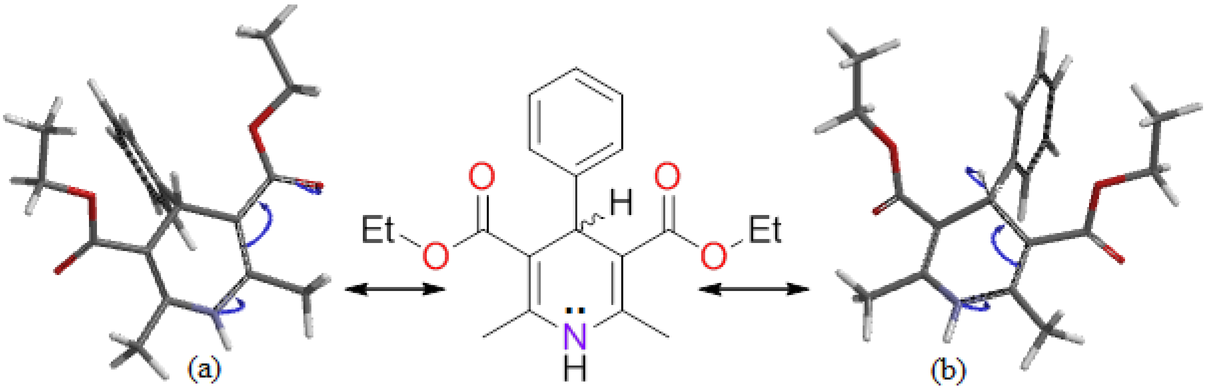

Fig. 1 Two models of resonance between atoms of 1,4-dihydropyridine. (a) Resonance with carboxylate (b) anomeric effect

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Experimental and Theoretical Studies on the Protection of aldehydes with diols and dithiols

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Keywords: Protection of aldehydes, Acetalization, Nano magnetic catalyst, Hyperconjugation, Theoretical studies.

Protection of carbonyl compounds is an important at the multistep total synthesis of the enantiomerically pure natural and non-natural compounds. Acetals and thioacetals were well known as the protecting intermediates [1, 2]. The nano magnetic $Fe_3O_4@SiO_2@(CH_2)_3NHSO_3H$ catalyst was used for the protection process of aldehydes with diols and dithiols [3]. To determine the most stable structure of the products were applied DFT-B3LYP/6-31G* method. The obtained theoretical results on the synthesized products have shown that the structure of the products of diols in compare with dithiols demonstrated different electronic properties. The diols and dithiols both have two conformers. There are interesting result, due to the hyperconjugation effect between C-H and aromatic ring in diols and also hyperconjugation between π-electrons of aromatic ring and *3d* orbital space of S-atoms in dithiol derivatives. The different interesting aspects of this experimental and theoretical investigation will be presented and discussed [4].

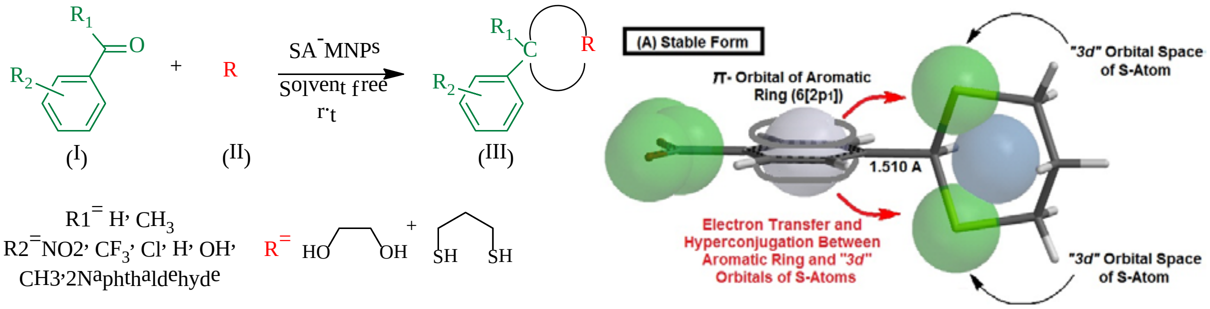

Fig. 1 The process of reaction and figure of hyperconjugation between π-electrons of aromatic ring and *3d* orbital space of S-atoms

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Synthesis and properties of epoxy resin networks containing polyethylene oxide unites

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Keywords: Epoxy thermoset, Diglycidyl ether of bisphenol A, Diglycidyl ether of polyethylene oxide, Isophorone diamine, amine-functionalized polyethylene oxide.

Epoxy resins are thermosetting resins, which are cured using a wide variety of curing agents via curing reactions. Their properties depend on the specific combination of the type of epoxy resins and curing agents used.[1] Because of their excellent mechanical properties, high adhesiveness to many substrates, and good heat and chemical resistances, currently epoxy resins are intensively used across a wide range of fields, where they act as fiber-reinforced materials, general-purpose adhesives, high-performance coatings, and encapsulating materials.[2,3] In this study, three epoxy thermosetting materials possessing polyethylene oxide units are prepared starting from polyethylene glycol. To improve the mechanical strength of the epoxy materials, alongside the flexible units of polyethylene oxide, rigid aromatic and alicyclic moieties arised from two popular monomers are also present into the structures obtained. Thus, epoxide-functionalized polyethylene oxide (EFPEG) and/or diglycidyl ether of bisphenol A (DGEBA) are cured by amine-functionalized polyethylene oxide (AFPEG) and/or isophorone diamine (IPDA) in various proportions while keeping the stoichiometry of the epoxy/amino hydrogen groups constant (table 1). The samples were characterized by the FTIR spectral analysis and thermal behaviour of the cured samples was evaluated with thermogravimetric analysis (TGA).

Table 1. cods and molar ratios of the networks obtained**.**

Cods	Samples			
	DGEBA	EFPEG	AFPEG	IPDA
1	0.5	0.5	0.5	0.5
2	1.0	0.0	0.5	0.0
3	0.0	1	0.0	0.5

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Preparation nanocellulose based composite as a flowable dental composite

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Keywords: Nanocellulose, Flowable dental composites, Compressive strength, Dental materials

Dental composite resins due to their aesthetic properties are replacing with amalgam, that operate as same as natural tooth but dental composites are prematurely fracturing when placed in stressful areas and this leads to their short longevity. [1,2] When a little amount of herbal fibers incorporated in the composites lead to increase in their physical and mechanical properties.[3] Cellulose has known as one of herbal fibers that we can used in composites for reinforcement. In this report, we have prepared nanocellulose by treating microcrystalline cellulose with sulfuric acid and added to flowable composite for evaluating its compressive strength by ISO 4049 six experimental groups included. Five resin composites containing nanocellulose at different concentrations of 1, 2, 3, 4 and 5 wt% and a control group without any additive have been prepared. The results shown that adding 2% of nanocellulose in flowable dental composites can be increased compressive strength about 74%.

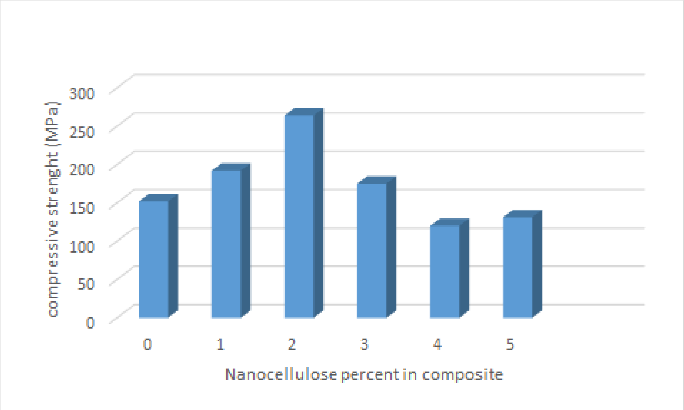

Fig.1 Investigation of nanocellulose concentrations on compressive strength of flowable dental composites

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Fabrication of co-delivery systems based on graphene-g-cyclodextrin/ chitosan nanofiber

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Keywords: Nanofiber, Graphene oxide, Chitosan, Curcumin and Gallic acid

Nowadays, co-loading of therapeutic drugs into one drug delivery system has revolutionized in the medical field to improve the therapeutic activity.[1-3] Combination therapy provides an effective strategy to achieve high therapeutic concentration compared with single drug therapy, In this regard, polymer nanocarriers with core–shell nanostructures are the most prevalent carrier in these applications.[4] Here, we designed co-loaded delivery systems, composed of curcumin loaded cyclodextrin-graphene oxide core (Cur@CD-GO) and gallic acid loaded chitosan shell (Ga@Cs) nanofibers (Cur-Ga NF), which can promote the therapeutic efficiency of drugs. The synthesized nanofibres were fabricated by electrospinning technique with the coaxial system. It was demonstrated that the nanofibers were successfully prepared, and the drugs in the core and shell of nanofibers were released in a controlled and sustained manner. MTT assay, antibacterial activity, antioxidant activity, and the anti-inflammatory assay were used for evaluation the performance of nanofibers. The produced Cur-Ga NF, providing improved anti-cancer activity, antimicrobial activity, antioxidant activity and anti-inflammatory outcome as compared to single drug-loaded NFs (Cur@CD-GO NF). Our investigations showed that such co-delivery fiber systems could be employed as a promising nanocarrier for therapeutic applications.

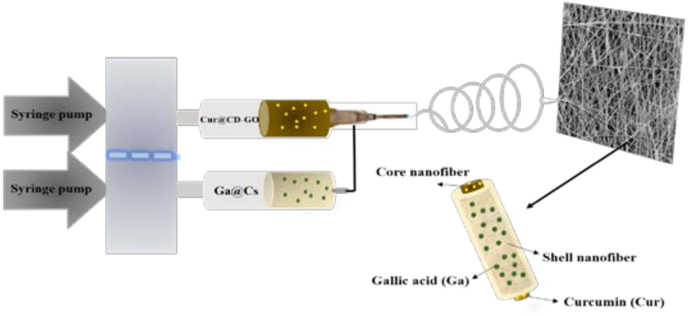

Fig. 1 Electrospinning setup of the fabrication of Core-Shell nanofiber.

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Curing of epoxy resin cross-linked in the presence of two different diamine hardeners

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Keywords: Epoxy thermosets, diglycidyl ether of bisphenol A, Isophorone diamine, polyetheramine.

Epoxy resins have been widely used for coatings, electronic materials, adhesives, and matrices for many composites because of their outstanding mechanical properties, high adhesion strength, good heat resistance, and high electrical resistance. The final properties of cured epoxy resins are affected by the type of epoxy resin, curing agent, and curing process.[1,2] Moreover, the choice of a hardener depends on the required performance of the thermosets or on the type of processing tool used to make pieces like thermosets composite parts.[3,4] In this work, an epoxy resin diglycidyl ether of bisphenol A (DGEBA) is cross-linked with the help of alicyclic amine isophorone diamine (IPDA) and polyetheramine by different reactivities (Fig. 1). The ratio of the two amines is varied while keeping the stoichiometry of the epoxy/amino hydrogen groups constant. The epoxy-amine systems were characterized by the FTIR spectral analysis and thermal behaviour of the cured samples was evaluated with thermogravimetric analysis (TGA).

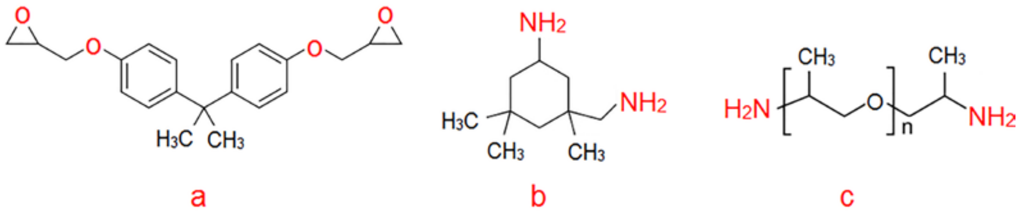

Fig. 1 Structures of DGEBA (a), IPDA (b) and polyetheramine (c).

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A new liquid immobilized on nanoporous SiO_2 as an efficient and reusable catalyst for the synthesis of pyrano[3,2-*d*]pyrimidine derivatives

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Keywords: Nanoporous SiO_2, Ionic liquid, Pyrano [d-3,2]pyrimidine, (Thio) Barbituric acid.

Pyrano [d-3,2]pyrimidine is one of the most important classes of (thio)barbituric acid derivatives that show considerable pharmaceutical activities, including antitumor, antibacterial, antiallergic, liver protector and blood pressure reduction properties. [1, 2] The most simple and straightforward protocols for the preparation of pyrano[2,3-*d*]pyrimidinones is based on three-component reactions of substituted aldehydes, malononitrile, and (thio) barbituric acid. Various conditions for these reactions have been reported.[3] Although these procedures are better than other methods, they have disadvantages such as long reaction times, harsh reaction conditions, the need for excess amounts of reagents, the use of organic solvents and toxic reagents, and non-recoverability of the catalyst. The development of simple, efficient, and mild procedures using easily separable and reusable solid catalysts to overcome these problems is therefore needed.

In this work, a green and efficient procedure is reported for the preparation of pyrano[d-3,2]pyrimidine derivatives using nanoporous SiO_2 containing an ionic liquid. The procedure gave the products in excellent yields in very short reaction times. The reusability of the catalyst is the other important feature of the reported method (Fig. 1).

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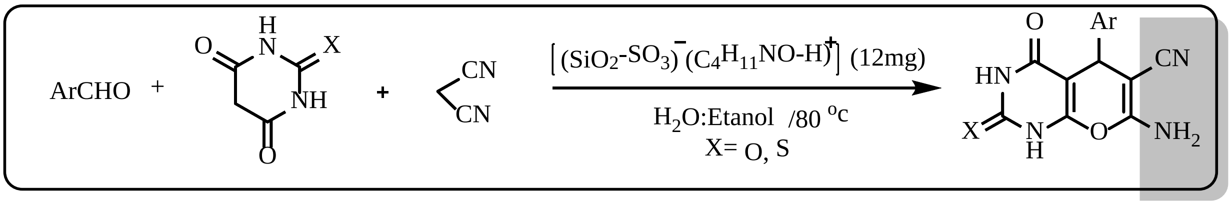

Fig. 1 Synthesis of Pyrano [d-3,2]pyrimidine (thio) barbituric acid derivatives catalyzed by $(SiO_2\text{-}SO_3)^-$ $(C_4H_{11}NO\text{-}H)$.

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Anchoring of nickel (II) 4-pyrone Schiff-base complex in functionalized nano-silica MCM-41 matrix: A highly effective novel heterogeneous catalyst for the catalytic clean synthesis of dihydropyrano[3,2-*b*]chromenediones

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Keywords: Silica-MCM-41-4-pyrone-Ni, Nanocatalyst, Three-component condensation reaction, Dihydropyrano[3,2-*b*]chromene-4,9-diones

The discovery of nanoporous silica-MCM-41 ordered molecular sieves has introduced it as an ideal heterogeneous catalyst support, in inclusion compounds as host materials, and separation media which has been reported in various synthetic routes.[1, 2] The multi-component (three reactants or more) reactions (MCRs) have been developed in organic chemistry and modern drug discovery owing to the generation of biologically active products e.g. chromenes.[3] Accordingly, the providing of an eco-friendly, simple, efficient, clean, convenient, and excellent yielding synthetic procedure of chromene derivatives utilizing an environmentally and recyclable novel catalyst is desired. Thus, the Ni complex on 4-pyrone-functionalized MCM-41 nanostructures has been immobilized and utilized as a promising nano-catalyst for the clean production of dihydropyrano[3,2-*b*]chromene derivatives using the 3-CR of KA, dimedone, and aromatic aldehydes in an efficient solventless and green procedure. Nano-silica-MCM-41-4-pyrone-Ni was prepared by the post-grafting method and characterized using XRD, ICP, EDX, BET, FT-IR, TGA, SEM, and TEM analyses.

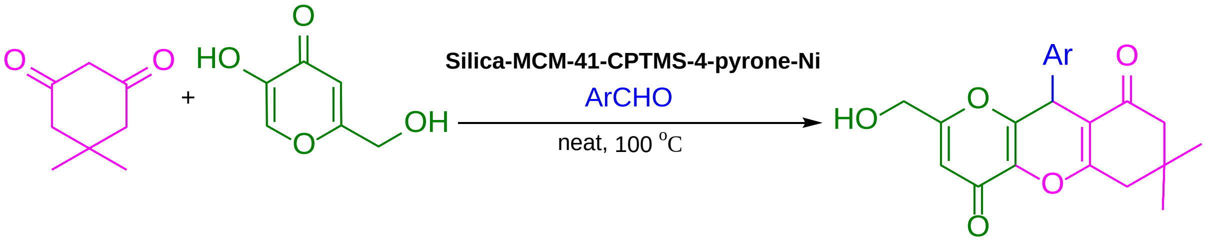

Fig. 1 MCM-41-4-pyrone-Ni-catalyzed the clean production of dihydropyrano[3,2-*b*]chromenediones

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Modification of Chitosan with Enrofloxacin

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Keywords: Enrofloxacin, Chitosan, Drug delivery.

Enrofloxacin (EF) is a fluoroquinolone antibiotic used in veterinary against both Gram negative and positive bacteria. It is generally administered at high concentrations which can cause molecular stacking and crystal formation affecting many organs with undesirable side effects. Recently, loading of biologically active compounds on biocompatible polymers has attracted great deals of attention to increase their efficiency in low loading. In continues of our interest in deposition of drugs on polymers,[1-3] herein enrofloxacin anchored to chitosan to obtain new polymer supported enrofloxacin for biological applications. The reaction was carried out via amidation reaction between amine groups of chitosan and carboxylic acid group of enrofloxacin. The new compound was characterized with common instruments such as FT-IR, elemental analysis, and energy dispersive spectroscopy.

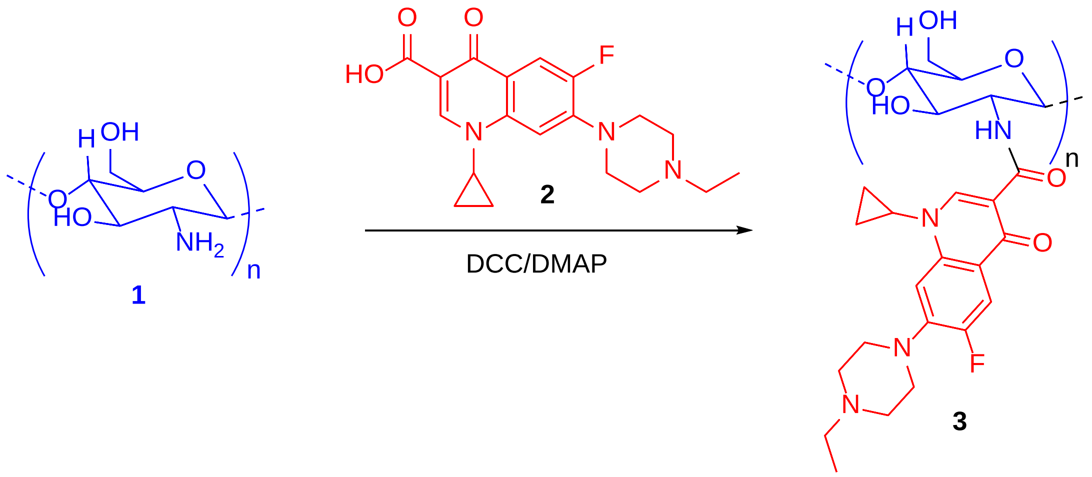

Fig. 1 Modification of chitosan with enrofloxacin

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Study of reactive Yellow 145 removal by Ag/GO nanocomposite using response surface methodology

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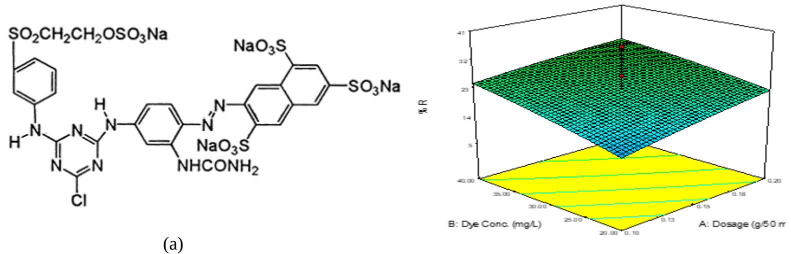
Azo dyes are organic compounds bearing the functional group R−N=N−R′, in which R and R′ are usually aryl. They are a commercially important family of azo compounds, i.e. compounds containing the linkage C-N=N-C. Azo dyes are widely used to treat textiles, leather articles, and some foods. Chemically related to azo dyes are azo pigments, which are insoluble in water and other solvents. Azo dyes should be removed from water resources since they are highly resistant under aerobic conditions and their anaerobic reduction gives aromatic amines, which are intrinsically carcinogenic and mutagenic.[1] Azo dyes are highly carcinogenic, mutagenic and resistance against biodegradation.[2] Therefore, they must be to remove from water and wastewater. Different physical and chemical processes have been employed to remove of azo dyes.[3-4] Adsorption is a efficiency method to removal of pollutants. In recent years, interest in composite based on graphene oxide (GO) with silver species has increased. Response surface methodology (RSM) is a useful technique for evaluation of several input variables that affect the efficiency or the qualitative properties of interest. Also, this method is a beneficial tool for optimization studies.[5] RSM proposes a second- or higher-order function to relate the response to the experimental parameters. This study aims to investigate removal of the Reactive Yellow 145 azo (RY 145) dye by the Ag NPs /GO nanocomposite and evaluate the effect of pH, RY 145 concentration, contact time and catalyst dosage on RY 145 removal. Structure of RY 145 is shown in Fig. 1. Performance of the process is predicted and optimized using a second-order equation by RSM.



(a)

(b)

Fig. 1 Structure of RY145 dye (a) and Effect of initial dye concentration and catalyst dosage (b)

As shown, RY145 removal was increased by increasing the dosage of catalyst. Increasing the dosage of the catalyst increases the active surface area and enhancement of RY145 adsorption. consequently, removal of a of RY 145 was increased.

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A New Hybrid Self-healing System for Industrial Coatings

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Keywords: Self-healing, Anticorrosion coating, Aqueous environment, Organosilane

Polymeric coatings are used to protect metal surfaces against corrosive materials. However, over time or with damage occurring in the coating or creation of micro-cracks, the metal is exposed to air or corrosive environments [1]. Self-healing coatings as a new generation of intelligent coatings are introduced to solve this problem [2]. Mixing of capsules containing self-healing agent with the polymeric coating is a common mechanism in order to prepare self-healing coatings [3]. When cracks are created in a coating, these capsules break down and release the healing agent at the site of the crack. The healing agent forms a protective layer and corrosion resistant is improved [4]. In the current study, self-healing organic coatings containing capsules with water reactive organo-silane compounds was used. In fact, when the damage occurs, the self-healing agent reacts with water or moisture and creates a protective hydrophobic layer that protects the metal against further corrosion attacks. The performance of fabricated coatings was investigated by EIS, FESEM, XRD and adhesion tests.

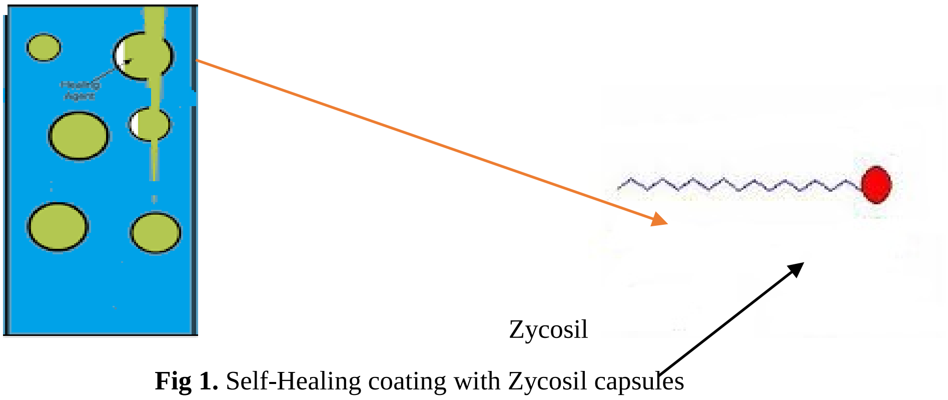

Fig 1. Self-Healing coating with Zycosil capsules

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A Convenient Synthesis of Spiroindolo[2,1-*b*]quinazoline-6,2′-[1,3,4]oxadiazoles from Tryptanthrin and Nitrile Imines

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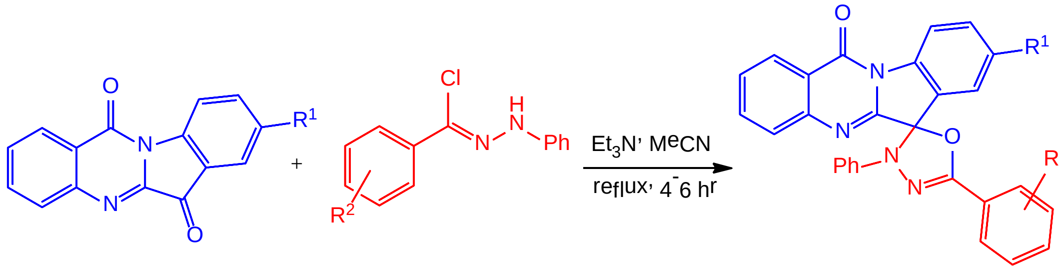
Keywords: Spirocompound, 1,3-Dipolar cycloaddition, Tryptanthrin, 1,3,4-Oxadiazole.

Development of heterocyclic synthesis has always been an important area in synthetic organic chemistry. Spiro heterocycles are regarded as a privileged framework because of their rigidity, three-dimensional geometries, and wide distribution in various natural products and synthetic molecules. Currently, these spirans are attracting considerable interest in organic chemistry because of their molecular structure and diverse biological activities.[1] In particular, spiroindoles represent important structural motifs that can be found in many biologically active synthetic compounds and natural products.[2,3] Herein, we report the synthesis of new 5′-aryl-3′-phenyl-3′*H*,12*H*-spiro[indolo[2,1-*b*]quinazoline-6,2′-[1,3,4]oxadiazol]-12-ones **3** from the reaction between tryptanthrins **1** and hydrazonoyl chlorides **2** in MeCN at 80 °C in the presence of Et_3N (Figure 1).[4] All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^1H and ^{13}C NMR and IR spectroscopic data.



1 2 3

Fig. 1 A Convenient Synthesis of Spiroindolo[2,1-*b*]quinazoline-6,2′-[1,3,4]oxadiazoles

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Theoretical studies on the molecular switch of ortho-triphenyl

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Keywords: π-Conjugated, *O*-Terphenyl, Triphenylene, Photosensitive, 1,4-Dihydrotriphenylene.

In research electron-transport properties of o-terphenyl and products of its electrocyclization reaction is investigated with the nonequilibrium Green function combined with density functional theory. o-terphenyl is a photosensitive π-conjugated molecule, whose electronic and geometric structures can be changed upon photoirradiation. By photoexcitation, o-terphenyl give triphenylene through transient intermediate, 1,4-dihydrotriphenylene. The two isomers of this photocyclization reaction differ in their geometrical and electrical structures. The steric hindrance between hydrogen atoms prevents the o-terphenyl from assuming a planar structure. As a result, in the open-ring isomer, the π-electrons are localized in the two aryl groups and π-conjugation is decreased. Geometry optimizations of these molecules have been performed with the Gaussian 09 program at the hybrid density functional B_3LYP level of theory combined with the 6-31G(d,p) basis set. We performed electron-transport calculations with the ATK 13.8.1 program.

By conducting recent experiments on molecular wires, where a molecule is placed between two electrodes and passes through the electric current, such as the conductivity of some of the alkanes that can act as a wiper, is very much taken into consideration. This important feature of molecules can occur in response to a change in applied voltage difference. [1-3]

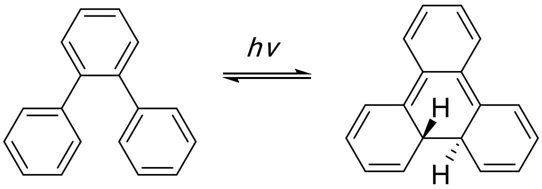

Fig. 1 The image of the molecule of the ortho-triphenyl switch that turns into light in the form of a packet.[4]

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Efficient synthesis of α-aminonitriles using ultrasonic irradiation

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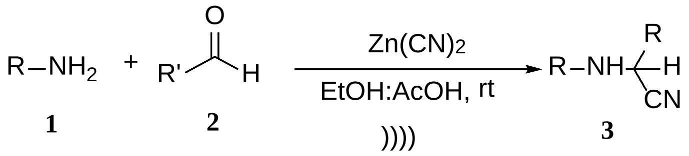
Keywords: Strecker reaction, Amine, Aldehyde, $Zn(CN)_2$, Ultrasouics

Strecker reaction[1], the oldest known synthesis of α-aminonitriles, is one of the most general methods potentially useful for synthesis of aminoacids and other bioactive compounds including natural products. α-aminonitriles constitute a major class of naturally occurring compounds of great interest displaying remarkable biological activities.[2] In recent years, several modifications have been reported using a variety of cyanating agents such as HCN, KCN, TMSCN, Bu_3SnCN, MeCOCN.[3] Herein, we report the synthesis of α-aminonitriles **3** from the reaction between amine **1** and aldehyde **2** in the presence of zinc cyanide by ultrasouics irradiation. This new methodology provides good to excellent yields in short reaction times (15-20 min) at room temperature. All the new synthesized compounds are stable solids whose structures were determined on the basis of their IR, ^{1}H-NMR and ^{13}C-NMR spectroscopy data.



R = 4-Me-C6H4NH2   R'= 4-OMe-C6H4   Yeild 85%

Fig. 1 Synthesis of α-aminonitriles

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Iron(III) decorated magnetic Fe_3O_4/chitosan-dithiocarbamate for aqueous oxidation of benzylic alcohols at room temperature

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Keywords: Magnetic Fe_3O_4/chitosan-dithiocarbamate, Aqueous oxidation, Benzylic alcohols.

Heterogeneous catalysts play an important role in the field of organic transformations [1]. On the other hand, since catalysts are one of the key components "green chemistry", the design and use of environmentally benign catalysts is one of the urgent challenges for chemists [2]. Fe_3O_4 nanoparticles have been extensively studied because of structural and functional elements have various novel applications [3]. In this work, Fe(III) were complexed by a modified Fe_3O_4-CSDTC composite as a stable catalyst **Figure 1**. Separable Fe_3O_4-CSDTC/Fe^{+3} demonstrated excellent performance with high yields for various benzylic alcohols in the presence of H_2O_2 at ambient temperature, so that Fe_3O_4-CSDTC was recovered and reused several times without significant decrease in activity.

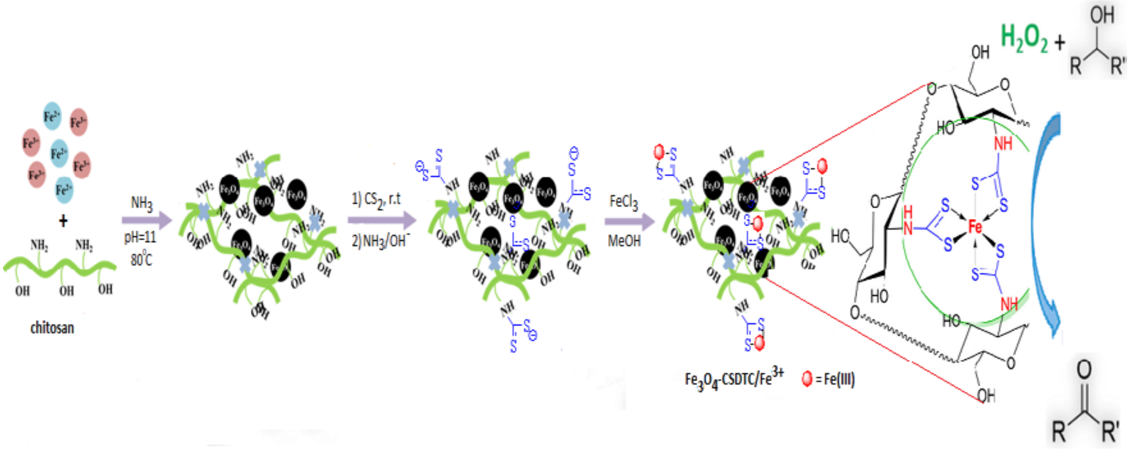

Fig 1. Preparation of Fe_3O_4-CSDTC/Fe^{3+} for the aqueous oxidation of benzylic alcohols.

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Docking the newly designed anti cancer molecules and studying their effect on Hypoxia –inducible factor-1 (HIF-1) compared to the LW6 molecule.

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Keywords: HIF-1, Molecular docking, LW6, Anticancer drug.

Molecular docking is a superb established computational technique that often used to predict the binding orientation of small molecule drug candidates to their protein targets in order to forecast the affinity and activity of the small molecule [1]. Hypoxia –inducible factor-1 (HIF-1) is a pivotal transcriptions factor, which strongly correlated with angiogenesis, tumor survival, metastasis, and cell proliferation. Docking results are as follows:

1- Adamantyl group is essential for inhibition. Molecules without adamantyl group have much less inhibitory effect. 2- O, N, amide groups that are located in a particular position of this molecule are at their best position. 3- The length of the molecule, if less or more than this amount will greatly reduce the inhibitory effect. 4- The effect of indene's group is high for inhibitor [2].

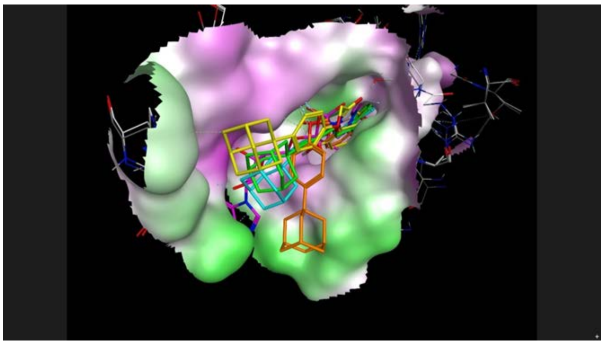

Fig 1. Schamatic of HIF-1 inhibtor.

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Study of synthesis of a novel series of inden pyrazole derivatives that possess anti cancer potential

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Keywords: HIF-1, LW6, Anti cancer, Adamantly.

Hypoxia inducible factor-1 (HIF-1) is a pivotal transcriptions factor, which strongly correlated with angiogenesis, tumor survival, metastasis, and cell proliferation.

In this work, we demonstrate novel series of multi functional chemical probes inclusive principal groups including, adamantly, inden at various locations of the parent compound LW6 and its relation to hypoxia inducible factor -1a (HIF-1) and malate dehydrogenase 2 MDH_2 [1]. Structure activity relationships showed that the adamantyl group was essential in maintaining activity as an HIF-1 inhibitor. The effect of indene's group is important for inhibitor [2].

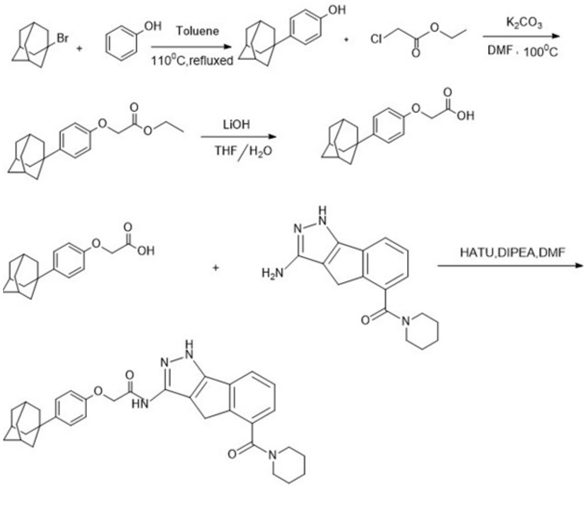

Fig 1. Synthesis of HIF-1 inhibitor.

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Pd-Biurea/MCM-41: As an efficient and recyclable nanocatalyst for one-pot three-component synthesis of dihydropyrano[3,2-*c*]chromene derivatives

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Keywords: Heterogeneous nanocatalyst, Multicomponent reactions, 4-hydroxycoumarin, Dihydropyrano[3,2-c]chromenes, MCM-41.

One-pot multicomponent reactions (MCRs) have proved to be very powerful and efficient bond-forming tools in organic and medicinal chemistry in the context of green chemistry.[1] Dihydropyrano[3,2-c]chromenes and their derivatives which have received significant attention due to their important biological and pharmacological properties, have been synthesized using the MCR system.[2] Along with other reaction parameters, the nature of the catalyst plays a significant role in determining yield and general applicability. In literature, various catalysts are used for the one-pot synthesis of chromene derivatives. In continuation of our previous work,[3] we report herein the application of Pd-Biurea/MCM-41**4** as a heterogeneous and easy recoverable catalyst in the eco-friendly synthesis of dihydropyrano[3,2-c]chromenes derivatives **5** via a one-pot three-component condensation of aromatic aldehydes **1** with malononitrile **2** and 4-hydroxycoumarin **3** in excellent yields. The synthesized derivatives were also characterized by melting points, FT-IR,^{1}H-NMR, ^{13}C-NMR, and this nanocatalyst was characterized using FT-IR, TEM, and BET techniques.

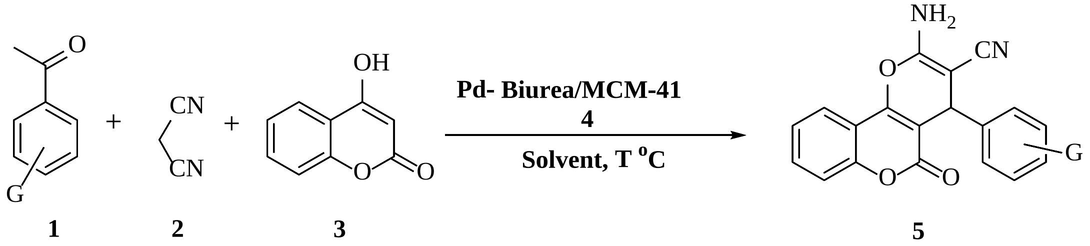

Fig 1. Synthesis of dihydropyrano[3,2-c]chromene using Pd-Biurea/MCM-41as recoverable nanocatalyst

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Synthesis of polyoxyethylene-crosslinked polystyrene network for preparation organic support via ATRP technique

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Keywords: solid-phase organic chemistry, polystyrene networks, polyoxyethylene units, surface-initiated ATRP technique.

Solid-phase organic synthesis (SPOS) continues to beimportant in the development of libraries of new molecules [1]. Microporous PS-DVB, with its high thermal stability, chemical inertness, and mechanical robustness, is an attractive support for solid-phase synthesis[2]. A drawback of the grafting approach, however, is that it reduces the functional group-to-mass ratio (polymer loading) by decreasing the number of free chloromethyl groups while increasing the resin mass. Replacing DVB with R,ω-bisfunctionalized PEG as the cross-linking agent represents a particularly intriguing approach as the propertiesof polymer networks are significantly influenced by thenature of the network junctions [3].

In the present study, a surface-initiated ATRP technique was used for the polyaddition of styrene monomer in the presence of a polyethylene glycol (PEG)-derived comonomer/crosslinker (α,ω-bis-4-(vinylbenzyl)ether of polyoxyethylene, denoted with STP) and the nanoparticles with anchored BnCl as the reaction initiator (Figure 1). The thermal behaviors of CPS and CPS/SNP's networks were thoroughly investigated by thermogravimetric analysis (TGA) and differential thermal analysis (DTA).

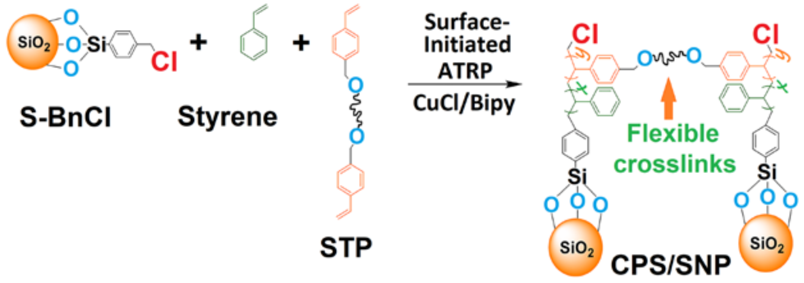

Fig 1. Synthesis of polystyrene-silica networks having polyoxyethylene crosslinks.

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Synthesis and Thermal Characterization of Polyurethane/Clay Nanocomposites Based on PTMO

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Keywords: polymer-clay nanocomposite, Montmorillonite, polyurethane, Organoclay.

Polyurethane (PU) is used for a variety of applications, from foams to elastomers and films, whose properties depend on the type and functionality of the polyols and isocyanates [1]. Polyurethanes have desirable properties such as high abrasion resistance, tear strength, shock absorption, flexibility and elasticity. Although they have relatively poor thermal stability, this can be improved by using treated clay [2]. Clays have also been used to improve properties of elastomeric and rigid PUs. polymer/clay nanocomposites have drawn considerable interest because of their enhanced properties, including flame resistance, mechanical properties, gas barrier properties, thermal stability and biodegradability, when compared to pristine polymers [3]. In this study, the synthesis and characterization of poly(tetramethylene oxide) (PTMO)-based segmented polyurethane using 4,4'-methylenediphenyl diisocyanate (MDI) and 1,4-buthylene glycol (1,4-BG) chain extender (Figure 1). Then the organically modified montmorillonite by the tetradecyltrimethylammonium bromide (TTAB-MMT) with the amount of 2.5 and 5 w% into the polyurethane matrix was dispersed in polymeric. the resulting nanocomposites are also investigated by TG/DTG and XRD measurements.

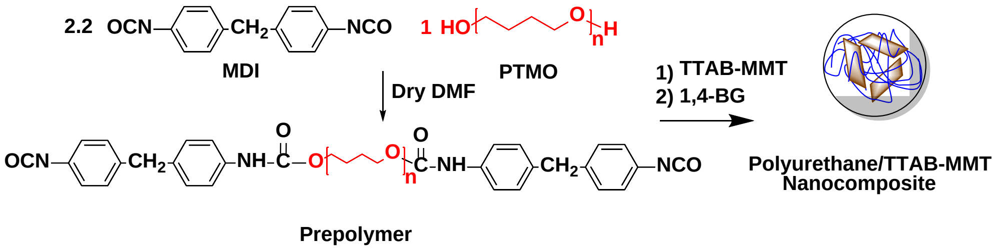

Fig 1. Two-step synthesis of segmented polyurethane/TTAB-MMT nanocomposites.

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Copper-phophine catalysted arylation of aromatic aldehydes

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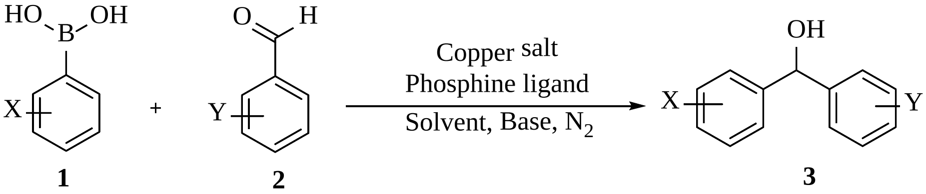
Keyword: Phosphine ligand, Aldehyde, Arylation, Copper salt, Homogenous catalysts.

Alcohols are very important compounds in the synthesis of drugs, chemicals, flavors and materials used in the agricultural industry.[1] They also play as intermediary compounds.[2] There are numerous ways for the preparation of secondary alcohols **3** that among them, reduction of diaryl-ketone or addition of organic-metallic reagents to carbonyl-containing compounds are the most important reactions of C-C bond formation in organic syntheses.[3] The use of boron reagents **2** as a source of aryl through the exchange of the aryl group between boron and metal is one of the most commonly used methods for aldehyde arylation.

In this research, we have investigated the arylation of aromatic aldehydes **1** using high economical, available, active and selective homogeneous catalytic system with copper salts and phosphorus ligands (Scheme 1).

The structure of the prepared products was characterized by melting point and spectral analysis techniques IR, ^{1}HNMR, ^{13}CNMR.



Scheme. 1 Copper-phophine catalysted arylation of aromatic aldehydes

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Synthesis of amidoalkyl napthols derivatives in the presence of nano-catalyst KCC-1/SA

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Keywords: Green chemistry, Nano-catalyst, Solid acid, Amidoalkyl napthols, Multicomponent reactions.

The use of nanomaterials as heterogeneous catalysts has attracted a lot of attention due to its economic, environmental, structural features and high levels of catalytic activity.[1-3] Solid acid catalysts play a prominent role in organic synthesis under heterogeneous conditions.[4] Herein, we report the synthesis of amidoalkyl napthols **(4)** from the reaction between B-naphthol **(1)**, aromatic aldehyde **(2)** and acetamide **(3)** in the presence of KCC-1/SA in solvent-free conditions (Fig.1). The KCC-1/SA NPs were thoroughly characterized by using SEM and FT-IR. The results showed that the catalyst has a high activity, is environmentally friendly, heterogeneous and easy to recover from the reaction mixture without losing its catalytic activity.

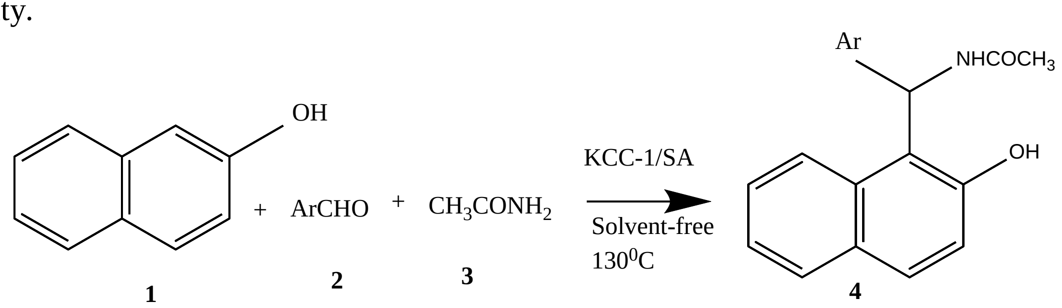

Fig. 1 KCC-1/SA Catalyzed synthesis of amidoalkyl napthols.

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Synthesis of 3,4-dihydropyrimidine-2(1*H*)-one derivatives in the presence of nano-catalyst $Fe_3O_4/SiO_2/SO_3H$

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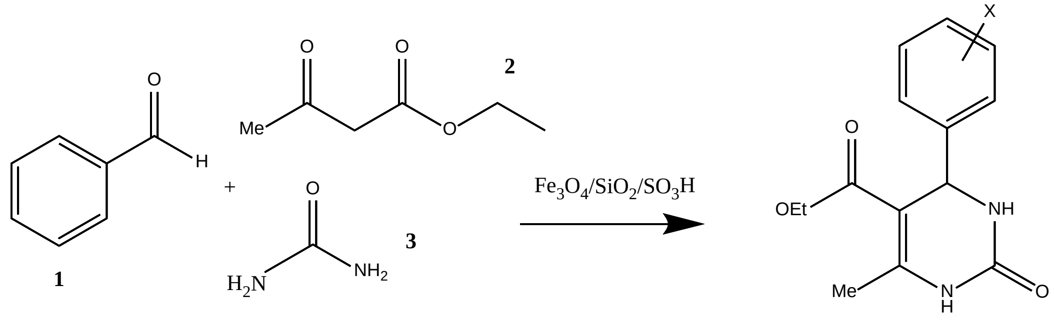
Keywords: Multicomponent reactions, Green chemistry, Nano-catalyst, Solid acid, $Fe_3O_4/SiO_2/SO_3H$.

The heterogeneous acid catalysts were introduced owing to their unique properties such as ease of separation and recovery, low toxicity and non-corrosive nature from the viewpoint of green chemistry.[1] The use of recyclable solid acids in organic reactions is often considered to follow the principles of green chemistry since these catalyzed processes consume less energy and reagents, and minimize waste.[2,3] Moreover nanostructured solid acids exhibit higher activity and selectivity than their corresponding bulk materials.[4] Herein, we report the synthesis 3,4-dihydropyrimidine-2(*1H*)-ones (**4**) from the reaction between aromatic aldehyde (**١**) Ethyl acetoacetate (**2**) and Urea (**3**) in the presence of nano-catalyst $Fe_3O_4/SiO_2/SO_3H$ NPs (Fig.1). The $Fe_3O_4/SiO_2/SO_3$ NPs were thoroughly characterized by using SEM and FT-IR. The results showed that the catalyst has a high activity, is environmentally friendly, heterogeneous and easy to recover from the reaction mixture without losing its catalytic activity.



X=4-Cl, 4-Me, 4-MeO

4

Fig. 1 Multicomponent synthesis of 3,4-dihydropyrimidine-2(*1H*)-one.

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Synthesis and characterization of magnetic graphene oxide as a solid support for metal nanoparticles

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Keywords: Graphene oxide, Magnetic, Solid support, Metal nanoparticles

Graphene oxide, a derivative of graphene, due to many exceptional properties such as large specific surface area, chemical stability and numerous functional groups on its surface has become a hot topic in recent years.[1] It has been remarkable option as noted candidates for supported of metal nanoparticles such as TiO_2,[2] Pd,[3] Ag,[4] and Pt.[5] Magnetic Fe_3O_4 has been widely investigated for several applications such as drug delivery,[6] biosensors,[7] and bioseparation.[8] Recently, the combination of magnetic Fe_3O_4 with other material has gained considerable attention in separation science. In this study, we report the preparation of magnetic graphene oxide supported metal nanoparticles with relatively high yield and characterization is undertaken by various selected techniques, including SEM, EDX, TGA, XRD and FT-IR.

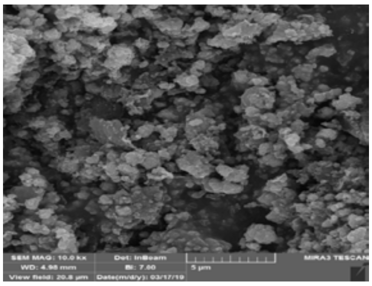

Fig. 1 SEM image of magnetic graphene oxide

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Effective removal of cationic methylene blue and crystal violet dyes on a novel magnetic Fucus vesiculosus (brown algae)

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Keywords: Magnetic; Fucus vesiculosus; Adsorption; Cationic dyes.

In this project, a new magnetic Fucus vesiculosus (m-FV) nanoparticle with a high adsorption capacity of cationic dyes was prepared. To achieve a high effective nanocomposite, Fucus vesiculosus (FV) modified using ultrasound and then, the magnetic property induced via *in situ* co-precipitation of iron ions in the presence of FV[1]. The produced m-FV examined to remove cationic methylene blue (MB) and crystal violet (CV) dyes from aqueous solutions. The effect of contact time revealed a fast removing of MB and CV, reaching equilibrium at 10 and 5 minutes, respectively. Adsorption process Kinetics modeled and the results presented the best fit of experimental data for pseudo-second-order (PSO) than that of pseudo-first-order (PFO) kinetic model in MB and CV adsorption processes[2]. Analyzing equilibrium isotherm data carried out using Langmuir and Freundlich models and the results revealed a better fitting to the Langmuir model for MB and CV adsorption processes. According to the Langmuir model, the maximum adsorption capacity of m-FV obtained 577 and 1062 $mg.g^{-1}$ for MB and CV, respectively[3]. Easy recovery, good recyclability, pH and temperature-independent properties of m-FV nanoparticles, moreover than high adsorption capacity, could be employed as an effective and low-cost adsorbent in the removal of dye pollutions[4]**.**

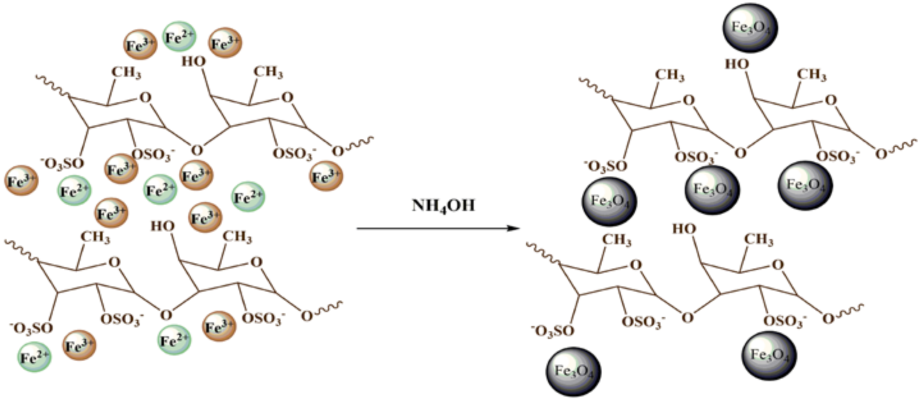

Fig. 1 A simple scheme showing the used steps for preparing magnetic FV nanoparticles.

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Computational Fluid Dynamics Modeling of Single-Phase Seawater Flow Inside a Reverse Osmosis Process Spiral Module

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Keywords: Reverse Osmosis, Spiral Wound, Membrane, Single-Phase Modeling, Concentration Polarization, Permeation Flux, Shear Rate.

In this study, computational fluid dynamics modeling of the single-phase in the spiral wound membrane is presented for water desalination through the reverse osmosis (RO) process. single-phase Level Set method using the last version of CFD package, COMSOL Multiphysics 5.3 was employed to understand, qualitatively and quantitatively, the details of fluid flow and mass transfer. The 2D model proposed, considers hydrodynamic and convection-diffusion equations.

Finally, the impacts of some effective operating variables such as feed concentration, feed velocity, trans-membrane pressure, water permeation flux, shear rate and osmotic pressure on the walls as well as outlet salt concentration.

Results show that in the laminar single-phase flow, concentration polarization the whole spacer micro-channel including near the membrane wall and nodes, Flux reduction and Increased osmotic pressure and Reduced membrane efficiency.

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Removel of cationic dyes from water by solvent extraction using amphiphilic polyurethane reverse micelles

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Keywords: Amphiphilic polyurethane, Reverse micelle, Liquid/liquid extraction, Removel of dyes.

Several methods (e.g., adsorption, UV/H_2O oxidation, precipitation) are normally employed to remove organic dyes and purify water.[1] Recently liquid/liquid extraction technique using reverse micelle approach were gained more attention.[2] The reverse micelles are nanometer-sized aggregates of amphiphilic molecules in nonpolar solvent. In this approach, to investigate removing organic dyes from water using a novel amphiphilic polyurethane reverse micelles(APU), experiments were conducted by mixing a know quanity of dye in aqueous phase and solvent-containing APU in a vial. The dye is solubilized in the hydrophilic core of the reverse micelles, which are present in the organic solvent phase. While phase transferring and receding the dye in aqueous phase, the organic phase was colorized. The oil layer was separated for a UV-vis measurement. The removel of different cationic dyes (e.g., methylene blue, malachite green, Nile blue and Rhodamine B, fuchsin) , and the anionic dyes including methyl orange (MO), Congo red and methyl blue (MeB) were studied by conducting experiments. The obtained results demonstrated that the lowest encapsulation were for the anionic guests, while the cationic dyes due to the ionic interactions between the dye and the APU was successfully encapsulated and transferred to organic phase, Fig 1.

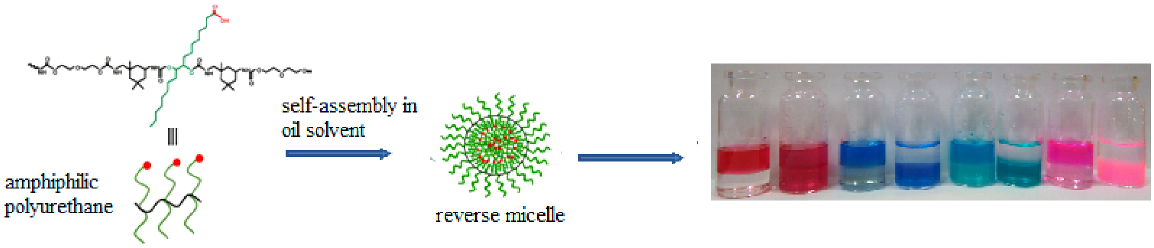

Fig. 1 Reverse miellization of APU and dyes transferred from the water phase into the $CHCl_3$ phase

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Modeling the Amount of Ferric Chloride in the Treatment Plant (Case Study: Lowshan Power Plant)

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Keywords: Water treatment, Ferric chloride, Modeling, GMDH –NN, Power plant.

The water in the nature is not applicable directly as feed water for boiler of the thermal power plant due to the precipitating of its insoluble materials on the thermal installations and it must be purified under physical and chemical treatment before use. One of the most important parts of the treatment process is consumption of the chemicals during the coagulation process. For this purpose, the modeling with GMDH neural networks was applied to predict the amount of ferric chloride used in the coagulation unit using the input-output data set collected from the Lowshan power plant during the six-month period from September 2018 to February 2019. The GMDH neural network was used to modeling, which is a self-organized and one-sided network consisting of several layers in which each layer includes several neurons, and all neurons have the same structure[1,2]. Experimental data sets were divided into two groups for modeling: 70% for network learning and 30% for model testing. After modeling, the model results were compared to experimental data (Fig. 1) and tested with the statistical parameter (the coefficient of determination) of $R^2 = 0.9989$, which the results show a good agreement with experimental results.

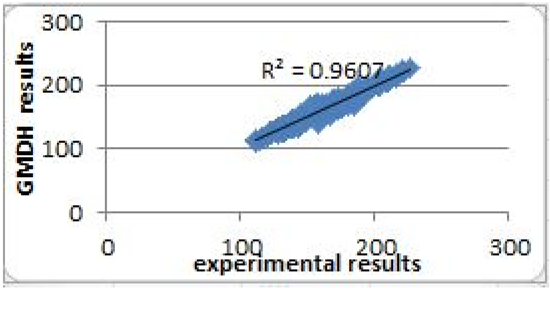

Fig. 1 Comparison the real results and modeled outputs in GMDH Modeling.

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Synthesis and valuation of novel nanohydrogel for the Dual-Drug Delivery of methotrexate and cisplatin

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Keywords: RAFT synthesis, Nanohydrogel, EDTA, Methotrexate, Cisplatin, Dual drug delivery.

Co-delivery of two drugs in one nanoparticle is increasingly used to overcome for example multi-drug resistance in cancer therapy and therefore suitable drug carriers need to be developed. In this work, using reversible addition–fragmentation chain transfer polymerization method a novel nanohydrogel based on poly (hydroxyl ethyl methacrylate), PEGDA and EDTA, was employed as a reactive scaffold for the attachment of methotrexate (MTX) and cisplatin prodrug. The synthesized structure was confirmed by Fourier-transform infrared spectroscopy and proton nuclear magnetic resonance methods. The pH responsive behavior of the synthesized particles was checked by size measurement in two different pH values (5.5 and 7.4) by dynamic light scattering and transmission electron microscopy. The release profiles of nanoparticles carrying drug molecules were checked in two different simulated pH of healthy organs (7.4) and tumor site (5.5). Despite lower release in pH of 7.4, an increased drug release was obtained in pH of 5.5. The *in vitro* toxicity assay was performed on SW 480 as a colorectal cancer cell line, which showed a time dependency cellular entrance, an enhanced cytotoxicity by the drugs loaded nanoparticles. The suitable size (<200nm), pH responsive behavior and anti-proliferative activity in cancer cells and hemocompatibility were the noticeable features of the developed dual drugs adsorbed nanoparticle, which introduced this formulation as an ideal vehicle in anti-cancer drug delivery.

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Water-based organic synthesis: Recent development of green organic reactions

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Keywords: Water-based organic synthesis, Multicomponent reactions, Surfactants, Ionic liquids carbohydrate catalysts

By progress of green chemistry, solvent-free and aqueous organic reactions have progressed as the sustainable transformations[1], while water is a unique, most abundant, and environmentally friendly solvent for *in-vitro* bio mimic and biochemical processes in cells[2]. However, the water-based organic reactions categorized to two fields of “in-water” and “on-water” reactions by Sharpless and co-workers concept[3], although most of these reactions are “on-water” transformations[4] that profits from hydrophobicity of organic materials on water. Anyway, “in-water” or “on-water”, organic reactions are more profitable by joining to multi-component reactions (MCRs)[5-7]. Due to the extra advantages, modern processes have turned to the collaboration of the synthetic methods with the beneficial MCRs in aqueous medium. To develop the water-based organic synthesis, we have recently developed new catalytic approach to promote of the water-based organic reactions using cationic/anionic/magnetic surfactants, carbohydrate catalysts, enzymes, and ionic liquids. Therefore, various types of in-water” and “on-water” organic reactions using green catalysts surfactants are reviewed in this work.

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Comparison of natural minerals for treatment of drug pollutant wastewaters by Heterogeneous Fenton process

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Keywords: Advanced Oxidation Process, heterogeneous Electro-Fenton, iron mineral clays, drug pollutants, wastewater treatment

The drug pollution combined with other environmental pollution agents resulted in the spread of pollution in a local to global scale.[1] Gemcitabine hydrochloride as a drug contaminant is an antitumor agent with LD_{50}=500 mg/kg. So, presence little amount of this drug in the water released from hospital effluents to the environment can cause serious and long lasting effects on humans and other creatures.[2] This research aimed to present a green, simple, cheap and also efficient method for degradation of drugs and wastewater treatment. Some iron minerals from the nature can be useful catalysts as a source of required iron for the Fenton reaction.[3] Production of H_2O_2 in situ play another main role to present a safe and cost effective treatment method.[4, 5] Herein, present study applied heterogeneous Electro-Fenton catalyzed by 5 iron minerals such as Limonite, Hematite, Magnetite, Siderite and Pyrite. In this study, the amount of TOC was investigated for five minerals at certain times. In addition, removal efficiency, reaction rate constants and amount of iron ions produced in the solutions were determined for all mineral catalysts. As a result, pyrite with the maximum amount of rate constant (k = 8 .0. 10^{-3} min^{-1}) and efficiency of degradation (75%) was the only mineral able to degrade Gemcitabine in aqueous solution considerably in the same condition. The major asset of this study is that using pyrite prevent solution increasing pH during the reaction and hence provide the best condition of acidic pH for Fenton reaction.

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Click Synthesis of Bis(1,2,3-triazole) Anchored Noroxymorphone

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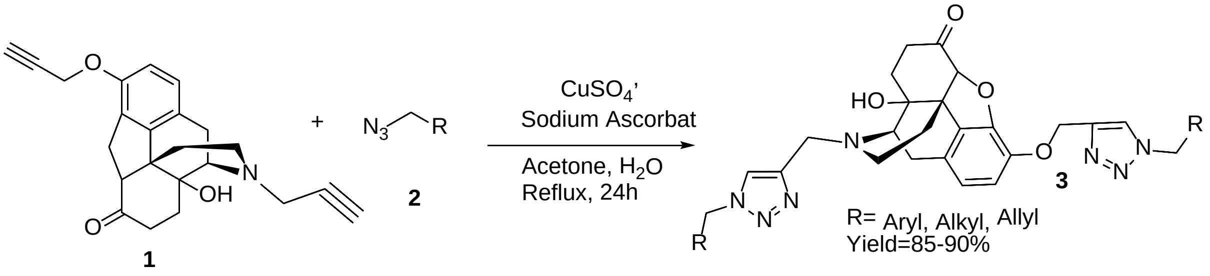
Keywords: Click Chemistry, CuAAC, Triazoles, Alkaloid Modification

Alkaloids are long known for their distinguished properties suitable for medical and pharmaceutical uses, inspiring impulse research interest in several scientific communities.[1] Triazoles are also proved to be highly valuable heterocyclic moieties exerting notable biological propertiers.[2]

Click chemistry is a term used for a group of reactions recognized to be fast and simple automated, and selective, while rendering high yielding transformations. Copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddition of azides and terminal alkynes (CuAAC) for acquisition of regioselective triazoles is the most conducted "click" reaction.[3]

Herein, click synthesis of bis(1,4-triazole) anchored noroxymorphone scaffold (**3**) is presented via a reaction of a bis-alkynyl noroxymorphone derivative (**1**) with azides (**2**). The reaction delivers high yields in presence of *in situ* produced Cu(I) catalyst under reflux conditions. The scope of the reaction is successfully extended to an array of aromatic, aliphatic, and allylic azide compounds.



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Study the reaction of β-enaminonitriles and perhalopyridines

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Keywords: Synthesis, β-Enaminonitriles, Perhalopyridines.

β-enaminonitriles or β- amino acrilonitriles serve as important building blocks in the synthesis of a wide variety of unique heterocyclic systems such as pharmaceuticals, fungicides, and solvatochromatic dyes.[1-3] Recently, a number of papers and patents concerning the importance of β-enaminonitriles in the synthesis of biologically active compounds, dihydropyridines analogous to nifedipine and amlodipine as potential calcium channel blockers in the treatment of angina and hypertension have been found.[4] They are generally prepared by base-catalyzed Thorpe reaction. Various bases such as sodium alkoxides, lithium ethyl anilide, and lithium diethyl amide are reported for the synthesis of b-enaminonitriles via coupling of aromatic/aliphatic nitriles with active methylenecarbonitriles.[5] perhalopyridines as Aromatic heterocycles are widespread and valuable synthetic templates for the preparation of new compounds with specific biological or material properties.[6] The structure of compounds were identified by IR, ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectroscopy.

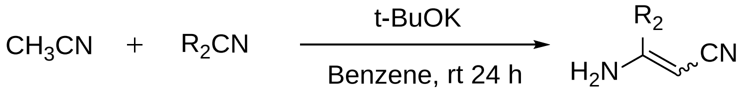

Fig. 1 Synthesis of β-enaminonitriles

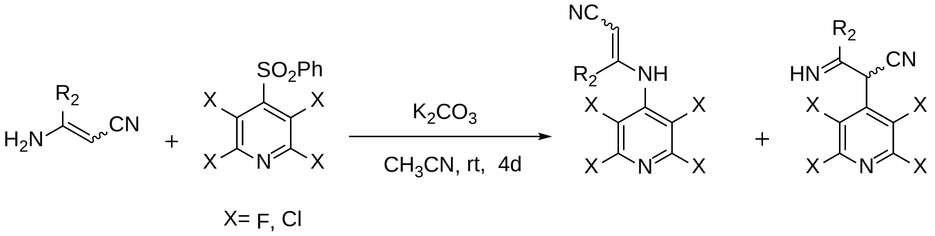

Fig. 2 Reaction of β-enaminonitriles and perhalopyridins

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Fabrication of magnetic nanocomposite based on ZrO_2 and investigation of structural properties

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Keywords: Nanocomposite; Hydrothermal; Structural; Magnetic**.**

Magnetic nanocomposites are multi-component materials, typically containing nanosized magnetic material to trigger the response to an external stimulus. Up to now, the search for novel nanocomposites has led to the combination of different materials with various types of magnetic particles. In this study, $CoFe_2O_4/ZrO_2$ nanocomposite was prepared by hydrothermal approach and then structural properties was investigated[1].

At the first, ZrO_2 nanoparticles, $Co^{2+}$and $Fe^{3+}$with a mole ratio of 1:2 were dissolved in distilled water. Then Ammonium hydroxide solution was added drop wise to resultant suspension to attain the pH=11 and stirred continuously for 1 h, followed by a hydrothermal treatment at 180◦C for 10h. The products were washed with deionized water and dried in oven at 60°C[2].The characterizations of the synthesized nanocomposite were carried using powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR).

The XRD and FTIR patterns of the nanocomposite are shown in Fig.1 and Fig.2, respectively.Fig.1 indicates the diffraction peaks situated at, 30.17, 28.175, 50.474, 45.85, 35.125 correspond to (111) , (101) , (110) ,(211) ,(202) planes of ZrO_2 and the peaks at 30.42◦, 35.925◦, 57.525◦and 62.875◦ correspond to (220), (311) ,(511) and (440) planes of $CoFe_2O_4$. [2,3]. From figure 2, peaks observed at 501 and 582 cm^{-1} are due to the Zr–O vibration mode and the absorption bands at 574.76 and 877.57 cm^{-1} are assigned to the stretching mode of Fe-O and Co-O bands[3].

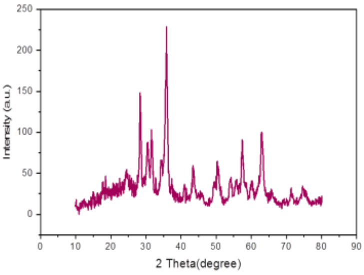

Fig. 1 XRD pattern

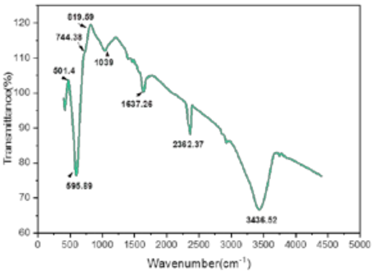

Fig. 2 FTIR pattern

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Synthesis and catalytic application of a novel phosphonium based ionic liquid for the preparation of pyridine derivatives

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Keywords: Phosphonium-based ionic liquids, Pyridine derivatives, Multicomponent reactions, Cooperative vinylogous anomeric based oxidation.

Phosphonium-based ionic liquids (PILs) represent varied merits such as more thermal and chemical stability, over other types of ionic liquids such as imidazolium and pyridinium-based ionic liquids. Therefore, PILs have varied applications in academic and industrial processes[1].

On the other hands, improvement of the reaction efficacy, atom and step economy, synthesis of complex molecules through a simple route, reduction of waste production and avoidance of utilization of hazardous organic solvents have become crucial issues for chemists. Multicomponent reaction strategy, can resolve these concerns[2].

One of the most important scaffolds of heterocyclic structures is pyridine systems. The versatile molecules can be found in several pharmaceutical active structures. It is reported that some pyridine derivatives applied as IKK-b inhibitors, A_{2A} adenosine receptor antagonists, inhibitor of HIV-1 integrase[3].

In this work, we reported the synthesis and catalytic application of a novel phosphonium based ionic liquid for the preparation of pyridine derivatives under mild reaction conditions (Fig 1).

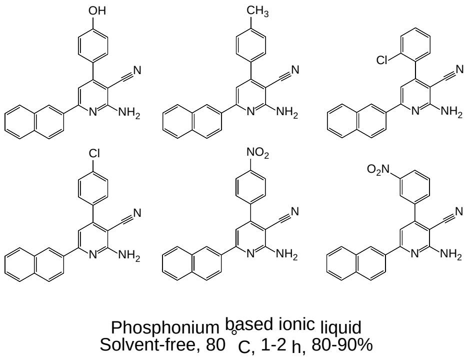

Fig. 1 Synthesis of pyridines using $Fe_3O_4@SiO_2@(CH_2)_3$-urea-benzimidazole sulfonic acid as catalyst

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Theoretical studies of anomeric amids on enzme inhibitors

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Keywords: Anomeric effect, anomeric amid, DFT-B3LYP/6-31G* method.

Anomeric effect has found its influential position in the field of chemistry and it can be defined as stereoelectronic stabilizing effect that favor the placement of electronegative substituents in the axial, rather than equatorial, position in a pyranoid ring system at C1[1]. Recently, our research groups have introduced a new mechanistic outlook for the oxidative aromatization of some heterocyclic compounds based on anomeric effect and present the term of "anomeric based oxidation (ABO)" as an explanation for the final step of aromatization mechanism[3-5]. The modeling and the appropriate calculations on the structures (A-D) (enzme inhibitors of 5-lipoxygenase) have undertaken by DFT-B3LYP/6-31G* method in the vacuum state[2]. The theoretical studies on anomeric amids in the structures show that amid groups are not planner and amid resonance are not described as a HOMO-LUMO interaction. In this structure amid groups constitute a class of "twised amid". The obtained data will be presented.

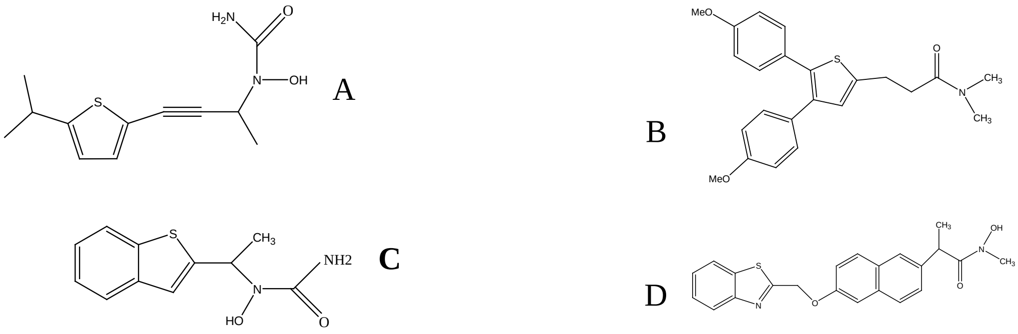

Fig. 1 The structures of enzme inhibitors of 5-lipoxygenase

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Removal of Pb^{+2} and Cd^{+2} pollutants using $B_{12}N_{12}$ Nanocage: A DFT Study

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Keywords: Adsorption, Pb^{+2} and Cd^{+2} Pollutants, B12N12 nanocage, DFT calculations.

Lead poisoning can cause severe injuries to central nervous system, kidney, liver and reproductive system due to its multiple toxicity and progressive accumulation[1]. A variety of syndromes, renal function hypertension, hepatic injury, lung damage and teratogenic effects may result from cadmium toxicity[2] . Adsorption of Pb+2 and Cd+2 pollutants ions on the exterior surface of B12N12 nanocage[3] is scrutinized using Density functional theory (DFT) calculations to investigating its potential as chemical adsorbent. DFT calculations at the B3LYP3 /6-31G*level were performed in terms of energetic, geometric, and electronic properties. The most favorite position for adsorption of the studied cations are a top of N atoms of B12N12. The strongest interactions are obtained when Pb+2 and Cd^{+2} are located a top of N atom with the adsorption energies of -1.07 eV and -1.25 eV, respectively. In water media, adsorption energy of ions is reduced due hydration of ions and nanocage. IR spectra confirm sensing ability of B12N12 for adsorption of Pb+2 and Cd+2 pollutants ions. It is expected that B12N12 acts as new potential adsorbent for Pb+2 and Cd+2 pollutants ions from environmental systems.

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One-pot synthesis of tetrahydro-4*H*-chromene derivatives catalysed by Fe_3O_4@CNTs@TiO_2 nanocomposite

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Keywords: tetrahydro-4H-chromenes, dimedone, CNTs, TiO_2, Fe_3O_4, nanocomposite,

Nanoscience is one of the most prominent research and development areas in modern science. Carbon materials such as carbon nanotubes (CNTs) show great capabilities to serve as substitutes for conventional catalyst or catalyst supports owing to their large surface area.[1] Magnetic nanoparticles such as Fe_3O_4 are often considered to follow the principles of green chemistry.[2] Among nanomaterials, TiO_2 is a biocompatible and environmentally benign catalyst.[3] Heterocyclic compounds are momentous skeleton which widely used for the synthesis of important chemical compounds.[4] Among the hetrocycles, functionally substituted 4H-chromenes have recived considerable attention.[5] Herein, we report the one-pot synthesis of tetrahydro-4H-chromene derivatives **4** via a three component reactions of aromatic aldehyds **1**, malononitrile **2** and dimedone **3** catalysed by Fe_3O_4@CNTs@TiO_2 nanocomposite as a novel, magnetic and recoverable heterogeneous catalyst.

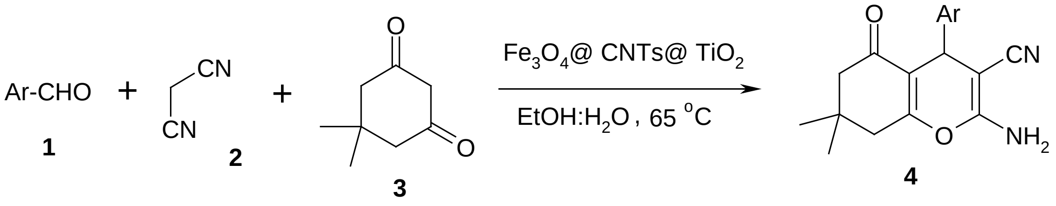

Fig. 1 synthesis of tetrahydro-4H-chromene derivatives

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Synthesis, Identification and the Biological Evaluation of New Mono and Bis Cyclohexen - on Derivatives Basead on Chalcone.

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Keywords: Biological effects, Mono and bis derivatives, Cyclohexene – one, Chalcone

Cancer is a complex and life-threatening disease associated with uncontrolled cell division. Despite the advances made in the field of chemotherapy for cancer, there is still no broad and effective anticancer drug that can target cancer cells specifically. Therefore, it is imperative to design and discover new anti-cancer drugs with high efficacy and specificity. Chalcones have a variety of activities, such as anti-inflammatory effects, anti-leishmaniasis, antimalarials, antiviruses, antifungals, and others[1]. The most important effects of chalcones are their anti-cancer effect, which is done by a variety of mechanisms[2]. Chalcone compounds of natural origin which are of high synthetic diversity for the design of new biologically active compounds, particularly anti-cancer drugs. Recently, it has been shown that many chalcones can inhibit many human cancers through induction of apoptosis. In addition, many existing anticancer drugs, by disrupting the DNA, cause a major genetic toxicity, but chalcones may not develop such a complication due to a different mechanism. One of the most important anticancer mechanisms of chalcones is the induction of apoptosis in cancer cells. Although a large number of cholecystic compounds have been reported with cytotoxic and anticancer effects, in many cases, no mechanism has been investigated. Here, we try to synthesize mono and biass condensation reactions of chalcones and Methyl acetoacetate, synthesized new intermediate compounds such as inosulol, which have an optimal drug and anticancer property with high performance and specificity.

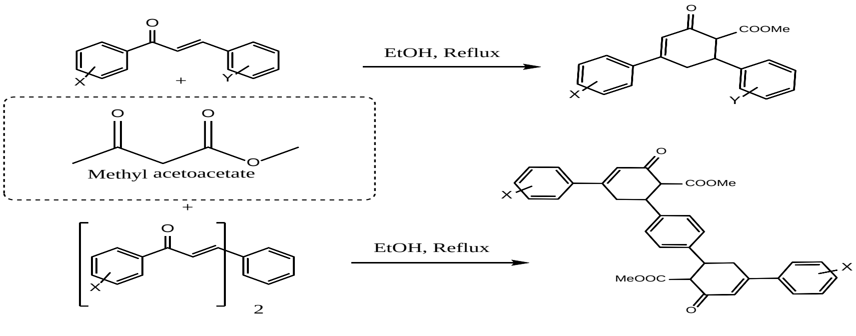

Fig. 1 Condensation Reaction Overview

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Analysis and comparison of Osmosed and non-Osmosed Aloe Vera gel drying kinetics in optimized condition

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** This article is extracted from the master thesis of Ladan Nikfarjam "Optimization of Aloe vera gel drying using osmotic dehydration" and supervised by Dr. Ahi at the Islamic Azad University of Bushehr.*

Keywords: Aloe Vera, Osmotic dehydration, Optimization, Drying kinetics.

The demand for nutritious food with longer shelf life and preservatives-free has increased significantly throughout the world. Today, processing of aloe vera gel plays a key role due to its application in the food industry.[1] Osmotic dehydration is the process of water removal with low energy consumption and temperature.[2] However, this process cannot provide products with enough low moisture content and long shelf life. Therefore, osmotic products need to be further dried by the air, vacuum or freeze dryer and so on.[3] In this study, 20 osmotic dehydration experiments were designed on aloe vera gel by using response surface methodology (RSM). Optimization of osmotic dehydration experiments was done based on maximizing water (WL) and minimizing solid gain (SG). After choosing an optimized osmotic condition, further drying experiments of aloe vera gel slabs were done in a tray dryer at different temperatures (50, 65, 80˚c). Thereafter, drying kinetics of osmotic and non-osmotic dried samples were evaluated (Fig.1). Results show that Osmotically dehydrated samples at all temperatures have dried in a shorter time than non-osmotic dried samples. As a result, with regard to the shorter drying time of Osmo-dried samples in comparison to non-Osmo dried ones and less probable heat damage to superficial and qualitative properties of final products, the Osmo-dried sample at 50˚c was chosen as the best sample.

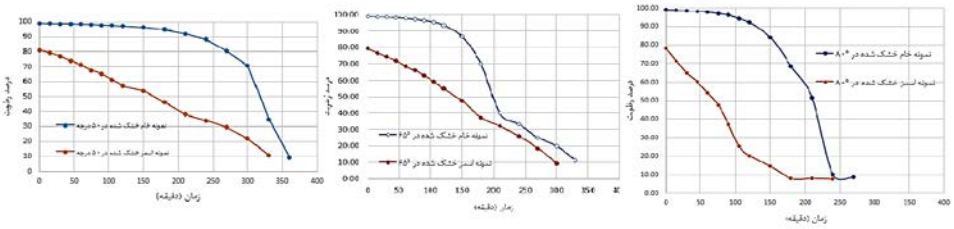

Fig. 1 Drying kinetics of Osmosed and non-Osmosed samples at 50, 65, 80˚c

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Synthesis of thiazepine derivatives using 2-(1, 3-dioxo-1*H*-inden-2(3*H*)-ylidene) malononitryl and thiosemicarbazone

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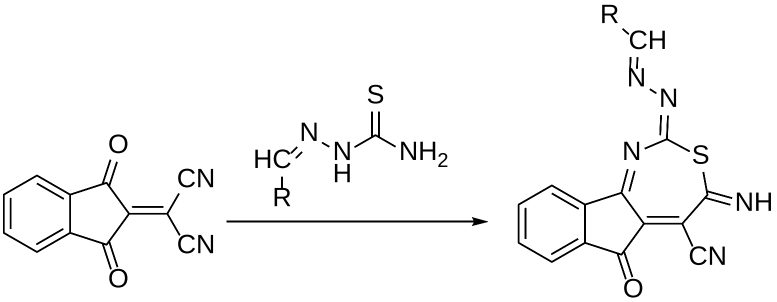
Keywords: Thiosemicarbazone, Malononitryl, Ninhydrin, Thiazepine.

Thiazepines and their derivatives are one of the most important heterocyclic compounds, due to the anticonvulsant, antiviral, anticancer, anti-HIV and antitumor effects.[1-3] In this study firstly, 2-(1,3-dioxo-1H-indene-2(3H)-yilidene) malononitrile was synthesized from reaction of ninhydrin with malononitril in the ethanol as a solvent at room temperature. Then this intermediate was used for synthesis of thiazepine derivatives using thiosemicarbazone derivatives (Scheme 1). Purification all of the compounds were achieved by recrystallization and were further identified by FT-IR, ^{1}H-NMR, ^{13}C-NMR spectra analysis.



R= Phenyl, 4-Cl-phenyl, 2-OH-phenyl, 3-NO_2-phenyl,
3,4-di OH-phenyl, 4-OMe-phenyl, 4-F-phenyl, 4-Br-phenyl, Me

Fig. 1 Synthesis of thiazepines derivatives.

References

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Investigation on the inhibition of $CaCO_3$ precipitation by an environmental friendly terpolymer of AA/AMPS/TBAA in artificial seawater

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Keywords: calcium carbonate, Antiscalant, acrylic acid: 2-acrylamido-2-methyl propanesulfonic acid: t-butyl acrylamide.

The formation of mineral deposits such as calcium carbonate (CaCO3) causes many problems in cooling water systems [1,2]. therefore in this study, the effect concentration of scale inhibition terpolymer of acrylic acid : 2-acrylamido-2-methylpropanesulfonic acid : t-butyl acrylamide (AA/AMPS/TBAA) on calcium carbonate precipitation in artificial seawater based on ASTM D1141 at cathodic potential of -0.9 V_{SCE} on carbon steel electrode is investigated by electrochemical methods. Increase inhibitory concentration leads to increase in scaling time (t_s) and residual normalized current density (i_{rn}). The Surface morphology characterization by using scanning electron microscopy and X-ray diffraction methods showed that presence of inhibitor to the amount of 2 ppm has not changed crystals morphology but cause decrease nucleation, delay in the crystal growth and increases dispersion on the electrode surface also reduced the percentage of coverage by $CaCO_3$ precipitation [3].

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Synthesis and characterization of (Fe_3O_4@ kryptofix @ Ni) as a heterogeneous nanocatalyst and using its catalytic efficacyor in the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones

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Keywords: Nanocatalyst, Ni-kryptofix[,2,2,2] complex, 2,3-Dihydroquinazolin-4(1H)-one.

The use of nanomaterials as support in heterogeneous catalysis is a growing field of research[1]. Due to their high surface/volume ratio, nanoparticles (NPs) as a supporting material provide the benefit of an increased active surface area, which allows for increasing reaction rates. NPs are now often considered as a bridge between heterogeneous and homogene catalyses[2] . Magnetic nanoparticles (mNPs) have attracted lot of interest in recent years in a wide range of disciplines due to their unique properties. They have been studied for example as nanofluids, in environmental remediation, in targeted drug delivery, in sensor applications, in imaging, in hyperthermia, and of course in catalysis[3]. Herein, In our studies on application of new heterogeneous and recoverable catalysts in organic transformations, we decided to prepare a novel heterogeneous catalyst (Fe3O4@ kryptofix @ Ni), and studied its application as in the synthesis 2,3-dihydroquinazolin-4(1H)-ones.The details of the synthesis 2,3-dihydroquinazolin-4(1H)-ones preparation procedure are presented by the concise route outlined in Fig 1.

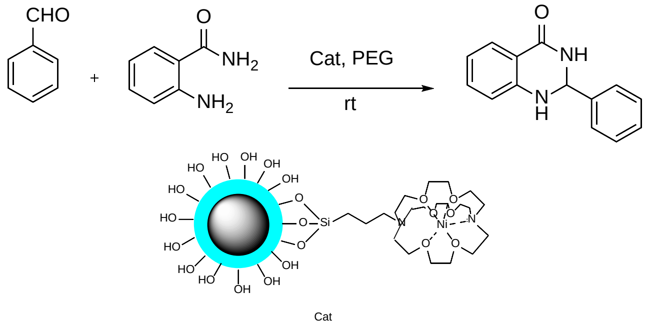

Fig. 1 synthesis 2,3-dihydroquinazolin-4(1H)-ones

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Synthesis, characterization and investigation of polybenzimidazoles containing ether linkages

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Keywords: Arylene bis-benzimidazole, Co-poly benzimidazole, Nitro displacement.

Benzimidazole polymers are important series of aromatic polymers because of their heat resistance, stability, and durability against oxidative reagents as well as proton conducting capability. [1] This ability of benzimidazole polymers have significantly attracted researcher's attention in the last decades. Based on structure-properties approach, co-polybenzimidazole synthesis by introducing the other functional groups presents many benefits. [2, 3] In this work, two diacid monomers were synthesized based on isophthalic and pyridine dicarboxylic acid. A nucleophilic nitro displacement reaction with 4-hydroxybenzoic acid was utilized in the preparation of arylene bis-benzimidazole dicarboxylic acid monomers. All of the synthesized compounds were identified with the IR, MS and NMR measurements. To synthesize the co-polymers, the monomers were reacted with different aromatic diamines (that contain flexible unites) along with equimolar amounts of adipic acid as comonomer. The gained polymers in the optimized conditions of temperature, time and concentration had a viscosity 0.34 to 0.51 dL/g. Thermal behavior and stability of the polymers were evaluated by TGA, DSC and DMTA techniques.

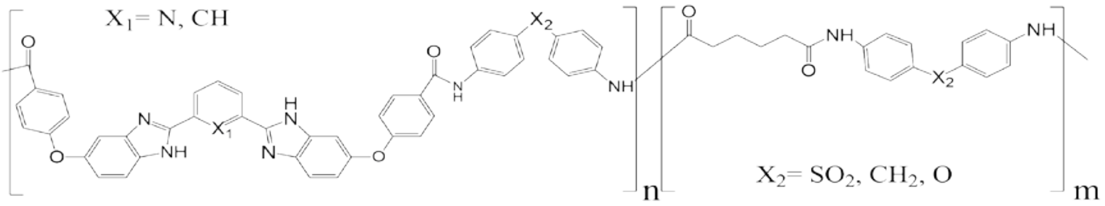

Fig. 1 Co-poly(benzimidazole-amide) structures

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Triethylammonium thiolate as an efficient reagent for synthesis of quinoxaline containing indandione skeleton *via* sequential one-pot multicomponent reaction

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Keywords: Triethylammonium thiolate, Methyl iodide, *O*-Phenylenediamine, Quinoxaline, Indandione motif, Multicomponent reactions

The nitrogen-containing heterocyclic compounds containing quinoxaline motif are well known for their biological activity[1]. So far, many synthetic methods have been reported for the preparation of quinoxalines. Most of these methods are conducted under harsh reaction conditions such as using acidic catalysts and oxidant reagents, reflux conditions, and microwave irradiation[2].

Considering the biological properties of the compounds containing quinoxaline and indandione skeleton (Indandione motif was found in pharmaceutical compounds and natural products[3]), we introduce the synthesis method of novel derivatives of 3-hydroxy-2-(3-phenyl-quinoxalin-2-yl)-1*H*-inden-1-ene **5** *via* a sequential one-pot three-component reaction between new triethylammonium thiolate salts **3**, methyl iodide and *o*-phenylenediamines **4** in EtOH at room temperature (Fig. 1).

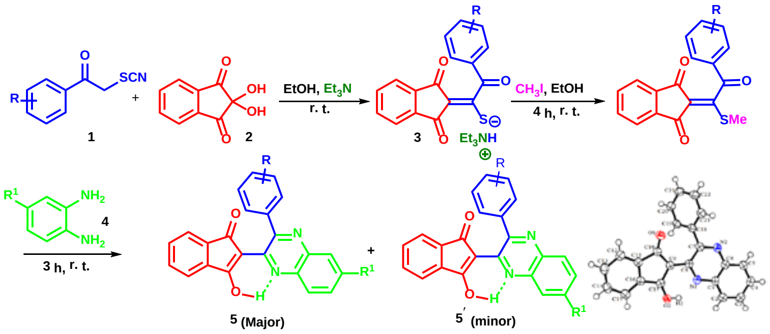

Fig. 1 The synthesis of novel derivatives of 3-hydroxy-2-(3-phenyl-quinoxalin-2-yl)-1*H*-inden-1-ene

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Synthesis and characterization of a magnetic nanocatalyst base on graphene oxide, Nickel and Cobalt and its activity in organic reactions

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Keywords: Ni, Co, Graphene oxide, Nanocatalyst, Cross-coupling reactions.

Today catalysts are widely used in the production of various materials. Nano-catalysts according to their importance have become one of the most important areas for nanotechnology research.[1] Development of magnetic catalysts for carbon-carbon and carbon-heteroatom coupling reactions are one of the most important issues in terms of applications to organic synthesis.[2] At present, many researches are focused on the construction of more active and more stable, heterogeneous Nano-sized metal catalysts, which can be recovered and reused.[3] Nickel and cobalt nanoparticles due to low prices, magnetic properties, and high chemical activity attracted particular attention.[2] In this work, nickel and cobalt nanoparticles were synthesized with a green and one-pot method on graphene oxide substrate for reduction reactions of 4-nitrophenol and Heck, Suzuky, Negishi, and Sonogashira cross-coupling reactions. Several characterization techniques such as FTIR, FESEM, XRD, and VSM were employed to characterize the Co and Ni nanoparticle reduced graphene oxide composites witch indicates that nickel and cobalt magnetic particles with a size of about 20-30 nanometers were uniformly anchored on graphene oxide nanosheets. In addition, results showed that incorporation of Co and Ni nanoparticles and GO produce much higher activity in cross-coupling and reduction reactions. The soft-ferromagnetic behavior of the RGO/Co_xNi_{100-x} nanocomposite demonstrated the easy separable from the reaction mixture and reusable several times without losing its catalytic activity, Hence, the RGO/Co_xNi_{100-x} composites can be a potential promising material to catalyze the cross-coupling reactions.

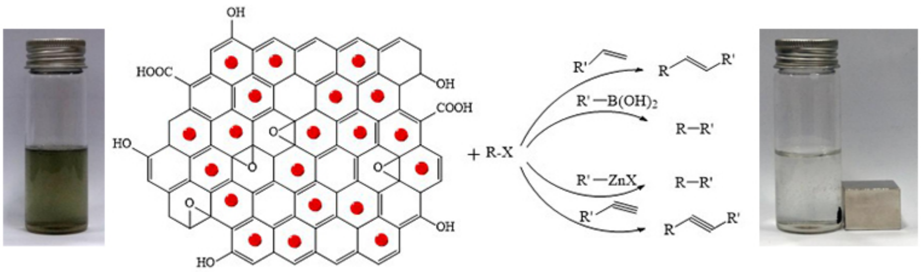

Fig 1. Functionalized graphene oxide with nickel and cobalt nanoparticle and its application in organic cross-coupling reactions

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Aerobic oxidation of alcohols to the corresponding carbonyl compounds in the presence of polyoxometalate@TiO_2/hydroquinone/palladium@MCF catalytic system

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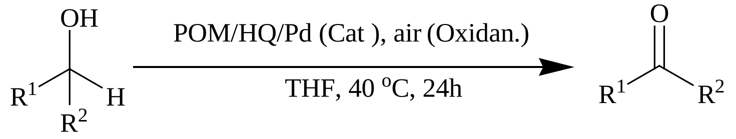
Keywords: Aerobic Oxidation, Cooperative catalytic system, Alcohols, Carbonyl compounds

The selective oxidation of alcohols to the corresponding carbonyl compounds is one of the most important reactions in chemical compounds because the corresponding carbonyl compounds are suitable intermediates for the composition of valuable organic compounds.[1] In the classic method for the oxidation of alcohol, toxic oxidizing stoichiometric values, such as permanganate and chromium salts, are used, which produce large amounts of toxic waste, and is not economically feasible.[2] Among the reported catalysts, palladium salts exhibit high catalytic activity for the reaction of aerobic oxidation of alcohols.[3] One of the limitations of these methods is the need for high temperature to react. To overcome this constraint, today researchers using the biometric model of molecules use electron transfer between the catalyst and molecular oxygen as oxidants.[4] In this work, for the first time, the selective aerobic oxidation of primary and secondary alcohols to the corresponding carbonyl compounds are investigated using air as an ideal oxidizing agent in the presence of POM@TiO_2/HQ/Pd@MCF as a novel cooperative catalyst system under mild conditions (Scheme 1). The main advantages of this method are the use of catalytic amount of supported palladium and polyoxometalate as heterogenuse which can be recycled for several times and the use of air as an abundant, cost effective and environmentally friendly oxidant.



R^1,R^2= Alkyl , Aryl, H

Scheme 1 POM@TiO_2/HQ/Pd@MCF catalyzed the selective aerobic oxidation of alcohols to the corresponding carbonyl compounds

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Chemoselective Reaction of Aaldehydes and 2-Methyl-5-pyrazolone in Different Basic and Acidic Choline chloride-based Deep Eutectic Solvents

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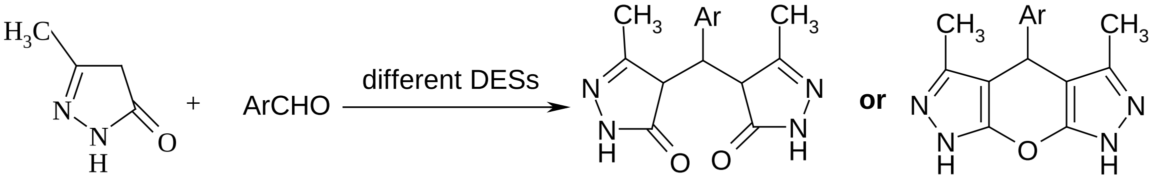
Keywords: Chemoselectivity, Deep Eutectic Solvents, Pyrazole, Choline chloride/$ZnCl_2$, Choline chloride/Triflouroacetic acid

Solvents play a key-role for the development of more efficient chemical transformations and industrial processes. A new generation of solvents, named Deep Eutectic Solvents (DESs), was presented as suitable alternative solvents compared to conventional and unconventional solvents, such as ionic liquids (ILs).[1,2] 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.[3] In this work, the chemoselectivity of the reaction of aromatic aldehydes and 2-methyl-5-pyrazolone, as active methylene compound, for the tandem synthesis of bis(pyrazolyl)methanes **1** and dipyrazolopyrane hybrids **2** in different basic and acidic Choline chloride-based deep eutectic solvents (DESs) has been investigated (Figure 1).



1 **2** **Fig.**

Fig 1. Chemoselective reaction of aldehydes and 2-methyl-5-pyrazolone in different DESs**.**

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Salen complex of Cu (II) supported on superparamagnetic Fe_3O_4@SiO_2 nanoparticles: an efficient and magnetically recoverable catalyst for the Synthesis is of 4-dihydropyridines

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Keywords: Nanocatalyst, 4-Dihydropyridines , Hantzsch Synthesis, Salten.

The Fe_3O_4@SiO_2/Salen-Cu(II) nanocatalyst is reported as a thermally and air-stable, economical, and magnetically recoverable heterogeneous catalyst for the selective and efficient 1,4-dihydropyridines Fig. 1. Only by adding a small amount of the catalyst (0.4mol% Cu) to the reactants and heating under air, the new presented method provides a variety of functionalized 1, 4-dihydropyridines in good to excellent yields within short reaction times.[1] The catalyst could be easily recovered with the aid of a permanent magnet and reused up to five consecutive runs without significant loss of activity. Also, the leaching of Cu was negligible after the fifth recycle.[2] Particularly, ethyl acetoacetate and aromatic aldehydes as agents and the need of only small amount of the magnetically recoverable heterogeneous copper-based nanocatalyst make this method low-cost, environmentally benign, and easy to use.[3]

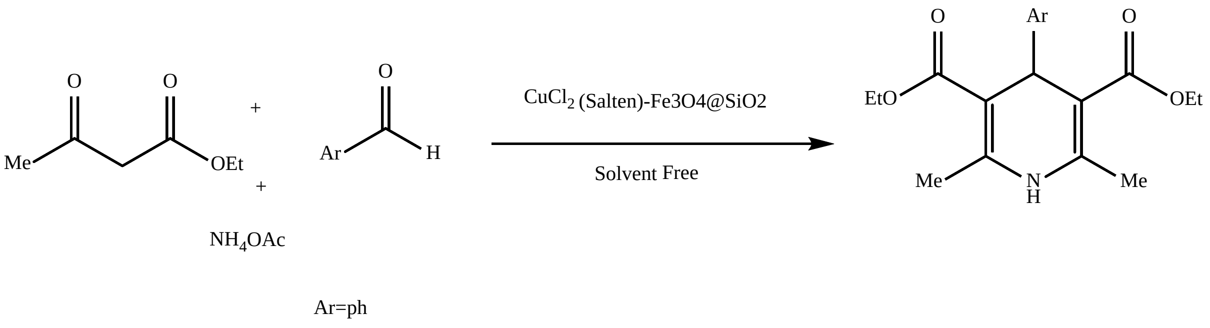

Fig. 1 Hantzsch synthesis of 1, 4-dihydropyridines Cu (Salten)- Fe_3O_4@SiO_2

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Synthesis of 2,4,6-triarylpyridine derivatives catalyzed by p-toluene sulfonic acid under solvent-free conditions

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Key word: 2,4,6-Triarylpyridine, Three-component reaction, One-pot, Solvent-free.

The heterocyclic compounds are very useful intermediates for the development of molecules in pharmaceutical or biological interest. The 2,4,6-triarylpyridines are applied as the useful intermediate in the synthesis of drugs, herbicides, insecticides, desiccants and surfactants and also prominent building blocks in supramolecular chemistry. So, designing of the new procedure for this transformation is highly desirable.[1-3]

In this work the reaction of aldehyde, acetophenone and ammonium acetate by using p-toluene sulfonic acid (TsOH) as efficient catalyst to afforde the 2,4,6-triarylpyridines under solvent-free conditione was reported.

After completion of reactin, the progress was monitored by TLC. Than, the reaction mixture was cooled to room temperature and the precipitated solid was collected, washed with cold ethanol, to give the pure product in excellent yields. Finally, melting point, ^{1}H NMR, and FT-IR techniques were recognized the structure of compounds.

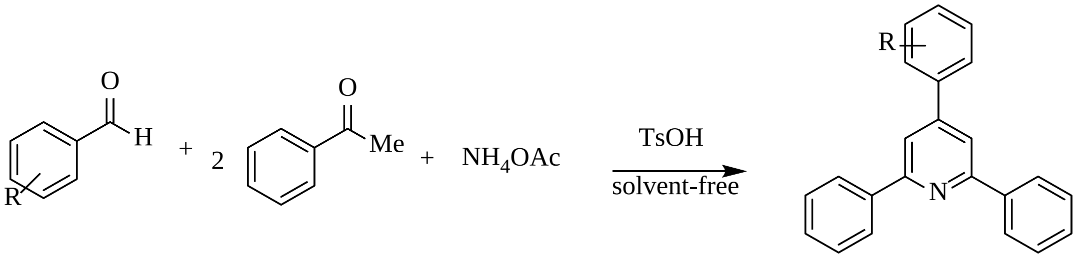

Fig 1. Synthesis of 2,4,6-triarylpyridine derivatives

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Antibacterial and Antioxidant Activity of Novel 2-Amino-4*H*-pyrans

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Keywords: Antibacterial, Antioxidant, Bioactive compounds, 2-Amino-4*H*-pyrans

Blocking the growth and multiplication of bacteria is an important action for antimicrobial agents. Many infectious diseases, caused by a variety of pathogens, can be controlled by antimicrobials[1]. Resistance to antimicrobial agents is increasing rapidly, and, therefore, designing new and potential antimicrobial agents with low risk of toxicity is a crucial issue[2]. The compounds possessing heterocyclic moieties have attracted much interest due to their biological and medicinal activities[3]. In the continuation of our research interest in the synthesis of potentially bioactive heterocyclic compounds[4], herein, we report evaluation antibacterial and antioxidant activities of novel 2-amino-4*H*-pyrans that prepared from three-component reaction.

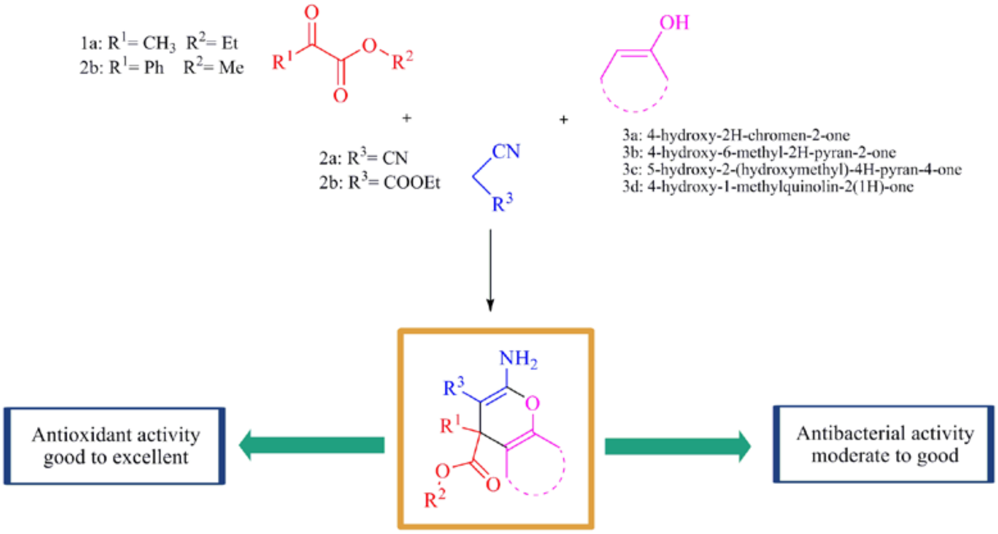

Fig. 1 Preparation of 2-amino-4*H*-pyran derivatives 4a-l *via* multi-component reaction.

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Synthesis of new derivatives of 2-amino-4*H*-pyran via three-component reaction

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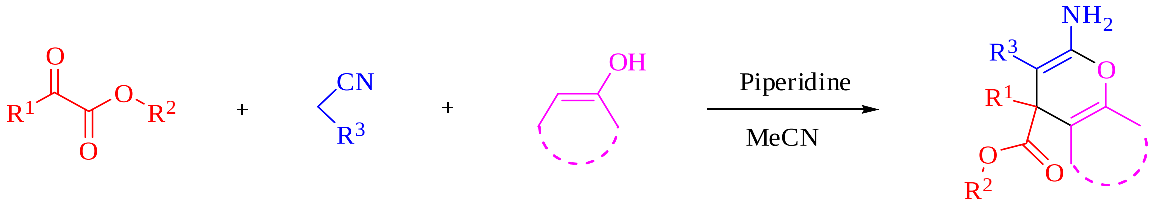
Keywords: Multicomponent reactions, 2-Amino-4*H*-pyrans, *OH*-acids, *α*-Ketoesters, Active methylenes

Multi-component reaction (MCR) can provide simplicity by reducing the synthesis steps and avoiding complicated purification processes [1]. In addition, it has high atom-economy and high selectivity, while saving time, energy and preventing the waste of reagents and solvents[2]. MCR is widely used for the synthesis of heterocyclic compounds such as 2-amino-4*H*-pyrans[3] and pyrano[3,2-c]pyran-5(4*H*)-one[4]. In continuation of our research in the synthesis of bioactive heterocyclic compounds[5], herein, we report synthesis of new derivatives of 2-amino-4*H*-pyran **4a-l** using some *α*-ketoesters **1a-b**, active methylene **2a-b**, and *OH*-acids **3a-d** in the presence of piperidine (Scheme 1).



1a: R^1= CH_3 R^2= Et
2b: R^1= Ph R^2= Me

2a: R^3= CN
2b: R^3= COOEt

3a: 4-hydroxy-2H-chromen-2-one
3b: 4-hydroxy-6-methyl-2H-pyran-2-one
3c: 5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one
3d: 4-hydroxy-1-methylquinolin-2(1H)-one

4a-l

Fig. 1 Preparation of 2-amino-4*H*-pyran derivatives 4a-l *via* multi-component reaction.

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Preparation and Evaluation of Mesalazine loaded Sodium Alginate/Nano Carboxy Methylcelloluse Beads for pH-Sensitive Drug Delivery

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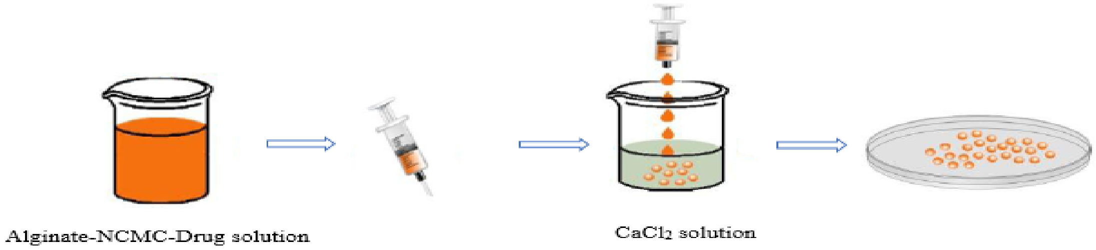
Keywords: Sodium alginate, Bead, Nano carboxymethyl cellulose, pH-sensitive drug delivery.

Controlled drug delivery systems are designed to deliver the drug at predetermined rate at a specific site thereby reducing the dose, dosing frequency, and side effects of the drug. One of such approach is the formulation of beads as drug carriers.[1] Beads have a wellordered size and shape, the huge surface area allowing for sufficient therapeutic coatings, and the high capability for encapsulation of various drugs and biomaterials.[2] Polymeric beads derived from natural sources are unique materials for controlled release due to inherent properties such as their non-toxic nature and biodegradation ability.[3] Sodium alginate (SA) and carboxymethyl cellulose (CMC) are biocompatible, biodegradable polymers and have finding widespread applications in pharmaceutical area.[4] The most attractive property of alginate is its gel formation simply induced by cross-linking with various divalent cations. Because of SA's ability to form a stable and bioadhesive gel with calcium ions, some sensitive drugs, protein, living cells, etc. could be encapsulated and released through alginate beads.[5]

The aim of this work is to produce alginate beads containing mesalazine as a drug model in order to control the drug release in the colon. The mesalazine loaded alginate-CMC bead were prepared using the ionotropic gelation method. The structure and surface morphology of the hydrogel beads were characterized by FTIR and SEM, respectively. The prepared beads were evaluated for swelling properties, entrapment efficiency, drug loading, and *in-vitro* drug release in simulated gastric (pH 1.2), intestinal (pH 7.4) fluids.



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Preparation and Characterization of New Porous Graphene Oxide-based Scaffolds for Bone Tissue Engineering

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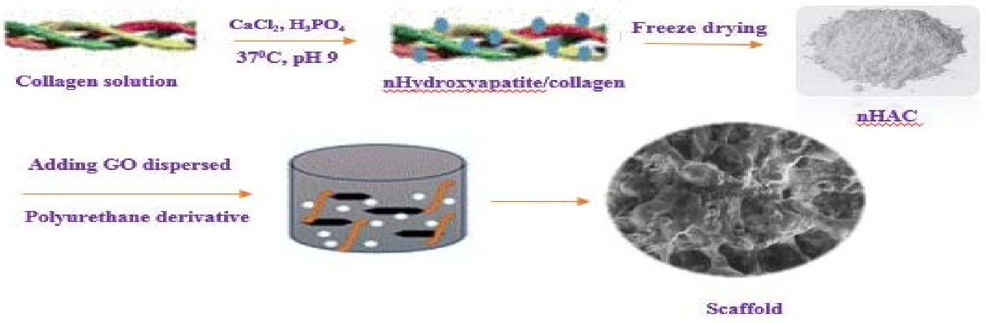
Keywords: Scaffold, Hydroxyapatite, Graphene oxide, Bone tissue engineering.

Scaffolds are a key requirement in bone tissue engineering, because can mimic the structure and function of the extracellular matrix (ECM) and support cell adhesion, proliferation and differentiation. In recent years, significant development has been achieved in the construction of artificial bone with ceramics, polymers and metals. Nano-hydroxyapatite (nHA) is an attractive bioceramic for hard tissue repair and regeneration due to its physicochemical similarities to natural apatite.[1] nHA with natural or biopolymer-basd composites containing chitin, collagen, gelatin, fibrin and with synthetic polymers such as polylactic acid, polycaprolactone, poly (lactic-co-glycolic) acid, polyurethane and polyhydroxybutyrate improve cellular attachment, viability, proliferation, and activity as well as mechanical properties.[3] Graphene and its derivatives such as graphene oxide (GO) have been considered as an attractive substrate for stem cell culture, as culture on these materials can enhance proliferation and lineage specification of the stem cell.[3]These unique properties make GO-based materials promising candidates as a scaffold for bone regeneration.

In this work, the porous GO-nHA/collagen/PU-polymer composite scaffolds containing different amount of GO were prepared. Interactions between in the individual components in the formation of the composits were confirmed by FTIR and XRD. The porous morphology of scaffolds was confirmed by SEM images. Osteoconductivity and biocompatibility of scaffolds were confirmed by *in vitro* MTT assay.



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Intramolecular Diels–Alder and [3+2] Cycloaddition Reactions in the One-Pot Synthesis of Epoxypyrrolo[3,4-*g*]indazoles

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Keywords: Isocyanides, Dialkyl acetylene dicarboxylates, 2-Furancarboxylic acid, Epoxypyrrolo[3,4-*g*]indazoles, IMDA, [3+2] Cycloaddition, Oxabicyclo Compounds.

Diels–Alder and [3+2] cycloaddition reactions are two dynamic tools for synthesis of diverse organic compounds. Recently employment of IMDA reaction in acetylene based isocyanide multicomponent reactions has found remarkable interests.[1] Additionally, in continuation of our previous works in acetylene-based isocyanide multicomponent reaction,[2] we were interested in the reaction of isocyanides **1**, dialkyl acetylene dicarboxylates **2** and 2-furan carboxylic acid **3**, which led to 1,3-dioxoepoxyisoindoles **4**. In the next step, we decided to investigate the reactivity of the double bond in the structure of 1, 3-dioxoepoxyisoindole **4** toward [3+2] cycloaddition reaction. To achieve this goal, hydrazonoyl chloride **5** with an equivalent amount of triethylamine were added to the reaction mixture and the reaction outcome was the epoxypyrrolo[3,4-*g*]indazoles **6/6′** in the form of two diastereomers, products were verified by mass, IR, ^{1}H NMR, ^{13}C NMR spectra and X-ray crystallography.

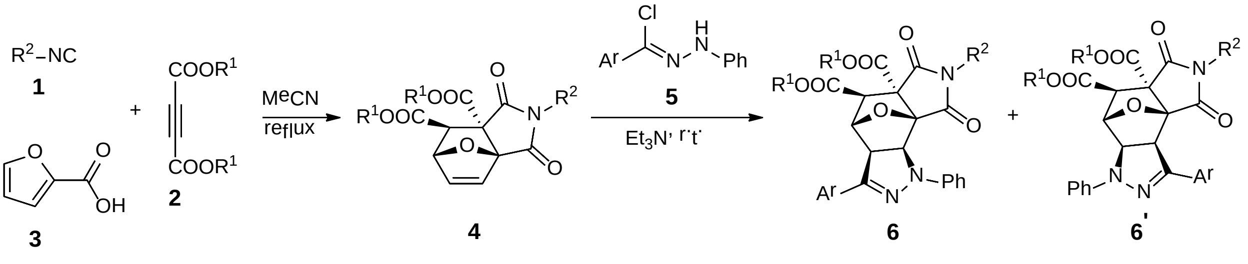

Fig. 1 Synthesis of epoxypyrrolo[3,4-*g*]indazoles

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Synthesis of green and high temperature stable palladium composite

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Keywords: Magnetic nanoparticles, Palladium, Kaolinite Clay, Green Chemistry.

Since the beginning of history, soils play an effective rule inhumane life. They are useful materials for many purposes such as constructing shelters, producing consumable goods, industrial and pharmaceutical applications. The large surface area, mechanical properties, high thermal stability, and other unique properties have caused that Kaolinite widely applied in adsorbents and composites.[1-3] Kaolinite has a potential for the catalytic carrier because their surface and special structure are very suitable for supporting transition metals.[4,5] This clay as a nontoxic, inexpensive, free available and abundant natural mineral was used to synthesize magnetic nanocomposite of palladium as a super stable and recoverable green catalyst (Fe_3O_4/Kaolinite-Pd). The catalytic activity of this system was evaluated in the reduction of Nitroarene compounds. Determination of novel nanoparticles structure was performed using FT-IR, XRD, VSM, TGA, and SEM –EDX spectral data.

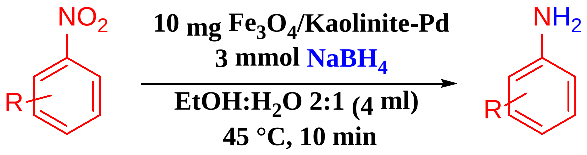

Fig. 1 Reduction of Nitroarene compound to aniline derivatives.

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Synthesis of 3, 4- dihydropyrimidine-2-(1*H*)-ones (thiones) in the presence of an efficient and eco-friendly solid acid catalyst under different conditions

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Keywords: Dihydropyrimidines, Biginelli reaction, Microwave irradiation, Grinding

Multiple-component reactions (MCRs) such as biginelli reaction are powerful strategies for the one-pot synthesis of organic compounds such as dihydropyrimidinone derivatives (DHPMs). The first biginelli-like reaction was reported by Wang.[1] Biginelli reaction involves the cyclo condensation of an aromatic aldehyde, α,β-ketoester and urea (thiourea). Biginelli products have potential in pharmaceutical applications such as anti-viral, anti-tumor, anti-bacterial, anti-inflammatory, anti-hypertensive and alpha antagonists.[2] Nano solid acid catalysts, which are bridges between homogeneous and heterogeneous catalysts, exhibit higher activity and selectivity than their corresponding bulk materials.[3] Heterogeneous catalysts have been applied in organic reactions in recent years. In this work, an efficient catalyst was used which is reusable, inexpensive, readily available, eco-friendly, without the use of harmful solvents. In this study, we report our results for the synthesis of 3,4-dihydropyrimidinones (thiones) via one-pot cyclo condensation of acetoacetates, aromatic aldehydes, and urea or thiourea using nanocatalyst under different conditions (Fig.1).

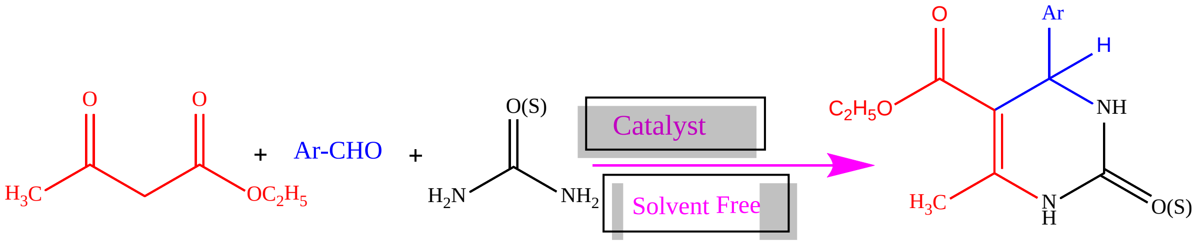

Fig. 1 Multicomponent reaction for the synthesis of 3, 4- dihydropyrimidine-2-(1*H*)-ones (thiones)

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Novel pH-sensitive nanocomposite hydrogels based on polyvinyl imidazole - graphene quantum dots for adsorption of congo red and methyl orange from aqueous solution

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Keywords: Nanocomposite hydrogels, N-Doped graphene quantum dot, Polyvinyl imidazole, Dye adsorption.

Recently, hydrogel adsorbents have attracted special attention for dye removal because of their three dimensional network structure and high swollen property, allowing the dye molecules to be easily absorbed in hydrogels[1]. Color removal from effluent is one of the most difficult requirement faced by the textile finishing, dye manufacturing, pulp and paper industries. The discharge of these to the river stream without proper treatment causes irreparable damage to the crops and living beings, both aquatic and terrestrial.

Dyes are classified in three broad categories: (a) anionic: direct, acid and reactive dyes; (b) cationic: all basic dyes and (c) nonionic: dispersed dyes. Congo red (CR) is an example of diazo dyes and is prepared by coupling tetrazotised benzidine with two molecules of napthionic acid. Methyl orange (MO) has been widely applied in the textile, printing, paper, food, research laboratory and pharmaceutical industries[2]. The pH sensitive hydrogels are extensively used in different fields such as medicine, pharmacy, agriculture, food industry and controlled drug delivery etc., but the removal of toxic dyes using pH sensitive hydrogel are rarely reported[3]. In this work, a series of pH-sensitive nanocomposite hydrogels (PVI/GQDs) based on polyvinyl imidazole (PVI) were synthesized using an imidazolium-based dicationic IL (DIL) as a crosslinker and N-doped graphene quantum dots (NGQDs) as a nanofiller with different feeding amounts. The obtained hydrogels containing 0.5 and 8% of NGQDs showed the removal efficiency above 95% for CR and MO with concentration of 100-600 ppm at pH=7, respectively. The synthesized PVI/GQDs hydrogels were characterized by FT-IR, TGA, XRD and SEM.

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Synthesis of spiropyrroles through multicomponent reaction

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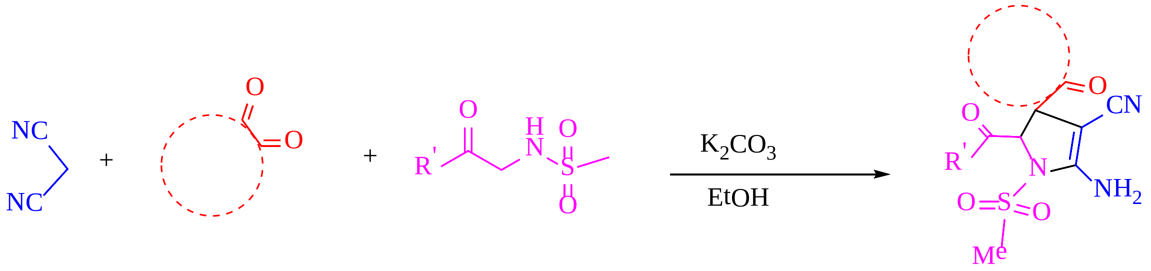
Keywords: Multicomponent reactions, Spiropyrrole, Active methylenes, α-Dicarbonyls

Multicomponent reaction (MCRs) is an emerging tool for the designing and developing new approach for the preparation of various bioactive heterocyclic compounds.[1] Nitrogen-containing heterocyclic compounds such as pyrroles are present in various biologically active alkaloids [2] and natural products [3] that show significant biological activities such as anti-cancer, antifungal, antiviral, antimicrobial, antitumor activities.[4] Herein, we report the synthesis of new tetrahydrospiropyrrole **4** from the multicomponent reaction of malononitrile **1**, α-diketones **2** and *N*-aryl methanesulfonamide **3** in the presence of K_2CO_3 as base **(Fig.1)**. The structure of the synthesized compounds **4** were determined on the basis of their mass spectra, ^1H and ^{13}C-NMR and IR spectra data.



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

Fig. 1 Synthesis of spiropyrroles through multicomponent reaction

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Preparation of dibenzylidenecyclohexanone compounds and the reaction of these compounds with N, N-dimethylbarbituric acid and dimedone free catalyst.

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Keywords: Spiro heterocycle, Michael Addition, *N*, *N*-Dimethyl barbituric acid, Dimedone, Dibenzylidenecyclohexanone, Free catalyst; Ethylene glycol.

The research carried out in this research work consists of three parts: in the first stage, the preparation of derivatives of dibenzylidenecyclohexanone was prepared based on Aldol density,[1] and in the second step, the reaction of dibenzylidenecyclohexanone compounds with dimethylbarbituric acid Based on the reaction of Michael's addition, in the third step, the reaction of the compounds of dibenzylidenecyclohexanone with dimedone, which is based on the reaction of Michael's addition. To prepare the compounds of dibenzylidenecyclohexanone was synthesized from cyclohexanone with benzaldehyde derivatives,[2] with a molar ratio of 1 to 2, all of which were derivatives as symmetrical reactions. These compounds were made of curcumin, which is produced by the change in the ketone group Also come into existence. The reaction carried out in ethylene glycol solvent at 110 ^{0}C in the absence of any catalyst to give high yields at short time.[3] All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H, and ^{13}C NMR and IR spectroscopic data.

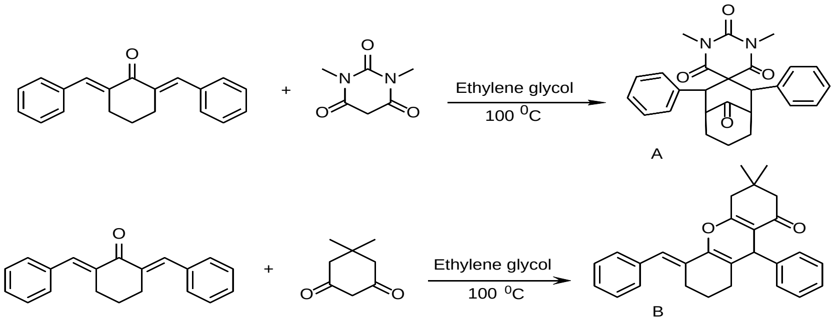

Fig.1 A: 1',3'-dimethyl-2,4-diphenyl-2'H-spiro[bicyclo[3.3.1]nonane-3,5'-pyrimidine]-2',4',6',9(1'H,3'H)-tetraone. B: (E)-5-benzylidene-3,3-dimethyl-9-phenyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-1-one

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[Bmim]HSO_4 loaded on graphene oxide: a green, reusable and nanocatalyst for the synthesis of polysubstituted pyrroles

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Keywords: Graphene oxide**,** Pyrroles, Multicomponent, [Bmim]HSO_4 / (GO)

Polysubstituted pyrroles are of paramount importance due to their antibacterial,[1] antiviral and antitumor,[2] antioxidant[3] activities and ability to inhibit the cytokine-mediated diseases.[4] Mention above and in course of multicomponent reactions (MCRs), one of the most important of MCRs is the synthesis of polysubstituted pyrroles.

In this research paper, a simple and convenient method for the synthesis of various polysubstituted pyrroles using mixture of the amines such as arylamines, 2-amino-4-methyl thiazole, adenine, aryl aldehydes, 1,3-dicarbonyl compounds and nitromethane in the presence of [Bmim]HSO_4 / GO as a green, reusable and nanocatalyst (Scheme 1).

The advantages of this protocol are the synthesis of some unprecedented polysubstituted pyrroles having fluorine atom and, containing thiazole and adenine nuclei that are very important in pharmaceutical and drug discovery research.

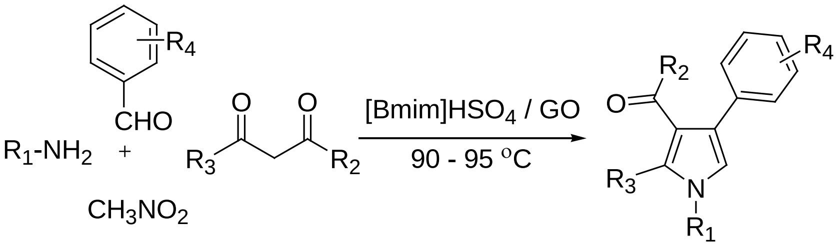

Fig. 1 Catalytic synthesis of polysubstituted pyrroles

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One-pot, four- components synthesis of 1,2,4,5-tetrasubstituted imidazoles using [Bmim]HSO_4 ionic liquid as a green catalyst

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Keywords: Benzil, Imidazole, Multicomponent, [Bmim]HSO_4

The imidazole ring system is one of the most important substructures found in a large number of natural products and pharmacologically active compounds.[1-3] In this communication, a number of methods have been also developed for the synthesis of 1,2,4,5-tetrasubstituted imidazoles.[4]

In this research paper, a simple and convenient method for the synthesis of various 1,2,4,5-tetrasubstituted imidazoles using mixture of the amines such as arylamines and aliphatic amines, aryl aldehydes, 1,2-dicarbonyl compounds and ammonium acetate in the presence of [Bmim]HSO_4 as a green, reusable catalyst in refluxing ethanol is described (Scheme 1).

The advantages of this protocol are the synthesis of tetrasubstituted imidazoles having fluorine atom, simple separation and workup and the use of reusable catalyst.

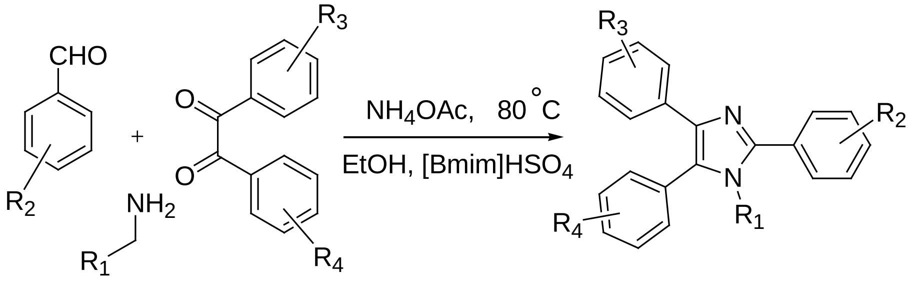

Fig. 1 Catalytic synthesis of tetrasubstituted pyrroles

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A green route for the synthesis of 2-amino-5,10-dioxo-4-aryl-5,10-dihydro-4*H*-benzo[*g*]chromene-3-carbonitriles using *L*-proline as a basic organocatalyst

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Keywords: Aryl-5,10-dihydro-4*H*-benzo[*g*]chromene, *L*-proline, Naphthoquinone

4*H*-Chromene derivatives were detected in natural compounds[1] and demonstrated pharmacological and biological activities.[2] Some synthetic approaches to 2-amino-4*H*-chromene derivatives via three components one-pot reactions involved such catalysts as triethylbenzylammonium chloride, DMF/AcOH, Et_3N, DBU, ionic liquids, NH_4OAc, KF, urea, and some the others reagents in literature.[3]

In this paper, a new procedure for the one pot synthesis of 2-amino-5,10-dioxo-4-aryl-5,10-dihydro-4*H*-benzo[*g*]chromene-3-carbonitriles using aryl aldehydes, 2-hydroxy-1,4-naphthoquinone and malononitrile in the presence of *L*-proline in refluxing ethanol is described (Fig.1).

The main advantages of the present synthetic protocol are eco-friendly catalyst, easy reaction work-up procedure and precedent some new derivative compounds. It is expected that the present methodology will find application in organic synthesis and industrial chemistry.

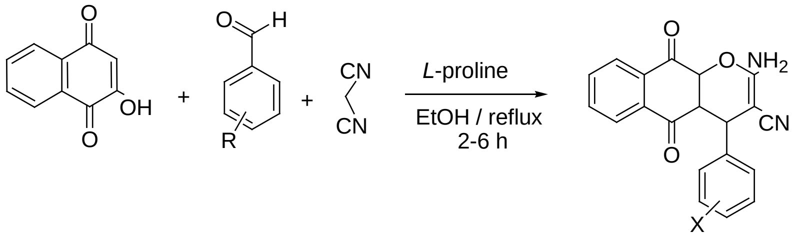

Fig. 1 Catalytic synthesis of 2-amino-5,10-dioxo-4-aryl-5,10-dihydro-4H-benzo[g]chromene-3-carbonitriles

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One-pot three-component synthesis of aminonaphthoquinones derived from lawsone using *L*-proline as an organocatalyst

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Keywords: Lawsone, *L*-proline, Naphthoquinone.

In regard to biological properties, the pharmacophoric quinone group receives great attention due to its extensive use and its presence in compounds with confirmed antitumour, molluscicidal, leishmanicidal, anti-inflammatory and antifungal activities,[1-2] as well as its industrial applications and their potential as intermediates in the synthesis of heterocyclic compounds. Lawsone is a *p*-naphthoquinone containing an enol group, which is susceptible to a multicomponent Mannich reaction.

In this study, environmentally friendly one-pot protocol was developed for the first synthesis of aminonaphthoquinones derived from 2-hydroxy-1,4-naphthoquinone (lawsone) via a multicomponent Mannich reaction in aqueous media using a catalytic amount of *L*-proline in refluxing ethanol (Fig.1)

The main advantages of the present synthetic protocol are eco-friendly catalyst, easy reaction work-up procedure and precedent some new derivative compounds. The system chosen for the multicomponent Mannich reaction is nontoxic and extremely inexpensive, which aligns with the concept of green chemistry.

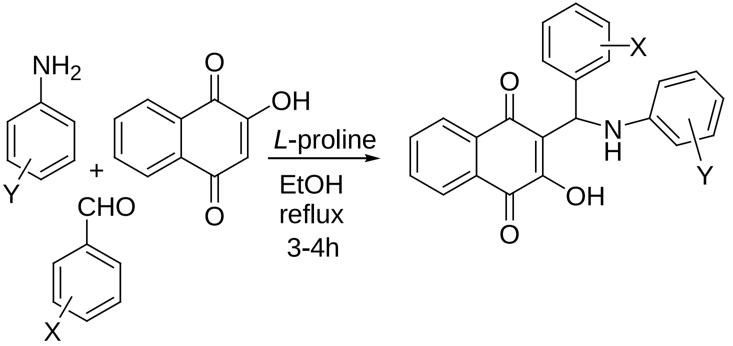

Fig. 1 Catalytic synthesis of synthesis of aminonaphthoquinones

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Boronic acid functionalized graphene platforms for diabetic wound healing

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Keywords: Graphene, boronic acid, diabetic wounds, dopamine, nematode, bacteria.

Graphene derivatives are two-dimensional platforms with a wide range of biomedical applications ranging from biosensors to tissue engineering[1,2]. To improve the antimicrobial activity of graphene derivatives, they should be equipped with functional groups that are able to attach to the membrane of pathogens strongly[3]. Due to the affinity of boronic acids towards cis-diol bearing biosystems[4], graphene sheets with this functionality were synthesized (Fig.1) and their covalent interactions with the bacteria and nematode were investigated. As expected, graphene platforms with boronic acid functionality (G-BA) were able to wrap bacteria and destroy it in a short time. Surprisingly, the body of nematodes was ruptured by graphene sheets and their viability decreased to 30% after 24 h incubation time. Because of their strong antibacterial and antiparasitic activities as well as their ability for wound dressing, graphene platforms with the boronic acid functionality were further investigated for diabetic wound healing. In vivo experiments showed that graphene platforms are more efficient than the commercially available drug, phenytoin, and restore both infected and non-infected diabetic wounds in ten days. The results indicate boronic acid functionalized graphene sheets are promising candidates for a broad range of future biomedical applications.

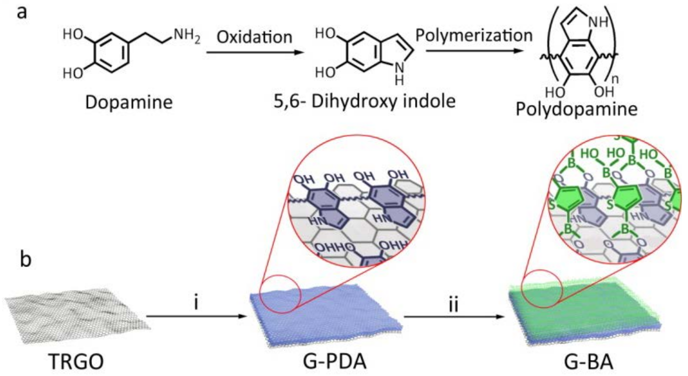

Fig. 1 a) Schematic representation of the self-polymerization of dopamine. b) Preparation of i) G-PDA and ii) afterwards attachment of 2,5-thiophenediylbis-boronic acid to its catechol groups to obtain graphene platforms with the boronic acid functionality (G-BA).

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Synthesis of responsive theranostic nanogels

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Keywords: Theranostic nanogel, Redox-sensitive, Doxorubicin

Theranostic nanogels simultaneously carrying both fluorescence-activable probes and therapeutic agents were primarily utilized to investigate drug delivery process. Targeted molecular imaging, an essential component of a theranostic system, can be used to image and track molecular targets involved in disease progression. Nanogels have the characteristics of hydrogels and colloidal nanoparticles such as blood transfusion capability, absorbing a large percentage of water, biocompatibility, high loading capacity and precision of active substances.[1-4] In this study, novel redox-sensitive nanogels with theranostic performance to significant abnormalities in the blood were synthesized. The performance of the theranostic system was evaluated in the measurement of hydrogen peroxide in the blood samples of cancerous patients using fluorescence technique. Results revealed that this theranostic nanogel can be used at treatment centers for early diagnosis and treatment of cancer.

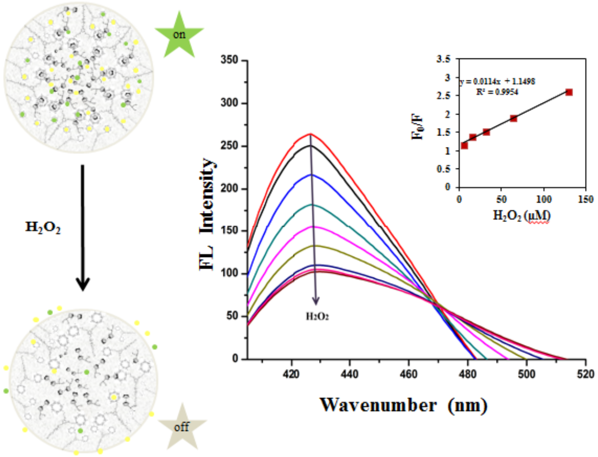

Fig. 1 Fluorescence-activable nanogel

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Large area synthesis of biodegradable two-dimensional polymer

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Keywords: 2D Polymers, Biodegradable, Drug delivery.

The two-dimensional polymers (2DPs) are topologically planar sheets that have repeat units rendering them crystalline in at least one confirmation. They are anticipated to be useful for a wide range of technological applications. The design and synthesis of two-dimensional (2D) polymers is a challenging task. Depending on their structure, such structures may find useful applications in many diverse areas including controlled drug delivery, chemical sensing and can also potentially act as well-defined 2D scaffolds for ordered functionalization or platforms for bottom up 3D construction.[1-3] We present the synthesis of a biodegradable 2D polymer in the micrometer lateral size regime through covalent bonds. Polymer is containing well-defined pores and is able to load and transport a high amount of therapeutic agents.

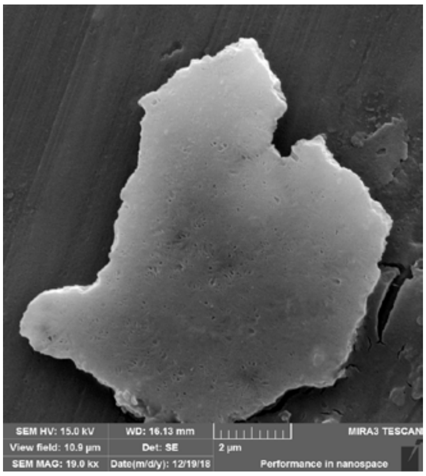

Fig. 1 FE-SEM image of biodegradable 2D polymer.

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Preparation of water insoluble β-cyclodextrin-co-thiourea polymer and its application as a new absorbent for removal Lead (II) ions from Wastewater

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Keywords: β-cyclodextrin-thiourea, Removal of heavy metal ions, Lead (II) ions.

A novel insoluble β-cyclodextrin-thiourea (β-CD-TU) polymer was synthesized from reacting thiourea with nanoporous β-cyclodextrin and epichlorohydrin. The structure of this polymer was characterized by fourier transform infrared (FT-IR), scanning electron microscope (SEM), thermal gravimetric analysis (TGA) and elemental analyses (CHNS). The prepared porous co-polymer was used as very attractive and effective adsorbents for the removal of heavy metal ions such as lead(II) ions from wastewater. The effect of contact time and initial adsorbent dose on the extent of adsorption was investigated. The equilibrium data obtained by experiments were well analyzed by adsorption isotherms which the results are well fitted with Langmuir model at ambient temperature. A maximum monolayer coverage capacity (q_m) 285.126 mg.g^{-1}. More importantly, the adsorption effectiveness of the β-CD-TU remained constant through five regeneration cycles.

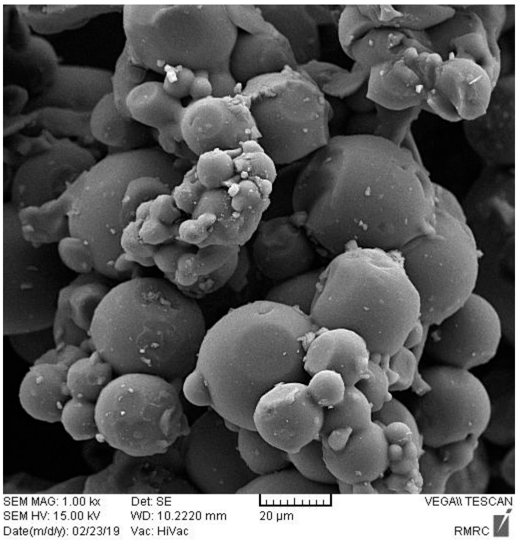

Fig. 1 FE-SEM image of cyclodextrin-thiourea

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Synthesis of diazo functional copolymers based on melamine-paraformaldehyde

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Keywords: Diazo polymers, Polymerization, Synthesis, Diazonium salt.

Polymeric architecture at different levels plays a key role to influence the photoresponsive behavior of azo polymers. In the past decades, azo polymers with different polymeric structures have been synthesized, such as sidechain polymers, main-chain polymers, dendritic polymers, crosslinked network, and block copolymers.[1,2] Typically, azo polymers can be prepared by radical polymerization and step-growth polycondensation.[3,4] In this work diazo functional copolymers based on poly melamine-paraformaldehyde was synthesized. For this purpose firstly the melamine- paraformaldehyde copolymer was synthesized with excess ratio of melamine to form a water soluble copolymer with $-NH_2$ end groups. Then the prepared copolymer was reacted with $NaNO_2/HCl$ to from diazonium salt. In the final step, the azo-functionalized copolymers were synthesized using phenol, aniline or 4-nitro aniline compounds. The synthesized compounds were characterized by spectroscopic methods and their properties were studied.

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SBA-15 supported acidic ionic liquid (IL-HSO_4@SBA-15) for clean oxidation of aromatic and aliphatic sulfide in water

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Keywords: SBA-15, Ionic liquid, Clean oxidation, Sulfide.

During the last decade, ionic liquids (ILs) are being more and more regarded as green catalysts and solvents due to their low volatility, negligible vapor pressure, reasonable thermal stability, outstanding recyclability and reusability [1]. In the recent years, the immobilization of ILs into mesoporous SBA-15 (IL@SBA-15) has attracted more attention in replacement of the conventional minerals amorphous silica based on their high surface area, high thermal and mechanical stability [2]. An important use of ionic liquids is the use of acid catalyst [3]. In this communication,ionic liquid functionalized SBA-15 were prepared and applied as an efficient and recyclable metal and halogen free catalyst for selective oxidation of broad range of aromatic and aliphatic sulfides with aqueous hydrogen peroxide. This ronsted acidic ionic liquid catalyst has been reused more than 10 runs. Figure 1 illustrates the proposed mechanism of the reaction.

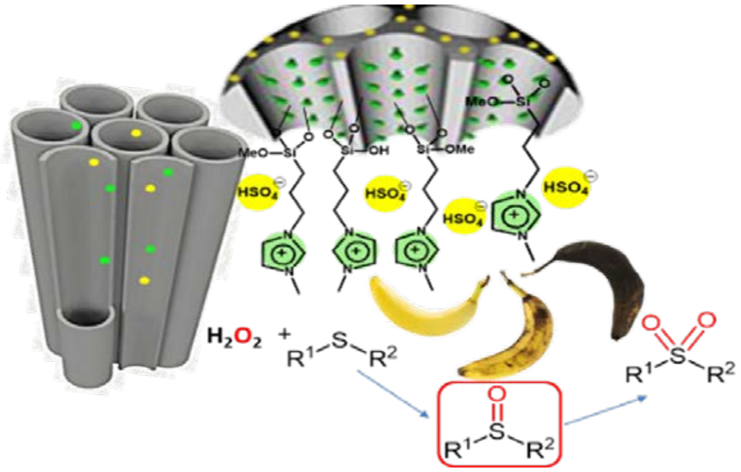

Fig. 1 preparation of IL@SBA-15 for the aqueous oxidation of sulfids.

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Design and synthesis of metal-organic frameworks of $Cu_3(BTC)_2$ microbelts for waste-free green oxidation of sulfides

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Keywords: Open metal site MOFs; $Cu_3(BTC)_2$, Microbelts (MBs), sulfide oxidation,

Metal oganic frameworks (MOFs) as porous coordination polymers are nanoporous materials prepared using the well-established principles of coordination chemistry [1, 2]. MOF-based structures demonstrate various advantages such as having high surface areas and simplicity of processability, and being tuneable and stable alternative materials [2, 3]. Herein, we report the synthesis of open metal site MOFs of $Cu_3(BTC)_2$ with microbelt morphology and a study of the catalytic oxidation of organic sulfides Figure 1. The proposed catalyst was found to be an efficient, selective and waste-free green heterogeneous co-catalyst for the green H_2O_2 catalytic oxidation of sulfides.

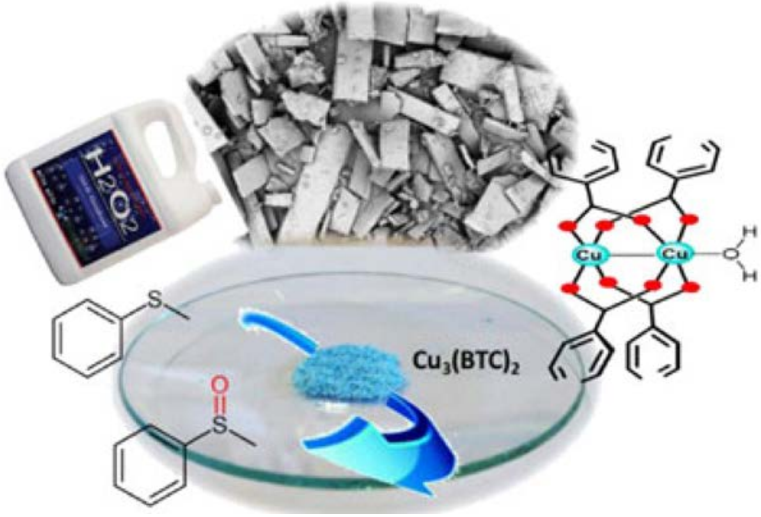

Fig. 1 $Cu_3(BTC)_2$-catalysed green sulfide oxidation.

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A green one‑pot synthesis of triazolo[2,1‑*b*]quinazolinones in choline chloride-based deep eutectic solvent

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Keywords: Multicomponent reactions, Choline chloride, Deep eutectic solvents, Triazolo[2,1‑ *b*]quinazolinones, Green organic synthesis.

Recently, research on deep eutectic solvents (DESs) as a new generation of eco-friendly solvent/catalyst systems has attracted strong interest in organic synthesis. DES consists out of two or three components which combine *via* hydrogen bond interactions to form eutectic mixtures, characterised by a melting point lower than that of each individual component. [1, 2] Quinazolinone derivatives are important class of heterocyclic compounds with various applications in pharmaceutical industries.[3] Hence, design and development of novel synthetic methods to the synthesis of the libraries of these compounds is an interesting field for many organic chemists. As a part of our continuing interest on designing environmentally benign methods for various chemical transformations, herein we have described an efficient and more practical route for the synthesis of triazolo[2,1‑ *b*]quinazolinones using modified ChCl based DES as a green catalyst. All reactions are performed during acceptable time with high efficiency.

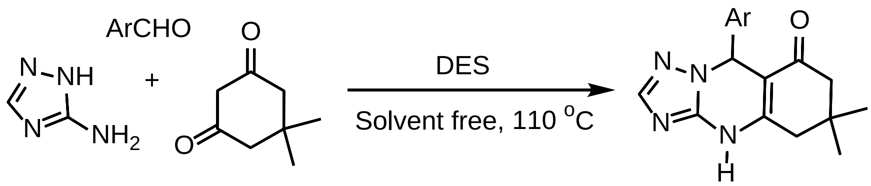

Fig. 1 DES catalyzed the synthesis of triazolo[2,1‑ *b*]quinazolinones

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Preparation and Characterization of New Inorganic-Organic Hybrid Catalyst and Its Application for Diastereoselective Synthesis of 2-Azapyrrolizidine Alkaloid Scaffolds

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Keywords: Organic-inorganic hybrid silica; Tetradentate ligand; Multicomponent reaction; Diversity-oriented synthesis.

Since the development of ordered mesoporous silicas [2], SBA-15 materials developed by Zhao and Stucky serve in many fields due to their interesting textural properties such as appreciable thermal and hydrothermal stability, large pore volume, uniform-sized pores (in the range 4-30 nm) and high special surface area (above 1000 m2/g) [3]. We are interested in the development of our research to prepare more effective catalyst to synthesize 2-aza analogue of pyrrolizidine and spirooxindole-2-azapyrrolizidine derivatives. Nano-catalyst W(IV)/NNBIA-SBA-15 was prepared by applying simple and cost-effective materials and also it was characterized as a new inorganic-organic hybrid catalyst. The one-pot reaction of aldehyde or isatin (1 mmol), malononitrile (1 mmol), and hydantoin (1 mmol) were catalyzed by W(IV)/NNBIA-SBA-15 in the water. All synthesized compounds are characterized by ^{1}H NMR and IR spectroscopy.

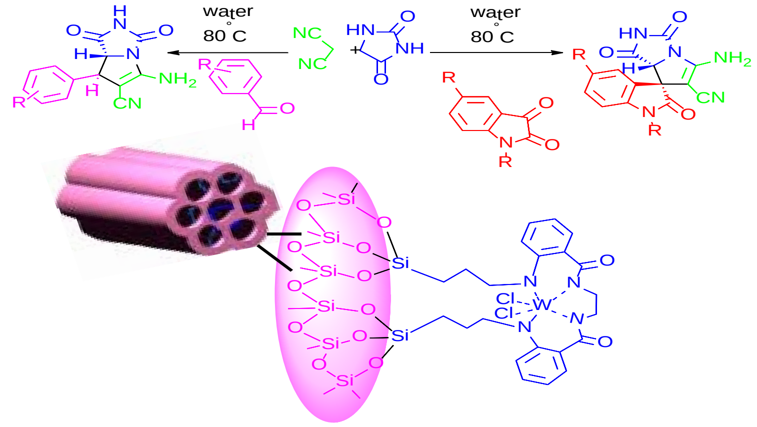

Fig. 1 Synthesis of the 2-aza analogue of pyrrolizidine and spirooxindole-2-azapyrrolizidine derivatives.

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Improvement of one-pot synthesis of benzothiazole by using methallophthalocyanine as catalyst under solvent-free and microwave conditions

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Keywords: Metallophthalocyanine, Benzothiazole, Condensation reaction, Microwave.

Benzothiazole derivatives are important heterocyclic compunds and due to their biological and pharmacological properties are used in organic and medicinal chemistry.[1-2] For example,benzothiazoles are used for antitumor,[3] anti-hepatitis C virus[4] drugs and industrial applications as vulcanization accelerators and antioxidants. Therefore, in recent years, researchers are interested in preparation and development of benzothiazoles. There are different methods for the synthesis of benzothiazoles. This article reports the condensation reaction between 2-aminothiophenol (1) and different aldehydes (2) by using metallophthalocyanine as efficient and acsessable catalyst and under microwave irradiation (Fig.1). All synthesized compounds characterized by using spectroscopic technique such as: mass spectrum, ^{1}H and ^{13}C NMR and FT-IR spectroscopic data.

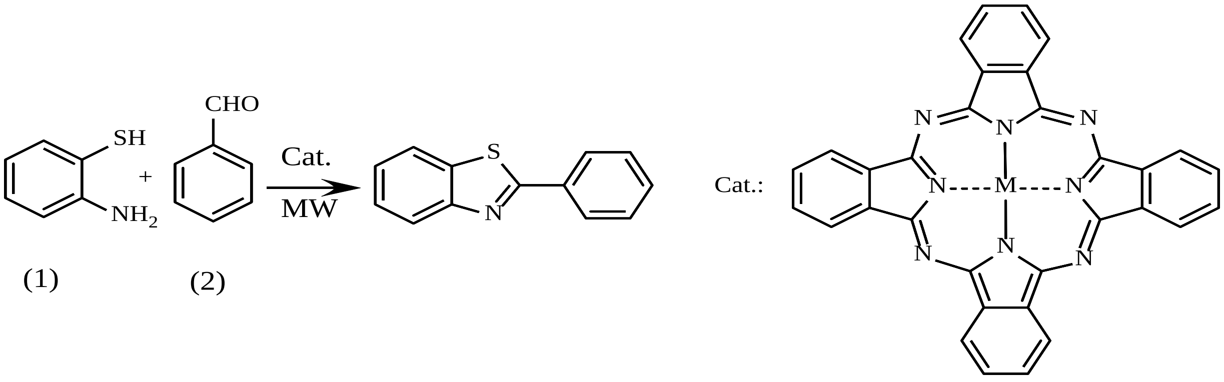

Fig. 1 Synthesis of some benzothiazole derivatives using metallophthalocyanines as catalyst

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Facile, efficient and one-pot synthesis of some metallophthalocyanines using microwave irradition

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Keywords: Metallophthalocyanine, One-pot, Phthalic anhydride, Microwave.

Phthalocyanines are planar macrocycles, small organic molecules with an 18-π electron system.[1] Phthalocyanine derivatives that have a similar structure to porphrins, are used as functional materials especially with regard to their properties as dyes. Phthalocyanines have important properties such as electron transmission ability, condensation and optical properties. Metallophthalocyanine complexes are used as blue-green pigments for printing inks, laserbeam printers in non_linear opticals, as photosensitizers,[2] as carrier generation material in near infrared (NIR),[3] photoconductors, electrical conductors, catalysts and in photodynamic therapy.[4] Metallophthalocyanines are usually prepared from the reaction between phthalonitrile, urea, metal salts and hexamethyldisilazane.[5] This article shows the use of phthalic anhydride (2), urea (3), metal salts (1) in the presence of hepta ammonium molibdate as catalyst under microwave irradiaton (Fig.1). The advantage of this method for the synthesis of metallophthalocyanine are high yield, solvent-free conditions, capability for scale-up and simple procedure. All synthesized compounds characterized by FT-IR spectroscopic data.

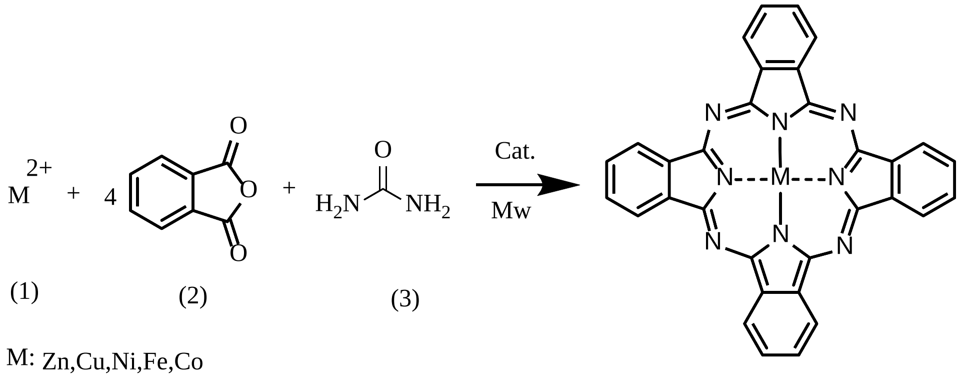

Fig. 1 Preparation of some metallophthalocyanines in macro scale

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Synthesis of 5-Arylidene barbituric acid derivatives using a bis compound of imidazole as an organocatalyst in water

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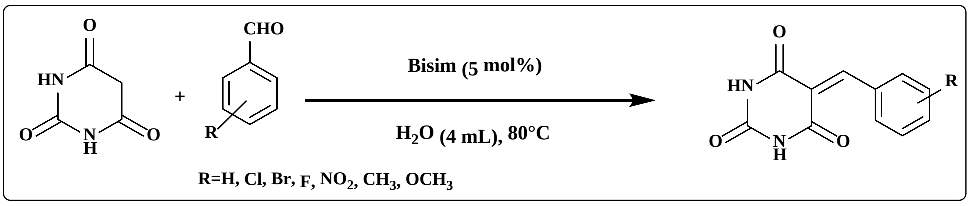
Keywords: Organocatalyst, Bis-imidazole, 5-Arylidene barbituric acid, Water

Organocatalysis term is referring to the promotion of the chemical reactions using catalytic amounts of an organic compound which only consist of hydrogen, carbon, nitrogen, oxygen, sulfur and phosphorus atoms without any metallic atoms or ions. The importance of these types of catalysts has been increasing due to their novelty, excellent selectivity and efficiency in the synthesis of more complicated compounds. Although it is not a long time of recognition of these compounds in the separated field in the catalysis, many advantages of their utilization in the organic reactions such as non-sensitive to moisture and oxidants, accessibility, low toxicity and price are unique and remarkable.[1-3]

Imidazole is a five-membered heterocycle containing two non-adjacent nitrogen atoms. This cyclic structure is available in many natural and bio-active compounds such as histidine, histamine and purine. Besides, a few drugs have been reported to have an imidazole ring in their structures.[4-5]

In continuation of our interest in the application of new catalysts in organic synthesis, we decided develop an efficient synthetic processes using green and eco-friendly methods for the synthesis of 5-arylidene barbituric acid derivatives in a Knoevenagel reaction of various types of aldehydes and barbituric acid in the presence a bis compound of imidazole as an organocatalyst (Scheme 1).



Scheme 1. Synthesis of 5-arylidene barbituric acid derivatives

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synthesis of pyrano pyrimidines using by guanidine as a base catalyst in aqueous media

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Keywords: Catalyst, Knoevenagel condensation, 1,3-dimethylbarbitoric acid ,Three-component reaction

Multi-component reactions (MCRs) achieve significant task in combinatorial chemistry due to the ability to prepare target compounds with more efficiency and atomic economy by the reaction of three or more compounds together in a single step. Moreover, MCRs increase simplicity and synthetic efficiency on the conventional organic transformations.[1-2]

Recently, pyran and substituted 4H-pyrans have attracted wide notices. They perform the major construction blocks of several natural products and form the core of noteworthy compounds are displaying broad biological activities such as; antimicrobial[3], antiviral[4] activities and antiprolife reation agents.

In this research, a mixture of dimethylbarbituric asid(1mmol), malononitril (1mmol) and aldehyde (1mmol) in the presence of guanidine as a base catalyst in queues media at room temperature to afford 7-amino-1,3-dimethyl-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydro-1*H*-pyrano[2,3-*d*] pyrmimidine-6-carbonitrile derivatives in high to excellent yields as target products.

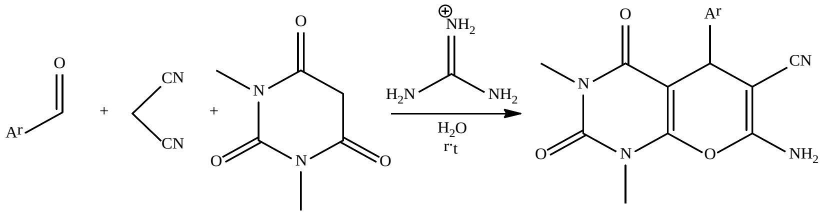

Fig. 1 Multicomponent synthesis of 7-amino-1,3-dimethyl-2,4-dioxo-5-phenyl-2,3,4,5-tetrahydro-1*H*-pyrano[2,3-*d*]pyrimidine-6-carbonitrile

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Computational studies on the Li-$B_{12}N_{12}$ as potential adsorbent for aniline from environment

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Keywords: Boron nitride nanocage, Aniline, Adsorbent, Electronic structures.

Aniline ($C_6H_5NH_2$) is an important organic compound due to its wide applications in the manufacturing of dyestuffs, rubbers, pesticides, plastics and paints [1]. Aniline is released throughout the environment by industrial wastewater and/or through degradation of some of the above mentioned compounds [2]. Adsorption of aniline molecule on the surface of Li-doped B12N12 nanocage is scrutinized using at Density functional theory (DFT) calculations to investigating its potential as chemical adsorbent. DFT calculations at the B3LYP [3] /6-31G*level were performed in terms of energetic, geometric, and electronic properties. People had shown that piristin nanocages are weak absorbents. In order to improve the properties of the nanocage adsorbent, Li doping process was investigated. The obtained results show that doping process changes electrical properties of B12N12 dramatically. It was found that aniline is more likely adsorbed via its nitrogen atom on the Li-B12N12 surface. The adsorption energy of aniline on the nanocage in the most stable state is -45.06 kcal/mol and about 0.28|e| is transferred from the aniline molecule to the nanocage. IR spectra confirm sensing ability of Li-doped B12N12 for adsorption of the aniline molecule. It is expected that Li-doped B12N12 acts as new potential adsorbent for toxic aniline molecules from environmental systems.

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Preparation of poly(glycidyl methacrylate) and its application as a good absorbent for removal of Ethyl violet

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Keywords: Poly glycidyl methacrylate, *p*-Aminophenylacetic acid, Adsorption of ethyl violet, Ring opening reaction

Organic dyes is one of the major groups of pollutants widely used in textile, plastic, medicine and many other industries, while the hazardous effects of organic dyes in waste water have been a major concern and now a major threat in the environment due to the substantial pollution problems caused by them. In this research a novel polymer was synthesized from glycidyl methacrylate. In suspension polymerization system, poly(glycidyl methacrylate) (PGMA) microspheres are firstly prepared. Then, ring opening reaction takes place when p-aminophenylacetic acid is bonded on PGMA microspheres to obtain functional PGMA-p-aminophenylacetic acid microspheres for first time. The prepared functionalized polymer characterized by transmission electron scanning electron microscopy (SEM), X-ray diffraction, and Fourier transform infrared spectroscopy (FT-IR) and applied investigated for the reduction of ethyl violet in an aqueous medium at 25 °C. The adsorption process monitored using UV-visible spectroscopy. The results show poly(glycidyl methacrylate) is an efficient absorbent for water purification and also useful to find numerous potential applications such as drug delivery systems.

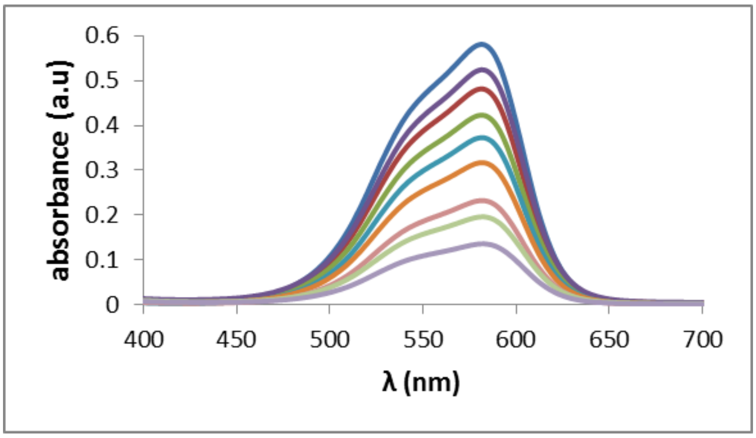

Fig. 1 UV-vis spectra for the adsorption of ethyl violet

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Tailor-made Thin Film Nanocomposite Membrane Incorporated with Boron Nitride Nanosheets for the Removal of Dye Water

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Keywords: Thin Film Nanocomposite; Interfacial Polymerization; Boron nitride; Salt Rejection

Two-dimensional (2D) layered hexagonal boron nitride nanosheets (h-BNNs), known as white graphene, is a fascinating class of nanomaterials with a high potential in catalysis, electronics, photonics, energy storage, and sensing. In this study, we report on a straightforward approach to modify the surface of BN with cyclopentadienyl and its application as a new absorbent for the removal of dye from water. Cyclopentadienyl-functionalized boron nitride (cpd-hBNNs) were characterized by FE-SEM and as well as BET analysis. Collectively, our results showed that cpd-hBNNs, with the high adsorption capacity and reusable property, is a promising candidate for the removal of pollutants from water. It is found that with the presence of BNCD, the TFN membranes exhibited higher surface hydrophilicity due to increment in Negative group and carboxyl groups in PA layer, hence, improved the attraction between water molecules and membrane surface. Upon incorporation of of BNCD, the resultant TFN membrane achieved 98% removal rate for MgSO4, respectively along with 31.4% higher water flux than the membrane contained no BN.

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One-step synthesis of three-dimensional graphene/polyaniline nanocomposite

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Keywords: 3D Graphene, Polyaniline, Nanocomposite.

Now days, three-dimensional graphenes have been attracting much attention since they not only preserve the intrinsic properties of 2D graphene flakes but also provide advanced functions with improved performance in various applications. In this study, we prepared a three-dimensional graphene/polyaniline nanocomposite via a One-Step hydrothermal process. The nanocomposite has been characterized by scanning electron microscopy (SEM), infrared spectroscopy (IR) and X-ray diffraction analysis (XRD). The results of XRD and FTIR indicated that the presence of polyaniline nanoparticles in nanocomposites, are in agreement with the SEM observation.

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Highly Efficient and Reusable MCM-41-Immobilized 2-(Methylthio)cyclohexanone Copper(I) Catalyst for the Sonogashira Coupling of Arylhalides with Phenylacetylene

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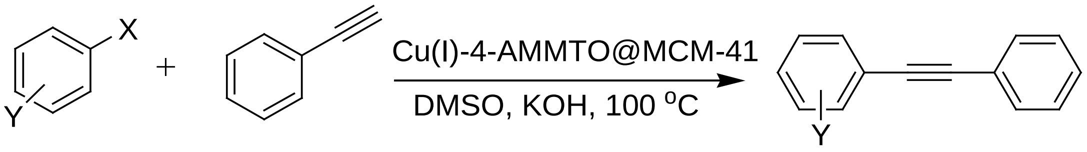
Keywords: Sonogashira, MCM-41, C-C coupling, Arylhalides, Heterogeneous

Catalytic methods including the C-C bond formation reactions have been appeared as most multipurpose and influential tool for the production of value added A useful and effective technique for carbon-carbon bond constructions is c opper catalyzed Sonogashira coupling reaction that plays a key role in contemporary synthetic chemistry. In fact Sonogashira coupling products that consist of a triple bond into aromatic systems are building blocks for an extensive range of natural and pharmaceuticals materials.

A highly efficient MCM-41-immobilized 2-(methylthio)cyclohexanone copper(I) complex [Cu(I)-2-MCH@MCM-41] was prepared from 2-(methylthio)cyclohexanone via immobilization on mesoporous material MCM-41, followed by reacting with CuI. The catalyst was applied for the C−C cross-coupling reaction of aryl halides with phenylacetylene. Corresponding products were produced in good to excellent yields in N_2 atmosphere. The catalyst could be recovered and recycled for several consecutive runs[1-3].



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A novel heterogeneous nanocatalyst: 2-Methoxy-1-phenylethanone functionalized MCM-41 supported Cu(II) complex for C-S coupling of aryl halides with thiourea

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Keywords: Copper(II) catalyst, C-S coupling, heterogeneous, MCM-41, thiourea

An environmentally friendly copper-based catalyst supported on 2-Methoxy-1-phenylethanone functionalized MCM-41 was prepared and characterized by FT-IR, FE-SEM, TEM, XRD, EDX, BET and ICP techniques. The catalyst was applied for the C−S cross-coupling reaction of aryl halides with thiourea. Corresponding products were produced in good yields in aerobic conditions. The catalyst could be recovered and recycled for several time[1-10]..

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Tetracycline as a pot life extender for high-filled polyurethane composites

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Keywords: pot life, pot life extender, viscosity build up, binder system, polyurethane composite

High-filled polyurethane composites based on hydroxyl terminated polybutadiene (HTPB) are widely used. The HTPB composite slurry should have a good viscosity at the end of the mixing to prepare convenient casting. The time available for casting after curative addition is called pot life.[1,2] Pot life extension is the topic of different researches recently. There are different methods to extend pot life which can be categorized to material and process approaches. Tetracycline addition is a new way to extend the pot life and called pot life extender. Studies showed that pot life of high-filled polyurethane composites based on HTPB can be considerably extended to 2-4 times by addition of tetracycline. Elamin et al. showed that the addition of 0.1% of tetracycline decrease viscosity build up rate or extend the pot life significantly (Figure 1). Moreover, mechanical properties of high-filled polyurethane composites based on HTPB containing tetracycline are better in comparison to without tetracycline.[3]

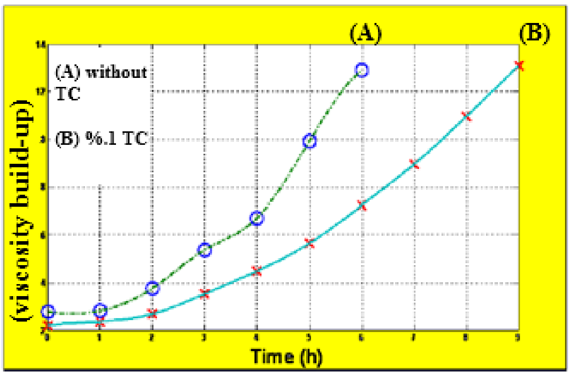

Fig. 1 Viscosity build up (reverse of pot life) vs. time after adding tetracycline for high-filled polyurethane composites [3]

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Synthesis of new triazolo[1,5-*a*]pyrimidine using ketene dithioacetals

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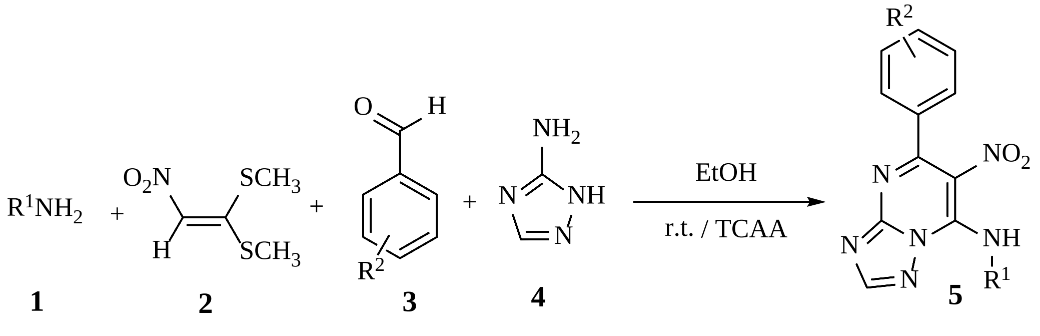
Keywords: 3-Amino-1,2,4-triazole, Nitroketene dithioacetals, Triazolo pyrimidine, Multicomponent reactions.

Triazole and its derivatives as highly significant nitrogen-containing heterocycles are attracted considerable attention in fields, such as medicinal and agrochemical research as well as in the material sciences due to their unique structure, hydrogen-bonding and dipole interactions.[1] Many substituted triazole compounds continue to be of scientific and engineering interest. The scaffolds containing triazole are promising candidates to inhibit acidic corrosion of steel. The interesting biological activities of triazole are versatile such as anticancer, anti-human immunodeficiency virus, antilieshmanial, antitrypanosomal, and antibiotic.[2] In the view of above-mentioned points, an interesting one-pot four-component reaction developed for the synthesis of *N*-methyl-6-nitro-5-phenyl-[1,2,4]triazolo[1,5-*a*]pyrimidine-7-amine **5** *via* reaction of primary aliphatic or aromatic amines **1**, nitroketene dithioacetals **2** followed by the subsequent condensation with aliphatic or aromatic aldehydes **3** and 3-amino-1,2,4-triazole **4** in the presence of trichloroacetic acid (TCAA) as a Brønsted-Lowry acidic catalyst (Scheme 1). The direction of heterocyclization and the structure of final products identified spectroscopically.



Scheme. 1 Synthetic scheme for the generation of triazolo[1,5-*a*]pyrimidine.

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The investigation of catalyst effect on curing kinetics of HTPB-TDI binder system by differential scanning calorimetry (DSC)

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Keywords: DSC, Heating rate, Catalyst, Released heat.

DSC method was used to investigate the curing kinetics of HTPB-TDI curing reaction like the other articles.[1-3] In this investigation, four heating rates (5, 10, 20, 40 ℃/min) were used to examine curing behavior of HTPB-TDI binder system, that just one of them (10 ℃/min) is demonstrated in figure 1-a. In the presence of catalyst (DBTDL), it's clear that the curing reaction has two different stages as two distinctive peaks has been observed (Figure 1-a). Two stages curing behavior exists in both catalytic and non-catalytic modes, but the different peaks are more obvious in the presence of catalyst. Peak separation and two-peak presence may be due to reduced activation energy as a result of using DBTDL catalyst. By calculating of the activation energy required for the formation of polyurethane, it is understood that activation energy for the non-catalyst state is about 36 kJ/mol more than the catalytic state. Since the use of the catalyst has reduced the activation energy, the rate of reaction has increased, and consequently, the released heat of reaction has increased. As shown in Figure 1-b, the amount of heat released decrease is more sensitive to heating rate for catalytic mode. It means that, when catalyst has been used in binder system, effect of heating rate on the released heat is negligible and therefore it may be predicted that the physical and mechanical properties will not mainly changed as the heat released during curing reaction is approximately constant.

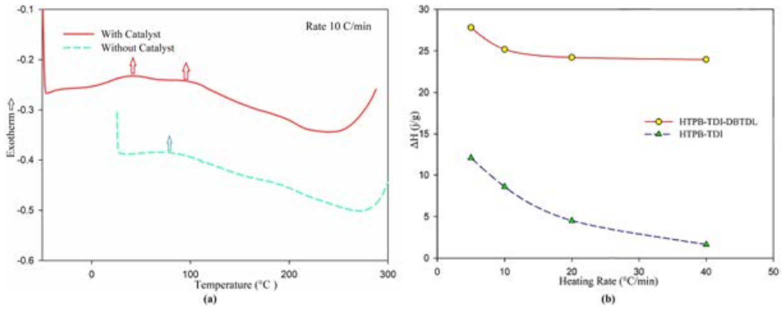

Fig. 1 Comparison of HTPB-TDI charts (a) and heat released (b) in two catalytic and non-catalytic states.

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The synthesis of poly substituted amino pyrazoles using *N*-heterocyclic sulfonic acid trichloro zincate

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Keywords: Multicomponent reactions, Amino pyrazole, Solvent-free.

Amino pyrazole derivatives is a class of pyrazole compounds which widely used in organic synthesis for the preparation of target compounds with high biological activity and also applied in the structure of drugs.[1] Various catalysts were reported for the multi component synthesis of poly substituted pyrazoles as significant medicinal heterocyclic compounds. These compounds were prepared by several catalysts such as ionic liquids,[2] molecular iodine,[3] piperidinium acetate [4] and $Cu(OAc)_2$.[5] In continuation of our previous projects involving the preparation and applications of acidic ILs and solid salts in organic transformations, we have prepared and characterized a new catalyst as a *N*-heterocyclic sulfonic acid trichlorozincate which S-N bond formation has been formed in a six members heterocyclic compounds and it was utilized for the synthesis of polysubstituted 5‑aminopyrazole‑4‑carbonitriles which exhibits many interesting properties (Scheme 1).

Fig. 1 The synthesis of 5‑ aminopyrazole‑ 4‑ carbonitriles.

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Synthesis of new indole substituted pyrazolo[3,4-*b*]quinoline via a sequential four component reaction

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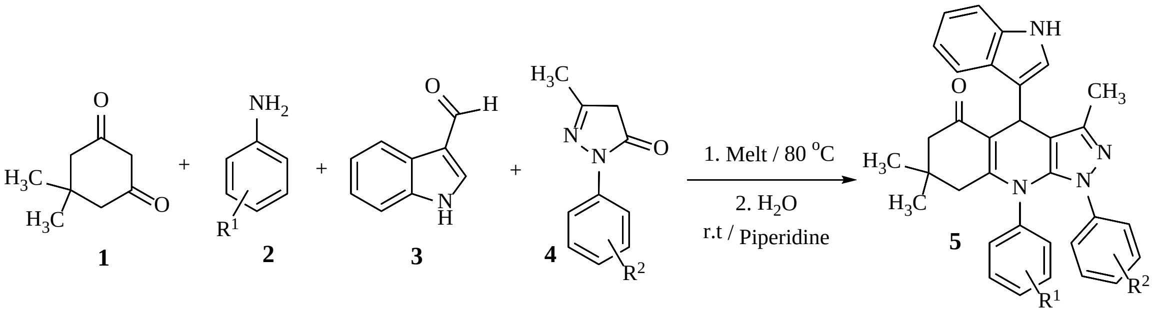
Keywords: Pyrazolo[3,4-*b*]quinoline, Indole-3-carboxaldehyde, Michel acceptor, Enamine.

Among nitrogen-containing heterocyclic compounds, pyrazolo quinolines have paid significant interest in medicinal chemistry due to uniqueness in biological activities such as antiviral, antimicrobial and antimalarial activities, and also used as optical brightener, dyestuff and as colorant.[1,2] In this paper, new pyrazolo[3,4-*b*]quinoline derivatives substituted with indole **5** have been prepared, based on the reaction of enamines and Michel acceptor *via* the one-pot, multicomponent reaction of dimedone **1**, various aniline **2**, indole-3-carboxaldehyde **3**, and pyrazolone as an enolizable C−H activated compound **4**, under mild conditions respectively in the stoichiometric melt and H_2O in the presence of piperidine (Scheme 1). In order to increase the therapeutic properties of pyrazolo[3,4-*b*]quinoline, we synthetically attached the indole ring with a broad range of biological activity in medicinal chemistry including antihypertensive, antiproliferative, antiviral, antitumor, analgesic, anti-inflammatory, antimicrobial and antifungal activities.[3]



Scheme. 1 Synthetic scheme for the formation of indol substituted pyrazolo[3,4-*b*]quinoline **5**

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Domino synthetic approach toward new spirooxindole pyran scaffolds

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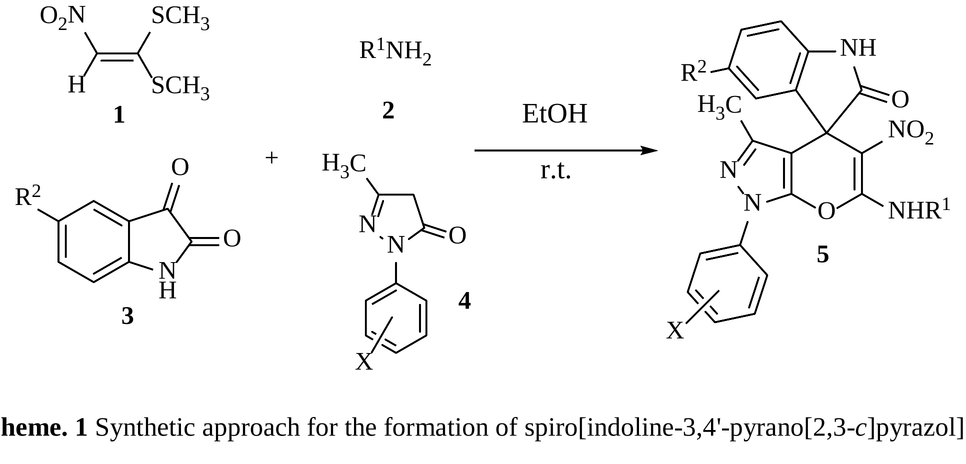
Keywords: Spirooxindole, Pyran, Catalyst-free approach, Nitroketene dithioacetals, Isatin.

Due to the necessary need of small molecules containing bioactive heterocycles for biological targets, access to wide compound collections with potential biological activities is highly desirable.[1] Heterocyclic spirooxindole pyran are attractive synthetic targets due to their biological activities such as antiviral, antibacterial, antifungal, anti-HIV, and anti-cancer activities.[2] With this background for the formation of molecular architectures with wide potential biological activities, here we designed and introduced a new protocol involves four-component reaction of the nitroketene dithioacetals **1**, alkylamine/benzylamine **2**, isatin **3** and pyrazolone **4** as an enolizable C−H activated compound under mild and catalyst-free conditions leads to new functionalized chiral spirooxindole pyrans named spiro[indoline-3,4'-pyrano[2,3-*c*]pyrazol] **5** in moderate to good yields (Scheme 1). Prominent advantages of this method are the diversity of molecular structure, easy workup, in the absence of a catalyst and operational simplicity.



Scheme. 1 Synthetic approach for the formation of spiro[indoline-3,4'-pyrano[2,3-*c*]pyrazol] **5**.

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Micellization and phase transfer application of a novel amphiphilic random polyurethane

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Keywords: Amphiphilic polyurethane, Polymer micelle, Encapsulation, Phase transfer

Amphiphilic polymers which are macromolecules with hydrophilic and hydrophobic moieties, explored as systems for nanoencapsulation, phase transfer, nano-reactors and catalysis[1]. Their amphiphilic core-shell structure provides good solubilization for hydrophobic or hydrophilic guest molecules in their micellar structure in polar aqueous or nonpolar organic media[2]. We have recently reported a synthesis of amphiphilic random polyurethane (APU) with hydrophilic and hydrophobic moieties (Fig. 1), while one would expect that this polymer behaves like a micellar host in a polar solvent. Here, the self aggregation and micelle formation of the APU was investigated using steady-state fluorescence spectra and dynamic light scattering (DLS). Also, the morphologies of the nanoparticles were investigated by scanning electron microscopy (SEM), ^{1}H NMR spectroscopy and water contact angle (WCA) measurements along with DLS. The ability of the copolymer to encapsulate, solubilize and transfer hydrophobic molecules (Nil red was usedas probe) through polar/nonpolar interface was evaluated.

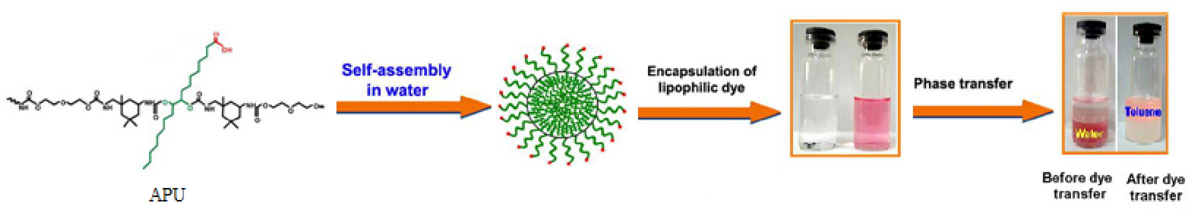

Fig. 1 Micellization of APU and dye transfer from aqueous phase into organic phase

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Immobilization of Cu species into the organosulfur modified channels of SBA-15 for green synthesis of tetrazoles

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Keywords: [3+2] cycloaddition reaction, Tetrazoles, SBA-15, mesoporous, Organosulfur.

The [3 + 2] cycloaddition of organometallic between nitriles and diverse form of azides was reported as common method for synthesis of tetrazoles which was recently studied *via* homogeneous and heterogeneous catalytic systems.[1] The ligands have inevitable role on the efficiency of metal catalysis. In this area, various copper/ligand catalytic systems were reported. The organosulfur-based ligands are one of the most important compounds which recently reported as a best functional group in coordination chemistry. Due to presence of nitrogen and sulfur atoms, these compound can be generate complex with different metals as a soft donor ligand.[2] In the present study, we have used SBA-15 silica mesoporous as a support for *in-situ* generation and stabilizing of Cu(I) species. The channels of SBA-15 were modified with organosulfur groups. This promising ligand into the SBA-15 led to the porous support with reductive nature. These well stabilized Cu(I) species into the nano-channels of SBA-15 were used for synthesis of various tetrazoles from sodium azide and aryl nitriles under green mild aqueous reaction conditions (Fig. 1).

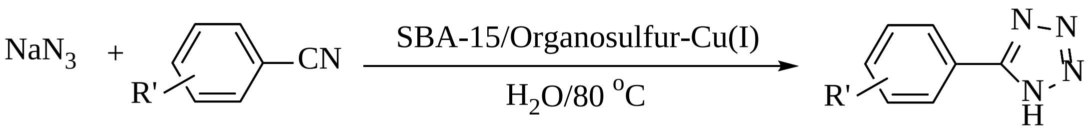

Fig. 1 Synthesis of substituted tetrazoles.

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Copper-catalyzed enantioselective esterification of allylic C-H bonds of olefins in the presence of heterogeneous oxazoline base ligands with aromatic substituents

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Keywords: Allylic C-H bonds oxidation, Heterogeneous oxazoline base ligand, Chiral allylic ester.

Asymmetric catalysis with chiral complexes has received considerable attention in recent years, and its contribution to the art of organic synthesis has become of leading importance. The ideal ligand, in principle, should offer the user a series of advantages: it has to be easily prepared, cheap and stable. It should also give very selective and flexible catalysts. Lately, oxazoline-based chiral ligands are considered as qualified catalysts by many of chemists.[1] The enantioselective allylic oxidation of olefins in the presence of copper catalysts is a topic of great interest and the reaction can be run using peresters to synthesize allylic esters (Kharasch-Sosnovsky reaction).[2,3] In this work, we prepared mesoporous silica MCM-41 and then functionalized by 3-chloro propyl trimethoxy silane. The synthesized chiral oxazoline ligands such as (*S*)-4-phenyl-4,5-dihydroxazole-2-amine and (*S*)-4-benzyl-4,5-dihydroxazole-2-amine immobilized on modified MCM-41. After that, we used the obtained chiral heterogeneous ligands in asymmetric allylic oxidation of alkenes.[4]

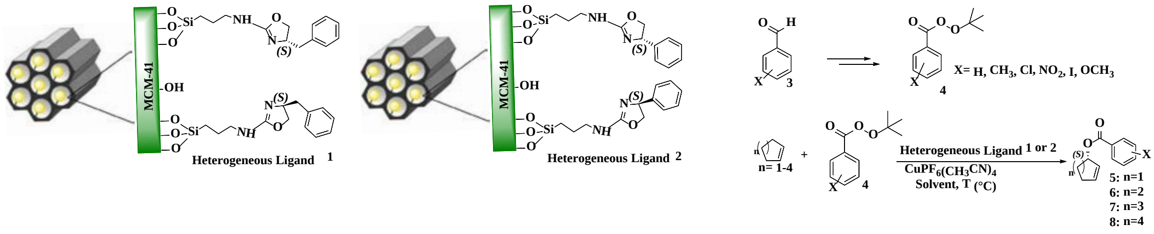

Fig. 1 Asymmetric oxidation of allylic C-H bond in the presence of heterogeneous chiral ligands and $CuPF_6(CH_3CN)_4$.

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Diastereoselective [5+1] double Michael reactions of thiooxindole with divinyl ketones: Synthesis of meso-spiro[cyclohexanone indoline-2-thione] by intramolecular induction with sulfur

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Keywords: Spiro-thiooxindole, Michael addition, Diastereoselective

The first diastereoselective synthesis of spiro-thiooxindole is reported *via* Michael reaction between thiooxindoles and divinyl ketones. The reaction was conducted without any catalyst or additive in ethanol as a green solvent at room temperature. This study showed the art of governing regioselectivity in which novel spiro frameworks were generated in high yields. In addition, simple purification process and diastereoselectivity make this protocol highly attractive. The structure of the products was investigated in the light of spectral data (IR, HRMS, ^{1}H-NMR, ^{13}C-NMR, NOESY, COSY, and X-ray diffraction). These compounds can be active biological substances and worthy of attention for the medicinal chemists.

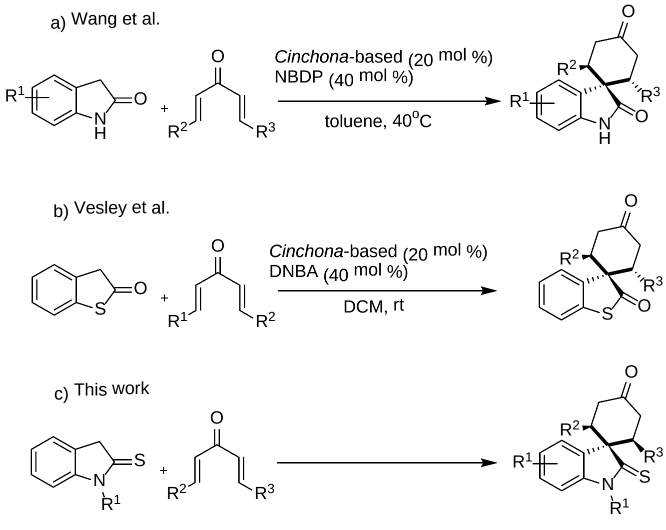

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Fig. 1 Comparison of different cascade [5+1] double Michael additions of divinyl ketones

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Measuring of Antioxidant Capacity and Phytochemical Evaluation of Two Genotypes of Hawthorn from Maragheh Region

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Keywords: Total phenols, Flavonoids, Anthocyanins, Ascorbic acid, Antioxidant

The antioxidant capability, total phenol, total flavonoid, anthocyanins, ascorbic acid contents, and reducing power contents of polar and non-polar extracts for two Genotypes of Hawthorn from Maragheh Region were evaluated in this work. The polar extraction of red type of Hawthorn had a higher total phenolic content as well as antioxidant the activity compared to that of the other subfractions. Antioxidant activities of the samples were determined by three various testing systems namely 2, 2-diphenyl-1-picrylhydrazyl (DPPH),[1] β-carotene/linoleic acid and reducing power assay.[2] In DPPH system, the highest radical scavenging activity was seen by the polar subfraction in of red type of methanol extract [44.05±4.52 (µg/ml)]. Our findings demonstrate that the methanolic extracts of two Genotypes of Hawthorn may be suggested as a new potential source of natural antioxidant.

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Manufacture of Thiophene Polymer Nanocomposite Coatings SBA15 and Its Application in the Extraction of Essential Oil of *Melissa officinalis* L.

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Keywords: Polythiophene, Hexagonally ordered silica nanocomposite, Solid-phase microextraction (SPME), Essential oil.

In this work, a highly porous fiber coated with polythiophene on hexagonally ordered silica nanocomposite (PT/SBA-15) was prepared and used for extraction of essential oils. The prepared nanomaterials were immobilized on a stainless steel wire for fabrication of the SPME fiber.[1] 40 compounds were separated and identified in *Melissa officinalis* which mainly included Geranial (34.4%), Neral (20.14%), Cis-Chresontynol (3.45%), and Trans Rose oxide (2.83%). The experimental results showed that the polythiophene/hexagonally ordered silica nanocomposite fibers were suitable for the semi-quantitative study of the composition of essential oils in plant materials and monitoring the variations in the volatile components of the plants.[2] In comparison to an HD method, the proposed technique could equally monitor almost all the components of the sample, in an easier way, shorter time and requiring a much lower amount of sample.

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Suzuki-cross-coupling reactions catalyzed by a new water dispersible Pd-NHC catalyst

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Keywords: Magnetically separable catalyst; Suzuki reaction, *N*-Heterocyclic carbene.

Transition-metal-catalyzed cross-coupling reactions have become a routine, straightforward, and powerful method for the preparation of carbon–carbon and carbon–heteroatom bonds in synthetic organic chemistry [1, 2]. Recently, *N*-heterocyclic carbene (NHC) ligands and their metal complexes have attracted many attentions in transition metal catalysis due to their ease of preparation, the strong σ-donor ability and effective binding strength to transition metals. The NHC transition metal complexes have been extensively used in organic transformations especially coupling reactions including Heck, Kumada and Suzuki– Miyaura.

Immobilization of homogeneous catalysts on the magnetic nanoparticles (MNPs) produces heterogeneous catalysts which can be easily isolated by using an external magnet. However, in most cases, the efficiency and selectivity of heterogeneous catalysts supported on MNPs are not desirable in water as a green solvent. To conquer this problem, micelles, surfactants or organic co-solvents have been used. A more desirable approach, which avoids using any additives, is designing water-dispersible MNPs. This allows reactions to be performed in pure water under near homogeneous conditions and also allows catalyst separation from the reaction mixture simply by an external magnetic field [3, 4]. In the work, we have synthesized a novel water-dispersible/magnetically recyclable Pd-NHC catalyst. The synthesized catalyst was characterized by FT-IR, XRD, XPS, EDX, TGA, VSM, TEM, and FE-SEM. We have successfully used this catalyst as a water-dispersible/magnetically recyclable Pd heterogeneous catalyst for Suzuki-cross-coupling reactions in neat water.

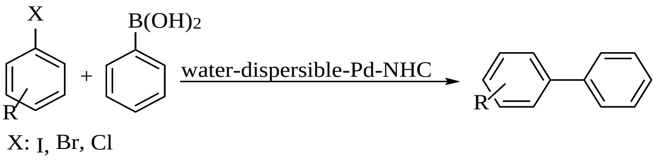

Fig. 1 Suzuki reaction of benzeneboronic acid with aryl halides catalyzed by water-dispersible-Pd-NHC

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Cobalt Complex of Metal–Organic Framework as an Efficient Visible-Light Photocatalyst for Oxidation of Alcohols

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Keywords: Metal-organic frameworks, Oxidation, Photocatalysis, Visible-light

Over the past two decades, the literature on metal–organic frameworks (MOFs) has increased rapidly. MOFs are a class of crystalline materials formed by transition metal-containing clusters as structural nodes bridged by organic linkers. Their intriguing aesthetic structures and outstanding properties such as high pore volume, high specific surface area, structural flexibility have led to the successful application of MOFs in gas adsorption, separation, chemical sensing, linear optical properties, as well as catalysis [1,2]. Recently, some attempts have been made to explore the potential of MOFs as a new class of photocatalysts. Of note, compared with the traditional photocatalysts, the superiority of MOFs is that the band gap which is closely related to the HOMO–LUMO gap, may be flexibly tuned by simply varying the connector and functionality of the organic linker. This would have a great influence on the optical absorption properties of the MOFs [3,4]. Despite the rapidly growing interest in MOFs, their photocatalytic performances have yet to be fully exploited.

In this article, Co-complex of metal-organic framework (MIL-101) was synthesized and characterized by a variety of techniques, including FT-IR, XRD, TGA, XPS, BET and ICP-OES analysis. This newly synthesized MOF was used successfully as a heterogeneous photocatalyst for the selective oxidation of alcohols to aldehydes under visible-light irradiation.

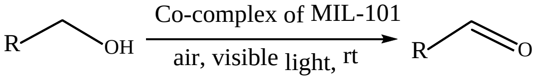

Fig. 1 Photocatalytic oxidation of alcohols by Co-complex of MIL-101

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Direct Conversion of Alcohols, Silyl and Tetrahydropyranyl Ethers to Oximes using Polyvinylpyrrolidone Supported Hydrogen Peroxide (PVP-H_2O_2) as a Catalyst

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Keywords: Alcohol, Ether, Oxime, Polyvinylpyrrolidone, Hydrogen peroxide.

Oximes are considered as very important and useful organic compounds due to their applications in various fields such as synthesis of agrochemicals and pharmaceuticals.[1] These crystalline and stable compounds can also be used in the synthesis of different other organic materials such as amides, nitro compounds, nitriles etc. In addition, oximation reaction is assumed as a very useful route for characterization and purification of aldehydes and ketones. Although the synthesis of these compounds from aldehyde and ketone sources is very well known, a few methods converting alcohols[2] or especially silyl (TMS) and tetrahydropyranyl (THP) ethers directly to oximes have been reported in the literature. Now, in the present work with the above description and in continuation of our pervious works about the oxime synthesis,[3] we report an efficient tandem oxidative method for the conversion of alcohols and TMS and THP ethers to oximes using a catalytic amounts of polyvinylpyrrolidone supported hydrogen peroxide (PVP-H_2O_2) as a mild, solid and stable oxidant[4] and hydroxylamine hydrochloride under solvent-free conditions (Scheme 1). This method follows "green chemistry" due to its tandem and catalytic nature and solvent-free operation and also can be used for characterization and purification of alcohols and the mentioned ethers.

$$ROX \;+\; NH_2OH{\cdot}HCl \xrightarrow[\text{solvent-free, heat}]{\text{PVP } H_2O_2 \text{ (0.1 equiv.)}} R'R''C{=}NOH$$

X = H, TMS, THP
R = primary and secondary aliphatic, benzylic, allylic and cyclic types

Scheme 1 Tandem oxidative conversion of alcohols, TMS and THP ethers to oximes catalyzed by PVP-H_2O_2.

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The removal of naphthenic acid from crude oil by the stringer method using a zinc oxide catalyst based on aluminum oxide

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Keywords: Crude oil , Naphthenic acid, Esterification, Acid removal, Catalyst

Most acids in petroleum are either naphthenic acids or fatty acids. Naphthenic acids are the primary contributor to the total acid number of the oil,[١] and they may cause serious corrosion to processing equipment as the temperature increases during oil refining.[٢-٥] In addition, naphthenic acids may cause emulsification during the refining process, which makes it difficult to separate water from the oil and decreases the oil yield. The thermal stability of petroleum products may also be reduced due to the presence of naphthenic acids. Therefore, the removal of naphthenic acids from crude oils is necessary.[٦-٧] The reaction equation of the esterification of naphthenic acids and the alcohols are shown below in Eq. (1).

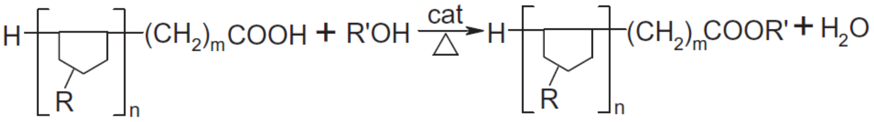

Fig. 1 String reaction equation for naphthenic acids and alcohols

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The effect of moisture on the creation of a physical/ chemical network in polyurethane/halloysite nanotube nanocomposites with shape memory behavior

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Keywords: Polyurethane, Shape memory, network, synthesis, Halloysite nanotube.

Polyurethane is an engineering polymer that has different applications such as adhesives, foams, coatings, fibers, and so on. This polymer is produced by a step-growth polymerization reaction between isocyanate and diol. Polyurethane is composed of covalent bonding of two hard and soft segments with different glass transition temperatures.[1] Shape memory behavior caused by this structure, which is why this polymer is considered in the field of smart materials. Smart materials are capable of responding to external stimuli such as temperature, light, pH, electricity, solvent and magnetic fields. Moisture is one of the environmental factors affecting the synthesis of polyurethane.[2] In this study, two samples were designed and tested to determine the effect of presenting moisture during synthesis on the polyurethane structure. The materials used were Hexamethylene diisocyanate (hard segment procreator), 1,4-butanediol and Poly (tetramethylene ether) glycol (soft segment procreator) and Dimethylacetamide (solvent) for synthesis. One weight percent of Halloysite nanotube was also added for improving shape memory and other mechanical properties. The first sample of polyurethane / Halloysite nanotube nanocomposite was synthesized in a moist environment. The second sample was synthesized in a moist environment. To investigation of the type of physical or chemical network in nanocomposite, a frequency sweep of rheological test was performed. The Dynamic mechanical analysis was used to study shape memory behavior. The results showed that the synthesis of polyurethane/ Halloysite nanotube nanocomposite in the presence of moisture, produced a chemical network in the polymer and had a more shape memory than the synthesized sample without moisture conditions. It was also noticeable that, the second specimen had physical network. From these tests it can be concluded that the presence of moisture in the synthesis environment is effective on the type of network and the behavior of shape memory. Considering that each of these types of polymer can have a special application in the industry, further research in this field and the examination of such effects on other properties of polyurethane is recommended.

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Au supported on graphene quantum dots/TiO_2 as oxidation catalyst

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Keywords: Graphene quantum dot, Metformine, Heterogeneous catalyst, oxidation reaction.

Heterogeneous photocatalysis has an industrial importance besides academic interest in the aerobic oxidation of organic molecules. In this regard, TiO_2 is a suitable candidate due to its low cost, non-toxicity, high photostability, and photocatalytic activity which benefits its industrial applications. In continues of our interest in developing the useful catalytic systems for oxidation of organic compounds,[1-4] herein titania nanoparticles combined with graphene quantum dots and Au nanoparticles was employed as a heterogeneous catalyst in the oxidation reaction of some alcohols and alkylarenes. Easy recovery, sustainability, high surface area, and chemical stability of the new catalyst make it attractive for the catalytic goals.

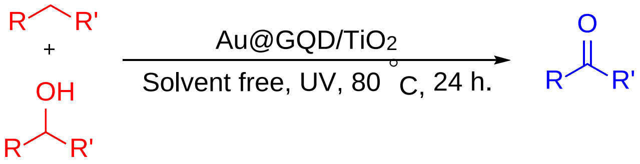

Fig. 1 Oxidation of alkylarenes and alcohols with heterogeneous Au catalyst

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Modified SBA-15 with Reductive Nature: a Robust Nanoreactor for Generation of Cu(I) Species for Synthesis of new Triazoles

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Keywords: Click reaction, SBA-15, Cu nanoparticles, Silica mesoporous.

In 2002 Sharpless and Meldal groups described a robust catalyst system based on Cu(I)-catalyzed 1,3-dipolar cycloaddition of organic azides and terminal alkynes (CuAAC reaction) term as a "click chemistry" to form a 1,2,3-triazole 5-membered heterocyclic compound.[1] After first report, many of heterogeneous and homogeneous catalysts based on direct addition of copper(I) or in situ reduction of Cu(II) by sodium ascorbate were developed for 1,3-dipolar cycloaddition of alkylazide and alkyne.[2]

In this work, a new modified SBA-15 with reductive nature was synthesized. For this purpose, the channels of SBA-15 were modified with poly-amine ligands. This porous material proved to be an effective host for the immobilization of inexpensive Cu(II) ions. The catalytically active Cu(I) species were generated automatically due to the reductive nature of modified surface of catalyst without use of any toxic reducing agents. The well stabilized Cu(I) species into the nano-channels of SBA-15 were used for synthesis of various triazoles from sodium azide, phenyl acetylene and alkyl/benzyl halides or alkyl epoxides under green mild aqueous reaction conditions (Fig. 1).

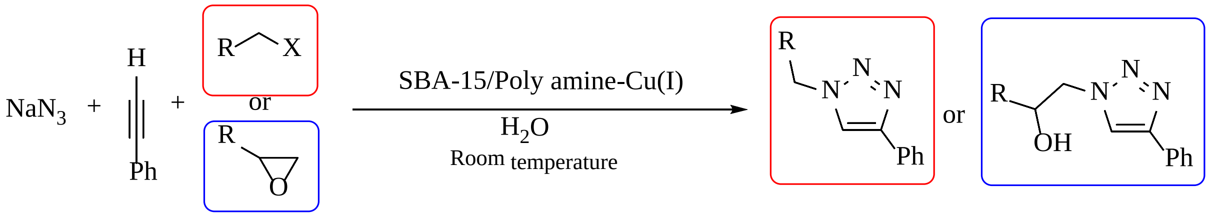

Fig. 1 Synthesis of substituted triazoles.

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Synthesis of β-Aminoketone Compositions by Mannich Three-Component with Nano Catalyst $Fe_3O_4/SiO_2/SA$

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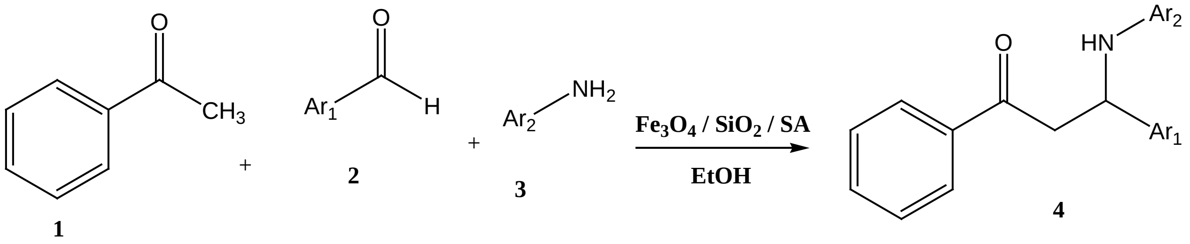
Keywords: $Fe_3O_4/SiO_2/SA$, Multicomponent reactions, Magnetic nano catalyst.

Nano-catalysts are important in chemical processes, producing energy, saving energy and also preventing the environmental pollution(1). In this study, the effect of magnetic nano catalyst $Fe_3O_4/SiO_2/SA$ for the synthesis of β-aminoketone compositions by Mannich three-component reaction with acetophenone **1**, aromatic aldehyde **2** and aromatic amines **3** have been studied.(2)The results showed that the reaction of β-amino-ketone and its derivatives functions better in the presence of the nano catalyst $Fe_3O_4/SiO_2/SA$, and also the nano catalyst $Fe_3O_4/SiO_2/SA$, in highest efficiency and the shortest possible time, leads to the production of the product, as well as the $Fe_3O_4/SiO_2/SA$ nano catalysts.(3)The purpose of this research is to replace the new acidic nano-catalysts rather than the other acid catalytic. In general, $Fe_3O_4/SiO_2/SA$ nano catalysts are one of the best catalysts for the reaction of β-amino ketone and its derivatives. The nano-magnetic catalyst was also characterized by BET surface area analyzer, FTIR and X-ray diffraction (SEM).



4a: $Ar_1 = C_6H_5$ $Ar_2 = C_6H_5$
4b: Ar_1 =4-BrC6H4 $Ar_2 = C_6H_5$
4c: $Ar_1 = 4\text{-}ClC_6H_4$ $Ar_2 = C_6H$
4d: $Ar_1 = 4\text{-}MeoC_6H_4$ $Ar_2 = C_6H_5$
4e: $Ar_1 = 3\text{-}MeoC_6H_4$ $Ar_2 = C_6H_4$
4f: $Ar_1 = 4\text{-}MeC_6H_4$ $Ar_2 = C_6H_5$

Fig. 1

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Synthesis of Tetrahydrobenzo [α] Xanthene-11-one Derivatives by One Pot three-component with Nano Catalyst

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Keywords: Multicomponent reactions, nanoparticle, catalyst, Xanthene.

Xanthene's derivatives have an important role in many biological activities as antibacterial, antivirals, bacteria play an important role in treating photodynamic therapy.[1] In PDT, photosensitizers are injected directly into malignant tissue and then light, of a specific wavelength, is used to excite the photosensitizer drug, which destroys the tumor cells and this compounds have also been investigated for agricultural bactericide activity and some other benzoxanthenes find application in industries such as dyes in laser technology and fluorescent materials for visualization of biomolecules.[2] The synthesis of these compounds is now very important and various methods for the synthesis of these compounds have been reported. The role of catalysts in the production of these compounds is undoubtedly important. So far, various catalysts have been used in the synthesis of these compounds, the most efficient of which are solid acid catlyst. The purpose of this study was to develop and introduce a KCC-1/SA Ns catalyst and its usage in one pot reaction to production of tetrahydrobenzo [α] Xanthene-11-one. The FTIR and SEM spectra of the composition were carefully evaluated and confirmed the product.

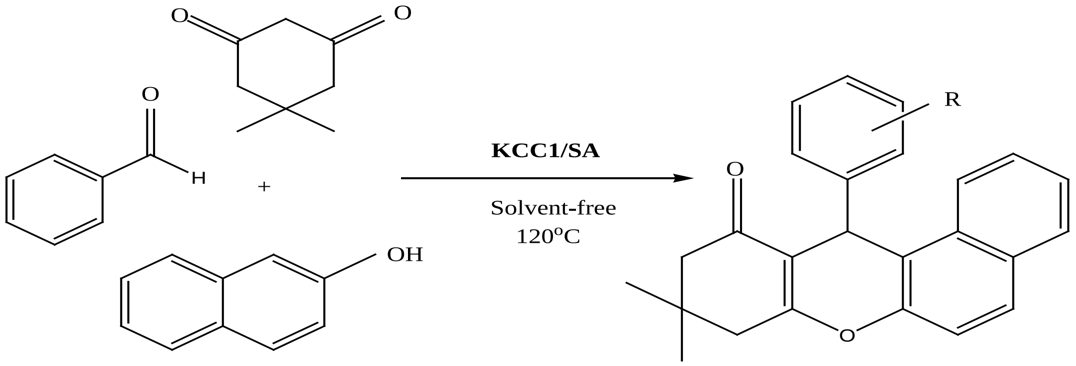

Fig. 1

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Magnetic Piperazine-Functionalized Reduced Graphene Oxide as a Heterogeneous Catalyst in the Pechmann Coumarin Synthesis

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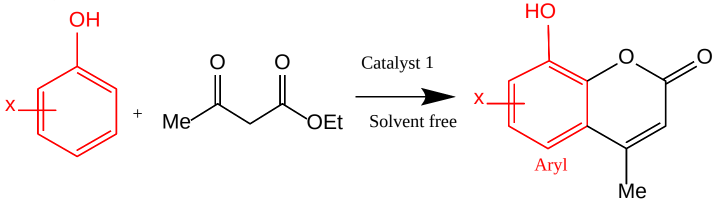
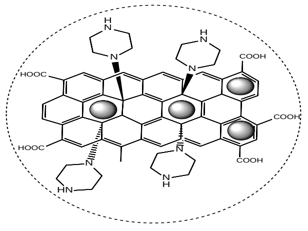
Keywords: Heterogeneous Catalyst, Reduced Graphene Oxide, Pechmann Reaction, Coumarins

Carbon nanomaterials have been ideal candidates for metal-free catalysts due to their inexpensiveness, easy availability, environmental friendliness and unique surface properties. Among them, the modified graphene oxide having a two-dimensional structure and prominent features has attracted a lot of attention(1). Chemical reduction of graphene oxide (rGO) is performed using hydrazine hydrate, which is also guided by the removal of oxygen and the recycling of two-way aromatic carbon and also has chemical active sites that make it noticeable as an active substance in molecular sensors (2) .

Coumarins play an important role in the natural products and organic synthesis To date, there are several methods for the synthesis of coumarines have been reported in the literature .Pechmann reaction is one of the best methods which include the condensation of phenols with β-ketoesters in the presence of various catalysts (3). In this work, the piperazine-functionalized reduced graphene oxide was initially synthesized, magnetized with Fe_3O_4, and was then used as a heterogeneouc catalyst in the Pechmann coumarin synthesis under solvent-free conditions. Also, effects of the various reaction parameters, including temperature, reaction time, mol% catalyst were studied. The yield results showed that the above magnetic catalyst efficienty catalyzed the Pechmann reaction





Catalyst 1

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Regio- and diastereoselective synthesis of pyrazolo[4,3-*e*]pyridines *via* multicomponent domino aza-Diels–Alder reactions in water

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Keywords: 5-Amino-pyrazole, Aza-Diels–Alder reactions, Regio- and diastereoselective.

Aza-Diels–Alder reactions (ADARs) are powerful processes that provide *N*-heterocycles in a straightforward method. Herein, we report a novel and efficient strategy for the synthesis of pyrazolo[4,3-*e*]pyridines **5** *via* a one-pot multicomponent intramolecular ADARs among benzoylacetonitrile derivatives **1**, phenylhydrazine **2**, salicylaldehyde derivatives **3**, and styrenesulfonyl or cinnamoyl chloride **4** in H_2O as a solvent.[1] Remarkable factors such as green, higher yields, regio- and diastereoselectivity, high atom-economy and easy isolation procedures are key features of this protocol.[2,3]

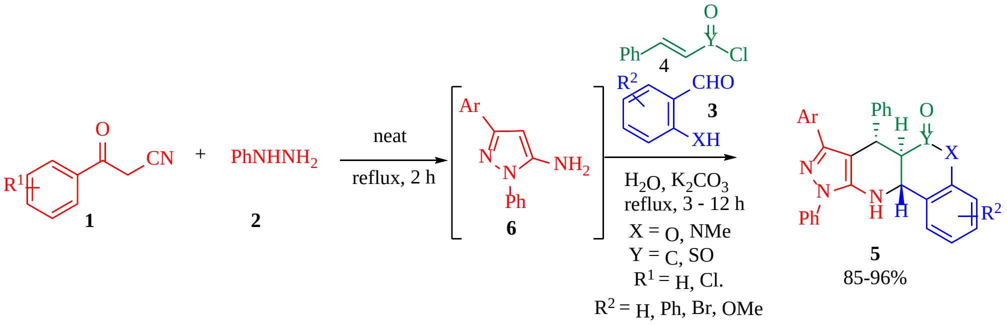

Fig. 1 Synthesis of pyrazolo[4,3-*e*]pyridine derivatives **5**

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The study of different methods of alizarin extraction from Madder for application in dyeing of handmade carpet

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Key words: Extraction of alizarin, Dyeing, HPLC, Color strength

Madder plant is a self- willed plant that has been used to attain the red shade of carpet industry since its earliest years. The roots of this plant contain anthraquinone derivatives that are soluble in water. In the root of Madder, alizarin with red shade and purpurin (orange and yellow) shade, which is widely used in cosmetic and food industries, and especially in the dyeing of handmade carpets. The widespread use of alizarin in the industry and the huge cost that imports of this pigment has imposed on the country's industry. In this research, the aim of this study is to investigate the use of alizarin and pyopurupurine by high performance liquid chromatography (HPCL) from Rhinos root. Then the dyeing of the wool product is performed and finally the color components, color strength, optical stability and washing of the samples are evaluated. The results of color strength of the samples show that the light and washing fastness of the sample are very good, as well as the color strength of the samples in direct and indirect extraction.

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Extraction of anthraquinone compounds from Rubia tinctorum plant

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Keyword: alizarin, anthraquinones, , madder. HPLC, quantitative analysis

The roots of Rubia tinctorum (madder) are the source of a natural dye and have been used to dye textiles in many parts of the world since ancient times. The dye components are anthraquinones with alizarin, the hydrolysis product of ruberythric acid, being the main dye constituent. Direct and indirect HPLC methods for the quantitative analysis determination of anthraquinones in dried madder root have been developed, validated and compared. In the direct method, madder root was extracted twice with refluxing ethanol–water.

This method allowed the determination of the two major native anthraquinone glycosides lucidin primeveroside and ruberythric acid. In the indirect extraction method, the anthraquinone glycosides were first converted into aglycones by endogenous enzymes and the aglycones were subsequently extracted with tetrahydrofuran–water and then analysed.

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Pd(II) Supported MIL-101(Al): A Heterogeneous, Efficient and Reusable Catalyst for Mizoroki-Heck Reaction

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Keywords: Metal–Organic-Frameworks, MIL-101(Al)-Pd(OAc)$_2$, Mizoroki-Heck reaction

Recently metal–organic frameworks (MOFs), porous materials of a crystalline structure comprising bridged organic ligands and metal centers, have been attracted significant attention in gas sorption average owing to their large pore volumes and surface areas. Several studies have been reported on MOFs utilization as support for heterogeneous catalysts,[1] and drug delivery [2]. These materials have been explored because of their intrinsic high surface area, tunable pores, and various functionalities.[3]

In this work, Pd(OAc)$_2$ was deposited on MIL-101(Al) particles, with a high surface area prepared by a hydrothermal method. The supported Pd(II) porous catalyst showed significant efficiency in the Mizoroki-Heck coupling reaction. The reaction parameters such as the type of base, amounts of the catalyst, solvents, temperature, and substrates ratios were optimized.

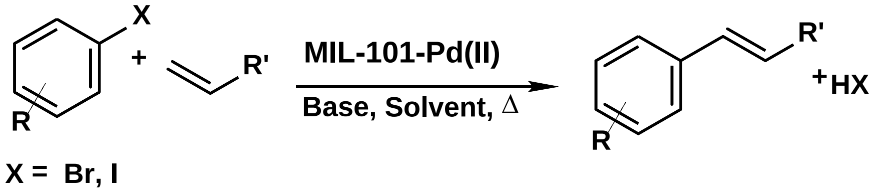

Fig. 1 The Heck reaction catalyzed by MIL-101-Pd(II)

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Synthesis of Fe_3O_4- Glycerol-Pd and its Catalytic Efficacy in C–C, C–N and C–O Coupling Reactions

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Keywords: Nanocatalyst، Fe_3O_4، Glycerol، coupling reactions، palladium.

Currently, nanocatalysts Perform an significant role in green chemistry and possessed much attention among the industrial and academic scientific community [1]. Nanoparticles have gotten remarkable attention in past two decades due to the interesting properties relevant to their size. In scientific realization, magnetite particles have been study extensively, because their synthesis is good known and convenient [2].

In novel organic chemistry, palladium-catalysed C─C bond have taken on an important role since their first expansion in the primary 1970s [3]. C─C coupling reactions catalysed by transition metals are among the most significant reactions in organic synthesis. between these reactions, C─C, C─O and C─N bond formations with palladium catalysts (e.g. Suzuki and Heck reactions) have become very efficient tools in the agrochemical, pharmaceutical and chemical industries [4].

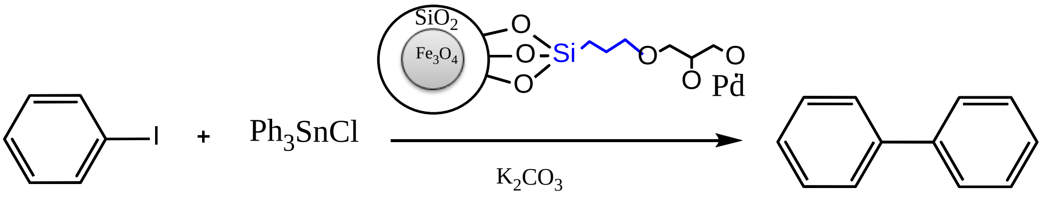

Fig. 1 Synthesis of coupling reactions with Fe_3O_4- Glycerol-Pd

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Synthesis of various cyclopropyl methyl bromide and its derivatives from ketones and/or aldehydes and some β-dicarbonyl compounds in the presence of BrCN and Et_3N

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Keywords: Ethyl cyanoacetate , One-pot reaction , 3-Alkyl-3-(bromomethyl)-1,2 dipropionylcyclopropane- 1,2-dicarbonitrile, Cyanogen bromide, Photochemical , Bromonium ion.

The ultimate goal in this paper has been developed for the synthesis of structurally various bromomethyl cyclopropane via an α-bromoketone and/or aldehydes with ethyl cyanoacetate or malononitrile and cyanogen bromide (BrCN) in the presence of Et3N to give products in excellent yields within about 3 s. The α-bromination of carbonyl compounds is an important transformation in organic synthesis chemistry. [1–2] There are several routes for the synthesis of cyclopropane ring frame in organic compounds, such as cyclopropanation of an aldehyde in the presence of BrCN and Et3N with β-dicarbonyl compound as malononitrile,[3] ethyl cyanoacetate.[4]

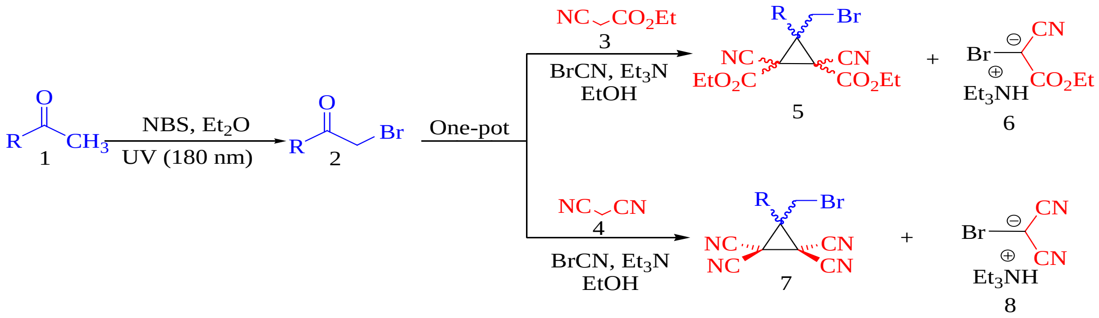

Fig. 1 Representatively, proposed afforded diethyl 3-alkyl/aryl-1,2-dicyano- 3-(bromomethyl) cyclopropane-1,2-dicarboxylate **5** and 3-(4-(bromomethyl)alkyl/ aryl)cyclopropane-1,1,2,2- tetracarbonitrile **7** under Et3N in excellent yields with short reaction time

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Synthesis of 3-(4-((2-(trimethylsilyl)ethynylthio) methyl) phenyl) cyclo propane -1,1,2,2-tetracarbonitrile in different temperature conditions

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Keywords: Ethyl cyanoacetate, One-pot reaction, 3-Alkyl-3-(bromomethyl)-1,2-dipropionylcyclopropane-1,2-dicarbonitrile, Cyanogen bromide.

Organosilicon compounds are widely encountered in commercial products. Most common are drug structures has been used to improve pharmacological potency, to modify selectivity toward a given target, to change metabolic rates, and to increase lipophilicity. Lipophilicity can provide several physiological benefits, including increased bioavailability and tissue and cell penetration Others important uses include agricultural plant control adjuvants such as herbicides and fungicides. [1–3]

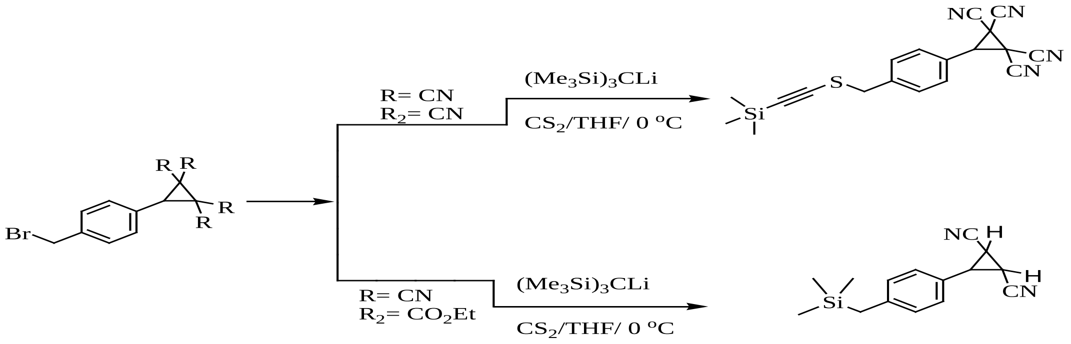

Fig. 1 Representatively, proposed afford 3-(4-((2-(trimethylsilyl)ethynylthio)methyl)phenyl) cyclopropane-1,1,2,2-tetracarbonitrile) and 3-(4-((trimethylsilyl)methyl)phenyl)cyclopropane-1,2-dicarbonitrile in different temperature conditions

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A First DFT and TD-DFT Study on Electron Transfer in Novel Non-Fullerene solar cells

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Keywords: PET, Metal-organic, donor-acceptor, Marcus theory.

Abstract: Recently, designing and producing organic solar cells are greatly increased because of flexibility, long life, low cost and recycling. In this work, four solar cells designed and investigated by the use of DFT and TDDFT computational methods[1]. The scandium (Sc) functionalized open edge boron nitride (Sc@BN) was used as acceptor[2] agent and α-sixithiophene that of donor ones. Using Hole-Electron calculation determined the efficiency of these solar cells[3], electron transport (ET) for the first five excitation states was obtained[4], which the systems with numbers **1**, **2** and **3** had the highest amount of ET in order and number **4** just locally excited. Natural bond orbital (NBO) analysis well explained charge distribution in both ground and excited states. At the end, using electron wavelength transportation and *Marcus* theory the potential difference created on either side of each system was determined.

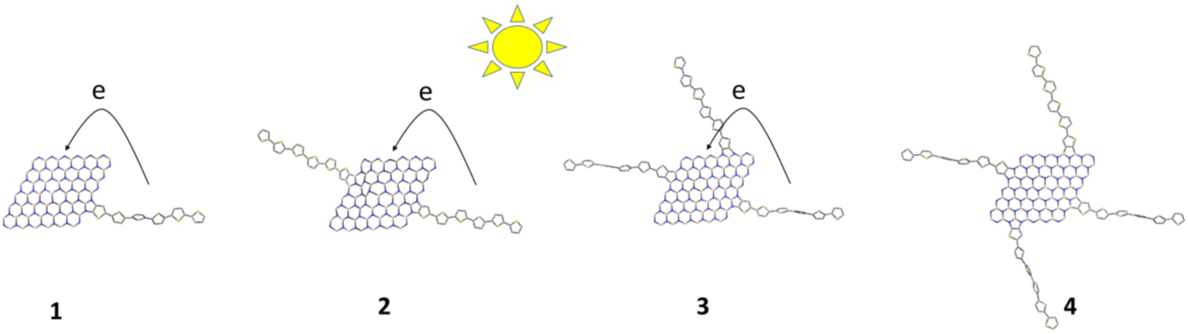

Fig. 1 Organic solar cells structure by Sc@BN and α-sixithiophene

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Theoretical DFT Study on Cubane Molecule and Its Reduced States ($C_8H_8^n$; n=0 and -1 to -4); A First Principle Study

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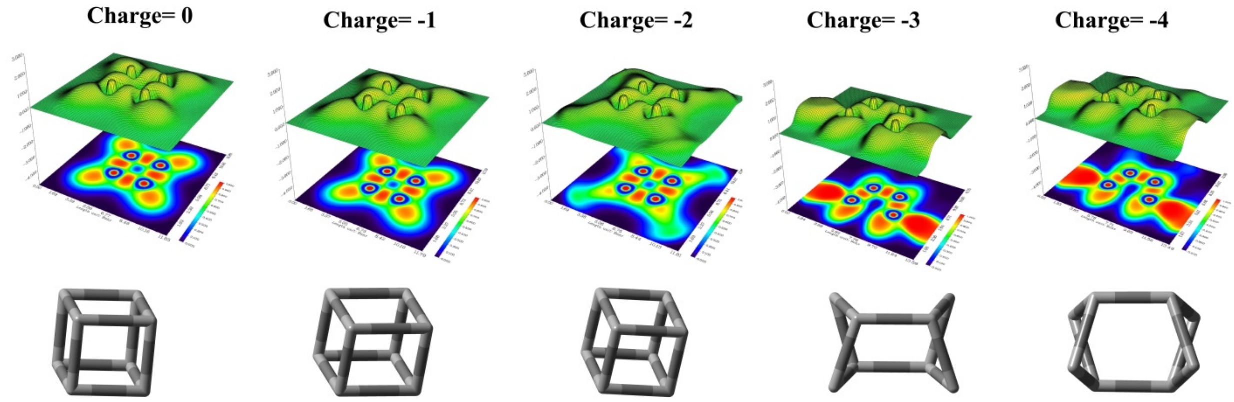
Keywords: DFT, Cubane, ELF, Reduced states

Abstract: The objective of this research is to study of cubane (C_8H_8) molecular deformation by stepwise reduced states ($C_8H_8^n$; n=0 and -1 to -4). In this study, the molecule of cubane was optimized to obtain minimize molecular geometry and the electronic structure by density functional theory (DFT, B3LYP) at the levels of 6-311G(d). Some important properties such as bond dissociation enthalpies, densities, frontier orbital energies, thermodynamic parameters, natural bond orbital populations, heat of formations and detonation parameters were calculated for $C_8H_8^n$ (n=0 and -1 to -4). The calculated spectra of IR and NMR of the structures ($C_8H_8^n$; n=0 and -1 to -4) were also computed. The results of the DFT investigations revealed that this compound exhibit excellent performance in its reduced form.

Structural distortions of cubane - Graphical abstract



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Investigation of Metal Free Organic Dye-sensitized and Their Application in Solar Cells

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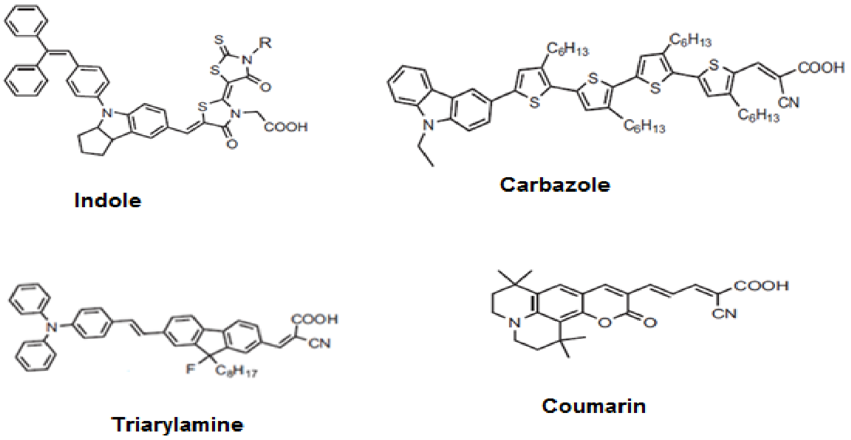
Keywords: metal free organic dye, dye-sensitized, solar cells

In recent years, extensive efforts have been made to synthesize and review the organic colors used in solar cells. These color sensors can be divided into two groups of polypyridine ruthenium complexes and metal free organic dyes-sensitized.

ruthenium-based paints have had disadvantages, so in recent years, studies have been made on a bunch of dyes-sensitized called metal free organic dyes for use in solar cells, such as triphonylamine, coumarin, squarine, indol, carbazole, perylene-based and others (Fig.1).

The results of the study showed that the molecular structure of organic dyes plays a very important role in the efficiency of the conversion of sunlight energy into electrical energy in dye-sensitized solar cells. In fact, an appropriate organic dye used in solar cells should have a range of absorption of its molecules in the visible region, the molecular extinction coefficient is high, so that light is better absorbed, the length of the resonant system is high in dye, and the molecules of dye should not be on the surface of the semiconductor (titanium dioxide) accumulate.(1,2)



Indole

Carbazole

Triarylamine

Coumarin

(Fig. 1)

References

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One-pot synthesis of benzopyrano[2,3-*d*]pyrimidine derivatives catalyzed by LDHs@Propyl-ANDSA

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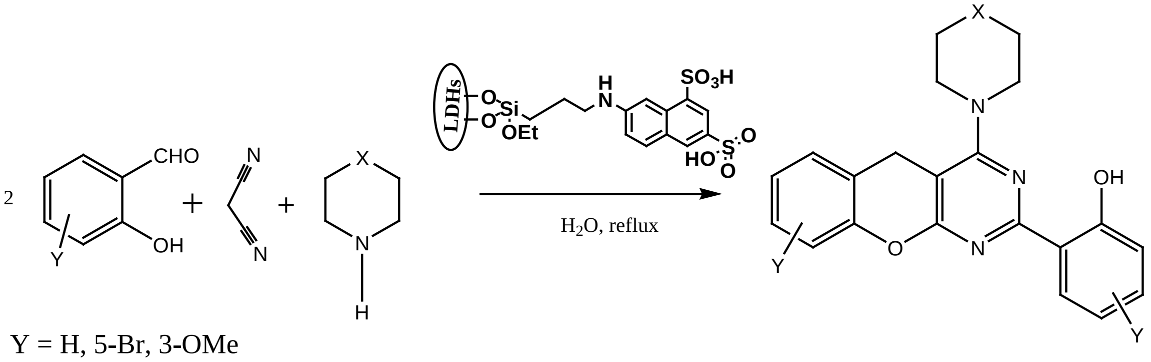
Keywords: Malononitril, Salicylaldehyde, *N*-Methyl pipyrazine

Development of new MCRs is an exciting research topic in organic chemistry, especially for the synthesis of heterocyclic compounds [1]. Benzopyrano[2,3-*d*]pyrimidines show interesting features which make them attractive targests for the synthesis *via* MCRS [2]. Benzopyrano[2,3-*d*]pyrimidine is a potentially important pharmacophere that exhibits in vivo antitumor activity, cytotoxic activity against cancer cell lines and can cause significant perturbation in cell cycle kinetics [3]. We report herein an efficient and simple synthesis a series of benzopyrano[2,3-*d*]pyrimidines in high yields *via* an one-pot, pseudo three component reaction between salicylic aldehydes, malononitrile and secondary amine in the presence of the layered double hydroxides functionalized by 7-aminonaphthalene-1,3-disulfonic acid (LDHs@Propyl-ANDSA), H_2O as green solvent under reflux condition [Fig.1].

Remarkable advantages of the present synthetic strategy over the others are shorter reaction times, higher isolated yields, reuse of catalytic system and simple work up procedure.



Y = H, 5-Br, 3-OMe

X = CCH_3, NCH_3, CH_2, O

Fig. 1 Synthesis of benzopyrano[2,3-*d*]pyrimidine derivatives using LDHs @Propyl-ANDSA as a catalyst

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Modification of chitosan aerogel with Fe(II)-phthalocyanine as the oxidation catalyst of organic substrates

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Keywords: Fe-Phthalocyanine, Chitosan aerogel, Heterogeneous catalyst, Oxidation.

Metallophthalocyanines (MPcs) are effective oxidation catalysts having high activity, rather cheap and facile preparation in a large scale, and chemical and thermal stability. Recently, many efforts have been focused on the preparation of novel catalytic methods using MPc. Fe(II)-Pc derivatives have been employed as the catalysts in the oxidation of various substrates such as methane,[1] cyclohexane,[2] cyclohexene,[3] and aromatic pollutant. Fe(II)-porphyrin as a structurally related compound to Fe(II)-Pc oxidaized alcohols to the corresponding aldehydes and ketones. In continues of our interest in developing the useful catalytic systems for oxidation of organic compounds,[4-6] phthalocyanines of Fe(II) was immobilized on chitosan aerogel *via* chemical binding. The catalytic activity of the composite was examined in the oxidation of alcohols. The oxidation of alcohols to the corresponding aldehydes or ketones was carried out with high yields and excellent selectivities.

Fig. 1 Oxidation of alcohols with Fe(II)-Pc supported on chitosan aerogel

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The chemistry of dithiocarbamates: from synthesis to their applications in synthetic organic chemistry

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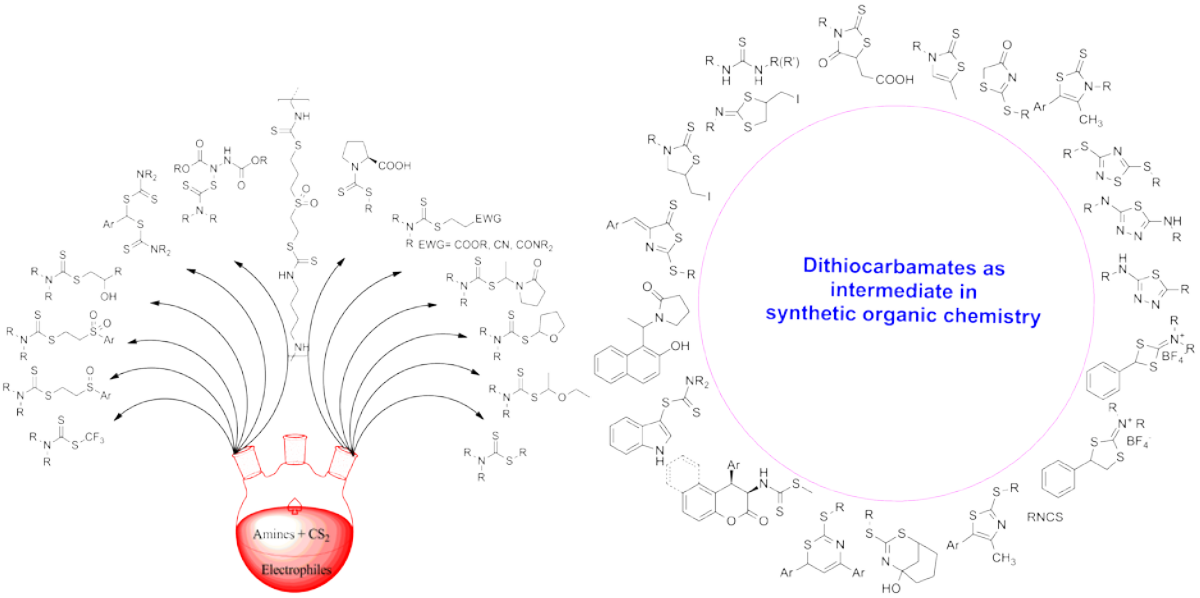
Keywords: Dithiocarbamate, Multi component reaction, Carbon disulfide

Dithiocarbamates are a well-known category of organic compounds with diverse applications in synthetic organic chemistry as intermediates, as fungicides and pesticides in agriculture, sulfur vulcanization in rubber manufacturing, radical chain transfer agents in the reversible addition fragmentation chain transfer (RAFT) polymerizations, and medicinal chemistry. Recent progress in the chemistry of dithiocarbamates from their synthesis to their applications in synthetic organic chemistry in my research group will be reported.



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Synthesis of microencapsulated palmitic acid with titania shell for thermal energy storage systems

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Keywords: Phase change materials, Thermal energy storage, Palmitic acid, TiO_2, Sol-gel

Nowadays, increasing energy consumption and the shortage of fossil fuels is a worrying issue for human society. Phase change materials (PCMs) which are used for thermal energy storage, are able to store a large amount of latent heat at their phase change temperature[1]. Encapsulation of phase change materials as micro/nano-capsules prevents thermal dissipation[2]. Fatty acids are one of the organic phase change materials that have a different melting temperature range that can be used depending on the application[3]. In this work, we prepared PCM microcapsules which contain PA (palmitic acid) as core and TiO_2 as shell materials. Microcapsules were synthesized using a sol-gel method, which is a physical-chemical method by changing the value of pH in the range of 9-10. The particle size and microstructure of microencapsulated phase change material (MPCM) were investigated by scanning electronic microscope (SEM). Fourier transformation infrared spectroscope (FT-IR) that examined chemical structure, illustrated that palmitic acid was well microencapsulated in TiO_2 shell. The thermal leakage test showed negligible leakage. The results show that microcapsules have good thermal stability and can be used to store thermal energy in a temperature range of 62-65°C.

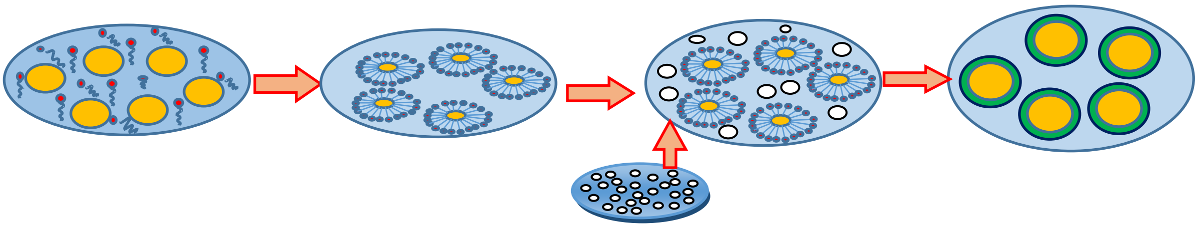

Fig. 1 preparation of microcapsules PA/ TiO_2

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Application of Fe_3O_4@HPG/Pd^0 NPs as an Innovative Semi-heterogeneous Catalyst in Suzuki Cross-coupling Reaction

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Keywords: Semiheterogeneous catalysts, Palladium nanoparticles, Hyperbranched polyglycidole, Suzuki–Miyaura coupling reaction.

Interest in catalysis by palladium nanoparticles is increasing dramatically due to the advantages offered by these “semi-heterogeneous catalysts” [1]. These advantages combine the characteristics of heterogeneous catalysis (recovery and recyclability) with those of homogeneous catalysis (relatively low catalyst loadings and good selectivity) [2]. Since the heterogeneous catalysis reaction occurs entirely on the surface of the metal particles, a high dispersion or size control is required to improve the catalytic activity and reduce the consumption of the catalysts [3]. Unfortunately, aggregation of naked nanoparticles often prohibits tailoring of particle size. For this reason, many attempts have been made to immobilize or stabilize Pd nanoparticles in a wide variety of supports, such as polymers, organic-inorganic hybrid materials, and glass-polymer composites, as well as on common inorganic substrates, such as carbon, silica, zeolites or carbon nanotubes [1-2]. Herein hyperbranched polyglycidole (HPG) is used as support, it also functions as reducing agent and stabilizer. We report green and innovative magnetic semi-heterogeneous efficient palladium catalyst system that has been immobilized hyperbranched polyglycidole (acting as support, reducing agent and stabilizer) coated magnetic Fe_3O_4 nanoparticles (**Fe_3O_4@HPG/Pd^0**) for effective palladium-catalyzed Suzuki–Miyaura coupling reactions in room temperature and aqueous media.

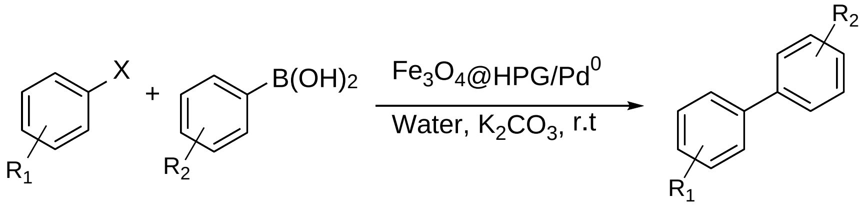

Fig. 1 Suzuki–Miyaura coupling reactions catalyzed by Fe_3O_4@HPG/Pd^0

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An alternative approach to the synthesis of new 2-substitueted-4,9-dimethyl-9*H*-pyrimido[4,5-b]indole derivatives

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Keywords: Pyrimido[4,5-*b*]indole, Hetretocyclic compound, pyrimidine

Pyrimido[4,5-*b*]indoles, fused tricyclic 6:5:6 compounds with three nitrogen atoms (2:1:0; positions 1, 3, and 9, and bicyclic 5:6 analogues, pyrrolo[2,3-*d*]pyrimidines), are of interest because of their extensive use as active ingredi-ents of pharmaceutical preparations.[1,2] Recently some of these compounds have been reported as useful new drugs in treatment of myocardial injury, pulmonary hyperten-sion, renal failure, Huntington's chorea, as well as neuro-degenerative disorders such as Parkinson's disease, Alzheimer's disease and focal ischemia.[2] So far, several synthetic methods have been reported for the preparation of pyrimido[4,5-*b*]indole ring systems. The most common synthetic routes involve ring closure of 2,3 functionalized indoles, e.g. 2-aminoindole-3-carboxylates or 2-aminoindole-3-carbonitriles with CN atom fragments such as formamide or cyanamide.[2,3] In this study we have reported a new methode for the synthesis of five novel of 2-substitueted-4,9-dimethyl-9*H*-pyrimido[4,5-*b*]indole (**3a-e**) catalyzed by Pd(0) wherein the biologically active indole moiety is fused to a potent pyrimidine ring across the 4, -positions (Scheme 1).

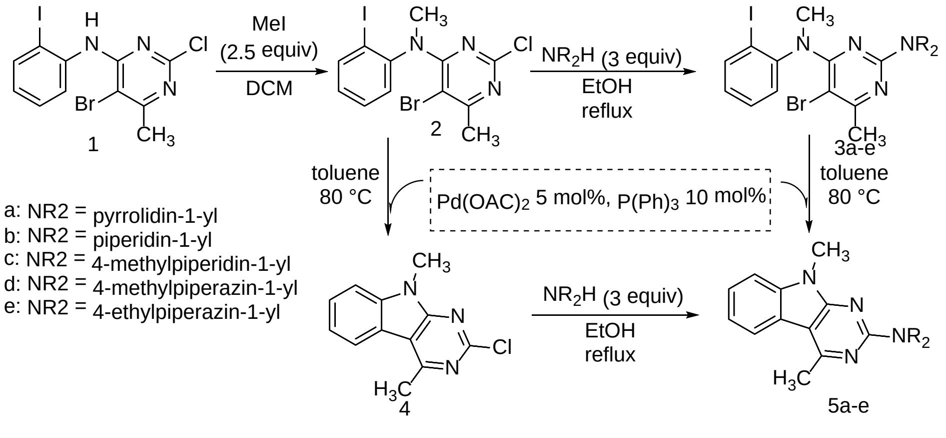

Fig. 1 General route for the synthesis of thiazino[2,3-*b*]quinoxaline

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2-Pyridine benzimidazole/Pd(II) complex supported on SBA-15: A new heterogeneous recoverable catalyst for the Heck reaction

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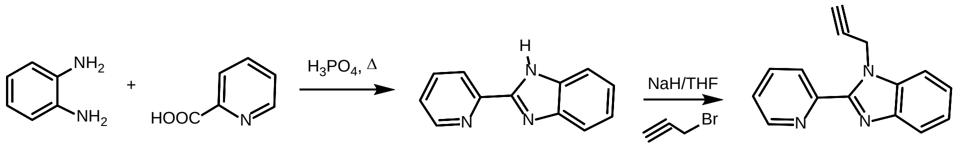
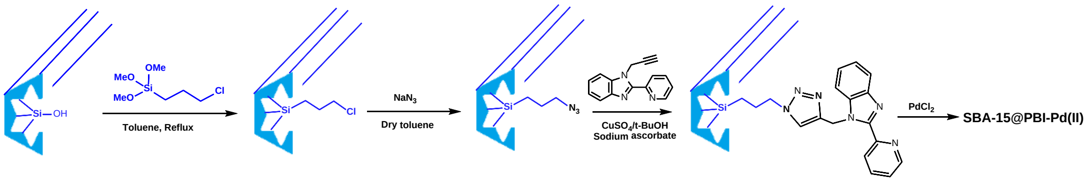
Keywords: mesoporous SBA-15**,** Heck cross-coupling reaction.

Palladium-catalyzed cross-coupling reactions, such as the Suzuki–Miyaura and Heck reactions, have become the standard methodologies for the synthetic organic chemists to construct useful organic compounds [1-2]. Among mesoporous silica nanoreactors, especially SBA-15, have been widely investigated due to its controllable size, composition and morphology, which are highly desirable for catalytic applications [3].

In this study, 1-propargyl-2-pyridine benzimidazole was synthesized, Scheme 1, grafted into SBA-15 via a click reaction (SBA-15@PBI), and then complexed with Pd(II) ions to afford SBA-15@PBI/Pd(II), Scheme 2. The supported Pd(II) mesoporous SBA-15 catalyst showed significant efficiency in the Mizoroki-Heck cross-coupling reaction. The reaction parameters, such as solvents, the type and amount of base, catalyst dosage, temperature, and substrates ratios were optimized.



Scheme 1: Synthesis of 1-propargyl-2-pyridine benzimidazole.



Scheme 2. Synthesis of SBA-15-PBI-Pd(II)

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Synthesis of 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives using magnetic nanoparticles functionalized with Cu(II) Schiff base complex as a new nanocatalyst

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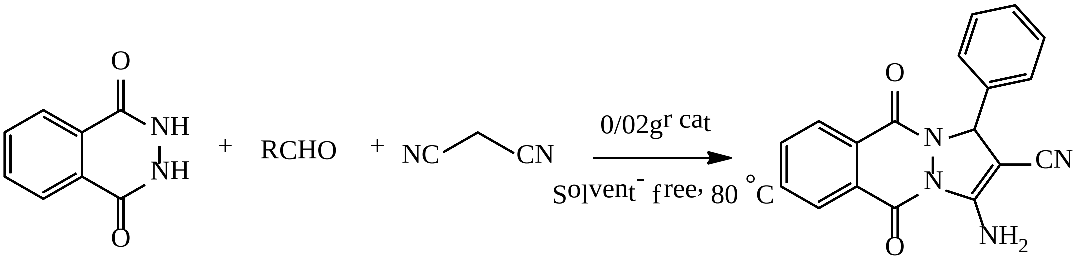
Keywords: Multi-component reaction, One-pot synthesis, green synthesis, malo-nonitrile, 1H-Pyrazolo[1,2-b]phthalazine-5,10-diones.

Given the goals of green chemistry, silica-coated magnetite nanoparticles (MNPs) open up new avenue to introduce an amazing and efficient system for facilitating catalyst recovery in different organic reactions.[1] The catalyst was characterized by infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), scanning electron microscope (SEM), X-ray diffraction (XRD) spectroscopy, and vibrating sample magnetometer (VSM).[2] capability of this nanomagnetic solid acid catalyst in the one-pot three-components condensation reaction of phthalhydrazide **1** , aromatic aldehydes **2** and malo-nonitrile **3** are also described. Use of easy reaction, conditions and simple magnetically work-up, short reaction times one of the most important features of this catalyst for the economic synthesis of 1H-Pyrazolo[1,2-b]phthalazine-5,10-diones **4**.[3]



1 2 3 4

Fig. 1 General scheme for the synthesis of 1H-Pyrazolo[1,2-b]phthalazine-5,10-diones.

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Effective degradation of acid orange 7 on silver chloride/bismuth iodide (Bi^{3+}: 4) hybrid nanophotocatalyst under simulated sunlight

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Keywords: Silver Chloride/Bismuth Iodide (Bi^{3+}:4), Acid Orange 7, Photocatalytic Degradation, Simulated Sunlight, Water Treatment.

By the development of industries, the amount of organic pollutants has also increased in the environment significantly. Dye contaminants which are more resistant are one of them[1, 2]. To tackle this issue, various forms of techniques are applied, but the photocatalytic approach has attracted a lot of attention as one of the most environmentally friendly method[2, 3]. Herein, degradation of acid orange 7 (AO7) with 100 mg/L concentration was studied during 180 min under simulated sunlight over plasmonic AgCl, silver chloride/bismuth iodide (Bi^{3+}:4) (25:75) (denoted as: plasmonic AgCl-BOI (25:75)) and bare bismuth iodide(Bi^{3+}:4) nanophotocatalysts that the photocatalytic degradation was obtained 43.2, 90.1 and 45.5%, respectively. Fig. 1 displays the absorption spectra of AO7 over plasmonic AgCl-BOI (25:75) at different irradiation time. Moreover, XRD, FESEM, and DRS analysis are used to demonstrate the true synthesis of nanophotocatalysts and the discussion of results gained.

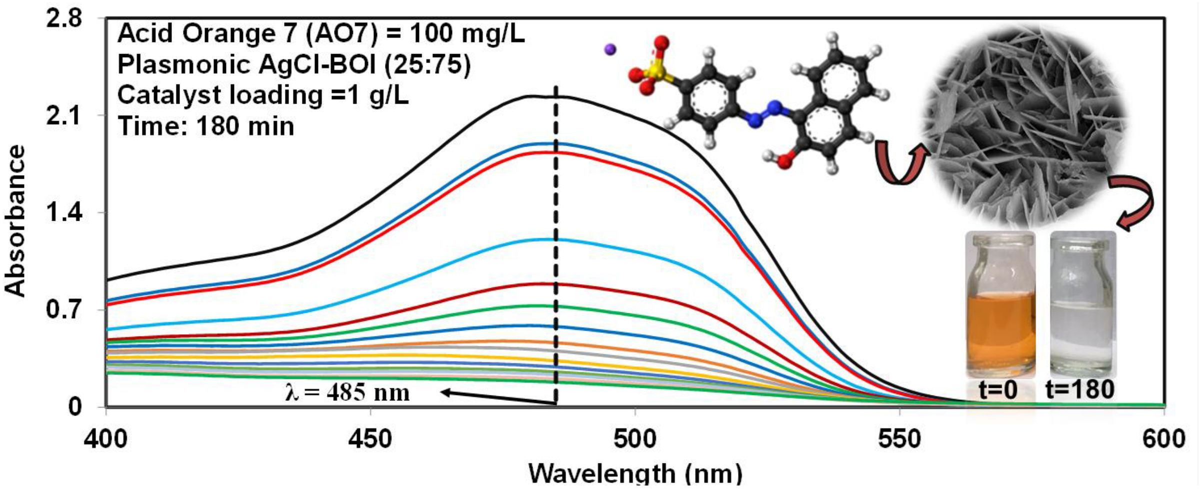

Fig.1 Temporal absorption spectral pattern of acid orange 7 over plasmonic AgCl-BOI (25:75) under simulated sunlight.

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Photocatalytic Elimination of Antibiotic Ofloxacin over Plasmonic AgBr Anchored with Co-Cr Layered Double Hydroxide as Solar-Light-Driven Nanophotocatalyst

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Keywords: Plasmonic AgBr Anchored with Co-Cr Layered Double Hydroxide, Antibiotic Ofloxacin, Solar-Light-Driven Nanophotocatalyst.

Currently, antibiotics, as non-biodegradable and emerging contaminants, are recognized as one of the most important environmental challenges[1]. Photocatalysis process is an effective method for the degradation of resistant contaminants[2] due to the low-cost and eco-friendly[3]. In this study, the elimination of the antibiotic ofloxacin was investigated using the novel plasmonic AgBr anchored with Co-Cr layered double hydroxide (denoted as: AgBr-CoCrLDH-P) nanophotocatalyst with 3:1 weighted ratio under simulated sunlight, and to further evaluate, pure AgBr-P and CoCrLDH samples were synthesized and employed in the ofloxacin degradation. For 25 mg/L ofloxacin solution, the photocatalytic efficiency of CoCrLDH, AgBr-P and AgBr-CoCrLDH-P after 120 min irradiation was found 11.4%, 65% and 83.6%, respectively (Fig. 1). XRD and FESEM analysis were used to characterize the photocatalysts. According to the results, the AgBr-CoCrLDH-P nanocomposite exhibited significantly enhanced photocatalytic performance due to a large specific area, low band gap and good charge separation.

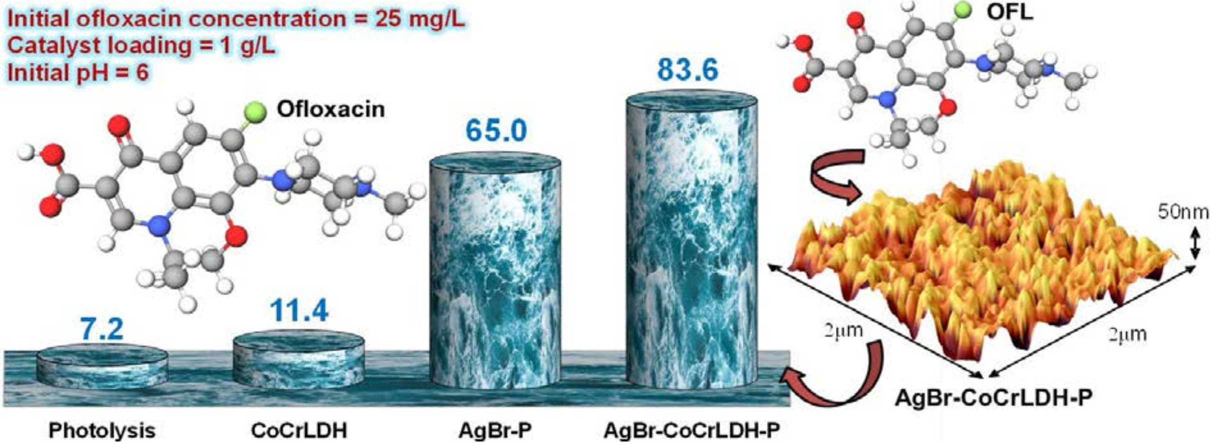

Fig. 1. Photocatalytic degradation of antibiotic ofloxacin over CoCrLDH, AgBr-P and AgBr-CoCrLDH-P under simulated solar light.

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Targeted design of three new amide-functionalized metal-organic frameworks for enhancement of the capability of epoxide ring-opening reaction catalysis

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Keywords: Metal Organic Frameworks; Ring opening of epoxide; Heterogeneous Catalysis.

Synthesis of MOFs compound with particular functionalized ligand is not always successful, and sometimes it cannot be synthesized easily and directly even using multiple methods. Hence, this limitation can be overcome by applying a post synthesis way which is swapping functional groups without changing the whole backbone of pillar ligand. Solvent-assisted functionality exchange (SAFE) is a post synthesis method which has been assisted to confront this challenge by replacing functional groups together. In this investigation, we tried to improved properties of the MOFs compound and increase their catalytic efficiency by importing a new functional group into their structures. N1, N3-di(pyridine-4-yl) malonamide linker (S) is one the pillar ligand which is not easily entering to the structure in order to synthesis MOFs compound. Therefore, to solve this issue , amide functionalized benzene-cored ligand derivatives were designed as linkers for manufacture of new 3D structures of $[Co(oba)(bpta)]\bullet(DMF)_2$ TMU-50, $[Co_2(oba)_2(bpfn)]\bullet(DMF)_{2.5}$ TMU-51 and one novel 2D $[Co(oba)(bpfb)]\bullet(DMF)_2$ TMU-49 , layered of compound via hydrothermal reaction. Also, their ability as catalysts was figured out in the methanolysis reaction of epoxides.

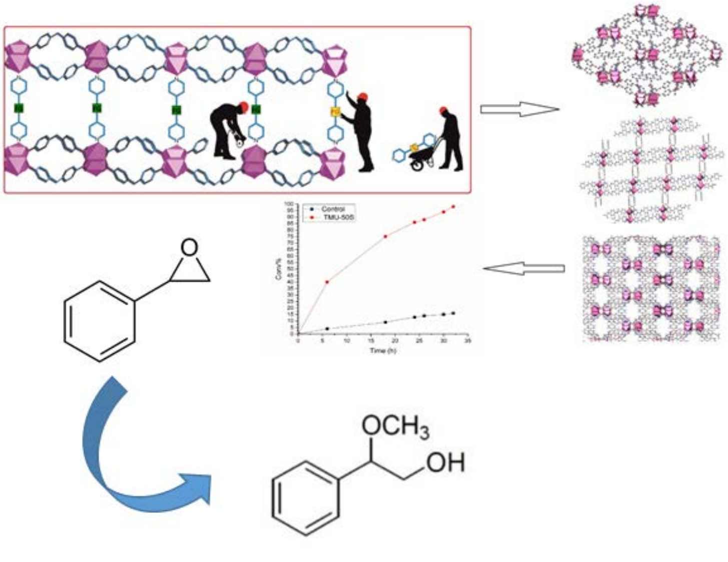

Fig. 1 synthesis of amide-based MOFs for ring opening reaction

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Solvent-free, facile, and an efficient synthesis of α-aminonitriles employing Halloysite nanotubes as an ecofriendly cyanating agent

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Keywords: Multicomponent reactions, α-Aminonitriles, solvent-free, Heterogeneous catalyst.

Synthesis of α-aminonitriles[1] has been an area of current interest for chemists as well as biologists because these are versatile precursors for the synthesis of pharmacologically significant molecules such as α-amino acids, amides, diamines, and various nitrogen and sulfur containing heterocycles such as thiadiazoles, imidazoles, etc.[2–5] Other biologically significant compounds such as saframycin A a natural product and phthalascidin a synthetic analogue, exhibit potent anti-tumor activity. Bruylants reaction and its Barbier version further crowned Strecker products as they serve as intermediate for the production of a variety of potent short-acting opioid analgesics. Halloysite nanotubes (HNTs) are clay minerals with a hollow nanotubular structure. Functionalized halloysite constitutes a valuable support for metal nanoparticles, promoting catalytic applications with tunable properties. Moreover, the presence of an empty lumen opens new perspectives for the production of nanoarchitectures with synergistic catalytic effects, due to the increase in local concentrations and confinement. The main focus of this review is the research on modified halloysite nanotubes for the preparation of an efficient synthesis of α-aminonitriles.

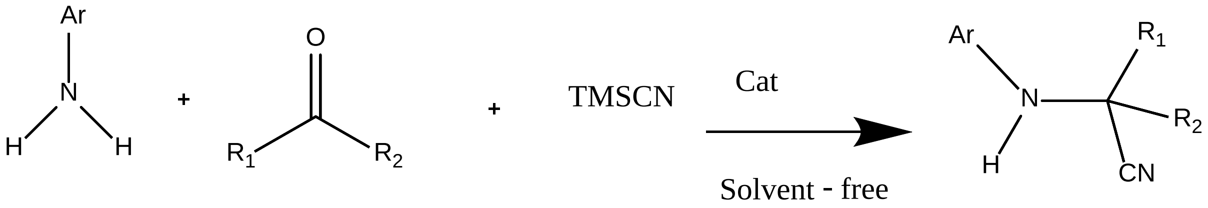

Fig. 1 Synthesis of α-aminonitriles

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Applications of Metal-Organic Frameworks (MOFs) in Organic Synthesis

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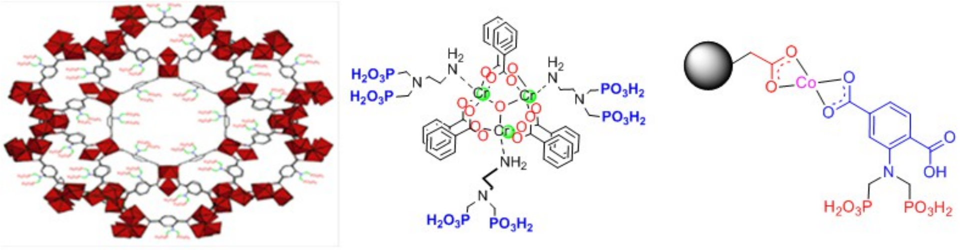
Keywords: Metal organic frameworks (MOFs), Multivariate MOFs (MTV-MOFs).

Nowadays, solid compounds with crystalline structure formed by inorganic clusters or metal ions (generally transition metal) linked by two or multifunctional organic units which called metal-organic frameworks (MOFs) [1]. In recent years, metal-organic frameworks (MOFs) are valuable materials because of their applications on the preparation of adsorption, catalysis, sensors, electronics, selective separation, fuel cells, petrochemistry, large scale of industrial products and drug delivery [2]. Some advantages of these materials nanoscopic and porous materials are high surface area, high thermal stability of their chemical structure [3]. Multivariate MOFs (MTV-MOFs), in which numerous nuclei, organic and linker features are merged into a framework, have introduced with many chances for modeling the complexity of the porous of MOFs in a logical method [4]. Therefore, task-specific and rational design of metal-organic frameworks (MOFs) with the goal to change the surface area, pore size, stability thermal and chemical improve performance is the major interest of various chemists around the world [5]. The catalytic activity of MOFs in cases of oxidation reactions, C-C bond formation and organic synthesis had been reported [6]. Recently, we have developed the modification of MOFs, as a significant system for preparing new functionalized frameworks [7]. Our research have focused on the synthesis of functionalized Cr, Co, Zr-based MOFs and their applications as task-specific, recyclable and reusable catalyst in organic synthesis (**Scheme 1**).



Scheme 1: Structure of various functionalized metal-organic frameworks (MOFs)

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Synthesis of novel UiO-66-SO$_3$H: Application in the synthesis of *N*-heterocycle compounds *via* vinylogous anomeric based oxidation

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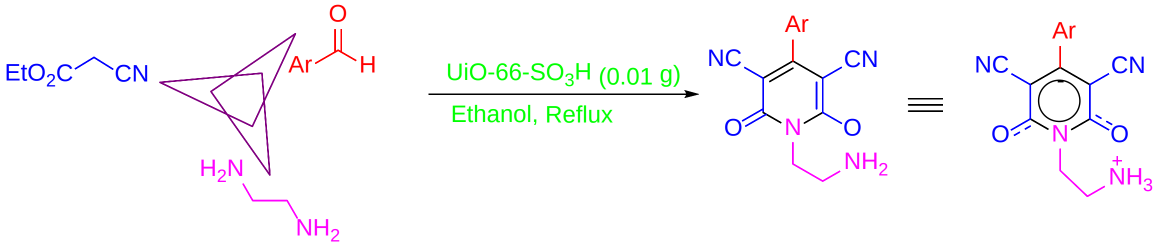
Keywords: *N*-heterocycle derivatives, Metal organic frameworks (MOFs), UiO-66-SO$_3$H.

Nowadays, one-pot multicomponent coupling 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. They also address fundamental principles of synthetic efficiency and reaction design, and show atom-economy and selectivity [1]. In this context, Hantzsch reaction for the synthesis of dihydropyridines (DHPs) shows interesting features of MCRs . More than a century ago, the first 1,4-DHPs were reported by Hantzsch [2]. After that a number of modified methods under improved conditions have been reported [3]. Hantzsch 1,4-dihydropyridine derivatives are often regarded as the models of the natural reduced nicotinamide-adenine dinucleotide (NADH) coenzyme which functions as redox reagent in the biological metabolism [4]. We have synthesized new UiO-66 containing sulfonic acid tags as catalyst for the regioselective synthesis of highly substituted 2-pyridones. A multicomponent reaction involving ethylcyanoacetate, aromatic or heteroaromatic aldehydes and amines to afford the hexasubstituted 2-pyridones in the presence of described catalyst (**Scheme 1**).



Scheme 1. Synthesis of hexasubstituted 2-pyridones catalyzed with UiO-66-SO$_3$H

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Silver nanoparticles decorated on thiol-modified magnetic hydrotalcite (Fe_3O_4/HT-Pr-S-Ag): a novel, efficient and magnetically nanocatalyst for oxidation of alcohols

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Keywords: Magnetic hydrotalcites, oxidation of alcohols, silver,

Organic synthesis under the conditions with respect to the principle of green chemistry still continues to be explored today. For this purpose, to improve the long-term durability and activity of catalysts, hydrotalicites (HTs) and magnetic hydrotalcites (MHTs) have been widely studied as promising supporting materials for catalysts in organic reactions[1-2]. Widespread attention has been focused on selective oxidation of alcohols into the corresponding aldehydes and ketones[3]. A number of new catalytic systems based on silver in combination with different ligands have been investigated in oxidation reactions[4]. In summary we have successfully synthesized Ag immobilized on functionalized magnetic hydrotalcite (Fe_3O_4/ HT-Pr-S-Ag) from readily available starting materials. The applicability of nanocatalyst was explored in oxidation benzyl alcohols to corresponding benzaldehydes using tert-butyl hydroperoxide (TBHP) as an oxidant in ethanol as a safe solvent at 60 °C.

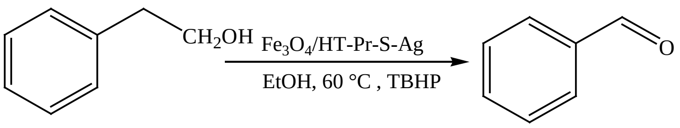

Fig. 1 Oxidation benzyl alcohols

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Synthesis of novel Lower-rim minoxidil substituted calix[4]arene: New sensitive and selective fluorescent sensor for Cu^{2+}

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Keywords: Supramolecular chemistry, Noncovalent interactions, Host-guest chemistry, Chemosensors, Calix[4]arenes, Minoxidil,

Supramolecular chemistry deals with reversible noncovalent interactions such as electrostatics, hydrogen binding, van der Waals and donor–acceptor interactions between two or more molecules or ions.[1] Macrocyclic hosts such as crown ethers, cryptands, cyclophanes, calixarenes and cucurbiturils have been synthesized and received much attention, opening a wide range of opportunities for new supramolecular chemistry.[2] Calixarenes are examples of metacyclophanes which are composed of phenol and methylene bridge units.[3] These cyclic oligomers are useful for the building-up of the functionalized host molecules. Minoxidil, a piperidinopyrimidine, was initially developed as an antihypertensive agent by The Upjohn company.[4] This molecule has an oxygen and five nitrogen atoms in an arraye which can make minoxidil such a suitable ligand to interact with various ions, in particular metal cations. Thus, we have used minoxidil to introduce two active site at the lower rim of calix[4]arene annulus which can selectively recognize Cu^{2+}. The synthesize of the target molecule has been summarized below. The structure of the product was determined by HRMS, ^{1}H and ^{13}C NMR and IR spectroscopic data.

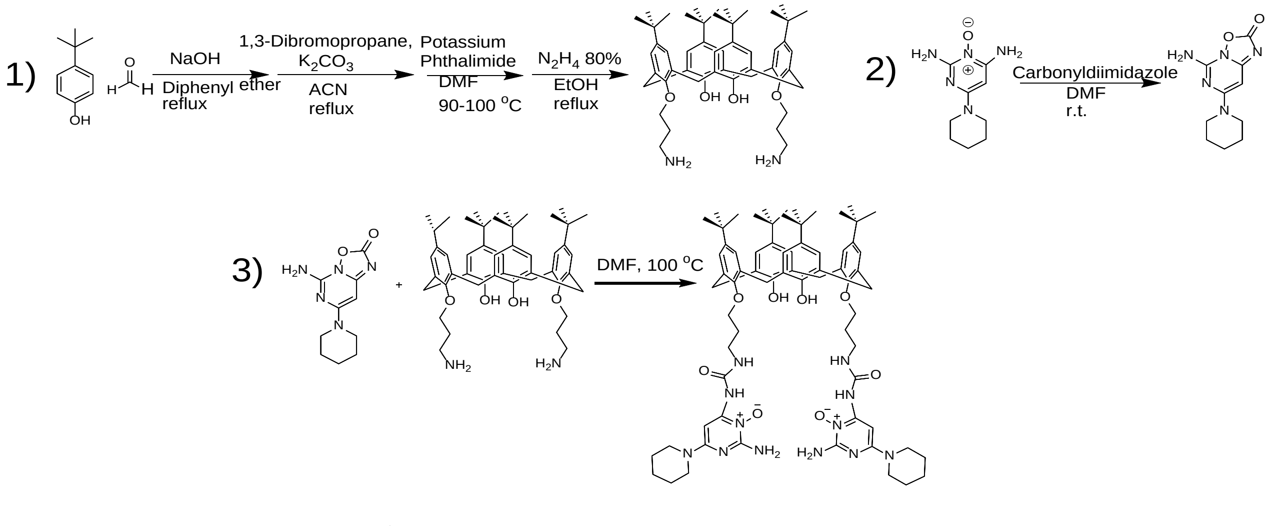

Fig. 1 Synthesis of Calix[4]arene di-substituted at the lower rim by minoxidil

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Organometallic Complex of Palladium on Boehmite Nanoparticles as Highly Efficient and Organic-Inorganic Hybrid Nanocatalyst for the C-C Coupling Reactions

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Keywords: Boehmite nanoparticles; Suzuki–Miyaura reaction; Mizoroki-Heck reaction; Palladium; C-C coupling reactions.

Boehmite is a cubic orthorhombic structure of aluminum oxide hydroxide which was prepared through addition of NaOH solution to $Al(NO_3)_3.9H_2O$ solution at room temperature. In this work, the surface of boehmite nanoparticles (BNPs) was modified by 3-choloropropyltrimtoxysilane (CPTMS) and further 1-methyl imidazole was anchored on its surface. Finally, an organometallic complex of palladium was supported on the surface of modified BNPs (Pd-imi@BNPs). These obtained nanoparticles were applied as efficient, recyclable and hybrid of organic-inorganic nanocatalyst in carbon-carbon coupling reactions under phosphine-free conditions at atmospheric pressure. Structure of this catalyst was characterized by SEM, TGA, XRD and ICP techniques. Heterogeneity and stability of Pd-imi@BNPs were studied by poisoning test and AAS technique which palladium leaching was not observed in reaction conditions. Therefore, this heterogeneous catalyst can be reused for several times. Also, all products were obtained in high TON and TOF numbers in the presence of Pd-imi@BNPs, which are reveal the high efficiency of this catalyst in C-C coupling reactions. Selectivity of this catalyst was studied in various aryl halides which are bearing different functional groups.

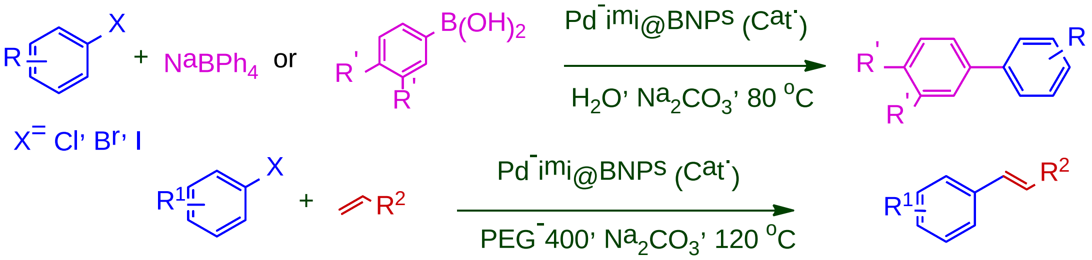

Fig. 1 C-C coupling reactions in the presence of Pd-imi@BNPs.

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Pd-adenine@boehmite as Efficient and Organic-Inorganic Hybrid Catalyst for Organic Reactions

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Keywords: Palladium, Boehmite nanoparticles, Suzuki reaction, Biphenyl, Tetrazoles, Adenine.

Boehmite (γ-AlOOH) is one of the polymorph phase of aluminum oxihydroxide and inorganic lamellar compound which was formed from octahedral units of six oxygen atoms around the central aluminum. Thermal stability, non-toxicity, ease of surface modification, high specific surface area are major advantages of boehmite nanoparticles for its catalytic application. Meanwhile, boehmite nanoparticles have been rarely applied as support for preparation of heterogeneous catalysts. Therefore herein we have reported a new procedure for the preparation of immobilized palladium catalyst on boehmite nanoparticles (Pd-adenine@boehmite), and successfully demonstrate its application as recoverable catalyst for carbon-carbon coupling reactions and synthesis of tetrazole derivative. All products were obtained in excellent yields and high TOF values which indicate the high efficiency of this catalyst. This catalyst was reused for several times without significant loss of its catalytic activity.

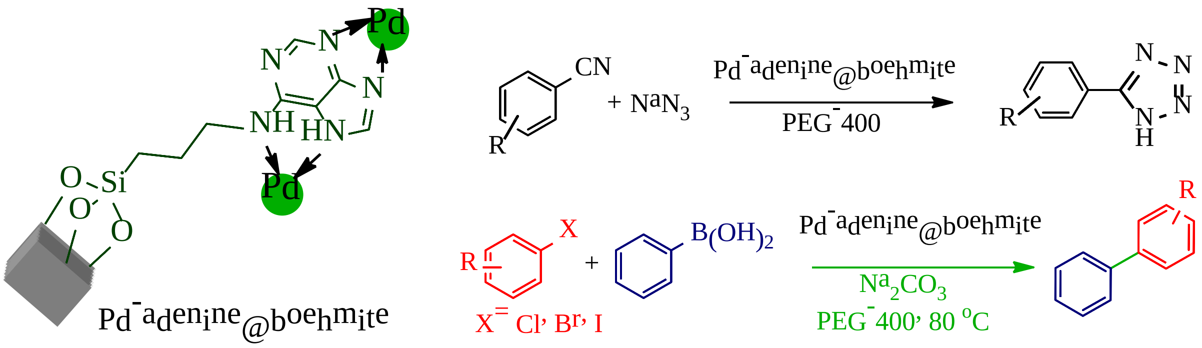

Fig. 1 Synthesis of tetrazoles and C–C coupling reaction in the presence of Pd-adenine@boehmite

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Modification of Boehmite Nanoparticles with Dithizone for the Immobilization of Copper as Organic–Inorganic Hybrid Nanocatalyst in Organic Reactions

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Keywords: Copper, Boehmite nanoparticles, Sulfoxides, Biphenyl, Polyhydroquinoline, Dithizone.

Boehmite nanoparticles are aluminum oxide hydroxide particles, which has large specific surface area and can be prepared using an inexpensive procedure in water. In this work, copper catalyst was immobilized on boehmite nanoparticles (Cu-dithizone@boehmite) using simple and inexpensive method and available materials. Further, this catalyst was characterized by SEM, EDS, WDX, XRD, AAS, FT-IR and TGA analysis. Cu-dithizone@boehmite was applied as highly efficient nanocatalyst in C-C coupling reaction (Suzuki reaction) under palladium-free and phosphine-free ligand. Also this catalyst was applied for the synthesis of polyhydroquinoline derivatives and selective oxidation of sulfides to sulfoxides. This catalyst was reused for several times without loss of its catalytic activity. Heterogeneity and stability of Cu-dithizone@boehmite was studied by hot filtration test.

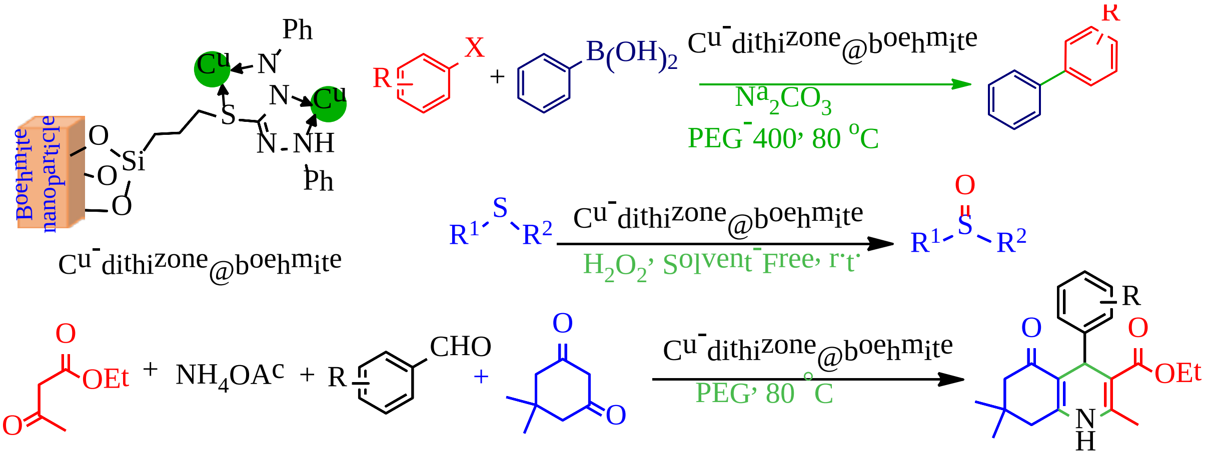

Fig. 1 Organic reaction in the presence of Cu-dithizone@boehmite

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Usage of 2-Methyl-5-isopropylphenol (Carvacrol) in the Preparation of Saturex Herbal Remedies to Prevent Stroke Caused by High Blood Pressure, Lipids and Blood Glucose

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Keywords: Carvacrol, Blood pressure , Inhibition, Saturex, Blood glucose

Carvacrol is the major compound of essential oils of many plants. In fact, it is an oxygenated monoterpene that widely found in the nature, and essential oil of plants acts an important role as protectors by exerting antibacterial, antiviral, antifungal, antioxidant, genotoxic, and free radical scavenging properties[1]. Several Satureja species are used in traditional medicine due to its recognized therapeutic properties that has anti-microbial and cytotoxic activities related to its chemical properties[2]. Carvacrol has formed more than 92% of medicinal plants essential oil structure and it was shown to possess antiseptic, antibacterial, antifungal antigen toxic, antitumor, antioxidant, and antispasmodic activities[3]. Pharmacological actions of the essential oils were suggested to be parallel to the carvacrol content of the essential oils[4]. Carvacrol absorbs destructive radicals, especially oxygen radical (endogenous), and radicals of food poisons such as; aflatoxins (exogenous), leading to a heartbeat reduction, arterial pressure and systolic and diastolic blood pressures. It has anti-oxidant properties in biochemical processes such as inhibition of lipid peroxidation, especially LDL. It prevents atherosclerosis and the occurrence of cardiovascular stroke.

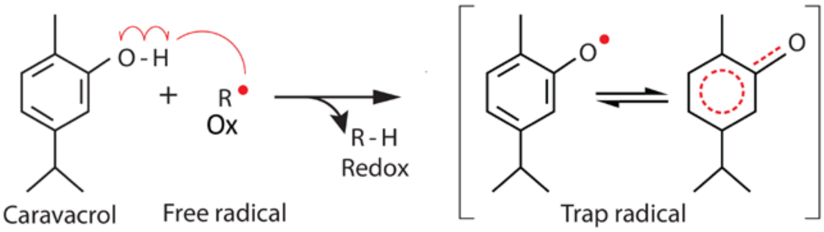

Fig. 1 Scavenging effect of carvacrol on free radical

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Synthesis of azo dyes in the presence of a solid acid catalyst under various conditions

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Keywords: Diazo coupling, Azo dyes, Solid acid catalyst, Aromatic amines

Azo dyes have been synthesized via coupling of diazotized aromatic amines with activated aromatic compounds[1]. Azo compounds are the most widely class of industrial synthesized organic dyes due to their versatile application in various fields[2]. In such new method, different kinds of aromatic amines, with electron-withdrawing groups as well as electron-donating groups, were rapidly converted to the corresponding azo dyes in the presence of $NaNO_2$ and solid acid catalyst at room temperature[3].

In this work we wish report the simple demonstrating and convenient method for the synthesis of azo dyes. Short reaction times, Simple reaction, high yields, clean process, simple methodology, conference system, easy work-up and green conditions are advantages of this protocol (Fig.1).

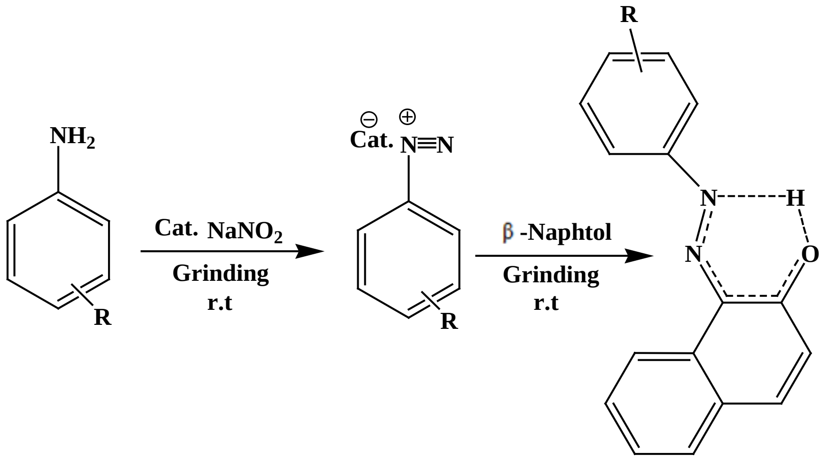

Fig. 1 Synthesis of azo dyes using solid acid catalyst at room temperature

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A simple green synthesis of $NiFe_2O_4$@ZnO magnetic nanocomposite and its use as an efficient catalyst for the synthesis of polyhydroquinoline derivatives under microwave irradiation

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Keywords: Multicomponent reactions, Polyhydroquinoline derivatives, Solvent free, Green synthesis.

Polyhydroquinolines are one of the most important classes of heterocyclic scaffolds providing major ligands for biological receptors. Polyhydroquinolines the source of some valuable drugs which are very important in pharmacy. For instance, they demonstrate activity for the treatment of angina pectoris and hypertension.[1-3] In this work, synthesis of $NiFe_2O_4$@ZnO nanocomposite was performed by the green sol–gel method using natural gel. The sample was characterized by Fourier transform infrared spectrophotometer (FTIR), X-ray powder diffraction (XRD), vibrating sample magnetometer (VSM), Transmission electron microscopy (TEM), Field emission scanning electron microscopy (FESEM) and energy dispersive X-ray analysis (EDX). $NiFe_2O_4$@ZnO nanocomposite was used as a reusable and robust heterogeneous catalyst for one-pot four component synthesis of polyhydroquinoline derivatives via the esteemed Hantzsch reaction using aryl aldehydes, ethyl acetoacetate, dimedone and ammonium acetate by microwave irradiation under solvent free conditions (Fig 1). The final product was investigated by ^1H NMR and ^{13}C NMR spectroscopy. This method has many advantages such as high yields, relatively short reaction times, mild reaction condition, easy work up, and using a highly recyclable catalyst.

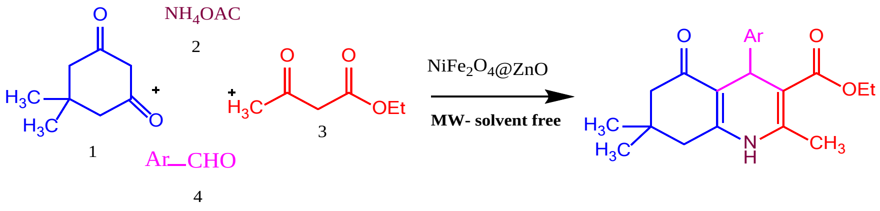

Fig. 1 Synthesis of polyhydroquinoline derivatives

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Preparing Biodegradable Hydrogel Based on Quince Seed Mucilage and Investigation as a Drug Delivery System

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Keywords: Polysaccharide-based hydrogels, Quince Seed Mucilage, Biocompatibility, Drug delivery.

The traditional drug delivery systems created side effects in the body, due to the lack of control in the amount and selectivity of drug release. So today, many scientists are interested in a controlle release drug delivery systems and much research is being done on it. Hydrogels are usually used for this purpose[1]. Hydrogels are three-dimensional network hydrophilic polymers that can absorb water several times more than their dry weight. This ability depends on the structure of the polymer and the environmental factors[1,2]. Polysaccharide-based hydrogels are currently attracting much interest for their unique properties, that is, high water-affinity, easy procedures, biocompatibility, biodegradability, renewability, and nontoxicity, which facilitates the applications in the pharmaceutical field[3]. Quince seed mucilage (QCM), composed of glucuronic acid and xylose (glucuronoxylan)-based biomaterial. Glucuronoxylan is an inexpensive and biocompatible polysaccharide hydrogel which is extruded from the seeds of different plants including quince (Cydonia Oblonga)[4]. In this research, the synthesis of polysaccharide extracted of quince seed graft to functionalized polyvinyl alcohol (APVA) and acrylic acid (AA) copolymer have been investigated, using ammonium persulfate (APS) as an initiator. Using *N, N'*-methylenebisacrylamide (MBA) as a cross-linked changed copolymer to Hydrogel. The optimization was carried out using to study the effect of AA and APVA, MBA amounts, initiator concentration, temperature and time reaction based on the water absorbency capacity. Drug loading and release behavior performed on hydrogel.

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Synthesis and Characterization of Biocompatible Hydrogel Nanocomposite Based on Quince Seed Mucilage

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Keywords: Quince seed hydrogel, nanocomposite, biocompatible, Metal oxide nanoparticle.

Natural polysaccharide-based hydrogels show unique properties such as biodegradability, biocompatibility, stimuli-responsive characteristics and biological functions making them a material of option for various applications. Actually, during the last few years, a number of biopolymers-based hydrogels have attracted great interest for different applications such as biomedical area, toxic ion removal and waste-water treatment, agriculture, biosensors, and tissue engineering. In order to improve the drawbacks related to hydrogels, nanocomposite hydrogels were extended by incorporating different types of nanoparticles in the hydrogel network. This research focuses on preparation of biodegradable chemically cross-linked hydrogels hybrid composites consisting of metal oxide nanoparticles (CuO-ZnO), two natural and synthetic polymers including the polysaccharide extracted of quince seed mucilage (QSM) and functionalized poly vinyl alcohol which are both inexpensive, and exhibits remarkable mechanical properties. QSM which is obtained from Cydonia Oblonga has been modified through graft copolymerization and network formation using APVA and acrylic acid (AA) as the monomers, ammonium persulphate (APS) as an initiator, and MBA as a cross-linker. Various reaction parameters such as amount of initiator and solvent, reaction time and temperature, pH, and monomer and cross-linker concentration, were optimized. A range of structural, mechanical and practical techniques were utilized to identify the hydrogels including, FTIR, UV/VIS, XRD, EDAX, TGA and swelling and hydrolytic stability.

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Synthesis of highly substituted pyrroles in the presence of cobalt phthalocyanine based catalyst

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Keywords: Synthesis of pyrroles, Cobalt phthalocyanine, Multicomponent reaction.

Among nitrogen containing heterocyclic compounds, pyrrole derivatives are one of the most interesting units in natural products, biological active molecules, and useful building blocks for various functional materials. On the other hand, multicomponent reactions protocol is one the most powerful strategy for the synthesis of versatile molecules through an economic manner. This key tool represents several merits such as good to high yields, minimizing waste, less time consuming and avoidance of costly purification steps, over step by step strategies. In recent times, phthalocyanine based catalysts with metal core, have found divers applications in different fields of science. This elegant position of phthalocyanine based catalyst is due to their thermal and chemical stability and distinct optical and electrical properties. [1-3]

Herein, we wish to report the synthesis of highly substituted pyrroles in the presence of cobalt phthalocyanine based catalyst (Fig 1).

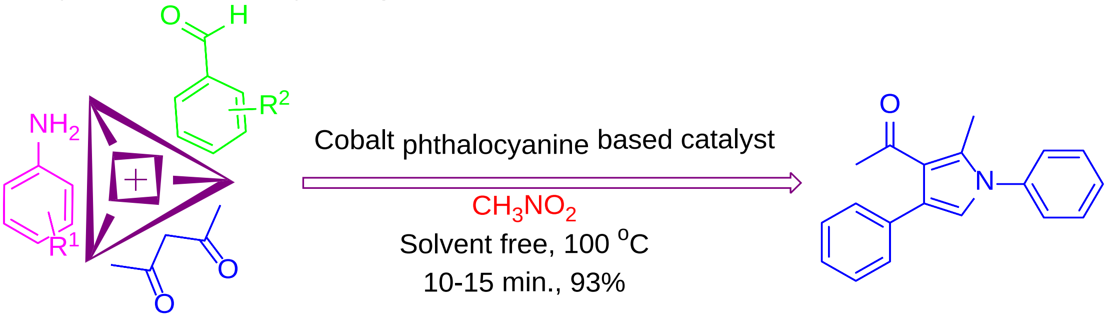

Fig. 1 Synthesis of highly substituted pyrroles by using cobalt phthalocyanine catalyst.

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Cobalt phthalocyanine based catalyst promoted the facile synthesis of cyclohexa-1,3-dienamines

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Keywords: Cobalt phthalocyanine, Cyclohexa-1,3-dienamines, Multicomponent reaction

Metal phthalocyanines as macrocyclic complexes, due to easy preparation and chemical stability are broadly used in organic functional group transformations. These structures, due to their elegant optical and electrical characteristic, have found various applications in material science. On the other hands, multisubstituted cyclohexa-1,3-dienamines are privileged structure which represent varied pharmaceutical applications in medicinal chemistry. These molecules, can applied as useful intermediates for synthesis of cyclophanes to create a large molecular cavity and host-guest complexes.[1-2]

In this investigation, we presented a multicomponent reaction manner for the synthesis of multisubstituted cyclohexa-1,3-dienamines through the reaction of aryl ketones, aldehydes and malononitrile in the presence of cobalt phthalocyanine based catalyst (Figure 1).

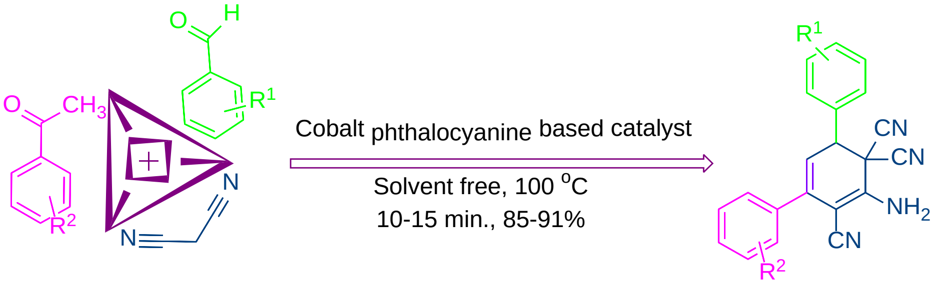

Fig 1: **Synthesis of multisubstituted cyclohexa-1,3-dienamines in the presence of cobalt phthalocyanine based catalyst.**

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Synthesis of fused benzoquinolines: Catalytic application of Co-phthalocyanine-SO_3H

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Keywords: Benzoquinoline, Co-phthalocyanine-SO_3H, Three-component reaction.

N-Heterocyclic compounds are a paramount important class of biological and medicinal candidates.[1] These scaffolds are found to be having several applications in agrochemicals, pharmaceuticals, dyestuffs, and functional materials. They have a wide range of biological activities including antitubercular, anticancer, antipsychotic, antimicrobial, anti-HIV, and for the treatment of neurodegenerative diseases.[2] Marinoquinolines are a class of fused quinolines isolated from the marine bacteria having antibacterial and antifungal activities. Fused quinolines and benzoquinolines core units are found in various alkaloids and commercial drugs.[3] In this work, we wish to report a clean method for synthesis of benzoquinoline derivatives via reaction of aromatic amin, dimedone and aryl aldehyde under refluxing CH_3CN using Co-phthalocyanine-SO_3H (10 mg) as an efficient nano-catalyst (**Scheme 1**).

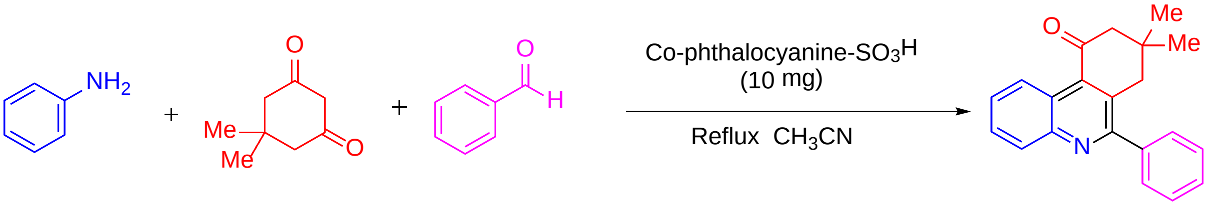

Fig. 1 Synthesis of benzoquinoline derivatives using Co-phthalocyanine-SO_3H

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One-pot synthesis of fused 1,2-dihydropyridines

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Keywords: 1,2-Dihydropyridines, Acetylenic esters, Triphenylphosphine, Alkylamines, Ninhydrin

Dihydropyridines (DHP) are among the most beneficial scaffolds that have revolutionised pharmaceutical research with unprecedented biological properties[1]. DHPs are versatile intermediates in the synthesis of various alkaloids and important bioactive products such as aza-sugar derivatives and anti-influenza drug Tamiflu. Major synthetic routes to 1,2-dihydropyridine derivatives include condensation reactions, reduction of and nucleophilic addition to pyridines and pyridinium salts, and ericyclic reactions[2,3]. The zwitterionic intermediates, generated *in situ* from triphenylphosphine and dialkyl acetylenedicarboxylates, are trapped by N-H acidic 2-(alkylamino)-2-(1,3-dioxo-1*H*-inden-2(3*H*)-ylidene)acetonitriles in refluxing toluene to afford dialkyl 2-alkyl-1-cyano-9-oxo-3,9-dihydro-2*H*-indeno[2,1-*c*]pyridine-3,4-dicarboxylates in good yields. Various features of these transformations will be presented and discussed.

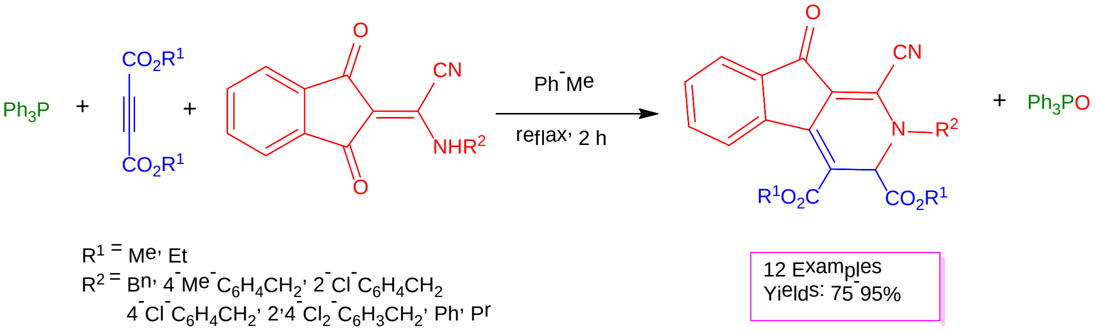

Fig. 1 Synthesis of fused 1,2- Dihydropyridine

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One-pot multicomponent synthesis of benzodiazepine derivatives

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Keywords: Asymmetric multicomponent reactions, benzodiazepines, cyclohexane 1,3-dione, 1,2-phenylenediamines.

Asymmetric multicomponent reactions (AMCRs) are chemical reactions in which three or more reactants produce products that they have some advantages containing simplicity of operation, high yields, easy purification1. Heterocycles containing benzodiazepine are a class of psychoactive drugs because of their biological activities related to the central nervous system2,3.

Herein, we report the synthesis of rigid seven-membered chiral heterocycles (benzodiazepines) from the reaction of cyclohexane 1,3-dione, 1,2-phenylenediamines, aldehyde derivatives in ethanol with L-proline at 80 °C.

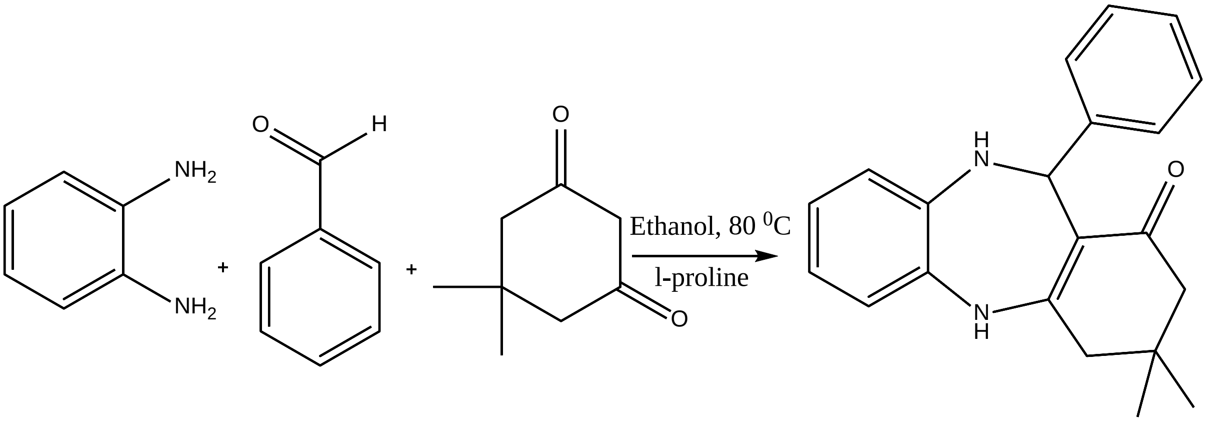

Fig. 1 synthesis of benzodiazepine derivatives

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Synthesis of 2,6-Diamino-4-arylpyridine-3,5-dicarbonitrile Derivatives of calix[4]aren via Multicomponent reaction

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Keywords: Multicomponent reactions, 2,6-Diamino-4-arylpyridine-3,5-dicarbonitrile, catalyst free, supramolecular chemistry, Calixarenes.

Six-membered aromatic rings such as pyridine have many useful applications such as drug structure, various biological activity and fluorescence properties.[1] 2,6-Diamino-4-arylpyridine-3,5-dicarbonitriles are specific category of substituted pyridine derivatives were synthesized by three-component reaction (MCR). The notable features of the conditions of reaction are simplicity, moderate, controllable, catalyst free and easy workup.[2]

The Calixarenes as rigid vase-like molecules are used widespread in several areas of supramolecular chemistry such as macrocyclic receptors for anions, cations, amino acids, small peptide and DNA recognition.[3,4]

In this research, we have focused on the synthesis of a novel lower rim pyridine-calix [4] arenes **4**, by the reaction between calix [4] aldehyde **1**, malononitrile **2** and ammonium acetate **3** in the reflux conditions. For this aim, the synthesized compounds were characterized by FTIR, ^{1}H NMR.

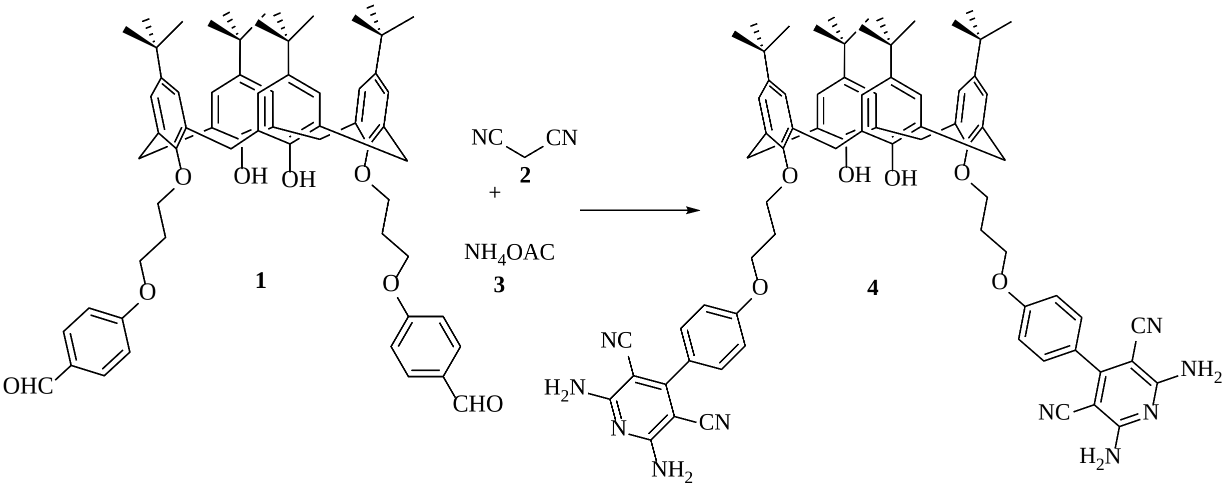

Fig. 1 Multicomponent 2,6-Diamino-4-arylpyridine-3,5-dicarbonitriles lower rim calix [4] arenes

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A synthesis of novel (arylthio-ethylidene)indolin-2-one derivatives via *S*-arylation of oxoindolin-ethanethiolates with aryl halides

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Keywords: Cu(I) iodide, *S*-Arylation, aryl halides, 1-aryl-2-thiocyanatoethan-1-ones, .

In recent years, Ullmann-type reactions have grown into a versatile tool for access to C−X (X = C, N, O, S, etc.) bonds.[1] Although several palladium, nickel, and cobalt catalysts have proven to be highly effective in such coupling processes,[2] copper reagents are favorable catalytic systems for C-X bond-forming reactions due to their low cost, low toxicity, and good functional group tolerance.[3] Among various cross-coupling reactions, *S*-arylation is comparatively less studied. However, given the prevalence of C-S bonds in a wide range of pharmaceutical compounds and polymeric materials, it is desirable to find novel catalytic procedures that provide efficient access to such useful organic products. In this investigation, we have reported a practical procedure for the copper-catalyzed *S*-arylation of triethylammonium [2-oxo-1-(2-oxo-1,2-dihydro-3*H*-indol-3-ylidene)-2-arylethyl]sulfides, which provides a new route to the synthesis of (*Z/E*)-3-(2-oxo-2-aryl-1-(arylthio)ethylidene)indolin-2-one derivatives in good yields.

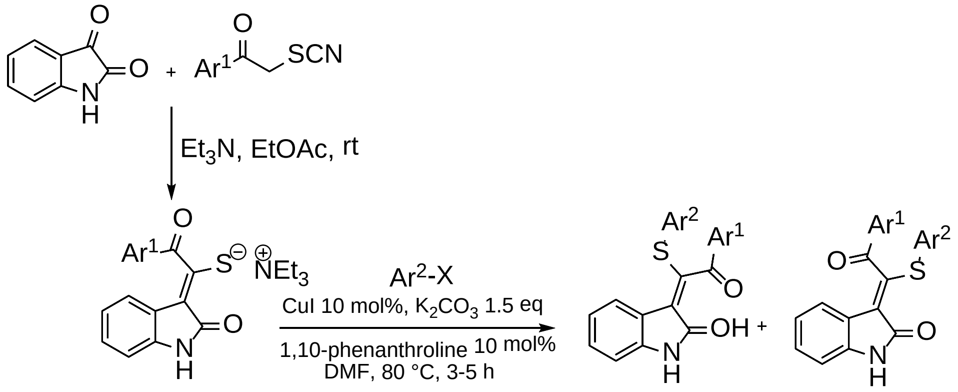

Fig. 1 Synthesis of (arylthio-ethylidene)indolin-2-ones

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Design and application of modified zeolite-Y as efficient nanocatalysts for the synthesis of heterocycles

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Keywords: Zeolite-NaY, Nanocatalyst, Heterocycle, Imidazole, Thiazole, Perimidine.

Recently, zeolites have attracted increasing interest as ideal supports for homogeneous catalysts due to their high surface area, high thermos-stability, nanoporous crystalline structure, persistence in all organic solvents, less or no corrosion, processes, *etc*. On the other hand, heterocycles are organic compounds that have atoms of at least two different elements as members of their rings. There are many synthetic heterocyclic systems that are indicative of their importance due to their biological activity and pharmaceutical applications. Herein, modified zeolite-NaY nano-porous were synthesized, characterized and applied for the synthesis of heterocycles such as perimidines, tri-substituted imidazoles, tetra-substituted imidazoles, 2-aminothiazoles, 2-arylbenzimidazoles, thiazolidinones, and chromenes,[1-4] respectively (Fig. 1).

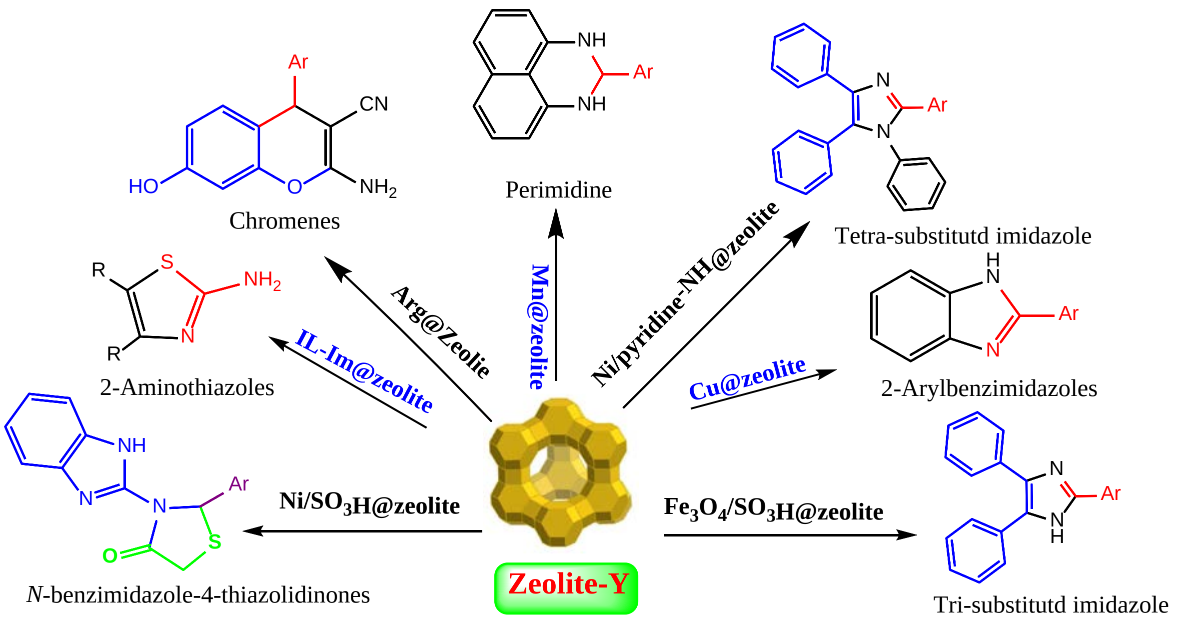

Fig. 1 Synthesis of organic heterocycles catalyzed modified zeolite-NaY

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Arginine functionalized zeolite-Y as a new nanocatalyst for efficient synthesis of 2-amino-4*H*-chromenes

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Keywords: Synthesis, Arginine, Zeolite-NaY, Nanocatalyst, Chromene.

Chromenes are widely used in pharmaceutical chemistry due to their potential biological properties and pharmacological importance such as psoriatic arthritis and rheumatoid and in cancer therapy. Among various types of chromene, 2-amino-4*H*-chromene heterocycles are of particular utility as they belong to privileged medicinal scaffolds serving for generation of small-molecule ligands with highly pronounced anti-coagulant, spasmolitic diuretic, and anti-anaphylactic activities[1-3]. Herein, further research on the synthesis of modified nano-zeolites[4], initial, *N*-(3-trimethoxysilylpropyl)-Arginine supported zeolite-NaY (Arg@zeolite-Y) based nanoporous materials were synthesized and their structures were confirmed using different characterization techniques such as FT-IR, FE-SEM, EDX, N_2 adsorption–desorption (BET), and TGA analyses. We also report the synthesis of 2-amino-4*H*-chromenes from aldehyde, malononitrile, and resorcinol in one-pot reaction at the percent of Arg@zeolite as high effective nonocatalyst, (Fig 1). The benefits of this work are mild reaction conditions, good yields, easy isolation of products, and simple operational procedures.

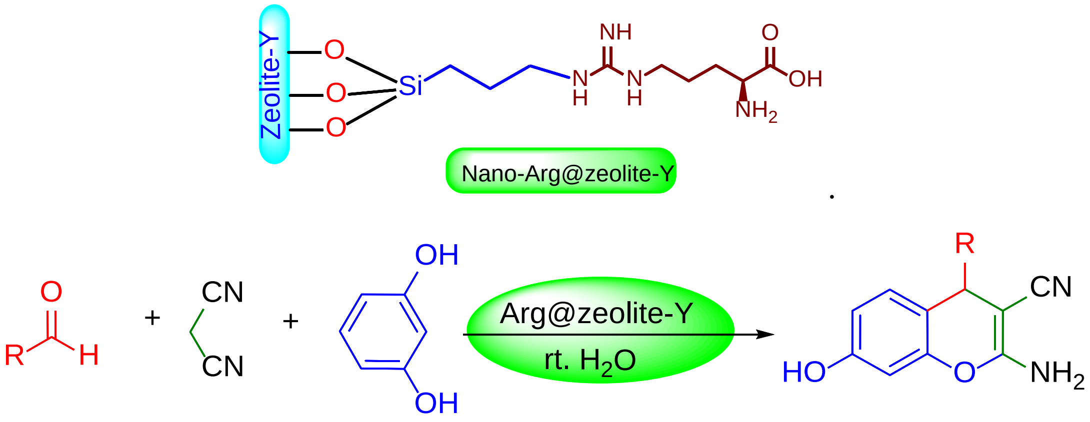

Fig 1. Synthesis of 2-amino-4*H*-chromenes using Arg@zeolite-Y

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Pseudopolymeric magnetic nanoparticles promoted the synthesis of pyrazolopyridines under mild reaction conditions

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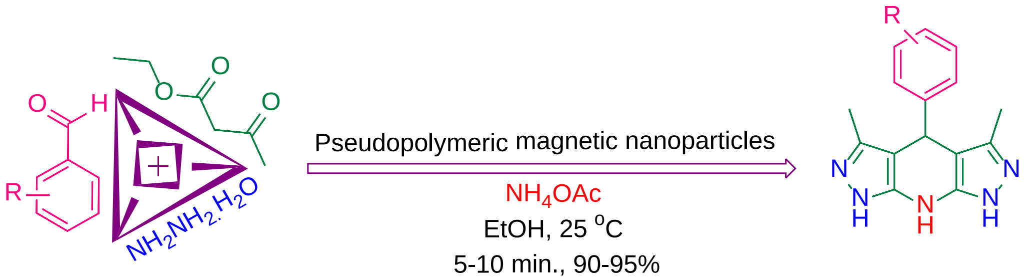
Keywords: Syntheis of pyrazolopyridine, Magnetic nanoparticles, Multicomponent reaction.

Due to unique features of magnetic nanoparticles such as high potential of reusability, low toxicity, large surface area, ease of separation and low cost, they were found an elegant role in different field of chemistry such as catalytic systems. Also, interesting characteristic of multicomponent reactions strategy such as tom economy, experimental simplicity and synthetic efficiency, makes it a powerful tool for chemists. On the other hand, pyrazolopyridine derivatives are biologically-active heterocyclic compounds which represent varied pharmacological properties such as antimicrobial and antiviral activities[1-3].

In this work, we presented the synthesis, characterization and catalytic application of novel pseudopolymeric magnetic nanoparticles for the synthesis of pyrazolopyridine derivatives (Fig1).



R : 4-Cl, 2-Cl, 4-Br, 4-CF$_3$’ 3,5-(F)$_2$’ 3-NO$_2$’ H, 4-Me, 4-OH, 2-OMe, 3,4,5-(OMe)$_3$, 4-Isopropyl, Pyridine-3-carbaldehyde, α-Methyl cinnamaldehyde

Fig 1: Synthesis of pyrazolopyridine derivatives by using pseudopolymeric magnetic nanoparticles

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Synthesis of cyclohexa-1,3-dienamines in the presence of pseudopolymeric magnetic nanoparticles under solvent free conditions

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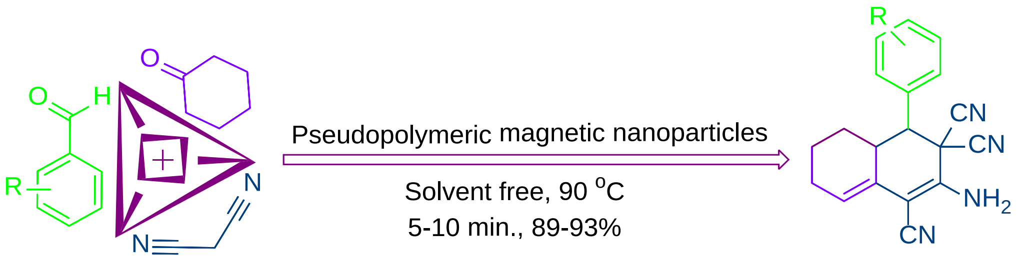
Keywords: Cyclohexa-1,3-dienamines, Pseudopolymeric magnetic nanoparticles, Multicomponent reaction.

Among heterocyclic scaffolds, multisubstituted cyclohexa-1,3-dienamines and their derivatives are unique. These heterocyclic molecules, represent diverse biological and pharmacological applications and well distributed in naturally-occurring compounds. Also, they are key synthetic intermediates. On the other hand, among heterogeneous catalytic systems, magnetic nanocatalysis presents a catalytic system which shows suitable activity, selectivity, easy separation and recovery. The paramount goal of one-pot multicomponent reactions, are the effective and rapid synthesis of target molecules accompanied with economic and ecological insight.[1-3]

In this study, we combined the merits of magnetic nanocatalysis and multicomponent reactions and represent a mild protocol for the synthesis of multisubstituted cyclohexa-1,3-dienamines by using a pseudopolymeric magnetic nanoparticles (Fig 1).



R= 4-Cl, 2-Cl, 4-Br, 3,4-F_2' 3,5-F_2' 3,5-$(CF_3)_2$' 4-CF_3' 3-NO_2' H, 4-Me, 3-OH, 4-OH, 3-OEt-4-OH, 2-OMe, 3,4,-$(OMe)_2$' 4-Isopropyl, Pyridine-4-carbaldehyde,Pyridine-3-carbaldehyde ، Pyridine-2-carbaldehyde

Fig. 1 Synthesis of cyclohexa-1,3-dienamines in the presence of pseudopolymeric magnetic nanoparticles

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Molecular Structure Investigation of Penicillins and Cephalosporins Antibiotics by DFT Method

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Keywords: Penicillin; Cephalosporin; β-lactamas; Acylation; β-lactam; pyramidality

The class of β-lactam antibiotics are the most successful medicines. They have a β-lactam reaction ring opening.[1] Penicillins and cephalosporins are both β-lactam antibiotics that interfere with the synthesis of peptidoglycan, which it is the main component of the bacterial cell membrane.[2] The molecular structures and the activities of β-lactam antibiotics are particularity importance in the emerging bacterial resistance to these medicines.[3] Here, some selected medicines from penicillin and cephalosporin antibiotics were discussed and the effect of pyramidality, carboxylate orientation and amide resonance (changes in the C-N and C=O length bond) have measured with quantum mechanics DFT/B3LYP/6-31G* method. The obtained values show that distance of the carboxyl with the carbonyl of the β-lactam is shorter in the active structures (Cohen distance between 3.0 to 3.9Å) as compared to those observed on the inactive geometries (more than 4.1Å Cohen distance). Also, the compared structural data of selected penicillins and cephalosporins were considered. The results show that the reduction of pyramidality values in cephalosporins is one of the reasons related to the acylation reaction by β-lactamase enzyme.

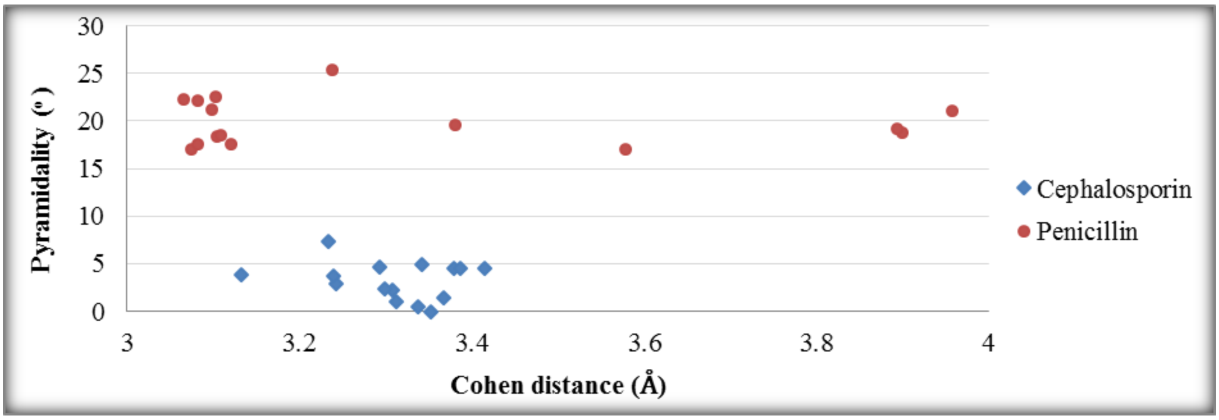

Fig. 1 Comparison of pyramidality and Cohen distance for penicillins and **cephalosporin**

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1)

Microencapsulation of Olive oil with gelatin and sodium alginate by complex coacervation

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Keywords: Microencapsulation, Complex coacervation, Olive oil, Gelatin, Sodium Alginate.

Most edible oils in spite of all proven health benefits are chemically unstable and sensitive to oxygen, light, moisture, and temperature. Hence, microencapsulation of active ingredients and their delivery need to be employed to stabilize the oil in order to fix the problem.[1] In the other hand, lipophilic drugs could not be encapsulated with water-soluble polymers as shell materials. To overcome this problem, olive oil which contains essential vitamins, fatty acids and other natural nutrients, is used as a solvent of these hydrophobic drugs.[2]

The present study aims at synthesizing gelatin A–sodium alginate complex coacervates and encapsulation of olive oil in the polymer system. Optimization of different reaction parameters such as pH and ratio between the polymers and cross-linker concentration was carried out to attain higher product yield.[3] The optimum ratio between gelatin and alginate and pH value in this study was set to 3.5 and 3.6, respectively. Microcapsules were crosslinked by sodium tripolyphosphate (PPT). Optical microscopy studies proved the formation of spherical microcapsules of different sizes. It was observed that the effect of using PPT as a crosslinker was desirable whereas increasing its amount in the case of a constant amount of polymer and oil caused the interruption of the electrostatic attraction between proteins and polysaccharides.[4] The optical microscopy analysis showed that the size of microcapsules was decreased with decreasing the amount of oil, polymer, and crosslinker. The oil content was sharply decreased with adjusting the PH value of TPP solution. Moreover, the encapsulation efficiency was increased by increasing the total amount of oil however it causes more surface oil.

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Schiff-base transition metal complexes fabricated on magnetic nanoparticles as efficient and reusable catalysts in Suzuki reaction

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Keywords: Zr, Cu Magnetic nanoparticles, Suzuki reaction, biphenyl, Schiff‑base.

Schiff- bases are widely studied because of increasing recognition of their role in catalytic systems. On other hand, magnetic nanoparticles (MNPs) can be used as heterogeneous support in catalytic reactions due to their unique features such as easy and clean separation of catalysts[1-3]. A simple, efficient, and less expensive protocol for the phosphine-free C-C coupling reactions has been reported in the presence of Schiff-base complexes of Zr or Cu ions supported on Fe_3O_4 MNPs (M–Schiff‑base@MNPs). The structure of these catalysts has been characterized by various techniques such as SEM, EDS, WDX, FT-IR, XRD, TGA, AAS, and VSM. The SEM images of this catalyst demonstrate that the particles size is less than 50 nm in diameter. The Suzuki reaction was carried out in green solvent using phenylboronic acid reagent. The formation of carbon-carbon bond have been frequently employed in the synthesis of natural products, agrochemicals, pharmaceuticals, biologically active compounds and advanced materials. VSM curve of the catalysts show that these catalysts can be recovered using an external magnet; therefore, these catalysts can be reused for several times without significant loss of its catalytic efficiency or metals leaching. Also, all products were obtained in high TOF numbers, which reveals these catalysts have high activity in the case of C-C coupling reactions.

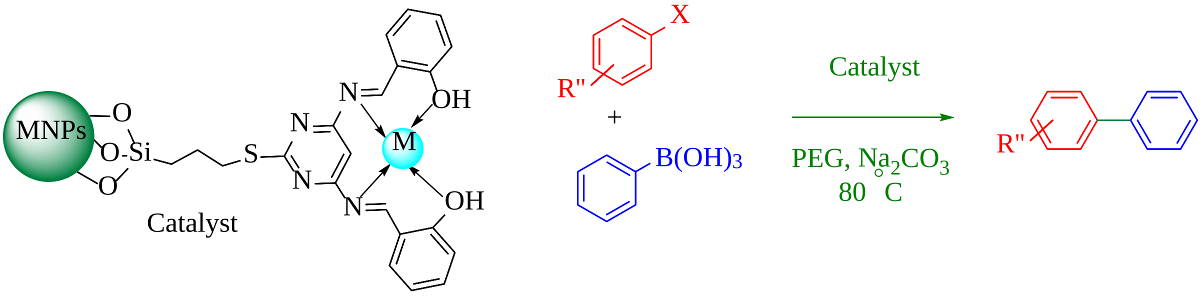

Fig. 1. Suzuki reaction in the presence of M–Schiff‑base@MNPs (M= Cu or Zr ions) as catalysts.

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Schiff-base complex of copper (II) fabricated on magnetic nanoparticles as practical and recyclable catalyst in organic reactions

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Keywords: Copper(II), Magnetic nanoparticles, Suzuki reaction, biphenyl, Schiff- base.

Schiff- bases are widely studied because of increasing recognition of their role in catalytic systems. On other hand, magnetic nanoparticles (MNPs) can be used as heterogeneous support in catalytic reactions due to their unique features such as easy and clean separation of catalysts. In this work, Fe_3O_4 MNPs was prepared via a chemical co-precipitation technique using Fe^{3+} and Fe^{2+} in aqueous ammonia solution. Then, the surface of MNPs was modified by 3-choloropropyltrimtoxysilane and further new Schiff-base was anchored on its surface. Finally, Schiff-base complex of copper (II) was stabilized on modified MNPs. Structure of this catalyst was characterized using FT-IR, VSM, SEM, EDS, WDX, XRD, TGA, and AAS techniques. The catalytic activity of this catalyst was described in the carbon-carbon coupling reaction and synthesis of nitrile derivatives. All the products were obtained in excellent yields and high TOF values which indicate the high efficiency of this catalyst. This catalyst was reused for several times without significant loss of its catalytic activity.

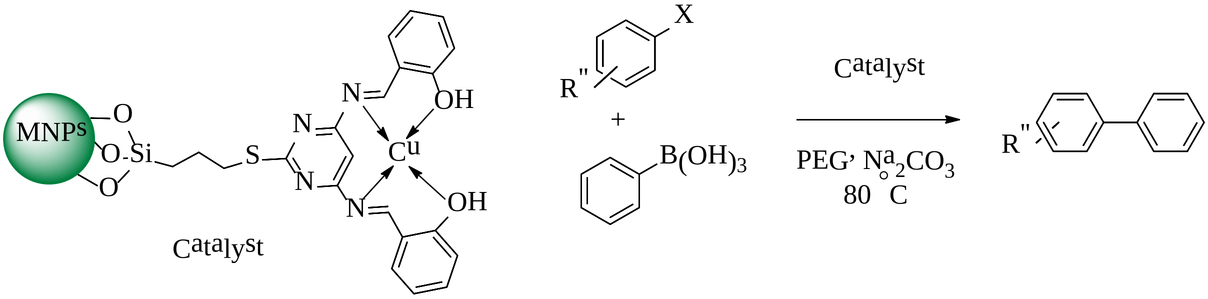

Fig. 1 C–C coupling reaction in the presence of Cu–Schiff- base@MNPs

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Four component synthesis of pyrano[2,3-*c*]pyrazoles using Ni@zeolite-Y as efficient and recyclable nanocatalyst

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Keywords: Ni@zeolite-Y, Nanocatalyst, Pyrano[2,3-c]pyrazole, Multi component reaction

The pyrano[2,3-c]pyrazoles are one important class of heterocyclic include nitrogen that exhibit a wide range of pharmacological activities and have broad applications in medicinal.[1,2] Additionally, these compounds have been acted as potential insecticidal.[3]According to importance of pyrano pyrazoles, up to now, different methods have reported for the synthesis of these compounds, the most of these methods despite have some benefit, include some limitations such as, use of toxic solvents, long reaction time, high reaction temperatures, low product yields, multi-stage processes and the use of toxic and expensive catalysts. Therefore, the development of a simple and environmentally benign approach is required to synthesis of this type of heterocyclic compounds. In this regard and looking for our research, [4] we report four-component synthesis of pyranopyrazole derivatives through the reaction between hydrazine, aromatic aldehydes, maleonitrile and ethyl acetoacetate, at 50-60 ℃ by application of mixture of ethanol and water as solvent (Fig 1) and using of Ni-supported on zeolite-Y as green and reusable catalyst.

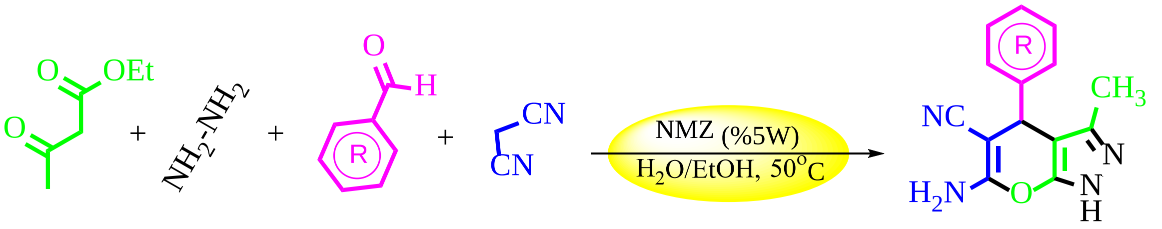

Fig 1: Synthetic method for pyranopyrazole derivatives

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SO_3H activated zeolite-Y as a nanostructured heterogeneous catalyst for synthesis of tri-substituted imidazoles

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Keywords: Imidazole, Zeolite, Nanocatalyst, Solid acid, Solvent-free.

Imidazoles are important *N*-containing heterocycles which have emerged as versatile biologically active compounds possessing applications. Tri-substituted midazoles or 2,4,5-triaryl-1*H*-imidazoles are generally synthesized in a one-pot three-component condensation of aldehydes, 1,2-diketones, and ammonium acetate. Although various catalysts have been proposed for tri-substituted imidazoles synthesis, exploration for greener and cleaner synthetic strategies still remains as an active research.[1-4] Herein, SO_3H@zeolite-NaY was used as a green and high active nanocatalyst for the synthesis of tri-substituted imidazole derivatives *via* solvent-free cyclocondensation of different aldehydes, benzil and ammonium acetate. (Fig 1) This economical chemical procedure has the advantages such as excellent yield in short reaction times, convenient manipulation and high purity of products, the use of nontoxic and heterogeneous acid catalyst with good reusability.

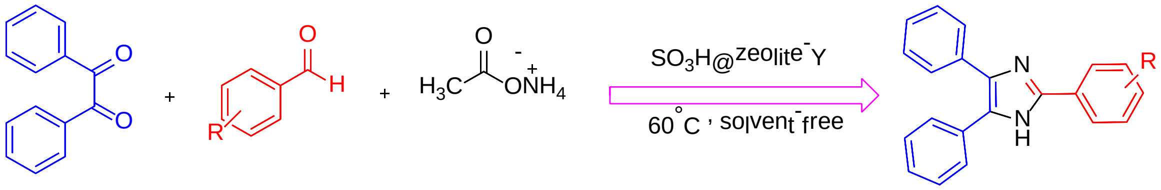

Fig 1: Synthesis of imidazole heterocycles using SO_3H@zeolite-Y.

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Synthesis of a new Series of Organophosphorus Aminopyrimidines under Solvent free Condition and Investigation of their Biological Activity

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Keywords: Multicomponent reactions, Antibacterial, Phosphonate.

Antibiotic resistance is a major global problem in both developed and developing countries.[1] The selection pressures on microorganisms when in contact with antibacterial agents underlies the emergence of resistance,[2] and the efficacy of first and second line antibiotics is decreasing at an alarming rate.[3] A series of novel unique structural organophosphorus aminopyrimidines were developed as potentially DNA-targeting membrane active inhibitors through an efficient one-pot procedure from aldehydes, phosphonate and aminopyrimidine. The biological assay revealed that some prepared compounds displayed antibacterial activities. In this report, we were able to find several new derivatives that have an inhibitory effect. Specifically, tyrosinase is a key enzyme, which catalyzes a rate-limiting step of the melanin synthesis, and the downregulation of tyrosinase is the most prominent approach for the development of melanogenesis inhibitors.

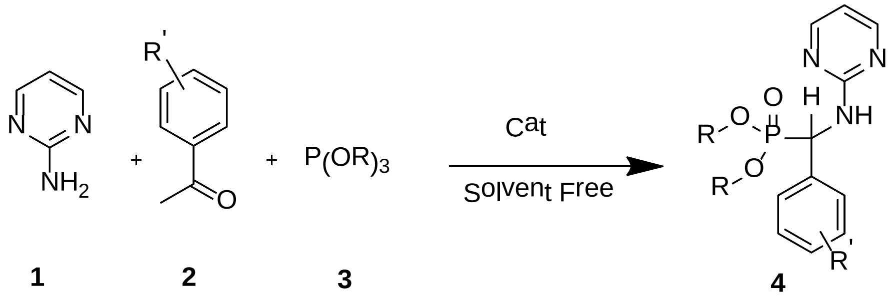

Fig. 1 Chemical procedure for the synthesis of organophosphorus aminopyrimidines.

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Synthesis, characterization and crystal structure of pyridine carbaldehyde thiosemicarbazone Schiff base ligand

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Keywords: Schiff bases thiosemicarbazone, Crystal Structure.

For decades, Schiff bases have been played an important role as chelating ligands in main group and transition metal coordination chemistry, due to their easy synthesis, wide availability and structural versatility associated with their potential applications in catalysis, electronics, and magnetism[1]. The semicarbazones and thiosemicarbazones usually behave as chelating ligands, which are versatile in both neutral and anionic forms[2]. Furthermore, the metal complexes of semicarbazones have demonstrated antimicrobial, anticancer, and antiviral activities[3]. Herein we synthesized and characterized a new thiosemicarbazone ligand from the reaction of thiosemicarbazide and pyridine carbaldehyde under reflux conditions. The HL is characterized fully. Furthermore, the structure of new ligand characterized by X-ray crystallography. The compound crystallizes in a *Monoclinic* system, with space group $P2_1/n$. Single X-ray crystal analysis reveals that new ligand consists of a Schiff base molecule and one methanol molecule. The self-assembly observed in the extended structure through several labile interactions.

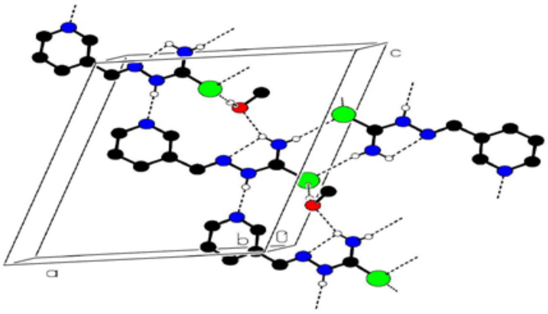

Fig. 1 pyridine 3-carbaldehyde thiosemicarbazone Schiff base ligand

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Synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives in the presence of a magnetic ionic liquid catalyst

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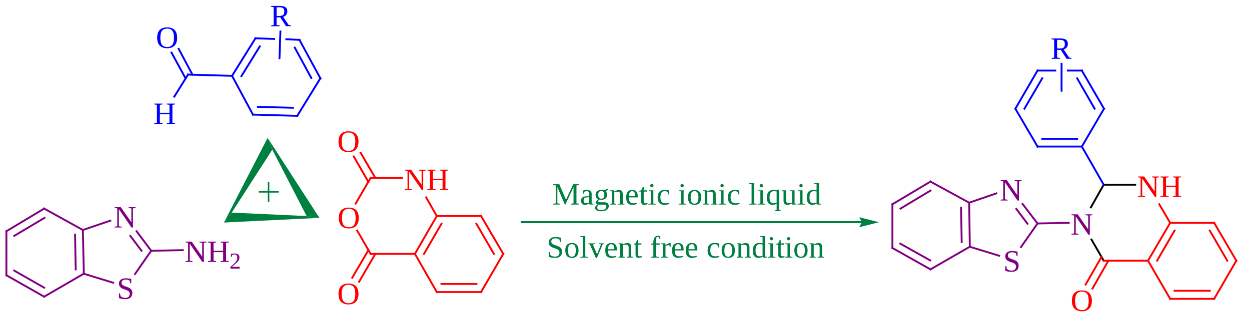
Keywords: Multicomponent reactions, Dihydroquinazolin-4(1*H*)-ones, Magnetic ionic liquid.

Dihydroquinazolin-4(1*H*)-one derivatives are an important class of heterocyclic compounds that possess important biological, pharmacological and physiological activities.[1] Using multicomponent reactions (MCRs) for the synthesis of organic compounds accompanied with economic and ecological insight is highly valuable.[2] On the other hands, ionic liquids as designable solvents, reagents and/or catalysts had been used for various purposes.[3] In this study, we would like to report the synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives via one-pot three-component reaction of arylaldehydes, 2-aminobenzothiazole and isatoic anhydride in the presence of magnetic ionic liquid as a highly efficient catalyst at 80 °C under solvent-free conditions. The structure of products were approved on the basis of their physical data , IR spectroscopic, ^{1}H and ^{13}C NMR.



R= H, 4-Me, 4-OMe, 3,4-(OMe)$_2$, 4-Cl, 2-Cl, 4-Br, 4-CF$_3$

Fig. 1 Synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives

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Synthesis of benzothiazolo[2,3-*b*]quinazolin-1-ones in the presence of a magnetic ionic liquid catalyst

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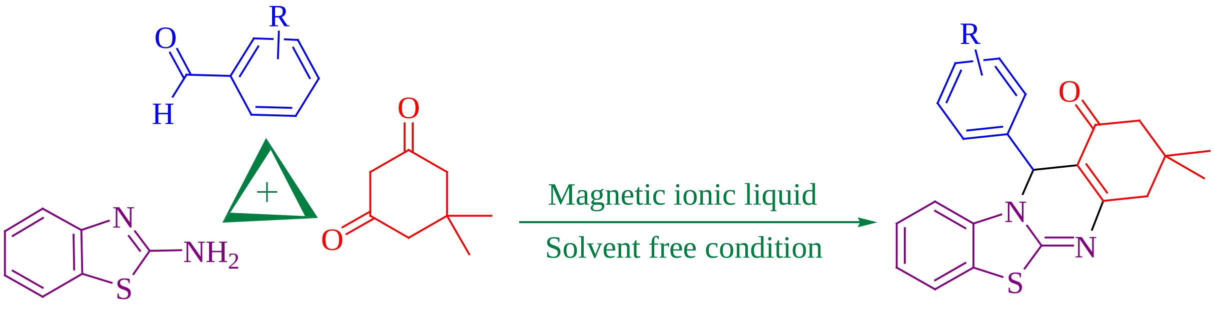
Keywords: Multicomponent reactions, Benzothiazolo[2,3-*b*]quinazolin-1-ones, Magnetic ionic liquid

Thiazoloquinazoline derivatives are a paramount important class of heterocycles that uses in drug research, as they have both of the property of thiazole and quinazoline which have shown anticancer activities.[1] On the other hands, multicomponent reactions (MCRs) have been applied to produce complex molecules and medicinal compound, and have attracted much attention from synthetic organic chemists.[2] Ionic liquids had been used as green catalysts because of its special chemical properties.[3] In this investigation, a green protocol will be report for the synthesis of benzothiazolo[2,3-*b*]quinazolin-1-one derivatives via one-pot three-component reaction of arylaldehydes, 2-aminobenzothiazole and dimedone using magnetic ionic liquid as catalyst under solvent free conditions The reported method represents varied merits such as high yields, short reaction time and simple workup procedure.



R= H, 4-Me, 4-OMe, 3,4-$(OMe)_2$, 4-Cl, 2-Cl, 4-Br, 4-CF_3

Fig. 1 Synthesis of benzothiazolo[2,3-*b*]quinazolin-1-ones.

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Synthesis of new pyrazolopyrano-quinolin-5-amine derivatives under ultrasonic conditions

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Keywords: Multicomponent reactions, 6-Amino-1,4-dihydropyrano-[2,3-c]pyrazole-5 carbonitrile, Alzheimer’s disease, Tacrine-Coumarins, 1,2,3-Triazole.

Tacrine which acts as a cholinesterase inhibitor is a well-known structure and was primarily studied for its antibacterial and later demonstrated various bilological properties.[1] The synthesis and pharmaceutical behavior of Tacrine is studied in detail and reviewed recently.[2]

In this work, we report the synthesis of a new series of tacrine-coumarin structures which are synthesized through a 4-component process combining ethyl acetoacetate, hydrazines, malononitrile, and vatrious aromatic aldehdes under ultrasonic conditions, followed by a condensation reaction with cycloalkanones to get to the final tetracyclic structures (Fig 1).

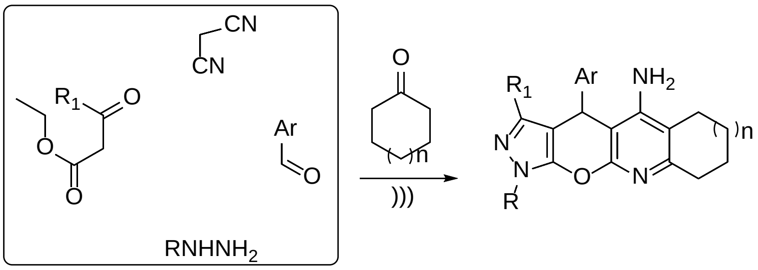

Fig 1

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Synthesis of piperazines derivatives by DABCO bond cleavage

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Keywords: Dithiocarbamate, DABCO bond cleavage, Piperazines.

Piperazine rings, as the main skeleton, play an essential role in the structure of many pharmaceutical and agronomic compounds. Also, these heterocyclic structures have been used as pesticides for the treatment of intestinal infections.[1] In addition to these structures, dithiocarbamate compounds have been used as fungicides for many years, and nowadays many scientists have taken note of their medicinal and biological properties.[2] Here in, we investigated the synthesis of substituted piperazine derivatives at positions 1 and 4 by using the breaking reaction of the C-N bond of the DABCO ring by dithiocarbamates as a nucleophile and various piperazine derivatives were synthesized in good to excellent yields.

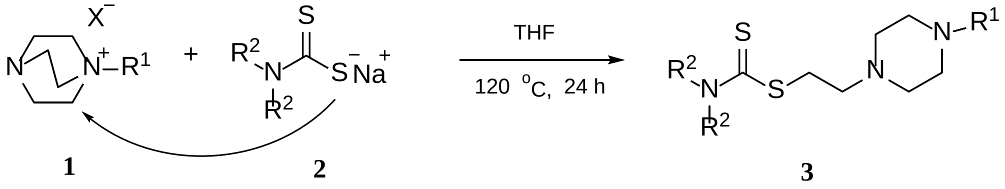

Fig. 1 Synthesis of 4-substituted 1-alkylpiperazines

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Design and synthesis of novel nano-magnetic Fe_3O_4 with phospherous acid tags: Its catalytic application at the synthesis of novel pyrimido[4,5-*b*]quinolines

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Keywords: C-P bonded phosphorous acid, $Fe_3O_4@SiO_2(CH_2)N(CH_2PO_3H_2)_2$, Pyrimido[4,5-*b*]quinolines, Task-specific catalyst.

Uracil and its derivatives, such as pyrimido[4,5-*b*]quinolines have received considerable attention over the past years because of their have biological activities such as, antibacterial, antiallergic, antimicrobial, tyrosine kinase, anti-inflammatory, analgesic, calcium channel antagonists, antihypertensive, tuberculostatic, antileishmanial, and antifungal. [1-3] In this work, nano magnetic particles of $Fe_3O_4@SiO_2(CH_2)N(CH_2PO_3H_2)_2$ as a novel and heterogeneous catalyst containing of phosphorous acid groups was synthesized and fully characterized by using various analysis techniques including. A good range of novel pyrimido[4,5-*b*]quinolines were prepared in the presence of $Fe_3O_4@SiO_2(CH_2)N(CH_2PO_3H_2)_2$ under solvent-free condition (Fig 1). Also, structure of desired products pyrimido[4,5-*b*]quinolones were fully characterized by using various analysis techniques such as ^{1}H-NMR, ^{13}C-NMR, mass spectrum, Fourier transform infrared spectroscopy (FT-IR).

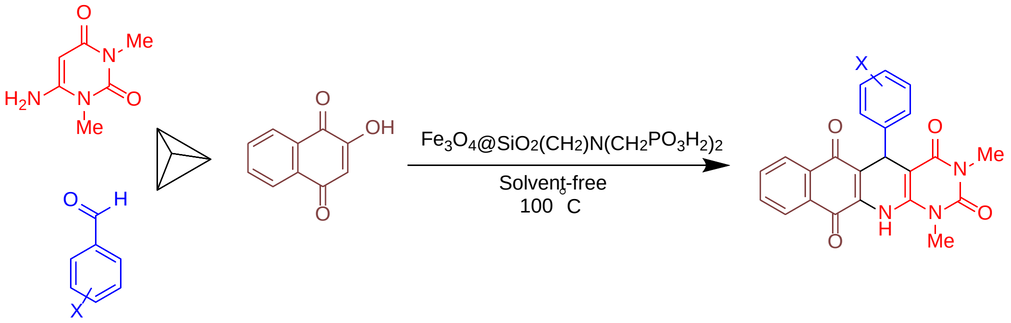

Fig. 1 Synthesis of pyrimido[4,5-*b*]quinolines catalysed by $Fe_3O_4@SiO_2(CH_2)N(CH_2PO_3H_2)_2$.

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New, stable and reusable magnetic Fe_3O_4/PEG@CPTMS-thioaminophenol@Ni nano catalyst for the synthesis of dispiro-cyclopropanes's Meldrum's acid

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Keywords: Fe_3O_4, Dispiro-cyclopropane, Meldrum's acid, 2-Amino thiophenol.

Fe_3O_4/polyethylene glycol (PEG-400), which is supply as a core-shell magnetic particles reason to their superficial space and immediate reclamation contain newly arisen as catalyst backings [1] Hybrid inorganic – organic magnetized nanoparticles had constantly reading case reason to their biomedical utilization, to protein separation [2] therapeutic transfer of DNA and drugs [3] inhibition their aggregation by build a clog barrier among they prepared biocompatibility, renderer probable for link aim region and avoid the reconnoiter [4] PEG is a biotic biocompatible polymer and is utilization as cover for nanoparticles which is an egregious between the more proper polymers because of its remarkable attribute for instance, greatly hydrophilic nature (hydrophilicity), flexibility and adaptability, dangerless and nonimmunogenicity [5].

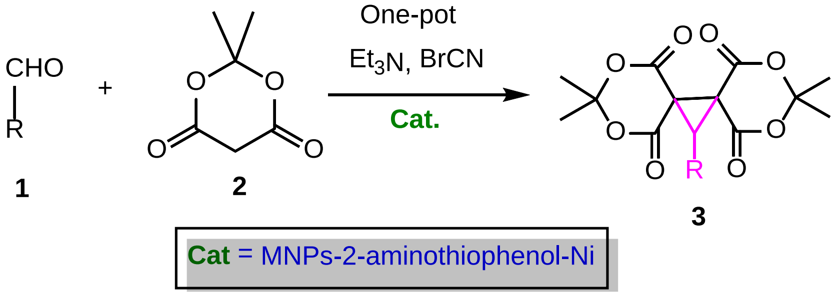

Fig. 1 Synthesis of compounds 3 with the reaction of various aldehydes 1with Meldrum's acid 2

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Synthesis and characterization of novel 4-(1-(pyrimidin-4-yl)ethyl)-12*H*-pyrimido[4',5':5,6][1,4]thiazino[2,3-*b*]quinoxaline derivatives

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Keywords: Pyrimido[4',5':5,6][1,4]thiazino[2,3-*b*]quinoxaline, Condensation reaction.

Development of straightforward and efficient methods for rapid construction of nitrogen and sulfur-containing heterocyclic compounds is an important target in synthetic, medicinal chemistry and in drug design.[1] For instance, heterocycles containing a 1,4-thiazine moiety as a class of pharmaceutically important compounds exhibit various pharmaceutical activities including antibacterial, antiprolifrative, anticancer, antiepileptic, anthelmintic, antihypertensive, antiviral, antifungal, antiinflammatory, antimalaria, and antithyroid. The first attempt to synthesize 1,4-thiazines was made by Charles Barkenbus in 1948.[2] Subsequently, other methods for the synthesis of 1,4-thiazine derivatives and heterocycles containing a 1,4-thiazine moiety have been reported in the literature.[1,3] Herein, we report an efficient one-pot synthetic approach to the synthesis of new 4-(1-(pyrimidin-4-yl)ethyl)-12*H*-pyrimido[4',5':5,6][1,4]thiazino[2,3-*b*]quinoxaline derivatives from 5-bromo-4-[1-(5-bromo-2,6-dichloropyrimidin-4-yl)ethyl]-2-chloro-6-methylpyrimidine **2** obtained from compound **1**[4] and 3-aminoquinoxaline-2-thiol **3** under mild conditions at room temperature.

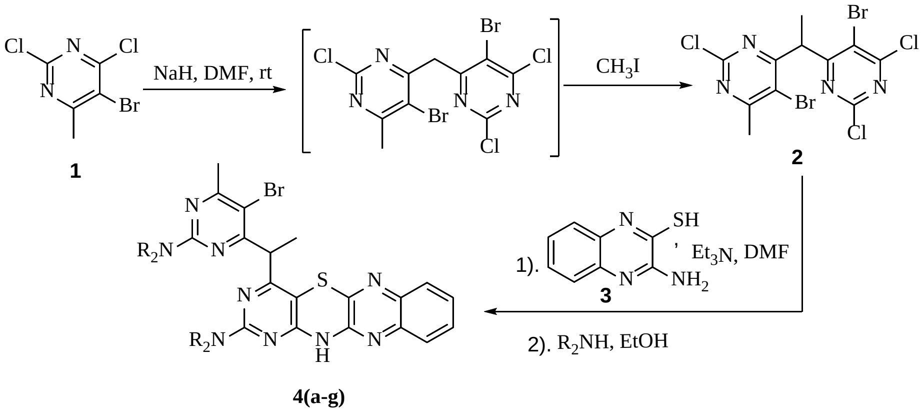

Fig. 1 Synthetic route for the synthesis of compounds (4a-g)

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Regioselective synthesis of new 5*H*,10*H*-dipyrimido[2,1-*b*:4',5'-*d*][1,3]thiazine as a novel heterocyclic system

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Keywords: Dipyrimido[2,1-*b*:4',5'-*d*][1,3]thiazine, Heterocyclization, Regiochemistry.

Pyrimidothiazines are a class of heterocyclic compounds that have been described as corrosion inhibitor for carbon steel in 1.0 M HCl, Filament temperature sensitive protein Z (FtsZ) inhibitors, 15-LO inhibitory activities, anti-inflammatory and antipyretic.[1] The main synthetic methods for the formation of various bicyclic pyrimidothiazines involve the reaction of pyrimidine-2-thiones with urea, 1,2-epoxy-3-chloropropane, 3-bromopropanoic acid derivatives, acetylene dicarboxylates or DMF-DMA and carbon disulfide.[2] In view of these observations and in continuation of our studies on developing the new routes for the synthesis of various fused heterocyclic derivatives containing pyrimidine core,[3] herein we report a simple and efficient method for the synthesis of new fused dipyrimido[2,1-*b*:4',5'-*d*][1,3]thiazines as a novel heterocyclic system. In addition, we present our findings on the regiochemistry of the reaction by performing x-ray analysis.

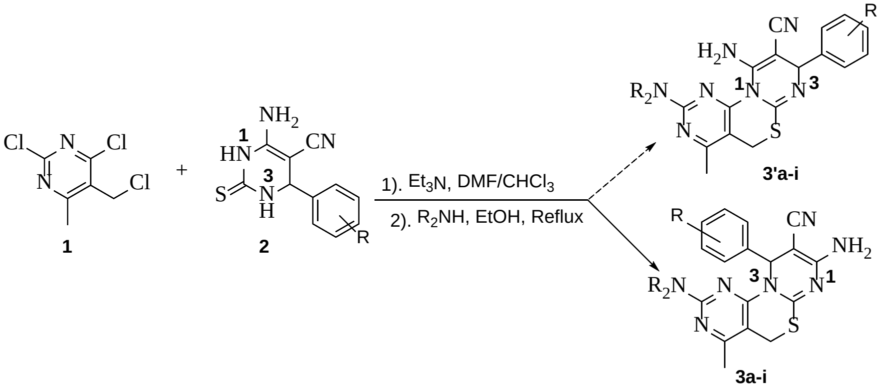

Fig. 1 Synthesis of 5*H*,10*H*-dipyrimido[2,1-*b*:4',5'-*d*][1,3]thiazine-9-carbonitrile 3a-i

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Eco-friendly synthesis of novel spiro dipyrazolo [3, 4-*b*: 4´, 3´-e] pyridine

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Keywords; eco-friendly, spirooxindole, medicinal, dipyrrazolopyridine

Green synthesis of spiro dipyrazolo[3,4-b: 4′,3′-e]pyridine has been reported via one-pot three-component reaction in H_2O in the presence of *p*-TSA as catalyst. Spirooxindoles display a wide range of biological and pharmaceutical activities such as anti-HIV, influenza virus, as inhibitors of the dengue virus and anti-cancer agents.[1] Dipyrrazolopyridines are much attractive in the synthetic and medicine target for researchers, owing to their significant fluorescence, biological and pharmacological activities such as anti-cancer agent, hypotensive, cytotoxic and anti-bacterial activity.[2,3] In additional, spiro[dipyrazolo[3,4-b′:4′,3′-e]pyridines system although less investigated exhibit also very promising biological agents, due to the spiro rigid framework and the presence of specific functional groups.[4]

As a part of our ongoing interest in this context, we reported a simple and facile synthesis of a new type of spiro dipyrazolo[3,4-b: 4′,3′-e]pyridine (4) in the presence of *p*-TSA as catalyst (Fig. 1) from starting materials pyrazol-3-one derivatives (2), pyrazol-5-amine derivatives (3), and 5,6-dihydro-1*H*-pyrrolo[3,2,1-*ij*]quinolone 1,2(4*H*)-dione (1) in environmentally friendly solvent H_2O.

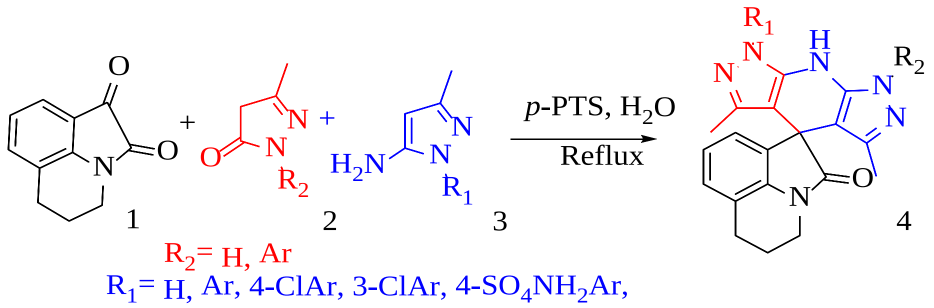

Fig. 1

All synthesized structures were determined on the basis of their ^1H and ^{13}C NMR and IR spectroscopic data.

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Synthesis of substituted pyridines in the presence of novel pseudopolymeric magnetic nanoparticles

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Keyword: Nanoparticles, Pseudopolymeric, Linked pyridine systems

Recycling of a typically applied catalyst is an important aspect of green chemistry. In recent years, magnetic separation appeared as a new strategy for catalyst separation. This manner omits problems connected to simple filtration of catalyst. *N*-heteroaromatic structures particularly linked pyridine systems are important scaffold of heterocyclic structures. These versatile molecules applied as anti-microbial, anti-tumor, analgesic, anti-inflammatory and antipyretic agents [1-3].

In this exploration, we reported the synthesis and catalytic performance of novel pseudopolymeric magnetic nanoparticles for the preparation of linked pyridine systems under solvent-free conditions (Figure 1).

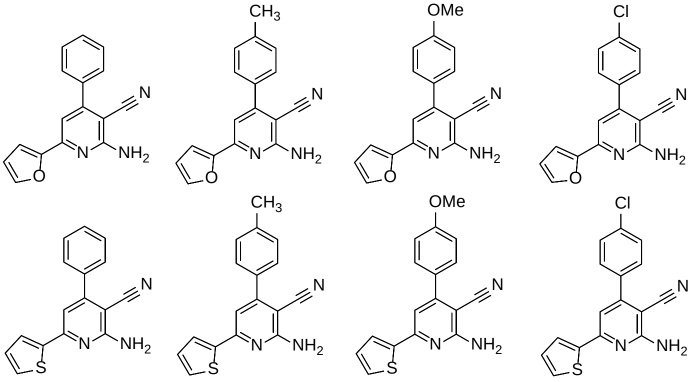

Fig. 1 Synthesis of substituted pyridines in the presence of pseudopolymeric magnetic nanoparticles

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Synthesis of fused *N*-hetrocycle compounds as biologically drug candidates by using novel Zr-based MOFs with sulfonic acid tags

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Keywords: Malononitrile dimer; *N*-Hetrocycle derivatives, Zr-based MOFs with sulfonic acid tags.

Polyfunctionally substituted nitriles are versatile reagents that have been extensively utilized as precursors for synthesis of functionalized heteroaromatic compounds.[1] Development of the synthetic routes for these compounds is a great demand.[2] 2-Aminoprop-1-ene-1,1,3-tricarbonitrile **(1)** has proved to be an excellent precursor to condensed pyridines, pyridazines, and pyrazoles.[3] Herein, we wish to report novel Zr-based metal organic frameworks (MOFs) with sulfonic acid tags as a nonporous catalyst. 6-Amino-2-(dicyanomethylene)-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitriles were prepared by reaction of 2-aminoprop-1-ene-1,1,3-tricarbonitrile **(1)**, aldehyde and malononitrile in the presence of Zr-MOFs-SO_3H at 110 °C in excellent yields and short reaction times (Fig 1).

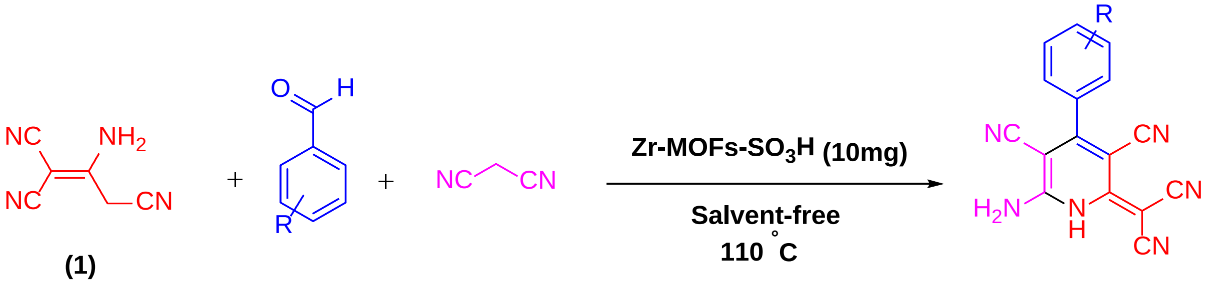

Fig. 1 Synthesis of fused *N*-hetrocycle by using Zr-MOFs-SO_3H.

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Waste Water Treatment via Adsorptive Removal of Antibiotics with Synthesized Carbon-based Adsorbent

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Keywords: Antibiotics, Resistant, Adsorption, CNT.

Because of the partial metabolism of antibiotics in human's body and the release of the effluent drug products, antibiotics have been noticed frequently from our environment. The presence of antibiotics in environment causes to growing antibiotics resistant bacteria and harmful effects on water value. Wastewater treatment generally involves many methods. Adsorptive removal is one of the most important and low-cost methods. Concerning the removal of antibiotics from wastewater, conventional treatment processes such as biological degradation and adsorption on wastewater have been demonstrated to be an effective method. Large surface area, micro-porous nature, high adsorption capacity, high purity and easy availability cause the treatment of sewage sludge with carbon-based materials is deliberated to be an effective method for the removal of antibiotics from wastewater. The nanosized behavior of the carbon nanotubes makes them more effective to use as an adsorbent in antibiotics from waste water solution. The scientist indicated that CNTs could be used as adsorbents in a wide pH range of 3–10 in qualitative agreement with experimental results. In this paper we synthesized the carbon nanotubes from natural gas via chemical vapor deposition method. The range of the carbon nanotubes size is in 10-35 nm. The surface area of the synthesized CNTs is calculated by BET method and it is about 870 cm^2/g. The adsorption capacity of the CNTs is 341 g/g. The adsorption process parameters in antibiotics removal process such as: temperature, time, mass loaded and initial concentrations are optimized. The adsorption kinetic modeling reveals that the pseudo second order is fitted the data. The adsorption isotherm model is Langmuir which appropriate the properties of the carbon-based adsorbents.

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Synthesis of the functional graphene in adsorptive removal of phenol from liquid streams

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Keywords: Graphene, Adsorption, Chemical bonding, Langmuir.

Industrial technology produces some different aromatic molecules which can be caused pollutant water due to negative impacts for ecosystems and humans' toxicity. Phenol is generated in large amount annually, with a significantly increasing trend. Phenolic products as industrial raw materials are very important in the production of certain artificial resins. Phenol can be produced from many industries such as petrochemicals, petroleum refineries, coke-oven, steel foundry, insecticides and herbicides. Due to the toxicity of the phenol even at low concentrations, the phenolic derivate is one of the most common organic water pollutants. The researchers evaluated the role of aromatic structure and –OH substitution in the polar aromatics carbon-based system. The adsorption of phenolic compounds by graphene was improved with increasing number of aromatic rings. In the other hand the –COOH substitution was enhanced the adsorptive removal of phenol from liquid streams. In this paper we synthesized the graphene as the base of the adsorbent then functionalized with –COOH. The solutions of the phenol as effluent model and graphene-COOH as adsorbents were chosen to evaluate the phenol adsorption mechanisms. Therefore, the Langmuir and Freundlich models are used to consider adsorption isotherms models. To complete our research, the effects of initial phenol concentration, contact time and adsorbent loaded are explored to adsorb phenol from aqueous stream by graphene-COOH. Scanning electron microscopy (SEM) images were taken from synthesized graphene, the surface area, pore volume and pore size distribution were measured by nitrogen adsorption at 77 K using an ASAP-2010 porosimeter from the micromeritics corporation GA. Fourier-transform infrared spectroscopy (FT-IR) was used to analyze the changes in the surface chemical bonding and structure in the frequency range of 4000–400 cm^{-1}.

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Catalytic improvement by open metal sites in a new mixed-ligand hetero topic metal-organic framework

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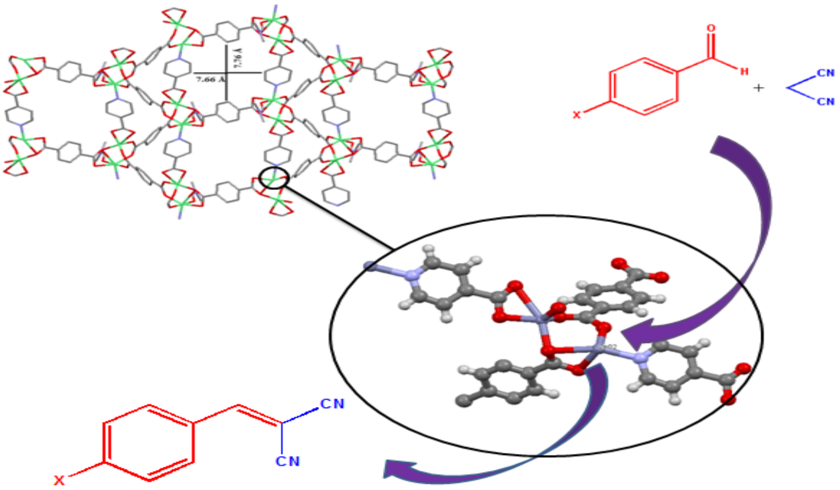
A new porous MOF, [$Zn_2(BDC)_{1.5}$(L)(DMF)].1.5DMF, [TMU-41] (L=pyridine 4-carboxylic acid), (BDC= benzene-1,4-dicarboxylate), has been synthesized and fully characterized by single-crystal X-ray crystallography, thermogravimetric analysis (TGA), X-ray diffraction (XRD), and N_2 adsorption-desorption isotherms. The values of surface areas obtained are in the range of 740 m^2/g after removing the coordinated DMF molecules. The standard procedure is to take the Zn_2 group as a single secondary building unit (SBU). Each of these is linked to five others to produce a 5-c net. The net is a high symmetry net with RCSR symbol bnn. Because of presence open metal sites (OMSs) in the Metal-Organic Framework, the framework exhibits specific properties, also the framework can act as a Lewis acid catalyst. In this study, due to the special properties of unsaturated metal sites which act as catalyst, tried to convert the structure with coordinated DMF molecules into open metal sites structure by removal coordinated DMF under a specific condition. Metal-organic framework with the open metal site (TMU-41 (OMS)) was used as a catalyst for the knoevenagel condensation reaction and the catalytic activity of this MOF was investigated in comparison to TMU-41. The result have showed that because of the availability of open metal site in this framework, (TMU-41 (OMS)) with the small amount catalyst (0.008 g), was more efficient than TMU-41 in these reaction.



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Synthesis of vinylidene-2-imino(iminium)1,3-dithiolanes via halocyclization reaction of S-propargyl dithiocarbamates

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Keywords: Dithiocarbamates, 1,3-dithiolanes

Dithiocarbamates have variety of applications in organic synthesis. In addition to their pharmaceutical properties and their applications in synthesis of pesticides, these compounds can act as important intermediates in the synthesis of other important organic compounds. For instance, in recent years, dithiocarbamates played an important role in the synthesis of 2-imino(iminium)1,3-dithiolane rings[4]. These sulfur heterocycles are of great importance and can be further used for protection of crop plants from the action of herbicides without reducing the herbicidal effectiveness against weeds. In this project, *S*-propargyl dihtiocarbamate (**3,5**) intermediates were synthesized from the reaction of amines, CS_2 and propargyl bromide **2**. In the next step, vinylidene 2-imino(iminium)1,3-dithiolanes (**4**,**6**) were prepared in a short reaction time by the iodocyclization reaction of *S*-propargyl dithiocarbamates (**3**,**5**) with I_2, under a mild reaction condition.

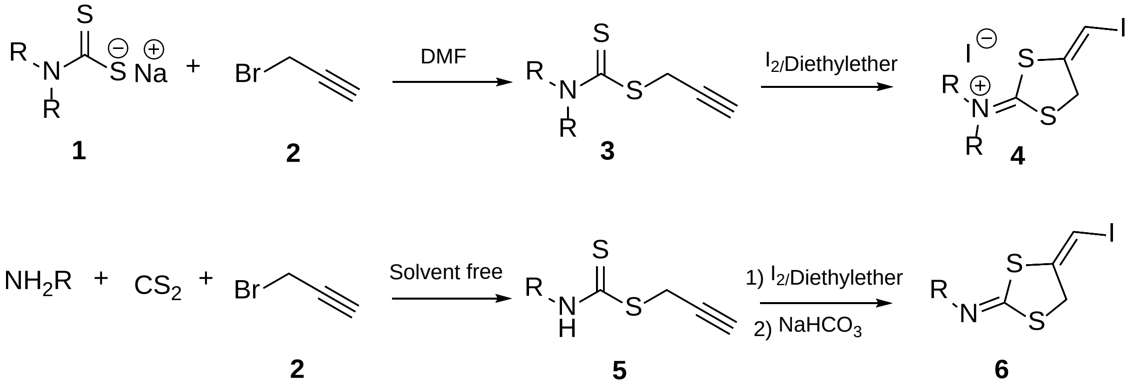

Fig. 1 Synthesis of vinylidene 2-imino(iminium)dithiocarbamates

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Construction of Alginat Cysteine Polymeric Based Nano Carries for Etoposide in Cancer therapy

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Keywords: Polymeric carbohydrate, L-Cysteine, Anticancer drug, Drug delivery.

Alginate is a naturally occurring, anionic copolymer of guluronic and mannuronic acids and is widely used in the bio encapsulation of drugs, proteins and cells. It is biodegradable, biocompatible, non-toxic properties; and has the ability to form a gel in the presence of divalent cations such as calcium[1]. To improve its properties, a variety of synthetic and natural polymers have been proposed for blending with alginate[2, 3]. In this study, etoposide, a typical chemotherapeutic agent, was selected as the model drug to evaluate of cysteine-modified sodium alginate nanoparticles to load drug. The structure of nanoparticles was elucidated by FTIR. The shape, and morphology were determined by SEM. The mean size, PDI and ZP of the obtained drug loaded nanoparticles were reported to be 355.4 nm, 0.309 and -27.7 mV, respectively. The in-vitro drug release was studied by using UV–Visible spectrophotometer at acidic environment and physiological pH and sustained release compared to the ETO alone. It was found that ETO drug is released much faster in pH 5.0 than in the pH 7.4. In addition, the cytotoxicity of the created nanoparticles was performed by using LDH assay analysis which showed that ETO loaded nanoparticles SA/Cys/ETO were toxic to MCF-7 cell line.

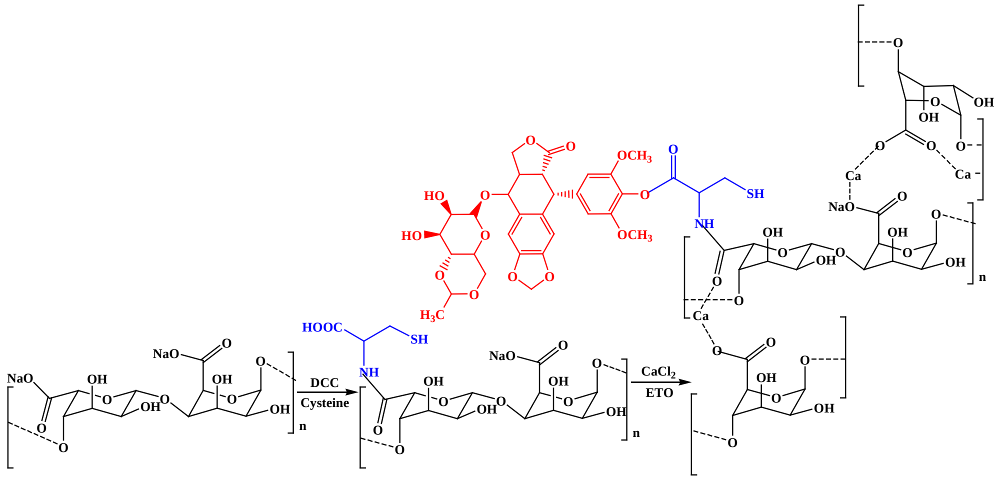

Fig. 1 Nanoparticle synthesis steps SA/Cys loaded with ETO

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A Synthesis of *N*-(1*H*-Pyrazol-5-yl)-1,3,4-thiadiazol-2(3*H*)-imines *via* Double Cycloaddition Reaction of Nitrile Imines with Erlenmeyer Thioazlactones

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Keywords: Pyrazoles, 2-Amino-1,3,4-thiadiazole, 1,3-Dipolar cycloaddition, Nitrile imines

Pyrazoles represent an important structural subunit in natural products and drug molecules. Due to their unique pharmacological properties and biological activities, they occupy an important position in heterocyclic chemistry. Many small-molecule drugs contain the pyrazole moiety. Currently, pyrazoles are employed as key constituents of ligands for transition metals, receptors in supramolecular chemistry, liquid crystals and polymers.[1] 1,3,4-Thiadiazole is a unique template that is associated with several biological activities. 2-Amino-1,3,4-thiadiazole occupy an important place in pharmaceutical chemistry. Some of the best-known drugs based on 2-amino-1,3,4-thiadiazole, are acetazolamide, methazolamide, and megazol.[2] During the course of an investigation aimed to the synthesis of pyrazole derivatives, we investigated the reaction between *N*-phenylbenzohydrazonoyl chloride (**1a**) and 4-benzylidene-2-(benzylthio)thiazol-5(4*H*)-one (**2a**) in the presence of Et_3N in MeCN. After work-up, the desired product *N*-(3,5-diphenyl-1,3,4-thiadiazol-2(3*H*)-ylidene)-1,3,4-triphenyl-1*H*-pyrazol-5-amine (**3a**) was isolated in 98% yield.

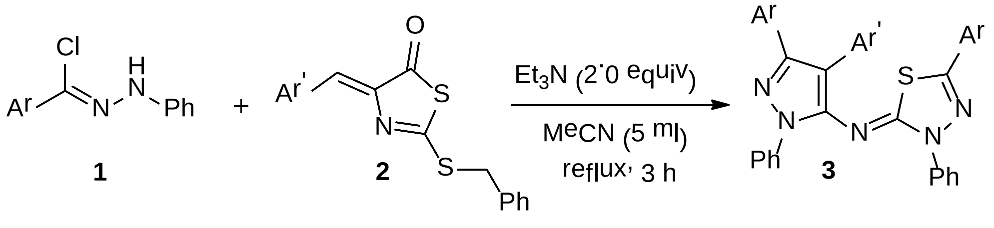

Fig. 1 Synthesis of *N*-(1*H*-pyrazol-5-yl)-1,3,4-thiadiazol-2(3*H*)-imines

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Synthesis of Fe_3O_4@4-amino-5-methyl-2*H*-1,2,4-triazole-3(4*H*) thion (AMTTO)@Cu and using catalytic efficacy in C–N and C–O reaction

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Keywords: Nanocatalys, Fe_3O_4, AMTTO, Copper, Coupling reactions.

Fe_3O_4@4-amino-5-methyl-*2H*-1,2,4-triazole-3(*4H*)-thion@cu has been introduced as a new catalyst,heterogeneous and reusable for formation of the bond C-O and C-N between different Aryl Halides.This heterogeneous catalyst exhibit significant recyclability and it can be used several times without losing its catalytic property.

Have been reported Anti-inflammatory and anti-fungal properties from amine and thione substituted triazoles [1] and 1,2,4-triazoles is important to have an extensive range of biological activities such as anti-tumor, antifungal and antibacterial drugs .[2]
The use of copper in Carbon-Nitrogen and Carbon-Oxygen coupling reactions has been reported as a powerful method [3,4]. and the use of Copper in coupling reactions has the advantage of having a plurality of substrate and mild reaction conditions in comparison to Palladium[5].

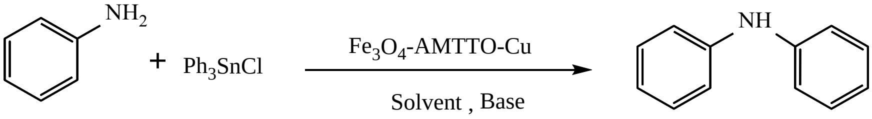

Fig. 1 Synthesis of coupling reactions with Fe_3O_4- AMTTO-Cu

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Synthesis and characterization of cooper complex immobilized on boehmite nanoparticles and its application in C-C coupling reaction

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Keywords: Boehmite; Suzuki reaction, Cu complex, C-C coupling

The immobilization of homogeneous catalysts on various support materials is of great interest in catalyst science[1-3]. However, immobilization of homogeneous catalysts usually decreases the catalytic activity or selectivity[2-4], This could be solved using nanoparticles as catalyst supports. Nanoparticulate supports can serve as an intermediate between homogeneous and heterogeneous catalysis[4,5]. However, nanoparticles are difficult to separate by filtration techniques. One of the most promising MPs supports for the development of high-performance catalyst supports is Boehmite nanoparticles[4], The notable advantages of boehmite MPs are simple synthesis, readily available, low cost, high surface area, low toxicity and high stability properties[5].

Therefore, we have prepared a novel nanoscale catalyst system composed of nanosized Cu catalysts immobilized on Boehmite nanoparticles. The catalyst is readily prepared from inexpensive commercially available starting materials and employed for C-C coupling reactions. Recovery of the catalyst by decantation of the reaction mixture using simple filtration is both convenient and efficient. The ease of recovery, combined with the intrinsic stability of catalyst components, allows the catalyst to be recycled for several times without any discernible loss in activity (Fig. 1).

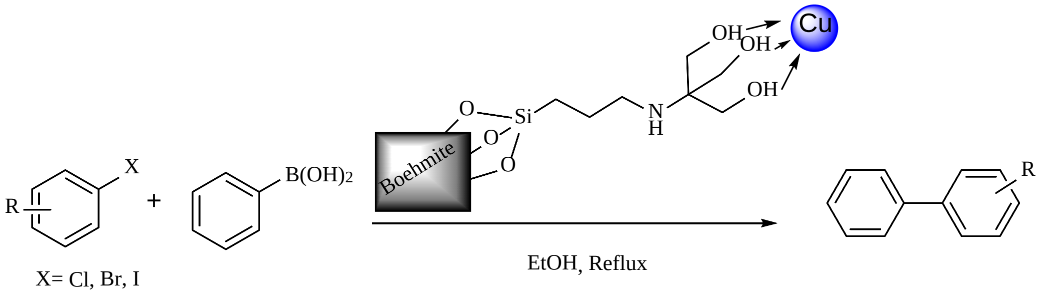

Fig. 1 Cu complex supported on Boehmite nanoparticles catalyzed C-C coupling reaction.

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Synthesis and characterization of Arginine-Ni complex supported on Hercynite magnetic nanoparticles ($FeAl_2O_4$@ Arginine-Ni) and it's applications in multi-component reactions

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Keywords: Hercynite; Arginine-Ni complex; 2,3-Dihydroquinazolin-4(1H)-one; Polyhydroquinoline.

In recent years, the improvement in nanotechnology led to an increasing insist for multifunctional materials owing to simplicity in operation, remarkable recyclability, high surface area of catalysts and ecofriendly nature[1]. In this regard, solid catalysts and magnetic composite nanoparticles are interesting for industrial and biomedical applications and, especially, in catalysis studies as a magnetically separable catalyst[2]. Different experimental methods for the synthesis of spinel ferrites have been reported in the literatures, such as: sol-gel, electrodeposition, reaction sintering, mechanochemical, single step solution combustion, co-precipitation, thermal decomposition, hydrothermal, electrochemical, and solvent deficient[3,4]. Among these procedures, co-precipitation method is an easy, versatile, and low-cost method for the preparation of $FeAl_2O_4$ nanoparticles[5].

In the development of greener and sustainable processes for the organic synthesis, Arginine-Ni organometallic complex supported on Hercynite magnetic nanoparticles $FeAl_2O_4$@ Arginine-Ni MNPs was prepared by simple procedure and applied as catalyst for the preparation of 2,3-dihydroquinazolin-4(1H)-one derivatives and polyhydroquinoline derivatives using expensive, green and available materials (Fig. 1).

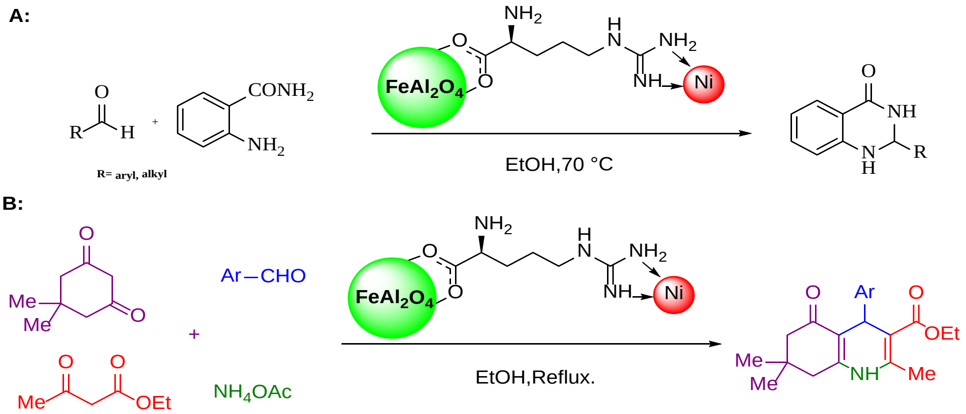

Fig. 1 $FeAl_2O_4$@Argenine-Ni magnetic nanoparticles catalyzed the synthesis of 2,3-dihydroquinazolin-4(1H)-one and polyhydroquinoline derivatives

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An isocyanide-based consecutive Bargellini/Ugi reaction: Synthesis of pseudopeptides containing three amide bonds

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Keywords: pseudopeptides, Bargellini reaction, Ugi reaction, multicomponent reactions, green chemistry.

Peptides and proteins perform essential task in both unicellular and multicellular organisms and living without them would be impossible. The therapeutic utilization of peptides and proteins is limited by their short time life, nonselective receptor binding and low absorption. Additionally, the synthesis of peptides comprises of difficult sequences, with a numerous residues such as active pharmaceutical ingredients. To overcome the disadvantages mentioned, chemists explored efficient methods to design pseudopeptides, which have better pharmacological properties and maintain the activities of original peptide.[1] In this work, a general method for synthesis of pseudopeptides containing three amide bonds has been developed *via* a novel isocyanide-based consecutive Bargellini/Ugi reaction. This approach is an efficient, environmentally friendly and simple procedure for direct access to wide ranges of pseudopeptides based on multicomponent reactions.[2-3]

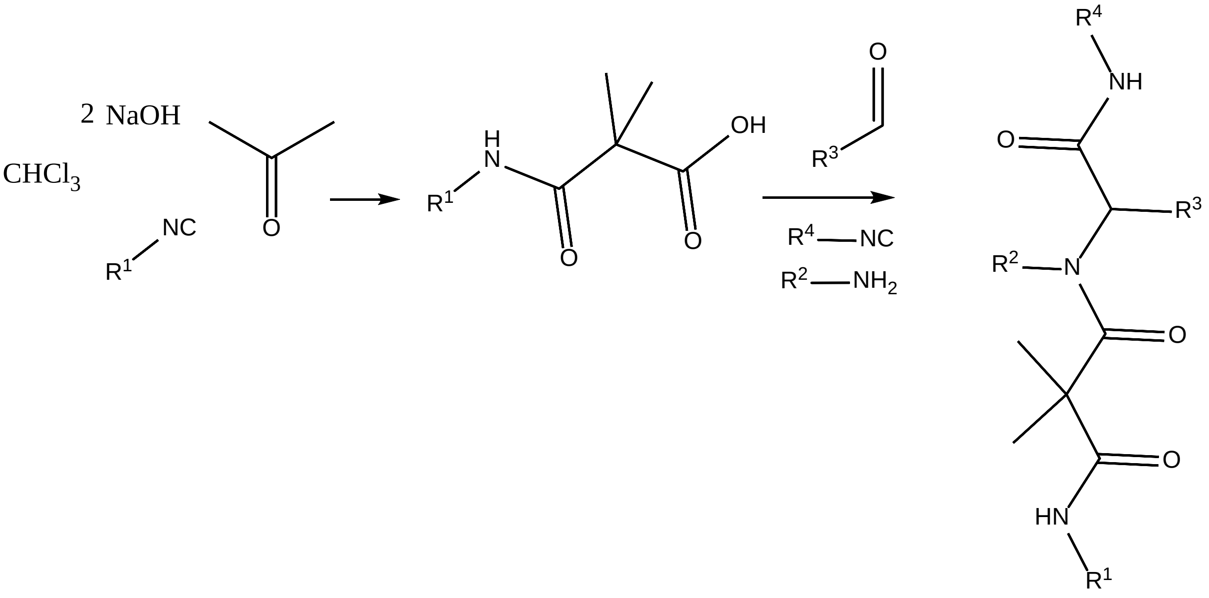

Fig. 1 Consecutive Bargellini/Ugi reaction.

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One-Pot Synthesis of Succinimide-3-Carboxamide Derivatives Using Microwave and Mechanistic insights and Kinetics analysis by Computational Method

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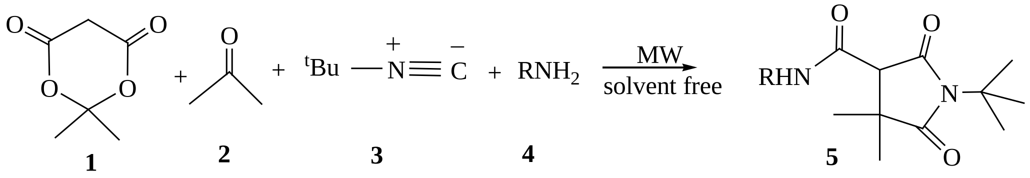
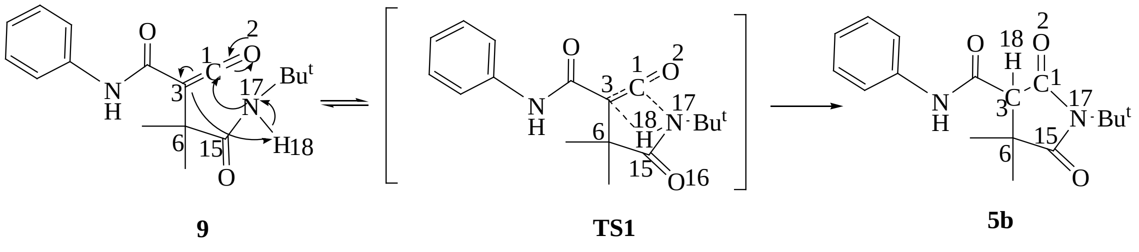
***Keywords*:** Meldrum’s acid, *tert*-butyl isocyanides, Mechanism, Theoretical and kinetics investigation, microwave irradiation, Two dimensional scanning, Amidosuccinimides

In the present work, one-pot and four-component condensation of Meldrum’s acid(**1**) and acetone(**2**) with *tert*-butyl isocyanides(**3**) in the presence of primary amines(**4**) under microwave irradiation which provided 1-*tert*-butyl-4,4-dimethyl-2,5-dioxopyrrolidine-3-carboxamides(**5**) in short time with high yields have been investigated. Also, multiple mechanisms have been studied theoretically for comparing formation of the amidosuccinimide with triamide products from intermediate **9** using ab initio molecular orbital theory in gas phase. The potential energy profile was constructed at the HF/6-311G (d, p) level of theory. Among four speculative proposed path only the pathway **A** (intramolecular reaction to formation amidosuccinimide product) was recognized as a desirable mechanism. Theoretical kinetics data involving k and activation parametres (E_a , ΔG‡, ΔS‡ and ΔH‡) were calculated for each step of the paths. In order to determine the possible nucleophilic sites for the N17, N33 local reactivity has been evaluated through Fukui indices.





Pathway **A**

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Synthesis and characterization of self-assembled three-dimensional graphene decorated with silica gel

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Keywords: Three-dimensional graphene -dye adsorption-Nano composite

Multicomponent reactions (MCRs), reactions involving at least three starting materials in a one-pot reaction, remain the most efficient method of synthesis of heterocycles.[1] Some reagents such as isocyanides are useful reagents for synthesis of organic structures.[2] There are many diverse cycloaddition reactions in which isocyanides play a key role for synthesis of different types of heterocycles.[3] Five-membered rings such as furan have many useful synthetic applications in drug structures.[4] Herein, we report the synthesis of new 2-amino-5-(cyclohexylamino)-4-arylfuran-3-carbonitriles **4** from the reaction between cyclohexyl isocyanide **1** and aldehydes **2** in the presence of cyanoacetamid **3** at room temperature. All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.

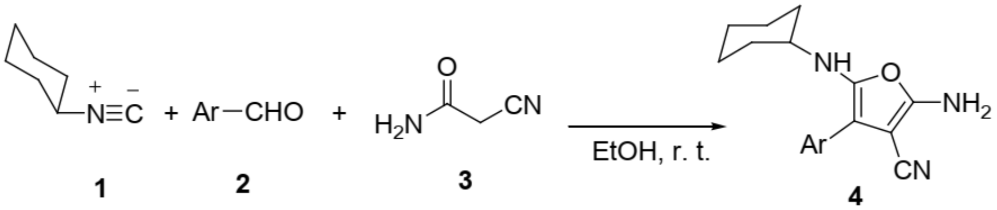

Fig. 1 Multicomponent 2-amino-5-(cyclohexylamino)-4-(aryl)furan-3-carbonitriles

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Fabrication of PVC/modified clay mixed matrix membranes with enhanced antifouling properties

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Keywords: Ultrafiltration, PVC, Modified clay, fouling, mixed matrix membrane.

Ultrafiltration (UF) membrane plays an important role in separation techniques such as water and wastewater treatment. Membrane fouling is the primary limitation of UF membrane that leads to flux decline. Increasing the membrane hydrophilicity is the main concern by numerous researchers in order to improve antifouling properties of membranes. Mixed matrix membranes have garnered considerable interest among researchers[1,2]. In mixed matrix membranes, the polymer acts as a matrix for the nano dimension inorganic additives and the interaction between these two materials led to variations in the structure and performance of membranes. Modified clay due to low cost can be a suitable additive for polymeric membranes. In this work, influence of modified clay on antifouling performance of poly(vinylchloride) (PVC) mixed matrix ultrafiltration membranes were investigated. Non-solvent induced phase separation method was applied to prepare neat and modified clay embedded membranes. Different amounts of modified clays were used. BSA fouling results in Fig.1 show that mixed matrix membranes can improve the fouling resistance of PVC membranes.

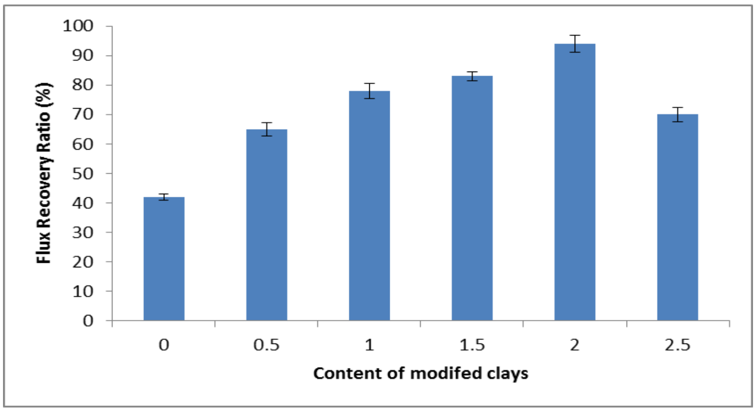

Fig. 1 Flux recovery ratio of mixed matrix membranes after BSA fouling.

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Effect of polyethylene crystallinity and extractant on the structure of membranes fabricated via thermally induced phase separation

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Keywords: Polyethylene, Membrane, Extractant, Phase separation, Crystallinity.

Polymeric membranes dominate the membrane separation field because they are well developed and quite competitive in separation performance and economics[1]. The thermally induced phase separation (TIPS) process is one of the most useful techniques to prepare the porous membranes. A lot of studies have been reported on the effect of different parameters on membrane structure fabricated via TIPS method. There is little research about the extractant effect on membrane morphology. In this work linear low density polyethylene and high density polyethylene were extracted by acetone and hexane extractants and their microstructures were compared. Fig. 1(a) and 1(b) show microstructure of linear low density polyethylene and high density polyethylene were extracted by acetone. Acetone has no effect on their structure and porous structures were obtained. As shown in Fig. 1 (c), LLDPE extracted by hexane is dense. Solubility parameter of hexane and polyethylene is close, so hexane can swell amorphous region of LLDPE. Swelling of polymer cause to closing the pores and dense structure obtained. Figure 1(d), shows the SEM images of HDPE by hexane. It seems that difference in HDPE and LLDPE crystallinity, causes that hexane change LLDPE structure. It can be concluded that in polymers with low crystallinity, solubility parameters of polymer and extractant should be different with each other.

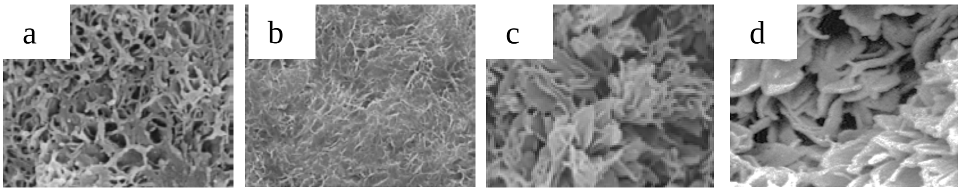

Fig.1 SEM images of LLDPE and HDPE extracted with acetone and hexane

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DFT study on mechanistic pathway of synthesis of 2-(indolyl)(phenyl)methyl)-indenedione

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Keywords: DFT, Mechanism study, Intermediate, Transition State

In recent years, an increasing interest has been focused on the synthesis of 2-substituted *2H*-indene-1,3-dione compounds owing to their significant biological activity[1,2]. It is well known that indandione and related compounds exhibit a wide range of biological activities such as antitumor, anticancer, sedative, hypertensive and neuromuscular blocking activities[3-6]. Computational chemistry is an important part of chemistry which studies the properties of compounds, their reactions and optimization of existing chemical methods by using advanced and specialized soft wares. One of the important area of study is to analyze of proposed mechanisms which this is done through theoretical methods. So, in continuation of our previous work,[5] herein, we specifically address the condensation of substituted benzaldehydes, 1,3-indandione and indole according to the three component reaction was investigated at the B3LYP/6-311G level to explore the reaction mechanism (Fig. 1). All of routes were studied and structure of intermediates were optimized and all of respective transition states were found. The calculation results proved that the proposed mechanism consists of four intermediates.

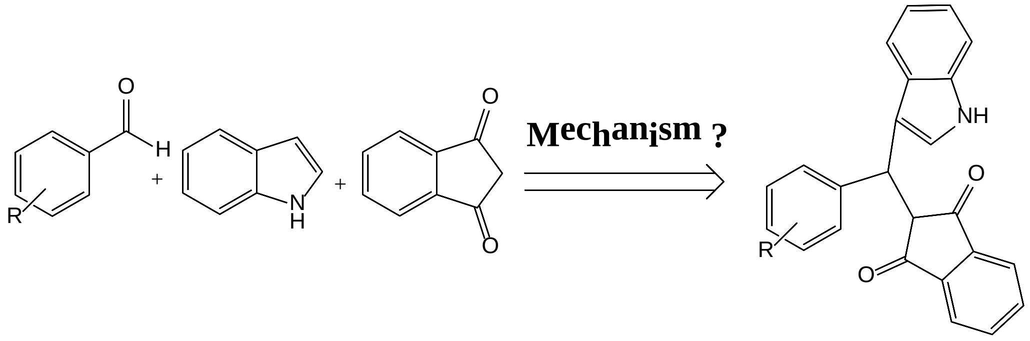

Fig. 1 various routes in synthesis of 2-(indolyl)(phenyl)methyl)-indenedione

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Labeled peptide synthesis: FAM-YYYYRRRR and study of its binding to para-sulfonatocalix[4]arene supramolecule as a pharmaceutical approach

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Keywords: Peptide synthesis, Supramolecular connection, Binding constant, Fluorimeter.

In recent decades, with the development of drug delivery, the synthesis of peptides in the solid phase has become important. Hence, the peptide FAM-Y_4R_4 was synthesized, consisting of four arginine (R) amino acids and four tyrosine (Y), and end capping with fluorescein dye. After separation and purification of the synthesized peptide (FAM-YYYYRRRR) by HPLC, a supramolecule para-sulfonatocaliX[4]arene (CX4), also known as the molecular basket, was connected to peptide. To calculate the constant binding of the labeled peptide to supramolecule, it can be measured by fluorimeter and obtain a constant binding. The purpose of this study was to estimate the amount of connection the branched chain of arginine to the CX4. It is expected to change from positive to negative, peptide CX4 to and increase the pathway of cell reabsorption and its permeability to eukaryotic cells. By binding the peptides to a fluorescence dye, it can also be evaluated in the cell for binding and transferring it. Supramolecules, known as carriers of smaller molecules, also have the potential to bind to peptides to transfer drugs into cells without causing toxicity.

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Tunable P-doped graphene oxide as a robust metal-free carbocatalyst for catalyzed selective oxidation of alcohols

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Keywords: Tunable P-doped graphene oxide ،thermal calcination ،Carbon nanomaterials ، selective oxidation of aromatic alcohols

Carboxylic acids as intermediates of several organic functionalities such as esters, amides, alkyd resin, medicines, and dyes are an important type of organic compounds.[5] Catalytic oxidation of primary alcohols is one of the most convenient methodology to synthesize the corresponding carboxylic acids. For selective catalytic oxidation reaction of primary alcohols, the noble or transition metals are reported previously.[6] Carbon nanomaterials as a type of metal free catalysts provide additional advantages because of their enrichment with reactants, environmental friendly, and biocompatible performance.[7] The structure of carbon materials can be fine-tuned by doping with heteroatoms like N, P, S, and B. The doping strategy led to the improved carbocatalytic activity. In this work, the P doped graphene oxide (P-GO) is prepared by thermal calcination method. The as-synthesized P-GO is proven to be an efficient catalyst in selective oxidation of aromatic alcohols to acids. The P-GO catalyst can be used to synthesize a variety of acids, and the catalyst recyclability has also been examined (Fig. 1).

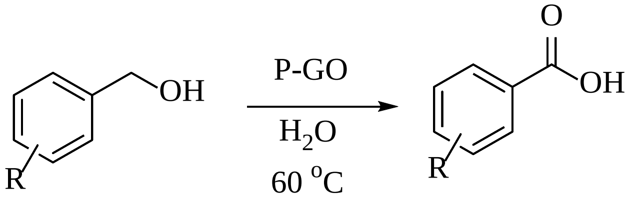

Fig. 1 Synthesis of substituted carboxylic acids.

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Synthesis and characterization of new potentially hexadentate (N_4O_2) Schiff base ligand

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Keywords: Hexadentate Schiff base, Tetraamine ligand, 2-Hydroxybenzaldehyde

Considerable attention has focused on the synthesis of new hetroacyclic ligands containing azo groups because of their role in the development of coordination chemistry as well as optical materials, dyes and so on.[1] Schiff base derived from the reaction of salicylaldehyde with primary amines represent a versatile series of ligand. In attention to importance of these compounds many literatures have been published in this field. In this work we want to report the synthesis and characterization of new type of hexadentate schiff base ligand. First we synthesis (2-2-2-aminobenzylideneamino)ethylimino)methyl)benzenamine and use to this tetraamine ligand and 2-hydroxybenzaldehyde to prepare new potentially hexadentate (N_4O_2) Schiff base ligand. Also this Schiff base was characterized by ^{1}H and ^{13}C NMR, elemental analysis, MS and IR spectroscopy (Fig 1).

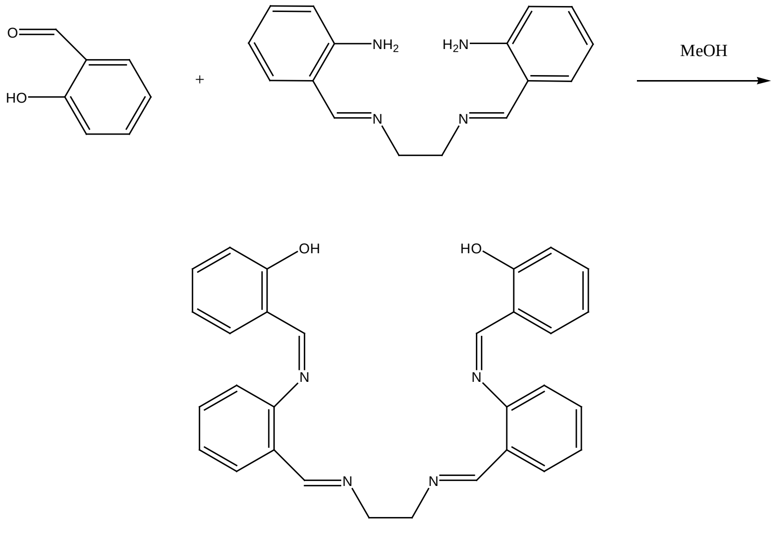

Fig. 1 Hexadentate (N_4O_2) Schiff base ligand

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Theoretical Investigation of 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepinium halids

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Keywords: Theoretical study, Electronic properties, Halids.

In this work, we have performed a computational investigation on the structural, electronic and spectroscopic properties of 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepinium halids [DBU][X] (X=F, Cl and Br)[1] which have been shown in Fig. 1. Considering that, density functional theory (DFT) is an electronic structure method which is widely used in chemistry and physics for theoretical study of various properties of many compounds and their derivatives[2,3], we used this method with B3LYP/6-311G(d,p) level of theory for investigation of [DBU][X].

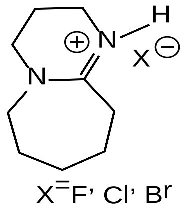

Fig. 1. The structure of [DBU][X]

Molecular orbitals (MOs) play a central role in electron transportation in molecular devices. Therefore, the calculated values of the HOMO, LUMO and the difference between HOMO and LUMO, known as HLG energies or E_{gap} for the [DBU]lX] were calculated and indicated in Table 1.

Table 1. The E_{HOMO}, E_{LUMO} and E_{gap} (in eV) for [DBU][X].

IL	E_{HOMO}	E_{LUMO}	E_{gap}
[DBU][F]	-6.107	0.992	7.101
[DBU][Cl]	-5.430	-0.994	4.435
[DBU][Br]	-5.060	-1.093	3.967

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DFT study of bis-2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepiniumethyl disulfate $[DBU]_2[EDS]$

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Keywords: Ionic liquid, DFT study, Spectroscopic properties.

Ionic liquids (ILs) are a class of organic salts, kind of new materials with unique physicochemical properties, therefore they have become increasingly attractive as green solvents for industrial applications and have considered attention of researchers.[1] Therefore, in this work, the molecular structures and vibrational spectra of bis-2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepiniumethyl disulfate $[DBU]_2[EDS]$ [2] were calculated. Since the B3LYP functional yields a good description of harmonic vibrational wavenumbers for the small and medium sized molecules[1], we choose this method with 6-311G(d,p) basis set for investigation of the structural, electronically and spectroscopic of the studied IL. Figure 1, displayed that the structure of $[DBU]_2[EDS]$. The computed geometry of this IL was verified to be minima by harmonic vibrational frequency calculations (no imaginary frequencies). As a result of MO orbitals, E_{HOMO}, E_{LUMO} and E_{gap} for $[DBU]_2[EDS]$ are -6.227, -1.034 and 5.192 eV, respectively. Additionally, total dipole moment of this compound is 38.211 Debye.

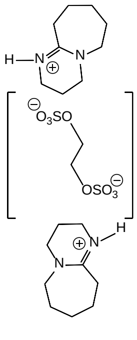

Fig. 1. The structure of $[DBU]_2[EDS]$.

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Synthesis of benzo[*g*]chromene derivatives in the presence of nano Cu-MOF

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Keywords: Multicomponent reactions, Benzo[*g*]chromene, Metal organic framework, Nanocatalyst.

The discovery of Metal Organic Framework (MOF), a new family of porous crystalline compounds, has attracted a lot of attention in the last two decades, as these compounds are capable of commercial application.[1] Recently, the use of MOFs as heterogeneous catalysts in organic reactions has been considered more than before because these compounds are unique in their structure due to the presence of metal and an organic ligand in their structures.[2] In order to the easy separation and recycling of heterogeneous catalysts, its use in multi-component reactions (MCRs) is of particular importance[3]. Herein, we report the synthesis of benzo[*g*]chromene derivatives **4** from the reaction between lawsone **1**, aldehydes **2** and Malononitrile **3** in the presence of nano Cu-MOF as catalyst in EtOH under reflux. The synthesized catalyst was characterized by SEM, PXRD, TGA and N_2 adsorption/desorption isotherms techniques.

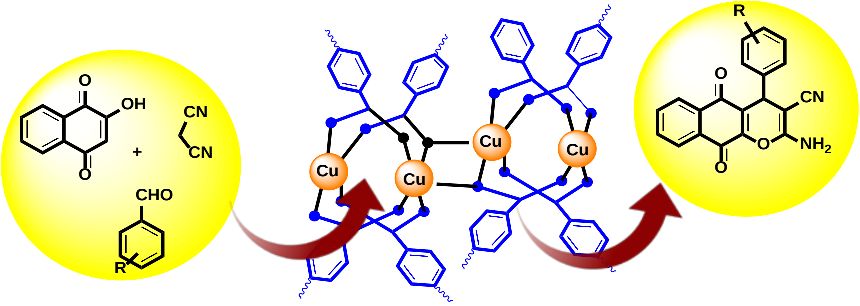

Fig. 1. Synthesis of benzo[*g*]chromene derivatives using nano Cu-MOF

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Synthesis of dihydropyrano[2,3-*g*]chromenes derivatives in present of nano Cu-MOF

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Keywords: Multicomponent reactions, Dihydropyrano[2,3-*g*]chromenes, Metal organic framework, Nanocatalyst.

In recent years, the synthesis and application of Metal Organic Framework (MOF) has attracted chemists, due to these compounds have unique properties in the field of catalyst and gas adsorbents[1]. Recently, the use of MOFs as heterogeneous catalysts in organic reactions has been considered more than before as the presence of metal and an organic ligand in their structures[2]. Chromenes and their derivatives are compounds that exhibit a good biological and antibacterial activity[3]. The chromene synthesis, in economical and optimal conditions, by recyclable heterogeneous catalysts is one of the perspectives examined by chemists. Herein, we report the synthesis of dihydropyrano[2,3-*g*]chromenes from the reaction between 2,5-dihydroxycyclohexa-2,5-diene-1,4-dione, aldehydes and malononitrile in the presence of nano Cu-MOF as catalyst in ultrasonic irradiation. The synthesized catalyst was characterized by SEM, PXRD, TGA.

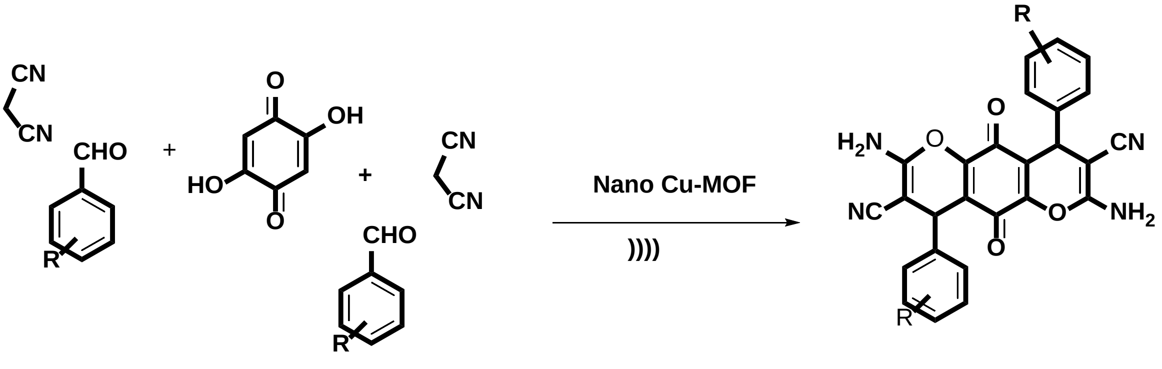

Fig. 1. Synthesis of dihydropyrano[2,3-*g*]chromene derivatives using Nano Cu-MOF

References

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2) Nagarjun, N. and Dhakshinamoorthy, A., *Mol Catal*, **2019**, *463*, 54.
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Facile synthesis of pyrano[2,3-*d*]pyrimidine derivatives using a morpholin-based ionic liquid immobilized on nanoporous SiO_2

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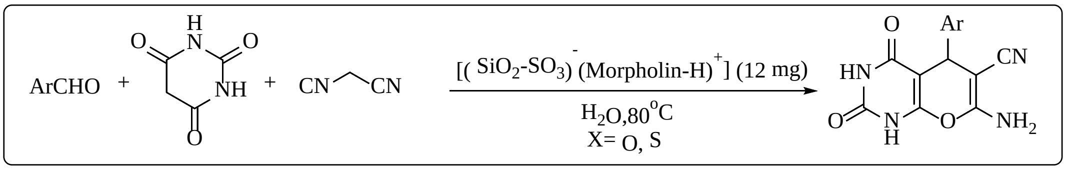
***Keywords*:** Nanoporous SiO_2, Ionic liquid immobilized, pyrano[2,3-d]pyrimidine

Multicomponent reactions (MCRs) have attracted considerable interest due to their ease of performance, high yield, and especially synthetic feasibility and efficiency.[1–3] MCRs include three or more starting materials reacting in a single flask to form a new product, where basically all the atoms contribute to the newly formed product. Pyrano [2,3-*d*] pyrimidine derivatives are examples where multicomponent synthesis can be used. Pyrano[2,3-*d*]pyrimidine structures have a wide range of biological activities such as spasmolytic, diuretic, antitumor, antiallergic, anticoagulant, anticancer, and antianaphylactic activities, as well as acting as potassium channel activators.[4] In this work, a green and efficient procedure is reported for the preparation of pyrano [2,3-*d*]pyrimidine derivatives using morpholin-based ionic liquids immobilized on nanoporous SiO_2. The procedure gave the products in excellent yields in very short reaction times. The reusability of the catalyst is the other important feature of the reported method (Scheme 1).



Scheme 1. Synthesis of pyrano[2,3-d]pyrimidine derivatives using morpholin-based ionic liquids immobilized on nanoporous SiO_2 [(SiO_2-SO_3)$^-$(Morpholin-H)$^+$]

References
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Synthesis of 2,4,6-triarylpyridines catalyzed by a novel magnetic nanocomposite on the basis of carbon nanotube

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Keywords: Triarylpyridine, Magnetic nanocomposite, Carbon nanotube, Multicomponent reactions.

Multicomponent reactions have been gained special attention in chemistry and pharmacology during the last decade, because they are simple, clean, quick and atom economic.[1] Pyridines are widely used in various sciences including biology, biochemistry and medicinal chemistry.[2] These compounds are used in chemical sensors[3] and photochemical reaction initiators.[4]

Herein, we wish to report a simple and efficient method for the synthesis of 2,4,6-triarylpyridines *via* the reactions of benzaldehydes, acetophenones and ammonium acetate in the presence of a new and recyclable magnetic nanocomposite. This nanocomposite has been made on the basis of carbon nanotubes and characterized by SEM, FT-IR, XRD, EDX and VSM analyses. Short reaction times, high yields of products, mild reaction conditions, easy work-up procedure, and the use of a highly efficient, non-corrosive, easy separable and reusable catalyst are noteworthy advantages of the present work.

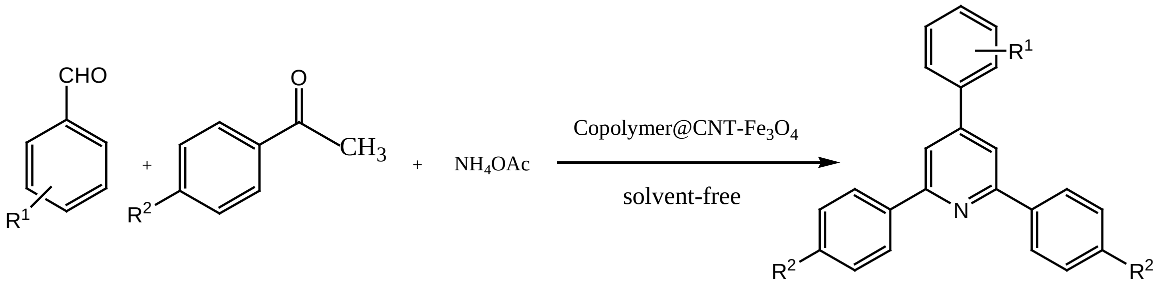

Fig. 1 Synthesis of 2, 4, 6- triarylpyridines in the presence of copolymer @ CNT-Fe_3O_4 nanocomposite under solvent-free condition

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Copolymer coated magnetic graphene oxide; a reusable catalyst for the preparation of triaryl pyridines in solvent-free condition

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Keywords: 2,4,6–Triaryl pyridine, Multicomponent reactions, Solvent-free conditions.

The pyridine rings have been found in the structure of many natural products such as nicotinic acid, vitamin B_6, and NAD nucleotides.[1] In recent years, various methods have been used for the synthesis of pyridine derivatives. But one of the best methods for the preparation of pyridine derivatives is the use of multicomponent reactions. In recent years, the synthesis of pyridine compounds has been carried out using various catalysts such as $H_{14}[NaP_5W_{30}O_{110}]$,[2] $Bi(OTf)_3$,[3] $MgAl_2O_4$,[4] $ZrOCl_2$,[5] $CoCl_2$ $6H_2O$.[6]

Although some of these methods are valuable, most of them have several disadvantages such as long reaction times, requiring large amounts of catalyst and the use of toxic or non-reusable reagent. Therefore, development of a facile and economical synthetic route to 2,4,6-triarylpyridines is still in demand. Herein, we apply a copolymer coated magnetic graphene oxide for the first time as a green and reusable nanocatalyst in the synthesis of these biologically active heterocycles from benzaldehydes, acetophenones and ammonium acetate in solvent-free conditions.

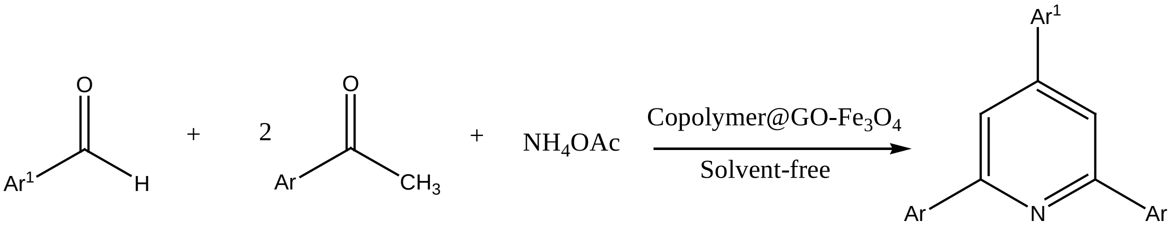

Fig. 1 Synthesis of 2,4,6- triarylpyridines in the presence of copolymer @ GO-Fe_3O_4 nanocomposite under solvent-free condition

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One-pot, solvent-free, and efficient synthesis of 2,4,6-triarylpyridines using Zeolite beta as a recyclable catalyst

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Keywords: Heterocycles, Multi-component reactions, 2,4,6-triarylpyridin, One-pot synthesis

Multi-component reactions are refered to one-pot processes, during which three or more substances are combined to generate a complex structure.[1] These reactions are highly efficient, quick, simple, clean, low cost and without side products.[2]

Pyridines are an important class of heterocyclic compounds and widely used in different fields.They are shown various pharmaceutical activites. For example; anti-inflammatory, anti-microbial and anti-HIV[3] properties have been detected for pyridine derivatives.

Zeolites are a group of crystalline and porous aluminosilicate compoands and have a tri-dimentional tetrahedral lattice constructed from SiO_4 and AlO_4 that create holes and canals in the structure of zeolite.[4]

Herein, we describe a clean and efficient method for the synthesis of 2,4,6-triarylpyridines from aldehydes, acetophenones and ammonium acetate in the presence of zeolite beta as a reasable catalyst.

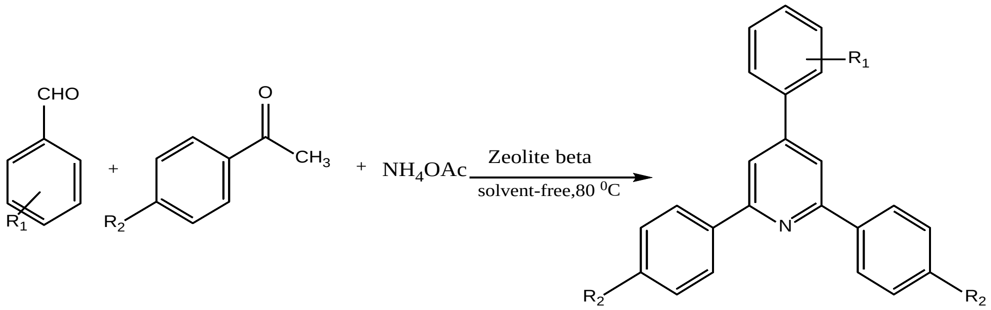

Fig. 1 Synthesis of 2, 4, 6- triarylpyridines in the presence of zeolite beta under solvent-free condition

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Synthesis of novel 1,2,4-triazole derivatives

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Keywords: 1,2,4-Triazoles, Hydrazonoyles, Dicyclohexylcarbodiimide, Cycloaddition reactions,

In this research, an efficient approach for the synthesis of some new 1,2,4-triazole derivatives is reported.[1] In relation to our research interest on the synthesis of *N*-heterocyclic compounds,[2] Various hydrazonoyles were reacted with dicyclohexylcarbodiimide *via* in situ formation of nitrilimines at reflux conditions. One of the intermediates has been isolated and identified by IR and NMR spectroscopy. A plausible mechanism for this transformation has been proposed and discussed. All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.

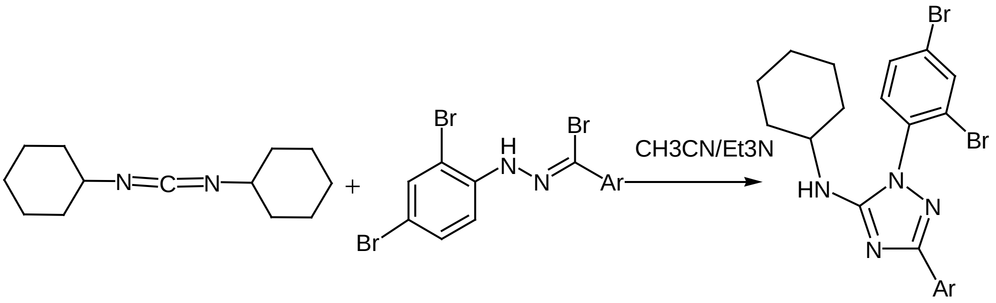

Fig. 1 Synthesis of 1,2,4-triazole derivatives from reaction of hydrazonoyl bromides (3a-g) with dicyclohexyl carbodiimide

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Ring expansion of aziridines to N-heterocyclic compounds

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Keywords: Aziridines, Oxazoles, Thiazole, Imidazolidine, Oxazolidinone.

Aziridines are well known to be useful reagents for the synthesis of many types of nitrogen-containing compounds. Aziridines are useful reagents for the synthesis of many types of nitrogen-containing compounds. In relation to our research interest on the synthesis of *N*-heterocyclic compounds,[1-8] various ketoaziridines were transformed to the variety of heterocyclic compounds All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.

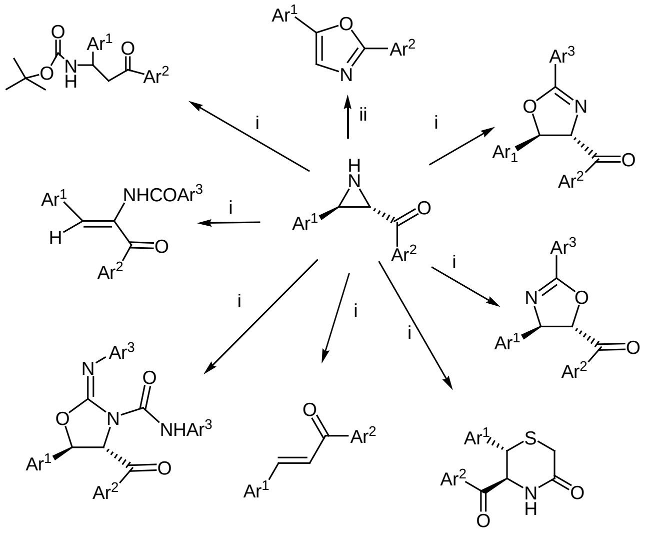
i) Via C-N bond cleavage   ii) C-C bond cleavage

Fig. 1 Reaction of ketoaziridines in C-C- bond cleavage and C-N bond cleavage

References

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An efficient synthesis of spiro-pyrimidine derivatives from malononitrile, isatin and amidine

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Keywords: Malononitrile, Isatin, Amidine, Spiro-pyrimidines derivatives.

Pyrimidine derivatives occupy a unique place in medicinal chemistry because of their presence in several bioactive substances such as antibacterial, antiviral, and anti-HIV agents.[1] Moreover, pyrimidine based spirocyclic systems have been of considerable interest due to their pronounced biological properties such as fredericamycine, acorenone, β-vetivone, and isocomene, which are isolated from plants.[2] A useful and simple strategy for the synthesis of spiro-pyrimidines derivatives *via* a three-component reaction between isatin **1**, malononitrile **2**, and amidine **3**, in the ethanol in the presence of 3 drop of Et_3N as a basic catalyst under reflux conditions is described in this study (Fig. 1). All the synthesized compounds were unknown to the best of our knowledge and were characterized by ^1H, ^{13}C- NMR, and IR.

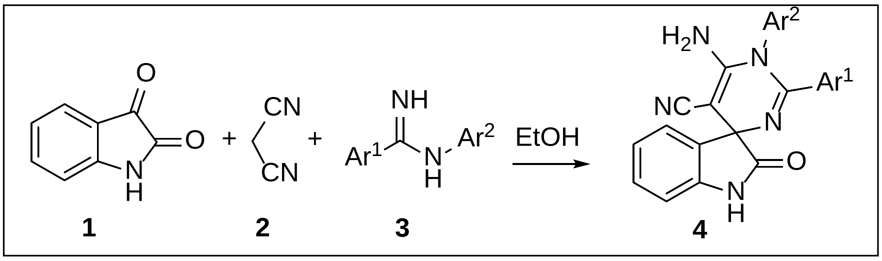

Fig. 1 Synthesis of spiro-pyrimidines derivatives

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Investigation of enterobacter aerogenes effects on heavy oil from biological degradation aspects by GCxGC technique

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Keywords: GCxGC, FT-IR, *Entrobacter aerogenes*, Heavy oil, Bioremediation.

Oil pollution affects the deterioration of the agrophysics soil characteristics, namely to the dysfunction of the water, air, thermal, oxidation-reduction and nutrient regimens. One of the methods to purify oil residue is bioremediation, in this way we investigate *Enterobacter aerogenes* effects on heavy oil by SARA, FT-IR, GC and GCxGC methods. The material required for the growth of *E. aerogenes* are carbon and phosphate. The *E. aerogenes* is injected with thioglycollate broth to crude oil which was distillated, and the samples were put for a month in an incubator. The results of this research illustrate that this bacterium has been able to survive in oil by isolating straight-run carbons with short and weak bounds from asphaltene and resin structures, as well as utilizing sulfur, nitrogen, and oxygen in the oil. In addition, it is found out this bacterium has had a positive effect on making light oil from heavy crude oil. Thereby, it is suitable for bioremediation in oil polluted sites and oil refinery for removing hydrocarbon pollutants from the environment.

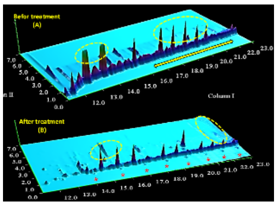

Fig. 1 Comparison of the spectra obtained from the GCxGC technique on saturate fracture. Spectrum A: before treatment, Spectrum B: after treatment.

Refrence:

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Synthesis of benzyl acetate by using supported polyoxometalate on magnetic nanoparticles as a heterageneous catalyst

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Keywords: Nanoparticle, Phosphotungstic acid, Polyoxometalate, Esterification, Acetic Acid, Benzyl Alcohol, Benzyl acetate.

Esterification of benzyl alcohol with acetic acid in the liquid phase using phosphotungstic acid stabilization on the substrate, benzyl acetate is used as a Jasmine essential oil. Carboxylic acid esterification is one of the basic reactions in organic chemistry, the speed of which can be increased by increasing the acidic catalyst to the reaction medium. In the reaction of esterification both homogeneous and heterogeneous catalysts can be used. Among the heterogeneous catalyst that can be used, phosphotungstic acid stabilized on magnetic nanoparticles used to esterification carboxylic acids with alcohols to prepare essential oils. The advantage of this is the very easy separation of catalyst from the reaction medium by the magnet. In fact, the application of magnetic nanoparticles in the catalysts as a catalyst base has been considered due to the good spread, the surface to volume ratio, the ease of surface modification, and the very easy and effective separation of the reaction medium. Polyoxometalate are used as a heteropoly acid catalyst on a solid bed that provides this opportunity to heteropoly acid to spread on a wider surface.

Solvotermal was used to synthesize magnetic iron oxide nanoparticles. Synthetic iron oxide nanoparticles are called MNP, which have a black color and magnetism. Then phosphotungstic acid، which is stabilized as polyoxometalate on iron oxide magnetic nanoparticles, is used for acidic catalysts. SEM and XRD were used to identify the catalysts, and IR and GC spectra were used for qualitative analysis of the product.

The performance of the catalyst in the stringer of benzyl alcohol with acetic acid was investigated. The effects of reaction parameters such as molar ratio of reactants, reaction temperature and optimal time to react, catalytic amount and catalyst reuse of the product were investigated.

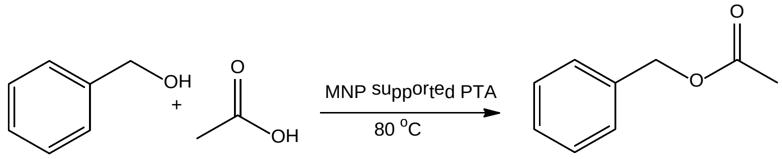

Fig. 1 benzyl alcohol acetic acid benzyl acetate

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Synthesis, characterization and catalytic evaluation of $NiFe_2O_4@SiO_2$@glucose amine for the synthesis of novel derivatives of thiazolidine-4-ones

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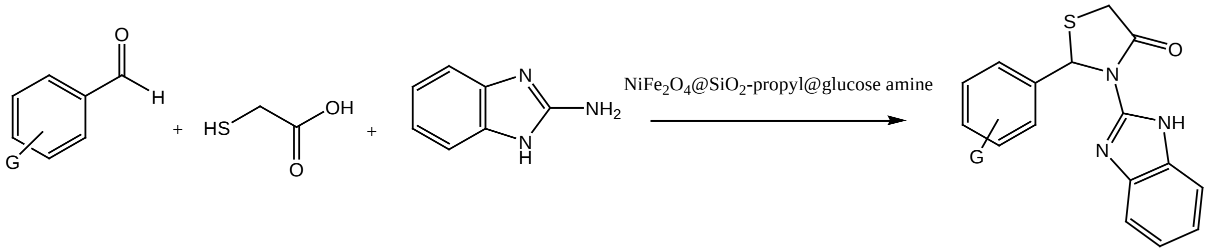
Keywords: Green Chemistry, $NiFe_2O_4@SiO_2$@glucose amine, thiazolidine-4-one

Thiazolidine -4-ones exhibit antitubercular, antimicrobial, antioxidant and antifungal activity and can be applied as COX-1 inhibitor, bacterial enzyme MurB inhibitor, non-nucleozide anzyme inhibitor of HIV-RT and antihistaminic agent.[1] For this reason, synthesis of novel derivatives of thiazoline-4-ones have attracted a lot of interest.

Traditional heterogeneous catalysts are limited in the nature of their active sites and their reaction scope abilities. Soluble organic catalysts can catalyse a variety of reaction more than traditional solid catalysts but suffer from their inability to be recycled. For this reason, synthesis of organic and inorganic hybrid composite to utilize the organic moiety as the active site and the solid to provide avenue to recovery and recyclability is attractive.[2]

In continuation of our previous work [3], herein, we specifically address the synthesis and usage of organic-inorganic hybrid materials based on $NiFe_2O_4@SiO_2$-propyl@glucose amine magnetic nanoparticle as catalyst for the synthesis of new generation of thiazolidine-4-ones. All of organic compounds are new and characterized by IR, ^1H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Multicomponent synthesis of thiazolidine-4-ones

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Design, synthesis and application of Ch-MoO as an efficient catalyst for the synthesis of Hantzsch 1,4-dihydropyridines

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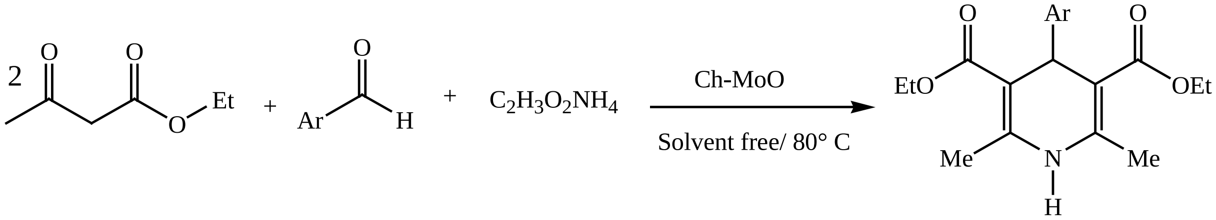
Keywords: Chitosan, 1,4-dihydropyridines, Hantzsch reaction.

In recent years, developing routs to produce materials based on green chemistry which minimizes pollution have been focused.[1] For this purpose these goals, the development of heterogeneous catalysts in the synthesis of organic compounds is highly investigated due to the ease of handling, reusability and simple work-up. Therefore, immobilization of metal on inorganic support to produce heterogeneous catalytic systems has been widely reported. Recently, chitosan (Cs) as a biological polymer has been found to be the most abundant natural amino polysaccharide that is usually obtained by deacetylation of chitin. It has attracted significant interest due to its green properties, safety, non-toxicity, biocompatibility, biodegradability, low immunogenicity, stability and ability of chelation.

In continuation of our efforts to synthesize of novel catalysts [2] for applying in the synthesis of heterocyclic ring, we wish to design and synthesis of molebdinium supported chitosan Ch-MoO as an efficient catalyst for the synthesis of 1,4-dihydropyridine through the condensation reaction of aldehydes, ethyl acetoacetate, ammonium acetate under solvent free condition at 80° C (Scheme 1).



Scheme 1: Synthesis of Hantzsch 1,4-dihydropyridines

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One-opt, four component synthesis of pyrano[2,3-*c*]pyrazoles catalyzed by [VO(TPPA)]SO_3H

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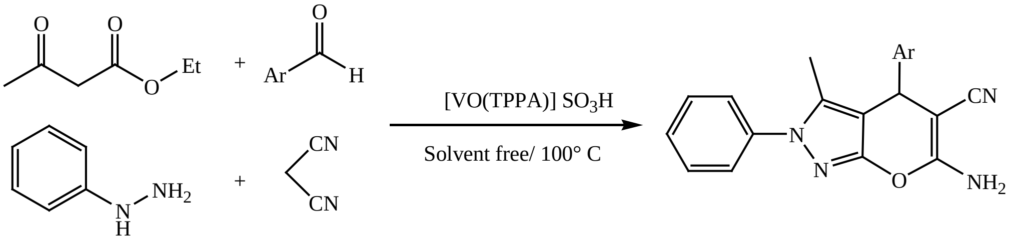
Keywords: Metallophthalocyanines (MPcs), Vanadium-oxo tetrapyridinoporphyrazine [VO(TPPA)]SO_3H, Dihydropyrano[2,3-c]pyrazole.

In the past decades, metallophthalocyanines (MPcs) employed as the efficient biomimetic catalysts with thermal and chemical stability and easy access.[1-2] In addition, poor solubility of metallophthalocyanines in common organic solvents can be considered as the most prominent point in their applications as the heterogeneous catalysts. In this regard, vanadium-oxo tetrapyridinoporphyrazine sulfonic acid was synthesized and fully characterized. Pyrazole derivatives are the significant kind of heterocyclic compounds that feature in several pharmaceutical targets and natural products of medicinal interest. Dihydropyrano[2,3-c]pyrazole derivatives have showed a wide variety of biological activities counting anticancer, antimicrobial, anti-inflammatory, insecticidal, and molluscicidal activities.

In continuation of our efforts to synthesize of novel catalysts in the synthesis of multicomponent reactions, we wish to report the synthesis of vanadium-oxo tetrapyridinoporphyrazine sulfonic acid [VO(TPPA)]SO_3H as an efficient catalyst for the synthesis of dihydropyrano[2,3-c]pyrazole through the condensation reaction of aryl aldehydes, ethyl acetoacetate, malononitrile, and phenyl hydrazine under solvent free conditions at 100° C (Scheme 1).



Scheme 1. Multicomponent synthesis of pyrano[2,3-c] pyrazoles

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A comparative ADME study of aminopterin derivatives and methotrexate as anti cancer drug

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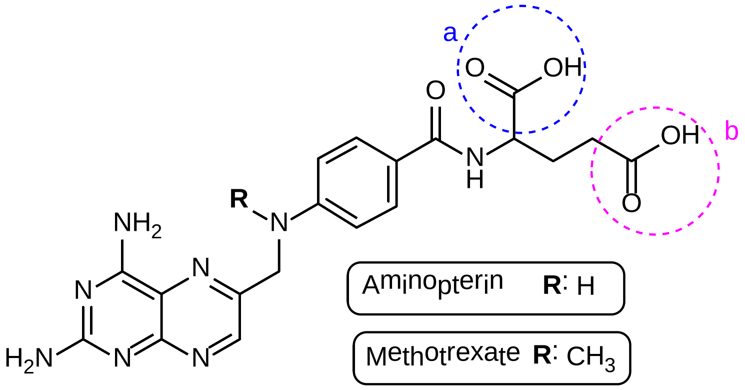
Keywords: aminopterin, methotrexate, ADME properties, in silico.

In designing new drugs, drug development includes the evaluation of efficacy and toxicity of the new drug candidates. Thus, precise data on the pharmacokinetics and metabolism must be available to determine the final success or failure of the compound. Screening absorption, distribution, metabolism and excretion (ADME) is necessary to decrease the cost and the ratio of failed compounds in clinical trials **1**. Methotrexate is an inhibitor of dihydrofolate reductase (DHFR), as a target for anticancer drugs **2, 3**. It acts by blocking the body's use of folic acid. As methotrexate can decrease the levels of folate, this leads folate deficiency **4** and additionally it concludes some other side effects such as liver damage which may lead to fibrosis or cirrhosis and severe skin rashes **5**. Thus, scientists try to find newer and safer replacements **6**. The present study incorporates ADME results of methotrexate and aminopterin derivatives as a less toxic replacement for methotrexate. All data were collected by swiss ADME prediction **7**. Herein the results of lipophilicity determination of aminopterin and some derivatives are investigated.



R	a	b	Log P
H	CO_2H	CO_2H	0.62
CH_3	CO_2H	CO_2H	1.53
H	CSOH	CO_2H	1.64
H	$CONH_2$	CO_2H	1.44
H	$CNNH_2$	CO_2H	1.08
H	$COCH_3$	CO_2H	1.56
H	CO_2H	$CO(CH_2)OH$	1.53
H	CO_2H	$(CH_2)_2CO_2H$	2.50

Fig.1 aminopterin and methotrexate structures and lipophilicities (Log P)

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DFT Study on DMNT biosynthesis as a defective plant-insect interaction

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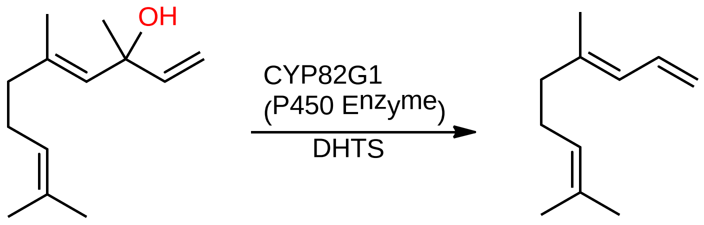
Keywords: DFT study, nerolidol, thermodynamic properties, B3LYP, STO-3G basis set.

The (*E*)-4,8-dimethyl-1,3,7-nonatriene (DMNT) biosynthesis has been proposed to occur via (*E*)-nerolidol as precursor **1-3**. Nerolidol is a sesquiterpene alcohol and a volatile organic compound constituent in the headspace of some flowers **4** and plants, which is converted to DMNT by cytochrome P450 enzyme catalysis **5**. Although DMNT is considered as one of the defensive volatile organic constituents involved in plant-insect interaction but the role of nerolidol as an active compound in plant defensive systems is ambiguous **6** and also the DMNT biosynthesis mechanism is not clearly known. Herein DMNT biosynthesis is thermodynamically investigated. The calculations were performed using Gaussian 09 with Gausview interface and the geometries were optimized at the DFT B3LYP level of theory with a STO-3G basis set. The thermochemical data such as entropy, gibs free energy, total energy data and also polarizability were calculated for both nerolidol and DMNT. Some of the results are tabled below.



(*E*)-Nerolidol

(3*E*)-4,8-Dimethyl-1,3,7-nonatriene
(DMNT)

ΔE_{tot} (kcal/mol)	**$1.42*10^5$**
ΔS (cal/mol-k)	**-20.92**
ΔG (kcal/mol)	**$6.75*10^5$**

Fig. 1 (*E*)- Nerolidol conversion to DMNT via cytochrome P450 enzyme catalysis

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Synthesis, characterization and catalytic evaluation of $Fe_3O_4@SiO_2$-pr@*L*-proline for the synthesis of novel derivatives of dihydropyridines

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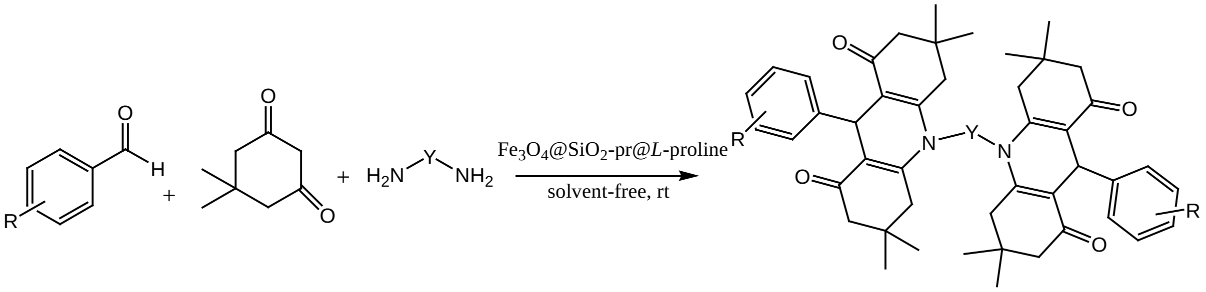
Keywords: Green Chemistry, $Fe_3O_4@SiO_2$-pr@*L*-proline, dihydropyridines

Compounds with dihydropyridines nucleus are a common and important substructures found in natural products and pharmacologically active compounds. They act as glucagon receptor antagonists, inhibitors of P38 MAP kinase, β-Raf kinase, transforming growth factor b1 (TGF-b1) type 1 activin receptor-like kinase (ALK5), cyclooxygenase-2 (COX-2), CB1 cannabinoid receptor antagonists, modulators of P-glycoprotein (P-gp)-mediated multidrug resistance (MDR), biosynthesis of interleukin-1 (IL-1). [1] For this reason, synthesis of novel derivatives of dihydropyridines have attracted a lot of interest.

Today, catalysts play a significant role in the production of chemicals and nanocatalysts have the potential for improving efficiency, selectivity and yield of the catalytic process. The higher surface to volume ratio means that much more catalyst actively participates in the reaction. Higher selectivity means less waste and fewer impurities, which could lead to safer and reduced environmental impact. [2]

In continuation of our previous work [3], herein, we specifically address the synthesis and usage of $Fe_3O_4@SiO_2$-pr@*L*-proline magnetic nanoparticle as catalyst for the synthesis of new generation of dihydropyridines. All of organic compounds are new and characterized by IR, ^{1}H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Multicomponent synthesis of bis dihydropyridines

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Unprecedented regiocontrol in synthesis of spirooxindolopyrrolizidines in both enantiomeric form *via* asymmetric [3+2] cycloaddition of azomethine ylides

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Keywords: 1,3-Dipolar cycloadditions, Azomethine ylides, Chiral spiroindolo pyrrolizidine, Asymmetric Synthesis.

Spirooxindoles and functionalized pyrrolizidines are an important class of naturally occurring substances characterized by highly pronounced biological properties and therapeutic applications. Thus, it might be expected that presence of a pyrrolizidine moiety at C-3 of the 2-indolinone system generates 3-spiroindolo pyrrolizidine that possess considerably enhanced biological activities. For example, horsfiline, elacomine and rhynchophylline, which exhibit significant biological activities.[1] We herein report a highly regio-, diastereo-, and enantioselective 1,3-dipolar cycloaddition reaction of (*R*)/(*S*)-camphorsultam cinnamate with azomethine ylides, which are generated from (*S*)-proline with isatins under optimized reaction conditions (**Fig. 1**). More importantly, for the first time an unusual regioselectivity was observed in this reaction, leading to the construction of novel 3-spiroindolopyrrolizidine derivatives in both enantiomeric form. The structures of cycloadducts were assigned from their elemental and spectroscopic analyses including IR, ^{1}H NMR, ^{13}C NMR, mass spectral data and by single-crystal X-ray analysis. The possible mechanism of the reaction was investigated using the DFT approach at the B3LYP/6-311G* level of theory.

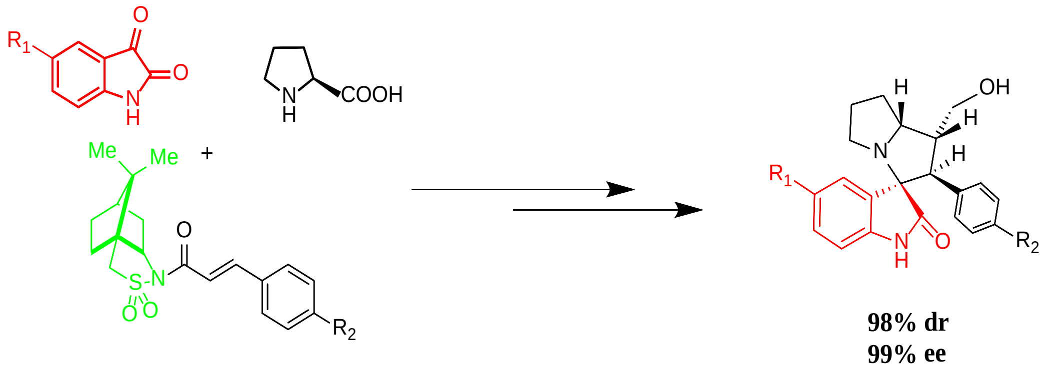

Fig. 1 Asymmetric synthesis of new chiral 3-spiroindolopyrrolizidine derivatives

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Synthesis of novel chiral dispiro pyrrolidines/pyrrolizidines *via* 1,3-dipolar cycloaddition and evaluation of their mechanism by DFT calculation

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Keywords: 1,3-Dipolar cycloaddition reaction, Azomethine ylide, Dispiropyrrolidines, Dispiro pyrrolizidines

Optically active spirooxindoles containing pyrrolidine and pyrrolizidines framework have been proven to have broad spectrum of considerable bioactivity and curative applications.[1] In this regard, spirooxindoles have received extensive attention in the last years and among all the developed synthetic methodologies, 1,3-dipolar cycloaddition has been found to be one of the most efficient and straightforward pathways, leading to rapid assembly of pyrrolidine and pyrrolizidine spirooxindole skeletons.[2] In continuation of previous our works[3], a variety of chiral dispiro pyrrolidines/pyrrolizidines have been synthesized in three and four contiguous and two quaternary stereogenic centers in generally high yields and excellent diastereo- and enantioselectivities (up to 99%). This new scaffold has been established *via* asymmetric 1,3-dipolar cycloadditions of acenaphthoquinone azomethine ylides with dipolarophiles which are generated from (*S*)-camphorsultam, as chiral auxiliary, with isatin-derived under optimized reaction conditions (**Fig. 1**). The structures of the products, after purification, were assigned and approved using NMR, mass, IR and single-crystal X-ray analysis. The reaction mechanism was discussed by quantum mechanical calculations.

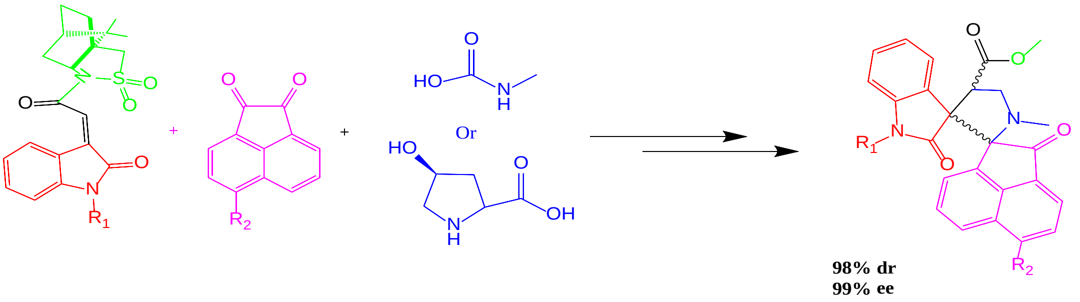

Fig. 1 Asymmetric synthesis of new chiral dispiropyrrolidine and pyrrolizidine derivatives

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Synthesis of new chiral spiroacenaphthyl-pyrrolidines/pyrrolizidines : Effect of two important chiral auxiliaries on their stereoselectivities

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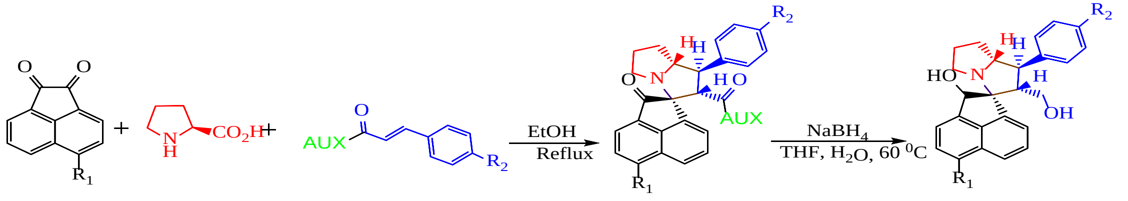
Keywords: Asymmetric 1,3-dipolar cycloaddition reaction, Azomethine ylide, Chiral auxiliary, Spiropyrrolizidines

Chiral spiro pyrrolidines/ pyrrolizidines have brought the surge of interest due to their highly pronounced biological significance and pharmaceutical applications. One of the powerful methods for the synthesis of a variety of natural products containing chiral spiro-pyrrolidine/ pyrrolidines structures is 1,3-DC reaction of azomethine ylides.[1] Stereocontrol in these reactions can be achieved through the use of chiral auxiliaries that are attached to the dipolarophiles. In continue of our laboratory purposes in the field of asymmetric 1,3-dipolar cycloaddition reaction (ADCR)[2], we report the easy preparation and characterization of new chiral derivatives of spiro pyrrolizidines based on acenaphthoquinone with a highly regio-, diastereo-, and enantioselectivity through of ADCR (**Fig. 1**). The absolute stereochemistry of cycloadducts, which was obtained by utilizing two types of chiral auxiliaries, was unambiguously established by X-ray crystallography and showed that all cycloadducts have same configuration. They were also clearly the result of endo-re addition of the dipoles to the dipolarophile. The possible mechanism of the reaction was investigated using the DFT approach at the B3LYP/6-311G* level of theory.



R_1 = H , Br
R_2 = Cl , F , Me , Br

Fig. 1 Asymmetric synthesis of new chiral spiro pyrrolizidine derivatives

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Synthesis, characterization and catalytic evaluation of Fe_3O_4@SiO_2-propyl@*L*-proline for the synthesis of novel derivatives of benzo[*d*]imidazoles

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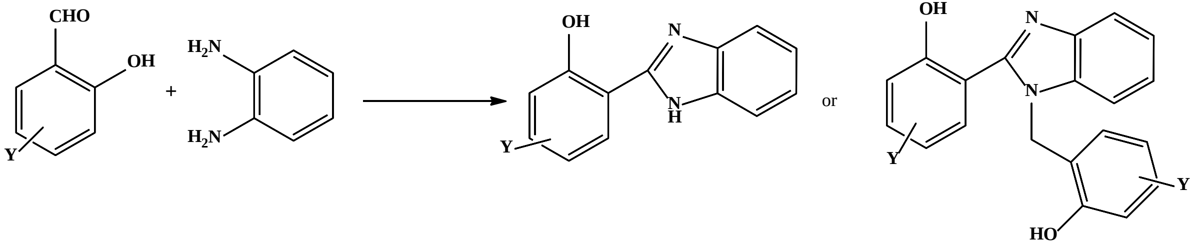
Keywords: Green Chemistry, Fe_3O_4@SiO_2-propyl@*L*-proline, benzo[*d*]imidazoles

Compounds with imidazole nucleus are a common and important substructures found in natural products and pharmacologically active compounds. They act as glucagon receptor antagonists, inhibitors of P38 MAP kinase, *β*-Raf kinase, transforming growth factor b1(TGF-b1) type 1 activin receptor-like kinase (ALK5), cyclooxygenase-2 (COX-2), CB1 cannabinoid receptor antagonists, modulators of P-glycoprotein (P-gp)-mediated multidrug resistance (MDR), biosynthesis of interleukin-1 (IL-1) [1]. There are a lot of reports for the synthesis of benzoimidazoles but they suffer from some serious defects, such as tedious workup and purification, significant amounts of toxic waste materials, highly acidic conditions, long reaction time, occurrence of side reactions, low yields, use of expensive reagents or catalysts, low selectivity and high temperatures in refluxing or microwave condition. Therefore, development of easy, green, effective, high yielding, and eco-friendly approaches using novel catalysts for the synthesis of imidazoles is an important.

In continuation of our previous work [2], herein, we specifically address the synthesis and usage of Fe_3O_4@SiO_2-propyl@*L*-proline magnetic nanoparticle as catalyst for the synthesis of new generation of benzo[*d*]imidazoles (Scheme 1). All of organic compounds are new and characterized by IR, ^1H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Green synthesis of benzo[*d*]imidazoles

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Synthesis of multicomponent hydrogel as a delivery system for anticancer drug doxorubicin

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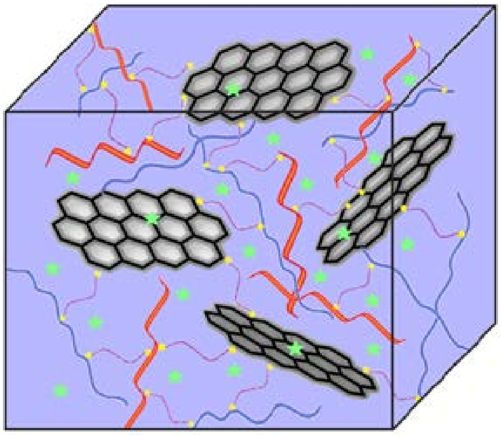
Keywords: Cellulose nanowhisker, Chitosan, Graphene, Hydrogel

Hydrogels are the three dimensional networks from hydrophilic polymers which can absorb a lot of water. Hydrogels are widely used in the various fields, including drug delivery [1] and dye absorption.[2] Cellulose and chitin are the abundant natural biopolymer from renewable sources and chitosan was obtained by alkaline deacetylation of chitin. These polysaccharides are non-toxic, biodegradable, and biocompatible and have different applications such as drug delivery systems.[3] Herein, we developed a multicomponent hydrogel by combination of chitosan, cellulose nanowhisker and graphene (Scheme **1**). A synthetic linker was applied as the crosslinking agent, which connect graphene sheets, chitosan chain, and nanowhisker together by forming a reversible linkage. The hydrogel was pH-responsive and was used for *in vitro* study of the anticancer drug doxorubicin delivery.



Scheme. 1 Multicomponent hydrogel by combination of chitosan, cellulose nanowhisker, and graphene.

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Synthesis of new curcumin derivatives and study of their medicinal properties

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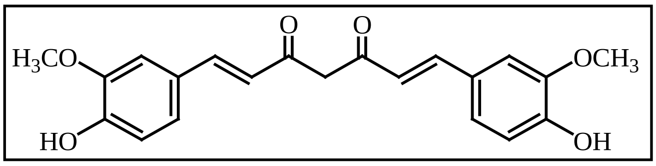
Keywords: Curcumin, Polyglycerol, Antibacterial, Antioxidant

Turmeric is a member of ginger family with the scientific name of *Longa Curcuma*. The most important components of turmeric are yellow pigments from the category of curcuminose. These compounds form about 3 to 5 percent of turmeric, and its main components are curcumin, demethoxycurcumin, and bisdemethoxycurcumin. Curcumin (Fig. **1**) has many biological properties, including antioxidant, antibacterial, anti-fungal, anti-inflammatory, and anti-tumor properties.[1-2] Curcumin also has the great therapeutic potential against all types of cancers.[3] Despite the extremely high therapeutic benefits of curcumin, the sustainability and bioavailability of this compound is very low. In recent years, many research groups have focused on improvement of biocompatibility and effectiveness of curcumin.[4] In this study, using hydrophilic polymer polyglycerol, new compounds of curcumin were synthesized, and then evaluated *in vitro* biological and medicinal properties and compared with primary curcumin.



Scheme. 1 The structure of curcumin.

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A novel and efficient synthesis of indoles by using a three-component reaction of arylamine, arylglyoxal, and 4-hydroxycoumarin

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Keywords: Indole derivatives, Arylamine, Arylglyoxal, 4-Hydroxycoumarin.

Indole cores are an important class of heterocyclic compounds found in natural products, drug molecules, and functional materials.[1] They have been attention in recently years due can be exhibit a wide spectrum of biological activity such as the anti-inflammatory,[2] anti-proliferative, and platelet aggregation inhibitory activities.[3] Herein, we describe efficient and novel method for the synthesis of indole derivatives **4** *via* appropriate arylamine **1**, arylglyoxal **2**, and 4-hydroxycoumarin **3** in ethanol solvent at reflux conditions for 12 h. (Fig. 1). Metal-free catalyst, eco-friendly solvents, and excellent yields (80-93 %) are advantages of the protocol. All the synthesized compounds were unknown to the best of our knowledge and were characterized by ^{1}H and ^{13}C- NMR, IR and melting points.

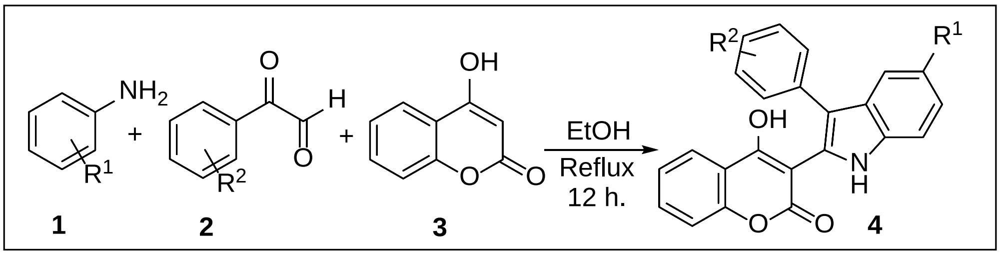

Fig. 1 Synthesis of indole derivatives

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Cu-Catalyzed regioselective synthesis of functionalized 4-benzoyl-5-cyanopyrazoles under mild conditions

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Keywords: 4-Benzoyl-5-cyanopyrazoles, Copper catalysis, [3+2] Cycloaddition, Phenacylmalononitrile, Hydrazonoyl chloride

The unsaturated cyanocarbonyl compounds provide an attractive entry into electron-deficient dienophiles employed in Diels–Alder cycloadditions.[1] To prepare these valuable substrates, several synthetic methodologies have been reported, including Wittig-type olefination of glyoxal derivatives, palladium catalyzed four-step procedure from alkenals, dehydrohalogenation of suitable substituted precursors, or five-step chemical modification of *trans*-styrylacetic acid.[2] These approaches are frequently long and cumbersome. To the best of our knowledge, there is no report regarding either *in situ* generation of benzoylacrylonitriles, or employing them as dipolarophile in the 1,3-dipolar cycloaddition reactions. We have described an unprecedented copper catalyzed regioselective synthesis of 4-arylcarboxo-1-phenyl-3-aryl-1*H*-pyrazole-5-carbonitriles *via* the [3 + 2] cycloaddition reaction between phenacylmalononitriles and hydrazonoyl chlorides (Figure 1). ^{13}C NMR spectra provide a useful clue to distinguish the product from its regioisomer. Thus, the ipso carbon to the cyano group in regioisomer is expected to appear below 100 ppm in ^{13}C NMR spectra while the ipso carbon to the CN group in the product is expected to appear at about 140 ppm. In line with the studies conducted in our research group centralized on the synthesis of different substituted pyrazoles,[3] we decided to carry out the multisubstituted pyrazole synthesis with the concomitant *in situ* generation of the dipole and the dipolarophile.

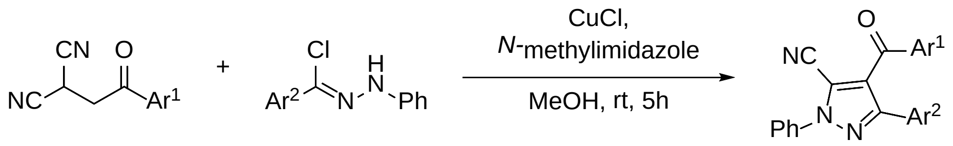

Fig. 1 Synthesis of 4-benzoyl-5-cyano-pyrazoles

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Synthesis of pyridine-3-carbonitriles using a novel and recoverable nanomagnetic catalyst via a cooperative vinylogous anomeric based oxidation

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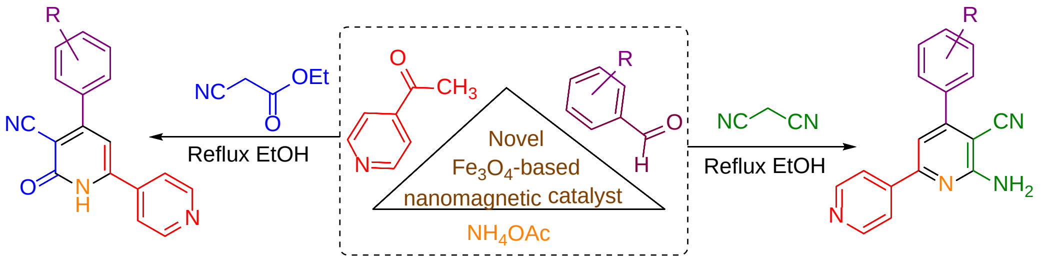
Keywords: Pyridine-3-carbonitrile, Recoverable nanomagnetic catalyst, Anomeric based oxidation , Multi component reactions, Vinylogous anomeric effect**.**

N-heteroaromatic structures particularly pyridine ring systems are ubiquitous in pharmaceutically active molecules and natural products. Among them, pyridine-3-carbonitrile derivatives represent fascinating biological characteristics. These compounds can apply as A_{2A} adenosine receptor antagonists, IKK-β inhibitors, inhibitors of HIV-1 integrase, antimicrobial, anti-tumour, analgesic, anti-inlammatory, and antipyretic agents.[1-3] Herein, we have developed a green, efficient and powerful protocol for the synthesis of pyridine-3-carbonitrile derivatives *via* a four-component reaction. The reaction was performed in the presence of a catalytic amount of nanomagnetic catalyst under reflux conditions (Fig.1). It is worthy to mention that the final step of the mechanistic pathway for the synthesis of target molecules has proceeded *via* a cooperative vinylogous anomeric based oxidation mechanism.



R= H, 2-Furyl, 4-Cl, 4-OH, 2-OH, 2,4-OH2

Fig.1. Preparation of pyridine-3-carbonitrile derivatives**.**

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Synthesis and characterization of new potentially hexadentate (N_4O_2) Schiff base ligand

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Keywords: Hexadentate Schiff base, Tetraamine ligand, 2-Hydroxybenzaldehyde

Considerable attention has focused on the synthesis of new hetroacyclic ligands containing azo groups because of their role in the development of coordination chemistry as well as optical materials, dyes and so on.[1] Schiff base derived from the reaction of salicylaldehyde with primary amines represent a versatile series of ligand. In attention to importance of these compounds many literatures have been published in this field. In this work we want to report the synthesis and characterization of new type of hexadentate schiff base ligand. First we synthesis (2-2-2-aminobenzylideneamino)ethylimino)methyl)benzenamine and use to this tetraamine ligand and 2-hydroxybenzaldehyde to prepare new potentially hexadentate (N_4O_2) Schiff base ligand. Also this Schiff base was characterized by ^1H and ^{13}C NMR, elemental analysis, MS and IR spectroscopy (Fig 1).

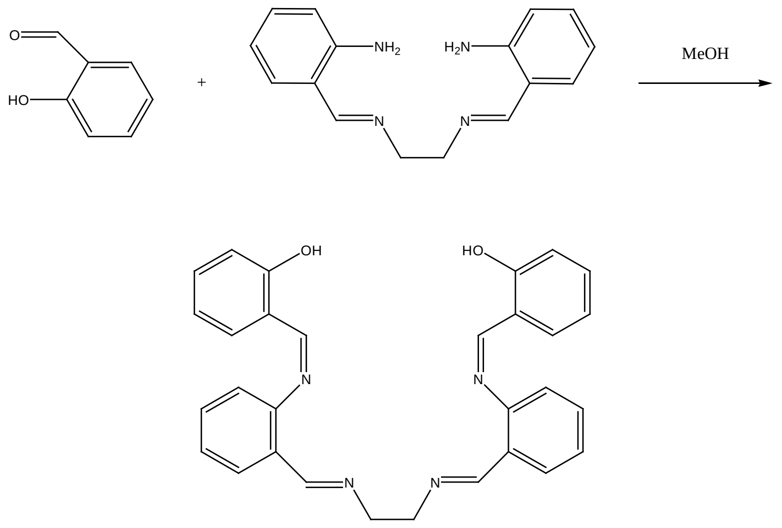

Fig. 1 Hexadentate (N_4O_2) Schiff base ligand

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Theoretical Investigation of 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepinium halids

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Keywords: Theoretical study, Electronic properties, Halids.

In this work, we have performed a computational investigation on the structural, electronic and spectroscopic properties of 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepinium halids [DBU][X] (X=F, Cl and Br)[1] which have been shown in Fig. 1. Considering that, density functional theory (DFT) is an electronic structure method which is widely used in chemistry and physics for theoretical study of various properties of many compounds and their derivatives[2,3], we used this method with B3LYP/6-311G(d,p) level of theory for investigation of [DBU][X].

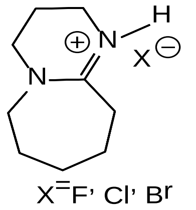

Fig. 1. The structure of [DBU][X]

Molecular orbitals (MOs) play a central role in electron transportation in molecular devices. Therefore, the calculated values of the HOMO, LUMO and the difference between HOMO and LUMO, known as HLG energies or E_{gap} for the [DBU]lX] were calculated and indicated in Table 1.

Table 1. The E_{HOMO}, E_{LUMO} and E_{gap} (in eV) for [DBU][X].

IL	E_{HOMO}	E_{LUMO}	E_{gap}
[DBU][F]	-6.107	0.992	7.101
[DBU][Cl]	-5.430	-0.994	4.435
[DBU][Br]	-5.060	-1.093	3.967

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DFT study of bis-2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepiniumethyl disulfate [DBU]*2*[EDS]

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Keywords: Ionic liquid, DFT study, Spectroscopic properties.

Ionic liquids (ILs) are a class of organic salts, kind of new materials with unique physicochemical properties, therefore they have become increasingly attractive as green solvents for industrial applications and have considered attention of researchers.[1] Therefore, in this work, the molecular structures and vibrational spectra of bis-2,3,4,6,7,8,9,10-octahydropyrimido[1,2-*a*]azepiniumethyl disulfate [DBU]$_2$[EDS] [2] were calculated. Since the B3LYP functional yields a good description of harmonic vibrational wavenumbers for the small and medium sized molecules[1], we choose this method with 6-311G(d,p) basis set for investigation of the structural, electronically and spectroscopic of the studied IL. Figure 1, displayed that the structure of [DBU]$_2$[EDS]. The computed geometry of this IL was verified to be minima by harmonic vibrational frequency calculations (no imaginary frequencies). As a result of MO orbitals, E_{HOMO}, E_{LUMO} and E_{gap} for [DBU]$_2$[EDS] are -6.227, -1.034 and 5.192 eV, respectively. Additionally, total dipole moment of this compound is 38.211 Debye.

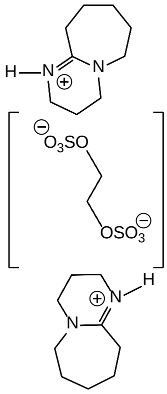

Fig. 1. The structure of [DBU]$_2$[EDS].

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Synthesis of benzo[*g*]chromene derivatives in the presence of nano Cu-MOF

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Keywords: Multicomponent reactions, Benzo[*g*]chromene, Metal organic framework, Nanocatalyst.

The discovery of Metal Organic Framework (MOF), a new family of porous crystalline compounds, has attracted a lot of attention in the last two decades, as these compounds are capable of commercial application.[1] Recently, the use of MOFs as heterogeneous catalysts in organic reactions has been considered more than before because these compounds are unique in their structure due to the presence of metal and an organic ligand in their structures.[2] In order to the easy separation and recycling of heterogeneous catalysts, its use in multi-component reactions (MCRs) is of particular importance[3]. Herein, we report the synthesis of benzo[*g*]chromene derivatives **4** from the reaction between lawsone **1**, aldehydes **2** and Malononitrile **3** in the presence of nano Cu-MOF as catalyst in EtOH under reflux. The synthesized catalyst was characterized by SEM, PXRD, TGA and N_2 adsorption/desorption isotherms techniques.

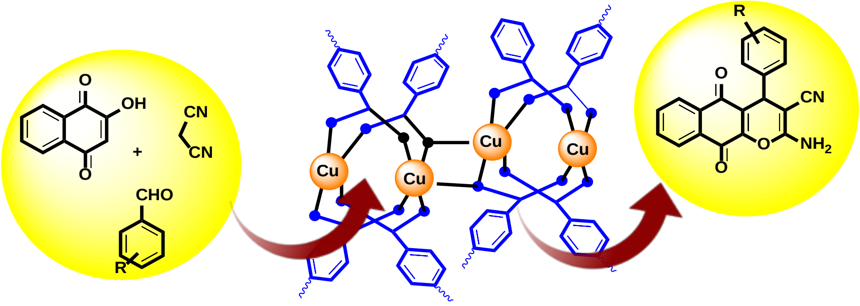

Fig. 1. Synthesis of benzo[*g*]chromene derivatives using nano Cu-MOF

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Synthesis of dihydropyrano[2,3-*g*]chromenes derivatives in present of nano Cu-MOF

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Keywords: Multicomponent reactions, Dihydropyrano[2,3-*g*]chromenes, Metal organic framework, Nanocatalyst.

In recent years, the synthesis and application of Metal Organic Framework (MOF) has attracted chemists, due to these compounds have unique properties in the field of catalyst and gas adsorbents[1]. Recently, the use of MOFs as heterogeneous catalysts in organic reactions has been considered more than before as the presence of metal and an organic ligand in their structures[2]. Chromenes and their derivatives are compounds that exhibit a good biological and antibacterial activity[3]. The chromene synthesis, in economical and optimal conditions, by recyclable heterogeneous catalysts is one of the perspectives examined by chemists. Herein, we report the synthesis of dihydropyrano[2,3-*g*]chromenes from the reaction between 2,5-dihydroxycyclohexa-2,5-diene-1,4-dione, aldehydes and malononitrile in the presence of nano Cu-MOF as catalyst in ultrasonic irradiation. The synthesized catalyst was characterized by SEM, PXRD, TGA.

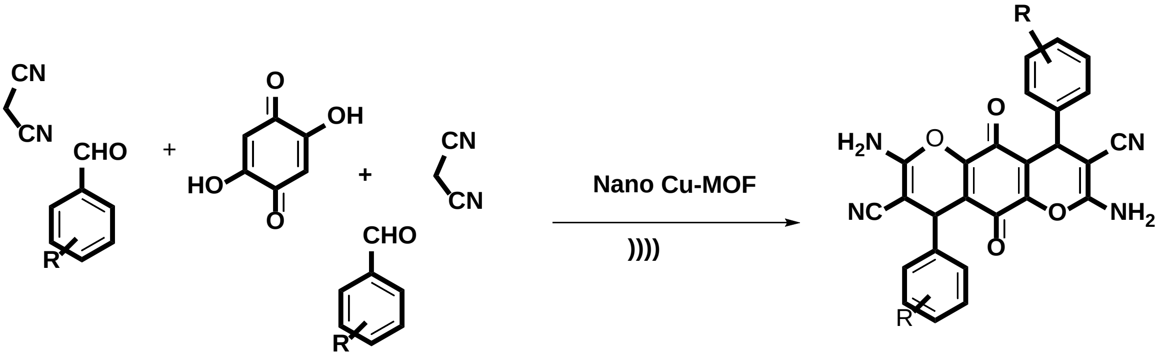

Fig. 1. Synthesis of dihydropyrano[2,3-*g*]chromene derivatives using Nano Cu-MOF

References

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Facile synthesis of pyrano[2,3-*d*]pyrimidine derivatives using a morpholin-based ionic liquid immobilized on nanoporous SiO_2

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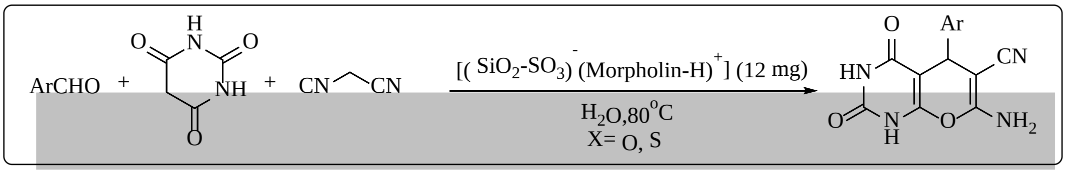
***Keywords*:** Nanoporous SiO_2, Ionic liquid immobilized, pyrano[2,3-d]pyrimidine

Multicomponent reactions (MCRs) have attracted considerable interest due to their ease of performance, high yield, and especially synthetic feasibility and efficiency.[1–3] MCRs include three or more starting materials reacting in a single flask to form a new product, where basically all the atoms contribute to the newly formed product. Pyrano [2,3-*d*] pyrimidine derivatives are examples where multicomponent synthesis can be used. Pyrano[2,3-*d*]pyrimidine structures have a wide range of biological activities such as spasmolytic, diuretic, antitumor, antiallergic, anticoagulant, anticancer, and antianaphylactic activities, as well as acting as potassium channel activators.[4] In this work, a green and efficient procedure is reported for the preparation of pyrano [2,3-*d*]pyrimidine derivatives using morpholin-based ionic liquids immobilized on nanoporous SiO_2. The procedure gave the products in excellent yields in very short reaction times. The reusability of the catalyst is the other important feature of the reported method (Scheme 1).



Scheme 1. Synthesis of pyrano[2,3-d]pyrimidine derivatives using morpholin-based ionic liquids immobilized on nanoporous SiO_2 [(SiO_2-SO_3)$^-$(Morpholin-H)$^+$]

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Synthesis of 2,4,6-triarylpyridines catalyzed by a novel magnetic nanocomposite on the basis of carbon nanotube

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Keywords: Triarylpyridine, Magnetic nanocomposite, Carbon nanotube, Multicomponent reactions.

Multicomponent reactions have been gained special attention in chemistry and pharmacology during the last decade, because they are simple, clean, quick and atom economic.[1] Pyridines are widely used in various sciences including biology, biochemistry and medicinal chemistry.[2] These compounds are used in chemical sensors[3] and photochemical reaction initiators.[4]

Herein, we wish to report a simple and efficient method for the synthesis of 2,4,6-triarylpyridines *via* the reactions of benzaldehydes, acetophenones and ammonium acetate in the presence of a new and recyclable magnetic nanocomposite. This nanocomposite has been made on the basis of carbon nanotubes and characterized by SEM, FT-IR, XRD, EDX and VSM analyses. Short reaction times, high yields of products, mild reaction conditions, easy work-up procedure, and the use of a highly efficient, non-corrosive, easy separable and reusable catalyst are noteworthy advantages of the present work.

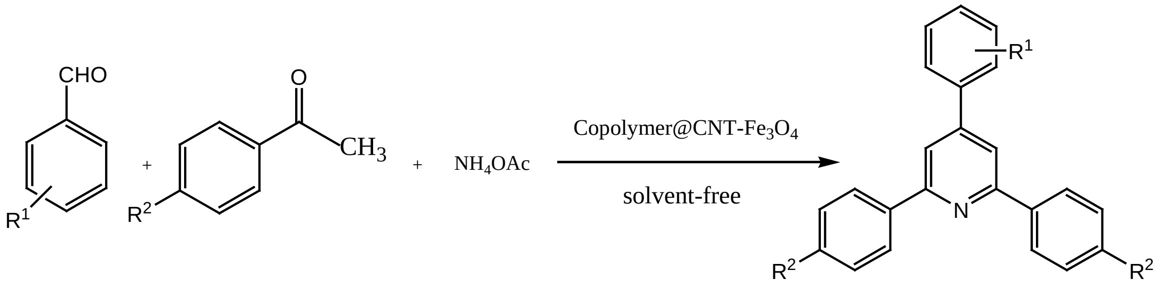

Fig. 1 Synthesis of 2, 4, 6- triarylpyridines in the presence of copolymer @ CNT-Fe_3O_4 nanocomposite under solvent-free condition

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Copolymer coated magnetic graphene oxide; a reusable catalyst for the preparation of triaryl pyridines in solvent-free condition

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Keywords: 2,4,6–Triaryl pyridine, Multicomponent reactions, Solvent-free conditions.

The pyridine rings have been found in the structure of many natural products such as nicotinic acid, vitamin B_6, and NAD nucleotides.[1] In recent years, various methods have been used for the synthesis of pyridine derivatives. But one of the best methods for the preparation of pyridine derivatives is the use of multicomponent reactions. In recent years, the synthesis of pyridine compounds has been carried out using various catalysts such as $H_{14}[NaP_5W_{30}O_{110}]$,[2] $Bi(OTf)_3$,[3] $MgAl_2O_4$,[4] $ZrOCl_2$,[5] $CoCl_2$ $6H_2O$.[6]

Although some of these methods are valuable, most of them have several disadvantages such as long reaction times, requiring large amounts of catalyst and the use of toxic or non-reusable reagent. Therefore, development of a facile and economical synthetic route to 2,4,6-triarylpyridines is still in demand. Herein, we apply a copolymer coated magnetic graphene oxide for the first time as a green and reusable nanocatalyst in the synthesis of these biologically active heterocycles from benzaldehydes, acetophenones and ammonium acetate in solvent-free conditions.

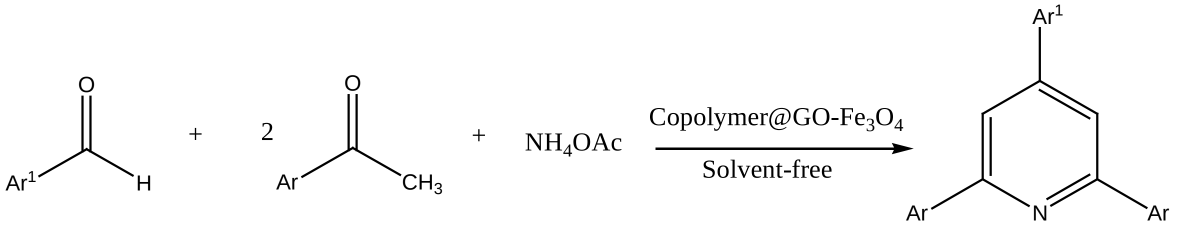

Fig. 1 Synthesis of 2,4,6- triarylpyridines in the presence of copolymer @ GO-Fe_3O_4 nanocomposite under solvent-free condition

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One-pot, solvent-free, and efficient synthesis of 2,4,6-triarylpyridines using Zeolite beta as a recyclable catalyst

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Keywords: Heterocycles, Multi-component reactions, 2,4,6-triarylpyridin, One-pot synthesis

Multi-component reactions are refered to one-pot processes, during which three or more substances are combined to generate a complex structure.[1] These reactions are highly efficient, quick, simple, clean, low cost and without side products.[2]

Pyridines are an important class of heterocyclic compounds and widely used in different fields.They are shown various pharmaceutical activites. For example; anti-inflammatory, anti-microbial and anti-HIV[3] properties have been detected for pyridine derivatives.

Zeolites are a group of crystalline and porous aluminosilicate compoands and have a tri-dimentional tetrahedral lattice constructed from SiO_4 and AlO_4 that create holes and canals in the structure of zeolite.[4]

Herein, we describe a clean and efficient method for the synthesis of 2,4,6-triarylpyridines from aldehydes, acetophenones and ammonium acetate in the presence of zeolite beta as a reasable catalyst.

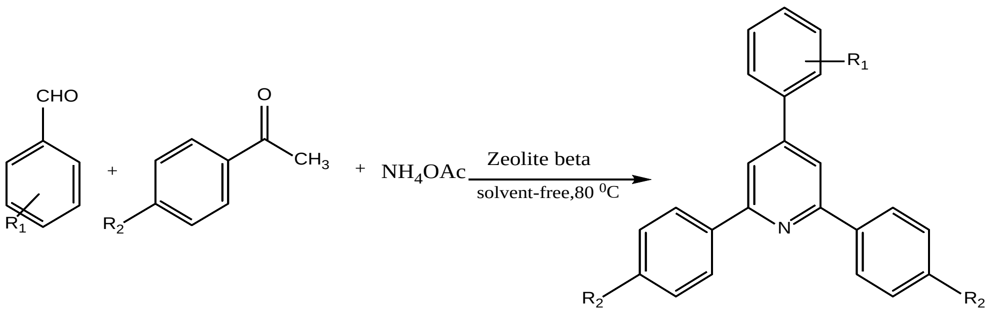

Fig. 1 Synthesis of 2, 4, 6- triarylpyridines in the presence of zeolite beta under solvent-free condition

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Synthesis of novel 1,2,4-triazole derivatives

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Keywords: 1,2,4-Triazoles, Hydrazonoyles, Dicyclohexylcarbodiimide, Cycloaddition reactions,

In this research, an efficient approach for the synthesis of some new 1,2,4-triazole derivatives is reported.[1] In relation to our research interest on the synthesis of *N*-heterocyclic compounds,[2] Various hydrazonoyles were reacted with dicyclohexylcarbodiimide *via* in situ formation of nitrilimines at reflux conditions. One of the intermediates has been isolated and identified by IR and NMR spectroscopy. A plausible mechanism for this transformation has been proposed and discussed. All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.

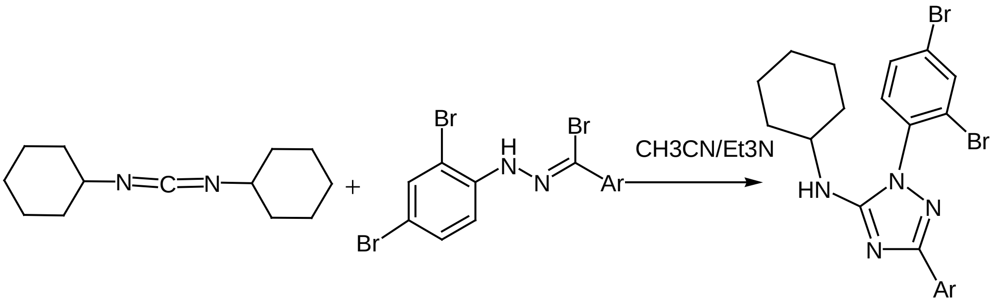

Fig. 1 Synthesis of 1,2,4-triazole derivatives from reaction of hydrazonoyl bromides (3a-g) with dicyclohexyl carbodiimide

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Ring expansion of aziridines to *N*-heterocyclic compounds

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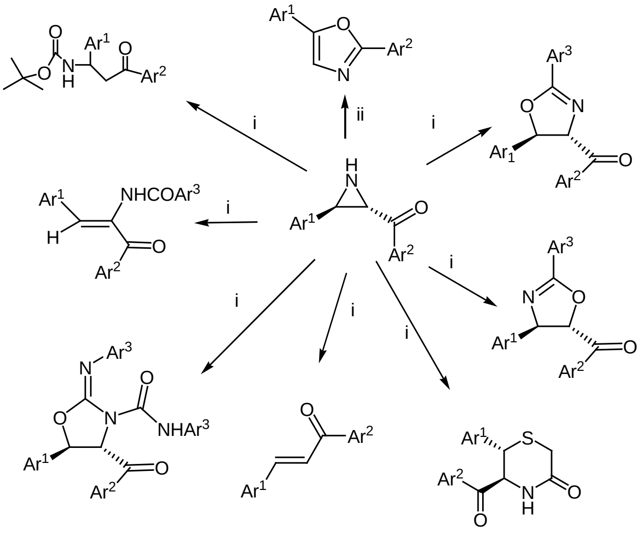
Keywords: Aziridines, Oxazoles, Thiazole, Imidazolidine, Oxazolidinone.

Aziridines are well known to be useful reagents for the synthesis of many types of nitrogen-containing compounds. Aziridines are useful reagents for the synthesis of many types of nitrogen-containing compounds. In relation to our research interest on the synthesis of *N*-heterocyclic compounds,[1-8] various ketoaziridines were transformed to the variety of heterocyclic compounds All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.



i) Via C-N bond cleavage ii) C-C bond cleavage

Fig. 1 Reaction of ketoaziridines in C-C- bond cleavage and C-N bond cleavage.

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2019

An efficient synthesis of spiro-pyrimidine derivatives from malononitrile, isatin and amidine

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Keywords: Malononitrile, Isatin, Amidine, Spiro-pyrimidines derivatives.

Pyrimidine derivatives occupy a unique place in medicinal chemistry because of their presence in several bioactive substances such as antibacterial, antiviral, and anti-HIV agents.[1] Moreover, pyrimidine based spirocyclic systems have been of considerable interest due to their pronounced biological properties such as fredericamycine, acorenone, β-vetivone, and isocomene, which are isolated from plants.[2] A useful and simple strategy for the synthesis of spiro-pyrimidines derivatives *via* a three-component reaction between isatin **1**, malononitrile **2**, and amidine **3**, in the ethanol in the presence of 3 drop of Et_3N as a basic catalyst under reflux conditions is described in this study (Fig. 1). All the synthesized compounds were unknown to the best of our knowledge and were characterized by ^1H, ^{13}C- NMR, and IR.

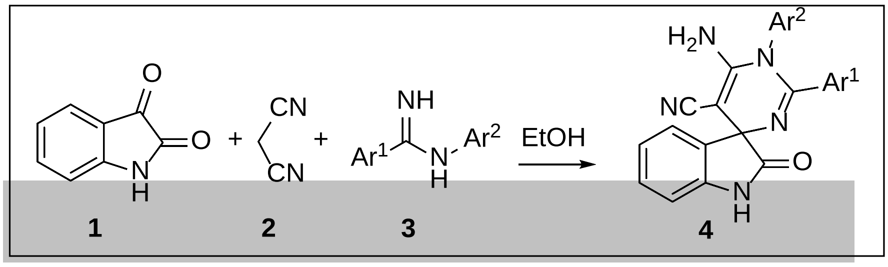

Fig. 1 Synthesis of spiro-pyrimidines derivatives

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Investigation of enterobacter aerogenes effects on heavy oil from biological degradation aspects by GCxGC technique

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Keywords: GCxGC, FT-IR, *Entrobacter aerogenes*, Heavy oil, Bioremediation.

Oil pollution affects the deterioration of the agrophysics soil characteristics, namely to the dysfunction of the water, air, thermal, oxidation-reduction and nutrient regimens. One of the methods to purify oil residue is bioremediation, in this way we investigate *Enterobacter aerogenes* effects on heavy oil by SARA, FT-IR, GC and GCxGC methods. The material required for the growth of *E. aerogenes* are carbon and phosphate. The *E. aerogenes* is injected with thioglycollate broth to crude oil which was distillated, and the samples were put for a month in an incubator. The results of this research illustrate that this bacterium has been able to survive in oil by isolating straight-run carbons with short and weak bounds from asphaltene and resin structures, as well as utilizing sulfur, nitrogen, and oxygen in the oil. In addition, it is found out this bacterium has had a positive effect on making light oil from heavy crude oil. Thereby, it is suitable for bioremediation in oil polluted sites and oil refinery for removing hydrocarbon pollutants from the environment.

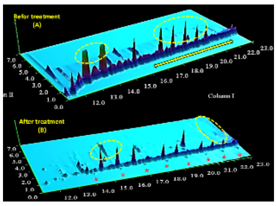

Fig. 1 Comparison of the spectra obtained from the GCxGC technique on saturate fracture. Spectrum A: before treatment, Spectrum B: after treatment.

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Synthesis of benzyl acetate by using supported polyoxometalate on magnetic nanoparticles as a heterageneous catalyst

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Keywords: Nanoparticle, Phosphotungstic acid, Polyoxometalate, Esterification, Acetic Acid, Benzyl Alcohol, Benzyl acetate.

Esterification of benzyl alcohol with acetic acid in the liquid phase using phosphotungstic acid stabilization on the substrate, benzyl acetate is used as a Jasmine essential oil. Carboxylic acid esterification is one of the basic reactions in organic chemistry, the speed of which can be increased by increasing the acidic catalyst to the reaction medium. In the reaction of esterification both homogeneous and heterogeneous catalysts can be used. Among the heterogeneous catalyst that can be used, phosphotungstic acid stabilized on magnetic nanoparticles used to esterification carboxylic acids with alcohols to prepare essential oils. The advantage of this is the very easy separation of catalyst from the reaction medium by the magnet. In fact, the application of magnetic nanoparticles in the catalysts as a catalyst base has been considered due to the good spread, the surface to volume ratio, the ease of surface modification, and the very easy and effective separation of the reaction medium. Polyoxometalate are used as a heteropoly acid catalyst on a solid bed that provides this opportunity to heteropoly acid to spread on a wider surface.

Solvotermal was used to synthesize magnetic iron oxide nanoparticles. Synthetic iron oxide nanoparticles are called MNP, which have a black color and magnetism. Then phosphotungstic acid، which is stabilized as polyoxometalate on iron oxide magnetic nanoparticles, is used for acidic catalysts. SEM and XRD were used to identify the catalysts, and IR and GC spectra were used for qualitative analysis of the product.

The performance of the catalyst in the stringer of benzyl alcohol with acetic acid was investigated. The effects of reaction parameters such as molar ratio of reactants, reaction temperature and optimal time to react, catalytic amount and catalyst reuse of the product were investigated.

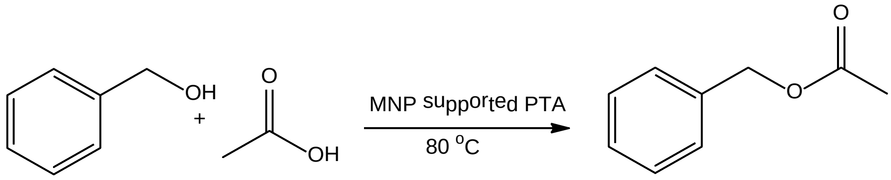

Fig. 1 benzyl alcohol acetic acid benzyl acetate

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Synthesis, characterization and catalytic evaluation of $NiFe_2O_4@SiO_2@$glucose amine for the synthesis of novel derivatives of thiazolidine-4-ones

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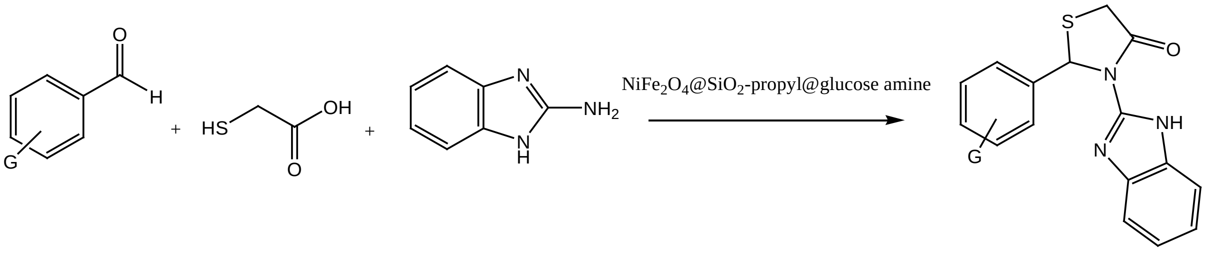
Keywords: Green Chemistry, $NiFe_2O_4@SiO_2@$glucose amine, thiazolidine-4-one

Thiazolidine -4-ones exhibit antitubercular, antimicrobial, antioxidant and antifungal activity and can be applied as COX-1 inhibitor, bacterial enzyme MurB inhibitor, non-nucleozide anzyme inhibitor of HIV-RT and antihistaminic agent.[1] For this reason, synthesis of novel derivatives of thiazoline-4-ones have attracted a lot of interest.

Traditional heterogeneous catalysts are limited in the nature of their active sites and their reaction scope abilities. Soluble organic catalysts can catalyse a variety of reaction more than traditional solid catalysts but suffer from their inability to be recycled. For this reason, synthesis of organic and inorganic hybrid composite to utilize the organic moiety as the active site and the solid to provide avenue to recovery and recyclability is attractive. [2]

In continuation of our previous work [3], herein, we specifically address the synthesis and usage of organic-inorganic hybrid materials based on $NiFe_2O_4@SiO_2$-propyl@glucose amine magnetic nanoparticle as catalyst for the synthesis of new generation of thiazolidine-4-ones. All of organic compounds are new and characterized by IR, ^1H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Multicomponent synthesis of thiazolidine-4-ones

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Design, synthesis and application of Ch-MoO as an efficient catalyst for the synthesis of Hantzsch 1,4-dihydropyridines

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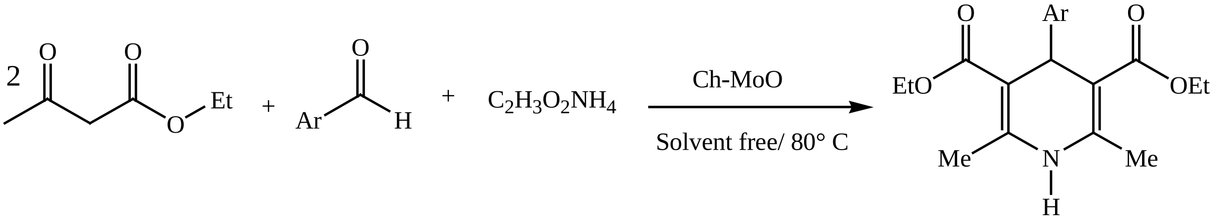
Keywords: Chitosan, 1,4-dihydropyridines, Hantzsch reaction.

In recent years, developing routs to produce materials based on green chemistry which minimizes pollution have been focused.[1] For this purpose these goals, the development of heterogeneous catalysts in the synthesis of organic compounds is highly investigated due to the ease of handling, reusability and simple work-up. Therefore, immobilization of metal on inorganic support to produce heterogeneous catalytic systems has been widely reported. Recently, chitosan (Cs) as a biological polymer has been found to be the most abundant natural amino polysaccharide that is usually obtained by deacetylation of chitin. It has attracted significant interest due to its green properties, safety, non-toxicity, biocompatibility, biodegradability, low immunogenicity, stability and ability of chelation.

In continuation of our efforts to synthesize of novel catalysts [2] for applying in the synthesis of heterocyclic ring, we wish to design and synthesis of molebdinium supported chitosan Ch-MoO as an efficient catalyst for the synthesis of 1,4-dihydropyridine through the condensation reaction of aldehydes, ethyl acetoacetate, ammonium acetate under solvent free condition at 80° C (Scheme 1).



Scheme 1: Synthesis of Hantzsch 1,4-dihydropyridines

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One-opt, four component synthesis of pyrano[2,3-*c*]pyrazoles catalyzed by [VO(TPPA)]SO_3H

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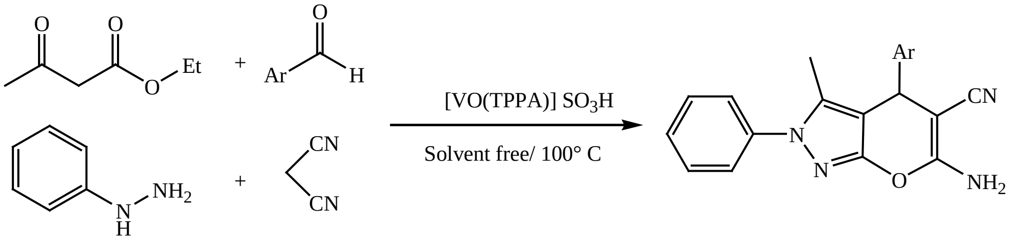
Keywords: Metallophthalocyanines (MPcs), Vanadium-oxo tetrapyridinoporphyrazine [VO(TPPA)]SO_3H, Dihydropyrano[2,3-c]pyrazole.

In the past decades, metallophthalocyanines (MPcs) employed as the efficient biomimetic catalysts with thermal and chemical stability and easy access.[1-2] In addition, poor solubility of metallophthalocyanines in common organic solvents can be considered as the most prominent point in their applications as the heterogeneous catalysts. In this regard, vanadium-oxo tetrapyridinoporphyrazine sulfonic acid was synthesized and fully characterized. Pyrazole derivatives are the significant kind of heterocyclic compounds that feature in several pharmaceutical targets and natural products of medicinal interest. Dihydropyrano[2,3-c]pyrazole derivatives have showed a wide variety of biological activities counting anticancer, antimicrobial, anti-inflammatory, insecticidal, and molluscicidal activities.

In continuation of our efforts to synthesize of novel catalysts in the synthesis of multicomponent reactions, we wish to report the synthesis of vanadium-oxo tetrapyridinoporphyrazine sulfonic acid [VO(TPPA)]SO_3H as an efficient catalyst for the synthesis of dihydropyrano[2,3-c]pyrazole through the condensation reaction of aryl aldehydes, ethyl acetoacetate, malononitrile, and phenyl hydrazine under solvent free conditions at 100° C (Scheme 1).



Scheme 1: Multicomponent synthesis of pyrano[2,3-c] pyrazoles

References

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A comparative ADME study of aminopterin derivatives and methotrexate as anti cancer drug

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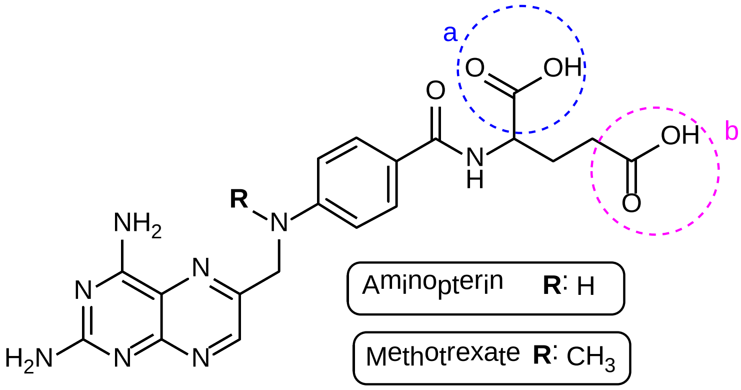
Keywords: aminopterin, methotrexate, ADME properties, in silico.

In designing new drugs, drug development includes the evaluation of efficacy and toxicity of the new drug candidates. Thus, precise data on the pharmacokinetics and metabolism must be available to determine the final success or failure of the compound. Screening absorption, distribution, metabolism and excretion (ADME) is necessary to decrease the cost and the ratio of failed compounds in clinical trials **1**. Methotrexate is an inhibitor of dihydrofolate reductase (DHFR), as a target for anticancer drugs **2, 3**. It acts by blocking the body's use of folic acid. As methotrexate can decrease the levels of folate, this leads folate deficiency **4** and additionally it concludes some other side effects such as liver damage which may lead to fibrosis or cirrhosis and severe skin rashes **5**. Thus, scientists try to find newer and safer replacements **6**. The present study incorporates ADME results of methotrexate and aminopterin derivatives as a less toxic replacement for methotrexate. All data were collected by swiss ADME prediction **7**. Herein the results of lipophilicity determination of aminopterin and some derivatives are investigated.



R	a	b	Log P
H	CO_2H	CO_2H	0.62
CH_3	CO_2H	CO_2H	1.53
H	CSOH	CO_2H	1.64
H	$CONH_2$	CO_2H	1.44
H	$CNNH_2$	CO_2H	1.08
H	$COCH_3$	CO_2H	1.56
H	CO_2H	$CO(CH_2)OH$	1.53
H	CO_2H	$(CH_2)_2CO_2H$	2.50

Fig.1 aminopterin and methotrexate structures and lipophilicities (Log P)

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DFT Study on DMNT biosynthesis as a defective plant-insect interaction

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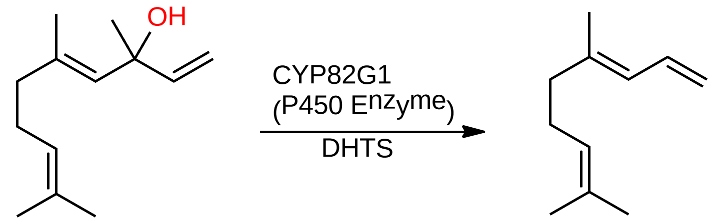
Keywords: DFT study, nerolidol, thermodynamic properties, B3LYP, STO-3G basis set.

The (*E*)-4,8-dimethyl-1,3,7-nonatriene (DMNT) biosynthesis has been proposed to occur via (*E*)-nerolidol as precursor **1-3**. Nerolidol is a sesquiterpene alcohol and a volatile organic compound constituent in the headspace of some flowers **4** and plants, which is converted to DMNT by cytochrome P450 enzyme catalysis **5**. Although DMNT is considered as one of the defensive volatile organic constituents involved in plant-insect interaction but the role of nerolidol as an active compound in plant defensive systems is ambiguous **6** and also the DMNT biosynthesis mechanism is not clearly known. Herein DMNT biosynthesis is thermodynamically investigated. The calculations were performed using Gaussian 09 with Gausview interface and the geometries were optimized at the DFT B3LYP level of theory with a STO-3G basis set. The thermochemical data such as entropy, gibs free energy, total energy data and also polarizability were calculated for both nerolidol and DMNT. Some of the results are tabled below.



ΔE_{tot} (kcal/mol)	**$1.42 * 10^5$**
ΔS (cal/mol-k)	**-20.92**
ΔG (kcal/mol)	**$6.75 * 10^5$**

(*E*)-Nerolidol

(3*E*)-4,8-Dimethyl-1,3,7-nonatriene (DMNT)

Fig. 1 (*E*)- Nerolidol conversion to DMNT via cytochrome P450 enzyme catalysis

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Synthesis, characterization and catalytic evaluation of Fe_3O_4@SiO_2-pr@*L*-proline for the synthesis of novel derivatives of dihydropyridines

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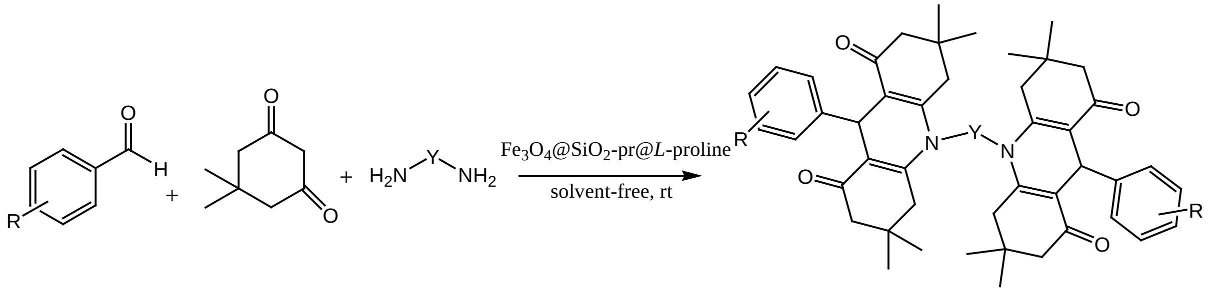
Keywords: Green Chemistry, Fe_3O_4@SiO_2-pr@*L*-proline, dihydropyridines

Compounds with dihydropyridines nucleus are a common and important substructures found in natural products and pharmacologically active compounds. They act as glucagon receptor antagonists, inhibitors of P38 MAP kinase, β-Raf kinase, transforming growth factor b1 (TGF-b1) type 1 activin receptor-like kinase (ALK5), cyclooxygenase-2 (COX-2), CB1 cannabinoid receptor antagonists, modulators of P-glycoprotein (P-gp)-mediated multidrug resistance (MDR), biosynthesis of interleukin-1 (IL-1). [1] For this reason, synthesis of novel derivatives of dihydropyridines have attracted a lot of interest.

Today, catalysts play a significant role in the production of chemicals and nanocatalysts have the potential for improving efficiency, selectivity and yield of the catalytic process. The higher surface to volume ratio means that much more catalyst actively participates in the reaction. Higher selectivity means less waste and fewer impurities, which could lead to safer and reduced environmental impact. [2]

In continuation of our previous work [3], herein, we specifically address the synthesis and usage of Fe_3O_4@SiO_2-pr@*L*-proline magnetic nanoparticle as catalyst for the synthesis of new generation of dihydropyridines. All of organic compounds are new and characterized by IR, ^1H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Multicomponent synthesis of bis dihydropyridines

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Unprecedented regiocontrol in synthesis of spirooxindolopyrrolizidines in both enantiomeric form *via* asymmetric [3+2] cycloaddition of azomethine ylides

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Keywords: 1,3-Dipolar cycloadditions, Azomethine ylides, Chiral spiroindolo pyrrolizidine, Asymmetric Synthesis.

Spirooxindoles and functionalized pyrrolizidines are an important class of naturally occurring substances characterized by highly pronounced biological properties and therapeutic applications. Thus, it might be expected that presence of a pyrrolizidine moiety at C-3 of the 2-indolinone system generates 3-spiroindolo pyrrolizidine that possess considerably enhanced biological activities. For example, horsfiline, elacomine and rhynchophylline, which exhibit significant biological activities.[1] We herein report a highly regio-, diastereo-, and enantioselective 1,3-dipolar cycloaddition reaction of (*R*)/(*S*)-camphorsultam cinnamate with azomethine ylides, which are generated from (*S*)-proline with isatins under optimized reaction conditions (**Fig. 1**). More importantly, for the first time an unusual regioselectivity was observed in this reaction, leading to the construction of novel 3-spiroindolopyrrolizidine derivatives in both enantiomeric form. The structures of cycloadducts were assigned from their elemental and spectroscopic analyses including IR, ^{1}H NMR, ^{13}C NMR, mass spectral data and by single-crystal X-ray analysis. The possible mechanism of the reaction was investigated using the DFT approach at the B3LYP/6-311G* level of theory.

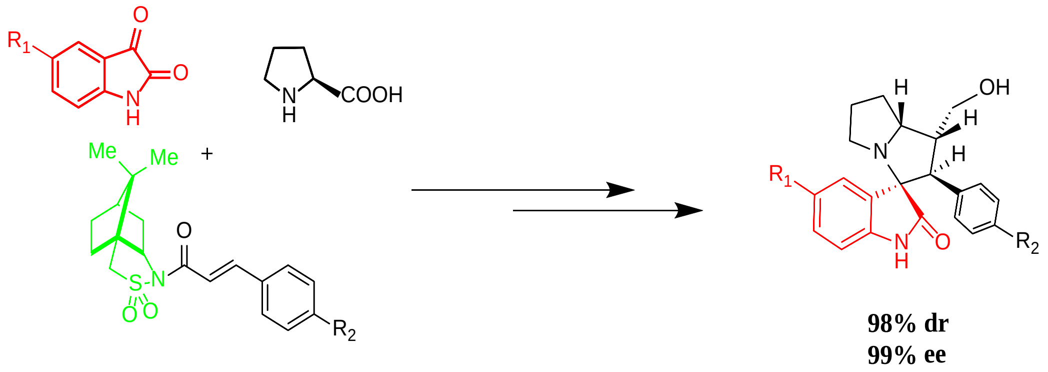

Fig. 1 Asymmetric synthesis of new chiral 3-spiroindolopyrrolizidine derivatives

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Synthesis of novel chiral dispiro pyrrolidines/pyrrolizidines *via* 1,3-dipolar cycloaddition and evaluation of their mechanism by DFT calculation

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Keywords: 1,3-Dipolar cycloaddition reaction, Azomethine ylide, Dispiropyrrolidines, Dispiro pyrrolizidines

Optically active spirooxindoles containing pyrrolidine and pyrrolizidines framework have been proven to have broad spectrum of considerable bioactivity and curative applications.[1] In this regard, spirooxindoles have received extensive attention in the last years and among all the developed synthetic methodologies, 1,3-dipolar cycloaddition has been found to be one of the most efficient and straightforward pathways, leading to rapid assembly of pyrrolidine and pyrrolizidine spirooxindole skeletons.[2] In continuation of previous our works[3], a variety of chiral dispiro pyrrolidines/pyrrolizidines have been synthesized in three and four contiguous and two quaternary stereogenic centers in generally high yields and excellent diastereo- and enantioselectivities (up to 99%). This new scaffold has been established *via* asymmetric 1,3-dipolar cycloadditions of acenaphthoquinone azomethine ylides with dipolarophiles which are generated from (*S*)-camphorsultam, as chiral auxiliary, with isatin-derived under optimized reaction conditions (**Fig. 1**). The structures of the products, after purification, were assigned and approved using NMR, mass, IR and single-crystal X-ray analysis. The reaction mechanism was discussed by quantum mechanical calculations.

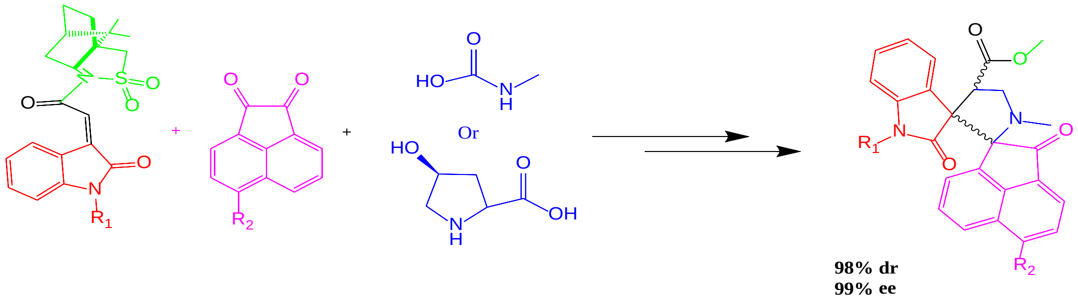

Fig. 1 Asymmetric synthesis of new chiral dispiropyrrolidine and pyrrolizidine derivatives

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Synthesis of new chiral spiroacenaphthyl-pyrrolidines/pyrrolizidines : Effect of two important chiral auxiliaries on their stereoselectivities

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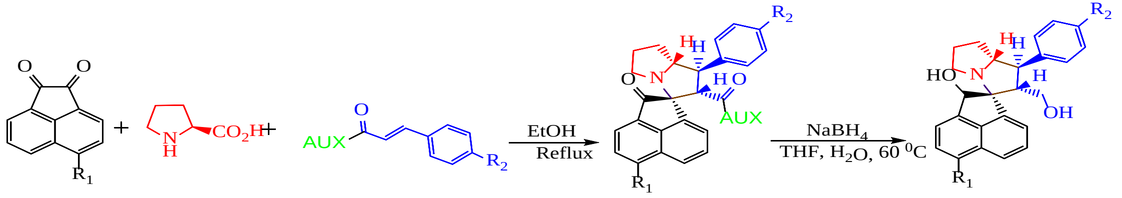
Keywords: Asymmetric 1,3-dipolar cycloaddition reaction, Azomethine ylide, Chiral auxiliary, Spiropyrrolizidines

Chiral spiro pyrrolidines/ pyrrolizidines have brought the surge of interest due to their highly pronounced biological significance and pharmaceutical applications. One of the powerful methods for the synthesis of a variety of natural products containing chiral spiro-pyrrolidine/ pyrrolidines structures is 1,3-DC reaction of azomethine ylides.[1] Stereocontrol in these reactions can be achieved through the use of chiral auxiliaries that are attached to the dipolarophiles. In continue of our laboratory purposes in the field of asymmetric 1,3-dipolar cycloaddition reaction (ADCR)[2], we report the easy preparation and characterization of new chiral derivatives of spiro pyrrolizidines based on acenaphthoquinone with a highly regio-, diastereo-, and enantioselectivity through of ADCR (**Fig. 1**). The absolute stereochemistry of cycloadducts, which was obtained by utilizing two types of chiral auxiliaries, was unambiguously established by X-ray crystallography and showed that all cycloadducts have same configuration. They were also clearly the result of endo-re addition of the dipoles to the dipolarophile. The possible mechanism of the reaction was investigated using the DFT approach at the B3LYP/6-311G* level of theory.



R_1 = H , Br
R_2 = Cl , F , Me , Br

Fig. 1 Asymmetric synthesis of new chiral spiro pyrrolizidine derivatives

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Synthesis, characterization and catalytic evaluation of $Fe_3O_4@SiO_2$-propyl@*L*-proline for the synthesis of novel derivatives of benzo[*d*]imidazoles

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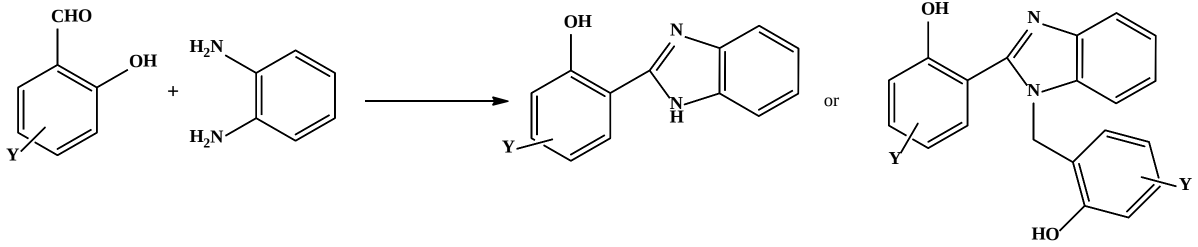
Keywords: Green Chemistry, $Fe_3O_4@SiO_2$-propyl@*L*-proline, benzo[*d*]imidazoles

Compounds with imidazole nucleus are a common and important substructures found in natural products and pharmacologically active compounds. They act as glucagon receptor antagonists, inhibitors of P38 MAP kinase, *β*-Raf kinase, transforming growth factor b1(TGF-b1) type 1 activin receptor-like kinase (ALK5), cyclooxygenase-2 (COX-2), CB1 cannabinoid receptor antagonists, modulators of P-glycoprotein (P-gp)-mediated multidrug resistance (MDR), biosynthesis of interleukin-1 (IL-1) [1]. There are a lot of reports for the synthesis of benzoimidazoles but they suffer from some serious defects, such as tedious workup and purification, significant amounts of toxic waste materials, highly acidic conditions, long reaction time, occurrence of side reactions, low yields, use of expensive reagents or catalysts, low selectivity and high temperatures in refluxing or microwave condition. Therefore, development of easy, green, effective, high yielding, and eco-friendly approaches using novel catalysts for the synthesis of imidazoles is an important.

In continuation of our previous work [2], herein, we specifically address the synthesis and usage of $Fe_3O_4@SiO_2$-propyl@*L*-proline magnetic nanoparticle as catalyst for the synthesis of new generation of benzo[*d*]imidazoles (Scheme 1). All of organic compounds are new and characterized by IR, ^1H NMR, ^{13}C NMR, Mass and elemental analysis.



Scheme 1. Green synthesis of benzo[*d*]imidazoles

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Synthesis of multicomponent hydrogel as a delivery system for anticancer drug doxorubicin

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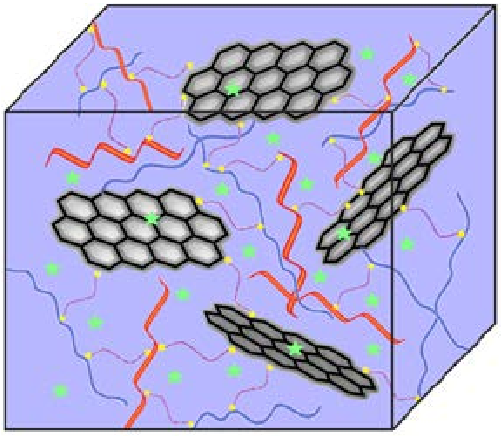
Keywords: Cellulose nanowhisker, Chitosan, Graphene, Hydrogel

Hydrogels are the three dimensional networks from hydrophilic polymers which can absorb a lot of water. Hydrogels are widely used in the various fields, including drug delivery [1] and dye absorption.[2] Cellulose and chitin are the abundant natural biopolymer from renewable sources and chitosan was obtained by alkaline deacetylation of chitin. These polysaccharides are non-toxic, biodegradable, and biocompatible and have different applications such as drug delivery systems.[3] Herein, we developed a multicomponent hydrogel by combination of chitosan, cellulose nanowhisker and graphene (Scheme **1**). A synthetic linker was applied as the crosslinking agent, which connect graphene sheets, chitosan chain, and nanowhisker together by forming a reversible linkage. The hydrogel was pH-responsive and was used for *in vitro* study of the anticancer drug doxorubicin delivery.



Scheme. 1 Multicomponent hydrogel by combination of chitosan, cellulose nanowhisker, and graphene.

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Synthesis of new curcumin derivatives and study of their medicinal properties

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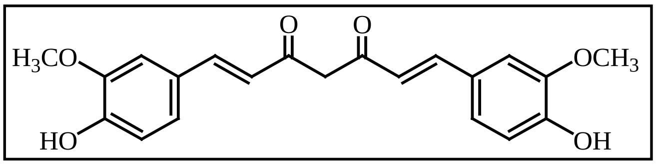
Keywords: Curcumin, Polyglycerol, Antibacterial, Antioxidant

Turmeric is a member of ginger family with the scientific name of *Longa Curcuma*. The most important components of turmeric are yellow pigments from the category of curcuminose. These compounds form about 3 to 5 percent of turmeric, and its main components are curcumin, demethoxycurcumin, and bisdemethoxycurcumin. Curcumin (Fig. **1**) has many biological properties, including antioxidant, antibacterial, anti-fungal, anti-inflammatory, and anti-tumor properties.[1-2] Curcumin also has the great therapeutic potential against all types of cancers.[3] Despite the extremely high therapeutic benefits of curcumin, the sustainability and bioavailability of this compound is very low. In recent years, many research groups have focused on improvement of biocompatibility and effectiveness of curcumin.[4] In this study, using hydrophilic polymer polyglycerol, new compounds of curcumin were synthesized, and then evaluated *in vitro* biological and medicinal properties and compared with primary curcumin.



Scheme. 1 The structure of curcumin.

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A novel and efficient synthesis of indoles by using a three-component reaction of arylamine, arylglyoxal, and 4-hydroxycoumarin

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Keywords: Indole derivatives, Arylamine, Arylglyoxal, 4-Hydroxycoumarin.

Indole cores are an important class of heterocyclic compounds found in natural products, drug molecules, and functional materials.[1] They have been attention in recently years due can be exhibit a wide spectrum of biological activity such as the anti-inflammatory,[2] anti-proliferative, and platelet aggregation inhibitory activities.[3] Herein, we describe efficient and novel method for the synthesis of indole derivatives **4** *via* appropriate arylamine **1**, arylglyoxal **2**, and 4-hydroxycoumarin **3** in ethanol solvent at reflux conditions for 12 h. (Fig. 1). Metal-free catalyst, eco-friendly solvents, and excellent yields (80-93 %) are advantages of the protocol. All the synthesized compounds were unknown to the best of our knowledge and were characterized by ^1H and ^{13}C- NMR, IR and melting points.

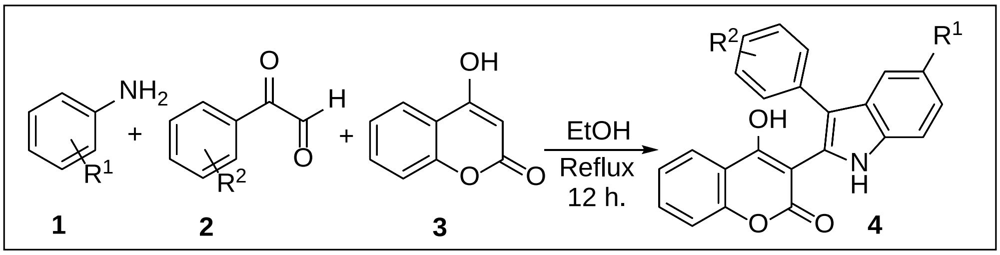

Fig. 1 Synthesis of indole derivatives

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Cu-Catalyzed regioselective synthesis of functionalized 4-benzoyl-5-cyanopyrazoles under mild conditions

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Keywords: 4-Benzoyl-5-cyanopyrazoles, Copper catalysis, [3+2] Cycloaddition, Phenacylmalononitrile, Hydrazonoyl chloride

The unsaturated cyanocarbonyl compounds provide an attractive entry into electron-deficient dienophiles employed in Diels–Alder cycloadditions.[1] To prepare these valuable substrates, several synthetic methodologies have been reported, including Wittig-type olefination of glyoxal derivatives, palladium catalyzed four-step procedure from alkenals, dehydrohalogenation of suitable substituted precursors, or five-step chemical modification of *trans*-styrylacetic acid.[2] These approaches are frequently long and cumbersome. To the best of our knowledge, there is no report regarding either *in situ* generation of benzoylacrylonitriles, or employing them as dipolarophile in the 1,3-dipolar cycloaddition reactions. We have described an unprecedented copper catalyzed regioselective synthesis of 4-arylcarboxo-1-phenyl-3-aryl-1*H*-pyrazole-5-carbonitriles *via* the [3 + 2] cycloaddition reaction between phenacylmalononitriles and hydrazonoyl chlorides (Figure 1). ^{13}C NMR spectra provide a useful clue to distinguish the product from its regioisomer. Thus, the ipso carbon to the cyano group in regioisomer is expected to appear below 100 ppm in ^{13}C NMR spectra while the ipso carbon to the CN group in the product is expected to appear at about 140 ppm. In line with the studies conducted in our research group centralized on the synthesis of different substituted pyrazoles,[3] we decided to carry out the multisubstituted pyrazole synthesis with the concomitant *in situ* generation of the dipole and the dipolarophile.

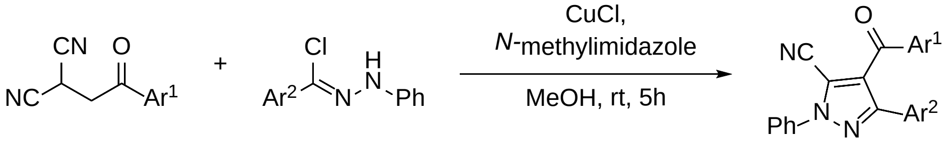

Fig. 1 Synthesis of 4-benzoyl-5-cyano-pyrazoles

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Synthesis of pyridine-3-carbonitriles using a novel and recoverable nanomagnetic catalyst via a cooperative vinylogous anomeric based oxidation

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Keywords: Pyridine-3-carbonitrile, Recoverable nanomagnetic catalyst, Anomeric based oxidation , Multi component reactions, Vinylogous anomeric effect.

N-heteroaromatic structures particularly pyridine ring systems are ubiquitous in pharmaceutically active molecules and natural products. Among them, pyridine-3-carbonitrile derivatives represent fascinating biological characteristics. These compounds can apply as A_{2A} adenosine receptor antagonists, IKK-β inhibitors, inhibitors of HIV-1 integrase, antimicrobial, anti-tumour, analgesic, anti-inlammatory, and antipyretic agents.[1-3] Herein, we have developed a green, efficient and powerful protocol for the synthesis of pyridine-3-carbonitrile derivatives *via* a four-component reaction. The reaction was performed in the presence of a catalytic amount of nanomagnetic catalyst under reflux conditions (Fig.1). It is worthy to mention that the final step of the mechanistic pathway for the synthesis of target molecules has proceeded *via* a cooperative vinylogous anomeric based oxidation mechanism.

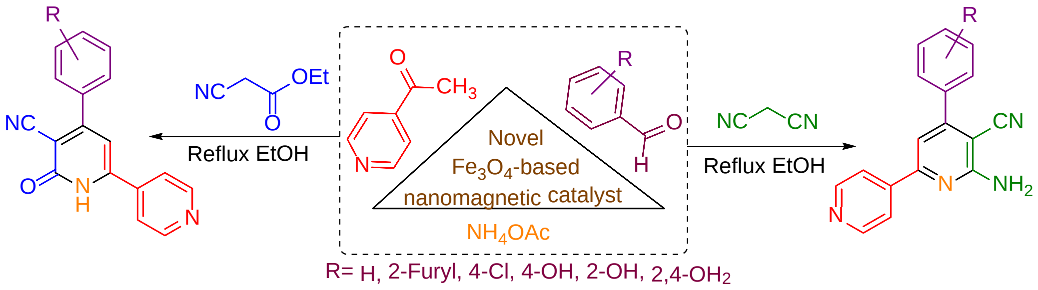

Fig.1. Preparation of pyridine-3-carbonitrile derivatives**.**

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Synthesis of the novel nanomagnetic catalyst and its application in the synthesis of benzo-[*h*]quinoline-4-carboxylic acids via a cooperative vinylogous anomeric based oxidation

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Keywords: Benzo-[*h*]quinoline-4-carboxylic acid, Anomeric based oxidation (ABO), Cooperative vinylogous anomeric effect, Multi component reactions, Reusable nanomagnetic catalyst.

In the last half-century, quinoline derivatives have been extensively investigated due to their biological and pharmaceutical activities. It has been reported that quinoline derivatives widely served as antagonists, analgesic agents, $5HT_3$, NK-3 receptors, and structural subunits of natural products. Quinoline-4-carboxylic acids are one of the most important series of quinoline derivatives because they have a variety of medicinal effects and are applied as active components in industrial antioxidants. [1-3] Herein, we designed a novel and reusable nanomagnetic catalyst, which was synthesized and its catalytic application was examined at the synthesis of benzo-[*h*]quinoline-4-carboxylic acid derivatives via a three-component reaction (Figuer 1). Resulting experimental data suggest that the final step of the plausible mechanism proceed *via* a cooperative vinylogous anomeric based oxidation mechanism. The presented catalyst shows excellent potential of recycling and reusing at the described multicomponent reaction.

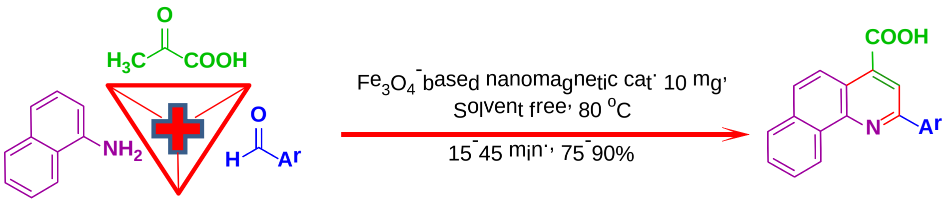

Fig. 1 Preparation of benzo-[*h*] quinoline-4-carboxylic acid derivatives.

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Removal of cationic methylene blue dye using magnetically anion–cationic surfactants modified montmorillonite

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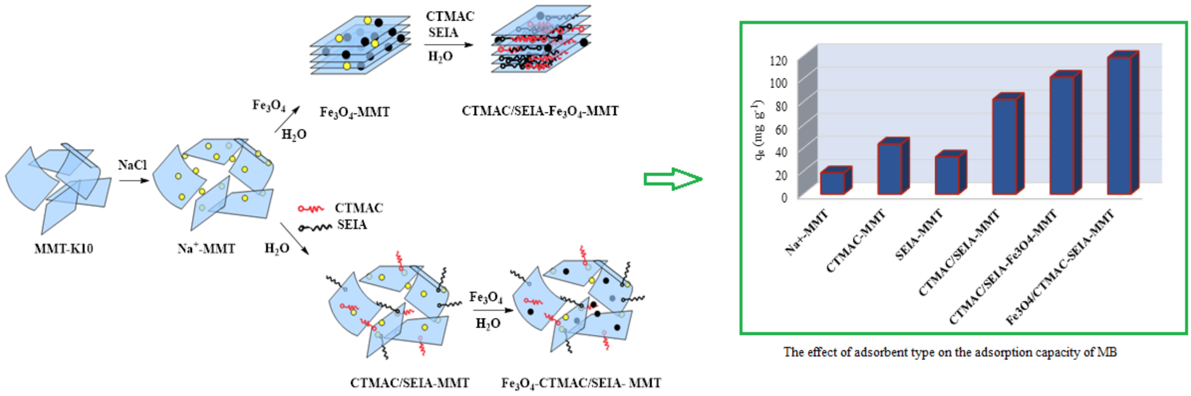
Keywords: Methylene blue, Montmorillonite, Nanocomposite, Removal, Surfactant

Organic dyestuffs in wastewater from many industries including textile, paper, leather, and plastics have been discharged to the environment causing serious soil and water pollution due to biological degradation, high chemical oxygen demand (COD) of the water body and inflected toxicity on humans [1]. Among various dyes, methylene blue (MB) as a toxic cationic dye is difficult to degrade due to its stability to light and oxidation reactions and is often employed as a model dye of organic pollutant [2]. Therefore, the removal of organic dyestuff from wastewater becomes environmentally important. Among the various methods of dye removal, adsorption technique is regarded as one of the ecofriendly and effective method because of simplicity design/operation, high efficiency and harmless to treated water [3]. In this study, we synthesized a novel magnetic organic-inorganic hybrid nanoadsorbent by incorporating anionic surfactant of sodium eicosenoate (SEIA), cationic surfactant of cetyl trimethylammonium bromide (CTMAB) and magnetic Fe_3O_4 nanoparticles into the interlayer of Mt. Subsequently, the modified Mt was used for the removal of MB from aqueous solutions and operational conditions for MB adsorption were studied.



The effect of adsorbent type on the adsorption capacity of MB

Fig. 1 Formation mechanism of CTMAC/SEIA-Fe_3O_4–Mt and Fe_3O_4–CTMAC/SEIA-Mt

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Antimony-Modified Nickel Ferrite: An Efficient Magnetically Nanocatalyst for Knoevenagel Condensation of Aryl Aldehydes with Malononitrile

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Keywords: Antimony, Benzylidenemalononitrile, Malononitrile, $NiFe_2O_4$

Benzylidene malononitriles (BMN) are one of the valuable organic intermediates which are utilized for synthesis of biologically active materials such as enzyme inhibitors, carbohydrates and heterocycles [1-3]. In addition, certain derivatives of benzylidene malononitriles have also been exhibited various optical, electrical and biological activities. BMN are generally prepared through the condensation reaction of aryl aldehydes with malononitrile in the presence of a catalyst. This subject prompted us to prepare $NiFe_2O_4/SbF_x$ as an efficient reusable nanocatalyst towards synthesis of benzilidenmalononitrils in refluxing ethanol (Fig. 1). This method has the advantages in terms of mild reaction conditions, short reaction times high yields of the products and reusability of the prepared catalyst system.

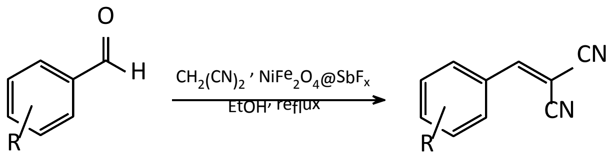

Fig. 1 Synthesis of Benzylidenemalononitrile with $NiFe_2O_4/SbF_x$

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Synthesis of new type of dendritic mesoprocesses silica and its applications towards elimination of some metal ions

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Keywords: Super-adsorbent, Removal of metal ions, Cysteine, Dendritic fibrous nanosilica.

L-Cysteine-modified dendritic fibrous nanosilica grafted by amine groups (Cys-DFNS-NH_2) have been synthesized by a novel hydrothermal method.[1] The N_2 adsorption-desorption isotherms analysis on the Cys-DFNS-NH_2 show that the average pore volume and surface area of the prepared fibrous Cys-DFNS-NH_2 were 2.2 cm^3 g^{-1} and 205 m^2/g, respectively. Also, average pore size is 6.06 nm.[2] Adsorption behavior of the Cys-DFNS-NH_2 for Cd^{2+}, Cu^{2+}, Ag^+, and Pb^{2+} was investigated by electrochemical methods. The results show that Cys-DFNS-NH_2 can selectively adsorb Cd^{2+}, Ag^+, and Pb^{2+} in different potentials. Finally, application of engineered adsorbent for the removal of Cd^{2+}, Ag^+, and Pb^{2+} from contaminated water samples was examined. This work provides a new platform to synthesis of Cys-DFNS-NH_2 with high specific surface area for efficient adsorbent of specific metal ions.

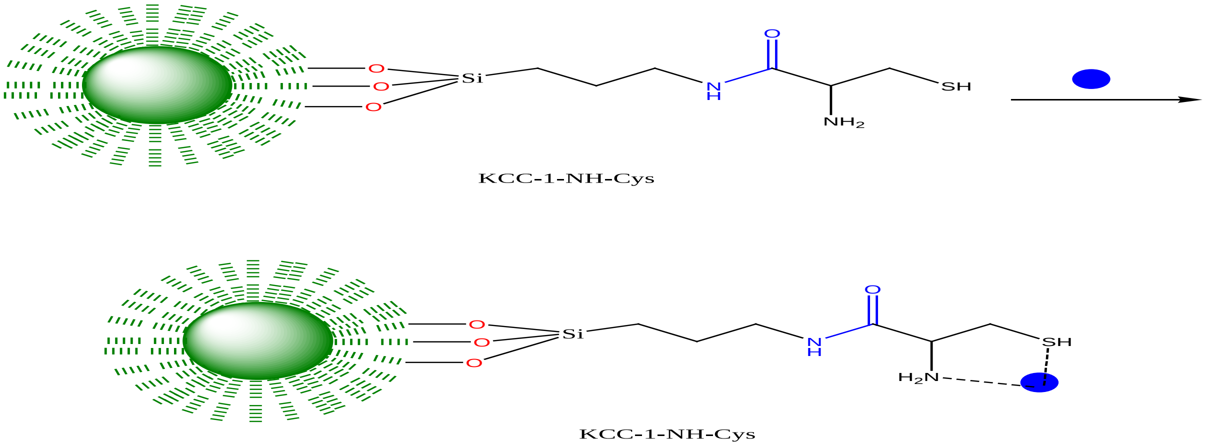

Fig. 1 Schematic representation of cations removal from aqueous solution using KCC-1-NH_2-Cys

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β- Cyclodextrin Functionalized KCC-1: A Novel Adsorbent for Separation of Organic Compounds

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Keywords: KCC- 1, β- Cyclodextrins, Organic compounds**.**

Dendritic nano silica fibers are of remarkable interest, which have been recently discovered by Polshettiwar et al [1]. These kind of nano materials possess high textural property and well defined morphology and are generally called as KCC-1. The aforementioned properties are a good stimulant to utilize this mesoporous material as a support for catalysis, adsorption of gas and solar energy, and bio medical applications [2]. These Nanomaterials have a convergent needle like morphology, which is demonstrated in Fig, 1 and has been compared morphologically with MCM-41 [3]. The present study is aimed to prepare β-Cyclodextrin functionalized KCC-1 and its utilization in removal of hazardous dyes such as malachite green. In order to study the morphology of the synthesized nano adsorbent, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) were achieved from the surface of the sample. Additionally, the functionalization of KCC-1 with β-Cyclodextrin was confirmed with Furrier Transform Infrared spectroscopy (FTIR). It should be noted that the adsorption capacity of the employed nano adsorbent was more than 95%, which could be attributed to high porosity of β-Cyclodextrin functionalized KCC-1. The textural property of KCC-1 was verified using nitrogen adsorption/ desorption analysis (BET equation). Specific surface area of the adsorbent was calculated to be 140 m^2/g. Consequently, it can be stated that the synthesized nano adsorbent has high removal efficiency.

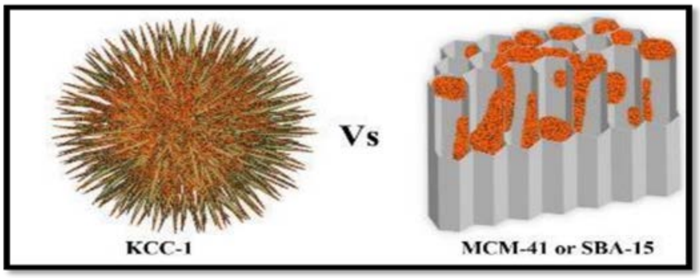

Fig. 1 The morphology of KCC-1 and its comparison with MCM-41 [3].

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Synthesis of graphene oxide based on alkyl vinyl imidazolinium chloride for removal of nitrate from water

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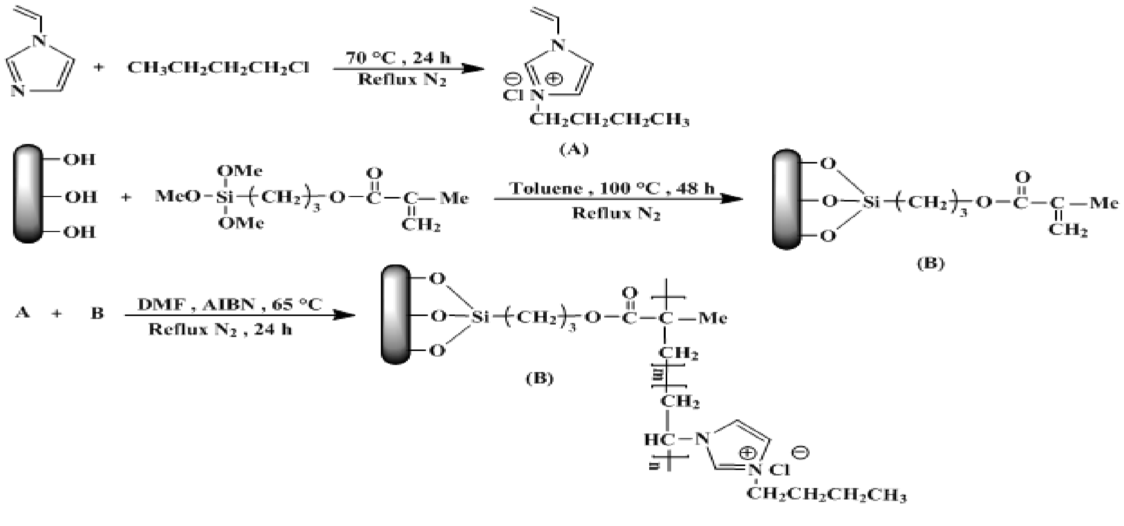
Keywords: Removal of nitrate, Nanocomposite, Graphene oxide, Ion exchange.

In last decades, the pollution of ground and surface water with nitrate has been observed in many countries.[1] Drinking water, high in nitrate condensation, can cause health problems and increase the rates of cancer.[2] Nitrate removal from environmental sources such as surface water and ground water is so necessary for prohibiting such issues.[3] In this work, we used of ion-exchange technology for removal of nitrate. At the first, a novel nanocomposite adsorbent was synthesized based on modified graphene oxide (Scheme1). The obtained adsorbent was investigated by FESEM, TGA and FT-IR spectra. The effects of solution pH, contact time, initial concentration of nitrate, adsorbent dosage, temperature and competing anions on nitrate adsorption was investigated. The maximum nitrate removal efficiency was achieved 92%. Antimicrobial and antifungal activity of adsorbent was carried out by disc diffusion method in vitro. Also, isotherm models, kinetic adsorption mechanism and thermodynamic parameters were investigated.



Scheme 1. Schematic synthesis of nanocomposite adsorbent.

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Synthesis of a novel magnetic nanoparticles with morpholine tags: Its catalytic application in the synthesis of 4,6-diarylpyrimidin-2(1*H*)-ones

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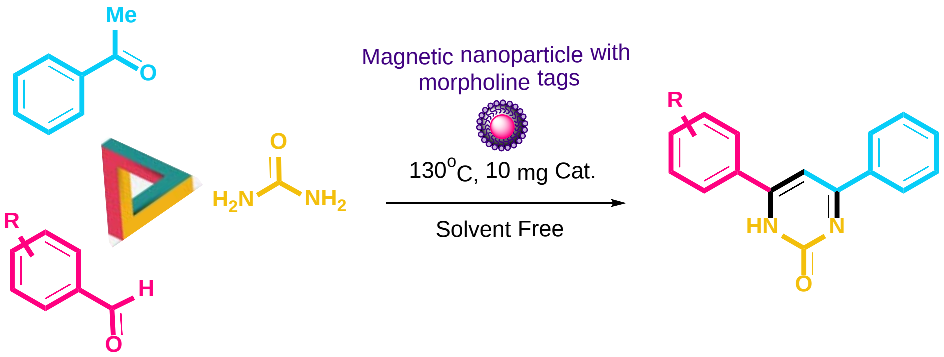
Keywords: Multicomponent reactions, Diarylpyrimidine, Magnetic nanoparticle, Morpholine.

Diarylpyrymidin-2(1*H*)-one (DAPM) belongs to one of the important class of heterocyclic compounds. DAPMs had been shown that a wide range of biological, medicinal, and therapeutic activities, such as: non-peptide antagonists, antiproliferative, cytodifferentiating activities and antihistaminic agents. On the other hands, semiheterogeneous catalysts such as magnetic nanocatalysts, present large surface-to-volume ratio which is a great solution to boost activity of a typical catalyst [1-3].

In this regard, we investigated the design, synthesis, characterization and catalytic performance of a novel magnetic nanoparticle with morpholine tags at the synthesis of biological active DAPM derivatives (Scheme 1).



Scheme 1: Synthesis of DAPM derivatives in the presence of magnetic nanoparticles catalyst

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A novel magnetic nanoparticle with morpholine tags as a multi-rule catalyst for synthesis of bis-dihydroquinazolinones

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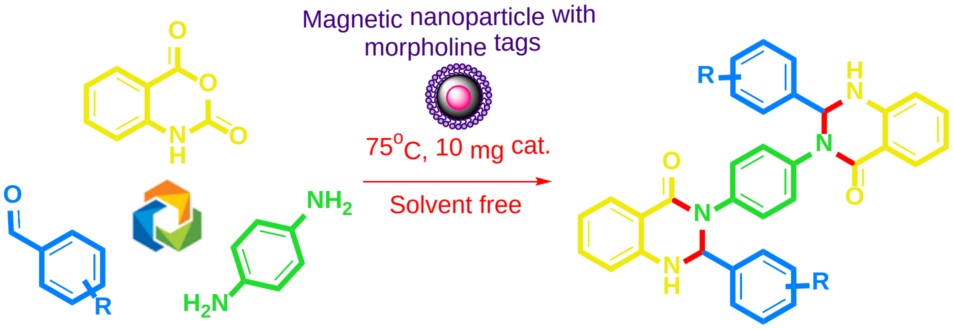
Keywords: Multicomponent reactions, Bis-dihydroquinazolinone, Magnetic nanoparticle, Morpholine.

In recent times, synthesis of dihydroquinazolin derivatives has attracted considerable attention from organic and medicinal chemists. Dihydroquinazolin derivatives showed a wide range of pharmacological and therapeutic properties such as antimalarial, antitumor, anticonvulsant, anti-inflammatory, and antimicrobial activities. Professional chemists are seeking catalytic systems which embrace "catalyst activity" and "catalyst separation together. Nowadays, by using magnetic nanoparticles, chemists can design and apply easy separable catalysts with high activity [1-3]

In this presentation, we will report the one-pot synthesis of bis-dihydroquinazolinone in the presence of a catalytic amount of magnetic nanoparticles with morpholine tags as a multi-rule catalyst (Scheme 1).



Scheme 1: Synthesis of dihydroquinazolin derivatives in the presence of magnetic nanoparticles with morpholine tags

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Synthesis of uric acid with phosphorus acid tags as a novel biological-based organocatalyst: Its application for synthesis of *N*-heterocycle

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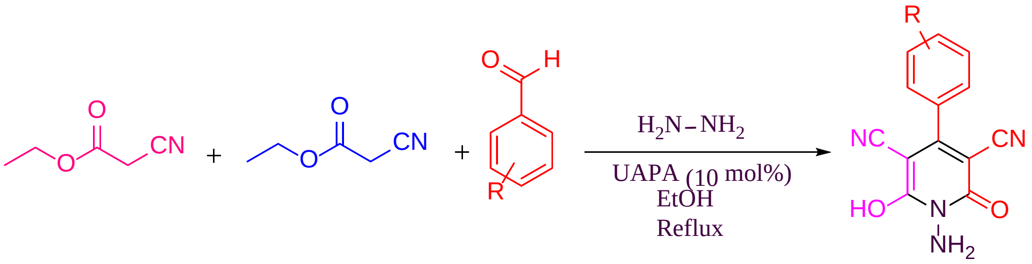
Keywords: *N*-heterocycle, (MCRs), phosphorus acid, uric acid with phosphorus acid tags.

Task-specific development of chemical methodologies for synthesis of target molecules may be achieved via rational design, applying a suitable procedure and reactants [1]. Heterocyclic moieties had been used as important building blocks within a wide range of medicinal and biological active molecules [2]. Among of oxygen and nitrogen hetreocycles, the *N*-amino-2-pyridones and pyrano [2,3-c]pyrazoles, had been shown, anticancer, anticoagulant, anticonvulsant, antimicrobial, anti-HIV, antimalarial, anti-tumor, antibacterial, antifungal and antitumor properties [3]. Biological-based uric acid with phosphorus acid tags (UAPA) as an efficient catalyst was successfully used for the synthesis of *N*-heterocycle *via* a multi-component reactions (MCRs) of various aromatic aldehyde, ethyl cyanoacetate and hydrazine under solvent free condensation (**Scheme 1**).



Scheme 1: Synthesis of 1-amino-6-hydroxy-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile catalyzed by UAPA

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Synthesis of novel magnetic metal-organic frameworks with phosphorous acid tags for the synthesis of pyrido[2,3-*d*]pyrimidine via vinylogous anomeric based oxidation

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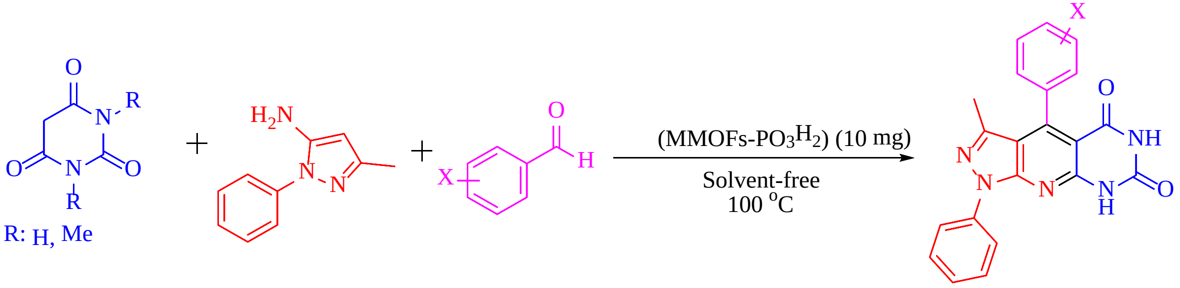
Keywords: Magnetic metal-organic frameworks, Organic compounds, Pyrido[2,3-*d*]pyrimidine.

Nowadays, porous and magnetic materials have been widely used in biotechnology, magnetic resonance imaging (MRI), catalysis, adsorption, gas separation and purification, optics, drug delivery and etc.[1-2] Metal-organic frameworks (MOFs) are widespread strategy for the expansion of new porous materials to reach with higher surface area. By selecting rational strategy, materials (metal centers and ligands) and suitable reaction condition can be precisely tuned and the spatial cavity arrangement precisely controlled. By joining of magnetic materials (Fe_3O_4) and metal-organic frameworks (MOFs) become powerful tools in the synthesis of new task-specific catalysts.[3] According to the above mentioned idea, we have synthesized MMOFs-PO_3H_2 as a nanoporous and magnetic catalyst. A good range of pyrido[2,3-*d*]pyrimidines were prepared by reaction of uracils, 3-methyl-1*H*-pyrazol-5-amine and aldehydes in the presence of described catalyst *via* a cooperative vinylogous anomeric based oxidation mechanism under solvent-free conditions (**Scheme 1**).



Scheme 1: Synthesis of pyrido[2,3-*d*]pyrimidine in the presence of MMOFs-PO_3H_2.

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Application of $Fe_3O_4@SiO_2@(CH_2)_3$-urea-benzimidazole sulfonic acid as a separable catalyst the synthesis of pyridines *via* a cooperative vinylogous anomeric based oxidation for

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Keywords: 2-Amino-3-cyano pyridine, Cooperative vinylogous anomeric based oxidation

Pyridine derivatives are one of the most important heterocycles which found in natural products, pharmaceuticals, and functional materials [1]. Among the pyridine systems, 2-amino-3-cyano pyridines are versatile structure which can be applied as intermediates towards the synthesis of varied heterocyclic molecules such as vitamins. They were also reported as novel IKK-b inhibitors, A_{2A} adenosine receptor antagonists, inhibitor of HIV-1 integrase [2]. On the other hand, urea and its derivatives are interesting biological structures which has ubiquitous role in the agriculture industry and pharmaceutical ingredients. In recent years, a series of separable nanomagnetic catalysts based on urea derivatives have been developed [3]. In this work, we applied $Fe_3O_4@SiO_2@(CH_2)_3$-urea-benzimidazole sulfonic acid for the synthesis of new 2-amino-3-cyano pyridines *via* a cooperative vinylogous anomeric based oxidation (Figure 1).

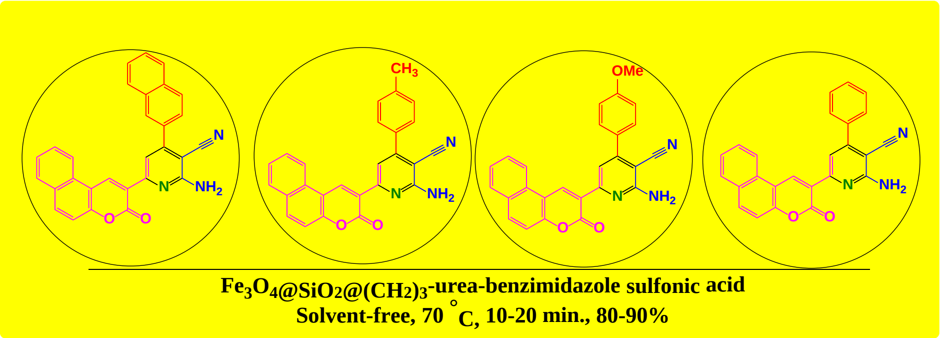

Figure. 1 Synthesis of pyridines using $Fe_3O_4@SiO_2@(CH_2)_3$-urea-benzimidazole sulfonic acid as catalyst

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Synthesis and catalytic application of imidazolium-based ionic liquid for the preparation of indole linked pyridines *via* a cooperative vinylogous anomeric based oxidation

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Keywords: Imidazolium-based ionic liquid, Indole linked pyridines,

Heterocyclic compounds are widely distributed in nature and have much biological and medicinal importance. Most of the drugs available in the market are heterocyclic structures. Among the heterocyclic structures, molecules containing pyridine motif are very important. The pyridine ring systems have emerged as integral backbones of over 7000 existing drugs [1]. Cyanopyridines are one of the most important derivatives of pyridine, which they have represent a wide variety of biological applications [2]. Ionic liquids (ILs) are persuasive areas of chemistry in the past decade. They have many advantages including negligible vapor pressure, designable properties, simplified separation of products and potential reuse [3]. In this study, we synthesized and applied an imidazolium-based IL for the preparation of new indole linked pyridine systems *via* a cooperative vinylogous anomeric based oxidation (Figure 1).

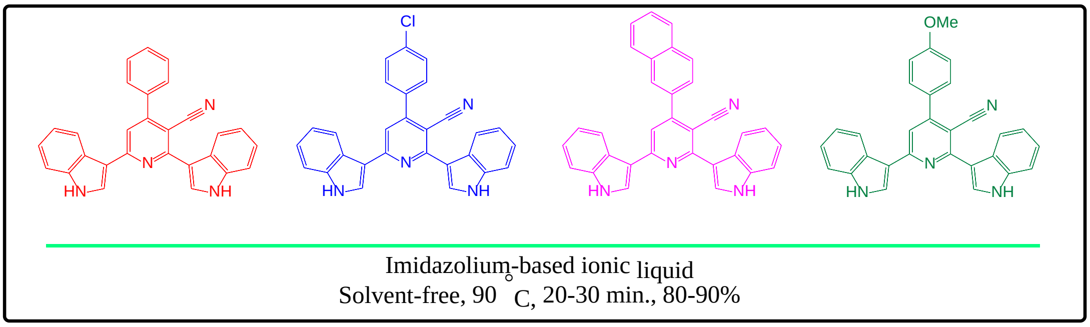

Figure 1: Synthesis of new indole linked pyridines using imidazolium-based ionic liquid as catalyst

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Investigation of arsenic removal from water using activated carbon produced from agricultural wastes

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Keywords: Adsorption, Arsenic, Walnut shell, Chemical Activation

In this study, activated carbon derived from agricultural waste was used as tertiary treatment. Activated carbon powder was used in laboratory-scale experiments and was performed for arsenic removal from synthetics samples.[1] physically activated carbon was obtained and then chemically activated by acidification. Characterization tests (i.e. XRD, FT-IR, BET and SEM tests) were carried out on both types of adsorbent.[2] Arsenic removal was carried out in batch experiments. Effect of laboratory parameters (i.e. contact time, pH, adsorbent dose and initial concentration) on removal process was studied.

Chemical activation, improved performance and characteristics of adsorbent.[3] The improvements was observed in chemical structure (reducing the number of phases and improve the chemical bonds of the material), increasing specific surface (from 1067.4 to 1437 m2/g), uniformity of pore size distribution, reduction of average pore size diameter (from 2.08 to 3.28 nm) and modified adsorbent pore network structure as shown in Table **1**. The results showed that in optimum conditions, removal efficiency was 100% and maximum capacity of adsorbent was 120 µg/g. Optimum conditions was pH=5 and equilibrium contact time of 10 minutes. Kinetic and equilibrium studies showed that adsorption process, followed of Langmuir isotherm and second-degree kinetic models.

Table 1. Special surface and mean diameter of absorbent holes in acidifies activated coal and without it.

Level of the highest diameter the cavities	Maximum diameter (nm)	Means of hole diameter (nm)	Total cavity volume (P/P0=0.990)(cm^3/g)	Special surface (m^2/g)	variable
256.37	>1.21	2.08	0.747	1434.6	Acid washing coal
12.97	>1.22	3.23	0.864	1067.4	Raw coal

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Pyridine ionic liquid coordinated Pd complex immobilized on SBA-15: A recoverable and efficient catalyst for the Mizoroki-Heck coupling reaction

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Keywords: Heck coupling, SBA-15, Palladium(II), Nanocatalyst, Ionid liquid

In recent years, intensive studies have focused on the preparation and supporting of palladium complexes with various types of ligands for coupling reactions. Such efforts have resulted in improving the efficiency of organic syntheses and decreasing processes time, reactions costs and generation of byproducts [1]. Heck reaction has a great potential for industrial applications, however, due to the properties and activities of the existing catalysts, limited industrial applications have been observed [2]. In this work a SBS-15 supported ionic liquid based on pyridine eas prepared and complexed with Pd(II), Scheme 1 [3].

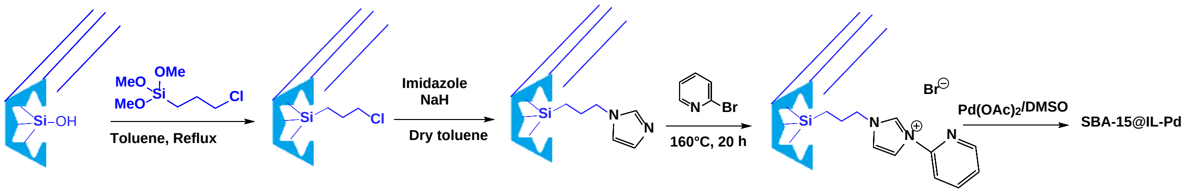

Fig. 1 Preparation of SBA-15 supported ionic liquid and Pd complex.

The reaction mixture cooled to room temperature and the gray solid catalyst was filtered in vacuum, washed with dicholorometan and dried. The Pd content of the catalyst was 7.9 wt.% as obtained by ICP-AES. The nanocatalyst was tested in Heck coupling reaction of iodobenzen and methylacrylate. The reaction conversion was increased up to 100%, as measured by GC analysis, by optimizing of the model reaction conditions.

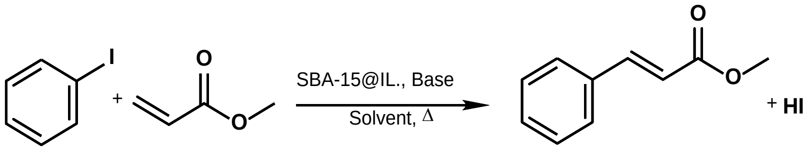

Fig. 1 The model Heck reaction

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Pd(0) nanoparticles supported on melamine functionalized SBA-15: An efficient catalyst for reduction of nitrobenzens

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Keywords: Nitro compounds, Pd(0) nanoparticles, Anilines, Reduction.

Aromatic amines are important intermediates in synthesis of several nitrogen containing biologically active compounds, agrochemicals, dyes, polymers, etc. Reduction of nitroarenes is a most common, short and facile route employed to prepare anilines and is one of the areas where major part of recent published work is targeted [1]. The catalytic process for hydrogenation of nitrobenzene is an industrially principal reaction for the synthesis of aniline. About 85% of all over aniline in the world is produced by catalytic routes [2].

In this work, we have used the nanocatalyst SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0) (Fig. 1) as a heterogeneous catalyst for reduction of nitroarenes to arylamines in ethanol, (Scheme 1).

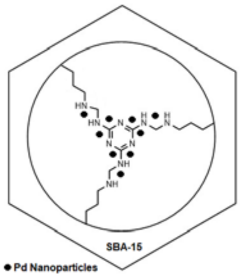
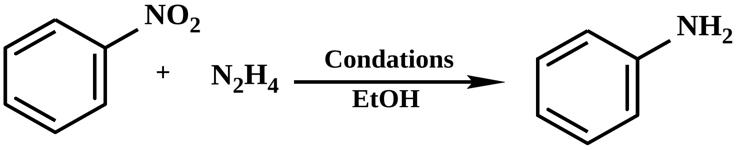


Fig. 1. SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0)

Remarkable reusability and easy separation of the nanocatalyst, high yields and mild reaction conditions as well as the benefits of using ethanol as a green solvent are the advantages which make this protocol a perfect candidate for the reduction of nitroarens.



Scheme. 1 The reduction of nitroarene with $N_2H_2.H_2O$ /SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0) system.

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Cu(II) salen@KCC-1 as a convenient heterogeneous catalyst for the one-pot multicomponent synthesis of 2-amino-4*H*-chromenes derivatives

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Keywords: Multicomponent reactions, Cu(II) salen@KCC-1 nanocatalyst, Heterogeneous catalysis, 2-amino-4*H*-benzochromenes.

One-pot, multicomponent reactions have emerged as an effective tool for being atom economic and synthetic by virtue of their convergence, productivity, facile execution and generation of highly diverse and complex products from easily available starting materials in a single operation.[1] These reactions are now being tailored for synthesizing various heterocyclic scaffolds for diverse applications. 2-Amino-4*H*-chromene derivatives have received significant attention in organic chemistry due to their biological and pharmaceutical properties such as antimicrobial,[2] sex pheromone[3] antitumor and cancer therapy.[4] The most straightforward synthesis of this heterocyclic system involves a three-component coupling of aromatic aldehyde, malononitrile and α/β naphthols. Herein, we report the synthesis of 2-amino-4*H*-benzochromenes derivatives with Cu(II) salen complex immobilized on KCC-1 nanosheets (Cu(II) salen@KCC-1) as a heterogeneous catalysis at 80° C within a very short reaction time having good to high yield (96%) when the loading of Cu was 0.48 mmol gr^{-1} based on Cu element analysis by ICP-AES (Fig.1).

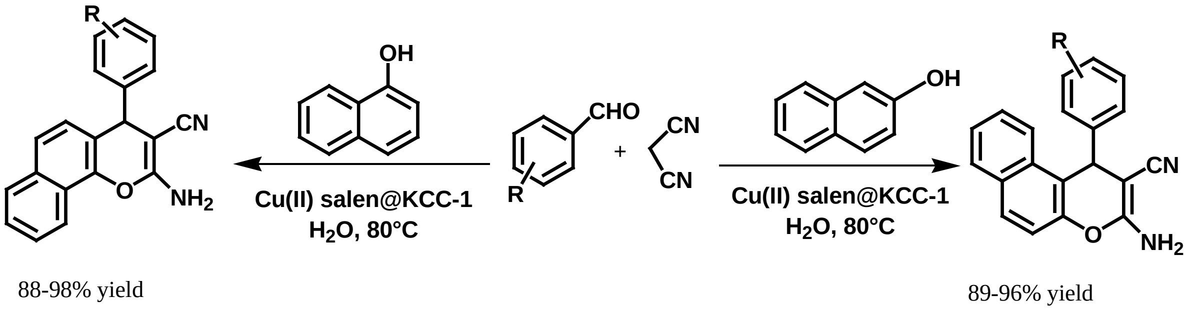

Fig. 1 Synthesis of 2-amino-4*H*-benzochromenes in the presence of Cu(II) salen@KCC-1

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Efficient and versatile acetylation of diverse alcohols and phenols with acetic anhydride catalyzed by nano-Fe_2O_3

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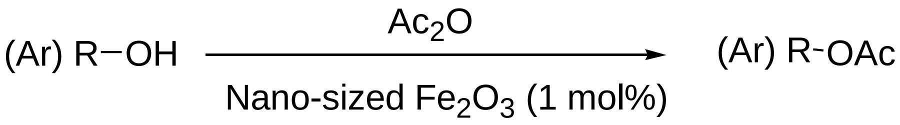
Keywords: Acetylation, Alcohol, Phenol, Acetic anhydride, Nano-sized Fe_2O_3 .

Amides and organic esters show a significant family of intermediates commonly used in the synthesis of industrial chemicals, medicines, cosmetics and food additives. Acetylation is one of the most applicable, beneficial and essential reaction in organic chemistry setting chemists to introduce reagents for this reaction. The protection of alcohols and phenols is one of the most widely used reactions in organic synthesis and is normally gained by acylation with anhydrides or acyl chlorides in the presence of tertiary amine bases like either triethylamine or pyridine,[1] Lewis or protonic acids[2] and solid acids.[3] Some of the reported methods for the acetylation of alcohols suffer from one or more drawback such as toxicity, cost, drastic reaction conditions, hygroscopicity, thermal stability, and the explosiveness of reagents.[4] Pyridine is a popular catalyst for the acetylation of alcohols using acetic anhydride, however it is toxic, has a bad smell and its high boiling point makes its removal after the reaction hard. Given those drawbacks, new, efficient, and eco-friendly methods are still in demand. Herein, we wish to report a mild, and efficient protocol for acetylation of alcohols and phenols using acetic anhydrides in the presence of Fe_2O_3-nano as catalyst (Fig.1).



$$\text{(Ar) R–OH} \xrightarrow[\text{Nano-sized Fe}_2\text{O}_3\text{ (1 mol\%)}]{\text{Ac}_2\text{O}} \text{(Ar) R-OAc}$$

Fig. 1 The Acetylation of Alcohols and phenols with Acetic Anhydride Catalyzed by nano-Fe_2O_3

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Synthesis of melamine functionalized with sulfonic acid supported on magnetic nanoparticle as reusable bifunctional heterogeneous catalyst, and its application in the preparation of 7,10,11,12-tetrahydrobenzo[*c*]acridin-8(9*H*)-ones

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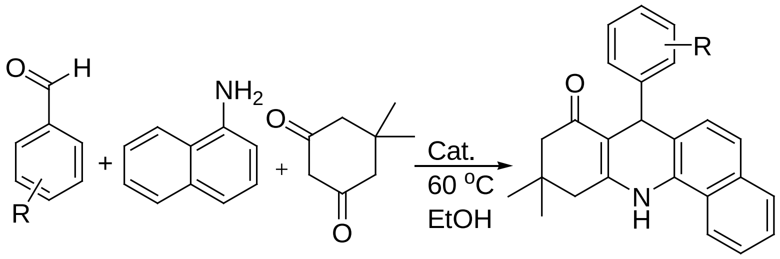
Keywords: Benzo[*c*]acridine, γ-Fe_2O_3@Si-$(CH_2)_3$@melamine@butyl sulfonic acid, Nanoparticle

Almost the heterocyclic compounds are of great interest in pharmaceutical chemistry. Out of these heterocyclic compounds, the tricyclic compounds containing acridine skeleton is an important pharmacophore and privileged structure in medicinal chemistry. Acridine derivatives have antitumor,[1] carcinogenic[2] and anti-malaria activities.[3] Thus the synthesis of acridine compounds is an important and principal task in modern organic chemistry.

In this communications, the present study describes the synthesis and characterization of melamine functionalized with sulfonic acid supported on the magnetic nanoparticle, γ-Fe_2O_3@Si-$(CH_2)_3$@melamine@butyl sulfonic acid nanoparticle as a green and reusable bifunctional catalyst. This catalyst was characterized by FT-IR, XRD, EDX, TEM analyses.

The catalytic activity of this new catalyst was studied for the synthesis of 7,10,11,12-tetrahydrobenzo[*c*]acridin-8(9*H*)-ones from aliphatic and aromatic aldehydes, 5,5-dimethyl-1,3-cyclohexanedione(dimedone) and 1-naphthylamine in excellent yields (Scheme 1).

This heterogeneous catalyst showed the advantages such as very simple and eco-friendly due to use from magnetic nanoparticle as high reusability of the catalyst, magnetically separable catalyst, excellent yield, and mild reaction condition.



Scheme 1: Catalytic synthesis of benzo[*c*]acridins

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A new key for old lock: Glycerol as an OH-acid catalyzed one-pot three-component and fully green synthesis of 3,4-dihydropyrimidin-2(1*H*)-one and thiones

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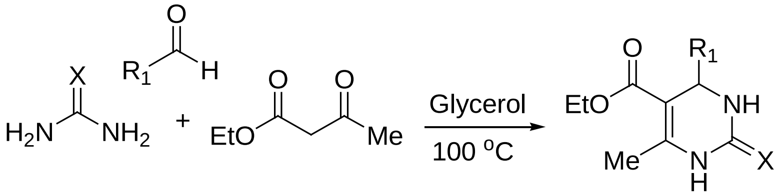
Keywords: Organo OH-Acid**,** Glycerol, Dihydropyrimidin-2(1*H*)-ones

Glycerol is a non-toxic, biodegradable and recyclable liquid that is highly inert, stable and also dissolves organic compounds that are poorly miscible in water. Glycerol has also been used, for other miscellaneous applications, as a single solvent, as co-solvent, being part of a deep eutectic mixture, or playing the double role of solvent and reagent [1], such as aza-Michael addition of aromatic amines to electron-deficient α,β-unsaturated ketones to achieve β-aminoketone [2], the utility of glycerol as solvent and reducing agent for the generation of metal nanoparticles[3] and the synthesis of vanillin-semicarbazone in crude glycerol [4] .In this study, the synthesis of 3,4-dihydropyrimidin-2(1*H*)-one and 3,4-dihydropyrimidin-2(1*H*)-thione derivatives (DHPMs) from aldehydes, ethyl acetoacetate and urea or thiourea using glycerol as an organo OH-acid, green and reusable catalyst is reported. The practical and simple protocol led to excellent yields of the dihydropyrimidin-2(1*H*)-one and thiones under mild reaction conditions and within short span of reaction times with easy reaction workup by maintaining excellent atom economy described (Scheme 1).



Scheme 1 Preparation of DHPMs in glycerol media

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Synthesis of Stenhouse salts from 4-((furan-2-yl)methylene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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Keywords: Stenhouse salts, Pyrazolone, Furfural, Donor acceptor Stenhouse adducts.

In recent years, Stenhouse salts (SSs) have attracted much attention as intermediates for the synthesis of cyclopenten-2- enones. These compounds were formed from the ring opening of furan derivatives by amines. This reaction uses in the identification of furfural in food products due to the intense color of these salts as a result of its conjugated triene structure.[1] Donor acceptor Stenhouse adducts (DASAs) are a new class of negative photoswitches. These compounds easily synthesized in two steps from commercially available starting materials.[2] DASAs were applied in smart materials, sensors, catalysis and also used as drug-carriers.[3] Furfural is a chemical product that can be derived from plant waste. It used as a readily available starting material to synthesize a wide range of materials.[4] Herein we design and synthesis of a new class of photochromes based on furfural, termed donor-acceptor Stenhouse adducts. We described DASAs containing alkyl-based amine “donors” (electron-rich) and pyrazolone “acceptors” (electron-deficient).

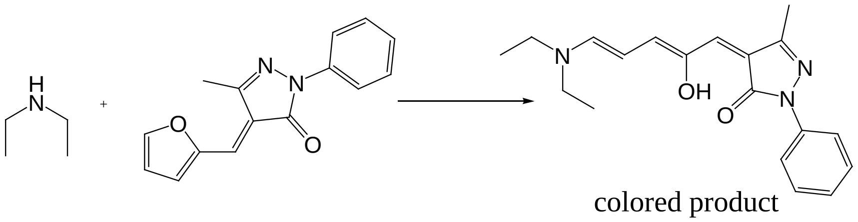

Fig. 1 Formation of Stenhouse salts from reaction of diethylamine with 4-((furan-2-yl)methylene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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Organic base-grafted on magnetic nanoparticles as a recoverable catalyst for the green synthesis of hydropyridine rings

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Keywords: 1,4-dihydropyridines; polyhydroquinoline; green chemistry; hybrid nanoparticles.

Organic-inorganic hybrid materials are of great interest as heterogeneous catalysts in organic synthesis, due to the functional diversity merged with thermal and mechanical stability of inorganic solids.[1] 1,4-Dihydropyridines (1,4-DHPs) are valuable heterocyclic compounds in view of pharmaceuticals and drugs development. [2] As part of our continuous effort to develop efficient heterogeneous magnetic nanocatalysts and green organic reactions [3], herein we describe the synthesis and characterization of 4-aminoquinaldine-grafted magnetite nanoparticles (MNPs-AQ) to give access to biologically interesting 1,4-dihydropyridines as a new eco-friendly method (Scheme 1). This newly design catalyst fulfilled our endeavor toward a heterogeneous system with a green synthetic aspects by avoiding the use of hazardous conditions for accessing target heterocyclic compounds.

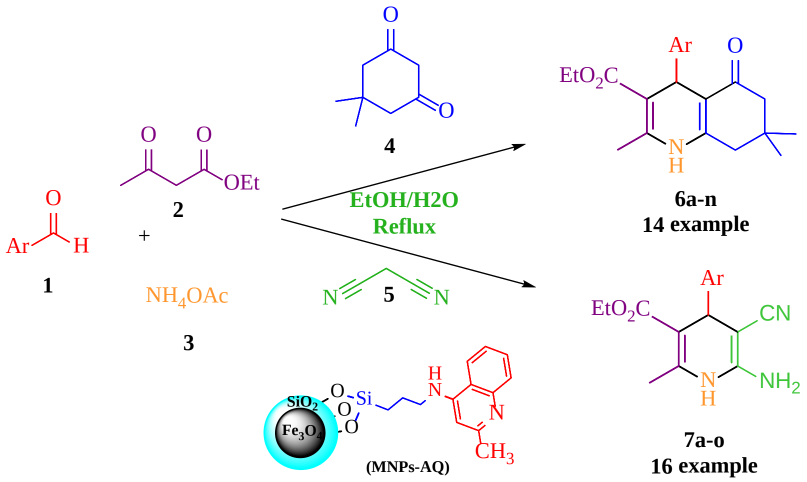

Fig. 1 Synthesis of 1,4-dihydropyridine derivatives using novel MNPs-AQ as catalyst

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Chemical Vapor Deposition and Activation Temperature on two important microporosity properties and density of methane storage capacity of active carbon based on anthracite

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***Keywords*:** Microporosity, Bulk density, Methane storage, Activated *carbon.*

Abstract

The present study investigates the effect of preparation variables of AC on the optimum amount of BET surface area and bulk density for methane adsorption purposes. All activated carbons samples were synthesized through the chemical activation method, using KOH chemical agent. The effect of preparation parameters including chemical impregnation ratio and activation temperatures was evaluated on two important characteristics of microporosity and bulk density. The best performance of the AC sample was observed at a KOH/anthracite chemical ratio of 3, activation temperature of 730ºC. At the optimum condition, the activated carbon acquired convenient microporosity in the matrix structure, with BET surface area of 2160 m2/g packing density of 0.53 g/cm3 and methane adsorption capacity of 175 V/V.

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Tunable porous doped carbon nanospheres as a robust host for immobilization of metal nanoparticles for aerobic oxidative synthesis of aryl nitriles

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Keywords: Tunable N-doped carbon spheres, Aryl nitriles, Porous carbon catalyst, Ag nanoparticles

Aromatic and aliphatic nitriles as a useful molecular scaffolds are an important part of pharmaceuticals, agrochemicals and fine chemicals. Up to now several nitrile-containing compounds were in clinical developments.[1] In the past decades, different transition metal-catalyzed protocols have been developed for the synthesis of aryl nitriles. Palladium, nickel and copper catalysts have shown to be effective for cyanation of aryl halides and organometallic reagents.[2] Various metal, metalloid-bound cyanide materials and nonmetallic "CN" units have been reported as CN precursors in the cyanation reactions. Recently, direct cyanation of aryl C-H bonds via transition metal-catalyzed process have been used as attractive method for the synthesis of organic nitriles.[2] We have prepared highly monodispersed, nitrogen-doped porous carbon nanospheres as a solid ligand for generation of Ag nanoparticles for oxidative synthesis of nitriles, directly from alcohols and ammonia as nitrogen source (Fig. 1). Synthesis of carbon spheres and nitrogen doping was proceeded in one step via hydrothermal method. Generally, nitrogen doping provide basic properties, which can enhance the interaction between substrates and carbon surfaces. Guanidine was used as nitrogen source in the doping procedure.

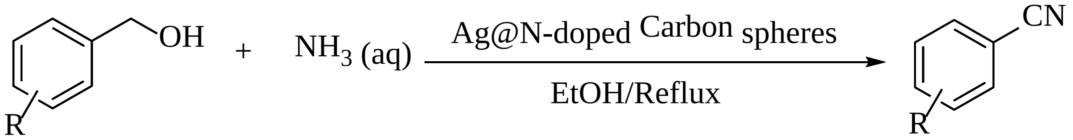

Fig. 1 Synthesis of substituted nitriles.

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Imidazole-aryl coupling reaction via C−H bond activation catalyzed by palladium supported on magnetic reduced graphene oxide in deep eutectic solvent

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Keywords: C-H arylation, Imidazole, Heterogeneous catalyst, Magnetic reduced graphene oxide, Palladium, Deep eutectic solvent.

The palladium-catalyzed direct C-H arylation reactions of heteroarenes with aryl halides have become as the extremely powerful method for the synthesis of biaryl or aryl-heteroaryl products compared to the traditional cross coupling reactions.[1] Major issue of Pd-catalyzed direct arylation in terms of green chemistry is related to the use of toxic and non-renewable solvents such as Dimethylformamide (DMF), Dimethylacetamide (DMA).[2] Deep eutectic solvents (DESs), have become more attractive in recent years due to their interesting properties and benefits, such as low cost of components, easy to prepare, tunable physicochemical properties, negligible vapor pressure, non-toxicity, biorenewability and biodegradability.[3]Also, despite the promising progress in C-H arylation reactions, the vast majority of C-H bond arylation of heterocyclic systems was achieved with homogeneous catalytic systems as it produces metal and ligand contamination.[4] herein, we report the first example of heterogeneous catalyst for C−H arylation reaction of imidazole with aryl bromide by using 2,6-diaminopyridine (DAP)-Pd^{II} complex immobilized on the magnetic reduced graphene oxide (MRGO@DAP-Pd^{II}). We also explore the possibility to use of DES as green and sustainable reaction media (Figure 1).

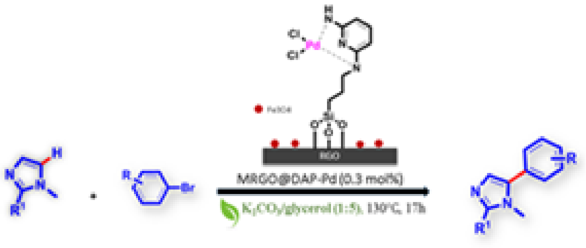

Figure 1. Cross coupling reaction of imidazoles with arylbromides via C-H activation catalyzed by MRGO@DAP-Pd^{II}

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Synthesis of diethyl-2-iminocoumarin-3-phosphonates

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Keywords: Knoevenagel Reaction, Horner-Wadsworth-Emmons Reaction (HWE), Diethyl cyanomethylphosphonate, Diethyl-2-iminocoumarin-3-phosphonate.

The organophosphorus compounds (OPCs) are important synthetic targets in modern organic synthesis. They have wide range of applications in different areas such as agriculture, medicine and industry.[1] In our knowledge the synthesis of the diethyl-2-iminocoumarin-3-Phosphonates haven't been reported previously. A survey of the literature show a lot of work have been done on the synthesis of Diethyl coumarine-3-phosphonate such as reaction of salicylaldehyde and triethyl phosphonoacetate in presence of $TiCl_4$[2] or Piperidene.[3] Nowadays phosphorylation of coumarine skeleton in the presence of $Mn(OAc)_3$,[4] Ag_2CO_3 [5] and NHC-Pd [6] as catalyst is used.

Herein, we report for the first time the synthesis of diethyl-2-iminocoumarin-3-Phosphonates from the reaction between salicyladehyde **1** and cyanomethylphosphonate **2** in presence of NEt_3 and $MgSO_4$ in toluene as solvent at 65 °C. We have been able to obtain the desired product **4** by using derivative of salicyladehyde with electonwithdrawing group. When we use salicyladehyde, the major product was the iminocoumaine **3** (Fig 1).

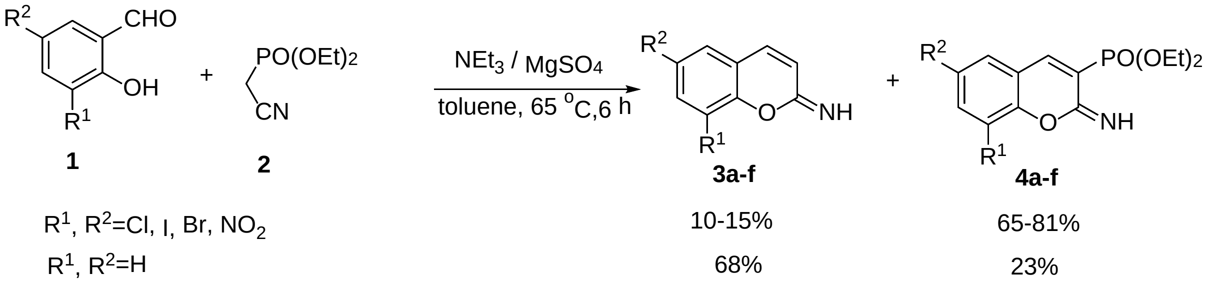

Fig.1

The structures of all synthesized compounds were determined on the basis of their HRMs, ^{1}H, ^{13}C, ^{31}P-NMR and IR spectroscopic data.

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Brönsted acidic ionic liquid-catalyzed multicomponent synthesis of pyrano[*c*]chromenes

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Keywords: Multicomponent reaction, [DABCO](SO_3H)$_2$(Cl)$_2$, Brönsted acidic Ionic liquid, Pyrano[*c*]chromenes.

Multicomponent reactions (MCRs) have emerged as an efficient and powerful tool in modern organic chemistry towards the generation of highly diverse and complex product from readily available substrates in a single operation without isolation of intermediates in minimal time with maximum selectivity, high atom-economy and high purity with excellent yields. MCRs have an outstanding status in medicinal chemistry and modern organic synthesis because they are one-pot processes that assemble three or more components. [1, 2]

Dihydropyrano[*c*]chromenes and their derivatives are of considerable interest as they possess a wide range of biological properties such as diuretic, analgesic, myorelaxant, anticoagulant, anticancer, anti-tumor, cytotoxicity and anti-HIV activities. They are also used as antimicrobial and anti-tuberculosis agents. [3-5]

In this study we have investigated the catalytic activity of a Brönsted acidic ionic liquid, [DABCO](SO_3H)$_2$(Cl)$_2$, in the synthesis of annulated pyrano[*c*]chromene derivatives to introduce a time- and cost-saving method using a recyclable catalyst (Fig 1).

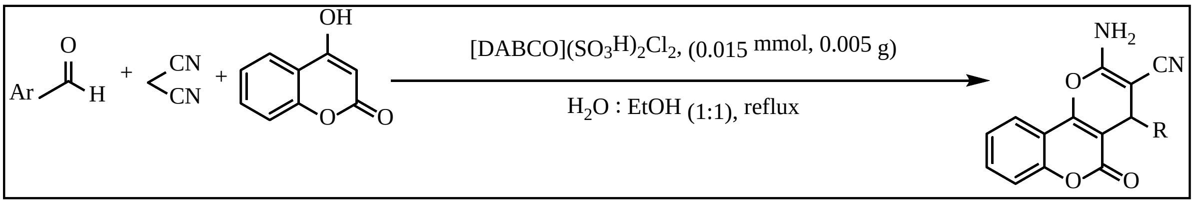

Fig. 1 Synthesis of pyrano[*c*]chromene derivatives using [DABCO](SO_3H)$_2$(Cl)$_2$ as catalyst

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Multi-component synthesis and study of biological effects of new passerini's derivatives based on Valproic acid

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Keywords: Multi-component reactions, Passerini, Valproic acid

Multicomponent reactions (MCRs), are powerful synthetic tools for the synthesis of complex and drivers molecules in a one-pot fashion from more than two starting materials.[1] Various reactions have been made to the multi-component reaction series. But recently, by replacing carboxylic acids in these reactions, synthesized various compounds of ester or amid macromolecules in a simple and efficient way.[2,3] In this study, a series of new passerini products valproic acid 1, aldehydes 2, isocyanide 3, in room temperature and water and dichloromethane as solvent. The structures of new product are determined on the basis of their mass spectrum ^{1}H NMR, ^{13}C NMR and IR spectroscopic data.

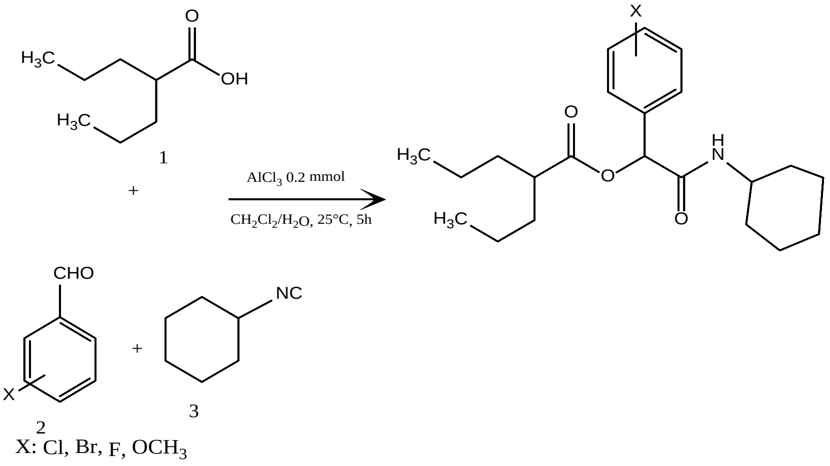

Fig1. Multicomponent product

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A novel amino acid-based deep eutectic solvent as a solvent-catalyst for the synthesis of pyrano[2, 3-*d*]pyrimidinone derivatives

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Keywords: Natural deep eutectic solvents, Amino acid, pyrano[2, 3-*d*]pyrimidinones, Choline chloride

Natural deep eutectic solvents (NADES) plays an important roles in extraction processes and organic syntheses. Exist hydrogen bond between molecules in these compounds change them to adequate alternatives for water in the organic transformations.[1]

In recent years, pyrano[2, 3-*d*]pyrimidinone derivatives are interested as widely experienced organic, heterocyclic compounds because of their biologically active properties such as antibacterial, antihypertensive, atoprotective, antiallergic antitumor, cardiotonic, vasodilator, bronchiodilators, analgesics, herbicidal, antimalarial and antifungal activities.[2] Different catalysts and methods were applied to synthesize these compounds in shorter times and milder conditions.[3,4] To avoid from the reported protocols problems, we are motivated to introduce a novel deep eutectic solvent as a solvent-catalyst (Fig. 1).

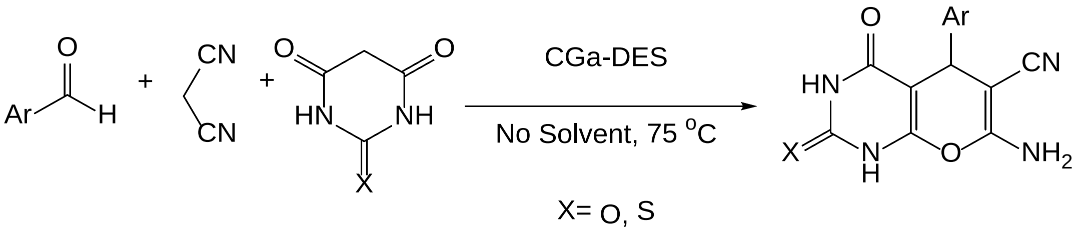

Fig. 1 Using amino acid based DES for the synthesis of pyrano[2, 3-*d*]pyrimidinones

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Asymmetric synthesis of Passerini reaction using a cheap and commercially available chiral amino acid as a catalyst

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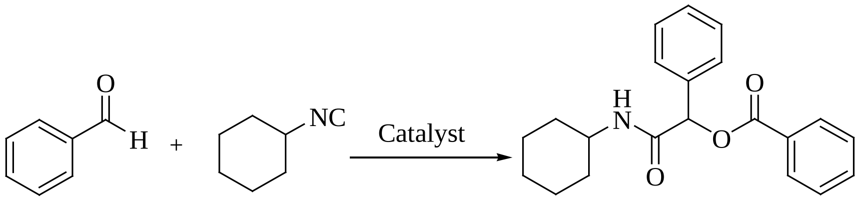
Keywords: Asymmetric synthesis, Isocyanides, Passerini reaction, Amino acid.

Today's chemistry focuses on the ways to accelerate organic reactions so that in addition to expediting reactions, high-yield products, easy workup and minimal environmental impact to be considered. For this purpose organo-catalysts have a prominent position in organic reactions, which carry many of the reactions in water that no longer requires traditional volatile organic solvents so that this aspect introduces green chemistry that focuses on technological approaches for the prevention of using and generating hazardous substances.

The Passerini reaction, one of the oldest multicomponent reactions, has been found useful for the construction of multifunctional α-acyloxyamide in a practical process with the concurrent generation of a stereogenic center. This reaction was often used as a key step in the total synthesis of natural products and the α-acyloxycarboxamide group is also a frequently recurring motif in biologically active compounds, for example, in the pharmacologically interesting depsipeptides.[1,2]

In this study an efficient enantioselective two component Passerini reaction in the presence of a chiral amino acid catalyst has been developed. This represents the general example of Passerini reaction with good to excellent enantioselectivies involving aromatic aldehydes under certain conditions. The feature of this method is highlighted by using a chiral reusable catalyst to brings about an aerobic oxidation of aldehyde for construction of widely useful complex compounds (Scheme 1).



Scheme 1. Asymmetric Synthesis of Passerini products using of a chiral amino acid.

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Synthesis, characterization and catalytic evaluation of $NiFe_2O_4@SiO_2@$glucose amine for the synthesis of novel derivatives of triazoles

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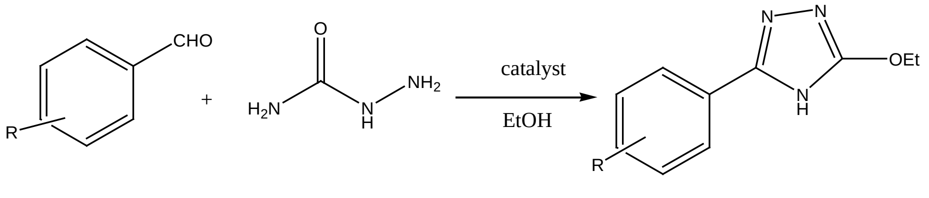
Keywords: Multicomponent reactions, triazoles, nanocatalyst

Triazoles and their derivatives are of great importance in medicinal chemistry and can be used for the synthesis of numerous heterocyclic compounds with different biological activities such as antiviral, antibacterial, antifungal, antituberculosis, anticonvulsant, antidepressant, anti-inflammatory and anticancer activities. They have been reported to be inhibitors of glycogen synthase kinase-3, antagonists of GABA receptors, agonists of muscarine receptors, be neuroleptic, and these compounds also show anti-HIV-1, cytotoxic, antihistaminic, and antiproliferative activities [1]. Thus, the design and synthesis of novel triazole derivatives are the prospective direction of medicinal chemistry for the scientists working in this field.In continuation of our previous work [2], herein, we specifically address the multicomponent synthesis of triazoles using $NiFe_2O_4@SiO_2$-propyl@glucose amine magnetic nanoparticle as catalyst .

The prepared nanocatalyst was characterized using Fourier Transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS), thermogravimetric analysis (TGA) and a vibrating sample magnetometer (VSM). All of organic compounds are new and characterized by IR, ^1H NMR, ^{13} C NMR, Mass and elemental analysis.



R = 4-Cl; 2-Cl; 4-CH_3; 4-OCH_3; H; 4-NO_2; 3-NO_2; 2-NO_2; 4-Br; 2,4- $(Cl)_2$

Fig. 1 Multicomponent synthesis of triazoles

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Preparation and charachterization of a new molecular nanomachine based on diamidic 18-crown-6 macrocycle as rotaxane

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Keywords: Nano-machine, Nano-motor, Rotaxane, Macrocycle, 18-Crown-6

A rotaxane is a molecular machine consisting of multiple docks on a chain around which a macrocycle is trapped by the bulky end stations, allowing only translational motion, which in this specific case happens upon excitation.[1] They like macroscopic machines, need energy to operate, the most efficient sources of energy for them are light and electricity.[2] In this paper, the preparation and identification of a new molecular nanomachine based on dimeidic 18-Crown-6 macrocyle as a type of rotaxane is discussed. Conversion of P-cresol in reaction with $SOCl_2$ converted to dicresyl solfoxide **(1)**. Dicresyl solfoxide in reaction with $ClCH_2CO_2Me$ diester was produced **(2)**. Macrocycle **(3)** was prepared from reaction diester **(2)** with proper amine. Reaction **(3)** with proper line was efforded to rotaxane **(4)** as nanomashine. The structures of all synthesized compounds were recognized by spectroscopic methods such as FT-IR, ^{1}H NMR, ^{13}C NMR, and Mass analysis (Fig. 1).

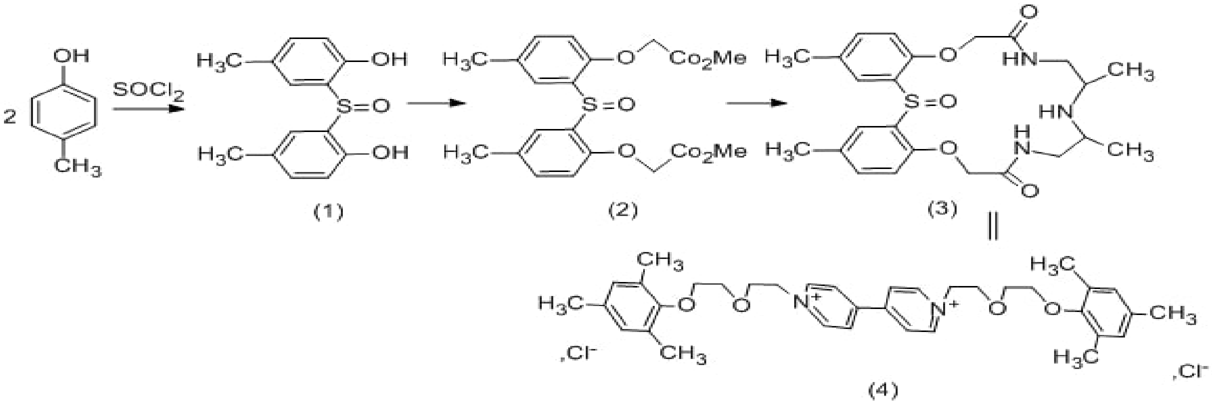

Fig. 1: Nanomachine based on diamidic 18-crown-6 macrocycle as rotaxane

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Synthesis and application Of magnetic nanoparticles coated with stearic acid and palmitic acid, and ionic and nonionic surfactants

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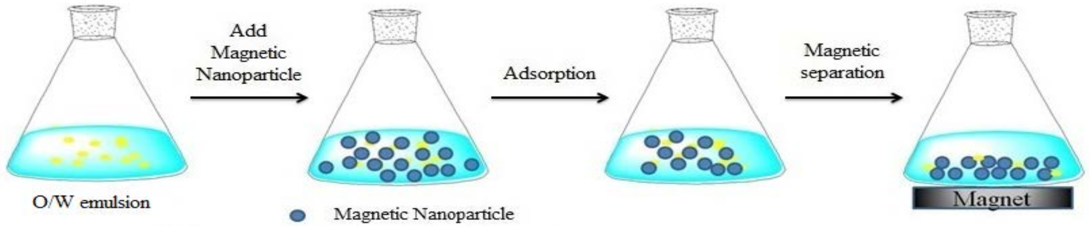
Keywords**:** Magnetic nanoparticle, Separation, Oil droplet, Demulsification,

Today, nanoscience and nanotechnology are considered as one of the most important research areas an extension of modern science. Nanoparticles magnetic have found many applications due to features such as a large special surface and simple separation with external magnetic field.[1]

Magnetic nanoparticles (MNPs) functionalized by organic and/or inorganic substrates have attracted much interest, because of their potential in medical resonance imaging (MRI)[2], drug delivery[3], magnetic recording media, catalysis[4], wastewater purification[5], and etc.

Magnetically driven separation is one of the major potential application areas for nanoparticles and has received considerable attention in the past decades.[6] Applying functional MNPs in oil-water multiphase separation and extraction have received increased recent attention.[7-9]

In this work, after synthesis of iron magnetic nanoparticles by co-precipitation, then, coating them with fatty acid of palmitic acid, as well as ionic and nonionic surfactants, their application were investigated especially, in demulsification for ligroin in water nanoemulsions. Finally, we compared the application of synthesized magnetic nanoparticles to demulsification of the crude oil-water emulsions.



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Synthesis of Novel Spiro-oxindole compounds by Reaction of 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione in green solvent

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Keywords: Multicomponent reaction, Spiro-oxindole compound, 6-aminouracil, Pyrazolone, Pyrazole, Green Solvents

Most Reactions concerted on useful tools for the synthesis of biologically active compounds. One of these reactions is the multi-step syntheses conducted in a one-pot fashion that can contain various compounds with biological effects. Multicomponent reactions (MCRs) can dramatically reduce the generation of chemical waste and reduce the cost of the starting materials.[1] The Uracil, Pyrazole, Pyrazolone and their analogs occupy a unique place in the field of medicinal chemistry as anticancer, anti-inflammatory, antiviral drugs and so all. [2-4] As a part of our continued interest in the synthesis of novel Spiro compounds,[5-6] we decided to demonstrate the one-pot reaction of 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinolone-1,2-dione **1**, 3-methylpyrazol-5-one **2** or 5-amine-3-methyl-pyrazole **3** with 6-aminouracil **4** in the green solvent such as Water, Ethanol and Ethanol/Water (1:1) (scheme 1). The resulting structure **5a** were produced in very good yields and the structures were confirmed by the ^{1}H & ^{13}C-NMR and FT-IR spectra’s.

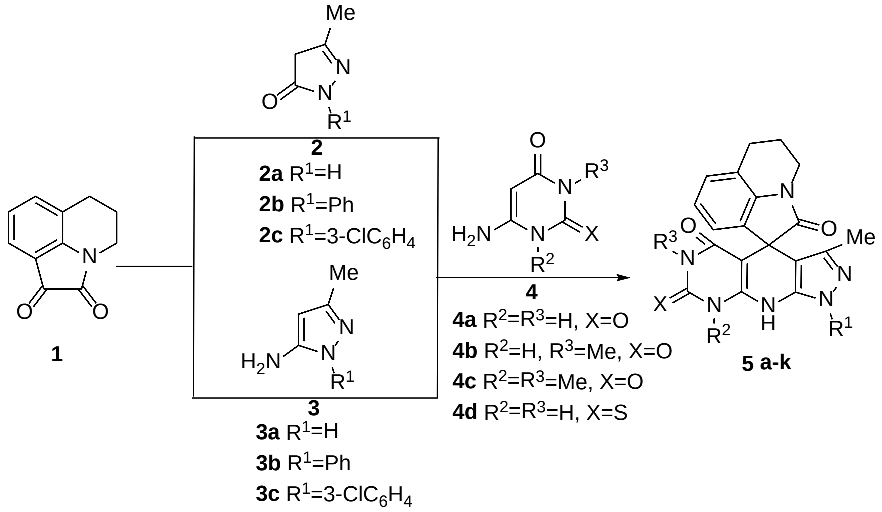

Fig 1: Synthesis of novel Spiro-oxindole

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The synthesis of Spiro-oxindole compounds by 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione, Pyrazole and Pyrazolone

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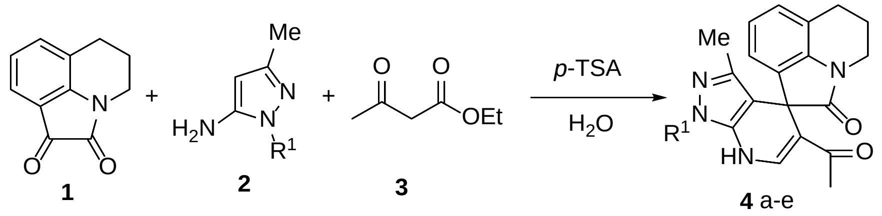
Keywords: Spiro Compound, Pyrazole, Pyrazolone, EAA, Water.

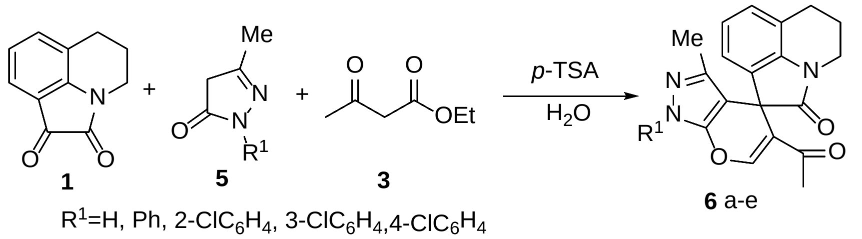
Recently, we have described a simple and straightforward preparation of novel spiro-oxindole by tricyclic and four cyclic Isatin.[1-5] Interest to the synthesis of novel spiro compounds, we have now demonstrated the *p*-TSA catalyzed and green synthesis of novel spiro-oxindole **4** by condensations of variously 5-aminopyrazole **2** with Ethyl acetoacetate **3** and 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione **1** (scheme 1).



R^1=H, Ph, 2-ClC$_6$H$_4$, 3-ClC$_6$H$_4$,4-ClC$_6$H$_4$

Fig 1: Reaction of 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione **1** with 5-aminopyrazole **2** and EAA **3**

In the other case of our work, we examined the reaction of 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione **1**, 3-methylpyrazol-5-one **5** and Ethyl acetoacetate **3** in H_2O (scheme 2).



R^1=H, Ph, 2-ClC$_6$H$_4$, 3-ClC$_6$H$_4$,4-ClC$_6$H$_4$

Fig 2: Synthesis of novel Spiro compound with 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione

The desired products were produced in good yields and their structures were determined on the basis of their spectroscopic analysis data.

Reference:

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Novel methodologies for the synthesis of indole derived scaffolds

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Keywords: Heterocycles, Indole, Indole derived scaffolds, Synthetic approaches.

Indole derivatives are very important heterocyclic compounds in the drug-discovery studies. They represent a very important class of molecules that play a major role in cell biology and are potential naturally occurring products. There has been an increasing interest in the use of indole derivatives as bioactive molecules against microbes, cancer cells, and various kinds of disorder in the human body.[1] In this case, indole often considered to be the pre-eminent heterocycle and this molecular scaffold has the greatest medicinal importance that attracted the attention of chemists and biologists.[2] In this presentation, we attempt to present new methodologies for the synthesis of indole, isoindole, benzoindole, fused Indoles, bis-indole, bis(indolyl)methanes, spiroindole, spirooxindole, indoloindole and also presented strategies for synthetic modification of indole *via* C2 functionalization, C3 functionalization and N functionalization of indoles (Figure 1). These new methods have been fragmented across the literature of organic chemistry.

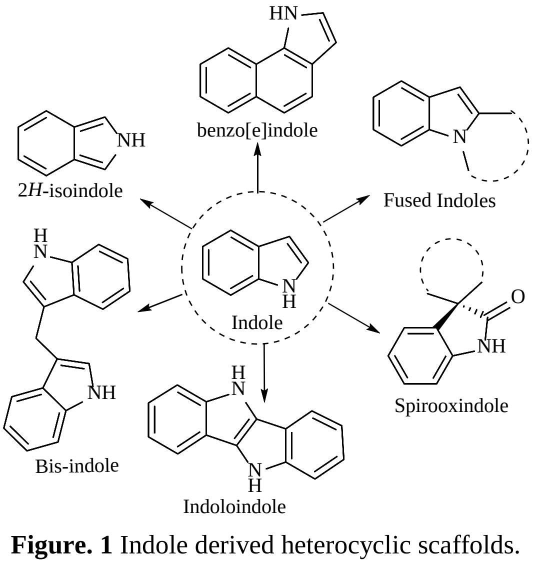

Figure. 1 Indole derived heterocyclic scaffolds.

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Application of trichloroisocyanuric acid and triphenylphosphine in the efficient one-pot conversion of benzylic silyl and tetrahydropyranyl ethers to gem-dichlorides

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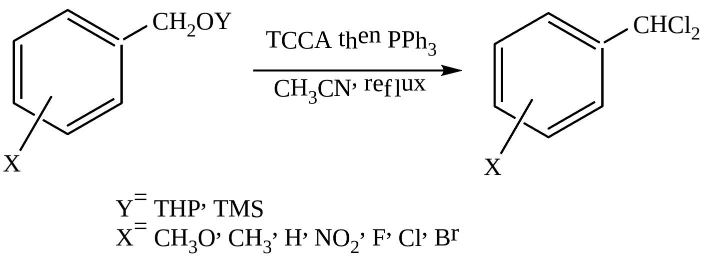
Keywords: Trichloroisocyanuric acid, Triphenylphosphine, Silyl ether, Tetrahydropyranyl ether, *gem*-Dichloride.

Geminal dihalides form an important group of organic compounds due to their applications in various fields such as pharmaceutical and agricultural industries or in organic synthesis such as synthesis of some biological active heterocyclic compounds[1] and polymers[2]. A known route for the synthesis of these valuable compounds is based on using aldehyde and ketone sources. Various methods have been reported in this area.[3] However, some these methods suffer from some disadvantages such as use of an unusual reagent with low accessibility, formation of undesired products, long reaction times, use of acidic conditions and low yields. On the other hand, the methods converting alcohols to *gem*-dihalides are very scarce[4] and as far as we know, there is not report on the one-pot and oxidative conversion of trimethylsilyl (TMS) or tetrahydropyranyl (THP) ethers to *gem*-dihalides in the literature. Now with the above descriptions and in continuation of our previous works on the synthesis of *gem*-dihalides,[4, 5] we describe for the first time an efficient one-pot oxidative conversion of benzylic both silyl and tetrahydropyranyl ethers to *gem*-dichlorides using trichloroisocyanuric acid (TCCA) and triphenylphosphine (PPh_3) in good to excellent yields under neutral conditions (Scheme 1). This method is tolerated by a variety of other functional groups.



Scheme 1. One-pot conversion of THP and TMS ethers to *gem*-dichlorides using TCCA and PPh_3.

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Preparation of Zein/CNT@PVA nano-fibers contains Chamomilla extract to electrospinning method for the treatment of wound and burn

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Keywords: Wound, Biocompatible, Biodegradable, CNT, Zein, Polyvinyl alcohol

Carriers of transfer Protein have many advantages over lipid carriers, carbohydrates, and synthesis polymers in terms of availability, biodegradability and high transplant capacity.[1] The electrospinning is a simple technique that is not for creating Ultra fine fibers in the form of a woven net. The fiber obtained from electrospinning can be used as novel carriers for targeted drug delivery and encapsulation of sensitive compounds.[2] An appropriate cover for wound should be biocompatible, biodegradable, accelerated of wound healing, and so on.[3] Zeine is the primary source of corn protein.[4] Chamomilla extract has several properties such as healer, Disinfectant, anti-inflammatory, Treat acne and anti-itching.[5] Polyvinyl alcohol is a biocompatible and biodegradable polymer that during adding to the materials, increases the hydrophilicity due to the carboxyl group.[6] Carbon Nanotubes (CNTS) have amazing and tremendous properties in various fields; the properties of nanotubes with functionalization are modified by chemical compounds. Using electrospinning, The nanofiber including zein, single wall carbon nanotube (SWCNTs), poly (vinyl alcohol) containing chamomile extracts and fiber properties were investigated using FT-IR, TGA-DTA, Zeta potential, tensile strength, MTT. The purpose of this study is to find a new method using nanotechnology and its effects on the process of wound and burn reconstruction.

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Synthesis and characterization of novel photoactive aromatic polyamides based on imidazole, xanthene and carbazole

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Keywords: polyamides-imidazole-xanthene-photoactive-carbazole

Polyamides are high-performance materials and occupy an important place in the world of polymers owing to their thermal and oxidative stability, flame permanence, and mechanical and dielectric properties.[1] Most of them are generally difficult to process which is led to high crystallinity, low solubility, high melting point, and limited application.[2] In recent years, many studies have been done to improve the polymer structure to increase solubility and its processing ability.[3] A group of new photoactive polyamides (PAs) based on imidazole with pendant group such as xanthene and carbazole was synthesized from new diamines and dicarboxylic acids. The structure of diamines and PAs were completely determined by FTIR and NMR. All of the polymers were good thermal stability and amorphous in nature, showed outstanding solubility and could be easily dissolved in amide-type polar aprotic solvents. Also, the antibacterial properties, optical activity and removal of heavy metal ions ability were studied.

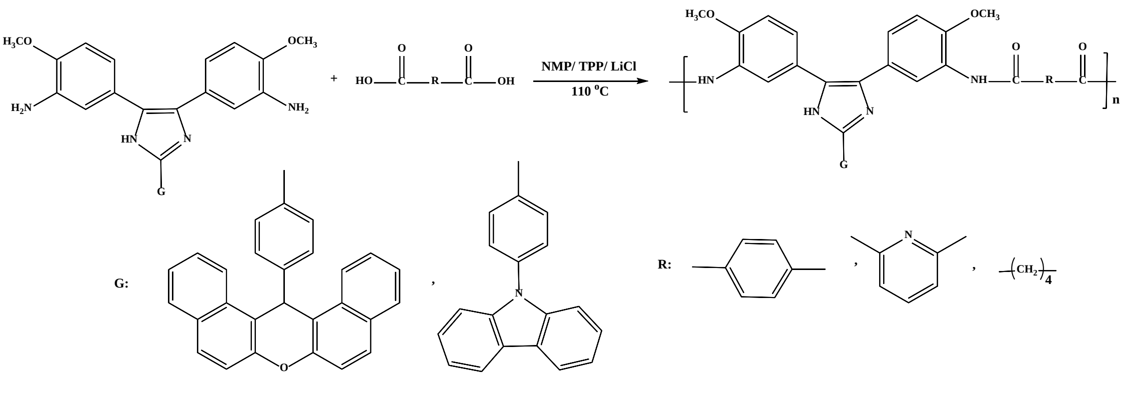

Fig. 1 Synthesis of PAs.

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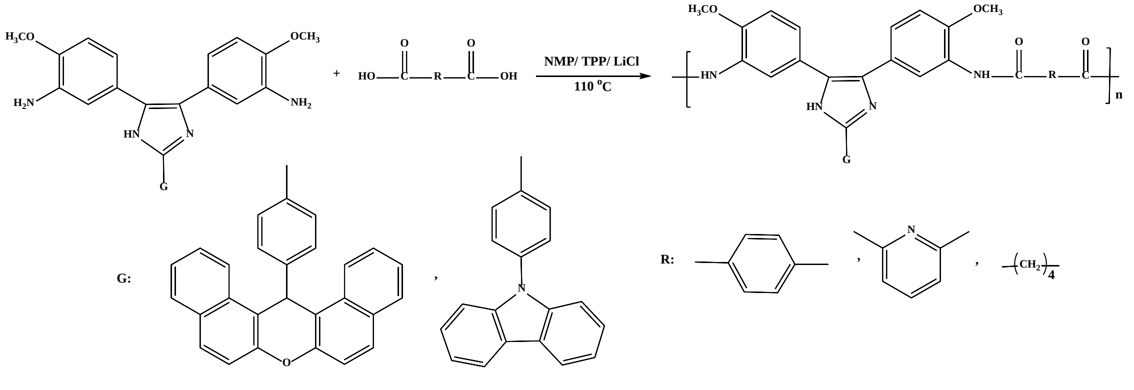

Scheme 1. Synthesis of PAs.

References,

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Application of novel Cu-based metal organic frameworks (MOFs): Application in synthesis of 7-amino-2-(1*H*-indol-3-yl)-5-phenylpyrazolo[1,5-*a*]pyrimidine-6-carbonitrile

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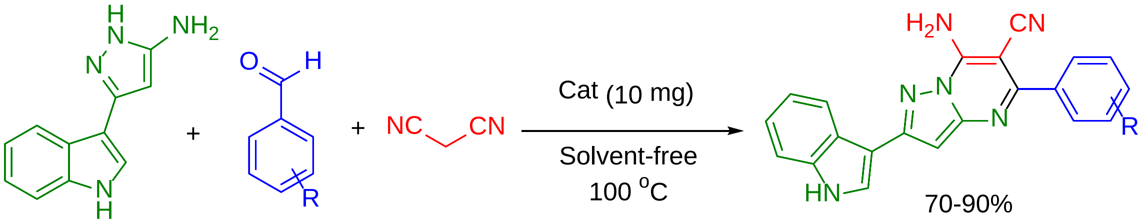
Keywords: Fused heterocyclic, Multi-component reactions, Metal organic frameworks (MOFs), Solvent free.

Pyrazolopyrimidines are fused heterocyclic ring systems which structurally can consider as bioisosteres of adenine, which is fundamental for every aspect of cell life. Pyrazolo[3,4-*d*]pyrimidine derivatives have been explored for their inhibitory activity towards various protein kinase enzymes and their role as anticancer agents [1]. On the other hand, metal organic frameworks (MOFs) as eco-friendly and green catalysts play an important role in the chemical processes. Easy recovery and reusability of these catalysts have led to their extensive use in the synthesis of a wide range of compounds [2-3]. MOFs based on the type of their ligands and functional groups on their surface exhibit different properties. Functional groups may initially be present in the organic ligand structure or after synthesizing MOFs are created. Herein, we wish to report a clean method for synthesis of the pyrazolopyrimidine derivatives under solvent free condition in the presence of MOF-Cu (10 mg) as an efficient nano-catalyst (**Scheme 1**).



Scheme 1: Multi-component reactions of 7-amino-2-(1*H*-indol-3-yl)-5-phenylpyrazolo[1,5-*a*]pyrimidine-6-carbonitrile

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Effect of preparation conditions on the catalytic performance of cobalt manganese catalysts for production ethylene and propylene

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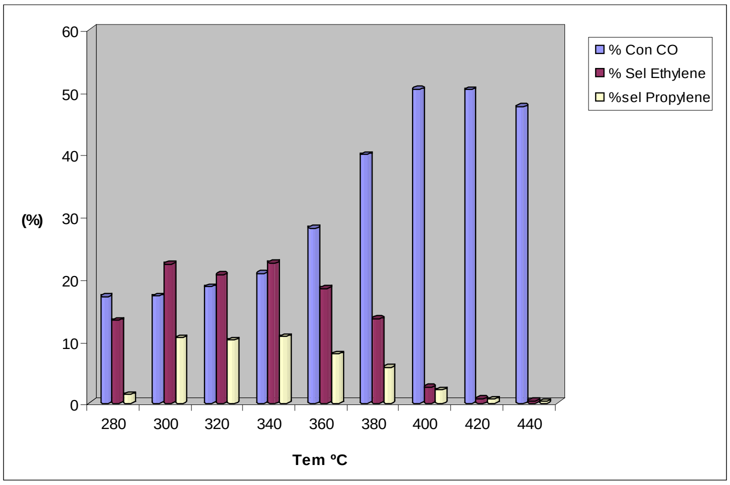
Keywords: Ethylene and propylene, Catalyst $[Mn(bpy)_3][Co(dipic)_2]/ SiO_2$, Synthesis gas

In this work cobalt manganese oxides are prepared using a new procedure and studied for the conversion of synthesis gas to light olefins (ethylene and propylene). Catalyst has been prepared from precursor of $[Mn(bpy)_3][Co(dipic)_2].18H_2O$ supported on silica. $[Mn(bpy)_3][Co(dipic)_2]/ SiO_2$ was calcined at 773 K for 5h. The activity and selectivity of prepared catalyst have been studied in a fixed microreactor under atmospheric pressure in a range of reactor temperatures using synthesis gas with different H_2:CO molar feed ratios. Bimetallic complex of $[Mn(bpy)_3][Co(dipic)_2].18H_2O$ and Co-Mn-SiO_2 catalyst were characterized by FT-IR, uv-vis, elemental analysis and atomic absorption spectroscopy and XRD, SEM, BET specific surface area and thermal analysis method.



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Properties of MDI-BP as wood adhesive

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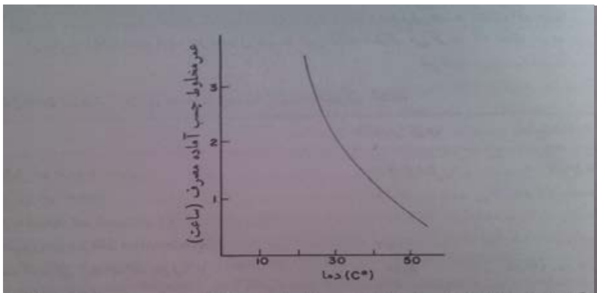
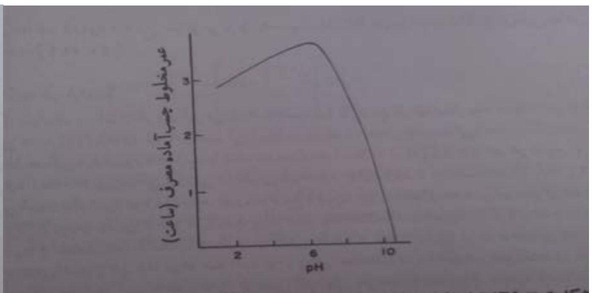
Keywords: MDI،Particleboard،Hydroxyl group،viscosity، Wood adhesive،Amide group

4.4 di-phenylmethane diisocyanate (MDI) is the superior diisocyanate for the production of particleboard.[1] This compound has a low vapor pressure at normal temperature and therefore increases the safety of its use.[۱]At normal temperature, commercially polymer MDI is a dark reddish brown liquid with a viscosity of 400 cp, which can be stored for up to 12 months.[2] MDI-BP is a very moisturizer and should keep it containers closed.[3]The reaction of MDI with hydroxyl groups is a constituent of wood to form the urethane bond between the wood and the adhesion line, and its reaction with water in wood to form polyurethanes is a major reaction that contributes to the function of this compound as a glue.[4] The effect of temperature and pH of the adhesive mixture on its life in ready-to-use mode is given in the following two graphs. [۵]



شکل ۶-۳ MDI امولسیون شدنی، عمرمخلوط چسب آمادهٔ مصرف به‌عنوان تابعی از دما



شکل ۶-۳ MDI امولسیون‌شدنی، عمرمخلوط چسب آمادهٔ مصرف به‌عنوان تابعی از pH

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Combination of Silver Nanoparticles with some new Monocyclic β-Lactams

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Keywords: *β*-Lactam, [2+2] Cycloaddition Staudinger reactions, Morpholine, Silver nanoparticles (AgNPs)

The scientists have been very interest in *β*-lactam compounds since the 1940s, when the antibiotic properties of the first semisynthetic the penicillins were discovered.[1] In the late 1970s and early 1980s, several monocyclic *β*-lactams with high antibacterial activity have been discovered in nature. It was believed that the biological activity of *β*-lactams is absolutely correlated to functional groups on 2-azetidinone ring.[2] Different research group studied biological activities of silver nanoparticles (AgNPs),[3] and also synthesized AgNPs combined with some antibiotics[4] as well as investigation of their antimicrobial activity. Our interest in *β*-lactam chemistry led us to study synthesis of some new *β*-lactams bearing morpholine ring and combination of some amino *β*-lactams with silver nanoparticles (Fig 1). The cycloadducts were characterized by spectral data, including ^{1}H-NMR, ^{13}C-NMR, IR, Mass spectroscopy and elemental analyses.

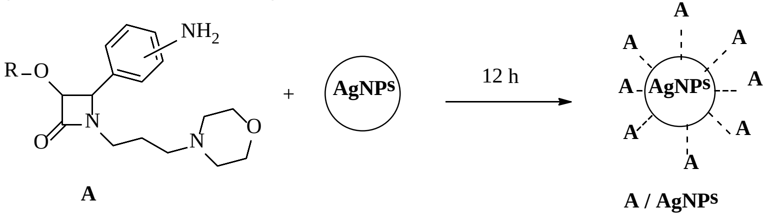

Fig. 1 *β*-Lactam "A" combined with silver nanoparticles

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Synthesis of 5-substituted 1H-tetrazoles by clean cabbage like silver crystals

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Keywords: Multicomponent reactions, 5-Substituted 1*H*-tetrazoles, Silver crystals, Catalyst.

Tetrazoles are synthetic heterocyclic compounds having one carbon and four nitrogen atoms in a five-membered ring.[1] They have widespread applications in materials science,[2] and medicinal chemistry.[3] Moreover, they can be served as lipophilic spacers and carboxylic acid substitutes.[4] One of the most significant aims of tetrazoles chemistry is searching for a new synthetic method as well as improvement of previous procedures. The most versatile used method for the syntheses of 5-substituted 1*H*-tetrazoles is [3+2] cycloaddition of nitriles and azide anion in the presence of various catalysts and solvent conditions. Several organic, inorganic, homogeneous, and heterogeneous catalysts have been used for this purpose. Herein we introduced our process as a highly efficient method for conversion of aldehydes into the corresponding 5-substituted 1*H*-tetrazoles using clean cabbage like silver crystals as reusable catalyst (Fig.1).

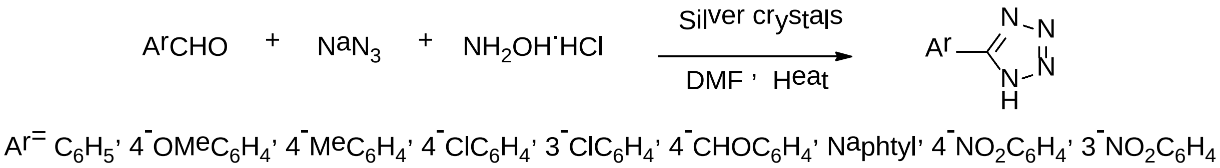

Fig. 1 The synthetic route to 5-substituted 1*H*-tetrazoles

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One pot synthesis of some new 2-((4-methylphenyl) sulfonamido) benzamide derivatives

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Keywords: Multi component reactions, Sulfonamide, 2-Aminobenzamide, 1,3-diketon

Multi component reactions are one of the most effective procedures for economical synthesis of structural diversity and molecular complexity in a simple process[1]. Sulfonamides as chemotherapeutic agents are known almost one hundred years. Recently, there has been increasing attachment to sulfonamides in connection with development of the application of these compounds that can interact with various targets[2]. The existence of donor and acceptor atoms in sulfonamide helps them to participate in the system of different hydrogen bond networks[3]. In this work, we wish to report synthesis of some new 2-((4-methylphenyl) sulfonamido) benzamide derivatives **4** by reaction of 2-aminobenzamide derivatives **1,** 1,3-diketon **2** and *p*-toluenesulfonic acid **3** in the absence of reagents.

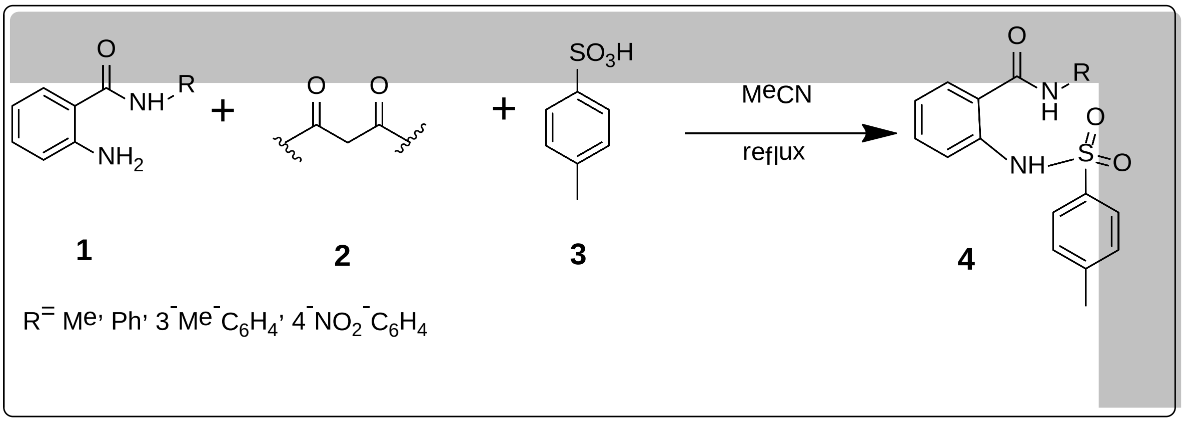

Fig. 1 Synthesis of 2-((4-methylphenyl) sulfonamido) benzamide

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Synthesis of thiopyranoindole derivatives in present of Nano Ni-MOF

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Keywords: Multi-component reactions, Knoevenagel condensation, Metal organic framework, Heterogeneous catalysis

Metal-organic frameworks or MOFs are porous compounds with special properties like controllability in terms of composition and structure coupled with high porosity.[1] These catalysts are recyclable. Multi-component reactions (MCRs) are known as very powerful procedure in synthetic organic and medicinal chemistry for the preparation of the complex materials in a one step from simple starting materials.[2] Thiopyran and fused-thiopyran derivatives are important classes of sulfur containing heterocycles because of their usefulness in accessing certain natural products [3]. Besides, they have valuable antipsychotic, anti inflammatory[4], antibacterial, anti-hyperplasia, and anticancer activities. Among the members of this family, thiopyranoindole-annulated analogs have found considerable utility as pharmaceutical agents demonstrating analgesic activity. Here, we report the synthesis of thiopyranoindole derivatives **4** from the reaction between thiooxindole **1**, aldehydes **2** and malononitrile **3** in the presence of Nano Ni-MOF as a Nanocatalyst in EtOH under reflux condition. The synthesized catalyst was characterized by SEM, EDX, XRD and FT-IR.

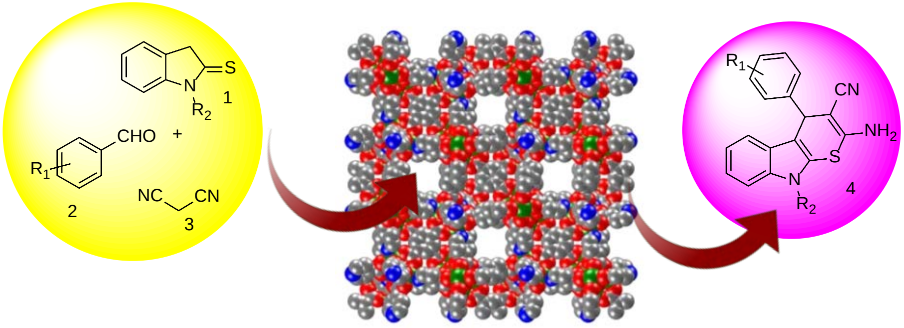

Fig. 1 Multi-component synthesis of dihydrothiopyrano[2,3-*b*]indole-3-carbonitrile

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Sulfur-containing nanocomposites based on polyurethane and cellulose

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Keywords: Polyurethane, Nanocomposite, Microcrystalline cellulose, Nanofiber.

Polymer-based nanocomposites reveal considerable improvements in mechanical, dielectric magnetic, thermal optical and acoustic properties compared to the pure organic polymers at very low-volume fractions of the reinforcing phase.[1-4] There is an increased use of cellulose nanocrystals as the loading-bearing constituent in developing inexpensive biodegradable materials owing to a high aspect ratio, a high bending strength of about 10 GPa, and a high Young's modulus of approximately 150 GPa.[5] Herein, we report the synthesis of new sulfur-containing polyurethane/cellulose hybrid nanocomposite films via dispersing different concentrations microcrystalline cellulose in a polyurethane matrix. The covalent and hydrogen bonds between the cellulose nanofibrils and the polymer matrix were improved the mechanical properties of the resulting nanocomposites. The obtained nanocomposites were characterized by fourier transform infrared spectroscopy, X-ray diffraction and transmission electron microscopy (TEM). The TEM results confirmed that the cellulose nanofibrils were dispersed in polymer matrix. Additionally, thermogravimetric analysis data showed an improvement of thermal stability of nanocomposite films as compared to the neat polymer. The superior properties of the novel bionanocomposite materials could have great potential applications.

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Chiral poly(amide-imide)/functionalized ZnO bionanocomposites containing L-alanine units

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Keywords: Poly (amide-imide), Bionanocomposite, L-Alanine, ZnO.

Organic-inorganic nanocomposites have attracted significant interest owing to unique combinaton desirable organic and inorganic properties.[1-3] The inorganic nanoparticles into polymer matrix provied high-performance materials that find applications in many fields such as semiconductor, sensor, fuel cell, drug delivery, rechargable batteries, etc.[4-6] In this study, optically active poly(amide-imide) (PAI)/ZnO hybrid bionanocomposite films with different weight percentages of ZnO nanoparticles were prepared via ultrasound-assisted technique. At the first a heteroaromatic diamine containing bulky phthalide group was successfully synthesized by a nucleophilic substitution reaction of phenolphthalein with *p*-bromonitrobenzene in the presence of K_2CO_3, followed by reduction of the dinitro compound by zinc dust and hydrochloric acid. Chiral diacid monomer, [*N,N′*-(4,4'-carbonyldiphthaloyl)]bis-L-alanine was synthesized through the reaction of 4,4′-carbonyldiphthalic anhydride and amino acid L-alanine in acetic acid in high yield. The direct polymerization reaction of the synthesized diamine with chiral dicarboxylic acid was produced a new optically active PAI. The obtained PAI and different weight percentages of functionalized ZnO nanoparticles (2, 4, 6, 8 and 10 wt.%) were used to prepare PAI/ZnO bionanocomposite films through ultrasonication assisted process. The PAI/ZnO bionanocomposite films were characterized by Fourier transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy and thermogravimetric analysis techniques.

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Formation of zwitterionic salts via three-component reaction of 2,6-dimethylpyridine, barbituric acid and dialkyl acetylenedicarboxylate

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Keywords: zwitterion, barbituric acid, 2,6-dimethylpyridine, dialkyl acetylenedicarboxylate.

A zwitterion, an ion pair where cation and anion are covalently tethered, is known to be a kind of salt. The charges on the different functional groups balance each other out, and the molecule as a whole is electrically neutral[1]. *N*-heterocycle zwitterions are reactive species that are widely used in organic synthesis, pharmaceuticals and bioinorganic chemistry.[2-4] Pyridine zwitterions are usually synthesized *via* the addition of pyridine derivatives to reactive double bonds or carbenes.[5-7] There are also some recent reports on the synthesis of *N*-heterocycle zwitterions by multi-component reactions.[8-10] Here we wish to report the result of our study on the reaction of 2,6-dimethylpyridine **1**, barbituric acid **2** and dimethyl or diethyl acetylenedicarboxylate **3** in dry acetonitrile as solvent lead to products **4** (Fig. 1). The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data and elemental analysiss.

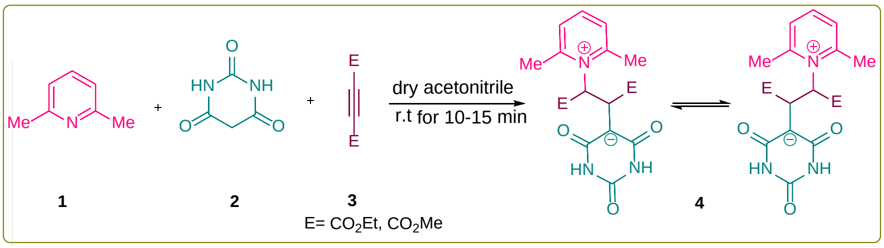

Fig. 1 zwitterionic salts **4**

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Optimization of the PMA@MIL-53 as a green catalyst for biodiesel production in the presence of ultrasonic illumination by using the CCD tab of the Design Expert Software

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Keywords: Biodiesel production, PMA@MIL-53(Fe), Esterification, Response surface methodology.

Due to environmental benefits such as lower air pollution, non-toxicity and biodegradability, biodiesel has become an extremely attractive biofuel.[1-3] Various methods have been reported for biodiesel production today.[4-5] In addition to the cost of raw materials, the main factor affecting the cost of biodiesel is the cost of processing. In this work, optimization of the PMA@MIL-53 as a green catalyst for biodiesel production in the presence of ultrasonic illumination were investigated using the CCD tab of the Design Expert Software. The factors were reaction time (5-20 Min), catalyst loading (50-200 Mg), PMA percentage (0-40 %), and Acid/Alcohol ratio (0.03125-0.15625). The catalytic activity of PMA@MIL-53(Fe) was investigated by using the esterification of oleic acid with propanol under ultrasound irradiation. The reaction was carried out at room temperature and catalyst was separated by centrifugation. The conversion of oil was analyzed with a GC-MS. The results show that the time of 20 minutes, the loading value of 100 mg of the catalyst and 30% of the heteropoly acid are the optimal reaction conditions. Comparison between the predicted data from the software and the actual (experimental), indicated that the proposed model well anticipated the interactions between the factors as well as their effects on the biodiesel production process by this method (Figure 1).

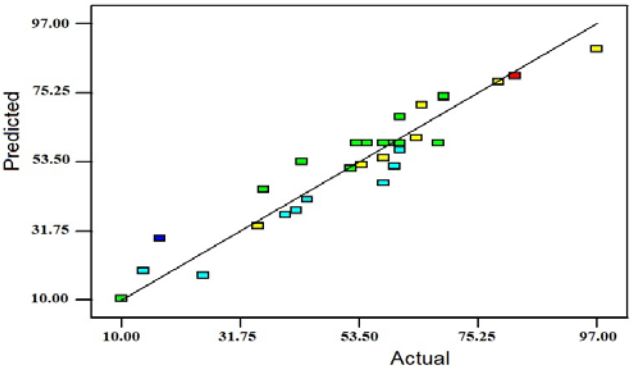

Fig. 1: comparison between the predicted data from the software and the actual (experimental).

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MoS_2-PNIPAM hydrogels as adsorbent for water purification

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Keywords: Hydrogel, Molybdenum disulfide nanosheets, Dye removal

MoS_2 is a prototypical two-dimensional (2D) transition-metal dichalcogenides (TMDs), which has emerged as a flagship material in the area of two-dimensional materials. 2D MoS_2 consist of atomic layers of Mo sandwiched between two layers of S atoms, through strong intralayer covalent bonding. [1-2] The functionalization of TMD is generally achieved at defect sites and is facilitated by electron transfer between the electron-rich metallic phase and electrophile reactants. Such reaction results in functional groups that are covalently attached to the chalcogen atoms of the TMD. Considerable efforts have been made to design functional hybrid TMD nanostructures by integrating of some of the unique properties of TMDs into polymeric materials to generate new functions and optimize their performance for varied applications.[3-4] In this work, N-isopropyl acryl amide (NIPAM) was polymerized at the surface of MoS_2 by stepwise reaction in the presence of *N*,*N′*-Methylenbisacrylamid. The obtained hybrid system was used to construct thermoresponsive filters by which different dyes could be specifically removed from water.

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Synthesize of hybrid membranes using Amylose modified MWCNTs as additives for potent HA removal

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Keywords: Polysaccharide, Am-MWCNTs-CA, Citric acid, polymeric membrane.

Up to now, a variety of polysaccharide additives materials such as cellulose, chitosan, starch, etc. were embedded in the casting solution of a polymeric membrane matrix to modify polymeric membranes. This result in improvement of the pore formation, the upgrading of surface hydrophilicity, enhancement of antifouling property as well as improved separation, reaction and sorption capacity.[1-2] Starch is specially one of the most promising natural polymers in many researches which was blended with various polymers and used for purpose of membrane fabrication.[3-4] In this work we were extracted amylose biopolymer from starch and used it for loading of MWCNTs by noncovalent interactions. Then their surfaces were modified with CA molecules by esterification reaction. Afterward, Am-MWCNTs-CA/PES mixed matrix membranes were fabricated. Finally, the effects of Am-MWCNTs-CA on the membrane properties such as performance, morphology, hydrophilicity, antifouling, and Humic acid (HA) removal were studied. AFM, SEM, ATR-IR etc. analyses have also been employed to characterize the obtained nanocomposite membranes.

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Synthesis new conductive copolymers based on aniline and melamine

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Keywords: Polyaniline, Melamine,Thermal conductive,Triphenylphosphate

Modifying the properties of polyaniline to improve its processability features is one of the wide researches in recent years. Polyaniline (PANI) is an organic conductive polymer and have recently attracted consideration because of their many applications in aerospace,[1] rechargeable batteries, solar cell, electrochromic switching, variable transmission, molecular sensors and non-linear optical materials.[2,3] In this research, copolymerization of aniline and melamine were carried out in different molar ratios in presence of ultrasonic irradiation. The SEM images from obtained copolymers showed that the size of particles was in nanometeric scale. The melamine is a low cast material with interesting properties and by introducing the melamine in polyaniline structure we expected to see new properties for conductive copolymers. The synthesized copolymer was characterized with different appropriate techniques such as FT-IR, SEM, CHN, TGA, DSC and PCFC. Also the obtained copolymers were studied by UV-Vis technique.

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Construction of alginate-arginine polymeric-based nano carriers for paclitaxel in cancer therapy

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Keywords: Arginine, sodium alginate, paclitaxel, drug delivery, breast cancer.

Nanoparticles of natural or synthetic biopolymers and polysaccharides have been developed and successfully employed for drug delivery applications. They are found to be the most promising and flexible drug delivery systems for transporting therapeutic agents into all parts of the body[1]. The sodium salts of alginic acid have emergedas one of the most extensively explored biomaterials for pharma-ceutical and biomedical applications[2,3]. In this study, paclitaxel, a typical chemotherapeutic agent, was selected as the model drug to evaluate of arginine-modified sodium alginate (SA) nanoparticles to load drug. The structure of nanoparticles was elucidated by FTIR. The shape, and morphology were determined by SEM. The mean size, polydispersity index (PDI) and zeta potential (ZP) of the obtained drug loaded nanoparticles were reported to be 342.2 nm, 0.360 and -12.2 mV, respectively.The in-vitro drug release was studied by using UV–Visible spectrophotometer at acidic environment and physiological pH and sustained release compared to the PTX alone. It was found that PTX drug is released much faster in pH 5.0 than in the pH 7.4. In addition, the cytotoxicity of the created nanoparticles was performed by using LDH assay analysis which showed that PTX loaded nanoparticles SA/Alg/PTX were toxic to MCF-7 cell line.

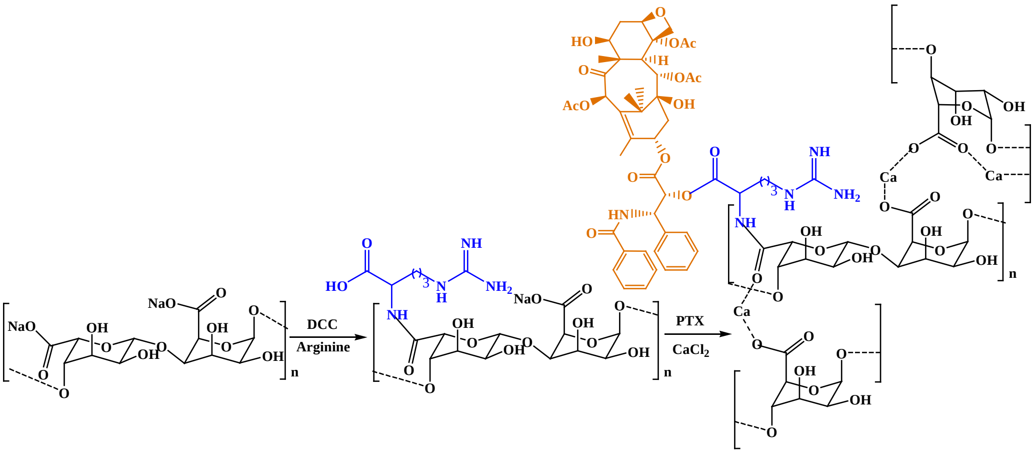

Fig. 1 Stages of synthesis of SA/Arg nanoparticles loaded with paclitaxel

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Synthesis of pyrido[2,3-d;6,5-*d*]dipyrimidine derivatives catalyzed by Methanesulfonic acid under solvent-free condition

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Keywords: Multicomponent reactions, 6-aminouracil, aromatic aldehydes, catalyst, solvent free.

Uracil is one of the five nucleobases and thus an important component of nucleic acids. Its chemistry and that of its derivatives, as these molecules can act as both nucleophiles and electrophiles, e.g. 6-aminouracil are very rich.[1] Uracils are widespread in natural products, because of their biological properties they are of interest. Uracil is an important component in helping enzymes carry out different reactions and the making of polysaccharides. 6-Aminouracils are used as raw materials for the synthesis of heterocyclic frames of biological significance, such as pyrido, pirrolo, and pyrimidopyrimidine.[2] Recent literature suggests that a new interest in the chemistry and biological properties of 6-aminouracil derivatives is indicative of improvement in several previous known reactions methods.[3]

In this research, in a reaction vessel, a mixture of 6-aminouracil (2mmol), and aldehyde (1mmol) in the presence of methanesulfonic acid (MSA) under solvent-free condition to afford pyrido[2,3-d;6,5-d]dipyrimidine derivatives in high to excellent yields as target products.

After completion of the reaction as followed by TLC, the reaction mixture was cooled to room temperature and then poured into cold water. The solid product was filtered and washed with boiling water to give the pure product in excellent yield.[4]

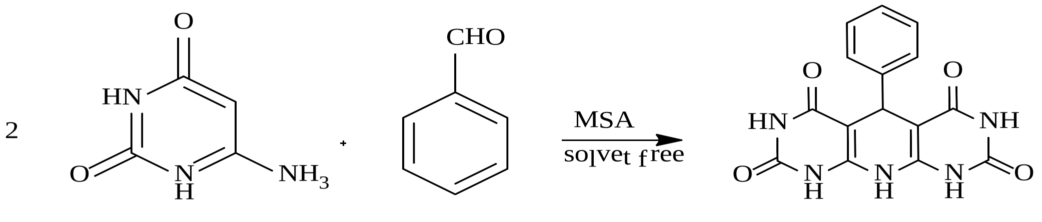

Fig1. Synthesis of pyrido[2,3-d;6,5-d]dipyrimidine derivatives

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One-pot Synthesis of the pyrimido[4,5-*d*]quinolones derivatives using methanesulfonic acid

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Keywords: Multicomponent reactions, 6-aminouracil ,aromatic aldehyde,
2-hydroxynaphthalene 1,4dione.

Uracil is an important component of nucleic acids and one of the five nucleobases. Its molecules can act as nucleophiles and electrophiles. [1] Uracil is an important component in helping enzymes carry out different reactions and the making of polysaccharides. Uracils are very common in natural products. 6-Aminouracils are used as raw materials for the synthesis of heterocyclic frameworks of biological significance. Recent literature shows 6-aminouracil derivatives leading to advancement in procedures of various already known reactions.[2],[3]

In a reaction vessel,a mixture of 6-aminouracil(1mmol),aldehyde(1mmol), 2-hydroxynaphthalene 1,4dione(1mmol) in the presence of Methanesulfonic acid (MSA) In H_2O/ETOH for 2hr afforded the pyrimido[4,5-d]quinolones. after complecction of the reaction as followed by TLC . the reaction mixture was cooled to room temperature and then poured in to cold water. The solid product was filtered and washed with boiling water to give the pure product in excellent yield.[4]

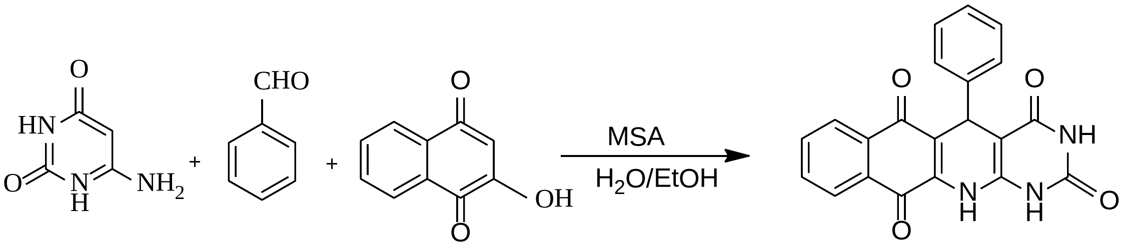

Fig. 1 Multicomponent reaction of pyrimido[4,5-d]quinolones derivatives

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Facile four component synthesis of pyrido[2,3-*d*:6,5-*d′*]-dipyrimidines catalyzed by [HNMP]$^+$[HSO4]$^-$ in water

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Keywords: Multicomponent reactions, Pyrido-dipyrimidines, Knoevenagel condensation, Aldehyde, 2-Thiobarbituric acid.

Multicomponent reactions (MCRs) are of importance in synthetic organic chemistry as they can produce complex molecules with greater efficacy and atom economy from three or more starting materials in a one step without isolation of intermediates[1-2]. MCRs have been shown to be environmentally friendly as they minimize the number of synthetic steps and workups, and eliminate isolation unstable intermediates. In addition, the synthesis of a broad range of complex products can be achieved by MCRs such as; knoevenagel condensation, and intermolecular cycloaddition, metathesis, aza-Wittig and Mitsunobu reaction thetic[2].

A simple, efficient method for the synthesis of pyrido[2,3-*d*:6,5-*d'*]dipyrimidine derivatives *via* one-pot four-component reaction of aromatic aldehydes (**1**), 2-thiobarbituric acid (**2**), ammonium aetate (**3**) in the presence of a catalytic amount of [H-NMP]$^+$[HSO4]$^-$ in water at room temperature is reported (Fig. 1). The process proved to be simple, environmentally friendly, efficient and high to excellent yielding. Moreover, some of the synthetic compounds were investigated and revealed important antimicrobial activity of prepared products.

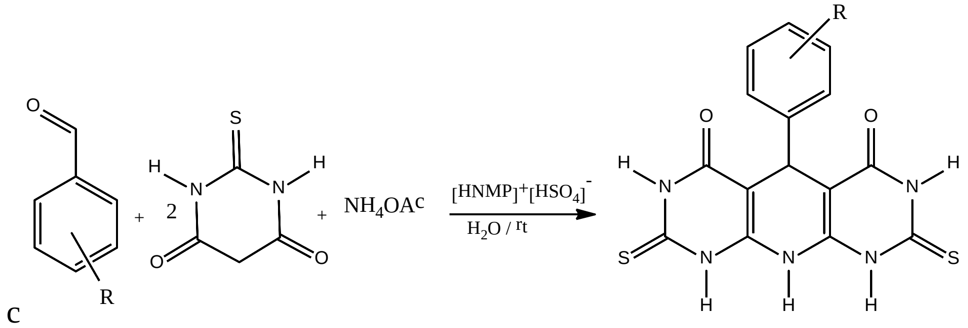

Fig. 1 Multicomponent reaction leading to the synthesis of novel pyrido[2,3-d]pyrimidine derivatives

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Highly efficient one-pot synthesis of *N*-(2,2-dicyanovinyl)-aniline in deep eutectic solvent

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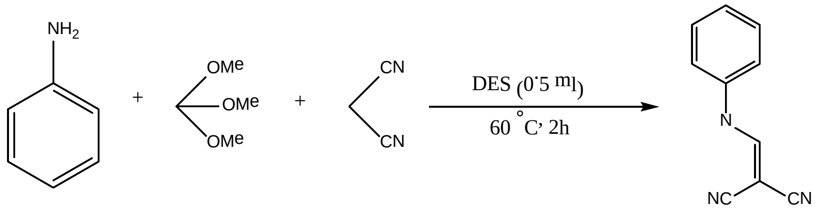
Keyword: *N*-(2,2-dicyanovinyl)-aniline, Alzheimer's Disease, Choline choloride/urea, synthesis of Tacrine

Alzheimer's disease (AD) is one of the most common diseases in the eldery. It is characterized by neuronal loss, synaptic damage, a deficit in neurotransmitter acetylcholine and vascular plaques. Still no precise explanation for the cause of this disease has yet been identified. The most recent method for the treatment of (AD) is suppresses acetylcholinesterase (AChE) to increase the acetylcholine (Ach) level in synapses. The available drug approved by the U.S food and Drug Administration (FDA) for the treatment Of AD are : Tacrine, Rivastigmine, Donepezil and Galantamine. One of the substance that is required for the synthesis of Tacrine is *N*-(2,2-dicyanovinyl)-aniline.[1,2]

In this research, we applied choline chloride/urea based deep eutectic solvent (DES) for three component synthesis of *N*-(2,2-dicyanovinyl)-aniline by the reaction of aniline derivatives and malononitrile and trimethylorthoformate at 60 °C. using DES has many advantages such as non-toxicity, cleaner and easier work-up procedures. This DES can be recycled four times without decrease in activity.



1 2 3 4

Fig.1: one-pot synthesis of *N*-(2,2-dicyanovinyl)-aniline in deep eutectic solvent

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Green multicomponent reaction for synthesis of α-aminonitrile in deep eutectic solvent

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Keywords: Strecker reaction, α-Aminonitrile, CH/urea

The Strecker reaction, discovered in 1850, has been recognized as the first multicomponent reaction published ever and has a central importance to the life sciences. Strecker reaction is an efficient method for producing a wide range of α-aminonitrile derivatives and is also one of the most important synthesis strategies for various types of α-amino acids and nitrogen cycles.[1]

In the classical Strecker method, acetaldehyde reacted with ammonia and hydrogen cyanide to produce α-amino acids. Due to the toxic and corrosive nature of hydrogen cyanid and the production of a wide range of by product, this approach was limited.

One of the modifications of the Streaker method is the use of cyanide agent such as trimethylsiloxynitrile and diethylphosphorocyanidates instead hydrogen cyanide.[2]

In this study, we used choline chloride/urea based deep eutectic solvent as a highly efficient reaction media and catalyst for greener synthesis of α-aminonitrile via one-pot three component reaction of aldehydes, amines and TMSCN under mild reaction conditions.

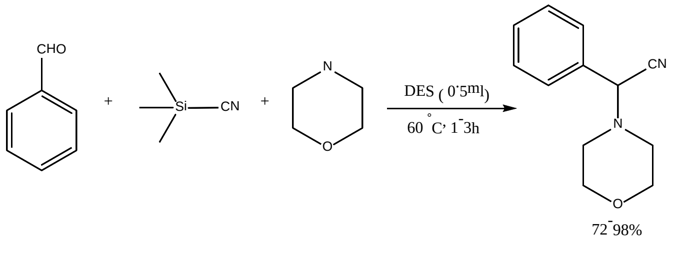

Fig. 1 one-pot synthesis of α-Aminonitrile in deep eutectic solvent

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An Efficient and One-pot Synthesis of Benzimidazoles Catalyzed via Nano-solid Acid Catalysts

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Keyword: *Benzimidazole, Solid acid catalyst, O-Diamine, Aldehyde*

Benzazoles such as benzimidazoles are considered as important class of heterocyclic compounds possessing interesting biological and pharmacological properties as anti-fungal, anti-oxidant, anti-inflammatory, anti-bacterial, anti-viral and anti-cancer agents [1]. The most attractive method for the synthesis of benzimidazoles[2] is the reaction of 1,2-phenelynediamine with aldehydes [3]. Recently reported methods mostly employed homogeneous catalysts which require special work-up and separation technique for the recovery and recycling form the reaction environment. Following our studies in this field[4] .In this research, $Fe_3O_4@SiO_2@COOH$ as a new, high efficient and green solid acid catalyst has been prepared and used for the synthesis of benzimidazoles under solvent free conditions. The recovery and reuse of a catalyst is highly desirable during its practical application. We were able to recycle this catalyst five times and use it in reaction, without reducing the efficiency of the product.

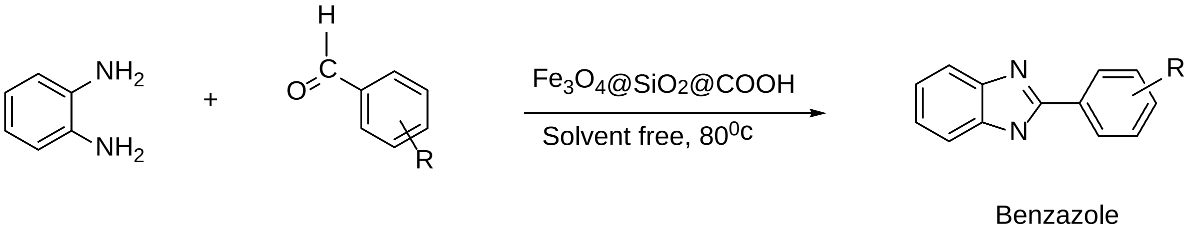

Fig. 1 Synthesis of benzimidazoles catalyzed via nano-solid acid catalysts

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An efficient and one-pot synthesis of benzimidazoles catalyzed via nano-solid acid catalysts

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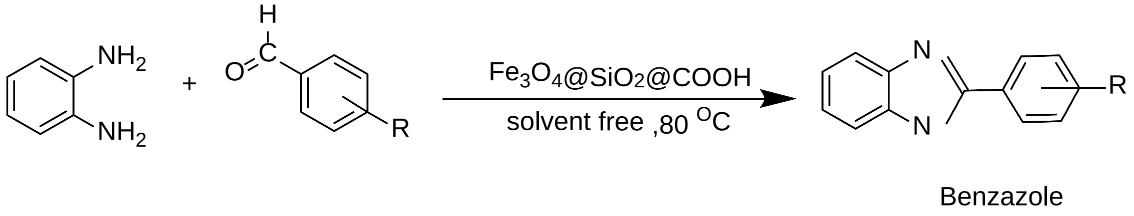
Keyword: benzimidazole, solid acid catalyst, O-diamine, aldehyde

Benzazoles such as benzimidazoles are considered as important class of heterocyclic compounds possessing interesting biological and pharmacological properties as anti-fungal, anti-oxidant, anti-inflammatory, anti-bacterial, anti-viral and anti-cancer agents [1]. The most attractive method for the synthesis of benzimidazoles[2] is the reaction of 1,2-phenelynediamine with aldehydes [3]. Recently reported methods mostly employed homogeneous catalysts which require special work-up and separation technique for the recovery and recycling form the reaction environment. Following our studies in this field[4] .In this research, $Fe_3O_4@SiO_2@COOH$ as a new, high efficient and green solid acid catalyst has been prepared and used for the synthesis of benzimidazoles under solvent free conditions. The recovery and reuse of a catalyst is highly desirable during its practical application. We were able to recycle this catalyst five times and use it in reaction, without reducing the efficiency of the product.



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Synthesis of DBU-based ionic liquids as the novel and green catalysts and use them in the synthesis of 1H-pyrazolo [1, 2-*b*] phthalazine-5, 10-diones under solvent-free conditions

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Keywords: Ionic liquid, 1,8-diazobicyclo [5.4.0] undec-7-ene-8-benzylium, ^{1}HNMR, FTIR.

Ionic liquids (ILs) are a fascinating class of low melting salts that generally are composed of large unsymmetrical organic cation and a weakly-coordinating inorganic or organic anion.[1,2] At first, we synthesized two aprotic ionic liquids composed of 1,8-diazobicyclo [5.4.0] undec-7-ene-8-benzylium ([Bn-DBU]$^+$) cation and $[CH_3CO_2]^-$ and $[CF_3CO_2]^-$ anions and characterized experimentally by the combined of ^{1}HNMR and FTIR spectroscopies, and thermogravimetric analysis (TGA).

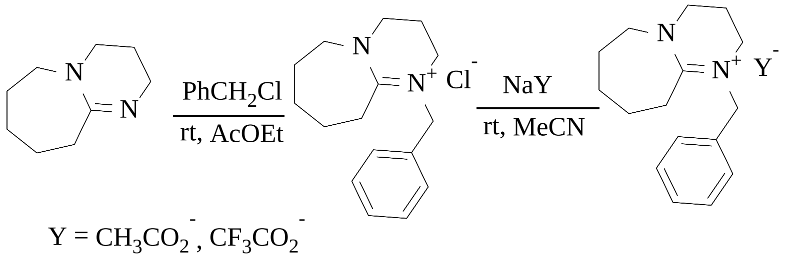

Fig. 1 synthesized Bn-DBU-based ionic liquid with above method.

The study of the various properties of N-substituted DBU-based ILs proved the advantages and uniqueness of these ILs as catalyst in different organic reactions.[3,4] In the following, we use the [Bn-DBU][Y_{1-2}], ($Y = CH_3CO_2$ and CF_3CO_2) ILs as catalyst in synthesis of 1*H*-pyrazolo [1, 2-*b*] phthalazine-5, 10-diones from reaction phthalhydrazid, aromatic aldehyde and malononitrile under solvent free condition at 100 °C.

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Superabsorbent polymers: materials, preparation and application

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Keywords: Superabsorbent, Hydrogel, Agriculture, Swelling, Water Absorbency.

Scarcity and misuse of water reservoirs is a major global issue excruciating by the increase in population and pose serious and growing threats to sustainable development and protection of the environment. Saving water in irrigation is a vital solution in protecting water reservoirs.[1] Superabsorbent polymers (SAPs) are lightly crosslinked hydrophilic hydrogels, which can absorb up to 2000 g/g water with reversible swelling properties.[2] In the past decade, many researchers have been focused in the field of particulate composites of hydrogels. Meanwhile, many of those have focused on superabsorbent hydrogel composites, and superabsorbent hydrogel nanocomposites.[3] Due to their unique properties, superabsorbent nanocomposites can find applications in different areas including agriculture, hygiene products, ion and dye removal, controlled release and sanitary products.[2-4] These smart materials and smart delivery systems helped the agricultural industries to increase the efficiency of pesticides and herbicides, allowing lower doses to be used and protect environment.[1] This report will review the key aspects of used superabsorbent polymers in agricultural area and highlighting the different classification and production background of superabsorbent polymers.

Fig. 1

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Synthesis of biaryls by chitosan-2-thiophenecarbaldhyde supported palladium complex under air conditions

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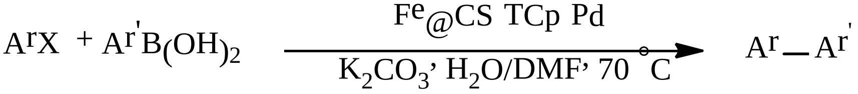
Keywords: Cross-coupling reaction, Palladium complex, Suzuki reaction, Chitosan, Thiophenecarbaldhyde.

Palladium catalyzed carbon-carbon bond-forming reactions have played a crucial role in synthetic organic chemistry. Heterogeneous catalyst in the Suzuki-Miyaura coupling of arylboronic acids and aryl halides represent as the most successful methods for the preparation of biaryls.[1] This reaction have shown to have widespread applications in the synthesis of natural products, biologically active molecules, and materials science.[2] Recently, polymers[3] especially biodegradable polymers[4] are used in the synthesis of heterogeneous catalysts. Herein, we have reported an environmental magnetic chitosan-2-thiophenecarbaldhyde based palladium complex (Fe@CS-TCp-Pd), which was efficiently used as a heterogeneous catalyst for Suzuki-Miyaura cross-coupling reactions in aqueous media under air condition. The catalyst shows not only high catalytic activity, but also offers many practical advantages such as thermal stability, and recyclability. The catalyst was reused for seven consecutive runs in Suzuki-Miyaura reaction with consistent activity. The excellent catalytic performance in aqueous media and the easy separation of the catalyst make it a good heterogeneous system and a useful alternative to other heterogeneous palladium catalysts. All the products were characterized by IR, ^{1}H, and ^{13}C NMR spectroscopy.



$$\mathrm{ArX} + \mathrm{Ar'B(OH)_2} \xrightarrow[\mathrm{K_2CO_3,\ H_2O/DMF,\ 70\ ^\circ C}]{\mathrm{Fe@CS\text{-}TCp\text{-}Pd}} \mathrm{Ar{-}Ar'}$$

Fig. 1 Suzuki-Miyaura cross-coupling reactions of aryl halides with arylboronic acids

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Covalently Bonded PIDA on SBA-15: A versatile new support for the synthesis of Palladium pre-catalyst

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Keywords: SBA-15, Suzuki reaction, Pd@SBA-15/PIDA, Heterogeneous catalyst.

Very recently, design of a heterogeneous catalyst with higher efficiency has been directed towards the development of stable supporting ligands, complexes and other catalytic species onto nanostructured materials [1, 2]. Among nanostructured materials, silica mesoporous materials (SBA-15) owing to their higher stability and surface area are most popular for such purposes [3]. I this study, we functionalized its analogue *N*-propyliminodiacetic acid (PIDA) onto SBA-15 (SBA-15/PIDA) as support of Pd^{II} ions to generate a Pd^{II}@SBA-15/PIDA catalyst Figure 1. Finally, performance catalytic Pd^{II}@SBA-15/PIDA was subsequently investigated in the Suzuki reaction with excellent conversion.

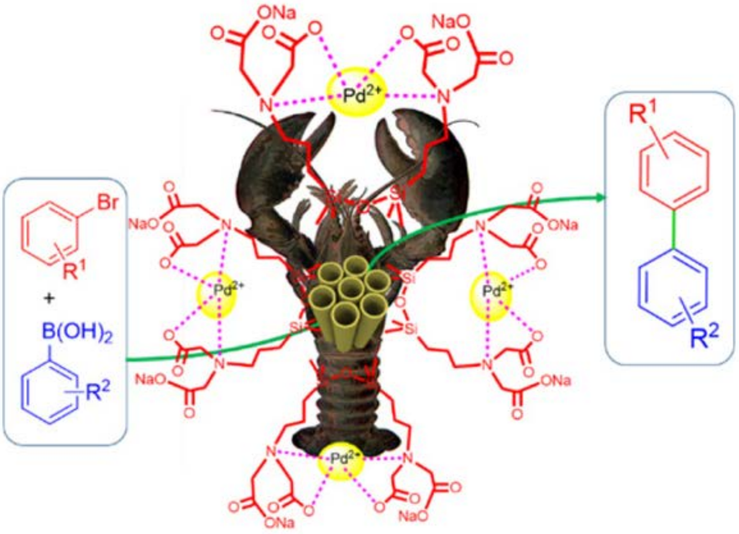

Fig. 1 Catalyst functionalisation Pd@SBA-15/PIDA for the proposed C-C couplings.

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Synthesis of a novel series of 1,4-dihyropyridine-triarylmethane hybrid derivatives

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Keywords: 1,4-Dihydropyridines, Three-Component reactions, Triarylmethanes, Hantzsch reaction, $ZrCl_4$/[Bmim][PF_6].

Over the past several decades, the synthesis of N-containing heterocyclic compounds has been a developing area of research within the realm of heterocylic chemistry.[1] Of N-heterocycles, 1,4-dihydropyridines (DHPs) are of great significance due to their wide range of chemical reactivity and broad spectrum of biological and pharmaceutical properties.[2] So far, many efforts have been devoted for the synthesis of various 1,4-dihydropyridine derivatives.[3] However, designing and synthesis of novel 1,4-DHPs is still in demand. In continuation of our research on triarylmethanes,[4] herein we wish to report the synthesis of novel 1,4-dihydropyridines bearing a triarylmethane moiety. The structures of the synthesized compounds were characterized by elemental analyses, and FT-IR, ^{1}H-NMR, and ^{13}C-NMR spectral data.

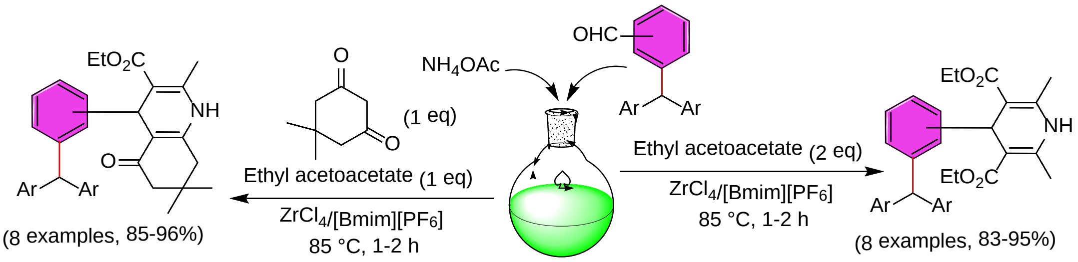

Fig. 1 Synthesis of novel 1,4-dihydropyridines-triarylmethane hybrid derivatives

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Synthesis of Co nanoparticles supported on cellulose: a magnetically recoverable and cost effective catalyst for the degradation of congo red and methyl orange

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Keywords: Cellulose, Degradation, Metal nanoparticles, Nanocomposite.

Dyes and pigments are important organic industrial raw materials which are widely used in textile, cosmetic, printing, drug and food-processing industries.[1] Most of the dyes are toxic to aquatic organisms. Thus, there is a drastic need to develop eco-friendly treatment methods for the elimination of these pollutants from the environment, because of their toxicity and carcinogenic properties.[2] Although conventional chemical and physical techniques such as precipitation, adsorption, and ozonation have been employed for the decolorization of dye effluents, they possess inherent limitations such as high cost, formation of hazardous by-products, and intensive energy requirements.[3] In recent years, metal nanoparticles (MNPs) have been used for the degradation of organic dyes due to their interesting structure, large specific surface area, strong electron transfer abilities and high catalytic activities.[1] Among various metal nanoparticles, cobalt nanoparticles have attracted particular attention because of their excellent electrical, magnetic and catalytic properties.[4] In the current work, we synthesis the magnetic cobalt nanoparticles supported on cellulose (Co NPs/Cellulose) (Scheme 1). The prepared nanocomposite was found to be highly efficient catalyst for the degradation of Congo red (CR) and Methyl orange (MO), with excess amounts of $NaBH_4$ in water at room temperature. Furthermore, the nanocomposite could be easily separated from the reaction media by an external magnet and reused three times without significant loss of activity.

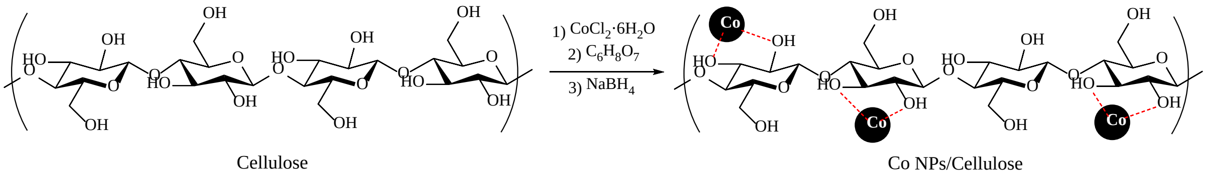

Fig 1. Synthesis of Co NPs/Cellulose nanocomposite

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Synthesis of new derivatives of Sulfones under solvent-free conditions

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Keywords: Organosulfur compounds, Sulfones, Michael reaction, Solvent-free reactions

A large variety of organosulfur compounds have been shown to having diverse biological effects such as antioxidant effects, anti-inflammatory properties, inhibition of platelet aggregation, reduction of systolic blood pressure, and reduction of cholesterol.[8] Sulfones are S, S-dioxides of ether and represented by general structural formula $R\text{-}S(O)_2\text{-}R$, where R and R are organic groups. The chemistry of sulfones has been explored due to their importance as synthetic intermediates for the production of a wide range of chemically and biologically active molecules.[2] The Michael reaction has been used widely in organic synthesis for the formation of carbon-carbon bond and carbon-heteroatom ability.[3] The conjugate addition of sulfur-centered nucleophiles to α, β-unsaturated carbonyl compounds or related derivatives, also regarded to as the sulfa-Michael reaction, is a powerful methodology for the formation of C−S bonds.[4] Solvent-free reactions obviously reduce pollution, and bring down handling costs due to simplification of experimental procedure, work up technique and saving in labor.[5] In this work, we describe a new, simple and efficient strategy for the formation of novel and valuable sulfone derivatives under solvent-free conditions.

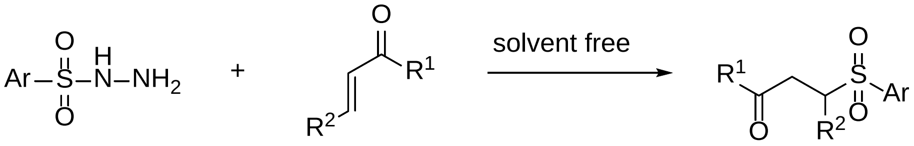

Fig. 1

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$H_3PW_{12}O_{40}$/[Bmim][PF_6]-catalyzed multicomponent synthesis of novel 1-amino- and 1-amidoalkyl-2-naphthol derivatives

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Keywords: Triarylmethanes, Naphthol derivatives, Multicomponent reactions, $H_3PW_{12}O_{40}$, [Bmim][PF_6].

Multicomponent Reactions (MCRs) are a fundamental tool in modern synthetic methodology, which are used to combine simultaneously three or more reactants in a single reaction vessel to form a new product.[1] MCRs have been widely used for the synthesis of amino- and amidoalkyl naphthols.[2] Triarylmethanes (TRAMs) have been used as dyes, protecting groups, photochromic agents, optical active devices, and therapeutic agents.[3] Although they can be prepared successfully using several methods, less attention has been paid to develop their synthetic applications until now.[4] In continuation of our research on TRAMs,[5] herein we wish to report the synthesis of novel 1-amino- and 1-amidoalkyl-2-naphthol derivatives employing a one-pot three-component condensation reaction of *β*-naphthol, formylated-triarylmethanes, and amine or amides in the presence of $H_3PW_{12}O_{40}$/[Bmim][PF_6] as Catalyst. The structures of the synthesized compounds were characterized by elemental analyses, and FT-IR, ^{1}H-NMR, and ^{13}C-NMR spectral data.

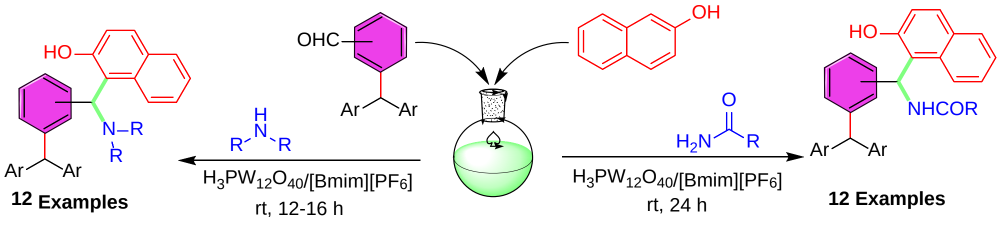

Fig. 1 Synthesis of novel 1-amino- and 1-amidomethyl-2-naphthol derivatives

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Catalytic performance of vanadyl pyrophosphate-KIT-6 on dehydration of glucose and fructose into 5-hydroxymethylfurfural

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Keywords: Biomass conversion**,** 5-hydroxymethylfurfural, Glucose and fructose dehydration, Mesoporous KIT-6 silica, VPO catalyst.

Vanadium phosphate oxide compounds (VPO) are heterogeneous catalysts having different phases and morphologies. Vanadyl pyrophosphate phase has been vastly applied in the industry for the oxidation of butane into maleic anhydride.[1] While application of VPO catalysts in oxidation reactions have been widely documented, there are a few reports on the application of these interesting materials as the solid acid catalyst. We synthesized a series of vanadyl pyrophosphate catalysts supported on the surface of KIT-6 in the mixture of benzyl alcohol/*iso*-butyl alcohol. The catalysts, as the solid acid, employed in dehydration reaction of fructose and glucose into 5-HMF, due to the importance of 5-HMF.[2,3] The catalysts were characterized by FT-IR spectroscopy, Raman spectroscopy, ICP-OES, XRD, BET, and NH_3-TPD techniques as well as SEM, TEM, and XPS. The current study obviously illustrated the role of surface area on the catalytic performance of these types of catalysts in the selective dehydration of fructose and glucose into 5-HMF.

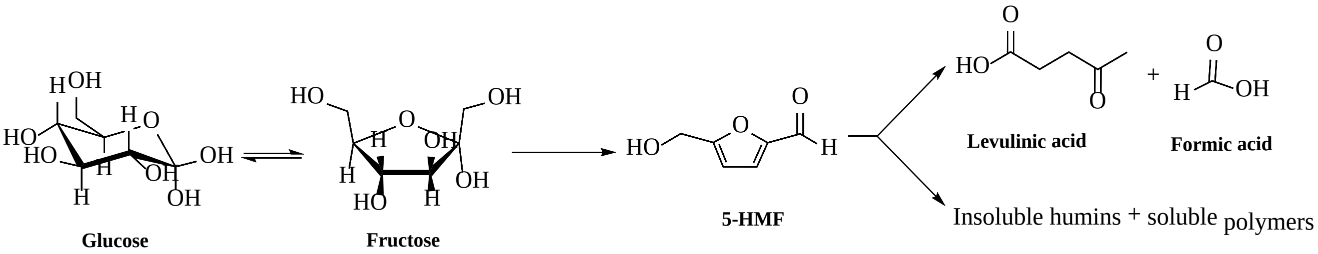

Fig. 1 Pathway of dehydration reaction of glucose and fructose into 5-HMF and other products.

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Synthesis of boron ester-containing additives for lubrication

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Keywords: Boron ester, Antiwear, Antioxidant, Lubricant, Additives.

Lubricating oil is a functional material applied for separating two surfaces. During the last decades, additives have been added to the lubricants to give them special properties and improve their lubrication performance.[1] Boron and boronate compounds are widely used in a range of tribological applications such as friction modifiers, antioxidants, antiwear additives, and in many cases as environmentally friendly lubricants oils and fuels. To improve the hydrolytic stability of borate esters, the addition of some amine compounds to produce additional molecular coordination is used.[2] added of electron-rich groups (such as nitrogen atom) into borate ester, to stabilize the electron-deficient of boron atom, and that can reduce the possibility of attack by some nucleophiles. More importantly, it can enhance antiwear performance for the synergetic effect between boron and nitrogen element.[3] Herein, we report the synthesis of boron ester-containing additives to improve the performance of a lubricating oil from the reaction between fatty acids and boric acid with secondary amine in toluene solvent at 250 °C. Finally, a reddish viscous liquid was obtained. It has the ability to dissolve in oil, as well as its antioxidant properties and viscosity. All synthesized compounds are stable materials whose structure is based on their mass spectra, ^{1}H and ^{13}C-NMR and IR spectroscopy data.

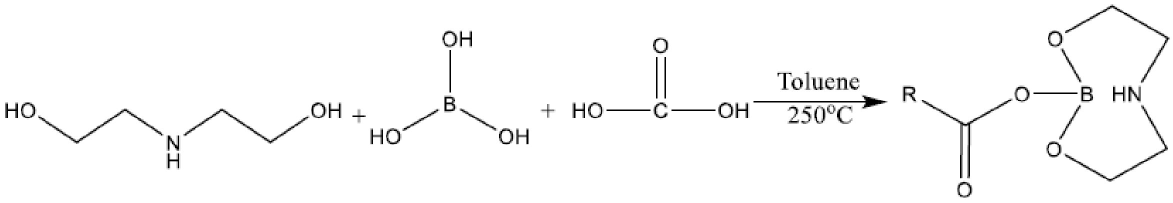

Fig 1. Schematic synthesis of boron ester-containing additives

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Synthesis and applications of boron-based ILs

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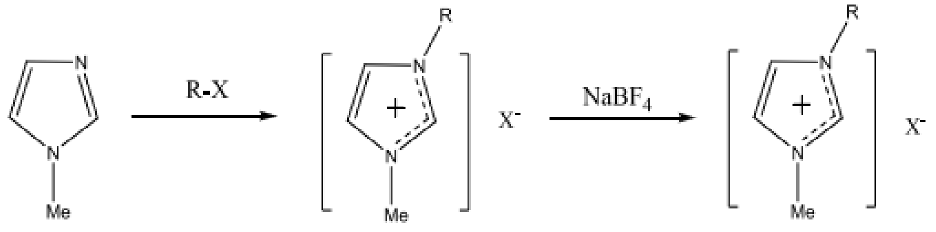
Keywords: Ionic liquids, Lubrican, Lubricants additives, Boron.

In spite of ILs appealing physicochemical properties that perfectly fit specifications for high-performance lubricants, they were not studied in tribological contacts until a decade ago. [1] Some researchers have shown that a small family of ILs can also be incorporated into non-polar base oils, replacing traditional anti-wear additives, with excellent performance of the neat IL being maintained.[2] Scientists have reported that BILs composed of $[BF_4]^-$ anion and various alkylimidazolium cations $[CnCmIm]^+$, n and m = 1, 2, 3. They concluded that alkylimidazolium tetrafluoroborates, [CnCmIm][BF4], have excellent lubricity in steel–steel, steel–aluminum, steel–copper, steel–SiO_2, steel–Si(100), steel–sialon, and Si_3N_4–sialon ceramic contacts, making them attractive alternatives to conventional liquid lubricants.[3] Most of the ILs successfully employed as lubricants in various ferrous and non-ferrous tribological contacts during the past decade and are predominantly based on the boronbased anion, $[BF_4]^-$. In this work, we report the synthesis and application of alkylimidazolium tetrafluoroborates of boron-based ILs. Initially, imidazole refluxed with sodium hydroxide in a THF solvent and 60 °C. The resulting product was refluxed with 1-bromobutane and the viscous yellow liquid was obtained. Then addition of a halide salt to obtained mixture in room temperature forms ionic liquid.



R = Alkyl
X = Cl, Br or I

R = Alkyl
X = BF_4, or PF_6

Fig 1. Preparation route for boron-based ionic liquid

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Asymmetric arylation of aldehyde in the presence of L-proline@Fe_3O_4

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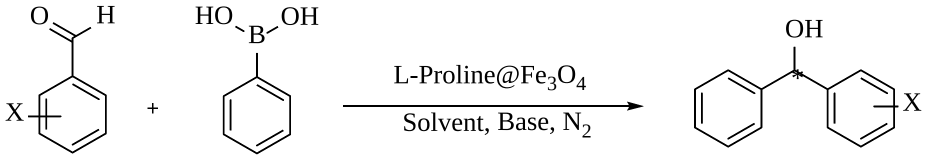
Keywords: Aldehyde, Chiral nanoligand, Asymmetric arylation, Alcohol

Recently, the investigation of chiral nanoligand for asymmetric synthesis is getting much importance. These nanoligands offer a powerful method for the preparation of optically active molecules that can act as precursors for other useful organic compounds.[1,2] In the other hands, the magnetic property, separation effect, and the high activity during cyclic utilization of Fe_3O_4 nanoligand are evaluated and indicated they could be used in various organic reactions.[3]

In this work, in order to develop an innovative approach toward the design of recoverable and reusable asymmetric nanoligand for C-C bond formation reactions, we have investigated the catalytic activity of L-proline-functionalized Fe_3O_4-nanoparticle catalyst on the arylation of aromatic aldehyde **1** by boron reagents **2** in the presence of prepared L-Proline@Fe_3O_4 which have proceeded with high enantioselectivity to produce the chiral diarylmethanols **3** (Scheme 1). The structure and morphology of prepared nanoligand L-Proline@Fe_3O_4 were characterized by scanning electron microscopy, and Fourier transforms infrared spectroscopy. The structure of chiral products are investigated by melting point, IR, ^{1}H NMR and ^{13}C NMR spectroscopies. The enantiomeric excess (ee) of chiral products is also detected by polarimeter.



1 **2** **3**

Scheme 1 Asymmetric arylation of aromatic aldehyde in the presence of L-Proline@Fe_3O_4

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A straightforward approach for the synthesis of diverse derivatives of a novel selenium containing heterocyclic system [1,3]selenazolo[4,5-d]pyrimidine-5(4*H*)-thione using phenyl isothiocyanates

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Keywords: Selenazoles, Phenyl isothiocyanates, One-pot procedure, Selenium containing heterocyclic system

In the recent years, selenazoles have been reported to have very unique chemical and biological properties such as inactivation of free radicals,[1] antioxidant,[2] cancer cell proliferation [3] and protein kinase activation [4]. In view of the importance of these heterocyclic cores, many synthetic methodologies have been reported in the literature [5]. Herein, we wish to report a one-pot procedure for the synthesis of various derivatives of [1,3]selenazolo[4,5-*d*]pyrimidine-5(4*H*)-thione as a novel selenium containing heterocyclic system. These potential pharmacologically active derivatives **3 (a-i)** were synthesized via heterocyclization of 4-amino-2-(*sec*-amin substituted)-5-carbonitrile-1,3-selenazoles **1 (a-c)** with various phenyl isothiocyanates **2 (a-c)** in the presence of pyridine in excellent yields. The structural assignments of all the newly synthesized compounds are based upon spectroscopic and microanalytical data.

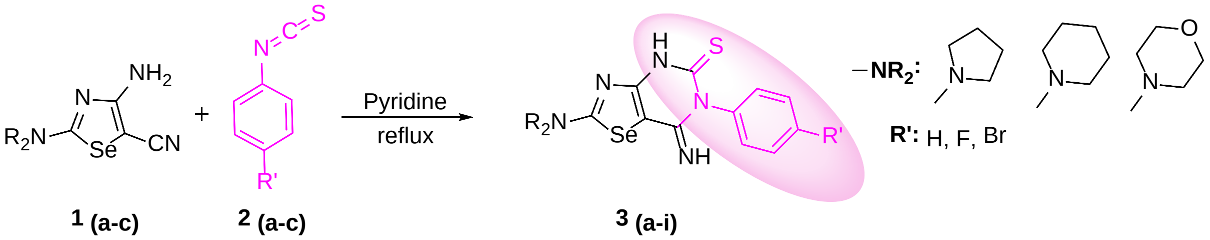

Fig 1. Synthesis of [1,3]selenazolo[4,5-*d*]pyrimidine-5(4*H*)-thione.

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Synthesis of various derivatives of [1,3]selenazolo[4,5-*d*]pyrimidine as a novel selenazolocondenced heterocyclic system

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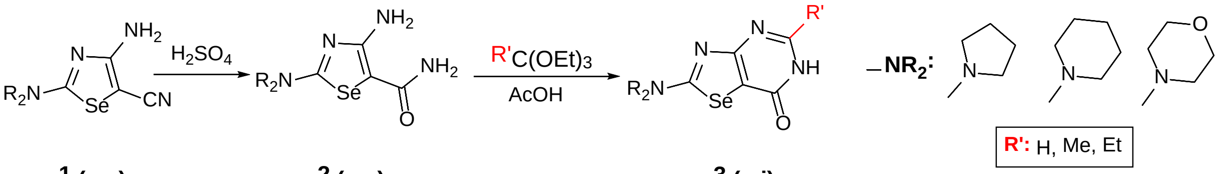
Keywords: Selenazolocondenced heterocyclic system, [1,3]Selenazolo[4,5-*d*]pyrimidin.

Selenium used to be considered as an essential nutrient, constituent of selenoproteins involved in self-defense mechanism against oxidative stress,[1] in reducing certain inflammatory processes and in detoxification processes [2]. Based on the benefits associated to the presence of selenium, the synthesis of many heterocyclic systems characterized by a large variety of biological activities was developed. Among them, amino-1,3-selenazole ring systems have received much attention from medicinal chemists worldwide because of their wide range of biological activity, such as antimicrobial, anti-HIV, antioxidant and anticancer, among others.[3,4] Due to widespread biological activities of 1,3-selenazols and our interest for the synthesis of selenazolocondenced heterocyclic systems, in the present protocol, concentrated sulfuric acid mediated hydrolysis of compounds **1 (a-c)** gave the corresponding 4-amino-1,3-selenazole-5-carboxamides **2 (a-c)** which subsequently underwent the heterocyclization reaction with some triethylorthoesters to yield various derivatives of a novel heterocyclic system of [1,3]selenazolo[4,5-*d*]pyrimidine **3 (a-i)** in excellent yields with potential biological activities.



1 (a-c) **2 (a-c)** **3 (a-i)**

Fig. 1 Synthesis of [1,3]Selenazolo[4,5-*d*]pyrimidin.

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Arylation of electron-deficient double bonds through metal-catalyzed reactions

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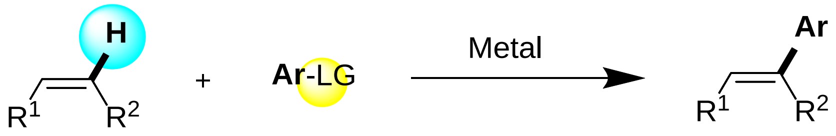
Keywords: Arylation, Carbon-carbon bond formation, C-H activation.

It has been quite a while that synthesis of organic frameworks through metal-mediated reactions has gained organic chemists' attention.[1] The underlying reason behind their wide application is that transition metals possess a special aptitude for C–H bond activation which facilitates practical and economical functionalization of organic molecules.[2]

Among all procedures being put forth in this area, molecules having to leave groups which produce only gaseous waste are highly satisfactory since they are in accordance with Green Chemistry postulates.[3] Thus, due to the superb attribute of these starting materials, we set our mind to take advantage of these substances and functionalize electron-deficient heterocycles by the aid of transition metals as promoters. The obtained moieties due to having double bonds in their building blocks can have wide applications ranging from biology to the materials sciences.



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Efficient synthesis of benzoimidazoquinoline derivatives

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Keywords: Benzoimidazoquinoline, Catalyst, I_2.

The benzoimidazoquinoline core is one of the most important heterocycles since it has not only found widespread applications in medicinal chemistry and drug synthesis but because it is also broadly used in material science.[1] Consequently, it has attracted considerable interest for synthetic chemists and stimulated the development of numerous methods for their preparation.[2] Hearin, we report synthesis of benzoimidazoquinoline derivatives **2** from the intermolecular reaction of 2-(1*H*-benzo[*d*]imidazol-2-yl)-3-phenylacrylonitrile **1** in the present of I_2/KI as catalyst in DMSO solvent (Fig. 1). All synthesized compounds are stable solids whose structures were determined on the basis of ^{1}H and ^{13}C NMR and IR spectroscopic data.

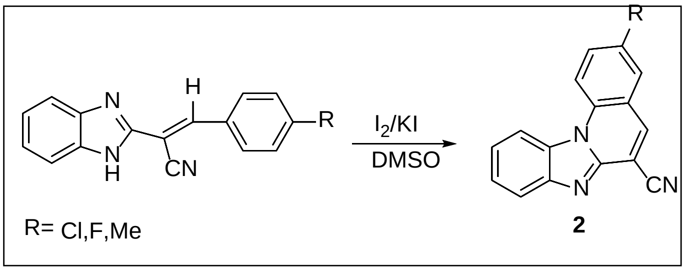

Fig. 1 Syntheis of benzoimidazoquinoline derivatives.

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Survey tri-components reaction of trifluoroacethymidoyl chloride, isocyanide and quinoline

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Keywords: Pyrimido[5,1-*a*]isoquinolines, Pyrimido[5,1-*a*]pyridines, Pyrimido[5,1-*a*]quinolines, N-Benzyl-2,2,2-trifluoroacetimidoyl chlorides, Cyclohexylisocyanide.

Amongst heterocyclic compounds, nitrogen heterocycles are very important. pyrimido[5,1-a]isoquinolines, pyrimido[5,1-*a*]pyridines and pyrimido[5,1-*a*]quinolines as the most stable, nitrogen-riched heterocyclic compounds show high levels of biological activities.[1] Nitrogen heterocyclic compounds contain trifluoromethyl substitute are very interesting due to the strong electron-withdrawing effect of the CF_3 group which contributes to a number of biologically properties.[2] These compounds are interesting as physiologically active agents.[3] Herein we wish to report, a highly efficient method for synthesis of triflouromethylated pyrimido[5,1-*a*]isoquinolines **4**, pyrimido[5,1-*a*]pyridines **5** and pyrimido[5,1-*a*]quinolines **6** derivatives from reaction of N-alkyl-benzimidoyl chlorides **1** (prepared in situ from the corresponding benzylamine, triphenylphosphine and CCl_4), with isoquinoline **3a**/ pyridine **3b** or quinolone **3c** and cyclohexylisocyanide **2** in present of base under reflux conditions in dry CH_3CN (Fig. 1).

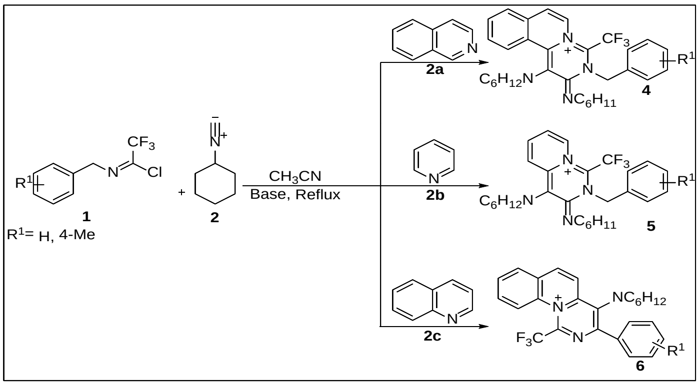

Fig. 1 Synthesis trifluoromethylate pyrimido[5,1-*a*]isoquinolines, pyrimido[5,1-*a*]pyridines and pyrimido[5,1-*a*]quinolones.

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Synthesis of anti-bacterial polymer based on polyvinyl alcohol

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Keywords: Antimicrobial, polymers, Isoquinoline, Polyvinyl alcohol.

The design and synthesis of antimicrobial polymers have gained increasing attention regarding concerns on microbial infection and safety.[1] Some of polymeric quaternary ammonium based on PVA have microbial properties and may be useful for many application such as biomedical devices, tissue engineering, wound dressing, surface coatings and additives for antifouling, paints and packaging containers.[2,3] Now, we report a new synthesis of a polymeric compound using PVA, isoquinoline and (3-choloropropyl) trimethoxysilane (Fig1). Examining this polymeric compound indicate very good antibacterial ability against E.coli, and S. aureus.

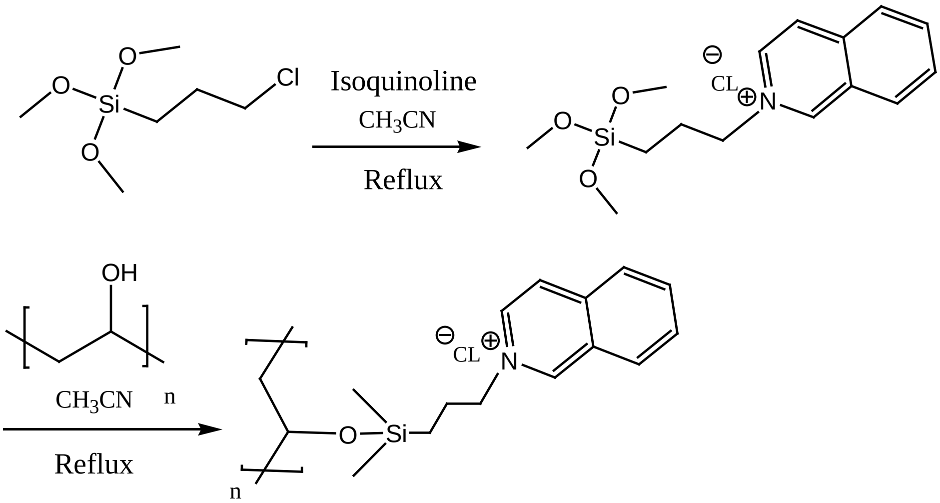

Fig. 1 Synthesis of anti-bacterial polymer based on polyvinyl alcohol

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Nef-isocyanide-Perkow access to novel pyrazolone derivations containing a cyclic ketene dithioacetal moiety

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Keywords: Pyrazolone, Nef-isocyanide-Perkow reaction, Cyclic ketene dithioacetal, CS_2, Polarized double bond

Pyrazolone compounds are privileged scaffolds in organic synthesis by virtue of their potential biological activities and wide-ranging utility as synthetic intermediates.[1] Bioactive compounds bearing pyrazolone systems have attracted much interest in medicinal chemistry. Recently, the construction of structurally diverse pyrazolone derivatives has attracted the research interests of synthetic chemists. As part of our current studies on developments of new applications of pyrazolone derivatives in heterocyclic synthesis,[2,3] we now report the formation of novel cyclic ketene dithioacetals containing a pyrazolone motif from the reaction between 2-pyrazolin-5-ones-CS_2 adduct and phosphorylated hydroxyketenimines [generated in situ from Nef-isocyanide Perkow reaction], in the presence of Et_3N as a base, at room temperature.[4] The structures of the products were determined by their spectroscopic data and X-ray crystallography. Various features of these transformations will be presented and discussed.

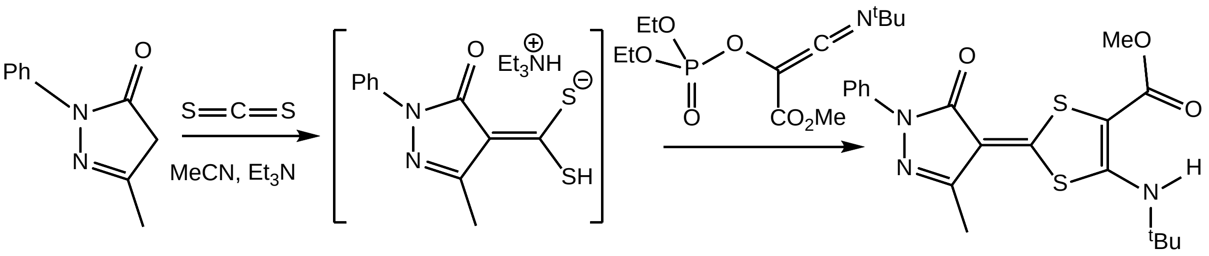

Fig. 1 Synthesis of alkyl (*E*)-2-(3-alkyl-5-oxo-1-phenyl-1,5-dihydro-4*H*-pyrazol-4-ylidene)-5-(alkylamino)-1,3-dithiole-4-carboxylates

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One-pot solvent-free synthesis of 3,4-dihydropyridin-2-(1*H*)-ones derivatives using a new acidic ionic liquid catalyst

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Keywords: Ionic liquids, Multicomponent reactions, Biginelli reactions, Knoevenagel condensation, 3,4-dihydropyridin-2-(1*H*)-ones.

Ionic liquids (ILs) are considered as powerful alternatives to conventional molecular organic solvents and catalysts and have various applications in the field of chemical synthesis. This is due to their particular properties such as non-flammable, recyclable, low vapor pressure, high thermal and chemical stability and the ability to dissolve the wide range of organic compounds [1,2].

Dihydropyrimidinones are important for their therapeutic and pharmacological properties. They are used in several calcium channel blockers, antihypertensive drugs and etc. Recently, dihydropyrimidinones have also been considered for the development of new anticancer drugs[3].

In this study, a new Bronsted acidic ionic liquid based on succinimide was easily prepared and characterized using various techniques. The reagent showed excellent activity in the promotion of the synthesis of 3,4-dihydropyridin-2-(1*H*)-ones derivatives. The use of this reagent has some important advantages, of which high purity of the products, short reaction times, reusability of the catalyst are the most important ones.

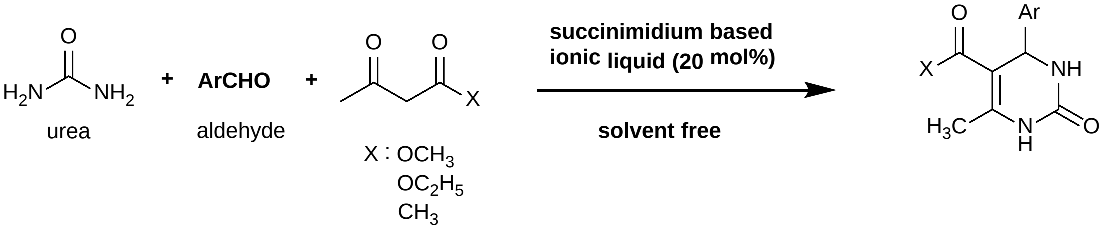

Fig. 1 Multicomponent synthesis of 3,4-dihydropyridin-2-(1*H*)-ones

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A magnetically recoverable copper-salen complex as a nano-catalytic system for amine protection via acetylation reaction using thioacetic acid

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Keywords: Thioacetic acid, Copper-salen complex, Magnetite, Nano catalyst, N-Acetylation reaction.

Amines are a beneficial class of compounds which are used as bioactive compounds, dyes and especially synthetic intermediates in the manufacture of many pharmaceutically active ingredients.[1] Due to the presence of a lone electron pair, amines can act as nucleophile. Hence, because of their significant nucleophilicity, it is unavoidable to protect amine functional groups in the presence of other nucleophilic functionalities (e.g., OH, S, P, etc.) to exclude side reactions. [2] Recently, thioacids have attracted considerable interest in peptide science, as well as in native chemical ligiation. Moreover, Gopi et al. reported selective acetyl protection of amines using thioacetic acid in the presence of copper(II) acetate as catalyst.[4] As the progress of our recent researches on environmentally friendly catalytic systems , we devised a nanocatalyst, taking advantage of the easy separation of magnetic nano-catalysts, the powerful complexing nature of Schiff bases, and the green character of chitosan, to heterogenize copper(II) ion to be applied in the acetyl protection of amines using thioacetic acid.

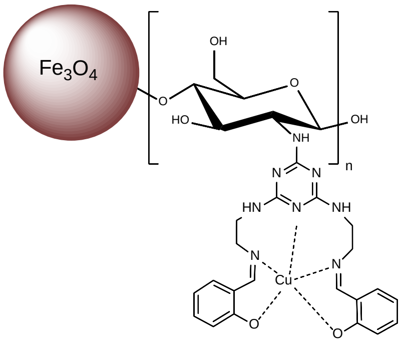

Fig. 1 Catalyst structure

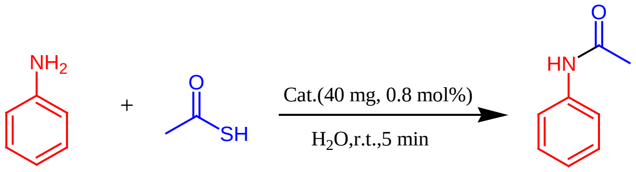

Fig. 2 Acetylation of Anilines

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Solvent-free synthesis of α,β-acetylenic ketones by chitosan-2-thiophenecarbaldhyde supported palladium complex under air conditions

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Keywords: Palladium complex, α,β-acetylenic ketones, Acylation Reaction, Chitosan.

During the last decade, acylation of terminal alkynes and acyl chlorides for synthesis of α,β-acetylenic ketones have attracted great attention.[1] Ynones or α,β-acetylenic ketones have applicated as intermediates for the synthesis heterocyclic compounds.[2] Moreover, ynones have been utilized in preparation biologically active molecules, natural products and pharmaceuticals.[3] Recently, the heterogeneous catalyst based palladium and copper have utilized for synthesis of α,β-acetylenic ketones. Moreover, magnetically recoverable nanoparticles have attracted much attention as heterogeneous catalysts due to their inherent properties, such as simple handling, large surface area, and recovery with magnetic separation in various organic reactions.[4] Herein, we have reported an environmental magnetic porous chitosan-2-thiophenecarbaldhyde supported palladium complex (Fe@CS-TCp-Pd), which was efficiently used as a heterogeneous catalyst for synthesis of ynones. The catalyst shows not only high catalytic activity, but also offers many practical advantages such as recyclability, simple separation with magnetic external and low catalyst loading without used from solvent. All the products were characterized by IR, ^{1}H and ^{13}C NMR spectroscopy.

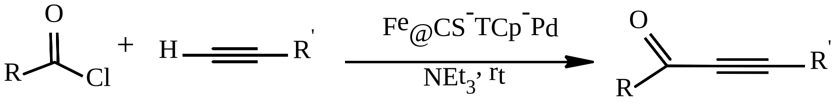

Fig. 1 synthesis of α,β-acetylenic ketone with acyl chlorides and terminal alkynes

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Ionic Liquids for the Synthesis of Pyrazolo[3,4-*b*]quinoline-3,5-diones

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Keywords: Multi-component reactions, pyrazolo[3,4-*b*]quinoline-3,5-diones, ionic Liquids.

Multicomponent reactions (MCRs) are considered as one of the best routes in organic and medicinal findings.[1,2] heterocyclic compounds containing quinoline and pyrazole ring systems, such as pyrazolo[4,3-*c*]quinoline[3] and pyrazolo[3,4-*b*]quinoline[4] play an important role in medicinal chemistry and drug discovery.[5,6] Among these compounds, pyrazolo[3,4-*b*]quinoline framework provides significant pharmacological activities such as antiviral,[7] antimalarial,[8] and anti-inflammatory.[9] A great number of reports on the synthesis of pyrazolo[3,4-*b*]quinoline by the multicomponent reactions have been published thus-far.[10]

Herein, we report the synthesis of pyrazolo[3,4-*b*]quinoline derivatives **4** by a multi-component reaction of dimedone **1**, 5-amino pyrazolone **2** and aromatic aldehydes **3a-i** in the presence of [Msim]Cl ionic liquid under solvent-free conditions (Fig. 1). Good yields of products, short experimental time, and low cost of the catalyst are advantages of this procedure.

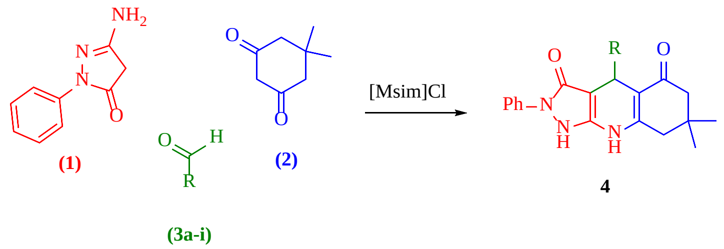

Fig. 1 Multi-component synthesis of pyrroles

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One-pot, three-component and green synthesis of diversely substituted *N*-aryl pyrroles

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Keywords: Multi-component reactions, *N*-aryl pyrrole, Sustainable, Green synthesis.

Today, green chemistry approaches have received considerable attention from chemists because of the reduction in by-products, produced waste and energy cost.[1] Because of the significant role of ionic liquids in green chemistry as a consequence of their unique properties such as offering enhanced rate,[2] ease of product recovery,[3] catalyst immobilization,[4] and recycling,[5] extraordinary consideration has been devoted to promoting organic reactions in ionic liquid media.

N-aryl pyrrole–containing compounds are an important class of *N*-heterocycles that are frequently found in many natural products,[6] and exhibit a wide array of biological activities such as antimycobacterial,[7] anticancer,[8] and anti-HIV [9] activities. Herein, we report the synthesis of substituted *N*-aryl pyrroles **4** from the reaction between nitroalkenes, 1,3-dicarbonyl compounds, and primary aromatic amines using [Et_3NH][HSO_4] ionic liquid under solvent-free conditions (Fig. 1).

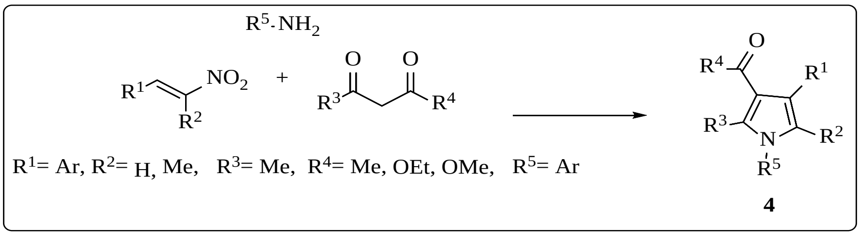

Fig. 1 Multi-component synthesis of pyrroles

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One-pot synthesis of pyrano[2,3-*d*]pyrimidinone derivatives using a new acidic ionic liquid catalyst based on benzimidazole

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Keywords: Pyrano[2,3-*d*]pyrimidinone, Barbituric acid, Multicomponent reactions, Benzimidazole

Multicomponent reactions (MCRs) by virtue of their convergence, productivity, ease of execution and generally high yields of products have attracted considerable attention from the point of view of combinatorial chemistry. The first MCR was described by Strecker in 1850 for the synthesis of amino acids. However, in the past decade, there has been tremendous development in three- and four-component reactions and great efforts continue to be made to develop new MCRs [1].

There is a continuous widespread interest in the synthesis of pyrano-pyrimidinones and coumarins because of the diverse biological properties associated with this system [2].

Uracil and its derivatives, such as pyrano[2,3-*d*]pyrimidinones have received considerable attention over the past years because of their several biological activities such as, antibacterial, antiallergic, antimicrobial, tyrosine kinase, anti-inflammatory, analgesic, calcium channel antagonists, antihypertensive, tuberculostatic, antileishmanial, and antifungal [3].

In this work, we have used a Bronsted acidic ionic liquid based on benzimidazole as a green and efficient catalyst for the preparation of pyrano[2,3-*d*]pyrimidinone derivatives. This method provided excellent yields during short reaction times. Also, the reusability of the catalyst was good.

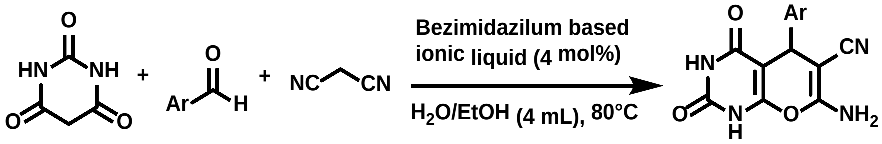

Fig. 1 Synthesis of pyrano[2,3-*d*]pyrimidinone derivatives.

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Asymmetric Synthesis of Amines by Nucleophilic 1,2-Addition of Organo Boron Reagents on C-N Double Bond of Aldimines

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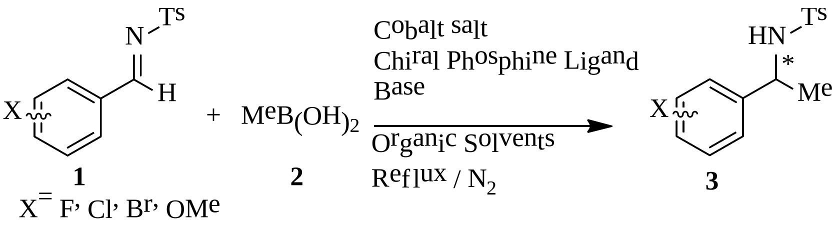
Keywords: Methylation reactions, Phosphine ligands, Cobalt catalysts.

Asymmetric synthesis of organic molecules such as amines are important in the pharmaceutical and agrochemical industries.[1] The efficient methods for the asymmetric methylation of imines have been reported. The breakthrough first methyl addition to an achiral imine using copper catalysts was reported by Tomioka *et al* in 1990.[2] Hoveyda *et al*. described a zirconium-catalyzed imine methylation using a peptide based chiral ligand to afford arylimines.[3] Hayashi and co-workers reported the first example of a rhodium catalyzed methylation of imines.[4]

Herein, we tried to prepare methyl amines **3** by addition of methylboronic acid **2** to aromatic aldimines **1** in the presence of phosphine-cobalt catalysts (Scheme 1). The desired products were produced in good yields and were characterized by IR, ^{1}H NMR and ^{13}C NMR. The enantiomeric excess (ee) of chiral products is detected by polarimeter.



Scheme 1. Methylation of aldimine derivatives by using methylboronic acid in presence of cobalt catalysts.

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Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones promoted by polystyrene sulfonic acid

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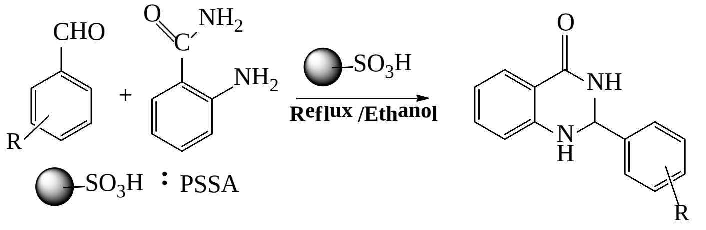
Keywords: polystyrene sulfonic acid, 2,3-Dihydroquinazolinone, Eco-friendly catalyst

2,3-Dihydroquinazolin-4(1*H*)-ones are an important class of nitrogen-containing heterocyclic One of the most important heterocyclic compounds in medicinal chemistry are quinazolinones that have many biological activities such as antifungal, cytotoxic and antimicrobial[1], antimalarial[2] and anticancer.[3] Quinazolinones are synthesized *via* condensation of 2-aminobenzamid with aldehydes in the presence of an acidic catalyst. Previously, this reaction have been catalyzed by I_2 [4], $ZnFe_2O_4$ [5], nano-$Fe_3O_4/TiCl_2$/cellulose[6] and ammonium chloride.[7] The application of inexpensive, ecofriendly and heterogeneous catalysts in organic synthesis have attracted to chemists. Therefor we have prepared a new solid acid catalyst *via* sulfonation of polystyrene which named polystyrene sulfonic acid (PSSA). We have used polystyrene sulfonic acid in the preparation of quinazolinone *via* reaction of 2-aminobenzamide and aldehydes (Scheme 1). The structures of obtained products were identified by FT-IR and ^1H-NMR. This project has some advantages such as high yield, short reaction times, simple separation of catalyst and easy workup.



Scheme 1 Synthesis of 2, 3-dihydroquinazolin-4(1H)-ones in the presence of polystyrene sulfonic acid

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Arylation of aromatic aldehydes in the presence of Cu doped Fe_3O_4 and phosphine ligand

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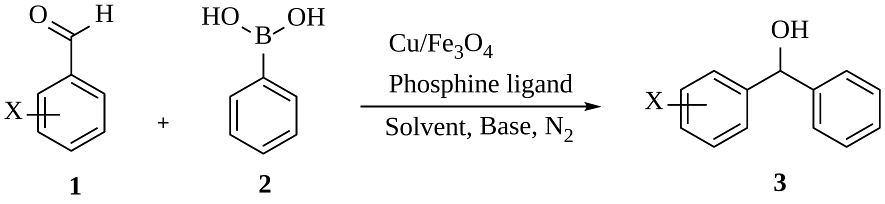
Keywords: Aldehyde, Nanomagnetic complex, Arylation, Phosphine ligand.

Metal nanoparticles exhibit excellent optical, electrical, and catalytic properties corresponding bulk materials, especially their high specific surface and surface defects. Among them, magnetic property, separation effect, and the catalytic activity during cyclic utilization of Fe_3O_4 nanometals are evaluated, indicating they could be used as an efficient degradation catalyst on organic reactions.[1] Other hand, copper nanoparticles because of suitable properties such as easy recycling, increasing number of access to the active site and being economically are used as a catalyst in various organic reactions.[2] In recent years, many attempts have been attracted to synthesis of diaryl methanol **3** through the addition of alkyl or aryl group to carbonyl groups in the presence of metal catalyst such as copper, silver, palladium, zinc, etc. Addition of organometallic reagents to aldehyde is one of the most important carbon-carbon bond formation, in this work wish to report the 1, 2-arylation of aldehyde **1** by boron reagents **2** in the presence of prepared Cu doped Fe_3O_4 and phosphine ligands (Scheme 1 and 2).[3] The prepared nanomagnetic Cu/Fe_3O_4 was characterized by scanning electron microscopy, and Fourier transform infrared spectroscopy and the structure of chiral products are investigated by melting point, IR, ^1H NMR and ^{13}C NMR spectroscopies.

$$Cu(NO_3)_2 + FeCl_3\cdot 6H_2O \xrightarrow[\text{Sodium citrate}]{\text{Urea, } H_2O} Cu/Fe_3O_4$$

Scheme 1. Preparation of Cu doped Fe_3O_4



Scheme 2. Cu doped Fe_3O_4 phophine catalysted arylation of aromatic aldehydes

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Synthesis, separation, purification and characterization of novel nano-derivatives of azo-compound thiazolidine dione

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Keywords: Thiazolidine-2,4-dione (TZD), Glitazone, Azo-compound, Nano-derivatives of phenyldiazenyl benzylidene thiazolidine-2,4-dione

Thiazolidine-2,4-dione (TZD) is an important heterocyclic ring system that exhibits a range of pharmacological activities, but not limited to, including anti-hyperglycemic, anti-cancer, anti-inflammatory, anti-arthritic, and anti-microbial, etc [1-3]. Among them, anti-hyperglycemic is the widely studied effect of TZD derivatives that has also been extended to the development of clinically used ‘glitazone’ drugs such as rosiglitazone lobeglitazone, pioglitazone, and troglitazone, etc [4-6]. In this study, a new nano-derivatives of phenyldiazenyl benzylidene thiazolidine-2,4-dione for the first time was prepared from premade azo-compound and thiazolidine dione and further was connected via alkyl-linkage on nanoparticles of gold, silver and copper to improve pharmaceutical effectiveness.

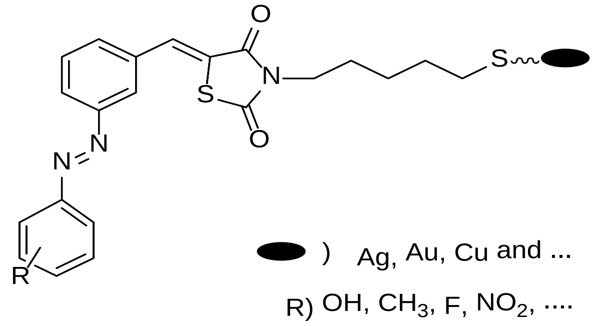

Fig 1. New nano-derivatives of phenyldiazenyl benzylidene thiazolidine-2,4-dione.

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Modification and functionalization of two-dimensional MoS_2 nanosheets by reversible addition fragmentation chain transfer (RAFT) polymerization

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Keywords: Two-dimensional nanosheets, Molybdenum disulfide (MoS_2), Reversible Addition-Fragmentation Chain Transfer (RAFT), polymerization

Two-dimensional (2D) layered transition-metal dichalcogenides (TMDs) are a fascinating class of nanomaterials that have garnered enormous interests because of their unique electronic, physical, and chemical properties. MoS_2 has been one of the most studied TMDCs and acts as an excellent model system to explore the chemistry of 2D TMDCs. To further modify their properties, and even broaden their application, the chemical functionalization of such layered materials is required.[1] Functionalization of the MoS_2 nanosheets with polymers has intensively investigated in order to enhance the compatibility of nanosheets with various matrices. Reversible Addition–Fragmentation Chain Transfer (RAFT) is a useful method for the modification of different nanomaterials, due to its versatility. This method is compatible with a wide range of monomers and can be used in all modes of free radical polymerization.[2,3] In this study, we present efficient grafting strategies to functionalize MoS_2 nanosheets with polystyrene (PSt) chains (MoS_2-CS_2-PSt) using RAFT polymerization. 1-bromoethylbenzene and CS_2 were grafted on the MoS_2 surface to synthesize RAFT agent (MoS_2-CS_2-Ph) and it was used for the controlled polymerization of styrene (Fig 1). MoS_2-CS_2-PSt was investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). This research provides an efficient route towards the design and development of functional MoS_2-PSt in gram large scale.

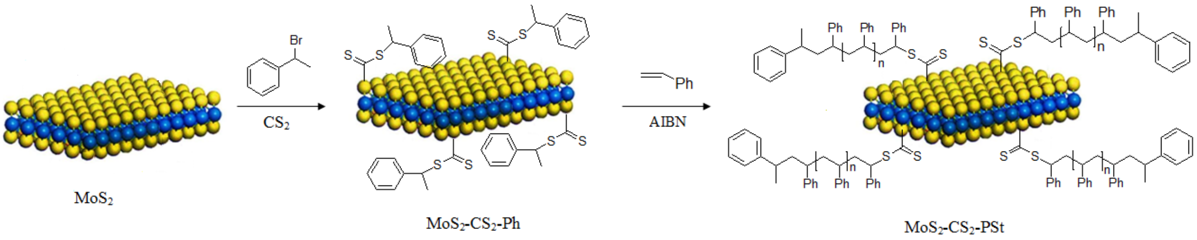

Fig. 1 Schematic representation of the synthesis of MoS_2-CS_2-Pst.

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Design and synthesis of new derivatives of 3-acetylcoumarin as 15-lipoxygenase inhibitors

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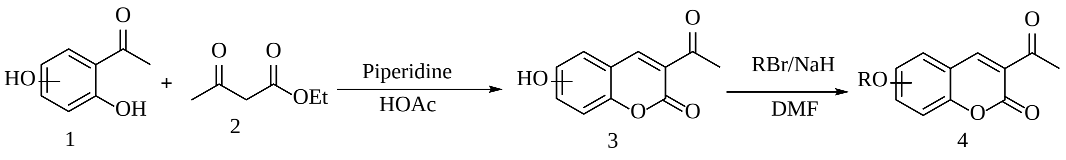
Keywords: Synthesis, inhibitors, 15-lipoxygenase, Knoevenagel condensation, alkylation.

15-Lipoxygenase (15-LOX) is one of the most important enzyme of lipoxygenase family in animals and plants. The critical role of the enzyme in creating human disease such as inflammatory disease of the respiratory system, sensitivity and also prostate cancer has been demonstrated.[2] In this research, with design and synthesis acetylcoumarin derivatives, we intend to evaluate their inhibitory potency against soybean 15-lipoxygenase. Herein, we report that new derivatives of compound **2** were synthesized through Knoevenagel condition of desired dihydroxybenzaldehyde **1** with ethyl acetoacetate. Then all of the O-prenylated 3-acetylcoumarins **3** were synthesized by hydroxyl3-acetyl coumarin with the desired prenyl bromide in presence of sodium hydride in DMF and their tension of inhibition are surveyed on soybean 15-lipoxygenase. In the following, these mentioned compounds were compared with prenyled coumarin derivatives in terms of inhibitory activity against on soybean 15-lipoxygenase enzyme.[3] All synthesized compounds structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.



R: Allyl, Isopentenyl, Geranyl, Farnesyl

Scheme. 1

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Synthesis of 4,4'-(aryl methylene)bis(3- methyl-1*H*-pyrazol-5-ol)s

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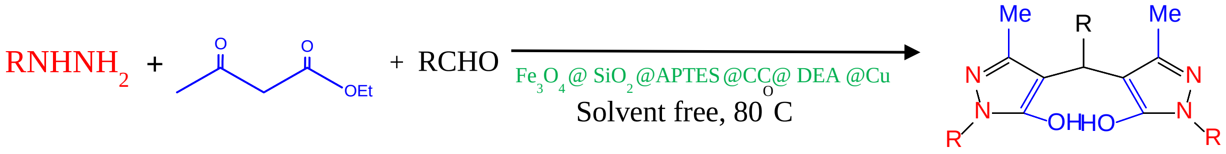
Keywords: one pot, nano- magnetic, heterogeneous catalysts, multi-component

Fe_3O_4 @ SiO_2 @APTES @CC@ DEA @Cu as a new green and recyclable solid catalyst was prepared. Green chemistry has led to the use of nano-magnetic catalysts, which are considered as heterogeneous catalysts in many of the multi-component reactions due to its high activity, easy separation and reuse. Magnetic nanoparticles are easily prepared and separated from the reaction medium by external magnetism, so the catalyst based on Fe_3O_4 nanoparticles can easily be removed from the reaction and reused. The catalytic activity of Fe_3O_4 @ SiO_2 @APTES @CC@ DEA @Cu was evaluated for synthesis of 4,4'-(aryl methylene)bis(3-methyl-1H-pyrazol-5-ol)s via one-pot reactions of phenylhydrazine/or hydrazine hydrate, ethylacetoacetate and aldehydes under solvent-free condition. 4,4′-(Aryl methylene) bis(1H-pyrazol-5-ol)s as an important class of heterocyclic compounds have been exhibited a wide range of biological activities such as antimalarial[1], antifungal[2], anti-inflammatory[3], antimicrobial. Also, they are used as important intermediates in organic synthesis.



Scheme 1 One-pot synthesis of 4,4'-(aryl methylene) bis(3-methyl-1H-pyrazol-5-ol)s catalyzed by Fe_3O_4 @ SiO_2 @APTES @ CC@ DEA @Cu

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Synthesis and characterization of new derivatives of iminosulfathiazoles

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Keywords: Sulfathiazole, Sulfonamide, Azo compounds.

Sulfonamides are a class of antibiotics that have many applications on medicinal. Sulfa drugs have a sulfonamide functional group. Sulfathiazole is one of the most important sulfa drugs that has antibacterial and antimicrobial properties and it can be effective in the treatment of viral and bacterial diseases.[1] Azo compounds have attracted much attention in both academic and applied research due to their versatile application in various fields, such as dyeing textile fiber, and advanced application in high technology areas such as laser, liquid crystalline displays, electro-optical devices, and ink-jet printers.[2-5]

Here, the reaction between sulfathiazole and various azo compounds was performed *via* the imine bond (Fig.1).Then the synthesized products were isolated, purified and the structures of the newly synthesized hybrid molecules were characterized by TLC, M.P., FT-IR, ^{1}H NMR, and ^{13}C NMR. Antibacterial, antioxidant, anticancer properties and other biological properties will also be considered.

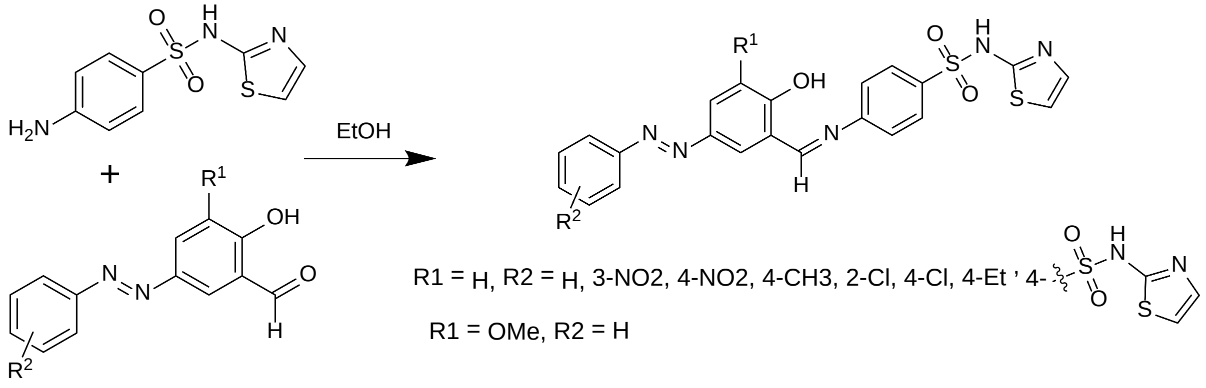

Fig 1. Synthesis of iminosulfathiazole derivatives.

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Synthesis of 4-((3-formyl-4-hydroxyphenyl)diazenyl)-*N*-(thiazol-2-yl)benzenesulfonamide as a new azo derivative of Sulfathiazole

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Keywords: Sulfathiazole, Azo compounds, Biological activity.

Sulfathiazole is one of the most important sulfa drugs. It is an organosulfur compound used as a short-acting sulfa drug with antibacterial and antiviral properties. This drug has many uses in the treatment of diseases.[1]

In this research, a new azo derivative of sulfathiazole was synthesized in one-pot *via* coupling of the corresponding diazonium salt with the salicylaldehyde (Fig.1). The crude product was recrystallized from EtOH to give an orange powder. The resulted azo-aldehyde product was characterized by TLC, M.P, FTIR and NMR. The synthesized azo-aldehyde is a good precursor to utilize as multicomponent one-pot reactions.[1-3]Antibacterial, antioxidant, anticancer properties and other biological properties in comparison to the standard sulfonamide will also be considered.

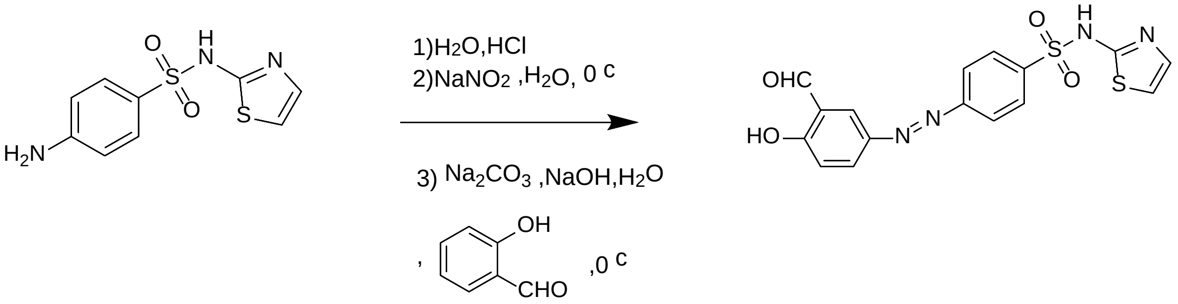

Fig. 1 Synthesis of a new azo derivative of sulfathiazole.

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Introduction of new ionic liquid and its application as a catalyst for the synthesis of pyrano[2,3-*d*]pyrimidinones

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Keywords: Ionic liquid, Bis-imidazole, Pyrano[2,3-d]pyrimidinones.

Since the first synthesized ionic liquid (IL) introduced in 1914, ILs have caused a drastic change in synthetic chemistry. Nowadays, ILs are known as environmentally benign and convenient catalysts or dual solvent-catalysts to improve and facilitate organic reactions by omitting traditional solvents. This is due to their particular properties such as negligible vapor pressure, ability to dissolve many organic and inorganic substances, recyclability, good thermal stability, tunable viscosity, and miscibility with water and organic solvents.[1] Pyran derivatives are common structural subunits in a variety of important natural products such as carbohydrates, alkaloids, polyether antibiotics, pheromones and iridoids. Pyrano[2,3-d]-pyrimidine derivatives have received more attention from chemists because of their biological activities such as, antiallergic, antihypertensive, cardiotonic, antibronchitic, antitumor hepatoprotective, antifungal, antimalarial, analgesic, antiviral evaluation, antibacterial, antileishmanial, vasodilator and herbicidal activities. In recent years, the use of acidic ionic liquid (*Lewis* and *Bronsted*) as catalyst has been a widely developed topic.[2] So according to the properties mentioned, a new ionic liquid based on bis-imidazole is designed and used as the catalyst. The applicability of this reagent is studied in the promotion of the synthesis of pyrano[2,3-d]pyrimidinone derivatives. This method possess some advance such as ease of preparation of the catalyst, short reaction time, excellent yields.

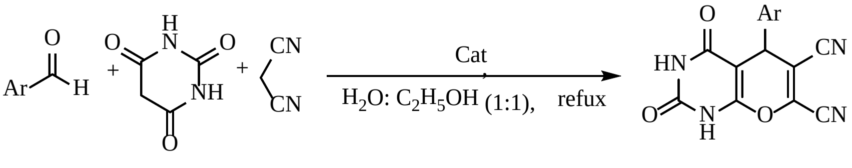

Fig. 1 synthesis of pyrano[2,3-d]pyrimidinone derivatives

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Synthesis and characterization of Fe_2O_3/CuO nanocomposite as a new photocatalyst for solar degradation of methylene blue dye in aqueous solution

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Keywords: Fe_2O_3/CuO nanocomposite, Photocatalyst, Methylene blue, Solar degradation.

Fe_2O_3/CuO nanocomposite were prepared using a Schiff base complex as precursor by solid state thermal decomposition method [1-4]. The nanocomposite was characterized by XRD, FT-IR, SEM, VSM and UV-Vis spectroscopy. Spherical particles of the nanocomposite (20-30 nm) were obtained. The band gap of superparamagnetic nanocomposite was estimated to be 4.2 eV. The photocatalytic performance of the nanocomposite was evaluated for degradation of methylene blue dye in aqueous solution (5 mg/Lit) at optimized condition (30 °C, 5 mg of catalyst, 20 mL H_2O_2 and pH =11) under solar light (average light intensity of 180 mW cm^{-2}). This nanocomposite destroyed this dye in 2 min with efficiency of 95%. The kinetics of MB degradation was obtained to be the pseudo-first order model, k= 0.038 cm^{-1}.

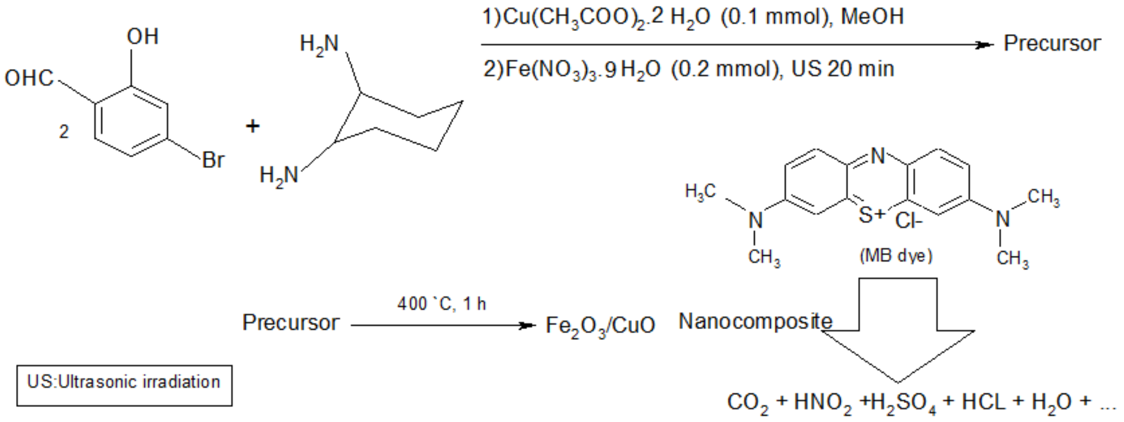

Fig 1. Steps of synthesis of Fe_2O_3/CuO nanocomposite

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New polyacid Catalyst Based on Nanoparticles as a highly effective and recyclable catalyst for the preparation of xanthenes under solvent-free condition

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Keywords: Xanthene, Solid acid Catalyst, Dimedone, Aldehyde

Xanthenes especially benzoxanthenes are an important class of organic compounds that attracted the attention of organic chemists because of their wide range of biological and pharmaceutical properties such as anti inflammatory, antiviral activity, and agricultural bactericide activity. Furthermore, these compounds are very important in the industry because they are used as a local-dyes, in fluorescent material for visualization of biomolecules, Photodynamic therapy (PDT) and in laser technologies [1-2]. Recently, solid acid catalyst has gained special attention as catalyst in organic synthesis because of the excellent solubility in water, uncomplicated handling, inexpensiveness, eco-friendly nature and readily available[3-4]**.**In this research, $Fe_3O_4@SiO_2@COOH$ as an effcient and reusable catalyst has been used for the one-pot preparation of 1,8-dioxo-octahydroxanthene derivatives via condensation between various aromatic aldehydes with dimedone under solvent-free and thermal conditions**.** We were able to recycle this catalyst ($Fe_3O_4@SiO_2@COOH$)five times and use it in reaction, without reducing the efficiency of the product.

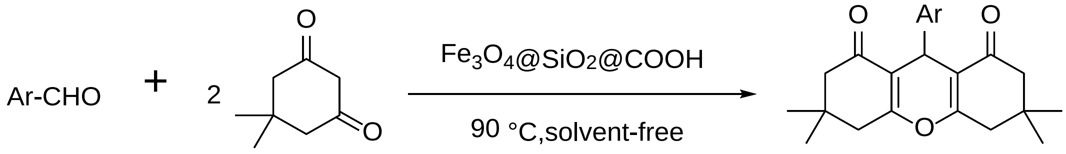

Fig. 1 Synthesis of 1,8-dioxo-octahydroxanthene catalyzed via nano-solid acid catalysts

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Synthesis of 1-(α-aminoalkyl)-2-naphthols using 3-methyl-1-sulfonic acid imidazolium trichloridocuprate

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***Keywords**:* Multi component reactions, 1-(α-aminoalkyl)-2-naphthol, Solvent-free.

One of the important classes of organic compounds is 1-(α-aminoalkyl)-2-naphthols which called Betti bases compounds.[1] The synthesis of substituted Betti base derivatives is an important part of organic chemistry because of their attractive catalytic [2] and biological properties.[3] The typical Betti reaction is a three-component reaction between an aldehyde, ammonia or urea and *β*-naphthol. Although, variations have been made to prepare Betti base derivatives through by quilinols, naphthols, alkyl amines to exchange ammonia, uncatalyzed in water, sulfanilic acid-functionalized silica-coatedmagnetite nanoparticles, *N*-heteroaryl amino naphthol and the addition of naphthols to preformed iminium salts has to be attained.[4] In the presented work, we have prepared 3-methyl-1-sulfonic acid imidazolium trichloridocuprate as a new catalyst for the synthesis of 1-(α-aminoalkyl)-2-naphthols which exhibits many important properties (Fig. 1).

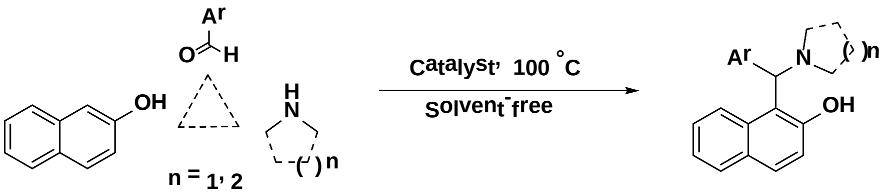

Fig. 1 The synthesis of 1-(α-aminoalkyl)-2-naphthols.

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Design, preparation and characterization of novel core-shell magnetic nanocatalyst based on amino-functionalized calix[4]arenes for one-pot three component synthesis of 2-amino-*4H*-chromene derivatives

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Keywords: Multicomponent reaction, Calixarene compounds, Functionalized magnetic nanoparticles, 2-amino-*4H*-chromene derivatives, Magnetic nanocatalyst.

One of the most common phenol-formaldehyde cyclic oligomers from hydroxyalkylation reactions with owning supramolecular chemistry are calixarenes.[1] These macrocyclic compounds are qualified to act as synthetic catalysts due to their specific features such as being able to form host-guest complexes and ease of chemical modifications with variety of functions on their rim.[2] In this research, a novel magnetic nanocatalyst based on Fe_3O_4 nanoparticles and their surface modification with different shells particularly the synthetic amino-functionalized calix[4]arene is propounded; as well as, its catalytic activity and considerable performance are evaluated in green and one-pot synthesis of 2-amino-*4H*-chromene derivatives **4** by utilizing substituted aldehydes **1**, dimedone **2** and malononitrile **3** at room temperature and using green solvent, ethanol. This novel magnetic nanocatalyst was characterized by spectroscopic and analytical techniques such as FT-IR, EDX, FE-SEM, VSM, XRD and ^{1}HNMR and also, the solid isolated products were identified by FT-IR, ^{1}HNMR and ^{13}CNMR spectral data.

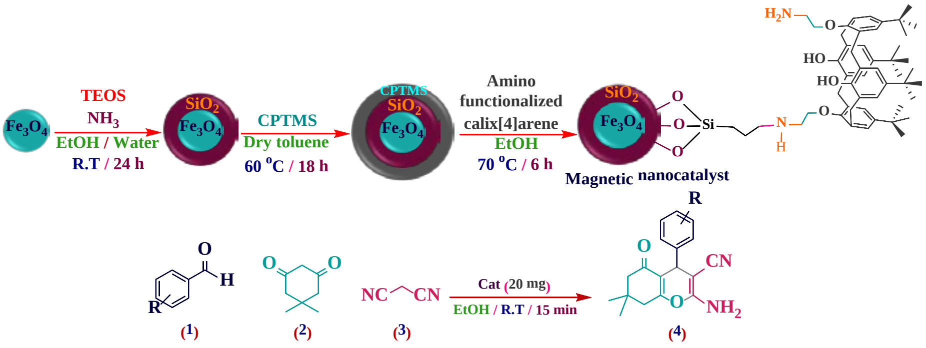

Fig. 1 Synthetic procedure of novel core-shell magnetic nanocatalyst and its applicability in one-pot three component synthesis of chromene derivatives

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Modification of covalent organic frameworks surface using thermal sensitivity polymers

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Keywords: Covalent organic frameworks (COFs), Boronic acid, Poly(N-isopropylacrylamide)

Covalent organic frameworks (COFs) represent an exciting new type of porous organic materials, which are ingeniously constructed with organic building units via strong covalent bonds. Boronic acids are one of versatile building blocks for the construction of complex molecular architectures.[1,2] Most notably, the formation of boronate esters has been used extensively in carbohydrate chemistry, where boronic acids have found applications as protecting groups or as receptors and sensors. Using reversible condensation reactions, it is possible to obtain macrocycles, cages, and dendritic structures. The creation of cage structures requires building blocks, which are able to connect more than two reaction partners. Molecular modeling showed that the cage has a cavity with approximate dimensions of 27A˚. Guest molecules such as monomers, fluorescein molecules, and drugs are able to encapsulate by the cage of COF.[3,4]

Here we synthesize 2D boronate ester-linked COF under conditions in which the monomers are fully soluble. Then, thermo-responsive poly(N-isopropylacrylamide) (PNIPAM) was growled inside the cavity of synthesized COF through radical polymerization. The as-prepared modified COFs integrated the individual advantages of two components, such as the thermal sensitivity of the PNIPAm terminal as well as pH sensitivity of the COF substrate. This smart COF has shown remarkable potential for intelligent strain sensors, textiles, actuators and on/off switches.

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Simple Synthesis of *bis*-*N*-Acetyl-1,2-Dihydro-(4*H*)-3,1-Benzoxazin-4-ones

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Keywords: 1,2-Dihydro-3,1-benzoxazin-4-ones, Antranilic acid, Schiff-base, Cyclization reaction.

4*H*-3,1-Benzoxazin-4-ones are valuable starting materials for the synthesis of a variety of heterocycles.[1] Also, they are used directly or indirectly in many clinical applications.[2] Contrary to the parent compounds 4*H*-3,1-benzoxazin-4-ones,[3] very few synthetic routes have ever been reported for *bis*-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones.[4] Here, a convenient synthesis of *bis*-*N*-acetyl-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones **4** are reported by first, a condensation reaction of anthranilic acid derivatives **1** with glyoxal **2** at room temperature and then, cyclization reaction of the produced Schiff-bases **3** with acetic anhydride under reflux conditions (Scheme 1). High yields of the desired products are obtained in high purity and simple work-up.

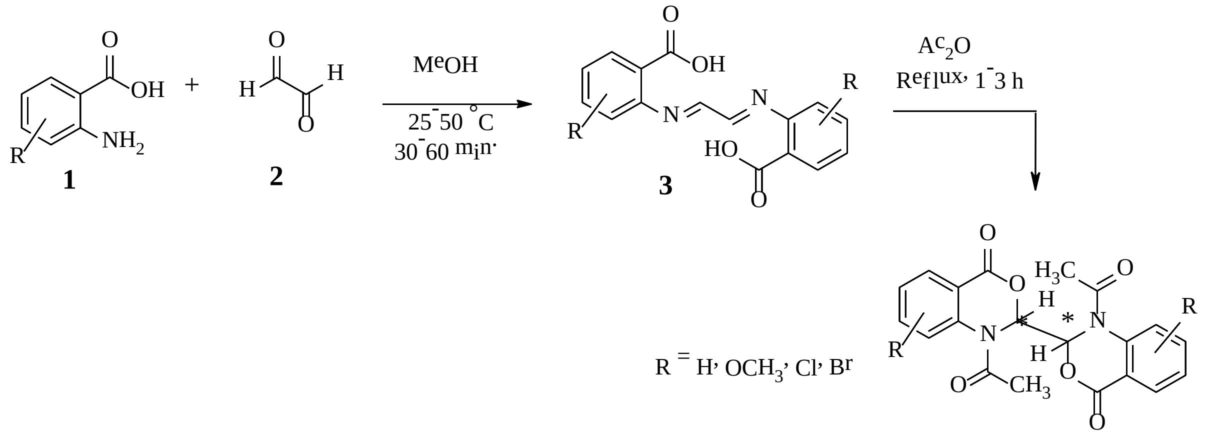

Fig. 1 Synthesis of *bis*-*N*-acetyl-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones

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Survey Friedel-Crafts reaction of *N*-aryltrifluoroacetimidoyl chlorides with aromatic compounds

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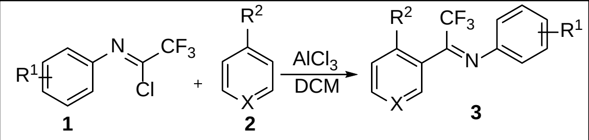
Keywords: Fluorinated compounds, N-Aryltrifluoroacetimidoyl chlorides, Friedel-crafts reaction.

Fluorinated compounds are most important organohalides in natural and medicinal chemistry.[1] In the most important drugs which are commercially available, at least one fluorine atom is present such as: antidepressant fluoxetine (Prozac), cholesterol-lowering drug atorvastatin (Lipitor) and the antibacterial ciprofloxacin (Ciprobay).[2] The trifluoromethyl group is becoming more and more important in both of agrochemical and pharmaceutical applications because of the influence of fluorine atom on physical, chemical, and physiological properties, stability, and lipophilicity of the molecule. In recent years, reactions of trifluoromethylation have been extensively investigated, in order to synthesis of new organofluorinated drugs.[3] Herein, we report a friedel-crafts reaction of N-aryltrifluoroacetimidoyl chlorides **1** and aromatic compounds **2** for synthesis of new N-aryltrifluoroacetimidoyl aromatic compounds **3** (Fig. 1). The FT-IR, ^{19}F-NMR, ^{1}H-NMR and ^{13}C-NMR confirm the structures of the products.



R^1= 4-Me, 4-OMe, 4-Cl, 4-F, 2-Cl, 3-CF_3’
2-Br-4-Cl, 3,4-diMe
X= C, R^2= Me (**2a**) or X= N, R^2= H (**2b**)

Fig. 1 Synthesis of new N-aryltrifluoroacetimidoyl aromatic compounds **3**.

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Cyclization of 2-(4-chlorobutanamido)benzoic acid to 2-(3-chloropropyl)-4*H*-benzo[3,1]oxazin-4-one using dehydrative cyclization agents

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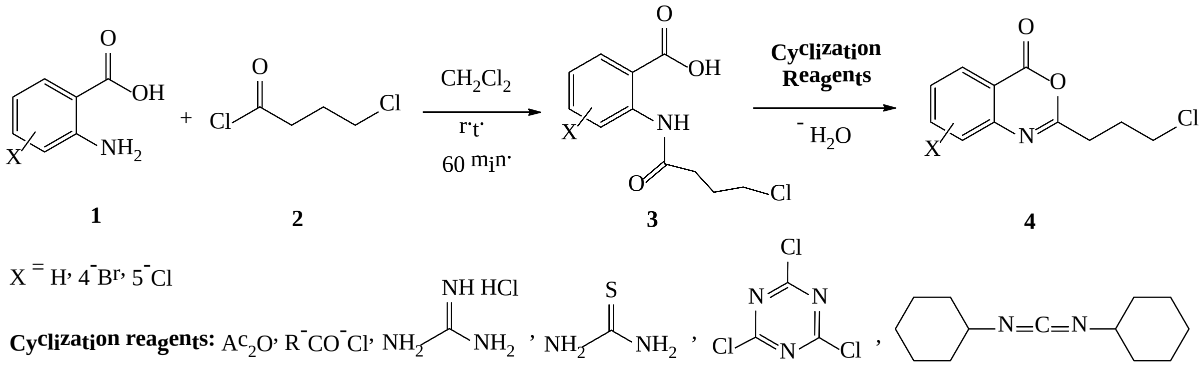
Keywords: 3,1-Benzoxazin-4-ones, Antranilic acid, 4-Chlorobutanoyl chloride, Cyclization agents

Functionalized 4*H*-3,1-benzoxazine-4-ones in 2-position have wide applications in synthesis of important heterocyclic compounds. Thus, development of simple and efficient protocols to prepare them using mild reaction conditions has received much attention.[1-4] In this work, efficient methods for the synthesis of 2-(3-chloropropyl)-(4*H*)-benzoxazin-4-ones under mild reaction conditions are described. The coupling reaction of anthranilic acid derivatives with 4-chlorobutanoyl chloride following with dehydrocyclization of the produced amides **3** with simple reagents such as 2,4,6-trichloro[1,3,5]triazine (cyanuric chloride, TCT), *N,N'*-dicyclohexylcarbodiimide (DCC) and acetic anhydride (Ac_2O) leads to the desired benzoxazin-4-ones **4** (Scheme 1). The notable advantages of these procedures are mild reaction conditions without need to use of any catalysts which produce high yields of the products with simple work-up of the reaction mixture.



Scheme 1 Synthesis of *2*-(3-chloropropyl)-(4*H*)-3,1-benzoxazin-4-ones 4

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Synthesis of *N*-(4-Chlorobutanoyl)-1,2-Dihydro-(4*H*)-3,1-Benzoxazin-4-one Derivatives

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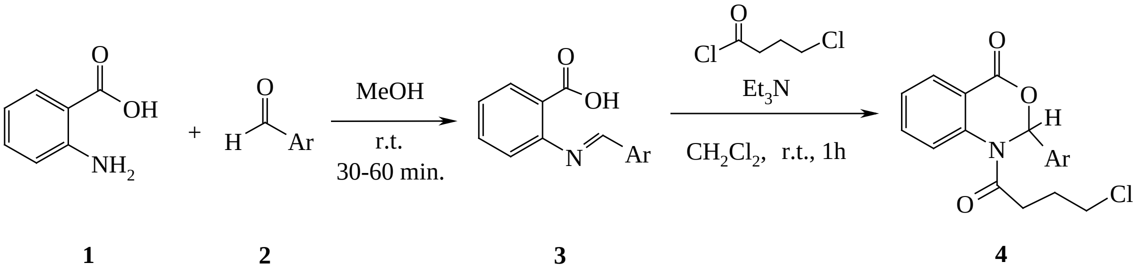
Keywords: 1,2-Dihydro-3,1-benzoxazin-4-ones, Antranilic acid, Schiff-base, 4-Chlorobutanoyl chloride.

3,1-Benzoxazin-4-one and their derivatives[1,2] are versatile intermediates in the synthesis of heterocycles with high pharmacological and biological activities.[3,4] Here, we report a practical and convenient synthesis of *N*-(4-chlorobutanoyl)-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones by cyclization reaction of Schiff-bases **3** (produced by condensation reaction of anthranilic acid derivatives **1** with benzaldehyde derivatives **2** at room temperature) with 4-chlorobutanoyl chloride at room temperature (Scheme 1). The presence of Cl in the end of butanoyl chain, makes the produced benzoxazine-4-ones **4** more reactive for further reactions against nucleophiles. The structures of all synthesized compounds were determined on the basis of their spectroscopic data.



Ar = C_6H_5, 4-Me-C_6H_4, 4-Cl-C_6H_4, 2-Cl-C_6H_4, 3-OH-C_6H_4

Fig. 1 Synthesis of *N*-(4-chlorobutanoyl)-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones **4**

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Synthesis of fluorinated imidazolopyridines from pentafluoropyridine

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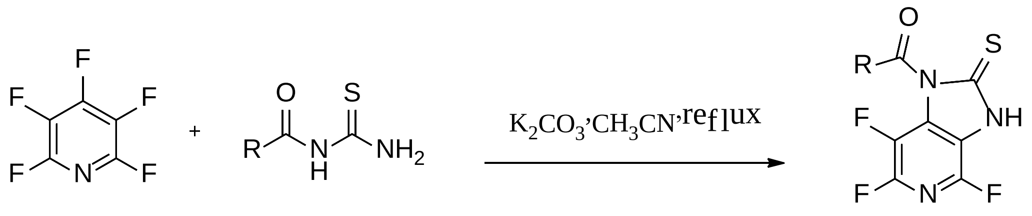
Keywords: Pentafluoropyridine, N-carbamothioylacetamide, Synthesis

Heteroaromatic systems have, of course, vast chemistry.[1] Perhalogenated heteroaromatic systems are an essential class of heterocyclic compounds with potentially various use in organic chemistry, biochemistry, and pharmaceutical chemistry. Many researchers are concerned about the reactions of different N, O, S, C, and P nucleophiles with perhalogenated compounds. The order of nucleophilic attack on pentafluoropyridine follows the sequence 4-F > 2-F > 3-F. Due to their high electronegativity, fluorine atoms are able to modify the physicochemical attributes of molecules drastically.[2-3] We report the synthesis of new 1-(4, 6, 7-trifluoro-2-thioxo-2, 3-dihydro-1H-imidazo [4, 5-c] pyridin-1-yl) ethanone **3** from the reaction between pentafluoropyridine **1** and N-carbamothioylacetamide **2** after heating together at reflux temperature in THF in the presence of potassium carbonate. All synthesized compounds are stable solids whose structures were determined on the basis of their ^{1}H and ^{13}C NMR and ^{19}F-NMR and IR spectroscopic data.



1 **2** **3**

Fig. 1 reaction 1-(4, 6, 7-trifluoro-2-thioxo-2, 3-dihydro-1*H*-imidazo [4, 5-c] pyridin-1-yl) ethanone

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Efficient synthesis of symmetrical anhydrides by cross dehydrogenative coupling of aldehydes over $CuFe_2O_4$ nanoparticles

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Keywords: $CuFe_2O_4$ NPs, Anhydride, Cross dehydrogenative coupling, Magnetic Nanocatalyst, Recyclable.

Carboxylic anhydrides are an important class of organic compounds used as versatile reagents in the preparation of carboxylic acid derivatives. They are also employed as reactive intermediate in various types of reactions.[1] Anhydrides are important, but less abundant in nature. Therefore, their synthesis is significant for organic chemists. In recent years, considerable attention has been attracted to the cross-dehydrogenative coupling (CDC) reactions because of their atom economy, step-economy, and the outstanding role in the formation of C–C, and C–X (X=heteroatom) bonds.[2] Aldehydes and other readily available materials are advantageous in CDC reactions.[3] These compounds have been used in significant organic transformations.[4] Due to copper is superior activity, in this study we report a novel CDC based approach for the synthesis of symmetrical anhydrides through oxidative activation of sp^2 C–H bond of aldehydes using TBHP as an oxidizing agent and copper ferrite nanoparticles ($CuFe_2O_4$ NPs) as the catalyst.

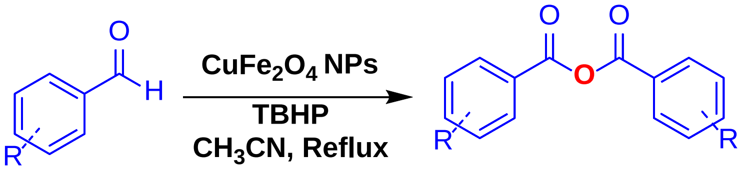

Fig. 1 Synthesis of anhydrides *via* CDC of aromatic aldehydes over $CuFe_2O_4$ NPs

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Green synthesis of dicoumarols by Cu (II) immobilized on Fe_3O_4@SiO_2@dimethylglyoxime as a novel and recyclable and nanocatalyst

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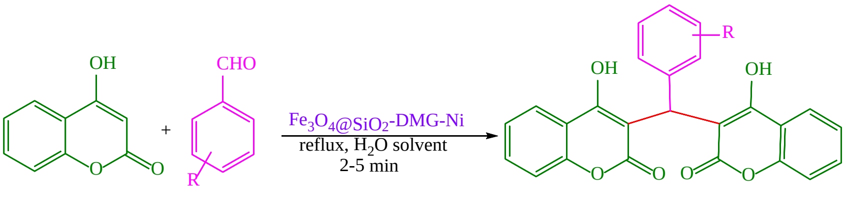
Keywords: Dimethylglyoxime, Magnetic nanoparticles, Core-shell, Dicoumarols.

In last years, catalysts of heterogeneous have been introduced as strategically vital in eco-friendly and various organic conversions due to their unparalleled aspects e.g. excellent catalytic activity, recyclability, low toxicity, and stability.[1,2]

In this work, we synthesized complex of Ni-Dimethylglyoxime immobilized on Fe_3O_4 of covered with SiO_2 by a post-grafting way and utilized as a novel[4], thermally stable, recoverable, and efficient for clean synthesis of dicoumarols[3] through the interaction of various aldehydes[5] with 4-hydroxycoumarin[6] in excellent yields and higher rate (Figure 1). Fe_3O_4@SiO_2-silylcyclopropyl-dimethylglyoxime-Ni superparamagnetic nanoparticles (MNP_s) were investigated by FT-IR, SEM, EDS, XRD, VSM, and BET technique. This nanocatalyst could be easily regained via the utilization of a magnet and reused for subsequent reactions for at least 7 times without any remarkable change and decrease in catalytic activity.[7]



1 **2** **3**

R= H, Cl, NO_2, CH_3O- , Br and OH

Fig. 1 Synthesis of dicoumarols [3] In the presence of Fe_3O_4@SiO_2-DMG-Ni nanocatalyst.

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Solvent-free three component synthesis of N-Acyl hydrazone derivatives from the reaction between aldehydes and α,β-unsaturated esters

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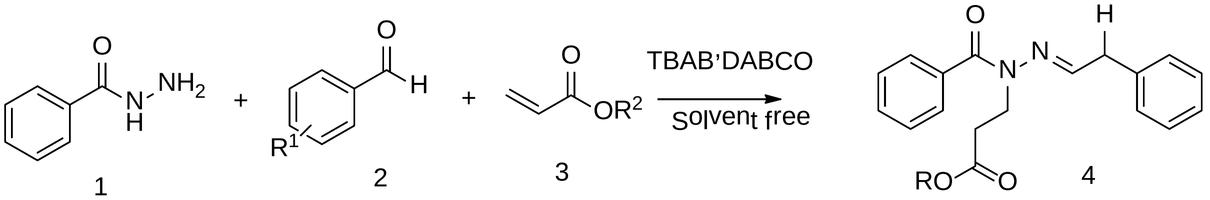
Keywords: *N*-Acyl hydrazine, Acyl hydrazide, Solvent-free reaction

Acylhydrazones are one of the most important Schiff bases and have been well documented to possess important pharmacological activities such as antitumor,[1] antibacterial,[2] antiviral, and antimalarial.[3] Due to the pharmacophoric character of acylhydrazone, this group framework has been widely exploited in the design of new bioactive compounds with different pharmacological profiles.[4]

At present study, we wish to introduce a novel, efficient and green method for the synthesis of new acyl hydrazide derivatives *via* reaction of various acylhydrazones with *α,β*-unsaturated esters (Fig. 1).

In this protocol, the desired benzoyl-2-(2-phenylethylidene)hydrazinyl)propanoates (**4**) were synthesized by the aza-Michael addition of hydrazide (**1**) and aldehydes (**2**) to activated acrylates (**3**) in the presence of tetrabutyl ammonium bromid (TBAB) –an ionic organic salt– and DABCO at 80°C under solvent-free condition.



R^1=NO_2' Cl' OH'NH_2' $N(CH_3)_2$

R^2=CH_3' CH_2CH_3' $(CH)_3$-CH_3' $(CH)_5$-CH_3

Fig. 1 Synthesis of acyl hydrazone derivatives

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Synthesis of new cyclophanes besed on calix[4]arene

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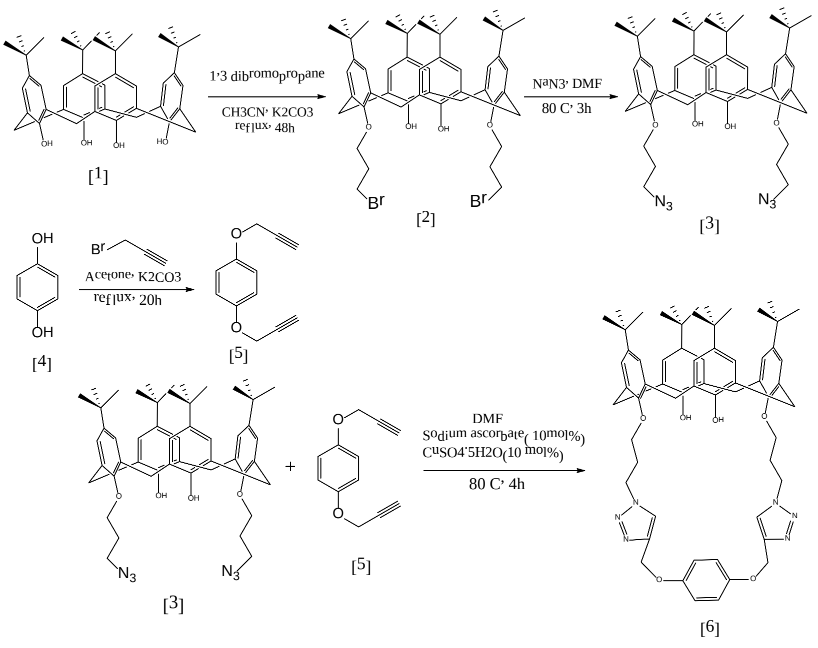
Keywords: Calix[4]arene, Click reaction, Capped calixarene

Calixarenes are well-known as one of the versatile and useful building blocks in supramolecular chemistry.[1] Several calixarene-based cavitands (capped and functional calixarenes) have been reported in the literature by using click chemistry methodology through the Cu(I)-catalyzed ligation of adequate bis-alkyne and bis-azide derivatives.[2] Herein, we report the synthesis of a capped calixarene by copper catalyzed azide-alkyne click reaction. As shown in Scheme 1, calix[4]arene **6** was synthesized in 3 steps. At each step, we confirmed the product with ^{1}H-NMR and the resulting calixarene were characterized by ^{1}H-NMR spectroscopy and mass spectrometry.



Scheme 1

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Synthesis and description characterization of triazole functionalized cellulose nanowhisker

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Keywords: Cellulose nanowhiskers, Click reaction, Calcium carbide, Triazole rings

Cellulose, the most abundant, polysaccharides in nature, is one of the natural and renewable resources of raw material for the increasing requirement for environmentally friendly and biocompatible products. By dissolving the amorphous or less ordered regions of the naturally occurring cellulose fibers by acid hydrolysis, cellulose nanowhiskers (CNW), are prepared as a new class of nano-materials. Compared to cellulose fibers, needle-like CNW possesses many advantages, such as dimensions in nanometer scale, good mechanical properties, unique optical properties, etc. However, the development of high-performance CNW-based materials is restricted by some limitations. Surface chemical modification via the reaction between the hydroxyl groups located at the surface of CNCs and a functional group from the organ modifying agents has been proposed as an approach to overcome this shortcoming.[1-3] Click reaction is one of the chemical modification methods which can be used for this purpose. This reaction can be performed under mild reaction conditions, shows high yields and has a good tolerance toward a wide range of functional groups and reaction conditions in the material science.[4,5] In In this study, cellulose nanowhiskers (CWs) extracted from cotton fibers were successfully modified with triazole rings through Click" reaction without using hazardous reagents(Fig.1). The surface modification of CWs was performed with calcium carbide, as cheap and commercially available precursors. In this reaction, calcium carbide provides acetylide linkages. These new synthesized biopolymeric nanoparticles were characterized by spectroscopic measurement methods such as IR spectroscopy, NMR spectroscopy, scanning electron microscopy, etc. Taking advantage of the straightforward and gram-scale synthesis as well as physical and chemical properties, prepared nanocomposite is of high interest for water pollutants and wastewater treatment.

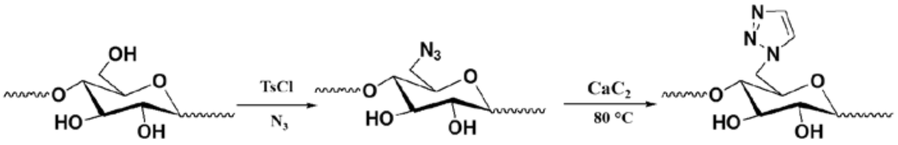

Fig1. Scheme of triazole functionalized cellulose nanowhisker.

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Application of triazole functionalized cellulose nanowhisker for dye adsorption from wastewater

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Keywords: Cellulosic nanowhisker, Click, Triazole ring, Adsorbents.

Nowadays, water pollution control has become one of the major environmental problems. The discharge of dye-contained wastewaters into ecosystem is a dramatic source of aesthetic pollution, eutrophication and perturbation in aquatic life as most of dyes are highly visible, stable and unaffected to chemical, photochemical as well as biological degradation.[1,2] A wide range of chemical and physical treatment technologies are available for dyes removal with different degree of accomplishment to minimize water contamination. However, the shortcomings of most of these methods are high operational and maintenance costs, generation of toxic sludge and complex procedure involved in the treatment.[3,4] Cellulose is one of the most abundant and significant fibrous material in nature which has high mechanical strength, high surface area, biodegradability, non-toxicity, and low cost.[5] In this study, the ability of triazole functionalized cellulose nanowhisker as adsorbents for the removal of the dyes from aqueous solutions was studied(Fig.1). The effect of factors affecting the absorption process such as pH, contact time, adsorbent dosage and temperature were examined. The equilibrium, kinetics, and thermodynamics of the adsorption process were also studied. The adsorption behavior of prepared adsorbents matches well with the pseudo-second-order model and Langmuir adsorption isotherm model.

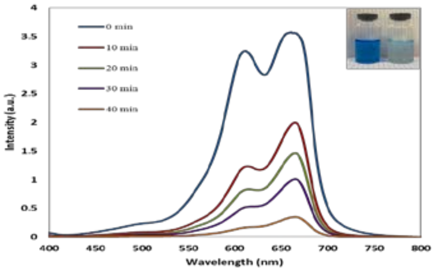

Fig.1 UV−Vis spectral changes for MB at different time intervals with triazole functionalized cellulose nanowhisker.

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A new application of Paal-Knorr reaction for synthesis of pyrrole by magnetic and highly efficient catalyst

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Keywords: Graphitic carbon nitride, C_3N_4/Fe_3O_4, C_3N_4/SO_3H, Paal- Knorr reaction, Pyrrole

The graphitic carbon nitride nanomagnetic catalyst (C_3N_4/Fe_3O_4 and C_3N_4/SO_3H) was prepared and characterized using various instrument methods. Iron oxide supported on graphitic carbon nitride and sulphonic acid supported on graphitic carbon nitride can act as well-organized nano-catalysts and can be easily separated from the reaction mixture using external magnetic fields. C_3N_4/Fe_3O_4 and C_3N_4/SO_3H catalysts is nontoxic and inexpensive catalysts and have particular advantages like a facile synthesis procedure, high activity, easy separation, and reusability. It has applied as efficient catalysts in the synthesis of some of the organic compounds such as pyrrole derivatives in Paal- Knorr reaction. Pyrroles are an important class of heterocyclic compounds, whose structural motif appears in many biologically active natural products, and serve as building blocks in the total synthesis of these compounds. Pyrrole derivatives are important intermediates not only in the synthesis of drugs, pigments, and pharmaceuticals but also for the development of organic functional materials. many methodologies have been developed for the construction of the pyrrole skeleton. Among them, the Paal-Knorr synthesis remains the most useful preparative method for generating pyrroles. This strategy has also been utilized for the preparation of pyrrole libraries, both in solution and on the solid phase. In this research, we applied C_3N_4/Fe_3O_4 and C_3N_4/SO_3H catalysts for synthesis of pyrrole derivatives. Pyrroles have been prepared via one-pot reaction from primary amine and 1,4-dicarbonyl compounds in ethanol at 60 ℃. This method has many advantages such as clean reaction condition, easy workup, and easy separated catalyst.

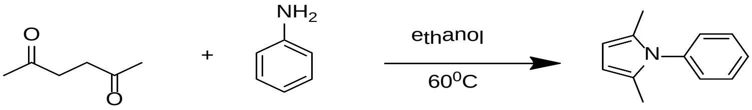

Fig. 1 Synthesis of 2, 5- Di Methyl 1- Phenyl 1-H Pyrrole

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Possible Sensing Study of Graphene-like BC3 and its Doped Derivatives on Diamondoid Antiparkinson Drug Amantadine by Computational Methods

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Keywords: Amantadine, Diamondoid, Sensor, Graphene-like BC_3, Density functional theory (DFT)

Diamondoids (also called nanodiamonds) are cage saturated hydrocarbon molecules that can be superimposed on the diamond lattice.[1] Thus diamondoids which resemble parts of the diamond lattice, are members of the carbon nanostructure family. The simplest of these diamondoids, with the common name “adamantane”, is a tricyclic $C_{10}H_{16}$ isomer. Diamondoids are very attractive nanoscale building blocks (0.5–2 nm).[2] The most widely known functionalized adamantane is 1-aminoadamantane (also known as amantadine), which is both an antiviral and anti-parkinson drug.[3]

In this work, the interactions between the amantadine molecule and nanoparticles including graphene, graphene-like BC_3, and Al-, Si-, P-, and Ga-doped BC_3 have been studied using the B3LYP method with a basis set of 6-31G(d) by Gaussian software 09. The results of calculations demonstrate poor energy interactions between graphene nanoparticles and amantadine. The E_{ad} (adsorption energy) and E_g (gap energy) of nanoparticles-amantadine complexes are as follows:

- The E_{ad} for nanoparticles-amantadine complexes follows the order of BC_3-Al/amantadine > BC_3/amantadine > BC_3-Ga/amantadine > BC_3-P/amantadine > BC_3-Si/amantadine > Graphene/amantadine
- The E_g for nanoparticles-amantadine complexes follows the order of BC_3-Si/amantadine > BC_3-Al/amantadine > BC_3-Ga/amantadine > BC_3/amantadine > Graphene/amantadine > BC_3-P/amantadine.

ΔE_g (%) were also calculated using the equation given below:

$$\Delta E_g = (E_g\text{-complex} - E_g\text{-nano}) / E_g\text{-nano} \times 100$$

The results show that the Si-doped BC_3 nanoparticle is the best sensor for amantadine drug.

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Multi-component synthesis and study of biological properties of new di-amide's Ugi derivatives based on ibuprofen

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Keywords: Multicomponent reaction, Ugi, Green chemistry, Isocyanides, Di-amide, Ibuprofen

Multicomponent reactions (MCRs) combine three or more reactants in a single operation to afford an adduct with a minimum loss of atoms.[1] The development of multi-component reaction [2] protocols for the synthesis of heterocyclic compounds has attracted significant interest from pharmaceutical groups. The Ugi four-component reaction (Ugi-4CR) is useful isocyanide- based MCRs that allow easy access to structurally varied and complex intermediates or scaffolds.[3] The use of water as a solvent for organic transformations offers several “green chemistry” benefits.[4-5] The product is formed by the synthesis of di-amid from cyclohexyl isocyanide 1, aldehyde 2, benzylamine 3, ibuprofen 4 in room temperature and water used as solvent. The structures are determined on the basis of their mass spectrum ^{13}C-NMR, ^{1}H-NMR, and IR spectroscopic data.

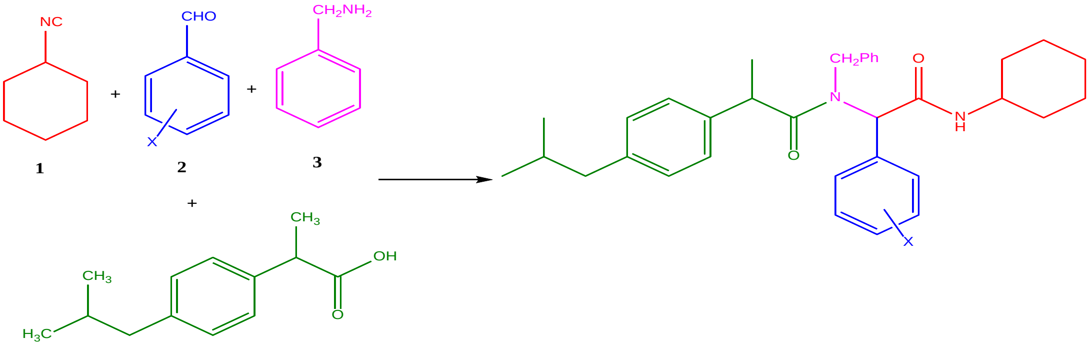

Fig1. Multicomponent product

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Synthesis and description characterization of hydrogels graphene oxide / molybdenum disulfide based nanosheets

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Keywords: Hydrogel, Molybdenum disulfide, Graphene oxide, Hyperbranched polyglycerol.

Nowadays, hydrogels has revolutionized in the wound healing field to improve the therapeutic activity. Various hydrogels made from natural or synthetic polymers have been widely used in this field due to their good biocompatibility, indicating a promising perspective in regenerative medicine.[1,2] Although many techniques have been devoted to promote the performance, physicochemical and therapeutic purposes of hydrogels, however, there are still many challenges in this area.[3,4]

In this study, novel 2D nanomaterials-gelatin hydrogels were synthesized by participation of the graphene (G) and MoS_2 nanosheets with multivalent functional groups (Fig.1). An effective strategy was applied to synthesize the multivalent functionalized MoS_2/G nanosheets by stepwise polymerization of glycidol on nanosheets surface (G/MoS_2-hPG) and conjugation of NH_2 groups to surface. The highest surface area of embedded two-dimensional (2D) nanomaterials in the gelatin hydrogel with the ability of covalent multivalent interactions significantly improved the mechanical and rheological properties as well as biological activity of hydrogels. Their structure and properties were systematically characterized by X-ray diffraction (XRD), thermo gravimetric analysis (TGA), Elemental analysis (CHNS), swelling experiments, scanning electron microscopy (SEM), mechanical and rheological tests.

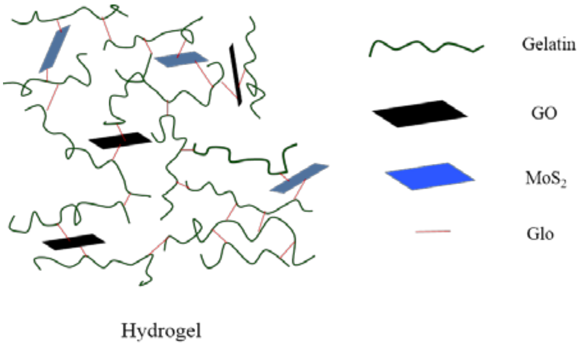

Fig. 1 Scheme of synthesis hydrogels graphene oxide / molybdenum disulfide based nanosheets.

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Release of Anticancer Sunitinib Drug from Chitosan Coated Magnetic Nanoparticle

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Keywords: Magnetic nanoparticle, Chitosan, Anticancer, Drug delivery, Sunitinib

The development of an effective method to treat advanced tumor infections remains a major challenge in cancer therapeutics.[1] In order to reach high therapeutic effects and reduce the side effects, active drug molecules should selectively accumulate in the disease area for a prolonged period with high controllability. Drug delivery refers to the approaches, formulations, technologies, and systems for transporting therapeutics in the body as needed to safely and efficiently achieve their desired therapeutic effects.[2] Sunitinib, an anticancer drug, released efficiently from magnetic carriers to acidic pHs environment. Considering that the nanoparticle size of magnetic carriers influences the release rate[3] as well as the magnetic nanoparticle size affected by the amount of chitosan, in this project, magnetic chitosan nanocarrier used to the controlled release of sunitinib. The magnetic nanoparticles synthesized by a special method and the produced samples dried by freeze-drying. The structure of the produced nanocarrier characterized by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and vibrating sample magnetometer (VSM) techniques. The release behavior of chitosan-coated nanoparticles investigated and revealed a pH and depended release profile. It showed good release at acidic media and at 25°C temperatures, which employed the chitosan-coated nanoparticles as an effective carrier.

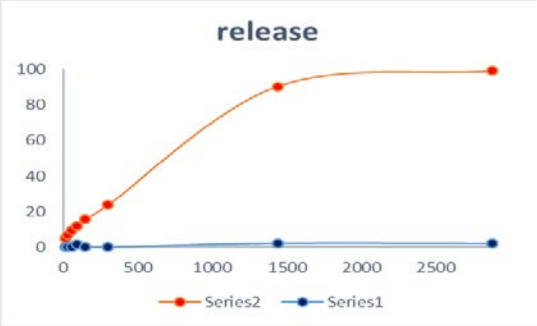

Fig. 1 Cumulative sunitinib release profiles from magnetic carriers at 25 °C and pHs=7.4 and 4.5 for 46h

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Magnetic polystyrene crosslinked by α,ω-bis-4-(vinylbenzyl)ether of polyoxyethylene: Synthesis through ATRP technique

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Keywords: Magnetic crosslinked polystyrene, Surface-initiated ATRP technique, Hydrophilic crosslinker.

Magnetic crosslinked polystyrene (CPS) is an appropriate choice for solid-phase organic chemistry (SPOC) such as organic solid supports in separating processes.[1] Divinylbenzene (DVB) is the most widely used crosslinker for preparing CPS thermosets.[2] However, in this study, we use an α,ω-bis-4-(vinylbenzyl)ether of polyoxyethylene (BVE) as the comonomer/crosslinker. The resulting magnetic CPS exhibited superior swelling and solvent absorption compared to the conventional DVB-crosslinked CPS. This macro-crosslinker could be synthesized from polyethylene glycol and 4-chloromethyl styrene in large excess amounts. In order to achieve magnetic BVE-CPS, the polyaddition reaction of styrene monomer and BVE crosslinker was performed using a surface-initiated atom transfer radical polymerization (ATRP). To attain this purpose, initiator-anchored magnetite nanoparticles (MNP's) were used. The core-shell structure of BVE-CPS/MNP's nanocomposites obtained was thoroughly characterized by Fourier transform-infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), field emission-scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), and vibrating sample magnetometry (VSM) techniques.

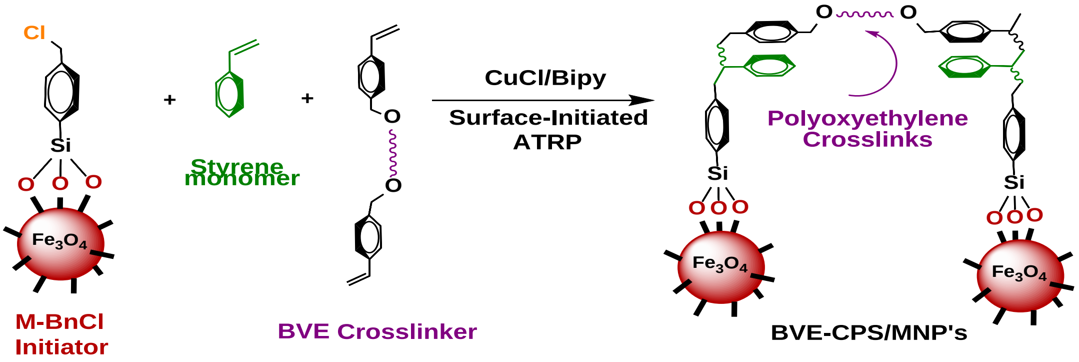

Fig. 1 Synthesis of magnetic crosslinked polystyrene by surface-initiated ATRP technique

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Synthesis, characterization and spectroscopic properties of some new heterocyclic azo dyes derived from 2-amino-4,6-dimethylpyrimidine

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Keywords: Diazo-coupling dyes, Heterocyclic azo dyes, Pyrimidine azo dyes, 2-Amino-4,6-dimethylpyrimidine.

Dyes play an essential role in human history and widely use in various fields, such as coloring fiber, cosmetics, pigments, photoelectronic and other advanced application industries. Among them, heterocyclic azo dyes attract considerable interest for their application as ligands which form complexes with transition metals, produce important colorimetric sensor for cations and anions, *etc*. In this class of azo dyes, pyrimidine and pyridone derivatives are relatively recent heterocyclic intermediates for the preparation of aryl-azo dyes.[1,2] In this study, a series of new azo dyes by linking 2-amino-4,6-dimethylpyrimidine (1) and various aniline derivatives was synthesized (Fig. 1). The structure of all compounds was confirmed characterized by Fourier transform-infrared spectroscopy (FT-IR), Proton magnetic resonance (^{1}H-NMR) and Ultraviolet-visible spectroscopy (UV-Vis). Comparison of absorption maxima (λ_{max}) by the introduction of substituents factors situation with ±I and ±M effects on diazonium salt component in two different solvents (Ethanol and DMSO) have been studied.

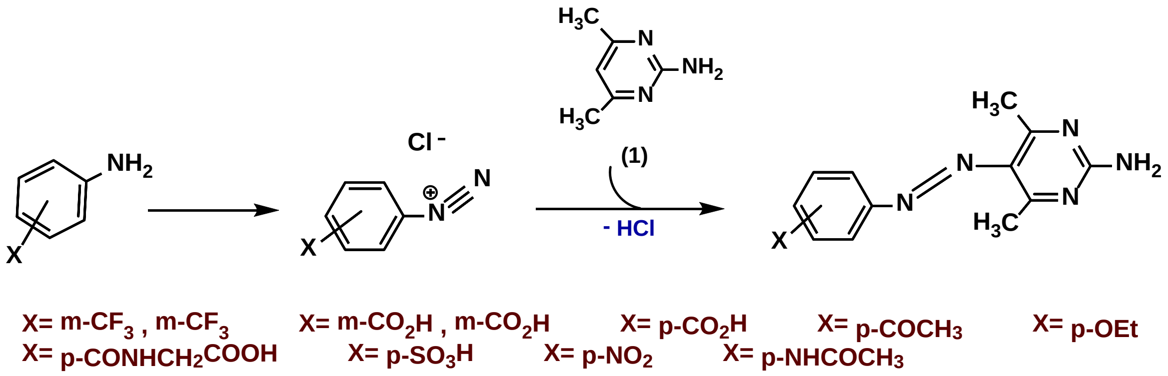

Fig. 1 Synthesis of azo dyes.

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School of experimental skills, theoretical aspects and computational abilities in chemistry; A bridge on limitations (II)

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Keywords: Chemistry; Experimental Skills; Theoretical Aspects; Computational Abilities.

The theory and mathematics of computational chemistry could be very specialized and tedious. Due to the endless applications of this established field, it gains a high reputation rapidly among all chemists around the world, even experimental chemist who call the computational software as “dry-lab”.[1-4] The statistical analysis of chemistry papers over the past two decades indicates continuous day to day grow in the proportion of chemistry researches. The main aims of this school is to introduce the computational chemistry as a significant and inseparable tool for chemists, and how this “dry-lab" could help researchers to supplement their experimental results.[5-9] The application of the items of this predicted school is very useful in the different scientific aspects, such as: benefits in science economy, time saving, boost scientific confidence, prevention of wasting time and energy of scientist and researchers, prevention of wasting expensive chemicals, improving of green chemistry aims, improving of safety, increasing the rapidity to gain the scientific results in pharmacology, medicinal chemistry, synthesis, physical organic chemistry, increasing the scientific efficiency aspects of chemical soft wares, increasing the economy efficiency from chemical soft wares, improving the rapidity of circle development of scientific in different aspects of chemistry, creation of new interdisciplinary sciences, construction of bridges on the scientific limitations and other effective aspects to improve the quality of life style of human.

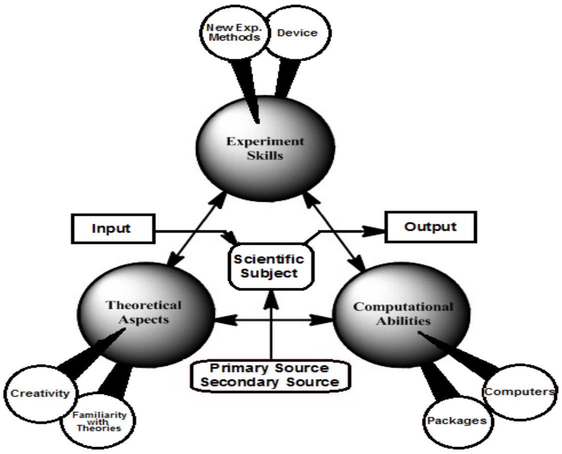

Fig.-1: Predicted School of Experimental Skills, Theoretical Aspects and Computational Abilities.

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Synthesis and assessment of PHEMA-st-PEG-DA nanohydrogels for controlled released of cisplatin

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Keywords: RAFT synthesis, Nanohydrogel, PHEMA, PEG-DA, Cisplatin, Drug delivery.

Nanohydrogels are novel and attractive carriers for various anti-cancer factors delivery. The objective of present study is development of a safe nanohydrogel for pH responsive delivery of cisplatin. Herein, poly (hydroxyl ethyl methacrylate) is utilized as the main structure, which is cross-linked with PEGDA and EDTA through reversible addition fragmentation chain transfer polymerization technique. After synthesis, the developed structure is characterized using different methods, including ^{1}HNMR, FT-IR, size exclusion chromatography, TEM and DLS. The results confirm successful synthesis of the nanohydrogel with acceptable yield and nano scale mean size of 196 nm. Cisplatin is conjugated with the EDTA of aforementioned structure through pH responsive esteric bond. The efficiency of the prepared nanohydrogel in loading and release of the anti-cancer drug, cisplatin, is tested. The developed nanohydrogel shows great potential in cisplatin loading, as well a faster release rate of cisplatin in acidic pH. The results of *in vitro* toxicity assessment on SW 480 as a colorectal cancer cell line reveal an improved cytotoxicity induction by the cisplatin loaded particles when compared with the free cisplatin molecules. The suitable size (<200 nm), great potential in loading and release of the cisplatin and cytotoxicity induction in cancer cells are the reliable features of nanohydrogel as an ideal anti-cancer vehicle.

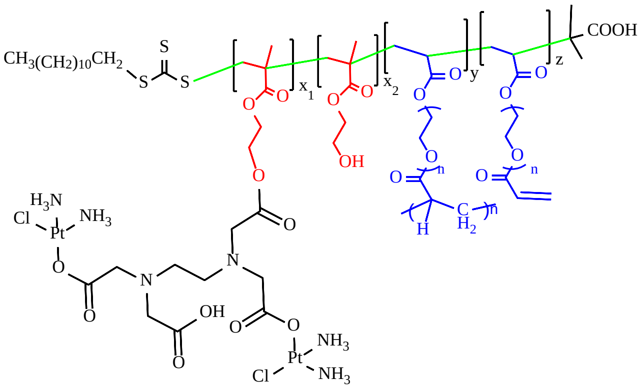

Fig. 1 Schematic presentation of the involved cisplatin and the final synthesized nanohydrogel structure.

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Magnetic mesoporous poly-melamine–formaldehyde: an efficient and recyclable catalyst for straightforward one-pot synthesis of α-Aminophosphonates

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Keywords: Multicomponent reactions, α-Aminophosphonates**,** mPMF@Fe3O4-SO3H, Green chemistry

Magnetically separable mesoporous poly-melamine–formaldehyde nanocomposite (PMF@Fe3O4-SO3H) has been synthesized and characterized by FTIR spectroscopy, SEM, XRD spectroscopy and EDS. The magnetically separable PMF@Fe3O4-SO3H catalyst had excellent efficiency for the synthesis a wide diversity of α-Aminophosphonates by a three-component reaction of a Amines, aldehyde and Trimethyl Phosphite in good-to-excellent yields within a short reaction time, through an environmental friendliness and straightforward procedure. The nanocomposite that is easily recoverable and also found to be reusable can be recovered and reused when the reaction is completed for several times without distinct deterioration in catalytic activity.

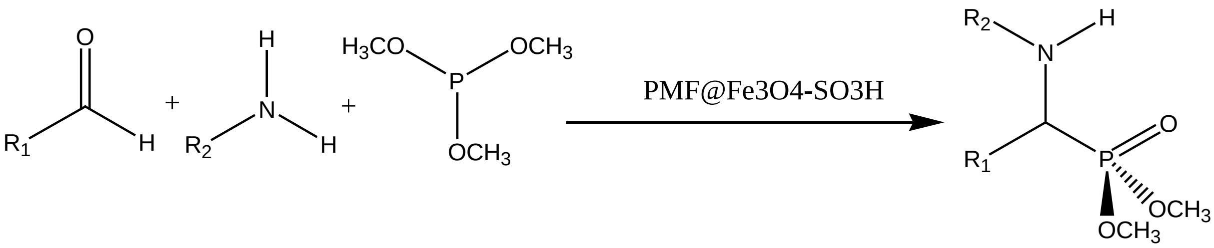

Fig. 1 Multicomponent α-Aminophosphonates

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Synthesis of 2-amino-4*H*- benzo[*h*]chromenes in the presence of Fe_3O_4/SiO_2/urea nanocatalyst

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Keywords: Multicomponent reactions, Nano catalyst, Fe_3O_4/SiO_2/urea, 2-Amino-4H-benzo[h]chromene-3-carbonitrile.

Nanoparticle Fe_3O_4-supported catalysts can be simply separated from the reaction mixture by an external permanent magnet. This strategy is typically more effective than filtration or centrifugation that become annoying for such small nanoparticles.[1,2] Herein, we report the synthesis of 2-amino-4*H*-benzo[*h*]chromene-3-carbonitrile **4** from the reaction between aromatic aldehyde **1**, malononitrile **2** and 1-naphthol **3** in the presence of Fe_3O_4/SiO_2/urea catalyst. All synthesized compounds are stable solids their structures were determined on the basis of their mass spectrum, ^1H and ^{13}C NMR and IR spectroscopic data.

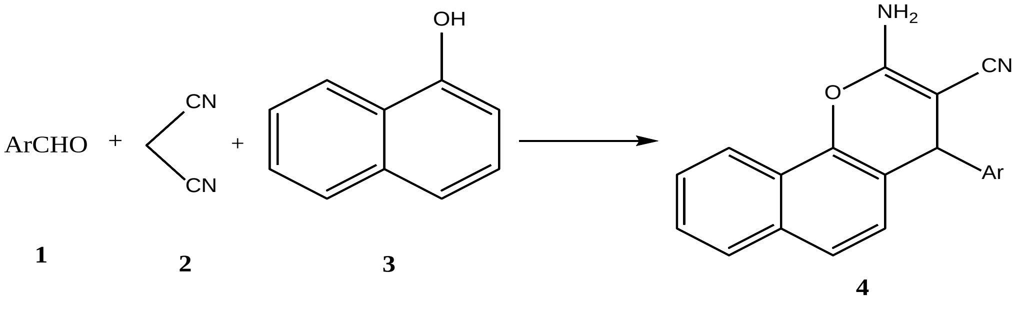

Fig. 1 Multicomponent 2-amino-4H- benzo[h]chromene-3-carbonitrile

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Synthesis of synthetic oils

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Keywords: Synthetic oils, Synthetic esters, Bio lubricants, Polyol ester

Lubricants have been used in various industries, such as drilling, aviation, automotive, factories, and food processing. The food grade lubricants that are available in the market are mostly produced from refined naphthenic mineral oil or white oil, which are not promisingly safe-based oils. Mineral oil-based lubricants are harmful to human beings and the environment, and also there is another issue of its poor biodegradability and toxicity which has led to health problems on a long term basis.[1] Synthetic polyol esters are used as environmentally acceptable base fluids in high performance lubricants. A very good low temperature behaviour, high thermo-oxidative stability of some types, very high viscosity index, good anti wear and low evaporation properties have led to their use in many lubricants. Compromise between viscosity, volatility and cost influences the choice of base stocks for their effective ecofriendly formulations.[2] Generally, ester-based biolubricants can be prepared via esterification reactions between polyhydric alcohols with fatty acids in the presence of acid catalyst.[3] Herein, we report the synthesis of the esters using polyhydric alcohols and carboxylic acids in toluene solvent at 250 ° C, whose structures were determined on the basis of their mass spectrum, ^{1}H NMR, X-ray, TGA, and IR spectroscopic data.

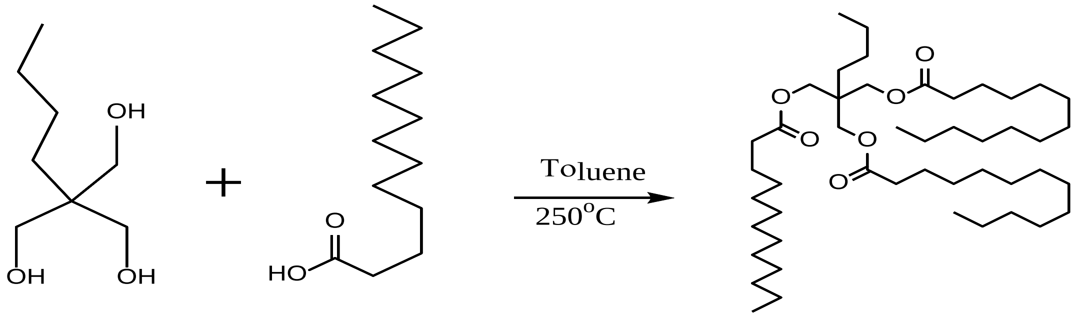

Fig.1 Schematic synthesis of esters-based synthetic oils

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Three-dimensional graphene/zeolite nanocomposite: Synthesis and characterization

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Keywords: 3D Graphene, Zeolite, Nanocomposite.

Huge amounts of study and development are currently underway in the arena of improving three-dimensional graphene and graphene oxide networks for use for a wide range of applications. The aim of this study is synthesis of three-dimensional (3D) graphene nanocomposites and loading of zeolite particles on three-dimensional graphene substrate. In this study, we prepared a three-dimensional graphene/zeolite nanocomposite via a simple in situ reduction method through simple cross-linking of graphene oxide (GO) using starch. The nanocomposite has honeycomb morphology and has been characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction analysis (XRD).

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pH-sensitive nanocomposite hydrogels scaffold based on polyvinyl imidazole -graphene quantum dots with antibacterial properties for tissue engineering

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Keywords: Nanocomposite hydrogels, N-Doped graphene quantum dot, 1-Vinylimidazole, Tissue engineering, Antibacterial properties.

Hydrogels are a form of 3D porous materials, which consist of polymer chains with either physical or chemical crosslinking. They represent an important class of biomaterials in biotechnology and medicine because many hydrogels exhibit excellent biocompatibility, causing minimal inflammatory responses, thrombosis, and tissue damage[1]. Hydrogels can also swell with large quantities of water without the dissolution of the polymer due to their hydrophilic but crosslinked structure, thus giving them physical characteristics similar to soft tissues. Hydrogel materials have been used extensively in medicine for applications such as contact lenses, biosensors, linings for artificial implants, and drug delivery devices and tissue engineering[2]. The pH sensitive hydrogels are extensively used in different fields such as medicine, pharmacy, agriculture, food industry and controlled drug delivery etc[3]. In this work, we synthesized two series of pH-sensitive nanocomposite hydrogels (PVI/GQDs) based on polyvinyl imidazole (PVI) and N-doped graphene quantum dots (NGQDs). The first series of nanocomposite hydrogels (PVI/NGQD-1) were synthesized using 1-vinyl imidazole (VI) monomer and N, N′- methylene-bis-acrylamide (MBA) cross linker with different molar ratios and different amounts of NGQD as a nanofiller. The second series of nanocomposite hydrogels (PVI/NGQD-2) were synthesized similarly only using an imidazolium-based dicationic IL (DIL) as a crosslinker. The compression test showed that the PVI/NGQD-1 hydrogels were more strength than the PVI/NGQD-2 hydrogels. Moreover, the PVI/GQD-1 hydrogels show more antibacterial properties in comparison with the PVI/NGQD-2 hydrogels. The synthesized PVI/GQDs hydrogels were characterized by FT-IR, TGA, XRD, SEM and compression test.

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Magnetically separable and recyclable mPMF nanocomposite catalyzed one-pot synthesis of substituted 3,4-dihydropyrimidin-2(1*H*)-ones

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Keywords**:** Multicomponent reactions, mPMF, mPMF@Fe3O4,Green chemistry, 3,4-dihydropyrimidin-2(1H)-ones

A green, reliable synthetic method and highly efficient one-pot three-component synthesis of 3,4-dihydropyrimidin-2(1H)-ones from urea, aldehydes and ethyleacetoacetate in the presence of recyclable magnetic poly-melamine–formaldehyde nanocomposite (mPMF@Fe3O4) has been developed. Various imidazole derivatives were obtained in moderate to excellent yields and high purity after recrystallization from ethanol. Interestingly, the low-cost mPMF@Fe3O4 a nontoxic and inexpensive catalyst showed excellent recyclability using an external magnet without loss of parent catalytic activity even after ten cycles and its provides new opportunities for the truly environmental friendliness methodology.

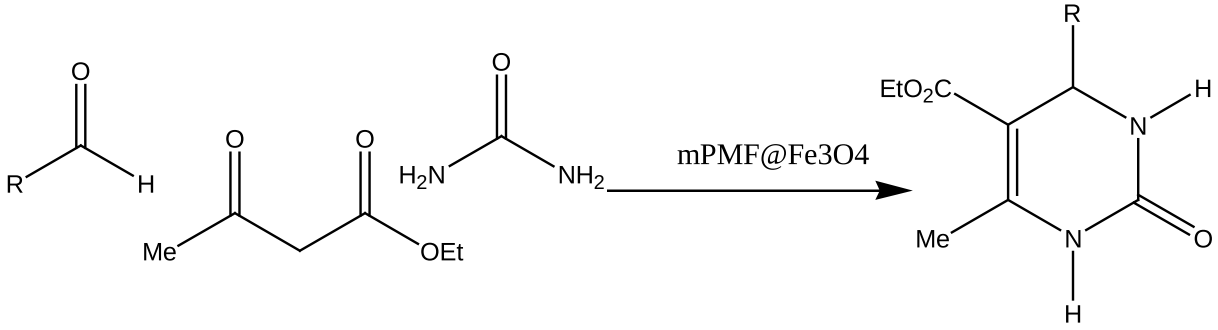

Fig. 1 Multicomponent 3,4-dihydropyrimidin-2(1H)-ones

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Synthesis of 2-amino-4*H*-benzo[*h*]chromenes in the presence of Fe_3O_4/SiO_2-APTES nanocatalyst

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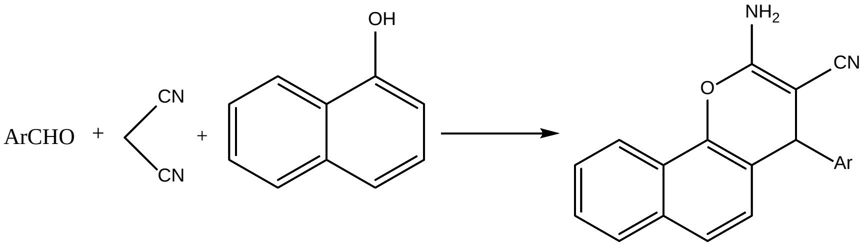
Keywords: Multicomponent reactions, Nano catalyst, Fe_3O_4/SiO_2-APTES, 2-Amino-4H-benzo[*h*]chromenes.

The use of environmentally benign, maintainable and efficiently reusable catalysts provides both economic and ecological advantages.[1] Recycling of homogeneous catalysts is a main draw back in large-scale production of chemicals.[2] Recently, nanoparticles have appeared as efficient catalysts and supports for the immobilization of homogeneous catalysts. [3-6] Herein, we report the synthesis of 2-amino-4H- benzo[h]chromene-3-carbonitrile **4** from the reaction between aromatic aldehyde **1**, malononitrile **2** and 1-naphthol **3** in the presence of Fe_3O_4/SiO_2-APTES catalyst. All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^{1}H and ^{13}C NMR and IR spectroscopic data.



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

Fig. 1 Multicomponent 2-amino-4H- benzo[h]chromene-3-carbonitrile

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Cellulose nanocrystals functionalized by folate-Conjugated cyclodextrin for targeted anti-cancer drug delivery system

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Keywords: Targeted drug delivery, Anti-cancer, Drug carriers, Cellulose nanocrystals, Natural polymers

Targeted drug delivery systems (TDDSs) have been exploited to improve the efficacy of anticancer agents by increasing their concentration in tumor cells relative to normal cells.[1,2] This leads to administration of required amount of drug with low toxicities which usually occur with conventional chemotherapeutic agents.[3] Herein, a TDDS based on nanoparticles transaminase of nanocrystalline cellulose (CNCs) which was prepared for cancer cell targeting. The nanoparticles transaminase then conjugated with carboxymethyl-β-cyclodextrin (CM-β-CD). The folic acid (FA) was then embedded into CD cavity via host guest interaction. Doxorubicin (DOX) an anticancer drug was introduced into nanocarier spheres. The properties of the prepared nanocarier were characterized by FT-IR, scanning electron microscope (SEM) and TGA. The in-vitro drug release and drug loading capacity were measured using UV spectroscopy.

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A targeted drug delivery system of anti cancer agents on Folate-Conjugated CM-β-CD and CNCs/APTMS

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Keywords: Nanotechnology, Targeted drug delivery, Cyclodextrin, Cellulose nanocrystals, Folic acid

Drug delivery systems can target the drug to specific tissues,[1,2] minimise side effects, overcome solubility problems and toxicity and be tailored to have the appropriate immunogenicity and metabolic stability [3,4]. In present research a qualified nanocarrier for targeted drug delivery to tumor cells based on Nanocrystalline cellulose (CNCs) was synthesized. The amino nanoparticles then conjugated with carboxymethyl-β-cyclodextrin (CM-β-CD) by aminopropyltrimethoxysilan (APTMS) as linker. The folic acid (FA) was then embedded into CD cavity via host guest interaction. Doxorubicin (DOX) an anticancer drug was introduced into nanocarier spheres. The properties of the prepared nanocarier were characterized by FT-IR, scanning electron microscope (SEM) and TGA, The in-vitro drug release, drug loading capacity were measured using UV spectroscopy.

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Synthesis Of Polyhedral Oligomeric Silsesquioxane (POSS) Derivatives

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Keywords: Polyhedral Oligomeric Silsesquioxane (POSS) Polymers, POSS Macromers, Thermoplastics, Thermosets, Thermal and Mechanical Properties.

The search for new nanofillers has led to development of new organic-inorganic hybrid materials such as polyhedral oligomeric silsesquioxanes (POSS).[1] POSS is a cubeoctameric molecule with an internal structure of silicon and oxygen that is covered outside by organic substrates. The POSS molecules having cubic inorganic core with the composition of $R_8Si_8O_{12}$ or $R_1R_7Si_8O_{12}$ are the most studied systems. R groups (organic shell) can be varied from hydrogen to alkyl (methyl, isobutyl, cyclopentyl or cyclohexyl, etc.), alkylene, or arylene.[2] Interest in POSS materials is based on the facts that their rigid framework closely resembles that of silica and that they offer a unique opportunity for preparing truly molecularly dispersed nanocomposites. The POSS chains act like nanoscale reinforcing fibers, producing extraordinary gains in heat resistance.[3] A novel octakis(3-propyl thiophenolate)-octasilsesquioxane was successfully synthesized via nucleophilic substitution on octakis(3-chloropropyl)octasilsesquioxane using sodium thiophenolate in aprotic dimethylformamide as a solvent. Complete substitution proceeded at room temperature product in high yield. The reaction products were characterized by ^1H, ^{13}C, and ^{29}Si NMR spectroscopy; confirming the structure of the cubic T_8 cage and demonstrating that the substitution reaction on eight side chains progressed smoothly under ambient conditions without any cage rearrangement or cage decomposition.

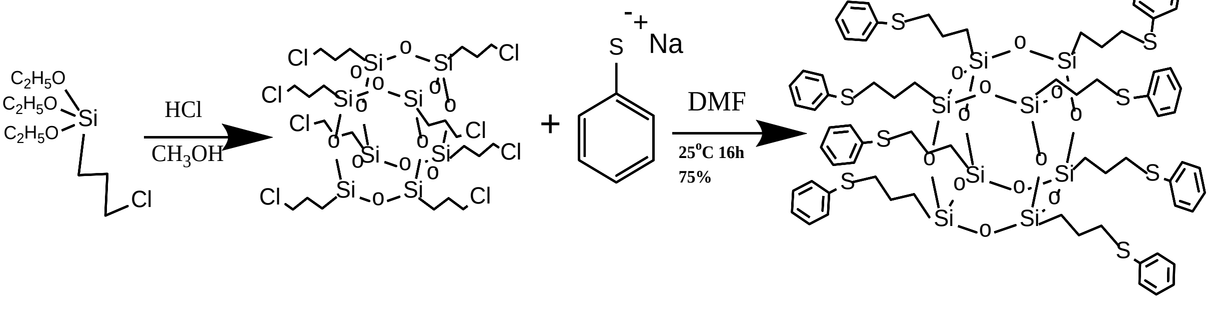

Fig. 1 Schematic of Octakis(3-propyl thiophenolate)octasilsesquioxane synthesis.

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pH-sensitive $Fe_3O_4@SiO_2@ CH_2=CHSiH_3$ magnetic nanocarrier for targeted anti cancer drug delivery labeled with carboxymethylcyclodextrin(CM-β-CD) and folic acid

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Keywords: Nanocomposites, Targeted drug delivery, Anti-cancer, Magnetic nanocarrier, Amino acid

Applications of Fe_3O_4 nanoparticles in the field of biotechnology involve targeted drug delivery,[1] magnetic resonance imaging (MRI),[2] contrast enhancement and hyperthermia reagents, biophotonics,[3] and detection, diagnosis, and magnetic field–assisted radiation treatment of cancerous cells [4]. In present research a qualified nanocarrier for targeted drug delivery to tumor cells based on magnetic mesoporous silica nanoparticles (MMSNs), consisting of Fe_3O_4 core coated with mesoporous silica and a pH-responsive shell of amino acid L-cystien conjugated carboxymethyl-B-cyclodextrin and folic acid was prepared (Fig.1). Doxorubicin (DOX) an anticancer drug was introduced into nanocarier spheres. The nanoparticles were characterized using various scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) thermogravimetric analysis (TGA), and vibrating sample magnetometer (VSM).

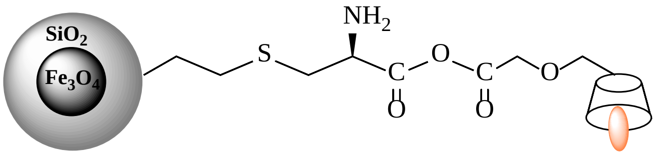

Fig.1 PH-sensitive magnetic nanocarrier for targeted anti cancer drug delivery

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Magnetic nanoparticle drug delivery systems for targeting tumor based on PEI -FA bonded Fe_3O_4@SiO_2@CPS nanoparticles

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Keywords: Targeted drug delivery, Anti-cancer, Nanocarriers, Magnetic nanoparticle

Magnetite Fe_3O_4 nanoparticles have widespread applications in the magnetic bioseparation,[1] drug delivery,[2, 3] and magnetic resonance imaging,[4] especially in targeted drugs. Herein we developed a targeted anticancer drug delivery system based on folate-conjugated rattle-type Fe_3O_4@SiO_2@CPS (3-chloropropyltriethoxysilian) hollow mesoporous spheres combining receptor-mediated targeting and magnetic targeting. Polyethylenimin -folic acid (FA) ligands were successfully grafted onto rattle-type Fe_3O_4@SiO_2 hollow mesoporous spheres via amide reaction (Fig.1). Doxorubicin (DOX) an anticancer drug, was introduced into nanocarier spheres. The nanoparticles were characterized using various scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) thermogravimetric analysis (TGA), and vibrating sample magnetometer (VSM).

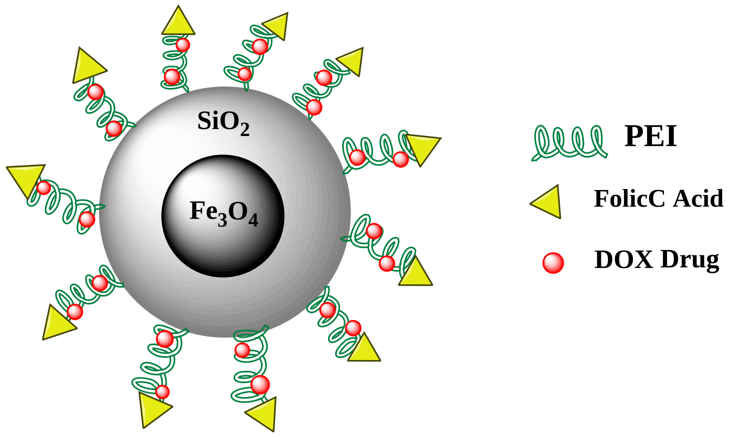

Fig1. Biocomptible and folat sensitive magnetic nanocarier with targeted drug deliveri

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One-Pot synthesis of stable phosphorus ylides

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Keywords: Phosphorus ylides, Triphenylphosphine, Arylglyoxals, 1,3-dicarbonyl compounds.

Phosphorus ylides are reactive systems, which take part in many reactions of value in organic synthesis.[1] The development of the modern chemistry of naturally and physiologically active compounds would have been impossible without the phosphorus ylides. These compounds have attained great significance as widely used reagents for linking synthetic building blocks with the formation of carbon-carbon double bonds, and this has aroused much interest in the study of the synthesis, structure, and properties of P-ylides and their derivatives.[2] Several methods have been developed for the preparation of phosphorus ylides. They are usually obtained by treatment of a phosphonium salt with a base; phosphonium salts are usually prepared from the corresponding phosphines and an alkyl halide.[3] Here we report an efficient synthetic route to stable phosphorus ylides using, arylglyoxals **1** and 1,3-dicarbonyl compounds such as barbituric acid **2** and triphenylphosphine **3** at boiling ethanol. All synthesized compounds are stable solids whose structures were determined on the basis of their ^{1}H and ^{13}C NMR and IR spectroscopic data**.**

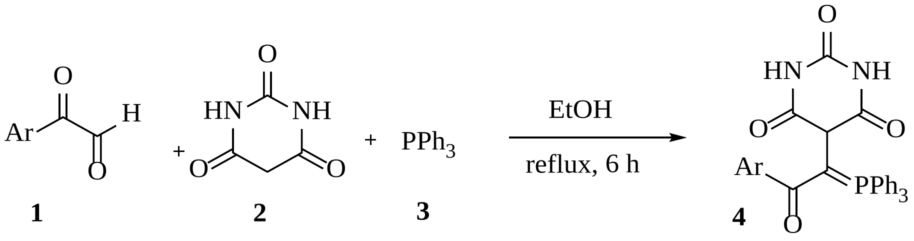

Fig. 1 Synthesis of stable phosphorus ylides

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Application of thiolate salts in the synthesis of heterocyclic compounds *via* multicomponent reactions

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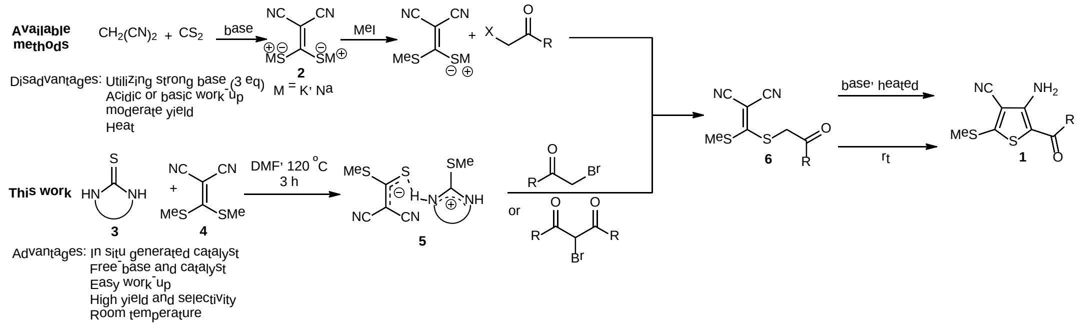
Keywords: Ketene dithioacetal, Triethylammonium thiolate, Methyl iodide, *o*-Phenylenediamine, Quinoxaline, Cyclic thiourea, Thiophenes, Indandione Motif, Multicomponent reactions

The available approaches to the synthesis of tetrasubstituted thiophenes include 5-acetyl-4-amino-2-methylsulfanyl-3-carbonitrile relies on generating inorganic salt of 2,2-dicyano-1,1-dithiolate from malononitrile and carbon disulfide, following reaction with α-haloketones in presence of base at heat condition.[1] However, these approaches suffer from significant limitations in terms of harsh reaction conditions, multitude operational steps, temperature adjustment, low yields, strong base, and difficult purification.

In line with the above statements, inventing a protocol that concomitantly lacks catalyst, acidic or basic media, and heating, which are three necessary obligations in all documented procedures for the synthesis of thiophene frameworks, would be a great innovation. Herein, the present study breaks the aforementioned boundary in a two-step reaction, harnessing organic salt **5** generated by cyclic thioureas and di(methylsulfanyl)methylenemalononitrile (Scheme 1).



Scheme 1 Synthetic methods for tetrasubstituted thiophenes **1**

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Cyclocondensation reaction of isatins with malononitrile and 4-hydroxycoumarin or 3,4-methylenedioxyphenol catalyzed by TiO_2 nanoparticles immobilized on carbon nanotubes

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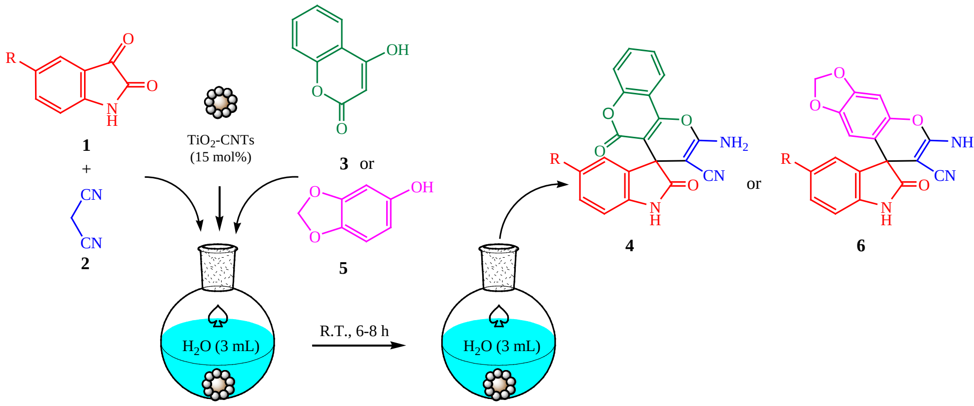
Keywords: Aqueous media, Environment-friendly procedure, 4-Hydroxycoumarin, Isatin, 3,4-Methylenedioxyphenol, TiO_2-CNTs.

During the past decade, the utility of metal oxide nanoparticles (NPs) as efficient heterogeneous catalysts in organic synthesis has been preferably expanded.[1-3] Due to the wide range of biological and medicinal activities the synthesis of spiro compounds has become a significant target over the past decade. in the present work, we report the efficient synthesis of spiro[3,4']1,3-dihydro-2*H*-indol-2-one-2'-amino-5'-oxo-4'*H*,5'*H*-pyrano[3',2'-*c*]chromen-3'-yl cyanides and spiro[3,8']1,3-dihydro-2*H*-indol-2-one-6'-amino-8'*H*-[1',3']dioxolo[4',5'-*g*]chromen-7'-yl cyanides catalyzed by TiO_2-CNTs as a useful recyclable heterogeneous catalyst in aqueous media at room temperature (Scheme 1).



Scheme 1 Reaction of isatins with malononitrile and 4-hydroxycoumarin or 3,4-methylenedioxyphenol in the presence of TiO_2-CNTs nanocomposite

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SiC hollow nanosphere as an efficient catalyst for oxidative desulfurization of model fuel

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Keywords: Silicon carbide, Nanosphere, Catalyst, Oxidative desulfurization.

The sulfur compounds in the oil products are one of the most important pollutants that must be removed due to the generation of the toxic sulfur.[1] There are several ways to remove the sulfur compounds from oil. Oxidation desulfurization (ODS) method is a favored approach due to its ability to reduce the aromatic sulfur compounds in mild operational condition.[2,3] In this research, SiC hollow nanosphere has been synthesized *via* two natural biopolymers as carbon sources and tetraethylorthosilicate as Si source. Low-temperature magnesiothermic method used to produce the special nanostructure. The prepared SiC catalyst was characterized by FT-IR, XRD, Raman, XPS, SEM/EDS, and BET/BJH methods and its catalytic activity was investigated in oxidative desulfurization of model fuels (thiophene, benzothiophene, dibenzothiophene, and 4,6-dimethyl dibenzothiophene). The results indicate that the SiC catalyst shows the good catalytic activity (99.5%, 20 min). The catalytic performance of this metal-free catalyst is comparable with the popular metal catalysts like MoO_3. Furthermore, the stability of catalyst was tested by recycling the catalyst. Result exhibits no remarkable decrease in activity of catalyst even after 5 runs.

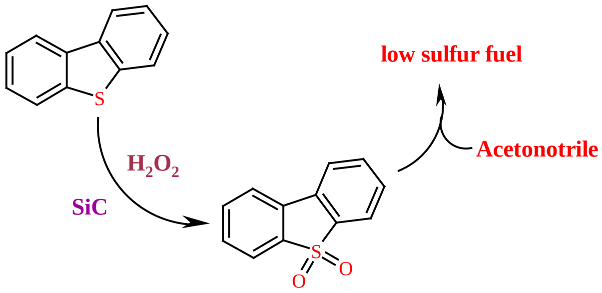

Fig. 1 Oxidative Desulfurization Reaction

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Design and synthesis of novel heterocyclic derivatives as soluble epoxide hydrolase inhibitors

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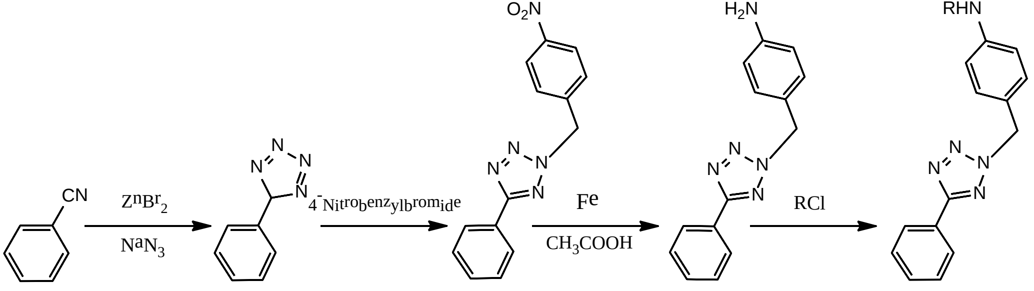
Keywords: Soluble epoxide hydrolase, Tetrazole, Synthesis.

Soluble epoxide hydrolase (sEH), is an enzyme belongs to serine hydrolase family. sEH inhibition provides a novel approach to treat common ailments such as hypertension and inflammation. We designed and synthesized novel inhibitors, having tetrazole core to improve pharmacokinetic profile and potency.[1] In this study, 5-phenyl-5H-tetrazole (**1**) was prepared by the reaction of benzonitrile and sodium azide using freshly synthesized $ZnBr_2$ as the catalyst.[2] Then N-benzylation of the compound **1** with 4-nitrobenzylbromide leads to crystalline compound **2**.[3] Then the compound **3** is resulted by reduction of nitro group of compound **2** with a mixture of iron powder, glacial acetic acid, ethanol and water under sonication for one hour.[4] The final products (**4**) were afforded by treating of 4-((5-phenyl-2H-tetrazol-2-yl)methyl)aniline (**3**) with different benzoyl chlorides at room temperature in dry tetrahydrofuran **(Fig. 1)**.[3]

Finally, some novel compounds bearing a tetrazole ring were designed. The designed compounds showed high affinity to the active site of the sEH enzyme and were synthesized in good yield and were characterized by IR, Mass, ^{H}NMR, and ^{C}NMR.



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

Fig. 1 The synthesis of the designed compounds.

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Preparation of Chitosan and Alginate Nano-Fibers in Delivery of Curcumin by Electrospinning

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Keywords: Chitosan, Nanofibers, Electrospinning, curcumin, Anticancer.

Electrospinning has been used to generate nanofibers via an electrically charged jet of the polymer solution. This process is established on a spinning technique, using electrostatic forces to produce fine fibers from polymer solutions. Nanofibers drug delivery systems have been developed for improving the therapeutic effects and to reduce the side effects of anti-cancer drugs. Curcumin is a natural compound extracted from the roots of Curcuma Longa L. and its cytotoxic properties were studied. Nanofibers of Chitosan (CS) alginate (ALG) loaded curcumin(CUR) were prepared by the electrospinning method. Their morphology was evaluated by Scanning Electron Microscopy. The drug loading and release rate of nanofibers (CS/ALG) were studied. Drug release rate dependence on pH and temperature. In vitro release rate was performed in acidic pH. The 56% of cells (the colorectal cell line HT-29) survived under MTT cytotoxic method after 72 hours exposed of (CS/ALG+ CUR) nanofibers.

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D-penicillamine functionalized Nano fibrous mesoporous silica and its application for the removal of heavy metal Pb^{2+} from the aqueous solution

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Keywords: Dendritic fibrous nanosilica, d-Penicillamine, Separation science**,** Absorbent

In this work, d-penicillamine-modified dendritic Fibrous Nanosilica grafted by amine groups (dPA-DFNS-NH_2) with specific surface area of 358 m^2g^{-1} have been successfully synthesized respectively by *in-situ* synthesis and post-modification methods [1]. Transmission electron microscopy (TEM) observations show that the average diameters of the prepared fibrous dPA-DFNS-NH_2 is 42 nm. The N_2 adsorption-desorption isotherms analysis on the DPA-DFNS-NH_2 show sharp peaks in the 15-22 nm range. After the -SH functional groups transformed to DFNS-NH_2, the adsorption behavior of the dPA-DFNS-NH_2 for Pb^{2+} was investigated [2]. The results show that the prepared dPA-DFNS-NH_2 can selectively adsorb Pb^{2+} in different potentials by some of electrochemical techniques. Finally, application of engineered adsorbent for the removal of Pb^{2+} from local natural ground water samples was examined. This work provides the methods to prepare dPA functionalized DFNS-NH_2 with high specific surface area and total pore volume, which has the potential to be applied as an efficient adsorbent for specific metal ions.

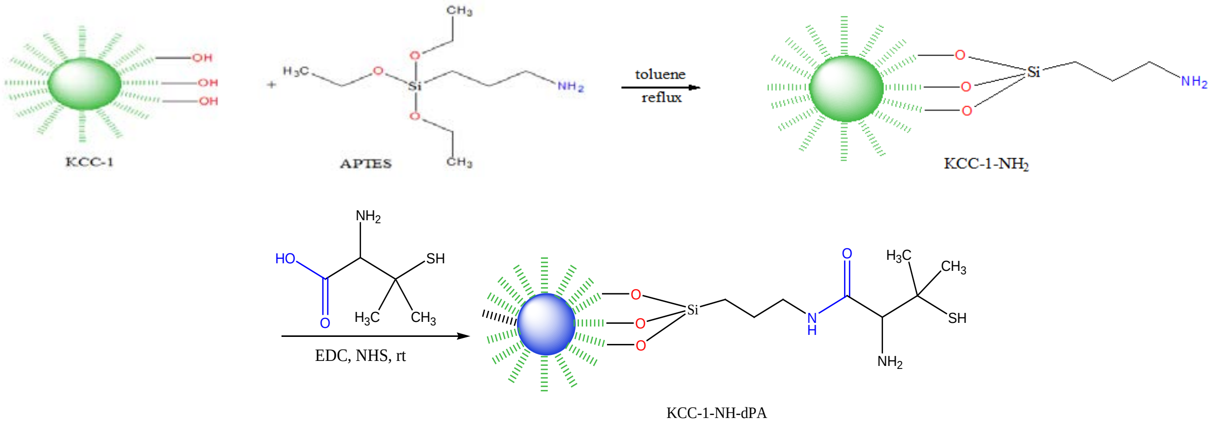

Fig.1 Synthesized procedure of KCC-1-NH_2-dPA

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Synthesis of carboxymethyl tragacanth coated Fe_3O_4@SiO_2 core–shell magnetic nanoparticles as a drug delivery system

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Keywords: Magnetic nanoparticles, Carboxymethyl Tragacanth, Methotrexate, drug delivery system, Core–shell.

In this study, chemically modified iron oxide nanoparticles with super paramagnetic behavior and biodegradable properties were prepared through the reaction of a polymeric layer with surface hydroxyl functional groups of magnetic nanoparticles (MNPs).[1] For this purpose firstly, Fe_3O_4@SiO_2 as a core magnetic nanoparticles were prepared by chemical coprecipitation of $FeCl_3.6H_2O$ and $FeCl_2.4H_2O$ in alkaline solution followed by silylation using triethoxy silane.[2] The MNPs was grafted with hexamethylene diisocyanate. Then, carboxymethyl tragacanth which was modified with the hexamethylenediamine (mCMT) as a shell was coated and reacted simultaneously on MNP-grafted hexamethylene diisocyanate to form a polymeric core–shell (MNP/mCMT). The structural, morphological, thermal, and magnetic properties of the synthesized magnetite nanocomposite were confirmed by Fourier transform infrared spectrophotometer, thermal gravimetric analysis, X-ray diffraction, vibrating sample magnetometer, and scanning electron microscopy.[3] Methotrexate (MTX) as a model anticancer drug was used. The in vitro release of MTX from the MNP/mCMT was investigated and indicated that the release speed of the MTX could be well controlled. Release profiles of the MTX and its loading capacity were determined by ultraviolet–visible spectroscopy absorption measurement at λ_{max} 307 nm.[4] The obtained results suggest that the prepared magnetite nanocomposite would be beneficial as a targeted anti-tumor drug carrier for pharmaceutical applications.

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Electrospinning of nanofibers based on carboxymethyl tragacanth-polyvinyl alcohol/nano-clay composite containing silver nanoparticals for wound healing applications

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Keywords: Electrospinning, Carboxymethyl Tragacanth, Polyvinyl Alcohol, Silver Nanoparticles, Wound Healing Applications.

The present article discusses a simple method to prepare antibacterial carboxymethyl tragacanth (CMT)/ polyvinyl alcohol (PVA) nanofiber mats containing silver nanoparticles (Ag NPs).[1] The nanofibers are fabricated by electrospinning of CMT/PVA/$AgNO_3$ blend aqueous solution with an $AgNO_3$ concentration of 10 mmol/L. Then the prepared composite was cross-linked with glutaraldhyde.[2] In electrospinning procedure, the Ag NPs with average diameter of 4.5 nm are obtained and separated from each other on the surface of CMT/PVA nanofibers.[3] At the next step nano-clay (NC) powder was added to the prepared nanocomposite structure with various mass ratio to enhance the chemical and mechanical stability of the prepared nanofibers. The prepared nanofibers are characterized by scanning electron microscopy (SEM), fourier transform infrared (FTIR) techniques. The formation and morphology of Ag NPs were investigated by Transmission Electron Microscopy and X-ray Photoelectron Spectroscopy. Finally, Ag release from the nanofibers was measured and the antibacterial behavior of the nanofibers against Escherichia coli was studied by bacterial growth inhibition halos and bactericidal kinetic testing. [4]

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Electrospinning of nanofibers based on carboxymethyl tragacanth-polyvinyl alcohol/nano-clay composite containing silver nanoparticals for wound healing applications

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The convenient one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones catalyzed by novel, green and recoverable MCM-41-CPTMS-DMG-Cu nanocatalyst

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Keywords: Nickel-dimethylglyoxime complex, MCM-41, Nanocatalyst, 2,3-Dihydroquinazolin-4(1*H*)-one

2,3-Dihydroquinazolinone derivatives are heterocyclic compounds with nitrogen atoms molecules that have been reported to possess a wide range of various pharmacological[1] and biological properties, antifertility, antibacterial, antitumor, antibiotic, analgesic, antihistaminic activities [2]. Not surprisingly, numerous efforts have already been made in direct preparation of quinazolinone[3]. the development of simple, efficient, clean, high yielding and environmentally friendly approaches using new catalysts for the synthesis of these compounds is an important task for organic chemists.

In this study, Ni-dimethylglyoxime complex supported onto organically modified MCM-41 was prepared and used as an efficient, heterogeneous, recoverable and thermally stable nanocatalyst for the one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)- ones from 2-aminobenzamide and aromatic aldehydes in ethanol solvent and under reflux conditions. This heterogeneous nanocatalyst was characterized using FT-IR, SEM, EDS, XRD, TGA and ICP techniques. The catalyst showed good recyclability and can be reused for at least six sequential cycles without significant loss of its catalytic activity.

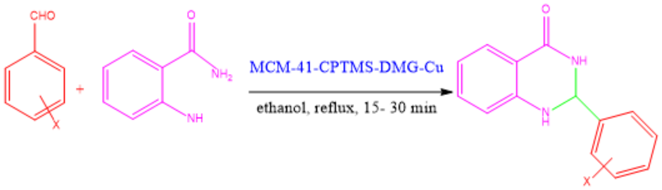

Fig. 1 MCM-41-CPTMS-DMG-Cu catalyzed the one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones in ethanol.

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Regioselective alkylation of indoles with α-pinene by $BF_3.Et_2O$ catalyst

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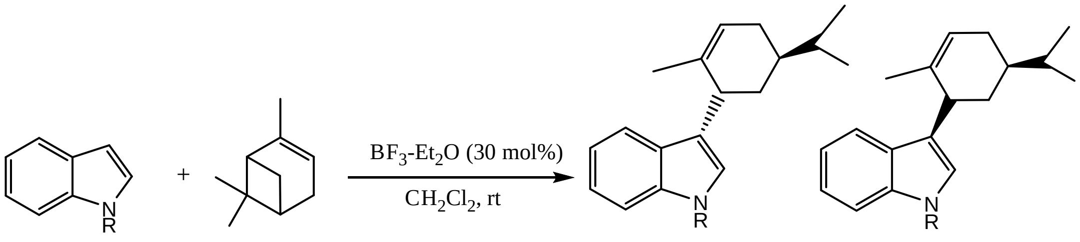
Keywords: One-pot reaction, Monoterpenes, Turpentine oil, α-Pinene, Indoles.

Monoterpenes are renewable resources that are widely used in the pharmaceutical, perfume, cosmetic and food industries.[1] Among them, α-pinene is a readily available and inexpensive raw material usually obtained from the pine gum. It is present to the extent of 85% in turpentine oil of pine. Several transformations of α-pinene, such as acetoxylation, hydration, isomerization and oxidation can be applied to produce a wide variety of added value products.[2,3]

Indole is the core structure of many pharmacological agents and natural products. Therefore, the synthesis and selective functionalization of indoles have been the focus of active research over the years.[4] Herein, we report the synthesis of 3-alkylated indoles by means of α-pinene as a starting material, which was separated from turpentine oil by distillation method. The indole derivatives undergo alkylation with α-pinene in the presence of $BF_3.Et_2O$ (30 mol %) in dichloromethane at room temperature to produce the corresponding 3-alkylated indoles in good yields with high *trans*-selectivity (Fig. 1). The products were obtained as oil and the structures were characterized on the basis of their mass spectrum, ^1H and ^{13}C NMR, and IR spectroscopic data.



1 **2** **3a** **3b**

R= H, CH_3, CH_2Ph major minor

Fig. 1 alkylation of indoles with α-pinene using $BF_3.Et_2O$ catalyst

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Synthesis of some silyl derivatives of graphene oxide

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Keywords: Graphene, Graphene oxide, Silylation, Silyl ether, Vinylsilane

Graphene is 2-D structure of a single-atom-thick sheet of sp^2-hybridized carbon atoms arrayed in a honeycomb pattern.[1] One specific branch of graphene research deals with graphene oxide (GO). Graphene oxide consists of a single-layer of graphite oxide and is usually produced by the chemical treatment of graphite through oxidation, with subsequent dispersion and exfoliation in water or suitable organic solvents. There are various oxygen containing functional groups in the GO. The oxygen functional groups have been identified as mostly in the form of hydroxyl and epoxy groups on the basal plane, with smaller amounts of carboxy, carbonyl at the sheet edges.[2] In this study Graphene oxide (GO) was prepared by a modified Hummers method ($KMnO_4$, $NaNO_3$, H_2SO_4) from natural graphite powder.[3] The structure of GO was characterized by X-ray diffraction (XRD), and Fourier transform infrared (FT-IR) spectroscopy. Then Graphene oxide (GO) was successfully silylated by various alkylchlorosilanes in the presence of Triethylamine (base) and Tetrahydrofuran (THF) as a solvent. The following reagents were used for silylation of GO, trimethylchlorosilane, triethylchlorosilane, Tert-Butyl dimethylchlorosilane, and Vinyl dimethylchlorosilane. The products were analyzed by X-ray diffractometry, FT-IR and TG measurements. Energy dispersive X-ray spectroscopy (EDX) was determine the silica composition in the samples. The results show that thermal stability and lipophilicity of silylated Graphene oxide were increased. This stability of silylated GO indicates that Si is strongly bonded to the GO layers via Si-O covalent bonding.

$$\text{Graphene oxide} \xrightarrow[\text{Base}]{R_3SiCl} \text{Silyl derivative of graphene oxide}$$

$$(R=Me_3,\ Et_3,\ \text{t-bu-}Me_2,\ \text{vinyl-}Me_2)$$

Fig. 1 Schematic Synthesis of silylated graphene oxide

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Applications of Ni-Biurea/MCM-41 as a powerful heterogeneous nanocatalyst in the Stille reaction

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Keywords: Nanocatalyst, Ni-Biurea/MCM-41, Coupling reactions, Green reaction conditions.

Carbon-Carbon coupling reactions catalyzed by transition-metals are among the most important reactions in the organic synthesis. Stille reaction, which is the cross-coupling of aryl halides and organotin compounds to give biaryl derivatives, is usually catalyzed by palladium.[1] However, inorganic supports are generally preferred due to their high stability as the polymeric supports are normally easy to swell under the reaction conditions which significantly affects the catalytic properties.

Biaryl products are an important class of compounds that are found in numerous natural products, polymers, and pharmaceuticals.[2] In literature, various catalysts are used for the synthesis of biaryl derivatives. In continuation of our previous work,[3] we report herein the application of Ni-Biurea/MCM-41 (**3**) as a powerful heterogeneous nanocatalyst in the synthesis of biaryl (**4**) via C-C coupling of aryl halid**e** (**1**) with Ph_3SnCl (**2**) in excellent yields (Fig.1). In addition, the application of Ph_3SnCl in the Stille coupling of aryl halides in the presence of Ni-Biurea/MCM-41 is discussed.

The structure of catalyst was characterized by different techniques such as TEM, FT-IR, and BET.

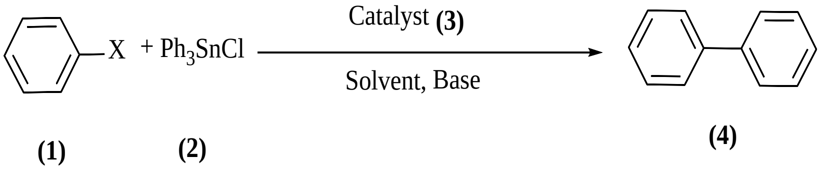

Fig. 1 Coupling of aryl halides with Ph_3SnCl catalyzed by Ni-Biurea/MCM-41 in the presence of PEG.

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Preparation, identification and application of 1,3-bis triphenylphosphonium propane peroxodisulfate in oxidation of benzylic alcohols

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Keywords: diphosphonium peroxydisulfate, oxidizing agent, X-ray crystallography, benzylic alcohols.

Oxidation of alcohols to carbonyl compounds is an organic functional group transformation and this is one of the most important basic reaction in synthetic organic chemistry.[1]

The peroxodisulfate ion has been shown to be a strong oxidizing agent for a variety of organic compounds. Some reported successful applications of this oxidant are oxidative decarboxylation of acids, aromatic hydroxylation, oxidation of alkyl benzenes, oxidation of carbon-nitrogen double bonds, alkenes, amines, alcohols.[2,3]

Herein, a new member of stable phosphorus-based peroxodisulfate family, 1,3 – bis triphenylphosphonium propane peroxodisulfate was easily prepared as a mild and efficient oxidizing agent for oxidation of various benzylic alcohols to their corresponding compounds in water under reflux condition as green chemistry.

It has been characterized by ^{1}H-NMR, ^{13}C-NMR, ^{31}P-NMR, FT-IR, single-crystal X-ray diffraction crystallography and differential scanning calorimetry, thermogravimetric analysis, and differential thermal analysis.

This salt represents different advantages such as thermal and Physico-chemical stability, good selectivity, simple working up, harmless in comparison to strong chromium oxides and permanganate ions.

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Preparation, identification and application of 1,5-bis triphenylphosphonium pentane peroxodisulfate in oxidation of benzylic alcohols

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Keywords: diphosphonium peroxydisulfate, oxidizing agent, X-ray crystallography, benzylic alcohols.

Oxidation of alcohols is the foundation of synthetic chemistry and a fundamental transformation in organic synthesis.[1]

The readily available peroxodisulfate ion, $S_2O_8^{2-}$,is an excellent and versatile oxidant for a variety of organic and inorganic compounds.[2] Some reported successful examples of oxidation with this oxidant are: oxidative decarboxylation of acids, aromatic hydroxylation, oxidation of carbon-nitrogen double bonds, oxidation of alkyl benzenes, alkenes, amines and alcohols.[3]

1,5 - bis triphenyl phosphonium pentane peroxodisulfate was synthesized as a new , mild and efficient oxidizing reagent and characterized by IR and NMR spectroscopy.

Physico-chemical stability, good selectivity and simple work up are some of advantages of this salt.

It has been used in oxidation of different benzylic alcohols to their corresponding carbonyl compounds and the result indicates that oxidation reaction takes place selectively with high yield and simple work up in short time.

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Preparation, identification and application of 1,3-bis triphenylphosphonium propane diborohydride in reduction of carbonyl compounds

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Keywords: diphosphonium diborohydride, reducing agent, reduction reaction, carbonyl compounds.

Reduction is one of the most fundamental and useful reactions in organic synthesis.[1] Sodium borohydride and lithium aluminum hydride are nucleophilic reducing agents which reduce polar multiple bonds.[2] In order to control the reducing power of the reagents, hundreds of substituted boron and aluminum hydrides have been described in chemical literature and many are now commercially available.[3]

Herein, 1,3- bis triphenylphosphonium propane diborohydride as a new, stable quaternary phosphonium borohydride is introduced and characterized by IR, NMR spectroscopy. This reagent is quantitatively prepared and used for reduction of variety of carbonyl compounds such as aldehydes, ketones, α, β-unsaturated carbonyl compounds and benzoil chlorides to their corresponding alcohols. Reduction reactions are performed in dry acetonitrile at room temperature or under solvent free conditions in good to excellent yields. In addition, this new reducing reagent indicates the chemoselective reduction of aldehydes over ketones.

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Preparation, identification and application of 1,5-bis triphenylphosphonium pentane diborohydride in reduction of carbonyl compounds

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Keywords: diphosphonium diborohydride, reducing agent, reduction reaction, carbonyl compounds.

In the past 40 years, metal hydrides, particularly sodium borohydride and lithium aluminum hydride, have emerged as preeminent reducing agents in modern organic chemistry.[1, 2] In order to change the reactivity of NaBH4, various structural modifications of NaBH4 are reported.[3] Herein, a new, efficient and stable reducing reagent, 1,5-bis triphenylphosphonium pentane diborohydride is introduced and characterized by IR, NMR spectroscopy. This new reagent is quantitatively prepared and used for reduction of variety of carbonyl compounds to their corresponding alcohols in dry acetonitrile at room temperature or under solvent free conditions. Chemoselective reduction of aldehydes over ketones, stability, high yields and rates of the reactions, working under aprotic reaction conditions or in the absence of solvent and ease of preparation of the reagent are some of advantages of this new reducing reagent.

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Preparation of Chitosan - Glutamic acid Nanoparticles in Drug Release of Curcumin

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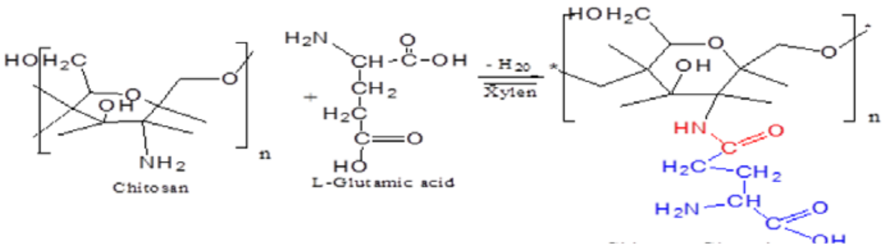
Keywords: Chitosan, Nanoparticles, glutamic acid, curcumin, Anticancer.

Curcumin as the active compound has antioxidative, anti_ inflammatory, antimicrobial and anticancer properties among others. However, its disadvantageous properties like low solubility, poor bioavailability under neutral or acidic pH conditions or when exposed to light limit its clinical application. These problems can be solved by preparing nanoparticles. The Present study deals with the chemical modification of chitosan by using click chemistry technique. We were prepared the poly(L-glutamic acid) (PLGA) and chitosan (CS) microcapsules and to study the release rate of hydrophobic curcumin. The PLGA/CS microcapsules show high loading capacity and sustained release behavior. Nanoparticles morphologies were evaluated by Scanning Electron Microscopy. The drug loading and release rate of nanoparticles (PLGA/CS/ALG) were studied. Drug release rate dependence on pH and temperature. In vitro release rate was performed in acidic pH. The 50% of cells (the colorectal cell line HT-29) survived under MTT cytotoxic method after 72 hours exposed of (PLGA/CS/ALG+ CUR) nanoparticles.



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Synthesis of amines through condensation of *p*-toluene sulphonamide with benzhydrol derivatives in the presence of copper-phosphine complexes

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Keywords: Benzhydrol, Amine, Copper complex, Phosphine ligand.

Amines employ an important role in biological, pharmacological and agricultural activities.[1,2] Amongst them, diaryl containing amines because this structural motif can be found in several drugs such as cetirizine, sertraline, rasagiline and rivastigmine,[3,4] which have attracted growing attentions. There are lots of various synthetic methods for the preparation of diarylamine, which amongst them arylation of aldimines employing various catalyst and aryl transfer reagents are realized due to high yield and activity. Because of the importance of carbon-nitrogen bonding in organic synthesis, the development of appropriate methods for the formation of these bonds is one of the most important goals of chemists.

In this work, diarylamines **3** were synthesized using *p*-toluenesulfonamides **2** with benzhydrol derivatives **1** in the presence of copper/bisphosphine complex yielding >98% under clean and mild reaction conditions. Use of available and cost-efficiency copper salts, short reaction time, high yield and rate of reaction highlighted this method. The structure of products are investigated by melting point, IR, ^{1}H NMR and ^{13}C NMR spectroscopies.

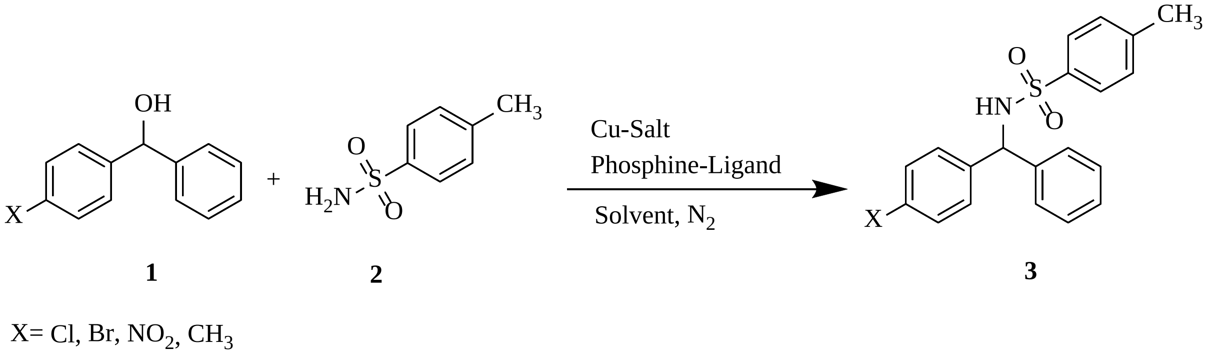

Fig. 1 Preparation of amine *via* condensation of *p*-toluene sulfonamide and benzhydrol derivatives in the presence of copper-phosphine complex

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Solvent-free one-pot synthesis of 4-(4-hydroxy-1,3-dithiolan-2-ylidene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-ones

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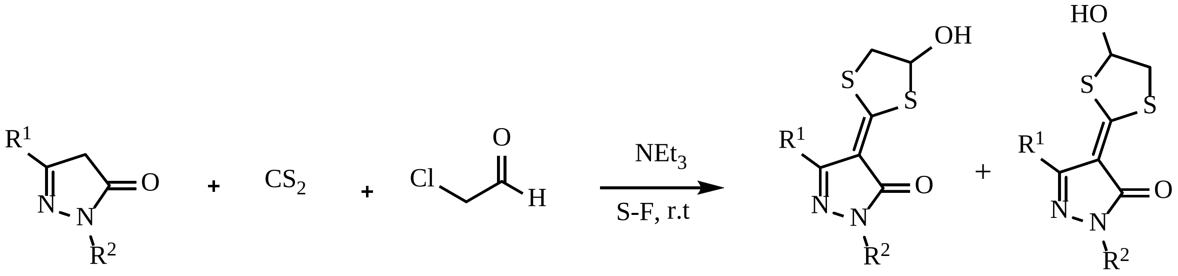
Keywords: Solvent-free reactions, heterocyclic, one-pot, Multicomponent, 4-(4-hydroxy-1,3-dithiolan-2-ylidene)-5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one.

Pyrazole derivatives possess diverse chemical reactivity and broad spectrum of biological activities. A number of substituted pyrazoles are used as fungicides, insecticide, pesticides, and herbicides in the field of agriculture.[1] They are used also as coloration of paints, varnishes, lacquers in the field of industry.[2] Herein, we report one-pot synthesis of *E* and *Z* form of 4-(4-hydroxy-1,3-dithiolan-2-ylidene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one derivatives **2** and **3** from the solvent-free reaction between pyrazole derivatives **1**, carbon disulfide, and α-chloroacetaldehyde in the presence of triethylamine at room temperature. All synthesized compounds are stable solids whose structures were determined on the basis of their IR, ^{1}H and ^{13}C-NMR, and Mass spectroscopic data.



1　　**2** (*Z*)　　**3** (*E*)

R^1: Me, Ph, CH_2CO_2Me, CH_2CO_2Et; R^2: Ph, H

Fig. 1 One-pot synthesis of *E* and *Z* 4-(4-hydroxy-1,3-dithiolan-2-ylidene)-5-methyl-2-phenyl-2,4-dihydro-3*H*-pyrazol-3-one

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Synthesis of a new superabsorbent copolymer based on acrylic acid grafted onto carboxymethyl tragacanth

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Keywords: Tragacanth gum, Superabsorbent polymer, Graft polymerization, Swelling behavior.

Superabsorbent polymer (SAP) materials are hydrophilic cross-linked networks that can absorb large quantities of water or aqueous solutions and hold it even under pressure. They can uptake water many hundred times more than their dry weight.[1] Three types of SAPs can be produced based on their origin: full synthetic (petrochemical-based), natural (e.g., polysaccharide and polypeptide-based), and hybrid (i.e. grafting synthetic monomers on the natural backbone).[2] Synthetic polymer-based SAPs have a high water absorbing capability but these materials can cause environmental problems due to their toxicity and non-biodegradability. As a recent result, SAPs based on the natural polymer have attracted more attention. Carbohydrate polymers such as cellulose, starch, chitin, alginates, etc. are commonly used to synthesize the biodegradable polymers.[3] In this study, we have also synthesized a novel hydrogel superabsorbent based on carboxymethyl tragacanth by grafting reaction of the acrylic acid (AA) onto the carboxymethyl tragacanth in an aqueous medium. Furthermore, we have investigated the effects of the reaction conditions on water absorbency and found the optimum conditions to synthesize the superabsorbent with the highest swelling ratio.

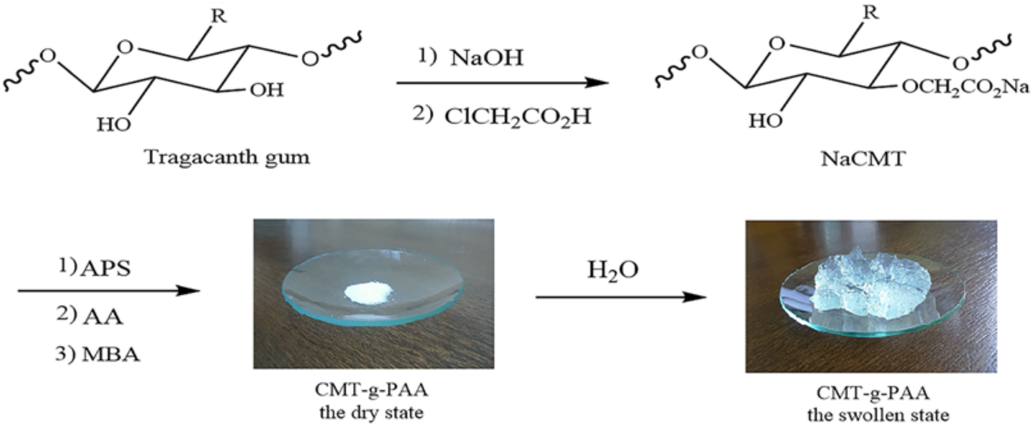

Fig. 1 Synthesis of the CMT-g-PAA superabsorbent polymer.

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Carboxymethyl tragacanth-based slow release system for urea delivery

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Keywords: Carboxymethyl tragacanth, Biodegradable superabsorbent, Slow release, Urea fertilizer.

Nitrogen is an essential nutrient for plant growth, and urea is also a nitrogenous nutrient that is widely used in agriculture due to its high nitrogen content (46%) and relatively low production cost. As urea is a neutral organic compound, it cannot be readily absorbed by the charged soil particles before hydrolysis, and thus a large fraction of urea is not absorbed by plant which causes serious environmental problems.[1] Moreover, due to the high solubility of urea in the water, a fraction of urea is also lost in leaching.[2] Volatilization is another harmful phenomenon that results in loss of urea.[3] One of the ways overcoming on the problems mentioned above is the use of slow or controlled release fertilizers (SRFs) containing the superabsorbent polymers (SAPs).[4] In the present work, we have also used a new type of low cost and eco-friendly slow release system based on the CMT with the function of superabsorbent. The CMT-based SAP is used as carrier of urea in the slow release system. To prepare of the SAP, we chemically modified the tragacanth gum by reaction with the monochloroacetic acid and then grafted acrylic acid on the CMT. We have applied the SAPs in order to water retention and slow-release of the urea fertilizer and the resulted data showed the proper effect of using these materials.

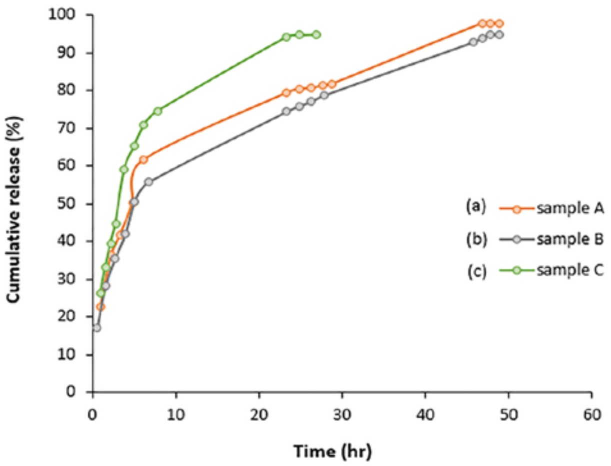

Fig. 1 Urea release in distilled water. samples with percentages of crosslinking agent a) 8%, b) 14% and c) 20%.

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Synthesis and identification of gelatin-polyvinyl alcohol hydrogel for use in the release of fluvoxamine maleate drug

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Keywords: Fluvoxamine maleate, Gelatin, Polyvinylalcohol, Hydrogel, Drug release.

Hydrogels are hydrophilic polymer networks which may absorb from 10–20% up to thousands of times their dry weight in water. Hydrogels may be chemically stable or they may degrade and eventually disintegrate and dissolve. They are called ‘reversible’, or ‘physical’ gels when the networks are held together by molecular entanglements, and/or secondary forces including ionic, H-bonding or hydrophobic forces.[1,2] The use of PVA based hydrogels as biomaterials has recently gained great importance in view of the low toxicity, non-carcinogenic, and high biocompatibility by many of them.[3] In this work gelatin-polyvinylalcohol cross-linked hydrogel was prepared using $K_2S_2O_8$ in aqueous media. Then, loading and release of fluvoxamine maleate drug was investigated using gelatin-polyvinylalcohol hydrogel. The effects of temperature and pH on the loading and release of fluvoxamine maleate drug in gelatin-polyvinylalcohol hydrogel were studied. The results showed that the highest loading of the drug was achieved at room temperature after 8 hours. Also, the highest drug release was observed after 6 hours at room temperature in pH = 7.

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One-pot three-component synthesis of 2*H*-thiopyrano[2,3-*b*]quinoline-2,3-dicarboxylates from 2-mercaptoquinoline-3-carbaldehydes, dialkyl acetylenedicarboxylates and Ph_3P

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Keywords: 2-Mercaptoquinoline-3-carbaldehyde, Intramolecular Wittig reaction, Tricyclic framework.

The presence of heterocyclic scaffolds in many natural and synthetic products endowed with biological properties is responsible for extensive research in recent years on the synthesis of useful polycyclic structures, that include one or more heteroatoms. The quinolines and quinoline-fused heterocycles are privileged structural units presented in numerous natural products and pharmacologically active compound.[1] Considering the importance of the above-mentioned applications and activities, methods for the synthesis of quinoline fused thiopyran structures are of great interest. In this study, our goal was to develop an improved procedure, including enhancing the reaction yield, of the biologically important thiopyran fused quinoline moiety. Following our research interest on the synthesis of quinoline-fused heterocyclic compounds[11,12] we herein used the same strategy reported in the literature for the synthesis of 2*H*-thiopyrano[2,3-*b*]quinoline-2,3-dicarboxylates using a one-pot three component coupling of 3-formyl-2-mercaptoquinolines, triphenylphosphine, and dialkyl acetylenedicarboxylate. The reaction was performed at room temperature within 15-30 minutes using DCM as solvent and afforded the products with excellent yields (80-90%).

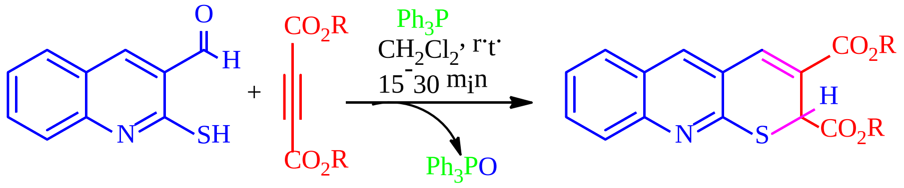

Fig. 1 Synthesis of 2*H*-thiopyrano[2,3-*b*]quinoline- 2,3-dicarboxylates

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Design, fabrication and catalytic study of OMS-MIL-100(Fe) as an Efficient Green Catalyst for the aza-Michael Reaction

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Keywords: Metal-organic framework, OMS-MIL-100(Fe), Organocatalyst, Aza-Michael reaction.

Porous coordination polymer as metal-organic frameworks (MOFs) have attracted significant attention during the past decade as promising nanoporous hybrid material for their potential application in gas storage and separation, sensors, drug delivery and catalysis [1, 2]. Recently, the aza-Michael reaction is a prominent reaction for forming carbon-nitrogen bond in synthesis of *β*-amino carbonyl/cyano compounds [3] and it was widely used as key reaction in synthetic chemistry and synthesis of antibiotics, anticancer, drugs and natural product [4]. Herein, we synthesized of a high porous open metal site MOFs of MIL-100(Fe) with new polygonal morphology as a suitable, efficient, and heterogeneous catalyst for the aza-Michael reaction **Fig 1**. Efficient transformation, mild condition, easy product isolation and the potential high recyclability of the organocatalyst are the key feature of this protocol.

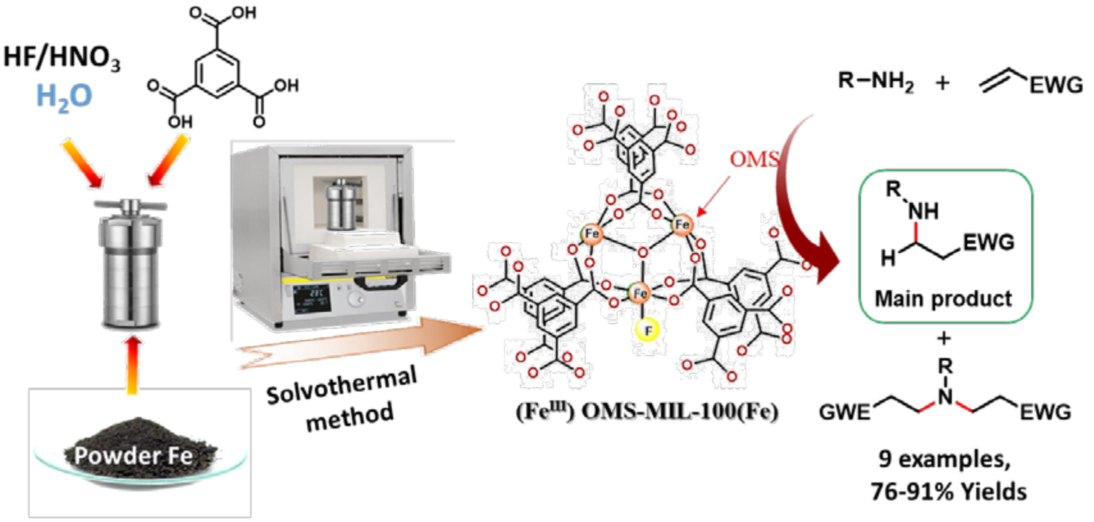

Fig. 1 Schematic synthetic process of OMS-MIL-100(Fe) for the aza-Michael reaction.

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Synthesis of functionalized terpolymer based on melamine-formaldehyde copolymer grafted by polyanilin for heavy metal removing from wastewaters

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Keywords: Polymeric adsorbent, Heavy metal**,** Wastewaters**,** Polymeric adsorbent**,** Nanocomposite.

Water pollution, especially heavy metal ion pollution, is currently one of the most serious environmental problems.[1,2] Heavy metal ions such as lead, copper, cadmium, zinc, nickel, and others are the most common pollutants found in industrial effluents.[3] The EDTA dianhydride (EDTAD), a ramification of EDTA containing two anhydride groups per molecule, can react with hydroxyl and amino groups of other materials. The use of EDTAD to treat baker's yeast biomass for producing biosorbents with high adsorption capacity of Pb^{2+} and Cu^{2+} ions has been reported in the literature.[4] In this work, melamine- paraformaldehyde copolymer was synthesized with excess ratio of melamine to form a water soluble copolymer with $–NH_2$ end groups. Then the aniline was graft polymerized on MF by oxidation polymerization in presence of amonium peroxy disulphate (APS). The prepared copolymer was functionalized by EDTA anhydride. The synthesized functional copolymer has a good capability for removing the heavy metal ions from wastewater. Atomic absorption spectroscopy was used in order to determine the amount of removed ion percentage. The requirements for the highest absorption were investigated and determined.

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One pot aqueous media synthesis of 1,3-oxazine derivatives catalyzed by reusable nano-$Al_2O_3/BF_3/Fe_3O_4$ at room temperature

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Keywords: Nano-$Al_2O_3/BF_3/Fe_3O_4$; 1,3-Oxazine; Magnetic catalyst; Lewis acid catalyst; Multi-component reactions.

The distinctive aspect of multi-component reactions (MCRs) is that the products contain all parts of substrates, creating almost no by-products. So, the applications of MCRs are very popular with only a minimum of endeavor and offer a wealth of products.[1] The 1,3-oxazine ring system has a structure which known as one of biologically-active heterocycles.[2] In addition, realizing the importance of naphthoxine compounds which has alterative prospect for the treatment of Parkinson's disease reported.[3] Previously, some is shown in protocols for synthesis of various naphtho[1,3]oxazines via a Mannich type condensation between a 2-naphthol, formaldehyde and a primary amine were reported.

In this work, we wish to report effective and eco-friendly procedure for the synthesis of 2-aryl/alkyl-2,3-dihydro-1*H*-naphtho[1,2-*e*][1,3]oxazine in the presence of nano-$Al_2O_3/BF_3/Fe_3O_4$. The obtained 1,3-oxazine compounds were characterized by various methods such as FT-IR, ^{1}HNMR and melting point.[4]

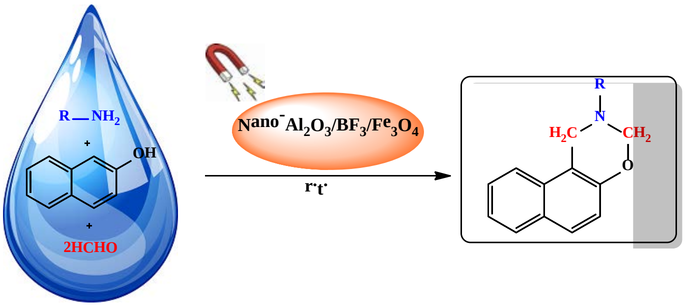

Fig. 1 Multicomponent 1,3-Oxazine Derivatives catalyzed by nano-$Al_2O_3/BF_3/Fe_3O_4$.

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Boehmite nanoparticles as support for preparation of heterogeneous catalysts in organic reactions

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Keywords: Boehmite nanoparticles, Organic reactions, Heterogeneous catalysts, Acidic catalysts, Basic catalyst, Metallic catalysts.

Boehmite nanoparticles are aluminum oxide hydroxide (γ-AlOOH) particles, which has large specific surface area (>120 m^2g^{-1}) and can be prepared *via* an inexpensive procedure in water using inexpensive commercial materials such as aqueous solution of $Al(NO_3)_3$ and NaOH. Boehmite nanoparticles are a cubic orthorhombic unites of aluminum oxide hydroxide that its structure is double sheets of octahedral of aluminum ions with cubic orthorhombic structure (Figure 1). Boehmite is stable in air atmosphere, high temperature, aqueous solution and it is inert in different chemical conditions, therefore boehmite is an ideal support for heterogenization of homogeneous catalysts. The surface of boehmite nanoparticles are covered with high density of hydroxyl groups, therefore it can be used as ideal support for heterogenization of homogeneous catalysts. But, despite of several studies on morphology, properties and preparation of boehmite, it was rarely employed as catalyst support. In order to reusing of catalysts with respect to green chemistry principles, we are reporting various acidic catalysts, basic catalyst and metallic catalysts on boehmite nanoparticles as efficient and reusable catalysts for organic reactions such as coupling reactions, oxidation reactions, multicomponent reactions, oxidative coupling reaction and also synthesis of organic compounds.

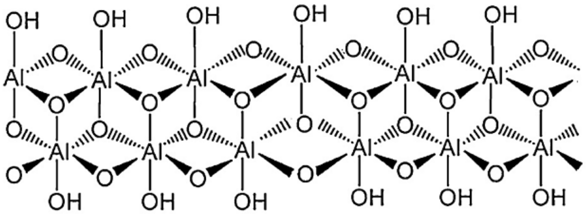

Fig. 1 The structure of BNPs boehmite nanoparticles.

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Modification of closite by glycidyl methacrylate and its effect on mechanical properties of flowable dental composites

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***Keywords**:* Closite, Flowable dental composites, Mechanical properties, Dental materials

Dental composites as dental restorative materials have weak mechanical and physical properties in stressful areas.[1,2,3] In this study, the closite surface modified with glycidyl methacrylate and investigated by IR spectroscopy and XRD analysis. Then, the modified closite was applied as a filler for preparation of flowable dental composites (Tetric Flow, Invoclar,Vivadent, USA) in different weight percent 0, 0.2, 0.5, 1, 2.5, 5 and 7.5 wt% at room temperature. Afterward, the physical and mechanical properties of prepared dental composites such as flexural strength, flexural modulus were investigated. Results shown that the modified closite by glycidyl methacrylate can improved strength and flexural modulus in flowable dental composites.

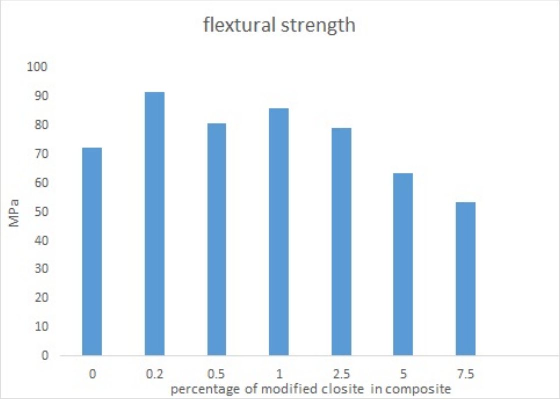

Fig1. Flexural strength of flowable dental composites containing different percentages of modified closite.

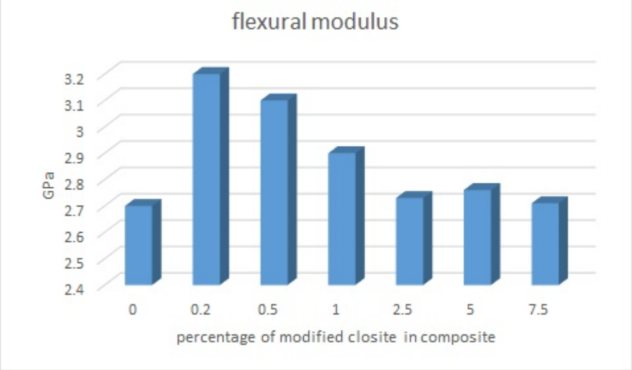

Fig2. Flexural modulus of flowable dental composites containing different percentages of modified closite.

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Efficient synthesis of new pyranopyrazole derivatives via a multicomponent approach

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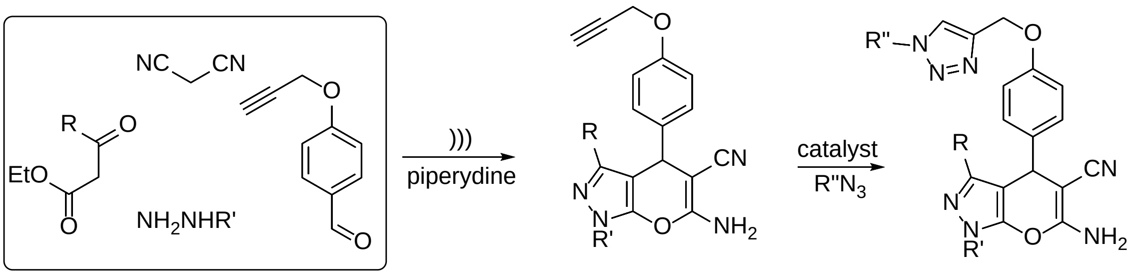
Keywords: Multicomponent reactions, pyranopyrazoles, Click reactions, ultrasonic reactions.

Preparation of molecules possessing various biological properties of interest through one-pot and multicomponent reactions has developed by far in recent decades.[1] This is because of the versatility associated with multicomponent reactions which allow rapid access to selectively build up complex target structures, while the atom economy, lower production of chemical waste. More efficient energy consumption, and convenient procedures are among other advantages of multicomponent reactions.[2]

An interesting group of heterocycles with desirable medicinal activities are pyranopyrazole derivatives, which are conveniently synthesized through four-component cyclocondensation of aldehydes, hydrazine derivatives, ethyl acetoacetate, and malononitrile.[3]

In the present work, a 4-component process is carried out in which ethyl acetoacetate derivatives combine with hydrazines, malononitrile, and propargylic aldehdes under ultrasonic conditions, followed by a click reaction in the second step to get to the final tetracyclic structures. (**Scheme 1).**



Scheme 1

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Co nanoparticles anchored on cellulose: a magnetically recoverable nanoadsorbent for removal of anionic congo red dye from aqueous solution

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Keywords: Adsorption, Cellulose, Congo red, Magnetic adsorbent, Removal.

Organic dyestuffs and dye-manufacturing wastewater are currently a major problem for environmental managers.[1] Various treatment processes such as adsorption, coagulation, flocculation, reverse osmosis, photo-degradation process and ion-exchange have been used to remove dyes from wastewater.[2] Because of its low cost and ease of operation, adsorption method has attracted many attentions to remove dyes.[3] The literature review shows that the application of magnetic adsorbents for removal of waste waters pollutants has been frequently documented. The magnetic adsorbents are easily separated from the solutions using an external magnetic field and therefore have the possibility of reusing for further examinations.[4] In this work, we report a facile approach to prepare the magnetic cobalt nanoparticles supported on cellulose (Co NPs/Cellulose). The prepared nanocomposite exhibited a perfect affinity towards removal of congo red (CR) from aqueous solutions and due to the magnetism of Co NPs is very easy to separate from treated solution.

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Three-component synthesis of novel spiro[4*H*-pyran-3,3´-oxindoles] using 5,6-dihydro-4*H*-pyrrolo[3,2,1-*ij*]quinoline-1,2-dione

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Keywords: Three-component reactions, Spirooxindoles, Cyanomethyl aryl ketones, Malononitrile, Ethyl cyanoacetate.

Spirooxindole systems are of great interest in a modern organic, medicinal, and natural product chemistry. This type of framework has been found as a core structure of many natural alkaloids with promising pharmacological activity, such as horsfiline, gelsemine, mitraphylline, spirotryprostatins A, B, and others. The pyrane/chromene-based heterocycles that fuse with an oxindole ring system represent a potentially promising subset of the tetrahydropyranone and pyrrolidinyl spirooxindole natural products.[1-3] Therefore, in this work, we report the synthesis of some new spiro[4*H*-pyran-3,3´-oxindoles] **4** by the three component reaction of keto-lactam **1**, substituted cyanomethyl aryl ketones **2** and malononitrile or ethyl cyanoacetate **3** in the presence of 4-(*N*,*N*-dimethylamino)pyridine (DMAP) in refluxing EtOH (Figure 1).

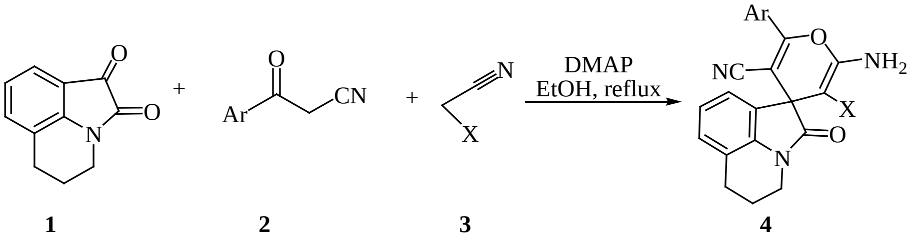

Fig. 1 Synthesis of some novel Spiro[4*H*-pyran-3,3´-oxindoles] **4**

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Acidic ionic liquid catalyzed Biginelli reaction under solvent-free conditions

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Keywords: Dihydropyrimidines, Multicomponent reaction, $[DABCO](SO_3H)_2(HSO_4)_2$, Ionic liquid.

Ionic liquids (ILs) are emerging as effective promoters and solvents for green chemical reactions. One of the most important advantages of ILs is the behavior of solvophobic interactions that generate an internal pressure, which promotes the association of the chemical reactants and reagents and also shows an acceleration of MCRs in comparison to conventional solvents.[1] Dihydropyrimidines are an important class of compounds exhibiting broad spectra of pharmacological activities such as antiinflammatory, anti-microbial, α-1a-adrenergic receptor antagonist, and antihypertensives.[2] The development of dihydropyrimidine templates as pharmacologically active compounds contributed toward Biginelli cyclocondensation applications in drug industry.[3] In this study and order to introduce an inexpensive and environmentally benign catalyst for this reaction, $[DABCO](SO_3H)_2(HSO_4)_2$ is used as a reusable catalyst in the synthesis of dihydropyrimidines through Biginelli reaction (Fig. 1).

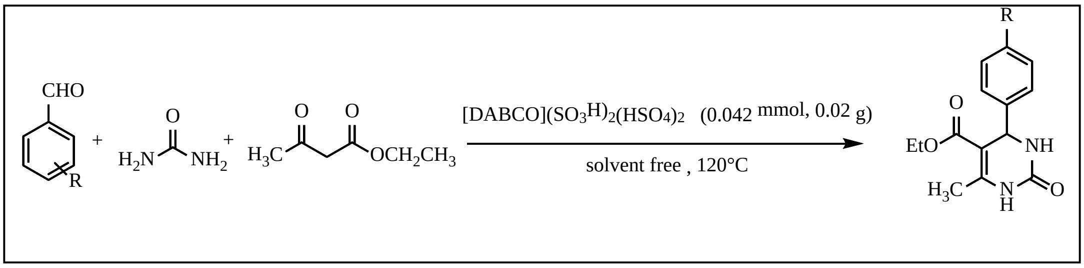

Fig. 1 $[DABCO](SO_3H)_2(HSO_4)_2$ catalyzed the synthesis of dihydropyrimidines

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Cu-4-Pyrone complex anchored to functionalized Silica-MCM-41: as a regioselective, reusable, and effective nanocatalyst for the clean synthesis of 1*H*-1,2,3-triazole compounds via Click reaction

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Keywords: Silica-MCM-41-4-pyrone-Cu, Nanocatalyst, 1,3-Dipolar cycloaddition, Click reaction, 1,2,3-Triazole.

Mobile Crystalline Material (MCM-41) of the family M41S prepared by a liquid templating mechanism and hydrothermal synthesis.[1] This material exhibits significant feature such as uniform shapes and nanopores with proper sizes that are well-ordered to possess arrays hexagonal channels.[2] Lately, the click reaction between a terminal alkyne and organic azide (CuAAC) has found in many uses in organic synthesis. This process suffers from one or some disadvantages such as tedious workup, harsh reaction conditions, and longer reaction time.[3, 4] Thus, we became concerned in the development of clean, efficient, simple, excellent yielding and eco-friendly method utilizing a novel catalyst for the synthesis of triazoles. Based on this, the Cu complex on 4-pyrone-functionalized the silica-MCM-41 nano motif has been immobilized and it is used as an excellent regioselective nanocatalyst for the synthesis of 1,4-disubstituted triazoles by click reaction. The structure of nanocatalyst was analyzed by ICP, BET, XRD, EDS, SEM, TGA, TEM, and FT-IR techniques.

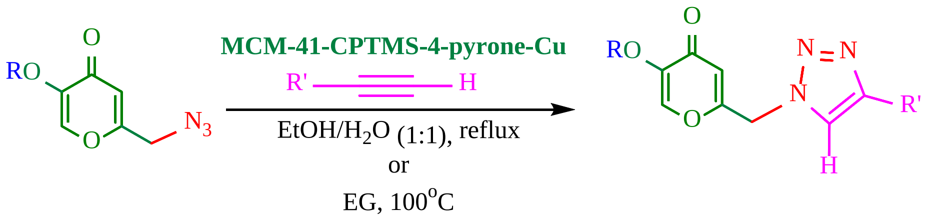

Fig. 1 Regioselective synthesis of 1,4-disubstituted 1,2,3-triazole compounds by catalytic amounts of silica-MCM-41-CPTMS-4-pyrone-Cu

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Synthesis of Novel Adamantly-containing Thiazolidinones

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Keywords: Adamantane motif, Diamondoid, Thiazolidinone.

Diamondoids are cage hydrocarbon molecules that can be described as fully hydrogen-terminated nanometer-sized diamonds. Adamantane is the smallest diamondoids.[1] The adamantyl group is present in seven compounds in current clinical use for the treatment of neurodegenerative disorders, viral infections and type 2 diabetes, and in many more substances that are in development as potential therapeutics. In many cases the adamantane motif, as a liphophile group, has been found to improve pharmacological properties of a parent compound, without increasing its toxicity.[2]Thiazolidinone is a five-membered heterocyclic ring with a broad spectrum of biological activities. This is a core structure in various synthetic pharmaceuticals.[3] In this work, novel adamantly containing thiazolidinones were synthesized in two steps. Firstly adamantly-contaning 1,3-disubstituted thioureas **1** were synthesized by the reaction of 1-aminoadamantane hydrochloride with phenyl isothiocyanate derivatives. Then reaction of thiourea derivatives **1** with dimethyl acetylenedicarboxylate (DMAD) **2** afford thiazolidinone derivatives **3** (Fig. 1).

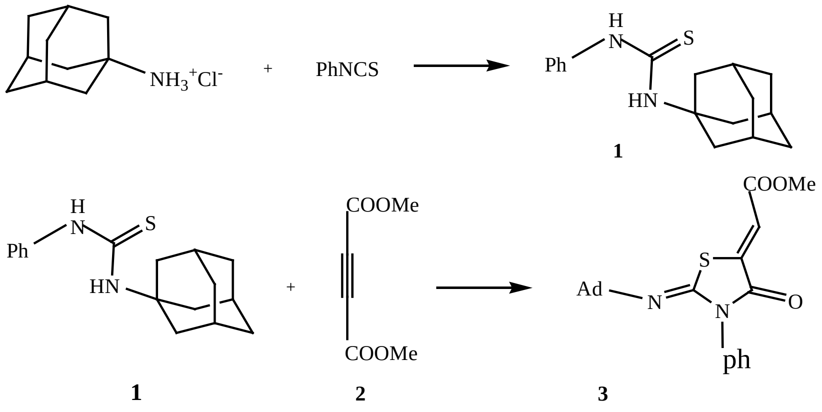

Fig. 1. Synthesis of adamantly-containing thiazolidinones

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DNA and RNA Building Blocks: Useful Scaffolds for the Synthesis of New Phosphodiesterase Type 3 Inhibitor Hybrid Compounds

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Keywords: nucleobase, molecular hybridization, phosphodiesterase type 3, anticancer agent.

Phosphodiesterases (PDEs) are characterized based on their affinities for cAMP and cGMP, their sensitivities to specific inhibitors, their biochemical and physical properties and their biological regulatory pathways.[1] Impaired cAMP and/or cGMP generation upon overexpression of PDE isoforms have been described in various cancer pathologies.[2] Selective inhibition of PDE isoforms, which raises the levels of intracellular cAMP and/or cGMP, may regulate the tumor microenvironment and induce apoptosis and cell cycle arrest in a broad spectrum of tumor cells. Therefore, development and clinical application of inhibitors specific for individual PDE isoenzymes may selectively restore normal intracellular signaling and provide antitumor therapy with reduced adverse effects.[3] Recent studies have shown that PDE3, PDE4 and PDE5 are overexpressed in cancer cells. In addition, inhibition of PDE3 along with other PDEs may lead to inhibition of tumor cell growth and angiogenesis.[4] Herein, inspired by the chemical structure of Cilostazol, a commercially available PDE3 inhibitor that is used as a medicine for the treatment of heart failures, some hybrid structures of nucleobases and tetrazole were synthesized. The cytotoxic effects of synthesized compounds on HeLa and MCF-7 cell lines were determined using MTT assay. PDE3 inhibitory effect of synthesized compounds was analyzed using an IMAP TR-FRET phosphodiesterase assay kit and cAMP as the substrate.

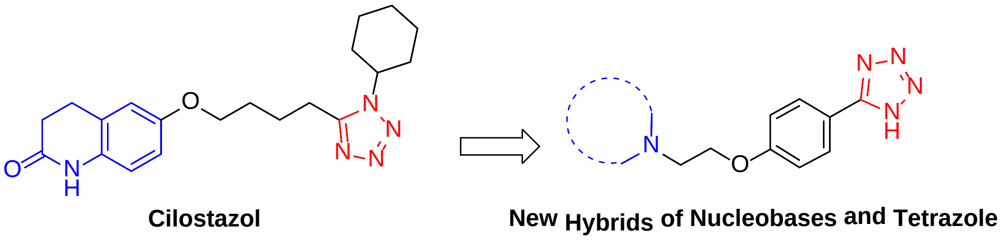

Fig. 1. The chemical structures of Cilostazol and synthesized new hybrids of nucleobases and tetrazole

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Graphene, material of the future

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Keywords: Graphene, Single layer material, Revolution

Graphene is a material made of a single layer of carbon atoms arranged in a hexagonal lattice[1]. Being a million times thinner than a human hair, it is the thinnest object ever created. Not only graphene is lightweight and flexible, it is also the world's strongest material, being 200 times stronger than steel[2].

Capable of increasing Internet speed 100 times and making its versatile and almost invisible clothes, graphene is already called by many in the scientific community as the “magic material” that will revolutionize several areas of technology. One million sheets of graphene are only one millimeter thick and many believe that this material can bring a new industrial revolution. It is the thinnest, the strongest and the toughest material ever made. At the same time, it is transparent, flexible and behaves very well in high heat and electricity conditions[3,4].

Given the extraordinary properties and functionalities of graphene in all areas of medicine and industry, the high cost of graphene production has been enormous in this regard, and certainly providing a simple and easy way to achieve graphene can revolutionize the world of graphene. Our research group, has developed a new method for achieving graphene in the shortest time and with the least use of chemicals.

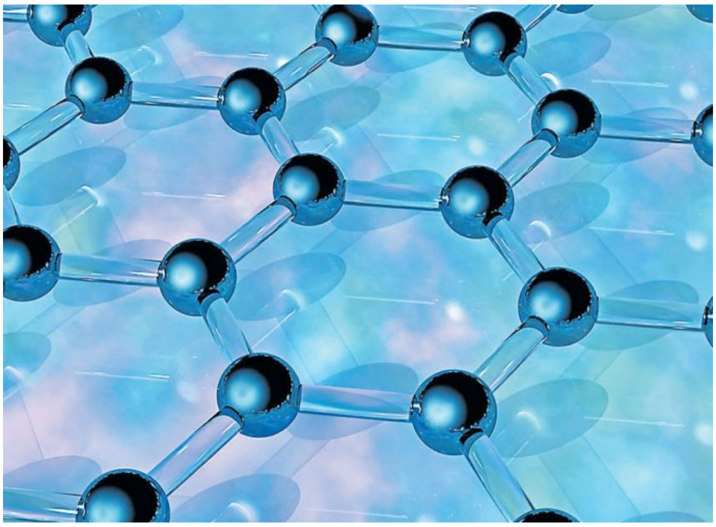

Fig. 1 Graphene: ‘Miracle matter’ of future

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Efficient synthesis of diverse heterocyclic scaffolds through post-transformation reactions

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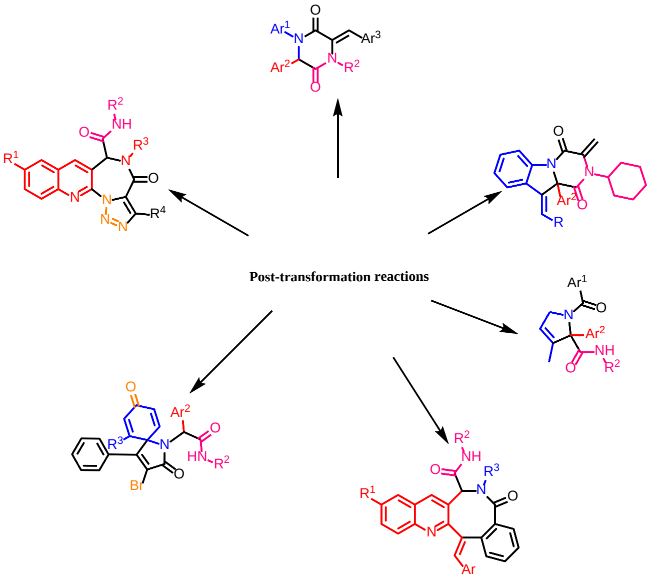
Designing of post-transformation reactions has become a useful tool for generation of complex and diverse molecular libraries with novel properties. The type of starting materials and putting secondary functional groups in the initial starting materials is an important point in designing of novel reactions. This approach drive for shorter and more efficient synthetic procedures as well as the quest for molecular diversity that has fueled the development of new reactions and catalysts that efficiently contributed to the selective syntheses of more complex systems. We have been recently involved in the development of various strategies based on different catalysts or other required reagents, which will be highlighted in the talk.



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Celebrating 150 years of the Mendeleev's periodic table

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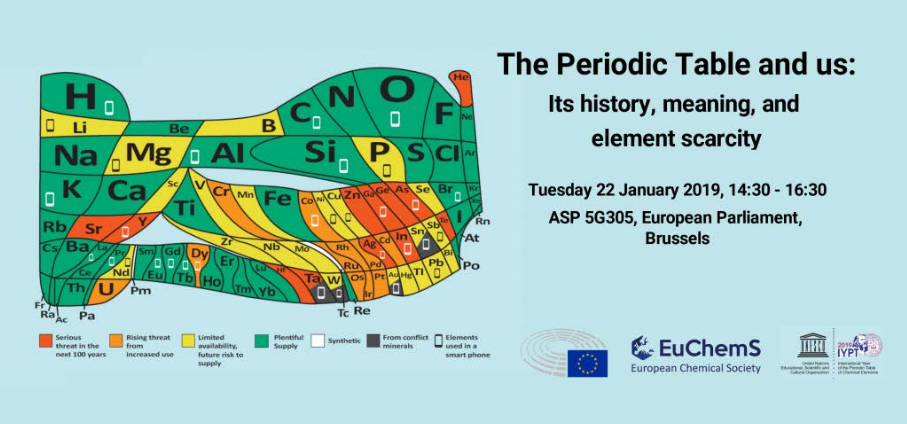
Keywords: Periodic table, Chemical elements, Periodic law

In chemistry, the Periodic Table of Elements is the map that outlines an ordered system of all the identified elements that make up everything in our universe. The chemical elements that make up the periodic table are the building blocks for water, plants, minerals and everything in nature. These elements also create the products and technologies that have shaped modern societies in countless ways – clean drinking water, effective medicines and technologies ranging from solar panels to electronics components, all rely on chemistry.

The Periodic Table represents more than 5,000 years of human discovery. The United Nations has declared 2019 the "*International Year of the Periodic Table of the Chemical Elements*," to celebrate the 150th anniversary of the first periodic table and recognize the important role chemistry plays today in promoting sustainable development and providing solutions to global challenges. Academic institutions, chemistry societies and industry will all be celebrating the periodic table throughout 2019. But you don't have to be a chemist or scientist to appreciate the periodic table.

In 1869, Russian chemist Dimitri Mendeleev wanted to see if there was a pattern to the chemical properties of the elements he knew. He found one by listing elements by their increasing atomic number and arranging them in a chart – creating the first periodic table. This structured order helped Mendeleev, and other scientists, identify similarities and differences among elements to help predict future chemical reactions. While Mendeleev's periodic table included **63** elements, he anticipated that others would one day be discovered, so he left open spaces in his table for additions. Today, the **118** chemical elements identified on the periodic table include the materials that make up all known objects in the universe.



The Periodic Table and us:

Its history, meaning, and element scarcity

Tuesday 22 January 2019, 14:30 - 16:30
ASP 5G305, European Parliament, Brussels

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Synthesis of super magnetic lipophilic graphene

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Keywords: Graphene, Magnetic, Lipophile, Lamellar structure, Friction and wear, 2D Materials

Friction and wear are the two major reasons for energy and material losses in mechanical processes. Lubrication is a principal issue to improve energy efficiency and mechanical durability[1]. Although graphene oxide (GO) is naturally hydrophilic, there are some ways to effectively adjust the characteristic of GO from hydrophilicity to super-hydrophobicity by grafting long chain alkanes on the GO surface[2]. As a promising and manipulable precursor, GO sheets provide active sites for chemical functionalization through hydroxyl, carbonyl, epoxy, and phenol functional groups attached onto the basal plane and along sheet edges[3,4]. In this work, in a typical experiment, GO was prepared by acid oxidation of graphite powder according to the modified Hummers method. we used the GO as an efficient oxidizing reagent to oxidize Fe^{2+} from $FeCl^2$ to form Fe^3O^4/rGO via the spontaneous *in situ* deposition of Fe^3O^4 nanoparticles onto the self-reduced GO surface. Then lipophilic magnetic graphene was synthesized.

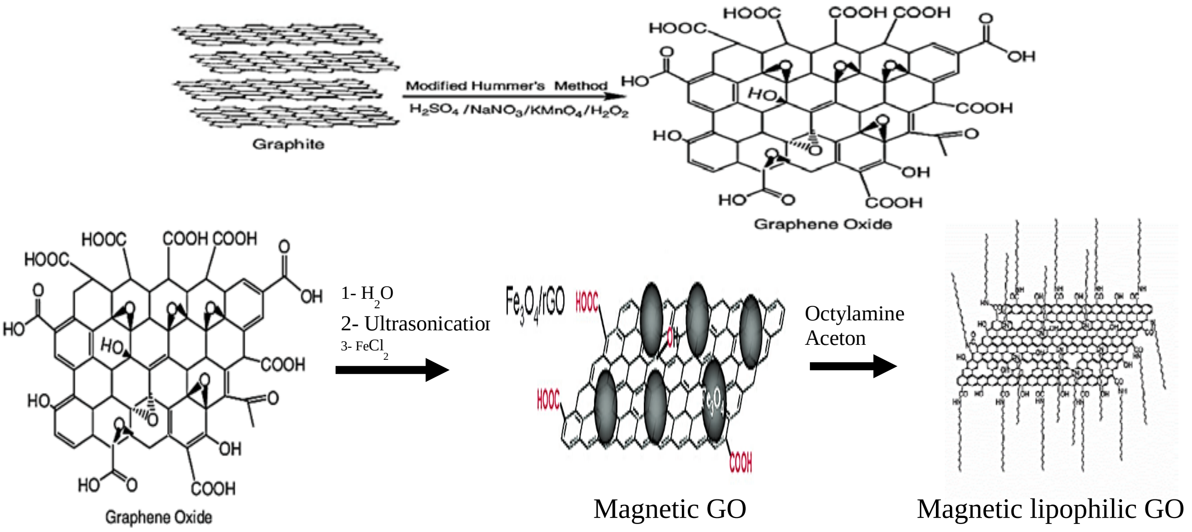

Fig. 1 Synthesis of magnetic lipophilic graphene

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Survey Friedel-Crafts reaction of *N*-aryltrifluoroacetimidoyl chlorides with aromatic compounds

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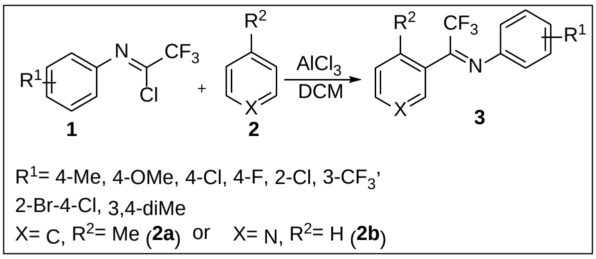
Keywords: Fluorinated compounds, N-Aryltrifluoroacetimidoyl chlorides, Friedel-crafts reaction.

Fluorinated compounds are most important organohalides in natural and medicinal chemistry.[1] In the most important drugs which are commercially available, at least one fluorine atom is present such as: antidepressant fluoxetine (Prozac), cholesterol-lowering drug atorvastatin (Lipitor) and the antibacterial ciprofloxacin (Ciprobay).[2] The trifluoromethyl group is becoming more and more important in both of agrochemical and pharmaceutical applications because of the influence of fluorine atom on physical, chemical, and physiological properties, stability, and lipophilicity of the molecule. In recent years, reactions of trifluoromethylation have been extensively investigated, in order to synthesis of new organofluorinated drugs.[3] Herein, we report a friedel-crafts reaction of N-aryltrifluoroacetimidoyl chlorides **1** and aromatic compounds **2** for synthesis of new N-aryltrifluoroacetimidoyl aromatic compounds **3** (Fig. 1). The FT-IR, ^{19}F-NMR, ^{1}H-NMR and ^{13}C-NMR confirm the structures of the products.



R^1= 4-Me, 4-OMe, 4-Cl, 4-F, 2-Cl, 3-CF_3'
2-Br-4-Cl, 3,4-diMe
X= C, R^2= Me (**2a**) or X= N, R^2= H (**2b**)

Fig. 1 Synthesis of new N-aryltrifluoroacetimidoyl aromatic compounds **3**.

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The synthesis of 2,3-dihydroquinazolinones in the presence of nano-biocatalyst

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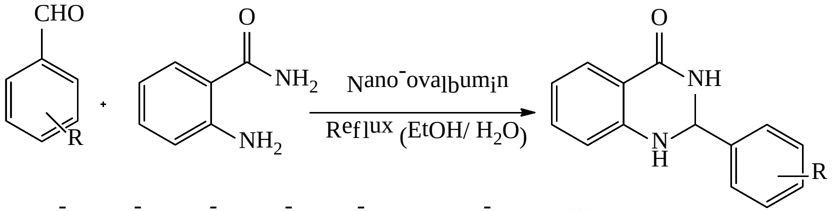
Keywords: Biocatalyst, 2,3-Dihydroquinazolinone, Eco-friendly catalyst, Nano-ovalbumin.

2,3-Dihydroquinazolin-4(1*H*)-ones are an important class of nitrogen-containing heterocyclic compounds which have attracted more attention in medicinal chemistry. They have extensive roles as key building units in the preparation of valuable drugs such as anticonvulsant,[1] antitumor,[2] and anticancer.[3]

Heterogeneous catalysts have been widely used in industrial and green chemistry because of their unique advantages such as easy separation from reaction media by simple filtration.[4] Nano-ovalbumin is a globular, biocompatible, non-toxic and biodegradable phosphoglyco protein that has been recently used as a heterogeneous and eco-friendly catalyst.[5]

We have synthesized 2,3-dihydroquinazolin-4(1*H*)-ones *via* condensation of 2-aminobenzamide and different aldehydes in the presence of nano-ovalbumin as a retrievable, metal-free and heterogeneous biocatalyst and in reflux (EtOH/H_2O) conditions (Fig. 1).



R: 2-NO_2, 3-NO_2, 4-NO_2, 4-Cl, 2,4-$(Cl)_2$, H, 2,4-$(MeO)_2$,…

Fig. 1 Synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives in the presence of nano-ovalbumin

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Enhancement of catalytic activity using two nano-structured Metal-Organic Frameworks (MOFs) synthesized via ultrasonic irradiation

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Keywords: Metal-Organic Frameworks (MOF); Ultrasonic irradiation; Knoevenagel condensation.

Facile and environmentally friendly nano-scale synthesis of two new zinc and cadmium-organic frameworks (MOFs)[1], $\{[Zn(NH_2\text{-}BDC)(4\text{-}bpmbp)].2DMF\}_n$ (**TMU-25**) and $\{[Cd(NH_2\text{-}BDC)(4\text{-}bpmbp)].2DMF\}_n$ (**TMU-26**), under ultrasonic irradiation at ambient temperature and atmospheric pressure has been explored. Ultrasonic irradiation is considered a green energy source because of shorter reaction times and higher yields in comparison to thermal energy sources.[2] Controlling the growth of Nanometer-sized particles of metal–organic frameworks is captivating to explore, since their inimitable properties are controlled by the large number of surface molecules, which experience a completely different environment than those in a bulk crystal. The effect of different parameters like concentrations of initial reagents and reaction times on size and morphology of compounds was investigated. Furthermore, the catalytic behavior of TMU-25 nano-structures toward the Knoevenagel condensation reaction was compared with its bulk form. The Knoevenagel condensation is a typical test reaction for the evaluation of basic catalysts[3], which is the most common used reaction for investigation of MOF containing basic functionalized structures due to its amenable reaction conditions and analysis.

Fig. 1 Overall presentation fabrication procedure

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Fabrication of chitosan hydrogels having phthalocyanine-colistin Conjugate as an antibacterial agent in photodynamic therapy

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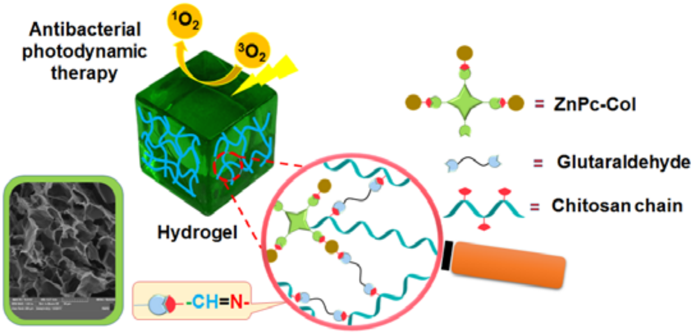
Keywords: Hydrogel, Phthalocyanine, Chitosan, Colistin, Photodynamic Therapy.

The preparation of a novel antibacterial system is a crucial therapeutic prerequisite to treat wounds affected by multidrug-resistant Gram-negative bacteria.[1] Antibacterial photodynamic therapy (APDT) is a hopeful therapy for bacterial infection.[2] However, the usage of most photosensitizers is limited by their low water solubility and their inadequacy in disruption of the outer membrane of Gram-negative bacteria.[3] In this context, zinc phthalocyanine-colistin (ZnPc-Col) conjugate as a new photosensitizer was prepared in the hope of modifying interaction of phthalocyanine with the surface of Gram-negative bacteria. Solving the problem of the poor solubility of phthalocyanine, was gained by the incorporation of ZnPc-Col into chitosan hydrogel. The weight percentages of ZnPc-Col and glutaraldehyde had significant influences in determining the hydrogel microstructure. Different spectroscopic methods, SEM, and rheological measurements were applied to investigate the properties of ZnPc-Col and fabricated hydrogels. The photosensitizing activity of the hydrogels was assessed by application of 1,3-diphenylisobenzofuran as a singlet oxygen chemical quencher. Hydrogels bearing zinc phthalocyanine-colistin adduct showed an enhanced APDT efficiency compared to hydrogels containing just zinc phthalocyanine component. This improvement has been seen against *P. aeruginosa*.



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Synthesis of triazine based 2D polymer

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Keyword: Triazine, Metal assisted, Nitrogen rich.

Covalent Triazine Frameworks (CTFs) are an exciting type of porous organic materials with unique physicochemical properties including high chemical and thermal stability, rich nitrogen contents, semiconducting behavior, high surface area, and defined pore size. Due to such properties, CTFs are attractive candidates for different applications such as separation and storage of gases, energy storage, photocatalysis as well as heterogeneous catalysis. These nanomaterials are synthesized by different approaches including ionothermal trimerization, phosphorus pentoxide (P_2O_5) catalyzed, amidine based polycondensation, superacid catalyzed and Friedel–Crafts reaction. However, the harsh conditions of these synthetic routes result in uncontrolled reactions, undefined structures and consequently low Processability.

In this work, we report a new method for the synthesis of CTFs at mild conditions. The synthesized materials were characterized by different spectroscopy and microscopy methods. Based on our results, metal has a crucial role in the direction of reaction and topology of the obtained nanomaterials.

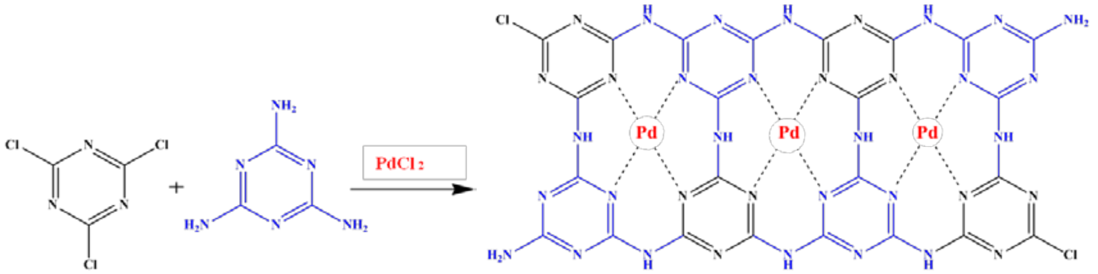

Fig. 1 Schematic representation of the synthesis of CTFs

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Adsorption study of penicillin onto single-walled carbon nanotubes from kinetics perspective

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Keywords: Adsorption, Kinetics, Penicillin, Carbon nanotubes.

Water is a precious environmental resource because it is used by nearly all living organisms; therefore, pollution of water resources may be a serious problem in all parts of the world. The pharmaceutical industry produces compounds that are toxic at trace concentrations if released to the environment in water or soil. Penicillin, selected as a model compound in the present study, is widely available in bulk drugs. It is recalcitrant and persistent towards biodegradation and is constituent intermediate of many pharmaceutical industrial effluents. The generation of penicillin containing aqueous wastes during formulation, distribution and field application of antibiotics is often unavoidable.[1] Hence, removal of penicillin from wastewater before its discharge is necessary in order to reduce this side effect on the environment and human health. In the last decade, various methods have been proposed to remove the penicillin.[2-5] The adsorption method appears to be the best strategy, especially for removal of the moderate and low concentration antibiotic compounds from effluent.

The adsorption kinetics data were described according to the integrated rate equations of pseudo-first order, pseudo-second order and Elovich (1-3), respectively:

$$\ln(q_e - q_t) = -k_1 t + \ln q_e \qquad (1)$$

$$t/q_t = 1/k_2 q_e^2 + t/q_e \qquad (2)$$

$$q_t = \beta \ln(\alpha\beta) + \ln t \qquad (3)$$

where q_e and q_t are the amount of penicillin adsorbed (mg/g) at equilibrium and time t (min). k_1 (1/min) and k_2 (g/mg.min) are the pseudo-first and pseudo-second order rate constants, respectively. α is the initial adsorption rate (mg/g.min) and β is the desorption constant during each experiment (g/mg).

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Photocatalytic degradation of Direct Blue 14 by Polyaniline/CdS nanocomposite

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Keywords: Polyaniline, Cadmium sulfide, Direct Blue 14, Photocatalyst.

There are different types of pollutants in water, soil and air that have harmful effects on human, plants and animals' health and affect the eco-environment. One of the major environmental pollutants is chromatic wastewater containing chemicals. The presence of dye in receiver water prevents light infiltration and causes eutrophication phenomenon that disturbs the photosynthesis process and inhibits the growth of aquatic organisms. In addition, studies have shown that dyes used in various industries have carcinogenic, mutagenicity and allergenicity properties.[1] Currently, the application of advanced oxidation processes (AOPs) for the removal of contaminants has a special place, especially from aqueous media.[2] Photocatalytic processes are efficient advanced oxidation processes to remove dye pollutants that play a role by a semiconductor photocatalyst and an energetic light source.[3] In this study, the role of polyaniline/cadmium sulfide (PANI/CdS) nanocomposite was evaluated as a photocatalyst for Direct Blue 14 (DB 14) dye removal from aqueous solutions. Experiments were designed using response surface methodology (RSM). Figure (1) shows the photocatalytic degradation of DB14 by PANI/CdS as a function of initial concentration of DB14-pH and PANI/CdS amount-irradiation time.

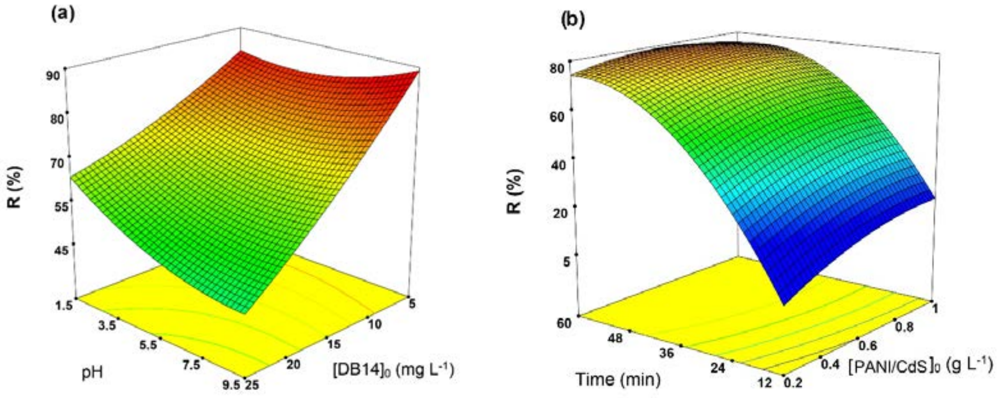

Fig. 1 Photocatalytic degradation of DB14 by PANI/CdS as a function of (a) initial concentration of DB14 and pH; (b) PANI/CdS amount and irradiation time.

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Pd(0) nanoparticles supported on melamine functionalized SBA-15: An efficient catalyst for reduction of nitrobenzens

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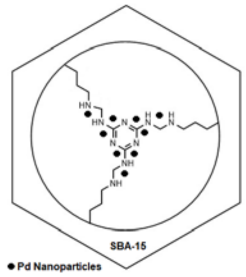
Keywords: Nitro compounds, Pd(0) nanoparticles, Anilines, Reduction.

Aromatic amines are important intermediates in synthesis of several nitrogen containing biologically active compounds, agrochemicals, dyes, polymers, etc. Reduction of nitroarenes is a most common, short and facile route employed to prepare anilines and is one of the areas where major part of recent published work is targeted 1. The catalytic process for hydrogenation of nitrobenzene is an industrially principal reaction for the synthesis of aniline. About 85% of all over aniline in the world is produced by catalytic routes 2.

In this work, we have used the nanocatalyst SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0) (Scheme 1) as a heterogeneous catalyst for reduction of nitroarenes to arylamines in ethanol.



Scheme 1. SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0)

Remarkable reusability and easy separation of the nanocatalyst, high yields and mild reaction conditions as well as the benefits of using ethanol as a green solvent are the advantages which make this protocol a perfect candidate for the reduction of nitroarens.

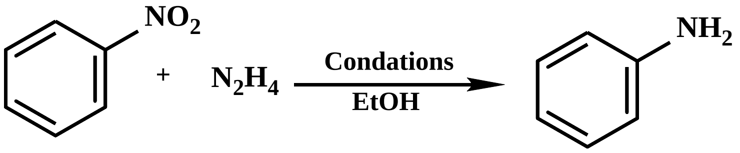


Fig. 1 The reduction of nitroarene with $N_2H_2.H_2O$ /SBA-15/Pr-NH_2-CH_2-Melamine@Pd(0) system.

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Relationship between hydrophobicity and basicity in the catalytic activity of isoreticular MOF catalysts

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Keywords: Metal-Organic Frameworks (MOF), heterogeneous catalysts, hydrophobicity, aldol-type condensation reaction.

Due to the structural diversity of metal–organic frameworks[1], MOFs, tailored engineering of these compounds is important for their use in catalytic processes. Among the MOFs tested as heterogeneous catalysts, there have been rare reports of size selective catalysts. In the present work, we could successfully indicate that subtle substrate selectivity can be induced in the catalytic system by designing a series of isoreticular MOFs with slight structural modifications. Four MOF catalysts possessing imine and/or amine basic N-donor pillars bearing phenyl or naphtyl cores showing different hydrophobic characters around the basic reaction center were prepared via a simple mechano-chemical synthesis. They were characterized thoroughly using TG, IR and PXRD analysis. For the first time, the aldol-type condensation reaction of malononitrile with ketone-functionalized carbonyl substrates was developed in the presence of the basic MOF organocatalysts.[2] Moreover, it has been successfully shown that a subtle substrate selectivity can be addressed during the reaction of three slightly different α-β unsaturated carbonyl compounds in contrast to the effect of size control barriers that commonly direct a heterogeneous reaction pathway.

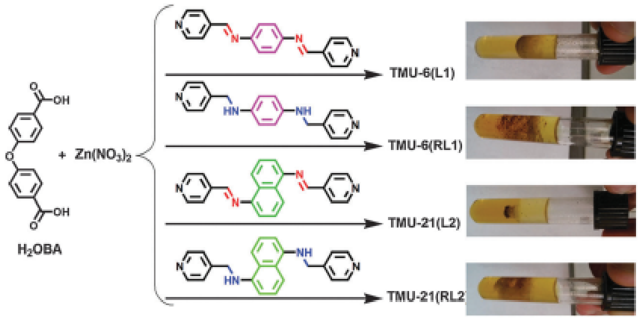

Figure 1. Structure of 4 MOFs synthesized in this work

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Immobilized palladium complex on to the OMS-Cu (BDC) metal-organic framework: sustainable development for the Heck coupling reaction

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Keywords: Metal organic frameworks, Heck reaction, Pd^{II}@Cu (BDC)/2-Py-SI, Nanocatalyst.

Within the field of nanoporous architecturing [1], metal organic framework (MOF) has attracted increased interest in the recent years because of their unique structural properties including high porosity, surface area and tenability [2]. MOFs are also the ideal platform for post synthetic modification chemistry to achieve multi-purpose materials [3]. I this communication, Pd ions were successfully immobilized within the pores of the open metal site (OMS) MOFs with Schiff-base (2-Py-SI) grafted in OMS-Cu (BDC) **Fig 1**. The proposed nanocatalyst is found to be very active, reusable, stable, an excellent reactivity and selectivity for Heck coupling reaction under very mild and sustainable reaction condition.

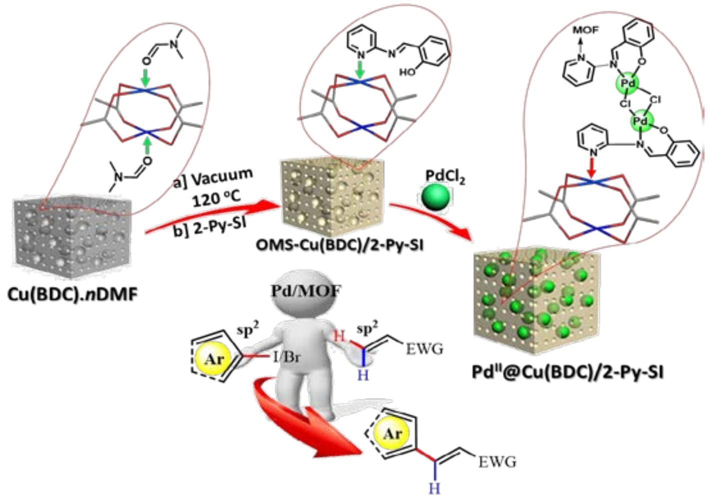

Fig. 1 Post modification immobilization of Pd ions onto the OMS Cu (BDC) for the Heck coupling.

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Synthesis of (*E*)-3,3´-bis(pyridin-4-ylmethyl)-2,2´-dithioxo-2,2´,3,3´-tetrahyro-4*H*,4´*H*-[5,5´-bithiazolylidene]-4,4´-dione as a potential ligand in MOF synthesis

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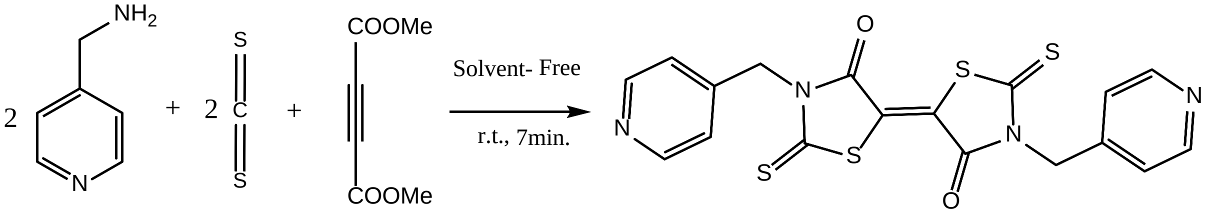
Keywords: MOF, birhodanines, organic ligands, 4-aminometyl pyridine

Metal-Organic Frameworks (MOFs) or porous coordination polymers (PCPs) were constructed by the linkage of metal ions or clusters and organic ligands. As advantages of these materials, high surface area, regular porosity, tunable structure, mild conditions of synthesis, and wide range of applications can be mentioned. Because of these compounds are preferred to other similar porous materials such as activated carbon and zeolites, are of most interest to chemists. The most important of organic ligands are 4,4-bipyridines and benzenedicarboxylates.[1,2] In this work we wish to report synthesis and characterization of (*E*)-3,3´-bis(pyridin-4-ylmethyl)-2,2´-dithioxo-2,2´,3,3´-tetrahyro-4*H*,4´*H*-[5,5´-bithiazolylidene]-4,4´-dione (1) that it has the potential to be used as a ligand in the synthesis of MOF's. The target ligand was synthesized through the one-pot reaction between 4-aminometyl pyridine as a primary amine and carbon disulfide in the presence of dimethylacetylenedicarboxylate under solvent-free condition.[3]



(1)

Fig. 1 Synthesis of ligand

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Preparation of polyurethane hydrogels based on polyethylene glycol/ ε-caprolactone/ methylene diphenyl diisocyanate in the presence of graphene oxide nanoplatelets

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Keywords: Polymeric networks, Polyurethane hydrogels, Graphene oxide nanoplatelets.

Polymeric hydrogels are tridimensional polymeric networks, capable of absorbing a high amount of water.[1] Due to their water uptake capacity, potential amphiphilic behavior, and biocompatibility or biodegradability, hydrogels have been intensively studied for applications in the biomedical, pharmaceutical, agriculture, oil recovery, and cosmetics fields as well as in the biotechnology, bioseparation processes, and as biosensors.[2,3] In this work, graphene oxide nanoplatelets (GNP's) were homogeneously trapped into a polyurethane (PU)-based hydrogel during its preparation (Fig. 1). The effect of the nanoparticles on the thermal behavior as well as the amounts of water uptake were thoroughly studied. Briefly, an azide-containing and polyoxyethylene (PEG)-based polyurethane (PU) was synthesized starting from PEG, ε-caprolactone (ε-CL), and methylene diphenyl diisocyanate (MDI). Next, dialkynyl PEG was used as the crosslinker in the presence of GNP's in 0.1, 0.2, and 0.5 wt.%. In this stage, a thermally-induced copper (I)-catalyzed 1,3-dipolar azide-alkyne cycloaddition (CuAAC) was performed. FT-IR, XRD, ^{1}H-NMR and FE-SEM techniques were used to characterize the samples obtained.

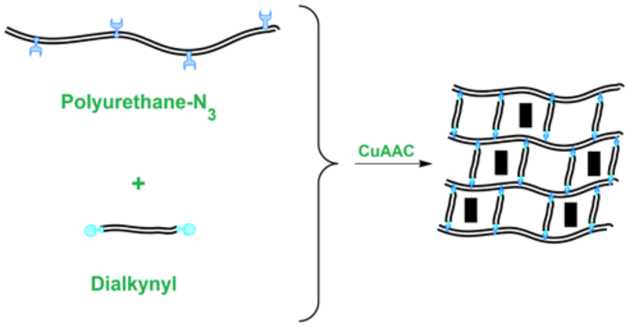

Fig. 1 Synthesis of new polyurethane hydrogel.

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Facile and novel method for graphite exfoliation and preparation of high-temperature stabilized product

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Keywords: Graphite, Graphene, Exfoliation, Bis-Tetrazole, Thermal treatment.

Exfoliation, i.e. individual separation of carbon sheets, is of great interest to produce single-layered graphene nanosheets. Chemical or thermal treatments are popular approaches to exfoliate graphite chunks. In general, these conventional methods are assisted with intercalation via covalent or non-covalent functionalization, expansion, and swelling, adsorption of organic molecules in gas phase, solid nanoparticle insertion or direct molecular exfoliation[1,2]. Exfoliation from bulk, stacked graphite is the most economical way to achieve large quantities of single layer graphene[3]. Development of a method for producing high-quality graphene in large quantities is essential for further investigation of its properties and applications[4]. Thermal exfoliation of graphite is considered as a promising strategy though it normally requires a high exfoliation temperature together with a fast heating rate. In this work, graphite was exfoliated through a thermal method in a way that graphite was dispersed in water and then bis-tetrazole was added and sonicated. Then intercalated graphite was heated on an electrical hotplate and exfoliated graphite obtained.

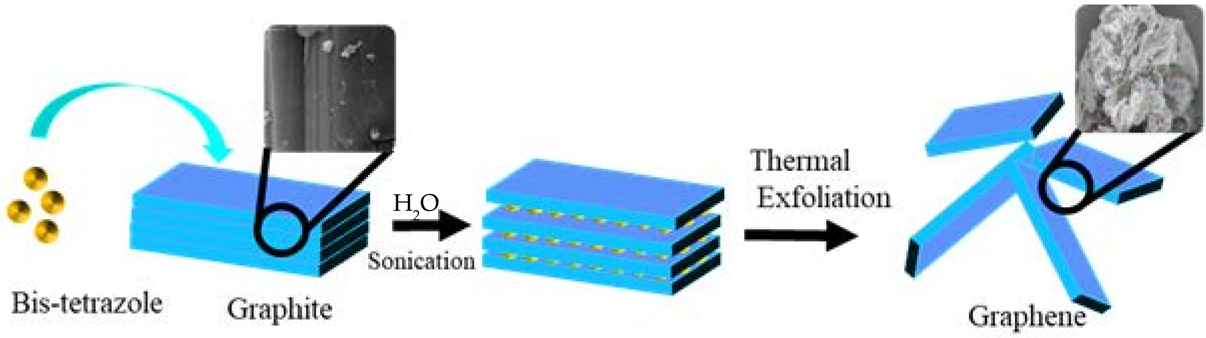

Fig. 1 Schematic of exfoliation of graphite with bis-tetrazole

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Synthesis of tetrazole-containing cyclopentenyl phosphanylidene dicarboxylates

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Keywords: Alkyl 3-phenyl-2-(1*H*-tetrazol-5-yl)acrylates, triphenylphosphine, Acetylenic diesters, Tetrazole, Triphenylphosphanylidene cyclopentene dicarboxylate.

Organophosphorus compounds have a special place in the synthetic chemistry.[1,2] Over the past decade, because of the nucleophilic property of triphenyphosphine, use of it in the presence of electron deficient substrates such as acetylenic esters has been gained more attentions for the synthesis of new carbocyclic and heterocyclic scaffolds.[3,4] Synthesis of highly functionalized carbocycles is interesting and important for industrial and biological sciences.[5] Herein, we report new chemo-selective reaction of triphenylphosphine and alkyl 3-phenyl-2-(1*H*-tetrazol-5-yl)acrylates **3** in the presence of dialkyl acetylenedicarboxylates **4** to produce tetrazole containing of triphenylphosphanylidene cyclopentene dicarboxylates **5** (Fig. 1).

All synthesized compounds are stable solids whose structures were determined on the basis of their mass spectrum, ^1H and ^{13}C NMR and IR spectroscopic data.

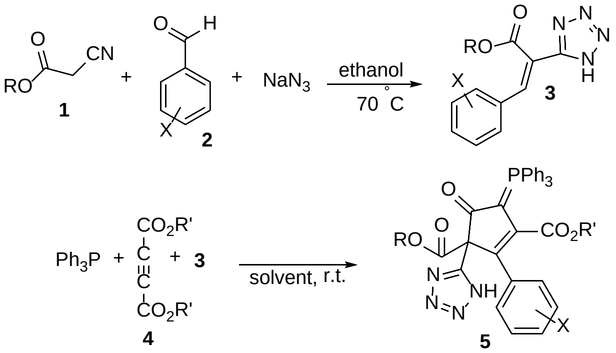

Fig. 1 Synthesis of alkyl 3-phenyl-2-(1*H*-tetrazol-5-yl)acrylates and 3-alkyl 1-alkyl 4-oxo-2-phenyl-3-(1*H*-tetrazol-5-yl)-5-(triphenyl-λ^5-phosphanylidene)cyclopent-1-ene-1,3-dicarboxylate

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Pyrrolidine-based acidic ionic liquid: An efficient and recyclable catalyst for the synthesis of 5-arylidene barbituric acid derivatives in aqueous media

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Keywords: Pyrrolidine, Brönsted acidic ionic-liquid, Barbituric acid, Aqueous media, Green organic synthesis.

Since many years, acid-catalyzed organic transformations have been used extensively to produce numerous organic products. In such transformations, mineral acids have mainly been employed. These acids are highly corrosive, toxic, and are responsible for environmental hazards. In order to solve these problems the subject of ionic liquids with acidic properties as potential green alternatives has been attended by organic researchers.[1,2] Barbituric acids and their derivatives have been widely used as sedative, hypnotic, anesthetic, anticonvulsant, antiosteoporosis, as well as antitumor agents. Arylidene barbituric acids as well as their 2-thio analogues are useful intermediates in the synthesis of important heterocyclic compounds.[3]
As a part of our continuing interest on designing environmentally benign methods for various chemical transformations, [4,5] herein we have described an efficient route for the synthesis of 5-arylidene barbituric acid derivatives using pyrrolidine-based acidic ionic liquid as an affordable and recyclable catalyst (Figure 1). The present protocol show some advantages such as high yields, reduced reaction times, no by-product, clean and simple work-up.

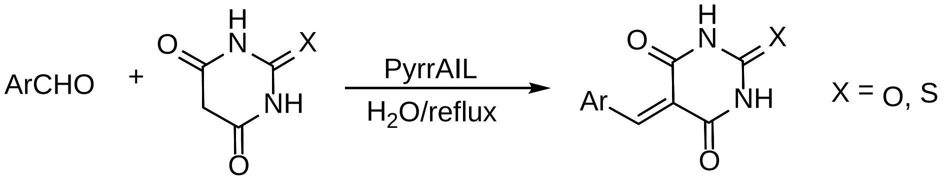

Fig. 1 PyrrAIL catalyzed the synthesis of 5-arylidene barbituric acid derivatives

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Synthesis and characterization of spinel $FeAl_2O_4$ (Hercynite) magnetic nanoparticles and it's applications in multi-component reactions

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Keywords: $FeAl_2O_4$; Hercynite, Magnetic nanoparticles, Benzo[a]pyrano[2,3-C]phenazine, Polyhydroquinoline..

Recent years, the improvement in nanotechnology led to an increasing insist for multifunctional materials owing to simplicity in operation[1–3], remarkable recyclability, high surface areaand ecofriendly nature. In this regard, solid catalysts and magnetic composite nanoparticles are interesting for industrial and biomedical applications and, especially, in catalysis studies as a magnetically separable catalyst [4,5]. Among the various MNPs, Fe_3O_4 has been widely considered as a catalyst[6]. In general, the spinel ferrite catalysts (AB_2O_4, B = Co, Fe, Ni, Mn, Mg, Al, Zr, Zn...) alloy (Fe-Co, Fe-Pt, Fe-Ru...) nanoparticles, and multifunctional nanoparticles have higher performance than the monometallic catalysts[1,7,8]. One of the most promising MNPs supports for the development of high-performance catalyst supports is superparamagnetic iron oxide. The notable advantages of spinel ferrite MNPs are simple synthesis, readily available, low cost, high surface area, low toxicity and superparamagnetism properties. Owing to the inherent advantages of recovery, in the context of green chemistry and reuse of catalyst, herein hercynite MNPs heterogeneous catalyst has been reported for one-pot synthesis of benzo[a]pyrano[2,3-*c*]phenazine and polyhydroquinoline derivatives (Fig. 1).

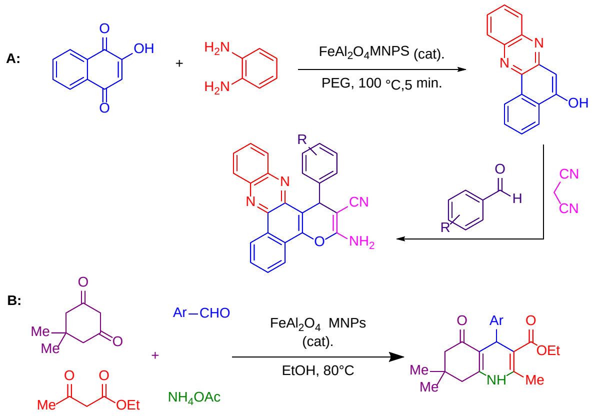

Fig. 1 Hercynite magnetic nanoparticles catalyzed multicomponent reaction

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Synthesis and characterization of L-Methionine-Pd complex supported on Hercynite magnetic nanoparticles ($FeAl_2O_4$@ L-Methionine-Pd) and it's applications in C-C coupling reactions

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Keywords: $FeAl_2O_4$@Methionine-Pd, Hercynite, Magnetic nanoparticles, Suzuki reaction, Heck Reaction.

Recently, separation and recycling of heterogeneous catalysts is employed in the various area. However, immobilization of homogeneous catalysts usually decreases the catalytic activity or selectivity[1]. This drawback can be overcome using nanomaterials as heterogeneous supports. When the size of the support is decreased to the nanometer scale, the surface area is substantially increased, which is combined with excellent accessibility of the surface-bound catalytic sites[2]. Among the various nano materials, the spinel ferrites (AB_2O_4, B= Co, Fe, Ni, Mn, Mg, Al, Zr, Zn...) alloy (Fe-Co, Fe-Pt, Fe-Ru.), and multifunctional nanoparticles have higher performance than the monometallic catalysts. The notable advantages of spinel ferrite MNPs are simple synthesis, readily available, low cost, high surface area, low toxicity and superparamagnetism properties. Owing to the inherent advantages of recovery, in the context of green chemistry and reuse of catalyst, and also rarely used in the isolation and recycling of expensive homogeneous catalysts [3,4].

In the present work, L-Methionine-Pd organometallic complex supported on Hercynite magnetic nanoparticles ($FeAl_2O_4$) with the size of 30–50 nm have been synthesized and its application was studied on the Suzuki and Heck C-C cross-coupling reactions (fig.1).

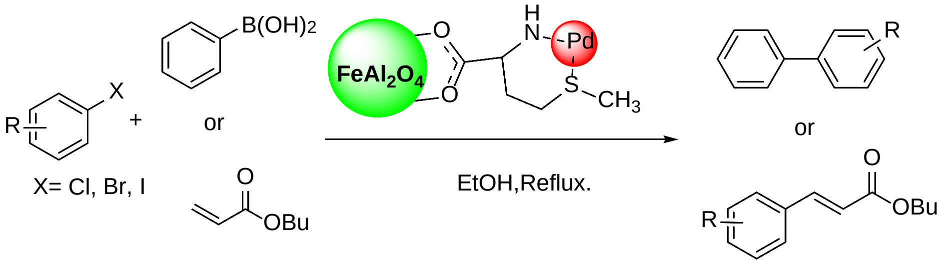

Fig. 1 $FeAl_2O_4$@Methionine-Pd magnetic nanoparticles catalyzed C-C coupling reactions

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Synthesis of boron nitride

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Keywords: Boron nitride, Hexagonal-BN, Cubic-BN, High-pressure high-temperature synthesis, Chemical vapor deposition.

Boron nitride (BN) - in all its various structures - is a synthetic product and not found in nature. Boron nitride is a extraordinary topic in the area of materials science. Boron and nitrogen are neighbors of carbon in the periodic table, and therefore BN phases are isoelectric to the corresponding carbon phases.[1] Due to the special bonding behaviors of boron and nitrogen the BN exists in many different structures. The well-defined crystallographic structures are hexagonal BN (h-BN), rhombohedral BN (r-BN), wurtzitic BN (w-BN), and cubic BN (c-BN).[2] Additionally, other crystalline and amorphous structures exist. Parts prepared of h-BN as well as c-BN are of great interest for industrial applications but also for materials science.[3] Hexagonal boron nitride (h-BN) is a structural analog of graphite lattice while consisting of an equal number of boron and nitrogen atoms.[2] It crystallizes similar to graphite in a hexagonal sheet layered structure, and therefore it is often referred to as "white graphite".[3] BN nanostructures, including nanoparticles, nanotubes, nanofibers, nanoribbons, nanosheets have attracted much attention in the past few decades due to their promising properties such as low density, excellent chemical inertness, superb oxidation resistance, high thermal conductivity, and unique catalytic properties.[2] In this study, the structures are synthesized using bottom-up, low-temperature (~300 ˚C), solid-state reaction of melamine and boric acid giving rise to porous and mechanically stable interconnected h-BN layers. synthesized compound are stable solid whose structures were determined on the basis of their X-ray, FT-IR, TGA, and EDS data.

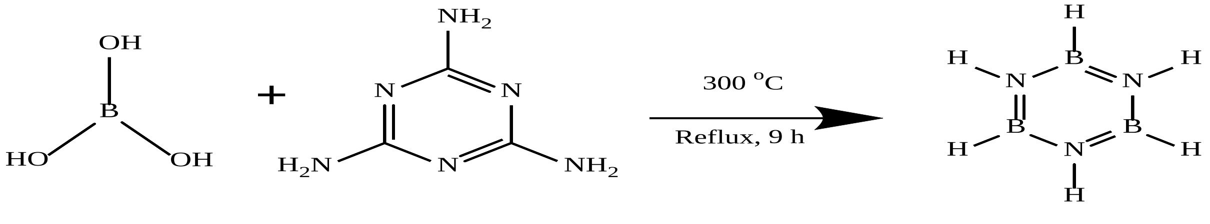

Fig. 1 Schematic of boron nitride synthesis

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Synthesis and characterization of trichloroarylsilanes

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Keywords: Trichlorosilane, Si–C coupling, Arylmethyltrichlorosilane

The chemistry of primary alkyl and aryl functionalized silicon compounds of the general formula $RSiH_nX_{3-n}$, (R = alkyl or aryl, X = halide) is well established.[1] Organotrichlorosilanes are widely used as starting materials in silicone industry and as coupling agents for the composites with inorganic materials in plastic. Over the last few decades, considerable effort has been made to develop a convenient route to organosilicon compounds such as Rochow direct process, the reaction of chlorosilanes with organometallic reagents, hydro- silylation, etc.[2] The classical synthetic procedure can be separated in the formation of a carbanion at the aryl carbon, forming an organolithium or a Grignard reagent. Herein, trichloro(naphthalen-1-yl)silane was prepared by an one-pot reaction of naphthalen-1-ylmagnesium bromide and tetrachlorosilane in THF and was isolated as a white solid.[3] We using aryl compound and tetrachlorosilane in THF solvent whose structures were determined on the basis of their mass spectrum, ^1H and ^{13}C NMR, X-ray, TGA and IR spectroscopic data.

$$\text{Ar}-\text{Br} \xrightarrow{\text{Mg, THF}} \text{Ar}-\text{MgBr} \xrightarrow[\text{THF,}]{\text{8eq, SiCl}_4\text{,}} \text{Ar}-\text{SiCl}_3$$

Ar = Naphthyl, 2,6-dimethylphenyl, Tolyl

Fig. 1 Schematic synthesis of trichloroarylsilanes

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Enantioselective synthesis of chiral dispiro-bisoxindole alkaloids via [3+2]-cycloaddition reaction in both enantiomeric form

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Keywords: Asymmetric 1,3-dipolar cycloaddition, Azomethine ylides, Enantioselective synthesis, Dispiro-bisoxindole alkaloids, Oppolzer's sultam chiral auxiliary

In this research, a highly diastereo- and enantioselective 1,3-dipolar cycloaddition of isatin-derived azomethine ylides with new chiral 3-arylidene-oxindoles, was described. Initially, we synthesized new chiral derivative of 3-arylidene-oxindoles equipped with (*S*)-Oppolzer's sultam chiral auxiliary for the first time and used it as dipolarophile in above asymmetric [3+2] cycloaddition reactions. The synthesis affords the desired chiral dispiro-bisoxindole alkaloids scaffold in excellent yields with high diastereo- and enantioselectivity under mild conditions. The other enantiomer of cycloadducts could be obtained utilizing (*R*)-Oppolzer's sultam and confirmed by HPLC analysis (Fig. 1). The stereochemistry of products was determined by single-crystal X-ray analysis.[1]

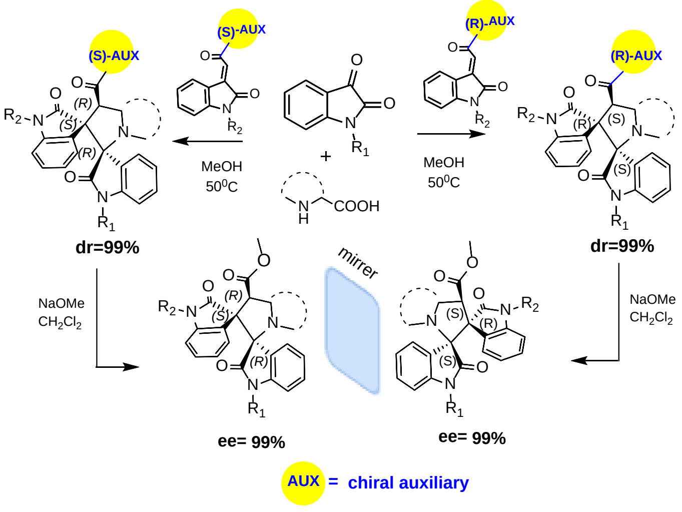

Fig. 1 Synthesis of dispiro-bisoxindole alkaloids in both enantiomeric forms

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Highly efficient acetalization and ketalization catalyzed by nano-kaolin/BF_3/Fe_3O_4 under solvent-free condition

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Keywords: Acetalization, Ketalization, Nano-kaolin/BF_3/Fe_3O_4, Solvent free.

The protection of carbonyl groups plays an important role in multi-step organic synthesis of compounds with multiple functional groups. Cyclic acetals and ketals are the most well-established and frequently used protective strategies for the carbonyl groups.[1] In addition, many acetals and ketals have wide applications in industrial manufacturing such as cosmetics, foods and fragrances, etc.[2] The most general method for the synthesis of acetals and ketals is the reaction of carbonyl compounds with an alcohol or diol. Traditionally, acidic catalysts like protic acid, Lewis acids, and heteropoly acids[3] were used to synthesize acetals or ketals. However, those methods suffered from several drawbacks such as corrosion, tedious work-up, environmental pollution and non-recoverability of catalysts. To solve these problems, a variety of solid acids, which were prepared by immobilization of acidic catalysts have been investigated.[4] Recently, transition metal complexes have been used to catalyze the acetalization and ketalization of carbonyl compounds.[5]

In this study, we report our results for the acetalization and ketalization of carbonyl compounds with diols under solvent-free conditions in the presence of nano-kaolin/BF_3/Fe_3O_4 as a magnetic catalyst (Fig.1). The advantages of this study involve in use of solvent-free condition, an easy experimental work-up system, rapidity, recyclable catalyst and green process.

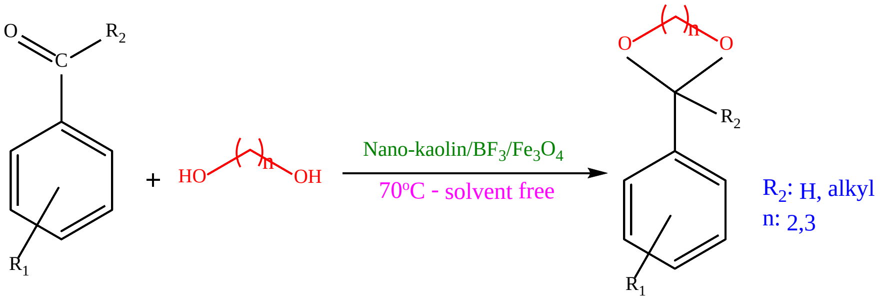

Fig. 1 Nano-kaolin/BF_3/Fe_3O_4-catalyzed acetalization and ketalization.

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Accelerated drug discovery: A combinatorial diversity oriented flow synthesis approach

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Keywords: Diversity oriented synthesis, Flow synthesis, Drug discovery, Combinatorial chemistry.

Drug discovery is exploring the chemical space aiming at finding chemicals which are able to interact with or regulate therapeutic biological targets[1]. However, development of an efficient and reliable synthetic method to produce a library of compounds which can represent a huge chemical space seems to be difficult and demanding. The present research aims at combining various synthetic strategies including diversity oriented synthesis, flow synthesis, combinatorial chemistry, multicomponent reactions and high throughput screening to suggest an accelerated method for sweeping and exploring the chemical space applicable to drug discovery.

Combinatorial chemistry comprises chemical synthetic methods that make it possible to prepare a large number of compounds in a single process[2]. These compound libraries can be made as mixtures, sets of individual compounds or chemical structures generated by computer software. Flow chemistry, sometimes referred to as “continuous flow chemistry”, is the process of performing chemical reactions in a tube or pipe[3]. Reactive components are pumped together at a mixing junction and flowed down a temperature controlled pipe or tube. Using a narrow tube in flow synthesis offer the merits of laminar flow and microfluidic effects which facilitate catalytic reactions and separation of the products. Applying combinatorial, diversity oriented methods on multicomponent reactions in flow greatly accelerate and facilitate synthesis of a large array of diversified functionalized chemical structures which ameliorate drug discover technics offering a programmable, modular and efficient method for drug discovery.

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Modification of Graphene quantum dots with metformine/Co(II) as an efficient oxidation catalyst

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Keywords: Graphene quantum dot, Metformine, Heterogeneous catalyst, oxidation reaction.

Nowadays, graphene quantum dots (GQDs) has drawn a lot of attention because of their properties like high accessible surface area, less cytotoxicity, high chemical stability, outstanding biocompatibility. It is believed that GQDs can attend as a platform for the development of other nanomaterial such as metals and metal oxides to use as catalysts. Thus, GQDs can be a superior candidate as a host for Co complexes to fabricate a heterogenous catalyst for selective oxidation. In continues of our interest in developing the useful catalytic systems for oxidation of organic compounds,[1-4] herein metformin employed as a ligand for connecting Co(II) to GQDs support to furnish a heterogeneous catalyst which enjoys from the high aspect ratio due to atomic distribution of catalyst on the support. Easy recovery, sustainability, high surface area, and chemical stability of the new catalyst make it attractive for catalytic goals. The catalyst was employed in the oxidation reaction of alkylarenes with high yields.

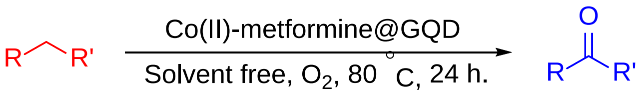

Fig. 1 Oxidation of alkylarenes with heterogeneous Co(II) catalyst

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Multicomponent reaction for synthesis of dihydropyrroles

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Keywords: Multicomponent reactions, Isocyanides, 2,5-dihydropyrrole-dihydropyrrole, Sultam.

Multicomponent reactions (MCRs) have become useful tools for diversity-oriented and complexity-generating synthesis of natural products and drug-like small molecules with novel properties.[1] Heterocyclic molecules are ubiquitous,s structural motifs in a wide range of biologically relevant molecules and natural products. Developing methods for rapid and efficient synthesis of structurally diverse heterocyclic molecules represents one of the major domains in both synthetic chemistry and drug discovery. In this context, dihydropyrrole represents one of the most important structural motifs presenting in biologically active molecules.[2] Herein one-pot synthesis of 2,5-dihydropyrrole-dihydropyrrole contain sultam carried out with good yield and cost-effective starting materials. In this regard at the first saccharin was used as acid in Ugi multicomponent reaction (after α-amino amide formed) sodium azide was added as nucleophile and 3-dihydropyrroles contain sultam (**6a-l**) synthesized. High atom economy, good yield and stereoselectivity is benefits of this procedure. The details about the synthesis will be further discussed in the conference (**Fig. 1**).

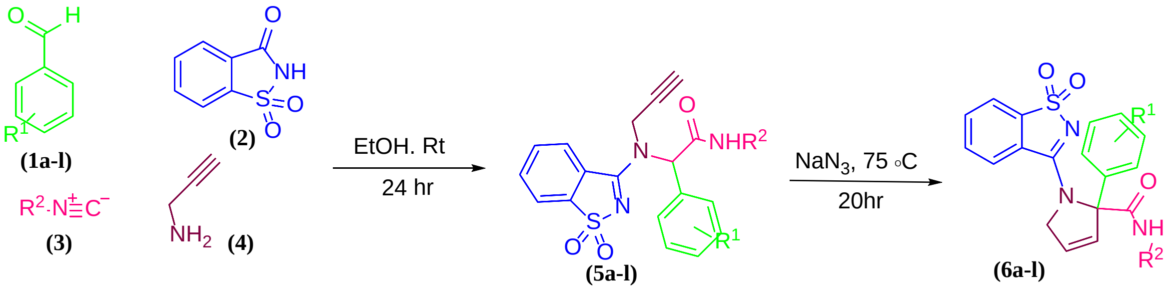

Fig. 1 One-pot five-component synthesis of 2,5-dihydropyrrole dihydropyrroles derivatives

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Synthesis of 5-(3-benzylbenzo[*d*]thiazol-2(3*H*)ylidene)1,3-dimethylpyrimidine-2,4,6(1*H*, 3*H*, 5*H*)-trion

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Keywords: 2-Chlorobenzothiazole, Benzyl bromide, 1,3-Dimethyl barbituricacid, Formation of C=C.

Benzothiazole ring belongs to the privileged scaffolds in modern medicinal chemistry.[1] Benzothiazole and its derivatives are extensively heterocyclics due to their wide spectrum of bioactivities. Among them, the imidazobenzothiazoles are pharmacologically important because of their anti-inflammatory, antifungal, antitumor, antibacterial, and other properties. [2, 3] On the other hand, benzothiazoles have industrial applications including serve as light-emitting materials in optical devices, fluorescent, electroluminescent, liquid crystal, semiconductor, optical sensors and photovoltaic cells.[4,5] In this work, synthesis of 5-(3-benzylbenzo[*d*]thiazol-2(3*H*)ylidene)1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trion is reported from reaction of 2-chlorobenzothiazole **1**, 1,3-dimethylbarbitoric acid **2** in the presence of benzybromide **3** in good yield.

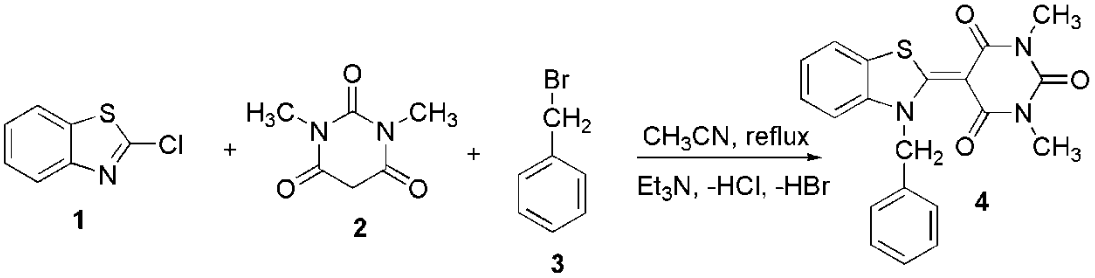

Fig. 1 5-(3-benzylbenzo[*d*]thiazol-2(3*H*)ylidene)1,3-dimethylpyrimidine-2,4,6(1*H*, 3*H*, 5*H*)-trion

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Synthesis and application of chelating resin based on poly (styrene-alt-maleic anhydride)(SMA) for metal ions removal

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Keywords: Adsorption, Chelating resin, 3-(4-Hydroxy phenyl) cyclopropane-1,1,2,2-tetracarboxylic acid, Metal ions, Poly(styrene-alt-maleic anhydride).

With the advent of new technologies and rapid development of the global industry, heavy metal ions are increasingly discharged into the environment. They are causing damages to the environment, human and plants life.[1] Various techniques have been used to remove metal ions from aqueous solution. Among related techniques, adsorption is considered to be the most promising process.[2] Recently, the synthesis of graft copolymers with synthetic and natural polymers of maleic anhydride copolymers which can chemically bind metal ions from aqueous solutions have been reported.[3] The aim of the present work is to study the adsorption characteristics of the prepared chelating resin toward metal ions under different experimental conditions. For this propose, first SMA copolymer was synthesized by free radical polymerization and prepared linear copolymer was modified with 3-(4-hydroxy phenyl) cyclopropane-1,1,2,2-tetracarboxylic acid (HPC) as a grafting and 1,2 diamino ethane as a crosslinking agent to obtain new chelating copolymer with multi-carboxylic acid cyclo propane functionalities in the pendant group. The functionalized copolymer showed strong adsorption ability to the Cu (II), with the maximum adsorption capacities at pH, 5. The high adsorption rate (<30 min) was seen. The synthesized resin and its metal ions chelates were characterized by FT-IR, thermogravimetric analysis (TGA) and atomic absorption techniques (AAS).

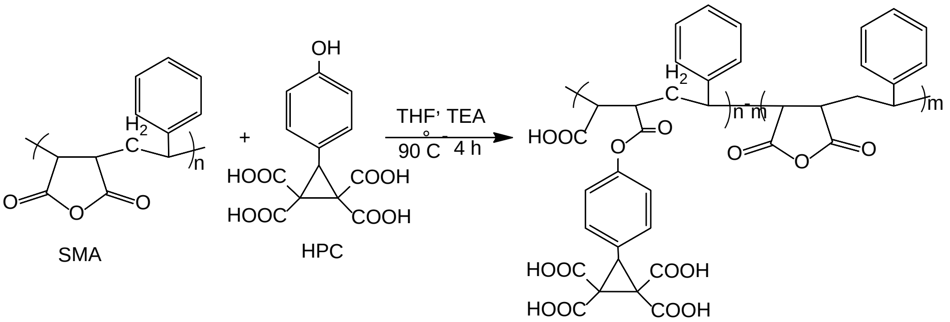

Fig. 1 Synthesis route of SMA-HPC

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Chemotherapy of breast cancer cells using novel pH-responsive chitosan-based nanomicelle

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***Keywords*:**Chitosan, Methotrexate, Nanomicelles, Targeted Drug Delivery, Cancer Chemotherapy

Conventional chemotherapy suffers lack of bioavailability, selectivity and multidrug resistance (MDR). Nano-sized drug delivery systems (DDS) is developing aimed to solve several limitations of conventional drug delivery systems. These systems have been offered for targeting tumor tissue due to their long circulation time and improved drug solubility, retention (EPR) effect, and enhanced permeability. So, the aim of this research was the development and design of novel targeted nanocarriers for cancer chemotherapy.[1-3] For this reason, *N*-phthaloyl-chitosan was first modified with 4-cyano, 4-[(phenylcarbothioyl) sulfanyl] pentatonic acid to prepare the macro initiator. Then, the macro initiator was copolymerized with DMAEMAQ and IA monomer via RAFT polymerization method to create CS-g-P(DMAEMA-co-IA). In the next step, fluorescein dye was entrapped into the core of nanomicelles during the synthesis with the dialysis method. Afterward, methotrexate anticancer drug (MTX) as an anionically charged drug was coupled to the cationic segment of nanomicelles. Additionally, owing to the folate-mediated endocytosis reaction of MTX, these developed nanocarriers can be potent for effective cell-uptake to provide the benefits of active targeting of NPs (Fig1).

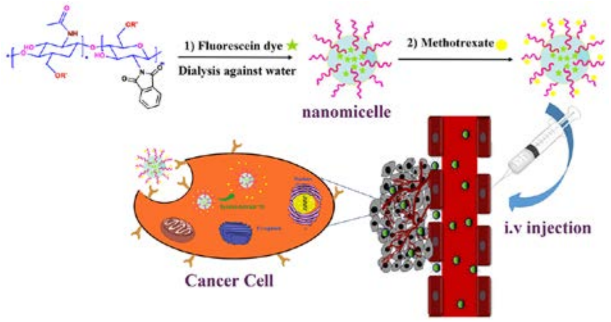

Fig. 1 Cell uptake mechanism for passive delivery of methotrexate (MTX) to the cancerous tissue.

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Investigation reaction of 1,6-dihydropyridine dicarbonitrils with indole arylbenzoiens

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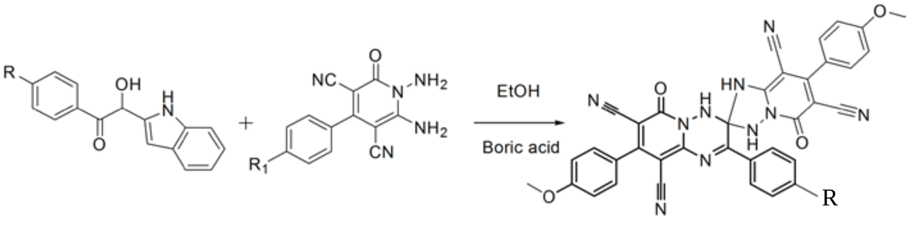
Keywords: Indole arylbenzoein, 1,6-Dihydropyridine dicarbonitrils

Triazole and triazine compounds containing three nitrogen atoms in the five and six-membered aromatic azole ring are readily able to bind with a variety of enzymes and receptors in biological system via diverse non-covalent interactions, and thus display versatile biological activities. The related researches in triazole and triazine-based derivatives as medicinal drugs have been an extremely active topic, and numerous excellent achievements have been acquired.[1]

α-(Indol-3-yl) carbonyl compounds are relevant precursors for the preparation of biologically active molecules such as tryptamines, β carbolines, carbazoles, and tryptophols, which are found in several natural sources and are useful intermediates in the synthesis of some biologically active compounds.[2]

In this research we investigated reaction of 1,6-diamino-4-aryl-2-oxo-1,2-dihidropyridine-3,5-dicarbonitrile with indole aryl benzoein derivatives. Indole arylbenzoein **1** was reacted with 1,6-diamino-4-aryl-2-oxo-1,2-dihidropyridine-3,5-dicarbonitrile **2** in ethanol under reflux conditions (24-48 hrs) and produced spiro-triazol triazine **3.** The structure of products were identified by ^{1}H-NMR, ^{13}C-NMR and IR spectroscopy techniques.



1 **2** **3**

R = Br,CH_3 R_1= H, OMe

Fig. 1 Reaction of 1,6-dihydropyridine dicarbonitrils with Indole arylbenzoiens

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Phytochemical study of *Nepeta racemosa* L.

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Keywords: *Nepeta racemosa* L., Isolation, Structure Elucidation, Total phenol and flavonoid content

The *Nepeta* genus is one of the great genera of the family of mint, accounting for over 250 species of this genus in the world.[1]This genus was first recognized with two species of *N. cataria* and *N. glechoma*. Various types of chemical compounds of this genus have been reported, such as monoterpenes, sesquiuterpenes, dipropenes, triplepenes, flavonoids, phenolic compounds, essential oils, and others.[2] Approximately 193 compounds have been identified in the *Nepeta* species, in which terpenoids and flavonoids are the dominant component of *Nepeta*. Different species of this genus were used for anti-inflammatory, asthmatic effects, anti-infectious and diuretic effects in traditional medicine.[3] *N. racemosa* L. species in the last survey of *Nepeta racemosa*, Iran identified 24 chemical compositions including beta-pylene, 4aα, 7α, 7aα-nepetalactone, 4aα, 7α, 7aβ-nepetalactone, 4aβ, 7α, 7aβ-nepetalactone and 8.1-pinole and has been isolated. In this study, *N. racemosa* L. species was collected from Sabalan mountain and extracted by n-hexane and ethyl acetate. Ursolic acid and oleanolic acid were isolated by column chromatography techniques and identified by ^{1}H-NMR and ^{13}C-NMR. Essential oil of this species was also studied by GC-MS. Major compounds were (*E*) -β-ocimene, 4aα, 7α, 7aβ-nepetalactone. The total phenol and flavonoid content of the studied species as well as the antioxidant properties were measured using DPPH reagent.

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Adsorption of crystal violet onto PVA-carrageenan/MMt nanocomposite

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Keywords: Hydrogel, Nanocomposites, Montmorillonite, Swell, Polyvinyl alcohol, Crystal violet

Currently, wastewater treatment due to loss of water resources, increasing waste and other hazardous materials has become a serious problem. The ultimate goal of environmental protection, the wastewater treatment by methods appropriate to the health of humans, animals and the environment has been evaluated. Different methods have been used for industrial wastewater treatment. Recently, due to the complexity of these industries and economical purpose, the adsorption method with low cost and ease of utilization has been studied. Introduction of new technologies to increase the availability of clean water is almost fifty years ago. Nanofiltration membranes were developed during the 1970s and 1980s. In the membrane process, using different types of membranes for drinking water production from seawater, brackish and saline water, wastewater, surface water and groundwater has expanded rapidly. The interaction of mineral powders with reactive site of natural polymers and monomers result in a superabsorbent composite. Superabsorbent composites based on synthetic polymers or natural polymers have been reported.

In this paper, we investigated the synthesis of nanocomposites based on poly (vinyl alcohol) in the presence of montmorillonite powder using carrageenan. The nanocomposite structure was confirmed using FTIR spectroscopy and the morphology of the samples was examined by scanning electron microscopy (SEM). The influence of the parameters, which can be altered gelation time as a parameter for assessing the optimal level of the resultant nanocomposites was investigated in details. The resulting nanocomposite was examined to remove cationic crystal violet dye from water. It was revealed that the by inclusion of montmorillonite nanoclay, the dye adsorption content of nanocomposite hydrogel (NH) was similar as clay-free hydrogel (H). But the rate of dye adsorption was increased.

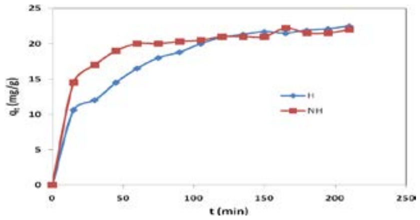

Fig. 1 Effect of contact time on the dye adsorption of hydrogel and nanocomposite hydrogel (adsorbent dose: 50 mg; volume of dye solution: 50 mL; Dye concentration: 25 mg/L)

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DFT geometry analysis of methylpentynol-azide H-bonding arrays to investigate H-bonding potential in regioselective 1,3-DC reactions

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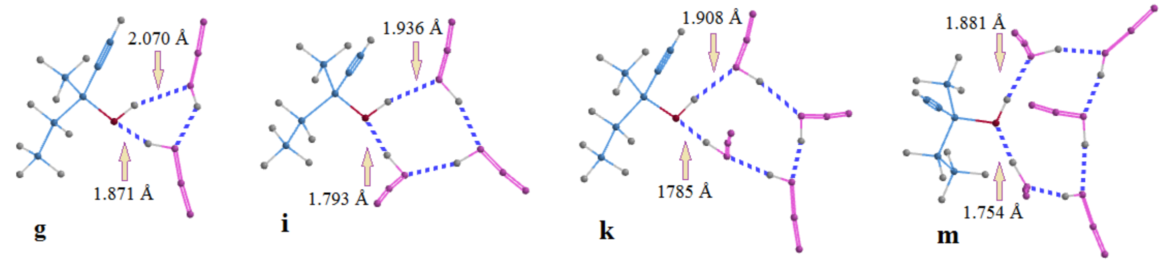
Keywords: H-Bonding Array, Cluster media, DFT/B3LYP/6-31G* method.

This study was focused on the geometries and properties of the structural isomers obtained from a random walk of the methylpentynol-HN$_3$ clusters. A-H$^{\delta+}$…:B form was applied to represent the isolated hydrogen bond in the HBNs.[1] Recently, extensive studies have been performed on the alcohol cluster structures,[2] which notably directs researchers' attention towards the clusters of different alcohols.[3] The obtained research data on the regioselectivity performance of 1,3-DC reactions have not been reported by using H-bonding array with a topology of the cluster. Here in, regioselectivity has reached by ‘‘silico modeling’’ via hydrogen-bonding networks (HBNs). The calculate method of B3LYP levels with the 6-31G* basis sets were applied to receive all structures’ geometries; and also the energy levels of the methylpentynol (**a**) as a dipolarophile and azide (**b**) as 1,3-dipoles, H-bonding arrays (**c-e**), and the methylpentynol-HN$_3$ clusters (**f-m**) were calculated and obtained by this method.

The H-bond lengths (Å) and angle (º) of N-H**…:**O and O-H**…:**N in **g**, **i**, **k** & **m** arrays (These H-bonded arrays are converged in the circular frame, which topology of them is shown in Figure below.).

Cluster	H-bond length of N-H**…:**O (Å)	H-bond length of O-H**…:**N (Å)	Angle of N-H**…:**O (º)	Angle of O-H**…:**N (º)
g	1.871	2.070	154.98	146.97
i	1.793	1.936	168.91	163.51
k	1.785	1.908	172.16	169.18
m	1.754	1.881	166.05	176.62



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Hydrogen bonding topology properties of methylpentynol and pargyline interaction with azide by DFT calculations

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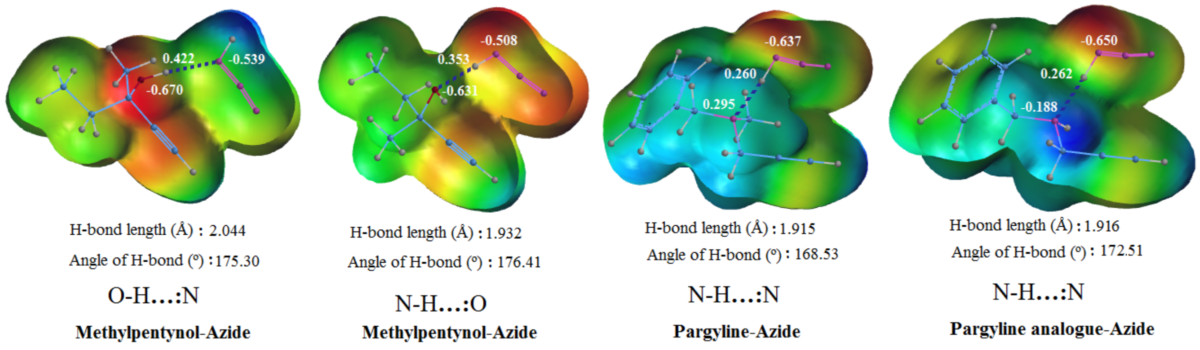
Keywords: H-Bonding Array, Hydrogen bond, DFT/B3LYP/6-31G* method.

The hydrogen bond strength and geometry is influenced by hydrogen acceptors.[1] Furthermore, the molecular environments and atoms hybridation are effective on the hydrogen bonding capabilities.[2] Recent studies of the hydrogen bonding are focused on water, alcohols, and homologues of them; which can form lots of attractive arrays.[3] In this study, methylpentynol and pargyline were chosen as hydrogen bond donor with different hydrogen acceptors (oxygen and nitrogen). However, in the case of pargyline, which hydrogen acceptor is nitrogen, the molecule is a third-degree amine. So, to have fairly matched conditions, analogue of pargyline with hydrogen instead methyl group was investigated too. Analyses of these data can help researchers to make more targeted reactions, for example regiochemical outcome on the 1,3-DC reactions is one of those assistance. All structures' geometries were optimized by DFT/B3LYP/6-31G* method.



H-bond length (Å) : 2.044
Angle of H-bond (°) :175.30
O-H…:N
Methylpentynol-Azide

H-bond length (Å) : 1.932
Angle of H-bond (°) : 176.41
N-H…:O
Methylpentynol-Azide

H-bond length (Å) : 1.915
Angle of H-bond (°) : 168.53
N-H…:N
Pargyline-Azide

H-bond length (Å) : 1.916
Angle of H-bond (°) : 172.51
N-H…:N
Pargyline analogue-Azide

Fig. 1 Electrostatic potential map of H-bonding arrays (Electrostatic charges of participating atoms in H-bonds were shown) & H-bond lengths (Å) and angle of H-bonds (°)

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Biomimetic supramolecular nanostructures based on polycaprolactone and nanosized calcium phosphate

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Keywords: Supramolecular polycaprolactone, Ureidopyrimidinone, calcium phosphate, Quadruple hydrogen-bonding, Bone tissue.

Nanocomposites based on polycaprolactone (PCL) and calcium phosphate (CaP) have recently been proposed for applications in bone repair and regeneration.[1,2] However, very limited studies have investigated the fabrication of 3D porous composites using the supramolecular PCL. Hence, in this study, ureidopyrimidinone groups (Upy) was first synthesized using 1,6-hexamethylene diisocyanate and 2-amino-4-hydroxy-6-methyl pyrimidine and then PCL with $\overline{M}_n$= 2000 g/mol and CaP with spherical morphology was functionalized by the as-synthesized Upy groups. Presence of UPy in the polymer structure was subsequently determined by Fourier-transform infrared (FTIR) spectroscopy according to the characteristic peaks observed at 1450 cm^{-1}–1690 cm^{-1}. Moreover, modification of CaP with UPy groups was again confirmed by FTIR; the NCO in UPy (2275 cm^{-1}) completely disappeared and the peaks at 1645, 1668, and 1697 cm^{-1} indicated the formation of a urethane linkages. The resulting modified CaP (CaPUPy) was finally conjugated with the supramolecular polymer to fabricate a new PCLUpy$_2$/CaPUpy nanocomposite. The results showed that mechanical properties can be significantly increased by incorporating appropriate orientation of hydrogen bonds in the supramolecular structure (Fig. 1). Accordingly, the nanocomposites reported here may provide a new opportunity to create supramolecular structures based on the reversible assemblies for the applications in bone tissue regeneration.

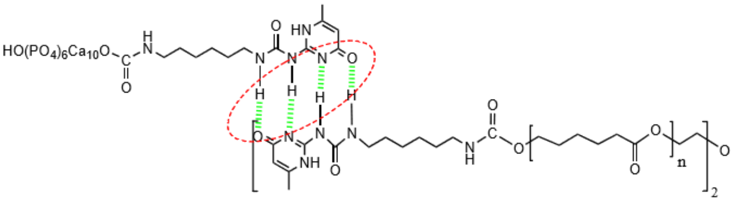

Fig. 1 Quadruple hydrogen bonding in supramolecular nanocomposite

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Application of design of experimental (DOE) for the synthesis of supramolecular polyesters

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***Keywords**:* Supramolecular polycaprolactone, Ureidopyrimidinone, Hydroxyapatite, Quadruple hydrogen-bonding, Design of experiments.

Design of experiments (DOE) is defined as a branch of applied statistics deals with planning, analyzing, and interpreting controlled tests to evaluate the parameters that control the value of a factor or group of factors. It allows for multiple input factors to be manipulated and finally to determine their effect on a desired output (i.e. response).[1] Hence, the aim of this study was to investigate the influence of reaction parameters on the properties of supramolecular polycaprolactone (PCLUPy$_2$) scaffolds according to a DOE approach. For this, Taguchi method was used to evaluate the statistically influential factors among those described in the literature for obtaining optimum conditions. The role of each experimental parameter was also discussed according to the degree of hydrogen bonds formation of quadruple motifs and the cooperative mechanism.[2] The results showed that among the selected variables, reagent ratio and solvent type were the most significant factors affecting the modification degree and hence the mechanical properties of the as-synthesized PCLUPy$_2$. This approach is therefore expected to provide opportunities to create a supramolecular assembly with a significantly higher mechanical strength in comparison with those reported in literature.

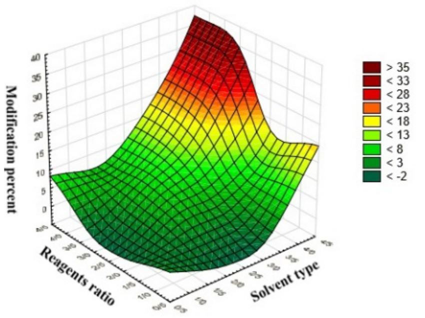

Fig. 1 Surface response of modification percent as a function of reagent ratio and solvent type.

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Synthesis of some heterocyclic compounds bearing nitrogen atom using magnetite nanoparticles supported on γ-$Al_2O_3/BF_3/Fe_3O_4$ under different conditions

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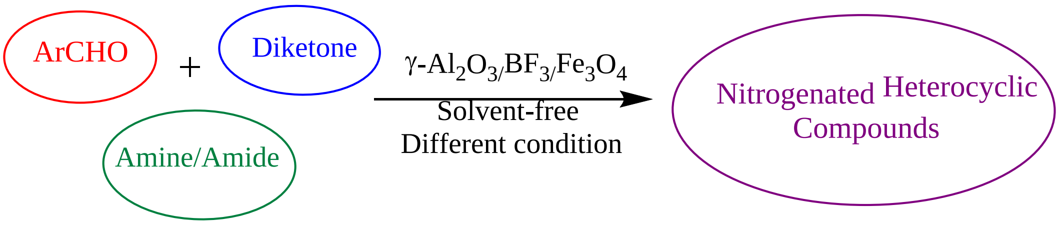
Keywords: Multicomponent reactions, Green chemistry, magnetite nanoparticle, γ-Al_2O_3/BF_3

In recent years, using nano-size solid acids in chemical reactions have been known as a principle in the development of green chemistry. The efficiency of heterogeneous and magnetite catalysts can be enhanced using nanosized catalysts because of their extremely small size and large surface to volume ratio and act as a bridge between homogeneous and heterogeneous catalysts.[1] On the other side, heterocyclic compounds containing nitrogen have received much attention for their biological activities and the extensive application in both pharmaceutical and industrial researches.[2] Therefore, the widespread application of solid acids, and magnetite nanoparticles structural and practical diversity of heterocyclic compounds containing N atom have prompted us to employ the novel and eco-friendly methods for the synthesis of heterocyclic compounds including: Indazolo-phthalazine-triones[3], 2,3-dihydro-1*H*-perimidines[4], Quinazolines[5], and Dihydropyrazines[6] using nano γ-$Al_2O_3/BF_3/Fe_3O_4$ as a green magnetite catalyst under different conditions. Firstly, nano γ-$Al_2O_3/BF_3/Fe_3O_4$ were prepared (Scheme 1). Its structure and properties were characterized through the conventional methods of determining materials such as FE-SEM, TEM, FT-IR, XRD, BET, VSM, and TGA. Then, the catalyst was used in the synthesis of some heterocyclic compounds bearing N atom. The obtained products have been characterized by FTIR, ^{1}H NMR, and ^{13}C NMR spectroscopy.



Scheme 1

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The first principle computational study for the comparison experimental and theoretical result for 2*H*-Indazolo[2,1-*b*]phthalazine-triones

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Keywords: Green reactions, Density functional theory, B3LYP/6-31G* method, Solvent-free, Molecular modeling

Experimental and computational studies in the synthesis of 2*H*-Indazolo[2,1-*b*]phthalazine-triones using γ-$Al_2O_3/BF_3@Fe_3O_4$ as a nanocatalyst under mild and solvent-free conditions were carried out.[1] The most important features of the present protocol are the easy preparation of the catalyst, short reaction times and environmentally benign, milder reaction conditions.[2,3] Also, the 2*H*-Indazolo[2,1-*b*]phthalazine-triones have been theoretically investigated by DFT-B3LYP/6-31G* method. The band gap of HOMO–LUMO orbitals, FT-IR and 1HNMR spectra, Electrostatic and Mulliken charge have examined for conformers of products.[4]

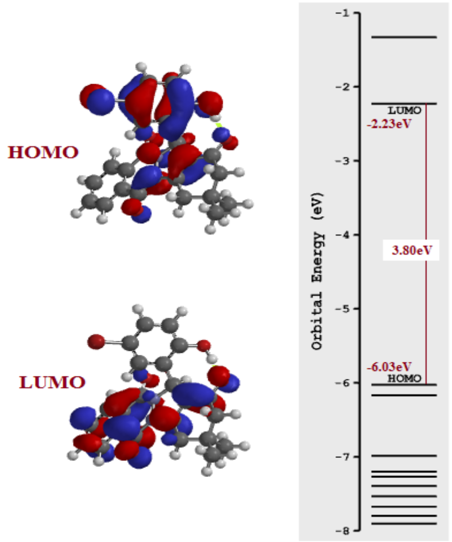

Fig. 1 Calculated HOMO–LUMO band gap ($\Delta E_{HOMO-LUMO}$) of the 3,4-dihydro-3,3-dimethyl-13-(2-hydroxy-5-bromophenyl)-2*H*-indazolo[2,1-*b*]phthalazine-1,6,11(13*H*)-trione

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Design and preparation of easily recycled Fe_3O_4@SiO_2@layered Zinc hydroxide as a highly efficient heterogeneous catalyst in Aza-Michael Addition

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Keywords: Layered Zinc hydroxide, Aza-Michael Addition, Tetrazole, Magnetic catalyst

The synthesis of tetrazoles has a special interest because of their broad biological activities.[1] The conjugate addition of heteroatom nucleophiles to α, β-unsaturated carbonyl compounds (i.e., Michael reaction) is one of the most important tools in organic synthesis for the construction of tetrazole derivatives.[2] In this study, Fe_3O_4@SiO_2@layered zinc hydroxide (LZH) nanoparticles as an efficient and novel catalysis system were synthesized and applied in Aza-Michael Addition. The catalytic activity of the catalyst was studied for the preparation of the new tetrazoles by the reaction of 5-substituted tetrazoles derivatives with cyclohex-2-eneone under reflux in acetonitrile. Therefore, this catalyst could be recycled and reused at least 5 times without significant loss of its activity.

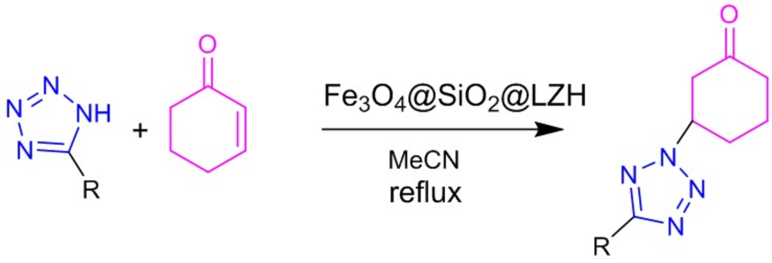

Fig. 1 Fe_3O_4@ SiO_2@LZH catalysed the aza-Michael reaction of 5-substituted tetrazoles with cyclohex-2-eneone

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Multicomponent synthesis of new derivatives of thiazolidine-4-ones in the presence of bis ionic liquid DABCO-diactate as a green media

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Keywords: Multicomponent reactions, ionic liquid, azo-thiazolidine-4-one

Thiazolidine -4-ones exhibit antitubercular, antimicrobial, antioxidant and antifungal activity and can be applied as COX-1 inhibitor, bacterial enzyme MurB inhibitor, non-nucleozide anzyme inhibitor of HIV-RT and antihistaminic agent[1] For this reason, synthesis of novel derivatives of thiazoline-4-ones have attracted a lot of interest. A multi-component reaction (MCR) can create highly complex molecules from readily available starting materials without complicated purification operations. Thus, MCRs are identified as time-effective, money saving, energy and raw material saving and economically favorable processes in diversity generation. They have benefits due to the creation of several new bonds in a one-pot reaction, a low number of reaction and purification steps, selectivity, synthetic convergence, high atom economy, simplicity and synthetic efficiency.[2] On the other hand, ionic liquids are suitable alternative instead of toxic solvents and volatile chemicals in the chemical and pharmaceutical industries, due to their proper emission and conductivity, thermal stability, reparability and recovery, high polarity and environmental friendliness and used as the green catalyst for organic reactions.[3]

In continuation of our previous work[2,3], herein, we specifically address the synthesis and usage of bis ionic liquid 1,4-diazabicyclo[2.2.2] octanium diacetate as an environmentally friendly green media for the synthesis of azo-thiazolidine -4-ones.

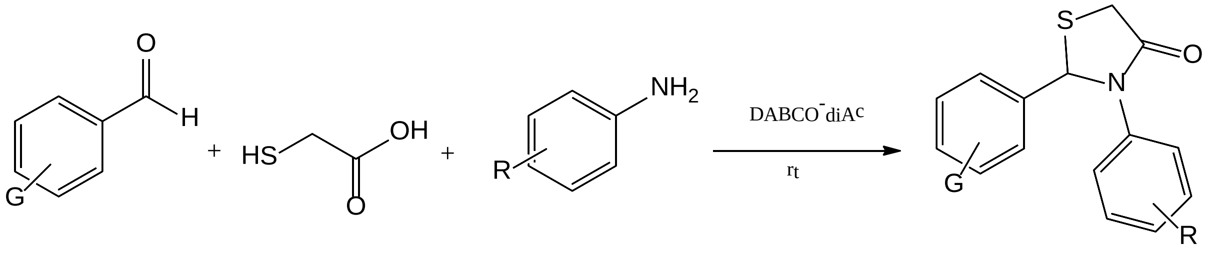

Fig. 1 Multicomponent synthesis of azo-thiazolidine-4-ones

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Preparation of MgO/SiO_2 nanoparticles as a base catalyst for synthesis of 1*H*-isochromenes

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Keyword: Nanocatalyst, 1*H*-Isocromene, Cyclohexanone, Malononitrile, Benzaldehyde.

The 1*H*-isochromene derivatives have an exceptional structural which appear in numerous natural and non-natural products[1]. 1*H*-isochromenes were represented as “advantaged structure” in various medicinally compound such as; their application as antitumor[2]. Some of these natural compounds are Dendrobium amoenum, Coelogyne Faccida and Faccidin that separated from the orchids[3,4].

In this study, we prepared the MgO/SiO_2 heterogeneous base nanocatalyst in several steps. Then, this nanostructure applied as a nanocatalyst for the synthesis of 1*H*-isocromenes from cyclohexanones, malononitrile and benzaldehyde in the ethanol solvent under mild conditions. In this reaction, the target products were obtained in excellent yields and short reaction times. At the end of the reaction, the nanocatalyst separated with simple filtration and reused in the other reactions.

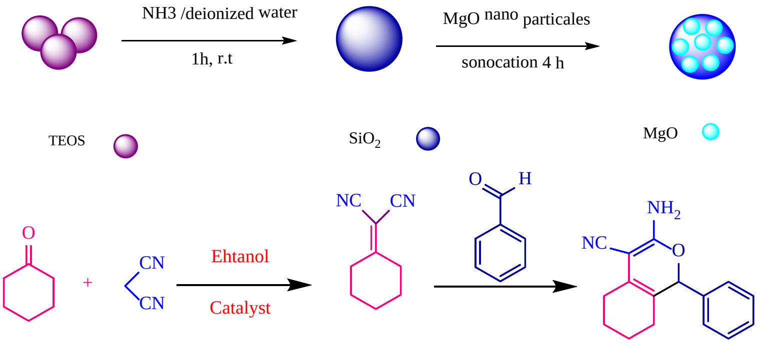

Fig. 1 Synthesis of 1*H*-isochoromene derivatives catalyzed by nano MgO/SiO_2

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Synthesis of a new superabsorbent copolymer Based on carboxymethylated polyvinyl alcohol

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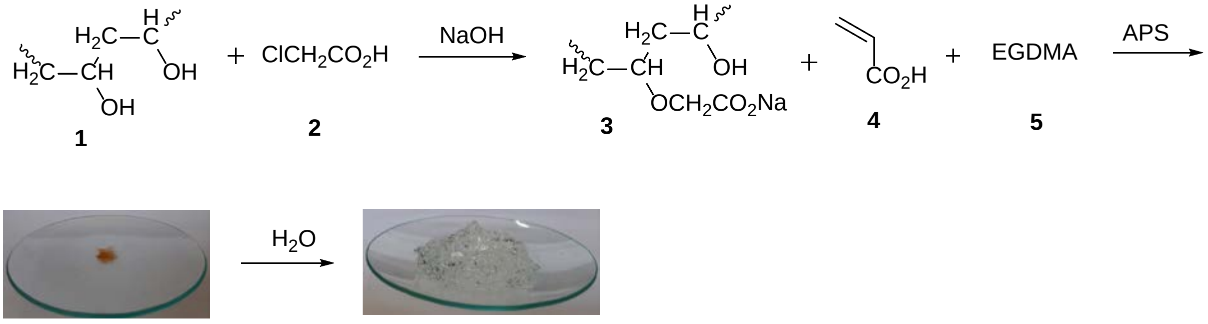
Keywords: Superabsorbent, Polyvinyl alcohol, Acrylic Acid, free radical polymerization.

Superabsorbent polymer (SAP) materials are hydrophilic crosslinked networks that can absorb large quantities of water or aqueous solutions and hold it even under pressure. They can uptake water many hundred times more than their dry weight.[1] Synthetic, semi-synthetic, or natural polymers are used separately or in combination for the synthesis of superabsorbent polymers.[2] In this research, a new superabsorbent copolymer **6** was synthesized based on the polyvinyl alcohol (PVA) **1**. For this purpose, firstly, the carboxymethyl polyvinyl alcohol **3** was synthesized by reaction of the polyvinyl alcohol **1** and the monochlroroacetic acid **2** in basic conditions. Then the acrylic acid **4** was grafted on the carboxymethyl polyvinyl alcohol **3** via free radical polymerization in the presence of ethylene glycol dimethacrylate **5** as a crosslinking agent. This superabsorbent polymer **6** can uptake water approximately three hundred times more than its dry weight. The synthesized copolymers were characterized by spectroscopic methods.



6 (The dry state) **6** (The swollen state)

Fig. 1 Overall procedure for synthesis of superabsorbent based on PVA

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Green synthesis of palladium nanoparticles and their catalytitc performance in acyl free copper sonogashira coupling

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Keywords: Green synthesis, Palladium nanoparticles, Tannic acid, Sonogashira coupling reaction, Multicomponent reaction.

The green synthesis of metal nanoparticles (MNPs) has made a broad spectral progress in recent times due to their novel electronic, chemical, catalytic, magnetic and optical properties.[1] The Sonogashira coupling reaction of terminal alkynes with acyl halides provides a powerful and versatile method for preparing ynones, which has been widely applied to multicomponent syntheses of heterocycles.[2] In this research, we investigated a one-step green method to generate nanoparticles of palladium (PdNPs) from palladium chloride ($PdCl_2$) by using polyphenolic compound: Tannic acid as a reducing and stabilizing agent. PdNPs were characterized by ICP-AES elemental analysis, UV-visible, XRD, EDX and SEM analaysis. The synthesized PdNPs@tannic acid was used as nanocatalyst in ligand and copper free Sonogashira coupling reaction under aerobic condition in order to multicomponent synthesis of heterocycles via ynones as intermediate. Typically, the coupling of benzoyl chloride **1** and phenylacetylene **2** in the presence of PdNPs@tannic acid gives 1,3-diphenylprop-2-yn-1-one **3** and followed by the reaction of **3** with 3-chloro phenylhydrazine hydrochloride **4** under basic condition produced 1-(2-chlorophenyl)-3,5-diphenyl-1*H*-pyrazole **5** (Figure **1**). The structure of product was confirmed by ^{1}H NMR and FT-IR spectroscopy.

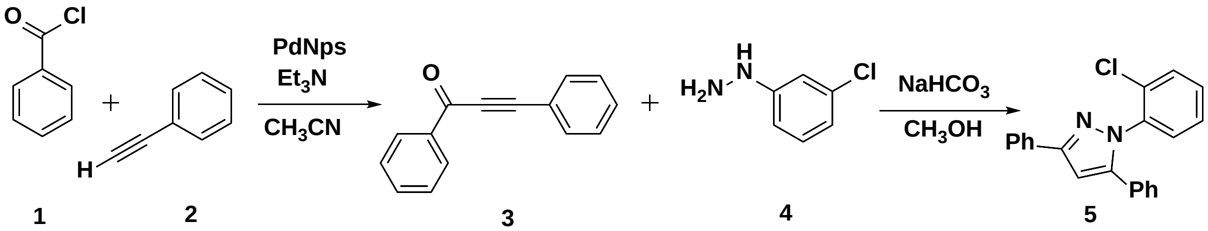

Fig. 1 Multicomponent synthesis of substituted pyrazole

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Green synthesis of novel 1,3-oxazine-2-thiones using NiFe$_2$O$_4$@amino glucosyl-SiO$_2$ as a recyclable catalyst

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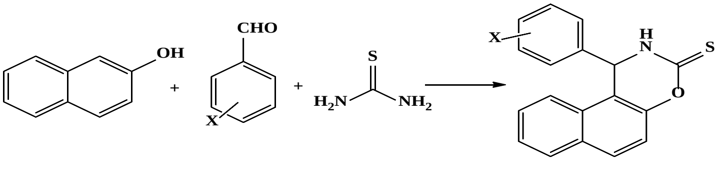
Keywords: Oxazine, Synthesis, Green reaction, Nano catalyst

The synthesis of 1,3-oxazine-2-thiones has attracted attention in the past because of their potential as antibiotics, antitumor, analgesics and anticonvulsants. One present significant area of new synthetic chemistry is the expansion of effective workable procedures that diminish the necessary reagents, solvents, cost time and separation courses for the preferred conversion and also minimize the creation of waste.[1,2] Multi-component reactions (MCRs) are powerful tools in modern medicinal chemistry, enabling straightforward access to large libraries of structurally related, drug-like compounds and thereby facilitating the generation of lead candidates compounds. Hence, combined with the use of combinatorial chemistry and high throughput parallel synthesis, such reactions have constituted an increasingly valuable approach to drug discovery efforts in recent years. On the other hand, nanostructures as efficient catalysts have been used in various organic catalytic reactions. Among the numerous metal oxides, Fe_3O_4 and $NiFe_2O_4$ have attracted most interest due to its special properties. Although iron oxide particles surface exhibits both Lewis acid and base properties, the nature of metal cation and surface area of the metal oxides have extensively amplified their catalytic properties. The reactivity of Fe_3O_4 and $NiFe_2O_4$ has been shown to increase greatly as their dimensions are reduced and they may undergo rapid biodegradation when exposed directly to biological systems. Suitable coating is essential to prevent such limitation. [3,4] In continuation of our research for the green synthesis of organic compounds, [3-6] we describe here synthesis and the use of acidic amino glucose-functionalized silica- coated $NiFe_2O_4$ nanoparticles ($NiFe_2O_4$@amino glucosyl-SiO_2) as a green, reusable and effective nano catalyst for the synthesis of 1,3-oxazine-2-thiones (Scheme 1). The structures of the synthesized 1,3-oxazine-2-thiones were confirmed by ^1H, ^{13}C NMR and FT-IR spectral data and elemental analyses.



Scheme 1. Multicomponent synthesis of 1,3-oxazine-2-thiones

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One pot synthesis of 4,6-diphenylpyrimidin-2(*1H*)-ones using of $NiFe_2O_4$@amino glucosyl-SiO_2 as a recyclable catalyst

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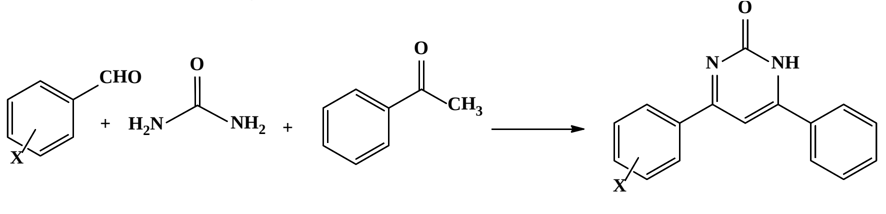
Keywords: Pyrimidine, Synthesis, Green reaction, Nano catalyst

The synthesis of arylpyrimidin-2(*1H*)-ones has attracted attention in the past because of their potential as anti-cancer, anti-microbial, anti-malarial, diuretic, anti-biotic, anti-hypertensive, anti-tubercular and anti-fungal anti-hypertensive and anti-viral activities One of the most widely used methods for the synthesis of diaryl-substituted pyrimidine-2(1H)-ol/-thiol derivatives involves starting from chalcone by cyclization with urea and thiourea. Chalcones are natural compounds and important precursors for the synthesis of many biologically active compounds.[1-3] Hence, combined with the use of combinatorial chemistry and high throughput parallel synthesis, such reactions have constituted an increasingly valuable approach to drug discovery efforts in recent years. On the other hand, nanostructures as efficient catalysts have been used in various organic catalytic reactions. Among the numerous metal oxides, Fe_3O_4 and $NiFe_2O_4$ have attracted most interest due to its special properties. Although iron oxide particles surface exhibits both Lewis acid and base properties, the nature of metal cation and surface area of the metal oxides have extensively amplified their catalytic properties. The reactivity of Fe_3O_4 and $NiFe_2O_4$ has been shown to increase greatly as their dimensions are reduced and they may undergo rapid biodegradation when exposed directly to biological systems. Suitable coating is essential to prevent such limitation. [4,5] In continuation of our research for the green synthesis of organic compounds, [4-7] we describe here synthesis and the use of acidic amino glucose-functionalized silica- coated $NiFe_2O_4$ nanoparticles ($NiFe_2O_4$@amino glucosyl-SiO_2) as a green, reusable and effective nano catalyst for the synthesis of arylpyrimidin-2(*1H*)-ones (Scheme 1). The structures of the synthesized arylpyrimidin-2(*1H*)-ones were confirmed by ^{1}H, ^{13}C NMR and FT-IR spectral data and elemental analyses.



Scheme 1. Multicomponent synthesis of arylpyrimidin-2(*1H*)-ones

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The effect of TiO_2 nanoparticles with different coating on the structure of DNA

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Keywords: Coated-Nanoparticles, DNA, Ethylene glycol, Ethanol, Titanium Dioxide Nanoparticles.

Over the past few years, nanoparticles (NPs) have become more and more significant for applications in biomedicine and bio-pharmacy.[1]Among the semiconductor nanoparticles, titanium dioxide nanoparticles (TiO_2NPs) has been utilized most broadly in the nanotechnology and medical industry due to its anti-rust and anti-tumor activities. It is currently believed that TiO_2NPs could be used as a medical agent.[2,3] Due to the advantages of TiO_2NPs in nanotechnology, the aim of this study is to evaluate the effects of ethylene glycol and ethanol coating on TiO_2NPs interaction with DNA by fluorescence spectroscopy, circular dichroism (CD) spectroscopy and zeta potential studies. The fluorescence data and binding constants showed that ethylene glycol-coated TiO_2NPs could interact with DNA more strongly and make structural changes compare with ethanol-coated TiO_2NPs. CD studies and zeta-potential analysis also confirmed the structural variations of DNA after interaction with ethylene glycol-coated TiO_2NPs strongly. Totally, the interaction of ethylene glycol-coated TiO_2NPs with DNA generated distinct DNA conformation variations. The results obtained from this study proffer a good strategy for designing new drugs and standardization in nanotechnology.

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Synthesis, characterization and antitumor activity of new Cu(II) mixed ligand coordination polymers at bulk-size and nanopowders

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Keywords: Coordination polymer, Nanopowders, Antitumor activity.

New cupper(II) mixed ligand coordination polymer at bulk and nanopowders [$Cu_3(\mu_3$-$BTCA)_2(Pyr)_3.3(H2O)]n$ [BDCA = Benzene 1,3,5-tree carboxylic acid and Pyr = Pyridine], has been synthesized by the reaction of a mixture Cu(II) acetate and BDCA in pyridine/water by simple branched tube and sonochemical method. The nanopowders of CuO was prepared from the calcinations of the NCP at air atmosphere. The structure of the CP and NCP (CP = Coordination polymers and NCP = Nano coordination polymers) were determined by X-ray crystallography, while nano-structural materials were characterized by X-ray powder diffraction (XRPD), thermal gravimetric analysis (TGA) and scanning electron microscopy (SEM). These binary complexes (CP and NCP) were tested in vitro as potential antitumor agents with Human Embryonic Kidney 293 cells. It was observed that the most stable NCP and CuO nanopowders exhibited a high antitumor activity respectively.

$$\mathrm{Cu(OAC)_2 + BTCA} \rightarrow$$

$$\rightarrow \begin{cases} \xrightarrow{\mathrm{(PYR/H_2O)\ in\ Branched-Tube}} \\ \qquad \mathrm{\{Single\ Crystal\ of\ [Cu_3(\mu^3 - BTCA)_2(PYR)_3.3(H_2O)]_n} \\ \xrightarrow{\mathrm{Ultrasond\ Irradiation + PYR/H_2O}} \mathrm{\{Nanoscale\ of\ [Cu_3(\mu^3 - BTCA)_2(PYR)_3.3(H_2O)]_n} \rightarrow\rightarrow \\ \qquad \xrightarrow{\mathrm{Calcination\ at\ 500-600^{\circ}C}} \mathrm{Nanoparticle\ of\ CuO} \end{cases}$$

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Sodium cyclamate-catalyzed expeditious and sustainable synthesis of 6-amino-5-cyano-3-methyl-4-aryl-1,4-dihydropyrano[2,3-*c*]pyrazoles

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Keywords: Aryl aldehyde, Green synthesis, Pyrano[2,3-*c*]pyrazole, Sodium cyclamate.

Pyrano[2,3-*c*]pyrazoles represent an important class of fused heterocyclic ring systems largely present in natural and synthetic organic compounds.[1] Several pyrano[2,3-*c*]pyrazole derivatives have been reported and they shows numerous biological properties, such as anti-inflammatory, analgesic, anti-bacterial, anticancer, vasodilator, antioxidant, antifungal, anti-microbial, inhibitory on human Chk1 kinase, antimalarial, hypoglycemic, hypotensive, insecticidal and molluscicidal activities.[2] They also find the applications in biodegradable agrochemicals and pharmaceutical ingredients.[3] Herein, we report an efficient synthesis of 6-amino-5-cyano-3-methyl-4-aryl-1,4-dihydropyrano[2,3-*c*]pyrazoles (**5a-n**) *via* four-component cyclocondensation of substituted benzaldehydes (**1a-n**), hydrazine hydrate (**2**), malononitrile (**3**), and ethyl acetoacetate (**4**) at 50 °C in the presence of catalytic amounts of an organocatalyst sodium cyclamate in water as medium. The structure of synthesized heterocycles characterized using melting points, ^{1}H and ^{13}C NMR and IR spectroscopic data.

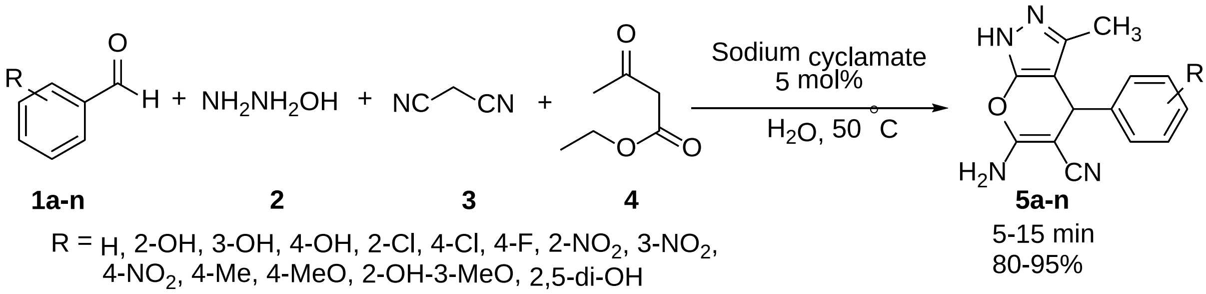

Fig. 1 Sodium cyclamate-catalyzed synthesis of 6-amino-5-cyano-3-methyl-4-aryl-1,4-dihydropyrano[2,3-*c*]pyrazoles

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Synthesis of 1,4-dihydropyridine derivatives in the presence of MNPs-trypsin as a biocatalyst.

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Keywords: 1,4-Dihydropyridine, MNPs-trypsin biocatalyst, Green chemistry, Enzyme

eworthy1,4-Dihydropyridine (1,4-DHP) ring is a challenging structural core in organic chemistry due to its biological properties, especially as calcium channel blockers. It is noteworthy that its range of application has been recently extended to other affections such as antioxidant, antidiabetic and antitumor agents.[1] A rapid, efficient and eco-friendly protocol has been developed for the preparation of various 1,4-dihydropyridine derivatives in the presence of biocatalyst. The process presented here is operationally simple, environmentally benign and has excellent yield. Furthermore, the biocatalyst can be recovered conveniently and reused efficiently.[2] For preparing the MNPs-trypsin biocatalyst, we first synthesized Fe_3O_4 magnetic nanoparticles (MNPs). Trypsin was then immobilized on the magnetic core-shell particles by using glutaraldehyde as a cross-linker.[3] We used this synthesized MNPs-trypsin biocatalyst in the reaction of 1,4-DHP and the results were amazing. Moreover, the ^1H and ^{13}C chemical shift and X-ray spectra values together with the structural parameters of 1,4-dihydropyridine have been computed and the scaled values have been compared with the corresponding experimental NMR and X-ray spectra. As a result, the calculated ^1H and ^{13}C chemical shift and X-ray spectra show a good agreement with the experimental results.

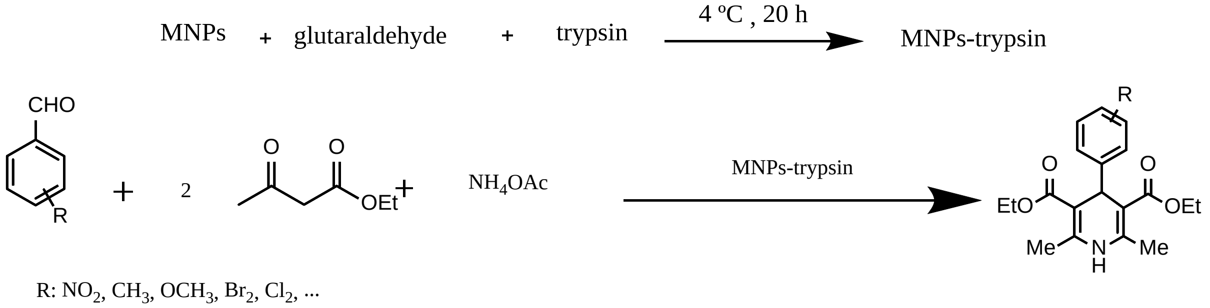

Fig. 1 Synthesis of 1,4-dihydropyridine derivatives in the presence of MNPs-trypsin as a biocatalyst.

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Synthesis and X-ray crystal structure of a new macrocyclic Schiff base ligand containing thiocarbonohydrazide unit

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Keywords: Thiocarbonohydrazide, Macrocyclic Schiff base ligand, Diamine.

Schiff base complexes have remained an important and popular area of research due to their simple synthesis, versatility and divers range of applications.[1] Schiff base condensations have long been used to form macrocyclic ligands from diamines and dicarbonyl compounds.[2] In this work, macrocyclic ligand (L) has been synthesized from thiocarbohydrazide and 2-[2-(2-formylphenoxy)propoxy]benzaldehyde. The new macrocycle was characterized by elemental analysis, MS, IR, ^{1}H and ^{13}C NMR spectroscopy and the structure of ligand was determined by a X-Ray crystallographic procedure and shows [2+2] cyclodondensation (Fig 1). In the IR spectrum of ligand a band at about 1603 cm^{-1} indicated the formation of C=N bonds, no peaks attributed to NH_2 and carbonyl groups implied that the condensation reaction have been completed.

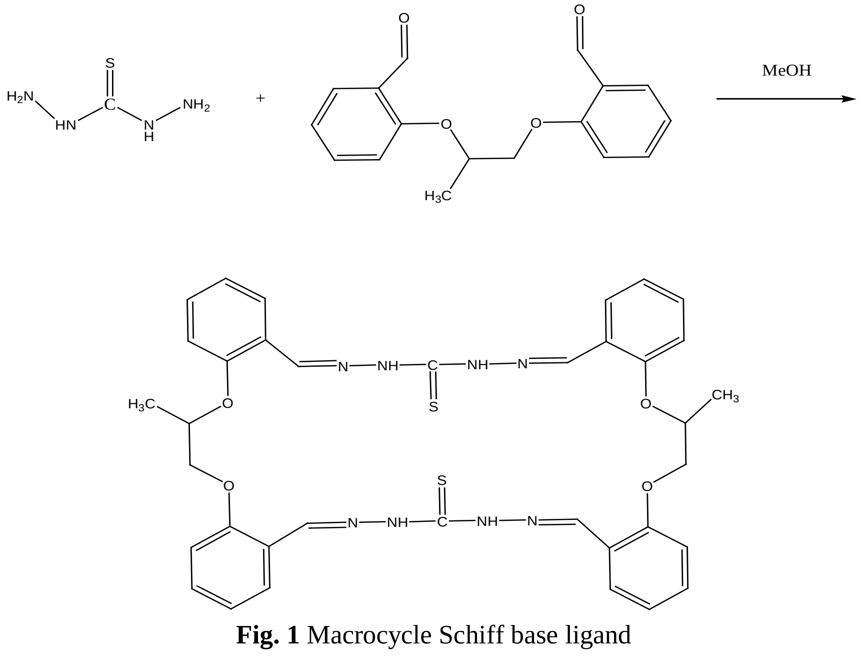

Fig. 1 Macrocycle Schiff base ligand

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Removal of cationic methylene blue dye using magnetically anion–cationic surfactants modified montmorillonite

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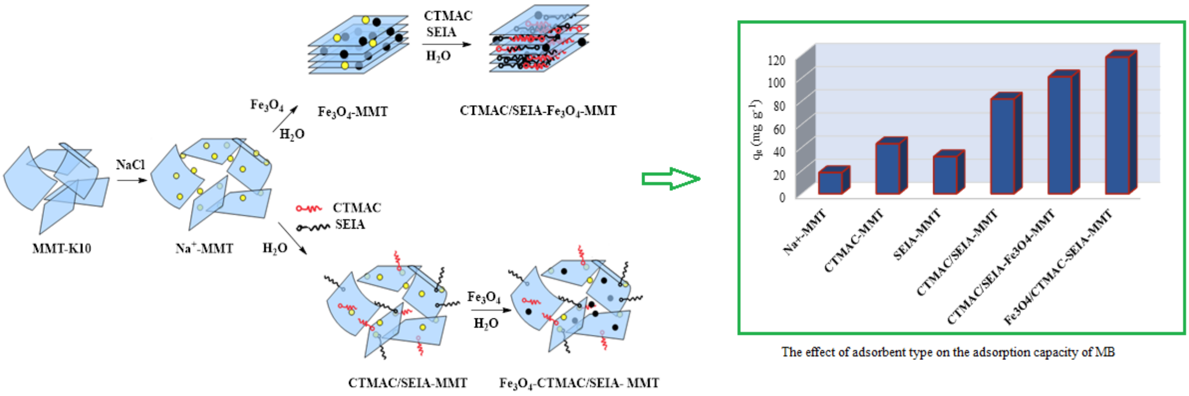
Keywords: Methylene blue, Montmorillonite, Nanocomposite, Removal, Surfactant

Organic dyestuffs in wastewater from many industries including textile, paper, leather, and plastics have been discharged to the environment causing serious soil and water pollution due to biological degradation, high chemical oxygen demand (COD) of the water body and inflected toxicity on humans [1]. Among various dyes, methylene blue (MB) as a toxic cationic dye is difficult to degrade due to its stability to light and oxidation reactions and is often employed as a model dye of organic pollutant [2]. Therefore, the removal of organic dyestuff from wastewater becomes environmentally important. Among the various methods of dye removal, adsorption technique is regarded as one of the ecofriendly and effective method because of simplicity design/operation, high efficiency and harmless to treated water [3]. In this study, we synthesized a novel magnetic organic-inorganic hybrid nanoadsorbent by incorporating anionic surfactant of sodium eicosenoate (SEIA), cationic surfactant of cetyl trimethylammonium bromide (CTMAB) and magnetic Fe_3O_4 nanoparticles into the interlayer of Mt. Subsequently, the modified Mt was used for the removal of MB from aqueous solutions and operational conditions for MB adsorption were studied.



The effect of adsorbent type on the adsorption capacity of MB

Fig. 1 Formation mechanism of CTMAC/SEIA-Fe_3O_4–Mt and Fe_3O_4–CTMAC/SEIA-Mt

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Synthesis of chiral oxazoline based ligands with aliphatic substituents and their application in Kharasch-Sosnovsky reaction

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Keywords: Chiral oxazoline based ligands, Heterogeneous catalysts, Chiral allylic ester, Kharasch-Sosnovsky reaction.

Allylic oxidation of alkenes is one of the most important reactions in organic chemistry, in this reaction double bond is remained unchanged while the second functional group is formed. The stereochemistry of this reaction can be controlled by the use of asymmetric methods.[1] Using chiral catalysts, especially heterogeneous chiral catalysts have drawn a lot of attention among all other methods because they can be separated easily and reused for the production of enantiorich compounds. One way to produce these catalysts is to immobilize chiral ligands onto mesoporous substrates.[2] For this purpose, chiral amino oxazoline ligands such (*S*)-4- isobutyl-4,5-dihydroxazole-2-amine and (*S*)-4-isopropyl-4,5-dihydroxazole-2-amine were synthesized from inexpensive and available amino acids and then immobilized onto Cl- MCM-41. The copper (I) complexes of the obtained chiral heterogeneous ligands were used in asymmetric allylic oxidation of alkenes with perseter as oxidant under different conditions. The chiral allylic esters were obtained in good yields and enantioselectivities.[3]

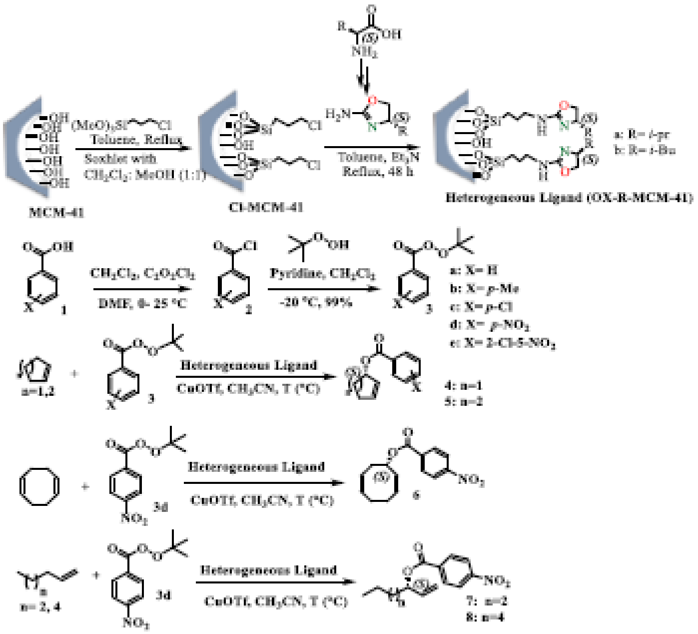

Fig. 1 Asymmetric Kharasch-Sosnovsky reaction in the presence of chiral heterogeneous ligands and CuOTf

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Atrp Fabricated dual sensitive based on pPDMAEMA-PCL-S-S-PCL-pPDMAEMA Triblock Copolymers for cancer targeting cells

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Keywords: ATRP, Bis(2-hydroxy ethyl) disulfide, ring opening polymerization, poly caprolacton, macroinitiator,

ATRP or atom transfer radical addition is one of the most often used synthetic polymerization methods to prepare well-define polymers with complex architecture. **1** functional copolymers prepared by ATRP were used for cancer targeting. **2** Herein, we report the synthesis of pPDMAEMA-PCL-S-S-PCL-pPDMAEMA Triblock Copolymers in three steps as shown in Figure **1**. In the first step, Bis(2-hydroxyethyl) disulfide prepared from oxidation of 2-mercaptoethanol in ETAC in presence of NaI and 30% H_2O_2. **3** In the second step, HO-PCL-ss-PCL-OH was synthesized by ring opening polymerization of ε-caprolactone using cystamine as initiator and tin (II) 2-ethylhexanoate as catalyst . In the third step, pPDMAEMA-PCL-ss-PCL-pPDMAEMA polymers were synthesized using ATRP. The viscous crude solution was purified by precipitation in cold diethyl ether twice and was characterized with IR and 1H NMR .

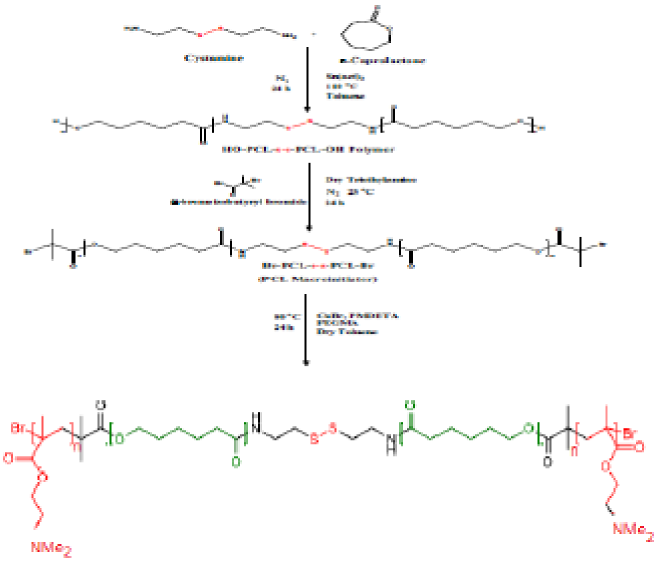

Fig. 1 pPDMAEMA-PCL-S-S-PCL-pPDMAEMA Triblock Copolymer

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Preparation of pH/redox responsive biodegradable poly beta amino esters for anticancer drug delivery

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Keywords: Michael Addition, Isocyanides, Poly(b-amino ester), 4-Amino butanol, Ethylenediamine.

Michael Addition Reaction is one of the most powerful methods in organic synthesis for C–C and C–X (X=O,N, S) bond formation. **1** We synthesized biodegradable poly(b-amino ester) (PBAE) polymers in a 2-step reaction procedure (Fig. **1**). Firstly, Acrylateterminated Poly(b-amino ester) (Acrylate-PBAE) was obtained via the Michael reaction with 1,4-butandial diacrylate and 4-Amino butanol at room temperature without eny solvent and catalyst. **2** In the second step of the reaction, base polymer was mixed with ethylenediamine overnight at room temperature. **3** In the third step, acrylated mPEG react with acrylate-PBAE with Michael type step polymerization successfully. The confirmation of synthesis and the composition of the prepared PBAEs were determined by 1H nuclear magnetic resonance and infrared spectroscopy data.

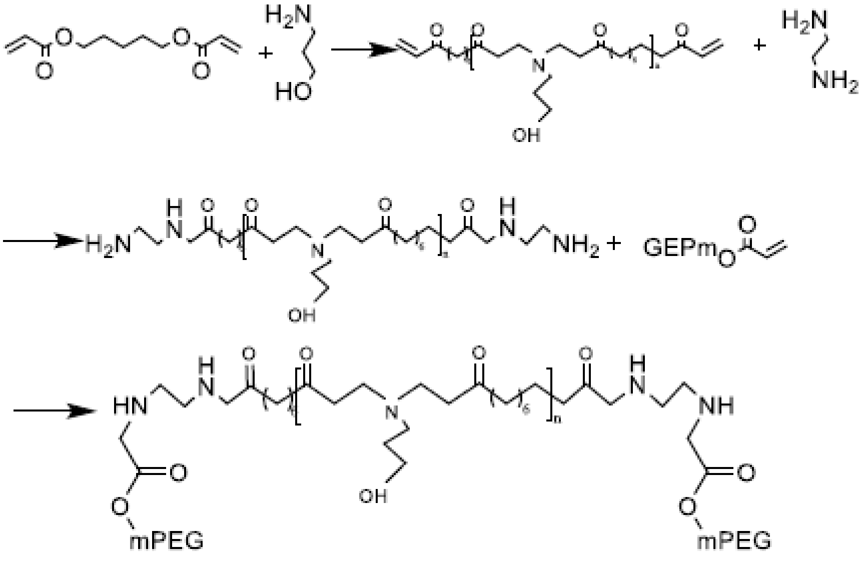

Fig. 1 PBAE synthesis scheme

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A Novel Nanomagnetic Catalyst for the Synthesis of 4*H*-Chromenes

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Keywords: Nanocomposite, Starch, Cross-Link, Iron Oxide, Silver, 4*H*-chromenes.

4*H*-chromene rings are an important class of oxygen heterocyclic that display a broad spectrum of interesting biological activities such as anti-bacterial, anti-cancer, anti-coagulant and anti-proliferative properties [1-4].

Herein, a new Ag/Fe_3O_4@starch nanocomposite was synthesized and used as a efficient catalyst for the synthesis of 4*H*-chromene derivatives using the reaction of benzaldehyde derivatives, malononitrile and cyclo-1,3-diketones (Scheme 1). The method of preparation of this catalyst is simple and has efficiency and short time in synthesis of various chromene derivatives. The remarkable magnetic properties of the nanocomposite made it easy to separate the catalyst from the reaction mixture without significantly reducing the catalytic properties of the nanocomposite.

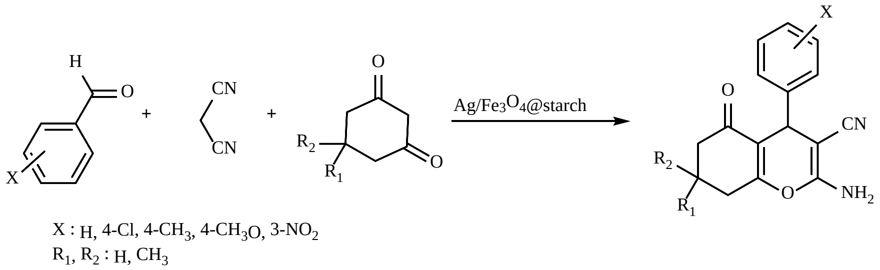

Fig 1. Synthesis of 4*H*-chromene derivatives

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