Abstracts

Natural biopolymers as a green catalyst for the synthesis of 3,4,5-trisubstituted 1,2,4- triazoles derivatives

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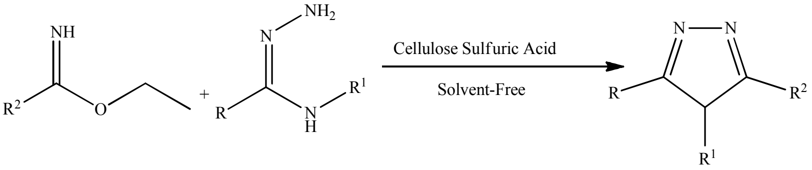
Cellulose sulfuric acid (CSA) has emerged as a promising biopolymeric solid support acid catalyst for acid-catalyzed reactions, such as the synthesis of α-amino nitriles, aryl-14H-dibenzo[a.j]xanthenes, 1,4-dihydropyridines, Pechmann condensation, thiadiazolo benzimidazoles, imidazoazines, quinolines and 3,4- dihydropyrimidine-2(1H)-ones [1, 2].

In general, 1,2,4-triazoles and 1,2,4-oxadiazoles have been attracting attention over the last decade due to their biological activities such as anti-inflammatory [3], antibacterial [4], antitumor [5], and antiviral [6].

We report a simple one-pot method for the synthesis of 3,4,5-trisubstituted 1,2,4- triazoles derivatives from 2,2,2-trichloroethyl imidates in the presence of a catalytic amounts Cellulose sulfuric acid at room temperature (Scheme 1).



Scheme 1

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The green synthesis of 2-amino-4*H*-chromene derivatives using Fe_3O_4-functionalized nanoparticles as a catalyst

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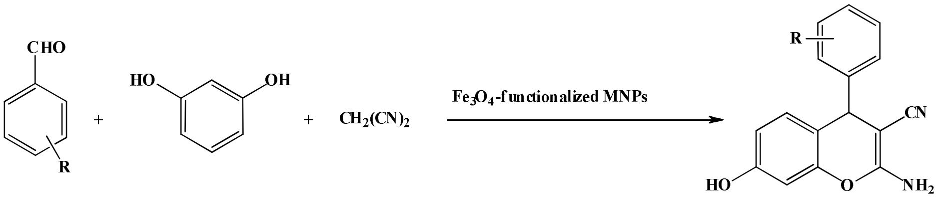
2-amino-4*H*-chromenes are of particular utility as they belong to privileged medicinal scaffolds serving for generation of small-molecule ligands with highly pronounced anticoagulant, and antianaphylactic activities [1]. The current interest in 2-amino-4*H*-chromenes arises from their potential application [2]. Many of the methods reported for the synthesis of these compounds are associated with the use of hazardous catalysts and long reaction time. Thus, development of an inexpensive, and reusable catalyst for MCRs remains an issue of interest.

Magnetic structures are great interest to research for their applications in different fields. After envoloping the Fe_3O_4 with silica, results expanded many applications of silica-coated magnetic Fe_3O_4 particle in chemical, biological and environmental fields [3-5]. Magnetic materials can be removed easily and recycled from the mixture of reaction by an external magnet.

In this study, We first prepared Fe_3O_4 nanoparticles using the massart's method based on the classical coprecipitation. Subsequently, magnetic Fe_3O_4 nanoparticles were fuctionalized. Fe_3O_4-functionalized nanoparticles as the green nanocatalyst were used for the one-pot synthesis of 2-amino-4*H*-chromenes (Scheme 1).



Scheme 1

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Synthesis of novel SBA-16 mesoporous silica functionalized with melamine based dendritic dithiocarbamate to remove Cd^{2+} cations from waste water

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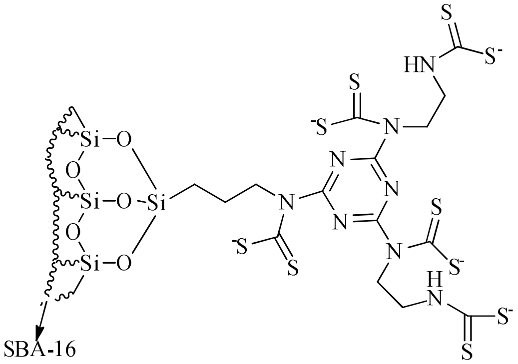
Mesoporous materials especially SBA-type has attracted a great attention for application to remove heavy metal ions from contaminated water for their large pore size, thick pore wall and high stability in harsh conditions [1]. Also, dithiocarbamates, a decent electron donor functional groups, have been studied as a heavy metal trapping agents in recent years [2]. Furthermore, dendritic materials, especially amine dendrimers are applied in various fields such as biotechnology and separation process due to high amount of function groups at low amount of used substance [3].

In our study, SBA-16 mesoporous silica was prepared and functionalized with amine groups; then it was reacted with cyanuric chloride and ethylenediamine in presence of base. After separation, amine groups were converted to dithiocarbamate and SBA-16 mesoporous silica functionalized with melamine based dendritic dithiocarbamate was obtained (Scheme1). Characterization of synthesized mesoporous silica was performed via FT-IR, N_2 adsorption-desorption, SEM, TEM and CHNS analysis. The synthesized mesoporous silica used for removing Cd^{2+} cations from contaminated water. The effect of different parameters such as pH, time and amount of used adsorbent on the adsorption efficient demonstrated optimum condition to remove Cd^{2+} cations in 60 to 100%.



Scheme 1

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Highly sulfonated multi and single-walled carbon nanotubes as reusable and regioselective catalysts for the *tert*-butylation of *p*-cresol under solvent-free conditions: acomparison study

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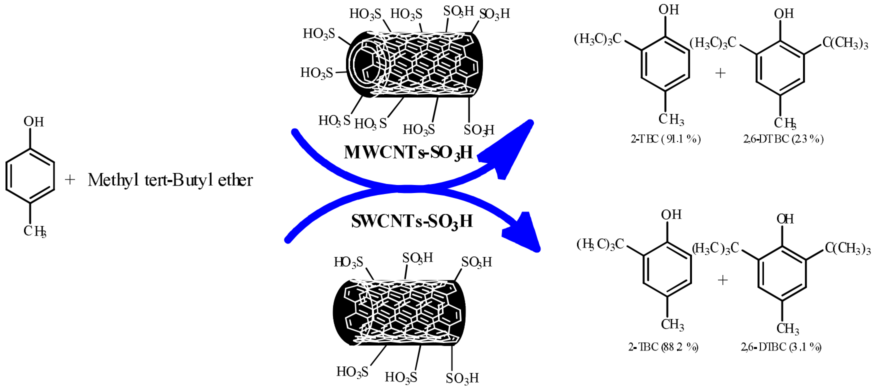
The synthesis of bulky organic molecules is an important area of search for industrial purpose. The *tert*-butylated benzene derivatives, typically bulky molecules are commercially important chemical intermediates. They have been used for the synthesis of antioxidants, antiseptics, agrochemicals, resins, UV absorber and stabilizer for the polymers [1]. *Tert*-butylatedbenzene derivatives, especially 2-*tert*-butyl-*p*-cresol (2-TBC) are widely employed for the synthesis of antioxidants such as 2,2′-methylene-bis-(6-*tert*-butyl-*p*-cresol) (A.O.2246) [2,3].

The present study describes the synthesis, characterization, and catalytic activity of sulfonated multi-walled carbon nanotubes and sulfonated single-walled carbon nanotubes in the *tert*-butylation of *p*-cresol. The sulfonated multi-walled carbon nanotubes and sulfonated single-walled carbon nanotubes have been used as efficient heterogeneous catalytic systems in the *tert*-butylation of *p*-cresol. The present study offers some advantages of high selectivity and yields, easy work-up, solvent-free conditions, and reusable catalyst.



Scheme 1

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A new method for the conversion of sulfoxides into sulfides by DBDMH/Ph_3P

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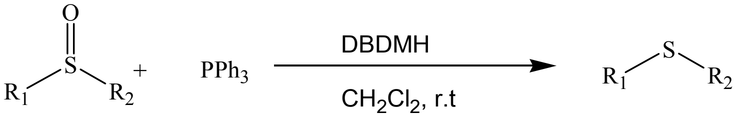
The reduction of sulfoxides to the corresponding sulfides is an important reaction, which has been found considerable utility in organic synthesis and in biochemical reactions [1,2]. So far, various methods for the deoxygenation of sulfoxides have been developed, such as metal hydride reagents ($LiAlH_4$, $NaBH_4$, etc.), low-valent metallic species ($SnCl_2$, VCl_3, etc.), halide ions (HI, TMSI, TiI_4, etc.) [3]. While numerous procedures are available for the deoxygenation of sulfoxides, they often suffer from serious disadvantages, such as the use of expensive reagents that are difficult to handle, functional group incompatibility, low efficiency of the reaction, long reaction time, difficult work-up procedures or harsh reaction conditions [4]. In order to, improve above mentioned limitations herein we report an efficient procedure for the reductive conversion of sulfoxides into sulfides using 1,3-dibromo-5,5-dimethylhydantoin in the presence of triphenylphosphine at room temperature (Scheme 1).



R_1,R_2 =aryl,alkyl

Scheme 1

References:

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Succinimide-*N*-sulfonic acid (SuSA): an efficient, eco-benign and recyclable solid acid catalyst for the one-pot addition of indoles to 3-formylchromone and aryl aldehydesunder solvent-free conditions

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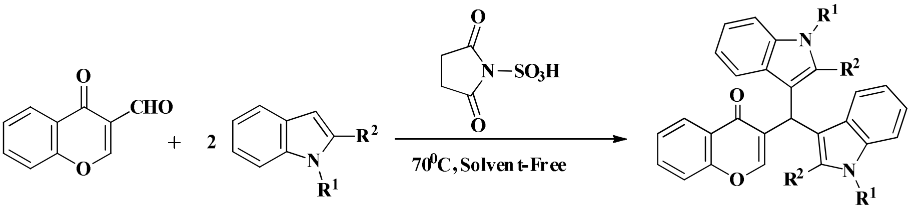
Indole is an important heterocyclic compound with a variety of natural and synthetic derivatives that have diverse pharmaceutical properties [1]. Indole core is also an important component in many of today's drugs for the treatment of chemotherapy-induced, nausea and vomiting or as antihypertensive, antineoplastic and antimitotic agents [2,3] Besides having the same 3-substituted indole nucleus as such fundamental biomolecules as tryptophan and melatonin.

At present, several general methods are known for the preparation of bis(indolyl)methanes, using various Lewis and protic acids [4] but inthis paper a convenient and highly efficient method is reported for the synthesis of (chromon-3-yl)bis(indol-3-yl)methanes and bis(indolyl)methanes by condensation of indolesderivatives and 3-formylchromone ordifferent aryl aldehydesin the precense of Succinimide sulfonic acid (SuSA) as efficient solid acid catalyst under solvent-free conditions.

Succinimide sulfonic acid (SuSA) as a stablereagent is easily prepared by the reaction of succinimidewith neat chlorosulfonic acid [5].



Scheme 1

Prominent advantages of this new methodology are the reusability of the catalyst, the experimental simplicity, and the high yields of product.

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Nanoporous MCM-41 materials modified with Copper(I)-salen type complex: as efficient and reusable catalyst for the synthesis of 1,2,3-triazoles

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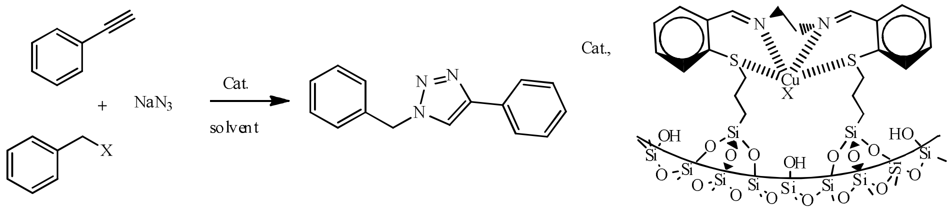
The development of new mesoporous organic–inorganic hybrid materials, as an example of heterogeneous catalysts, has played a key role in eco-friendly industrial processes.[1, 2] Immobilization of metal organic complexes on solid supports is highly desirable due to the facilitation both the isolation and recycling of the catalyst by simple filtration. Moreover, these catalysts exhibit a significant improvement in activity, selectivity and stability, which are attributed to contributions of isolated sites on the solid surface.[3-5]

The immobilization of copper complexes by covalent anchoring of the ligand on the surface of mesoporous MCM-41 has been described. Bis[2-(phenylthio)benzylidene]-1,2-ethylenediamine as a new N_2S_2-donor salen-type ligand was covalently anchored onto nanopores of MCM-41 followed coordinated with copper (I) halide. The organic-inorganic hybrid material was achieved readily using 3-mercaptopropyltrimethoxysilane as a reactive surface modifier. 2-nitrobenzaldehyde was reacted smoothly with the thiol moieties in order to form functionalized nanoporous silica with carbaldehyde groups. The resulting supported organic moieties were converted to thiosalen ligand and coordinated with CuX (X=CN, Cl, Br, I). The heterogenized catalyst was evaluated by the condensation reaction of benzylhalides, sodium azide and terminal alkynes. In this reaction, the corresponding triazoles were obtained as single products in good to excellent yields (scheme 1).



Scheme 1

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The study of transesterification sunflowers oil to biodiesel production in present of some chemical catalysts

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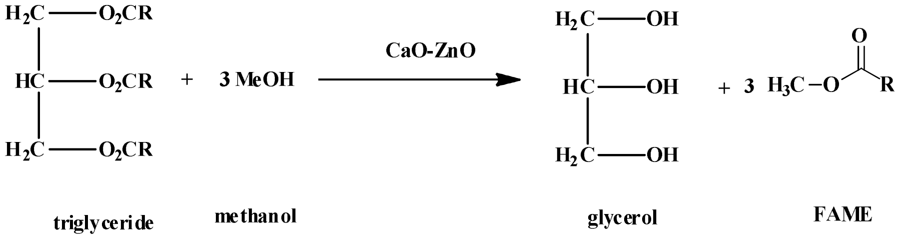
Industrial catalysis as a discipline, especially heterogeneous catalysis, has developed largely concurrently with the modern methods of industrial petroleum refining and has steadily allowed more sophisticated use of feedstocks for a growing range of and demand for petroleum products [1, 2].

The focus of this work the catalytic production of biodiesel from biomass, especially emphasizing catalytic conversion of waste vegetable oils and fats. Efficient, economical, and environmentally sound chemical production usually require the aid of catalysis to run at acceptable rates. Catalytic transesterification reaction of Sunflowers oil using synthesized CaO-ZnO catalysts with different of Ca:Zn ratio was performed. The process was presented in Scheme 1. When the Ca content rose from the ratio of 0.5 to 8.0, the FAME yield increased to the maximum value of 90 %. However, as the ratio was above 8.0, the FAME yield was dropped. By drawing on the results, the optimum loading amount of Ca content was ratio 8.0. The excess loading Ca content reduced the interaction between excess CaO with ZnO and thus the stability of the binary oxide system become weak.



Scheme 1

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Facile synthesis of 2-aryl-4,5-dicarbonitrile-1*H*-imidazoles using transition metal nitrates as an efficient catalyst

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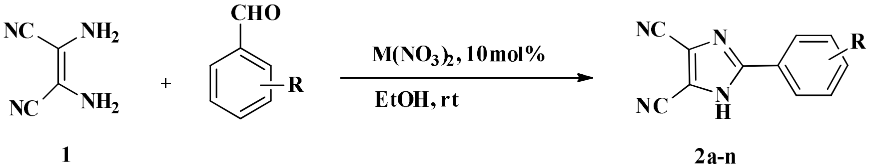
Imidazoles are vastly distributed in nature and known as biocatalyst and biological ligands. These compoundsplay a vital role in life activities. Based on several literature surveys, imidazole derivatives show a wide range of pharmacological activities [1,2]. Several methods have reported for the synthesis of these compounds. However, the most of these methods have some limitations including harsh reaction conditions, low yields, long reaction times and tedious workup procedure. Consequently, the introduction of new methods and/or further work on technical improvements to overcome these limitations is still needed. Recently, synthesis of organic compounds in the presence of heterogeneous or homogeneous catalysts has attracted special interest as they have many advantages [3].



1

2a-n

Scheme 1

In view of these points and as a part of our interest researches on the development of new methods for the synthesis of important heterocyclic rings [4],we wish to report a simple and practically procedure for the synthesis of 2-aryl-4,5-dicarbonitrile imidazoles through a one-pot condensation reaction of 2,3-diaminomaleonitrileand aromatic aldehydes in the presence of catalytic amount of $M(NO_3)_2$. $6H_2O$ in ethanol at room temperature (Scheme 1). Some of the major advantages of this practical procedure are use of available catalyst, high yields, short reaction times, and simplicity of the reaction and workup.

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A study upon the role of gallium oxide nanorod as an efficient & recyclable catalyst, a green approach

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We know very well that the crucial role of nanoparticles in organic transformations is their excellent catalytic activity, straightforward recoverability, better selectivity, criteria of evolution, and their versatile role in green chemistry. In this research, the main aim is studying the role of gallium oxide nanorod as an inexpensive, efficient and recyclable catalyst [1]. A feasible "NOSE" (nanoparticles-catalyzed organic synthesis enhancement) protocol has been developed for N,N-diformylation of bisuracil derivatives using nano-Ga_2O_3 rods as an efficient, inexpensive, and recyclable catalyst under solvent-free reaction condition at 40° C. The catalyst was reused up to the 4th cycle without affecting the rate and yield of the N,N-diformylation products appreciably. As indicated in Figure 1, the recycled nano-Ga_2O_3 revealed the aggregation of the particles responsible for reducing its surface area and hence deactivated the catalyst after 4th run which caused the lower yield of product [2,3].

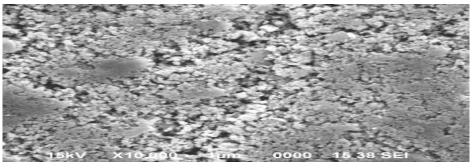

Figure 1

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A green, and efficient method for synthesis of 1,8-dioxo-octahydroxanthene derivatives using TSATA as a novel base catalyst

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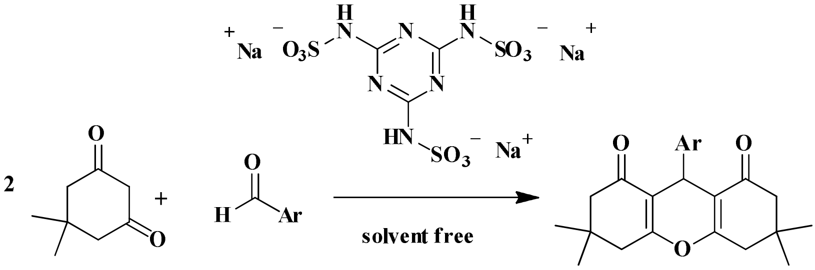
Use of heterogeneous catalysts has attracted considerable interest in recent years due to economic and inviromental considerations [1]. These catalysts have advantages such as, recoverability, easy sepration, long lifetime, eco-friendly, and non-corrosive [2]. And also according to recent searches, it can be seen that base catalytic reactions are one of the most widely reactions in organic chemistry [3].

On the other hand, hydroxanthene derivatives are known as an important class of organic compounds which shows useful biological, anti-flammatory, antiviral and pharmaceutical activities [4].

In present work, we offer TSATA as a novel base heterogeneous catalyst and use it for synthesis of 1,8-dioxo-octahydroxanthene derivatives via condensation reactions between aromatic aldehydes and dimedon under solvent free condition as a green method with high yields and short reaction times (Scheme 1).



Scheme 1

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Chemical composition of the essential oils from the flowers, stems and leaves of *pulicaria gnaphalodes*(vent.) boiss. using the head space solid phase microextraction method prior to gas chromatography-mass spectrometry

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The genus Pulicaria, family Asteraceae, is represented by ca. 100 species, more than 5 of which grow wild in Iran [1-2]. The Pulicaria species proved various activities such as anti-inflammatory, antilukemic, potential cancer chemopreventive and cytotoxic agents [2]. The plant material was collected from of south Khorasan Province, Iran. The present report deals with the analysis and comparison of composition of the volatiles component obtained by head space-solid phase microextraction (HS-SPME) procedures from the aerial parts of *Pulicaria gnaphalodes* (vent.) Boiss. The SPME head space volatiles were collected using a fiber coated with polydimethylsiloxane (PDMS).

The composition of the volatile essential oils from the flowers, leaves and stems of *Pulicaria gnaphalodes* was investigated by GC-FID and GC-MS. α-pinene (42.29%), 1,8-cineole (26.76%) and chrysanthenone (7.19%) were the main components in the flowers and 1,8-cineole (41.81%) and α-pinene (34.77%) were the main components in the leaves. 1,8-cineole (73.53%) and α-pinene (13.42%) were the other main components in the stems of *Pulicaria gnaphalodes* [3].

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Citric acid as real green, cheap and easy available catalyst for synthesis of cyanoacetamide containing compounds

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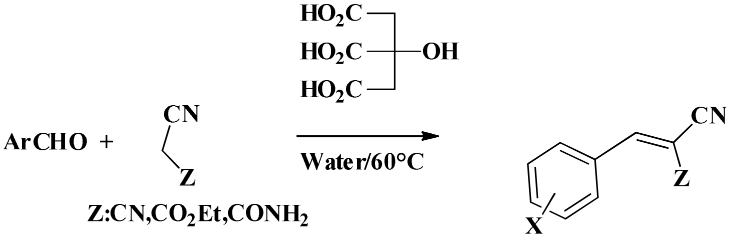
Green synthetic routes are the main concern of the present century and current synthetic efforts are directed to achieve this goal [1, 2].

Certainly there is increasing pressure on chemist to replace toxic catalysts and volatile solvents [3].

For aiming these purpose we utilized citric acid as a real green catalyst for promoting condensation reaction such as knoevenagel of cyanoacetamide with aromatic aldehydes in the best and ever green solvent (Water).



Scheme 1

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Fe_3O_4-SA-PPCA as novel and effective nanocatalyst for the synthesis of polyhydroquinoline derivatives

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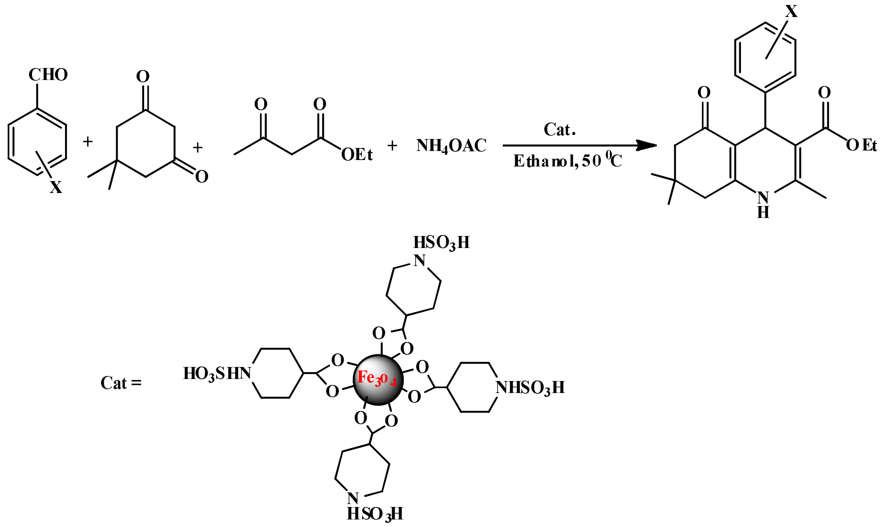
Nanoscale materials have been a subject of particular interest due to properties, which differ from their bulk counterparts [1]. They have been used extensively in chemistry [2], biology [3] and catalysis [4]. Magnetic nanoparticles (MNPs) have attracted great interest because of their multifunctional physical and chemical properties. Magnetic NPs have many unique magnetic properties such as superparamagnetic, high coercivity, low Curie temperature, high magnetic susceptibility, etc.

In this work, we report immobilization of sulfunic acid groups on the magnetic MNPs-PPCA, as a new heterogeneous catalyst for the synthesis of polyhydroquinoline derivatives *via* four component condensation reaction of dimedone, aldehydes, ethylacetoacetate and ammonium acetate in ethanol at 50 °C (Scheme1).



Scheme1

References:

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Magnetic nanoparticles Fe_3O_4 immobilized *N*-propylsulfamic acid (MNPs-PSA) as an efficient and reusable nanocatalyst for the synthesis of 1,8-dioxo-octahydroxanthenes derivatives

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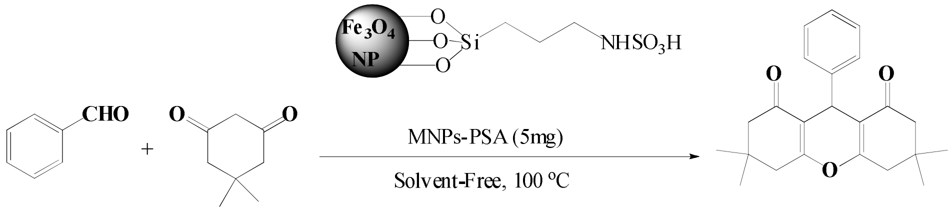
Magnetic nanoparticles are efficient, readily available, high-surface-area resulting in high catalyst loading capacity and outstanding stability heterogeneous supports for catalysts. Among the various magnetic nanoparticles used as the core magnetic support, Fe_3O_4 nanoparticles are arguably the most extensively studied because of their simple synthesis, low cost, and relatively large magnetic susceptibility [1].

Xantene derivatives such as octahydroxantene are an important class of organic compounds, which have been used as versatile synthons because of the inherent reactivity of the pyran ring. Furthermore, these compounds have recently received great attention because of the wide range of their therapeutic and biological properties such as antibacterial, antiviral and anti-inflammatory activities antinociceptive activities [2].

In continuation of our studies on magnetic nanocatalysts [3], herein, weinvestigated the synthesis of 1,8-dioxo-octahydroxanthenesderivatives in the presence of MNPs-PSA as a recyclable and green magnetic nanocatalystunder solvent-free conditions at 100 °C (Scheme 1).



Scheme 1

This method offers several advantages including high yield, short reaction time, simple work-up procedure, ease of separation, and recyclability of the magnetic nanocatalystwithout significant loss of their catalytic efficiency.

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Amino-functionalized nanoporoussilica (SBA-Pr-NH$_2$) in efficient One-pot synthesis of 2*H*-indazolo[2,1-*b*]phthalazine-trionederivatives

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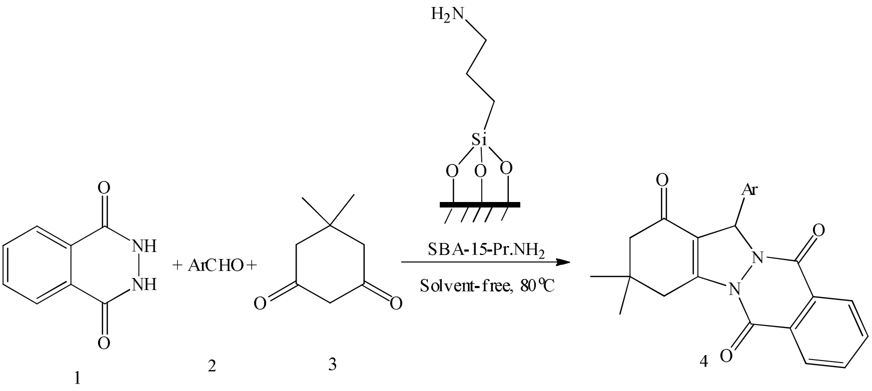
Heterogeneous catalysts have gained great importance due to their economic and environmental consideration [1]. Among the various heterogeneous catalysts, Santa Barbara Amorphous (SBA-15) is significant as a newnanoporoussilica with exclusive and important properties, such as hydrothermally stable and thick walls, profusely large surface area and huge pore volume. These properties render it as promising nano catalyst for wide range of applications [2] Moreover, integration of basic functional groups (e.g., NH$_2$) into SBA-15 has been explored to produce promising solid base catalysts which could enhance and optimize its catalytic activity [3].

Fused phthalazines were found to possess multiple biological activity such as anticonvulsant [4]. In this research we want to report the application of SBA-Pr-NH2 as a highly active nanoporous solid base catalyst in the three-component condensation of phthalhydrazide**1**, aromatic aldehydes **2**, and dimedone**3** to obtain 2H-Indazolo-[1,2-*b*] phthalazine-triones**4** under solvent-free conditions (Scheme 1).



Scheme 1

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5A Zeolite as an efficient and green catalyst for Knoevenagel condensation

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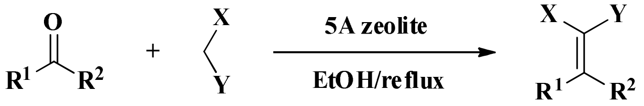
The Knoevenagel condensation is a useful carbon–carbon bond forming reaction with numerous applications in the synthesis of fine chemicals, hetero-Diels–Alder reactions and in the synthesis of carbocyclic as well as hetero cyclic compounds [1]. The reaction has been utilized in the preparation of coumarin derivatives, cosmetics, perfumes and pharmaceutical chemicals. Traditionally, this condensation has been carried out between a carbonyl compound and an active methylene compound. The condensation reaction could be catalyzed not only by bases, but also by acids or catalysts containing both acid–base sites [2].

Zeolite 5A is a class of microporous aluminosilicate materials, also known as 5A molecular sieve and commonly used as commercial adsorbents for gases and liquids. This compound is often utilized in the petroleum industry, especially for the purification of gas streams and in the chemistry laboratory for separating water of the compounds and drying reaction starting materials [3].

In this work zeolite 5A is used as catalyst for Knoevenagel condensation reaction in ethanol under reflux condition. Also, The reaction conditions are very simple, highly efficient and mild. The work-up procedure is very simple and the products do not require further purification.



R^1 & R^2 : H, Alkyl, Aryl
X & Y : CN, $CO_2C_2H_5$

Scheme 1

References:
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SPIONs-Bis(NHC)-palladium(II): powerful and efficient catalyst for Mizoroki-Heck and Suzuki-Miyaura reactions

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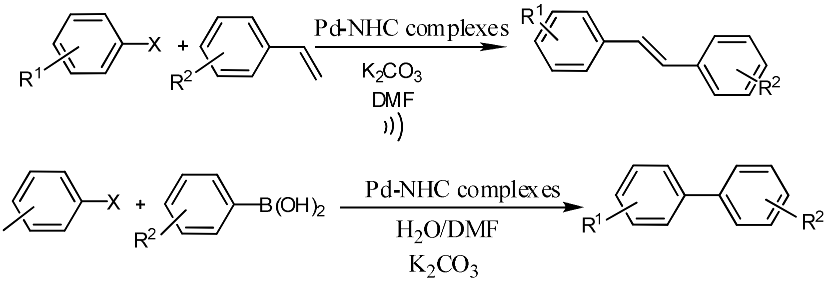
Recently, *N*-heterocyclic carbenes (NHCs) have emerged as an extremely useful and versatile class of ligands in homogeneous transition metal catalysis due to the strong σ-donor properties, ease of preparation and effective binding ability to any transition metal irrespective of their oxidation states [1]. Within this context, these compounds have attracted increasing attention in both academic and industrial fields owing to their unique catalytic activity [2]. NHCs complexes as homogeneous catalysts have been used in a number of organic transformations such as olefin metathesis, and C-C bond formation reactions [3].

In this study, preparation of new palladium NHC-Pd complex stabilized on magnetic nano-particles was investigated. In continuance of catalytic activity of the mentioned catalyst examined in the Mizoroki-Heck and Suzuki-Miyaura reactions (Scheme 1).



Scheme 1

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Efficient synthesis of β-enaminones and β-enamino esters catalyzed by carbon-based solid acid under solvent free conditions

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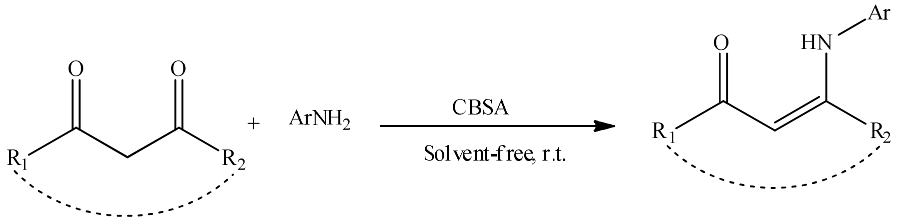
The enaminones and enamino esters are very stable structural motifs which are prepared by inexpensive raw materials. Hence they are considered as excellent starting materials in organic synthesis [1]. Condensation reactions of carbonyl compounds with amines in the presence of various acid are well reported for the synthesis of β-enaminones and enamino esters. However, these methods are associated with certain drawbacks. Thus, a search for a new catalyst and simple procedure is of practical importance [2].

The replacement of conventional, toxic, polluting liquid acid catalysts with environmentally benign reusable solid heterogeneous catalysts is an area of current interest. Carbon-based solid acids (CBSA) are conventional materials that have wide applications in chemical production [3].

Herein we report an efficient method for the synthesis of enaminone and enamino esters using CBSA. The reactions were carried out by treatment of equimolar amounts of primary amines and 1,3-dicarbonyl compounds with a catalytic amount of CBSA (0.05 gr) under solvent-free conditions at room temperature. (Scheme 1).



R_1,R_2= alkyl, cyxloalkyl, alkoxy

Scheme 1

References:

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Layer effectson benzimidazole derivatives in Trichomonosis' disease

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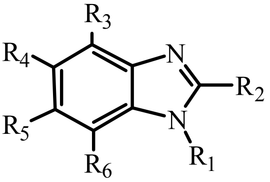
Trichomoniasis can increase the risk of getting or spreading other sexually transmitted infections. For example, trichomoniasis can cause genital inflammation that makes it easier to get infected with the HIV virus, or to pass the HIV virus on to a sex partner [1]. Quantitative structure activity relationships (QSAR) are the most important applications of chemometrics giving useful information for the design of new compounds acting on a specific target. A good QSAR model both enhances our understanding of the specifics of drug action and provides a theoretical foundation for lead optimization [2].

In this work, layer effects study has been done on benzimidazole derivatives in Trichomonosis' disease. Genetic algorithm (GA), artificial neural network (ANN) and stepwise multiple linear regression (stepwise-MLR) were used to create then on non-linear and linear QSAR models. In the gas phase the best root-mean square errors of the training set and the test set for GA–ANN model, were 0.1387 for layers [9, 1] and 0.7451 for layer [10, 1]. Also, the R and R^2 values in the gas phase were obtained 0.82, 0.67 from GA-stepwise-MLR model. The eight most significant descriptors which were selected by GA-stepwise-MLR are as follows: G (N..N), F04 [C-C], R5p, Mor30u, RDF090m, H5u, RDF095u and GATS6v. The general structure of the benzimidazole derivatives used in this study is shown in Scheme 1 [3].



Scheme 1

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Selective oxidation of alcohols with potassium permanganate supported on HA zeolite

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Compounds containing the ketone or aldehyde functional group are important in organic chemistry. They are common in nature and are often key intermediates in organic synthesis [1]. Despite numerous methods for preparation, the single most important method for preparation of both ketones and aldehydes is the oxidation of alcohols. Alcohols are among the most readily available organic compounds, and therefore, this method for preparation of aldehydes and ketones is extremely useful. The quest for effective catalytic system that uses clean, inexpensive oxidant is potassium permanganate supported on HA zeolite.

Zeolites, crystalline aluminosilicates, are widely used in separation and refinery industries as catalysts, adsorbents, membranes and ion exchangers. The significant catalytic activity and selectivity of zeolites are attributed to their large internal surface area and highly distributed active sites that are accessible through uniform pore size [2]. HA, a new heterogeneous catalyst is one of the crystalline zeolite which is acidic and we have discovered that it is an effective catalyst for selective oxidation of primary and secondary alcohols to aldehydes and ketones in ethylacetate under reflux condition.

$$\mathrm{RCH_2OH} \xrightarrow[\mathrm{EtOAc/reflux}]{\mathrm{KMnO_4/HA\ zeolite}} \mathrm{RCHO}$$

$$\mathrm{RCH(OH)R'} \xrightarrow[\mathrm{EtOAc/reflux}]{\mathrm{KMnO_4/HA\ zeolite}} \mathrm{RCOR'}$$

Scheme 1

References:

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Pentaaza tetraethylen modified polyacrylamide as an efficient catalyst for barbituric acid derivatives under green condition

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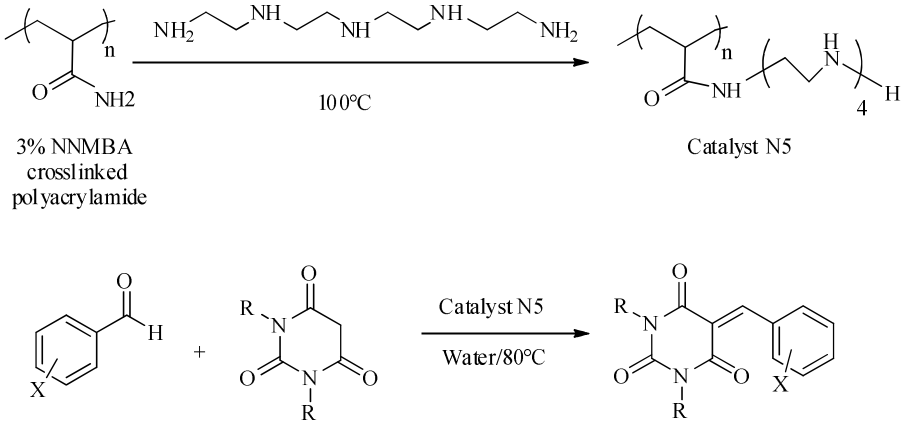
Usually homogeneous base catalysts are used for this kind of reaction. Heterogeneous catalysts have also been used for the Knoevenagel reaction thus; the reaction has been catalyzed by heterogeneous catalysts based on alumina, silica, zinc and magnesium oxides, resins and other catalysts with more or less success [1-3].

Inserting of *PATE* via transamidation root on 3%NNMBA-crosslinked polyacrylamide led to a novel and green basic catalyst for knoevenagel condensation of aromatic aldehyde with barbituric acid derivatives in absolutely green media: WATER. This catalytic activity in water is due to hydrophilic nature of polyacrylamide. Catalyst is reusable by mer filtration.



Scheme 1

References:

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Nano-$SnCl_4.SiO_2$ as an efficient catalyst for the synthesis of 1,4-dihydropyridine derivatives

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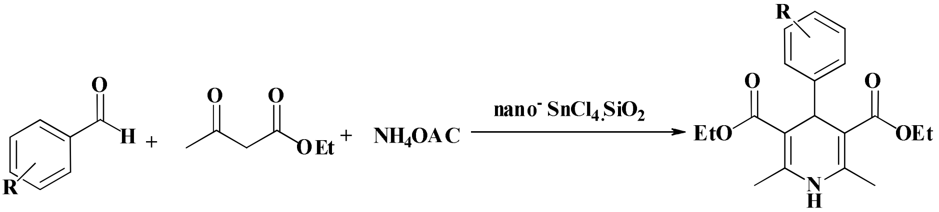
1,4-dihydropyridines (1,4-DHPs) are an important class of heterocycles with a wide range of pharmacological and biological activities such as anti-hypertensive, anti-anginal, antitumor, anti-inflammatory activity, antitubercular activity, analgesic activity [1,2]. Due to the biological importance of these compounds several methods have been reported for the improvement of 1,4-dihydropyridine ring and polyhydroquinoline derivatives [3,4]. 1,4-dihydropyridines are generally synthesized by classical Hantzsch reaction. Tin tetrachloride is a powerful Lewis acid which is, a liquid with a high specific gravity. The handling and the usability of $SnCl_4$in liquid form is laborious. Silica-supported $SnCl_4$ is a mild solid Lewis acid [5] and does not need special precautions for preparation, handling, or storage, which could promote acid-catalyzed organic reactions [6].

In this work,we have investigated the application of nano-$SnCl_4.SiO_2$ for the condensation of an aldehyde, ethyl acetoacetate and ammonium acetate. This method have some advantages such as good to excellent yields, mild reaction conditions, ease of operation and work-up, short reaction times and high purity products.(Scheme 1).



Scheme1

References:

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Synthesis and application of mono and bi nuclear cyclopalladated complexes

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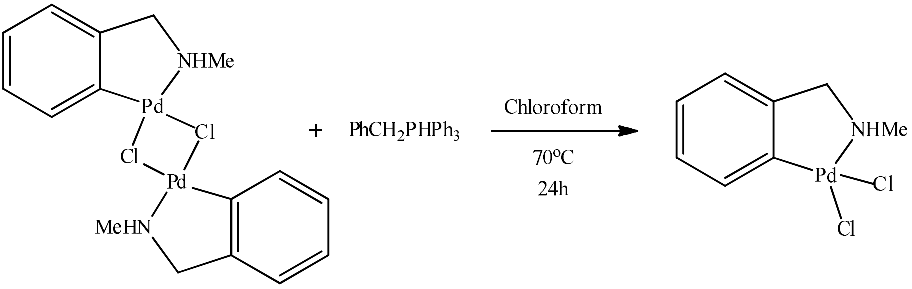
During the last years, transition-metal organometallic compounds have undergone an impressive growth as subjects for research and applications in organic synthesis. The interest in cyclopalladated complexes, cyclic species containing one Pd-C bond (alkyl or aryl) intramolecularly stabilized by at least one neutral donor atom, derived from N-donor ligands has increased considerably due to their extremely high catalytic activity in a variety of important C-C coupling reactions, versatile catalyst and speeds up hydrogenation and dehydrogenation reactions [1]. On the other hand, palladium complexes have been obtained aiming to produce drugs, due to its chemical similarity with platinum, and the fact that they showed excellent antitumoral and anti-infective activities *in vitro* and *in vivo* [2].

In this paper we present the preparation and structures of mono and bi nuclear palladacycles from secondary benzylamines. Reaction of bi-nuclear compound with benzyl triphenyl phosphonium salt in chloroform solvent afforded mono nuclear complex at 70 °C after 24 h. (Scheme 1). Theoretical data, IR spectroscopy, H, C and P NMR and crystallographically, show good agreement with the structure of complex.



Scheme 1

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Synthesis of sulfonamides as sulfa drugs under mild conditions

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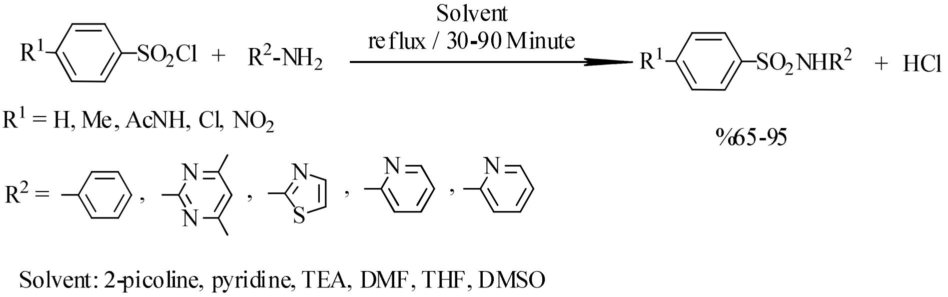
Sulfonamides play an important role in medicinal chemistry and being widely used as anticancer, anti-inflammatory and antiviral agents [1]. A general process for synthesis of sulfonamides is to perform the reaction in organic solvents and employ organic amine bases to scavenge the acid (HCl) that is generated [2-5].

Herein we disclose a simple synthesis of some sulfonamides as sulfa drugs. In this study, we have employed a simple procedure with simple work-up for manipulation of a variety of sulfonamides in organic solvents without any catalysts. The reactions are usually carried out under mild conditions with elevated yields and simple work-up. The best results was obtained in 2-picolin as solvent. Product isolation involves evaporation of solvent at the end of the reaction followed by purification of residue. Impure products were purified by dissolving the solid product in diluted alkali solution of sodium carbonate. The mentioned method examined with primary amines such as aniline, 2-aminothiazole, 3,5-dimethyl-2-amino pyrimidine, 2-amino pyridin, 2-amino pyrimidin, *etc* to synthesis sulfa drugs. Products are isolated in excellent yields by simple purification of the precipitated solid after evaporation of solvent. This method is applicable to a wide variety of amines, being a useful alternative over other methods in the literature. Sufathiazole, Sulfadiazine, Sulfadimidine, Sulfapyridine and Sulfasalazine, are among the sulfa drugs that were produced with this procedure (Scheme 1).



Scheme 1

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Sulfonated polynaphthalene (S-PNP) as a heterogeneous and chemoselective catalyst for trimethylsilylation of alcohols and phenols by 1,1,1,3,3,3-hexamethyldisilazane

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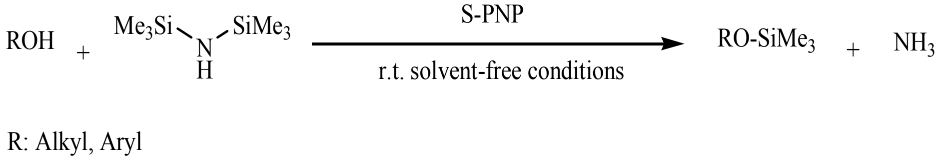
The principles of green chemistry and increasing concerns about environmental issues have stimulated the research for recyclable strong solid acids to replace of conventional toxic and corrosive acid catalysts, such as sulfuric acid [1]. Highly sulfonated polymers, which are used for acid catalysts, are of growing interest for many industrial applications [2].

The conversion of hydroxyl groups to their corresponding trimethylsilyl ethers is one of the popular methods used for protection of the hydroxyl group of alcohols and phenols. Hexamethyldisilazane (HMDS), as a cheap and commercially available reagent, is selected as one of the best candidates used for this purpose. But the low silylating power of HMDS is the main drawback for its application. So it is necessary to use a catalysts for the activation of HMDS [3].

In the present work, the investigation of the catalytic activity of sulfonated polynaphthalene (S-PNP) in selective trimethylsilylation of alcohols and phenols with hexamethyldisilazane is reported. (Scheme 1).



Scheme 1

Also the catalyst is of high reusability and stability, in that it was recovered several times without loss of its initial activity.

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Magnetic nanoparticle supported catalyst for synthesis of 2,3-dihydroquinazolin-4(1H)-ones

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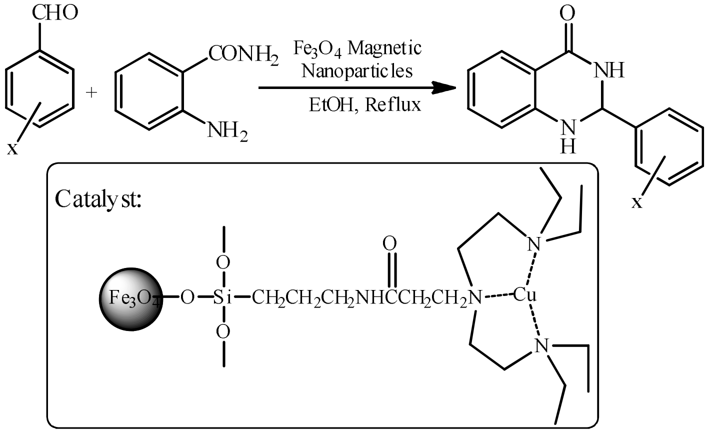
The synthesis of nanomaterials with uniformparticle size is a subject of intensive research inrecent time because of their fundamental scientificinterest as well as for the technological importance [1]. These nanomaterials exhibit veryinterestingelectrical, optical, magnetic, and chemical properties, which could not be achieved bytheir bulkcounterparts [2]. Nanomaterials mayalso be used invarious technological applications, viz. refrigerationsystems, medical imaging, drug targeting and otherbiological applications [3].

Hence, the development of clean, safe, effective, economicalbenign protocols is still desirable and is an important task for organic chemists.we became interested to develop a one-pot combination for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones, using by Magnetic Nanoparticle-Supported Catalyst$CuCl_2$/MNP-TEDETA. Therefore a variety of 2,3-dihydroquinazolin-4(1H)-ones have been prepared via combination ofaromatic aldehydesand 2-aminobenzamide.



Scheme 1

References:

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Nitrosation reaction of aromatic compoundsusing nano-$BF_3.SiO_2$ as an eco-friendlycatalyst under solvent-free conditions

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Nitrosation is a process converting organic compounds into nitroso derivatives. Nitrosation reactionsare widely used in medicine, dyestuff and fine chemical processes [1]. *C*-nitroso aromatic compounds play important roles in various biological metabolic processes [2,3]. Organic reaction under solvent free condition are of interest from both industrial and academic viewpoint. Mild reaction condition, ease of operation and workup, short reaction time are important advantages of this protocol.

In this work, a new strategy has been introduced for the preparation of nitroso aromatic compounds from the various aromatic compounds with sodium nitrite in the presence of a catalytic amounts of BF_3 supporting on nano SiO_2 as an efficient solid acid catalyst under solvent-free conditions in good to excellent yields (scheme 1).

$$\mathrm{ArH} \xrightarrow[\text{Solvent free}]{\text{nano - }\mathrm{BF_3\,.SiO_2\,,\,NaNO_2}} \mathrm{ArNO}$$

Scheme 1

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Functionalized-MCM-41 as a catalyst for oxidation of sulfides to sulfoxides under solvent free condition

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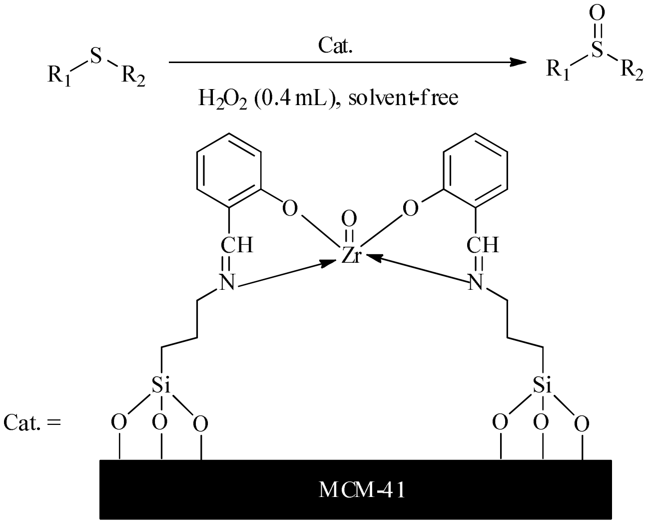
In recent years, mesoporous materials such as MCM-41 have attracted the attention of many scientists [1]. They enable to carrying high dosages of a variety of drugs in their mesopores. Furthermore mesoporous silica containing specific functional groups have highspecific surface areas and porosities that opened a wide field of applications. Thus they provide a suitable approach to the development of green chemistry principles

Sulfoxides are fine chemicals, pharmaceuticals and valuable intermediates in the synthesis of chemically useful and biologically active molecules [2]. Oxidation of sulfides is the most straight-forward method for the synthesis of sulfoxides. Concerning the green oxidant, hydrogen peroxide is one of the most powerful candidates besides molecular oxygen, because it is inexpensive, readily available, high atom efficiency, and water is expected as the only by-product to be generated from the reaction [3].

Herein we wish to report oxidation of sulfides to sufoxides using hydrogen peroxide in the presence of catalytic amount of functionalized-MCM-41 under solvent-free conditions at 35 °C.



Scheme 1

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Magnetic core-shellnanoparticles-supported sulfuric acid as a reusable catalyst for the synthesis of benzimidazoles and bis(indolyl)methanes

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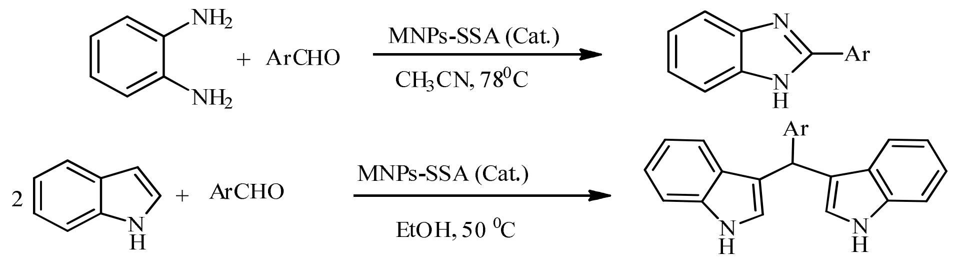
The catalysts supported on magnetic nanoparticles combine these advantages of heterogeneous catalysts (easy recovery and regeneration) and nanocatalysts (such as a large surface-to-volume ratio relative to bulk materials, excellent activity, great selectivity, and high stability) [1].

Benzimidazole derivatives and bis(indolyl)methanesare important class of heterocyclic active in the field of biological and medicinal chemistry [2-3]. Numerous methods have been reported in the literature for the synthesis of benzimidazoles and bis (indolyl) methanes [4-5]. Although these methods produce good results in many instances, there is still a demand to devolve new mild method for synthesis of benzthiazoles in the presence of cheap and bench top catalyst. In continuation of our studies on application of magnetically separable catalysts in organic reactions [6], herein, we synthesized and characterized the magnetic nanoparticle-supported silica sulfuric acid (MNPs-SSA) as aneco-friendly and reusable organic-inorganic hybrid catalystforthe synthesis of benzimidazoles and bis(indolyl)methanesfrom the condensation of o-phnylenediamines and indole with aromatic aldehydes respectively (Scheme 1).



Scheme 1

In summary, we have utilized MNPs-SSA as ananocatalystfor the synthesis ofbenzimidazole derivatives and bis(indolyl)methanesfor the first time. the significant advantages of these procedures are(a) the use of the eco-friendly,cost-effective,reusable and chemically stable catalyst, (b) mildreactionconditionsandvery easy work-up.

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One-pot and solvent-free synthesis of 3,4-dihydropyrimidin-2(1H)-one/thione using new synthetic recyclable catalysts via biginelli reaction

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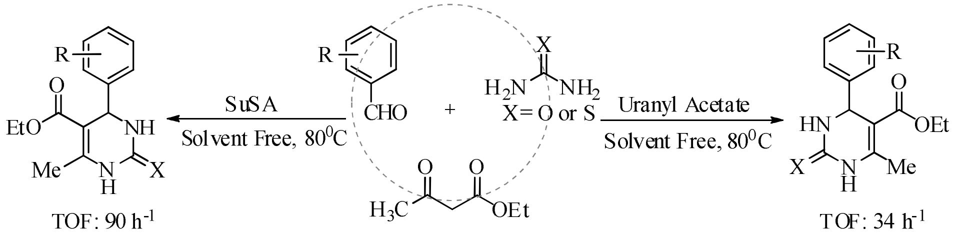
In 1893, and for the first time, the Italian chemist Pietro Biginelli reported the cyclocondensation of ethyl acetoacetate, urea, and an appropriate aryl aldehyde in the presence of an acid as a catalyst, to obtain 3,4-dihydropyrimidin-2(1*H*)-ones (DHPMs or Biginelli adducts) as major products [1]. Dihydropyrimidinones and their sulfur analogues have an important role in synthetic organic chemistry and natural products due to their extensive range of biological and pharmacological properties [2]. These compounds as a N-contained heterocycle attracted much attention due to activities of anticancer, anti-inflammatory, antibacterial, antifungal, anthelmintic, andantitopoisomerase [3].
For the Biginelli reaction, a large number of new techniques such as microwave-assisted synthesis, ultrasound irradiation, etc. and various catalysts have been reported [4].

In connection with our ongoing work on Biginelli reaction [5], herein we report afacile and rapid one-pot three component procedure for the preparation of 3,4-dihydropyrimidin-2-(1*H*)one/thione derivatives using aryl aldehydes, *β*-diketo compounds, urea or thiourea Catalyzed by Uranyl Acetate and Comparison of its Catalytic Efficacy with Succinimide sulfonic acid (SuSA)(Scheme 1).



Scheme 1

Both catalysts could be reused after a simple work-up and reused several times without noticeable reduction in the catalytic activity.

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TMSCl; Highly efficient and simple organo catalyst for the fast and clean synthesis of bis(indolyl)methanes at room temperature

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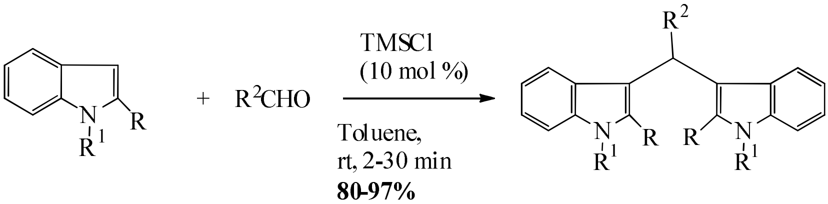
An operationally simple and highly efficient protocol for TMSCl catalyst reaction of indoles with aldehydes and simple ketons at ambient temperature with short reaction time and in good to excellent yields has been developed. There has been much interest to develop highly efficient and simple organocatalyst in organic transformations among the various organocatalyst [1]. TMSCl has received considerable attention as an inexpensive and readily available catalyst for various organic syntheses in recent years [2]. However, there is no example of bisindolylmethane synthesis using TMSCl as a catalyst. We herein report the use of TMSCl as catalysts in the electrophilic substitutions of indole and substituted indole with a variety of aldehydes and ketones to afford bis(indolyl)methanes at room temperature with excellent yields and short reaction times (Scheme 1



Scheme 1

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Application of sulfonated-Rice Husk Ash as a catalyst in the protection and deprotection of alcohols

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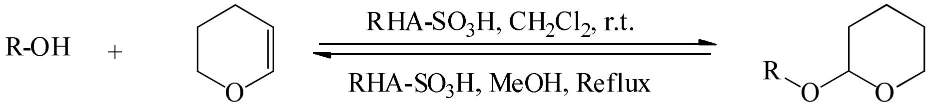
The protection and deprotection of the hydroxyl functional group can play an essential role in synthetic strategy. The tetrahydropyranyl (THP) group is one of the most frequently used groups to protect alcohols and phenols [1,2].

In this work, primary and secondary alcohols, as well as phenols, were converted to the corresponding tetrahydropyranyl (THP) ethers with short reaction times and high yields.

We have now found that the same catalyst also to be an efficient deprotection catalyst for THP ethers in the presence of methanol at reflux to provide the corresponding free alcohols in consistently excellent yields.(Scheme1)



Scheme 1

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A new approach to modified magnetic nanoparticles for synthesis of formazan dyes under solvent-free conditions

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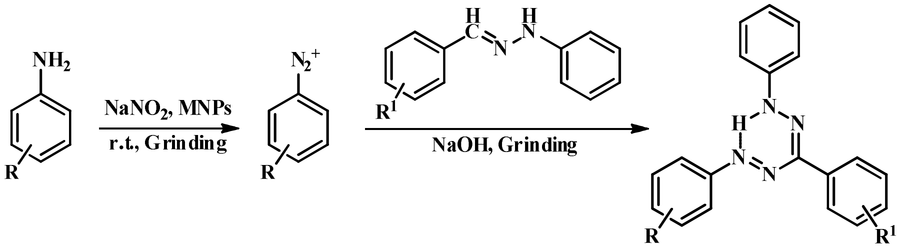
[b]*Department of Chemistry, College of Science, Yazd University, Yazd, Iran*
Email: bamoniri@kashanu.ac.ir

In recent years, magnetic nanoparticles (MNPs) have attracted a great interest due to their biocompatibility, easy of surface modification and unique superparamagnetism. MNPs can be functionalized by modifying their surfaces with various materials to achieve the special purposes especially in the field of catalysis [1-3].

Formazans form distinct class of organic dyes with characteristic properties. These compounds have received much attention for their applications in analytical chemistry, biological applications and as dyestuffs [4]. Formazans are usually synthesized by coupling of aryl diazonium salts and arylhydrazones at *p*H 10-12 and temperature below 5 °C [5-7].

Aiming to overcome the limitations of the previous reported methods, herein we wish to investigate the synthesis of formazan derivatives in the presence of a novel modified magnetic nano catalyst at room temperature in a solvent-free medium. This new catalytic system possesses both high separation efficiency and a relatively high catalytic activity for the synthesis of formazan dyes (Scheme 1).



Scheme 1

References:

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Synthesis and characterization of novel acidic ionic liquid supported magnetic nanoparticles as an efficient catalyst for the one-pot preparation of 14-aryl-14*H*-dibenzo[*a,j*]xanthenes and 1,8-dioxooctahydroxanthenes under solvent-free conditions

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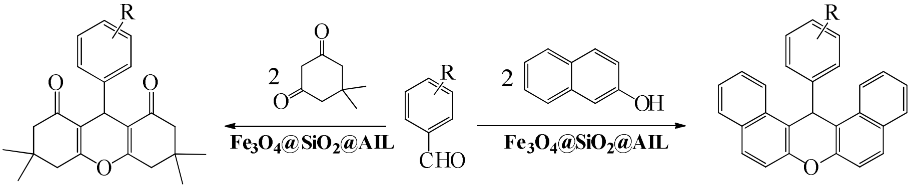
Supported-heterogeneous catalysts have garnered much attention in recent years and are actively pursued in the development of modern organic synthesis and greener reaction protocols. Homogeneous, flammable, and active protic acids have been immobilized on the solid support for deployment in organic reactions [1].

Surface functionalized iron oxide magnetic nanoparticles (MNPs) are a kind of novel functional materials, which have been widely used in biotechnology and catalysis. Good biocompatibility and biodegradability as well as basic magnetic characteristics could be denoted for functional organic materials grafted to MNPs [2].

Xanthenes derivatives, which have one oxygen atom in a fused ring system, possess antibacterial, antiviral, anti-inflammatory activities. Moreover, these compounds have been used as leuco-dyes, found application in laser technology, and also as sensitizers in photodynamic therapy. Thus the synthesis of xanthenes is of paramount importance in organic synthesis [3].



Scheme 1

References:

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Mesoporous silica nanoparticles as a catalyst for one-pot multicomponent synthesis of polyhydroquinolines and hantzsch 1,4-dihydropyridines

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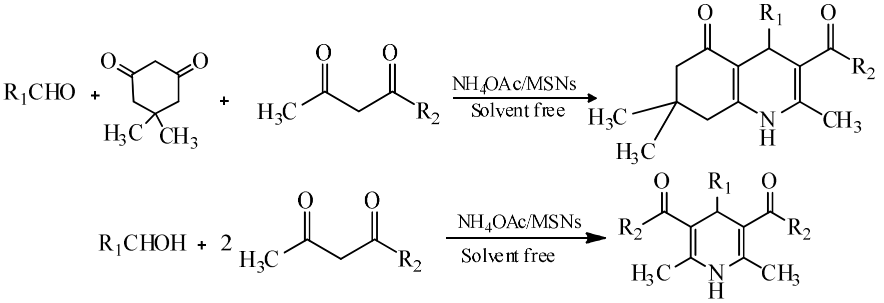
Polyhydroquinoline (PHQ) and 1,4-dihydropyridine (DHP) derivatives contain a large family of medicinally important compounds that have attracted much attention because of their diverse pharmacological and therapeutic properties. In view of the biological, industrial and synthetic importance of these compounds, several methods for their synthesis have been reported. Here we report a simple and efficient method for the synthesis of biologically active substituted Hantzsch 1,4-dihydropyridine and polyhydroquinoline using mesoporous silica nanoparticles (MSNs) as a green and reusable catalyst. The mild and neutral reaction conditions, excellent product yields, high reaction rates and easy recyclability of the catalyst make this a better alternative to the conventional process. In addition, our procedure enjoys an environmentally greener and safer synthetic protocol (Scheme1). The MSNs were characterized by XRD, SEM and FTIR.



Scheme 1

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Fast and efficient protocol for solvent-free acetylationof alcohols with Ac_2O/Zn(II) thiourea complex systems

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Hydroxy compounds are often converted to acetate derivatives for protection or characterization of the structure. For this purpose, acetic anhydride is the commonly used acetylating agent in the presence of an acid or basecatalyst. A literature review shows that most of the utilized methods suffer from disadvantages such as long reaction times, harsh reaction conditions,air sensitive and toxic reagents and formation of side products[1,2]. Therefore, the development and introduction of fast and more efficient methodsusing safer reagents is still in demand.

In this context, we found that the combination system of acetic anhydride and catalytic amounts of Zn(II) thiourea complexes [$Zn(OAc)_2(TU)_2$ and $ZnSO_4(TU)_3$] fast and efficiently converts different aliphatic and aromatic alcohols to their ester acetates.All reactions were carried out in an oil bath (45-50 °C) under solvent-free conditions giving the corresponding acetatesin high to excellent yields within 8-30 min (Scheme1).

$$\mathrm{ROH} \xrightarrow[\text{Oil bath (45-50 °C), 8-30 min, 90-97\%}]{\text{Ac}_2\text{O (11 mmol), Zn(II) Cat. (0.03 mmol)}} \mathrm{ROCOCH_3}$$

Scheme 1

References:

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Heterogenized copper nano catalysts for *N*-arylation of *N(H)*-heterocycles with aryl halides

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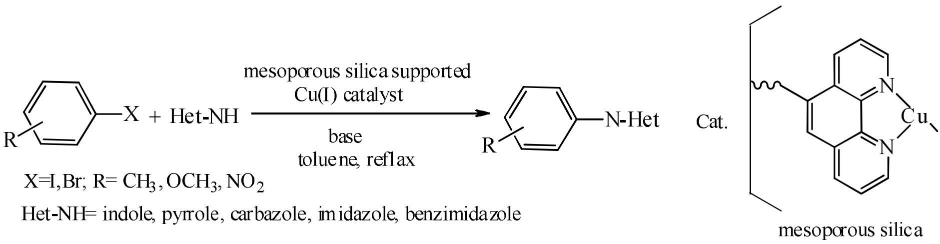
Transition-metal-catalyzed arylation of *N-H* heterocycles with aryl halides is a key tool for carbon–heteroatom bond formation in organic synthesis [1]. Among the reactions, copper and palladium catalyst combined with a ligand display high activity [2,3].

Most of the above methodologies are homogeneous in nature, where recyclability of the catalyst could not be achieved and moreover additional stabilizing ligand or metal is required.

Herein we report a recoverable and efficient mesoporous silica supported phenanthroline-Cu(I) catalyst, which exhibits a high catalytic activity in *N*-arylation of N-H heterocycles with aryl halides (Scheme 1).



Scheme 1

Typically, the mixture of aryl halides, *N-H* heterocyles, base and catalyst in toluene was stirred at 110°C for specified times. After the completion of the reaction, the catalyst was filtered off and the resulting residue was purified. Yields of the reactions were excellent and all the products were characterized by ^{1}H and ^{13}CNMR spectra.

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Selective mono α-bromination of acetophenone with NBS in presence of sulfuric acid immobilized on molecular sieve 4Å

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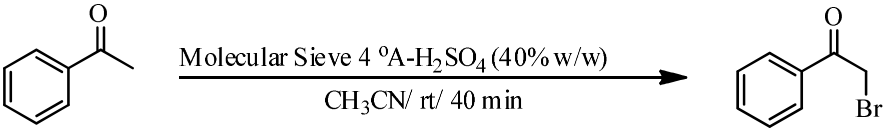
The α-bromination of carbonyl compounds containing α-hydrogen is an important transformation in synthetic organic chemistry [1]. Therefore, various α-bromination protocols of carbonyl compounds [2] have been developed including the basic method using Br_2 [3].

In this context, the unfriendly and dangerous nature of bromine, encouraged us to introduce a new protocol using N-bromosuccinimide under mild reaction conditions. So, we found that α-bromination of acetophenones could be successfully carried out in the presence of immobilized sulfuric acid on molecular sieve 4 Å (40% w/w) in CH_3CN at room temperature (25 °C). The corresponding α-brominated products were obtained in high to excellent yields during 40-90 min (Scheme1).



Scheme 1

References:

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Immobilized nanocrystalline TiO_2/Hydroxylapatite (HA) on magnetic BSA (Bovine Serum Albumin) (NCTHMB): a reusable and efficient green catalyst for the synthesis of pyranopyrazole derivatives in water

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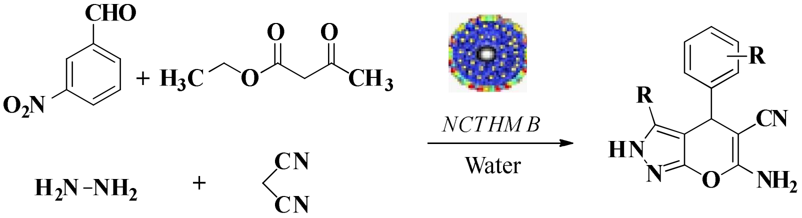
Heterogeneous catalysis is generally preferred to homogeneous catalysis mainly because of the easy recovering and possible recycling of the catalyst, simple experimental procedures, and minimization of chemical wastes as compared to the liquid phase counterparts. It seems that nanomagnetic can be a good candidate as a support material for heterogeneous catalysts, because of easy synthesis, high surface area, facile separation by magnetic forces, low toxicity and cost [1].

In this work, an efficient and ecofriendly four component condensation protocol in aqueous medium at room temperature in the presence of nanocrystallineTiO_2/HA based on magnetic BSA (NCTHMB) for the synthesis of pyranopyrazole derivatives has been reported. As shown in this study, NCTHMB catalyst displays high reactivity in preparation of pyranopyrazoles in water, and it can be further used for at least 5 runs. Operational simplicity, low cost, high yields, environmental friendliness, wide applicability and reusability of the catalyst are the key features of this methodology (Scheme 1).



Scheme 1

References:

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DABCO tribromide supported on magnetic nanoparticles as a new tribromide type catalyst for the synthesis of benzimidazoles

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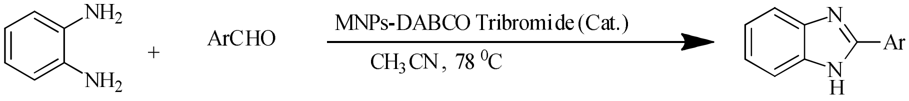
Magnetic nanoparticle-based materials (MNPs) are ideal supports for the immobilization of catalysts, since they can be recollected by using an external magnet [1].

As an alternative reagent or catalyst to the toxic liquid bromine, a wide variety of organic ammonium tribromides (OATBs) were designed [2]. However, recoverability and reusability of OTBs catalysts are high challenge for their application in organic reactions.

Benzimidazole derivatives are important class of heterocyclic compounds that exhibit a wide range of biological properties [3]. Numerous methods have been reported in the literature for the synthesis of benzimidazoles [4]. Although these protocols represent considerable progress, however, the recovery and reusability of the catalyst remains a major problem with reported method. Based on our previous experience about *N*-halo catalystas a source of halonium ion [5] and magnetically recoverable nanocatalyst [6], herein, we report the first example of magnetic nanoparticles-supported OTBs through the immobilization of a DABCO tribromide on magnetic nanoparticles Fe_3O_4 (MNPs-DABCO tribromide) as a magnetically recoverable OTBs catalyst. Also, the catalytic activity of MNPs-DABCO tribromide was investigated in the synthesis of benzimidazoles from the condensation of o-phnylenediamines with aromatic aldehydes respectively (Scheme 1).



Scheme 1

This procedure has several advantages: (1) The preparation and separationof MNPs-DABCO tribromide is simple (2) MNPs-DABCO tribromide is reused for several times (8 runs) with little loss of activity

Refrences:

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Fe_3O_4@CS-SO_3H NPs as an efficient and reusable magnetic catalyst for green synthesis of aminochromenyl phosphonates

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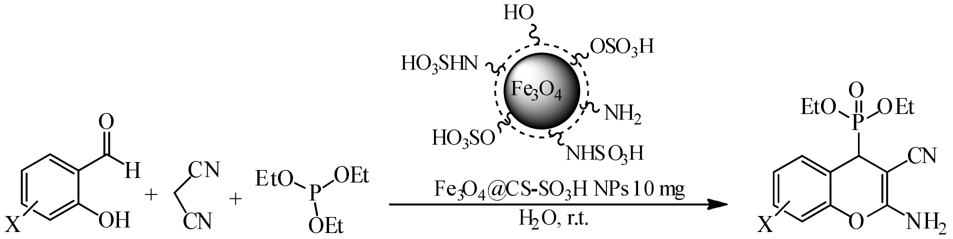
Highly dispersed chitosan-coated nano Fe_3O_4 core-shell structures (Fe_3O_4@CS NPs) are prepared simply through in situ co-precipitation of Fe^{3+} and Fe^{2+} ions via NH_4OH in an aqueous solution of chitosan [1-2]. Treatment of Fe_3O_4@CS NPs with chlorosulfonic acid leads to the formation of Fe_3O_4@CS-SO_3H NPs which exerts excellent catalytic activity toward one-pot, three-component synthesis of 2-amino-4H-chromen-4-yl phosphonate derivatives [3-4]. The core-shell structure and the composition of produced magnetic nanocatalyst are analyzed using FT-IR, XRD, TGA, VSM, ICP, SEM, TEM and BET. The results reveal that the unique heterogeneous Fe_3O_4@CS-SO_3H NPs appears as an excellent acid catalyst which produces high yields, impressive turnover number (TON) and turnover frequency (TOF) values with good recyclability without significant loss of the activity. Moreover, the proposed green synthetic method takes advantage of nontoxic reagents in an aqueous media through a simple procedure.



Scheme 1

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Peripherally substituted Cu-benzopyrazinoporphyrazines with red-shift in UV–Vis

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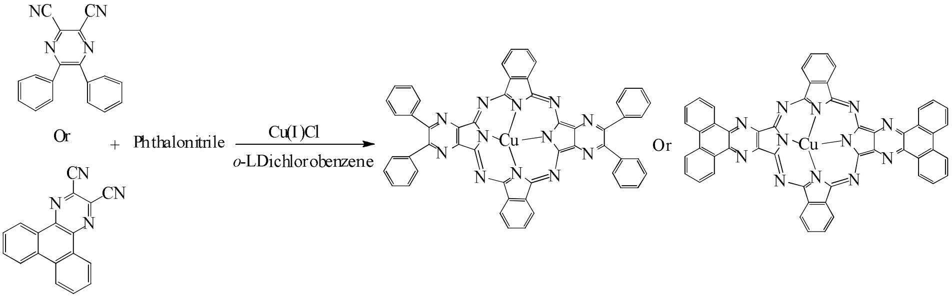
Synthesis, evaluation and application of porphyrazines (Pzs) and correlated structures modified by peripheral substituent attachments, particularly if be active in the visible or near-infrared region of light, have been a highly active research topic in recent years. Other improved methods such as; immobilization of metal complexes onto solid supports and binuclear annulations of porphyrazines as great interesting subjects have been reported too. These compounds have Main applications in diverse areas like photodynamic therapy (PDT), dyes, liquid crystals, photosensitizers, anticancer, anti AIDS, DNA cleavers, photochromism, photocatalyst and etc [1-8].

In the this work, some new Cu-benzopyrazinoporphyrazines with red-shifted λ_{max} and high yields, were synthesized using premade 2,3-dicyanopyrazine derivatives via an one-stage and synchronized cross cyclic-tetramerization way. Resulted complexes are estimated to be valuable photosensitizers and reagent for PDT (Scheme 1).



Scheme 1

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Synthesis of azines catalyzed by tungsten hexachloride-montmorillonite: green design methodology

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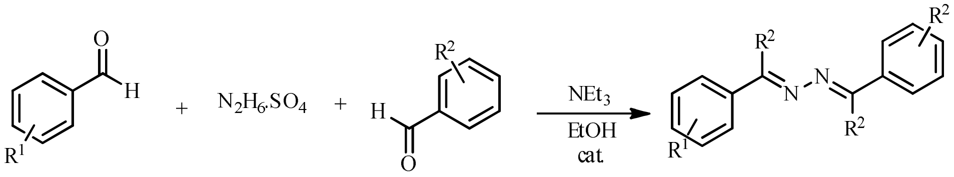
Azines, $R^1R^2C=N–N=CR^1R^2$ have attracted great attention in organic synthesis as they are good synthons to obtain heterocyclic compounds. Azine derivatives constitute an important class of compounds with unexpected biological activities [1,2]. A number of procedures have been reported for the synthesis of azines, but most of them require elevated temperatures and complex catalysts. Therefore, the search continues for a better catalyst for the synthesis of azine in terms of operational simplicity, reusability, economic viability, and greater selectivity [3].

Herein, we would like to report asymmetric azine derivative synthesis catalyzed by tungsten hexachloride-montmorillonite as a nanocatalyst. The attractive advantages of the present process are mild reaction conditions, short reaction times, easy isolation of products and good yields. (Scheme 1).



Scheme 1

References:

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The application of magnetically nanocatalysts for the synthesis of bis-indoles and protection/deprotection of alcohols as TMS-ethers

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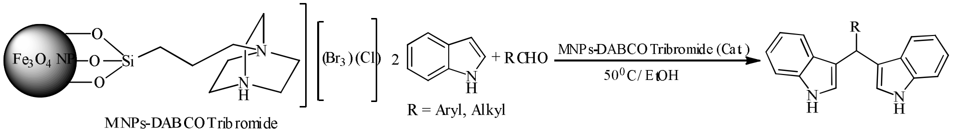
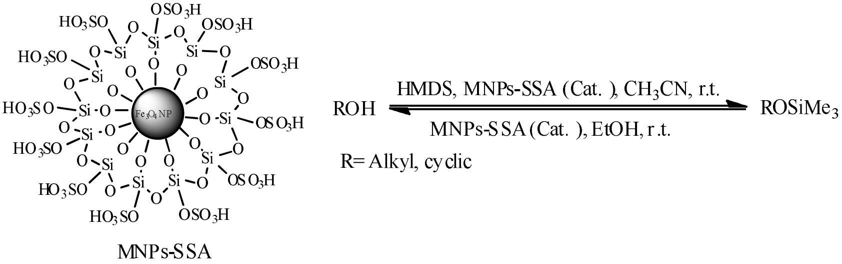
By using magnetic nanoparticles as heterogeneous catalyst bed separation and reuse makes it easier and more effective. Recently, due to the unique characteristics of the magnetic catalyst and its application in catalytic reactions has been discussed [1].

Bis-indoles improves estrogen metabolism and destroying the cancer cells [2]. As well as antibiotics used in the pharmaceutical field [3]. In this research, DABCO-Tribromide supported on magnetic nanoparticles Fe_3O_4 (MNPs-DABCO Tribromide) has been applied as a new magnetic nanocatalyst for the synthesis of bis(indolyl)methane (BIMs) via electrophilic substitution of indoles with aldehydes in CH_3CN at 50 °C (Scheme 1).



Scheme 1

Among the routinely employed methodologies for the protection of hydroxyl groups in organic chemistry, silylation undoubtedly plays a major role, from both analytical and synthetic point of views [4]. Silyl ethers are resistant to oxidation and are easily deprotected to provide the free alcohols [5]. In this research, a mild, simple and convenient procedure for the protection and deprotection of alcohols as TMS-ethers using silica sulforic acid supported on magnetic nanoparticles Fe_3O_4 (MNPs-SSA) as a reusable magnetic nanocatalyst under mild conditions was described (Scheme 2).



Scheme 2

In summery, the notable advantage of these catalysts are simple synthesis, non-toxic, high activity, recoverable and reusable by external magnet.

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The Mizoroki-Heck reaction catalyzed by multi-walled carbon nanotubes (MWCNTs) functionalized with a palladium (II)-Schiff base complex

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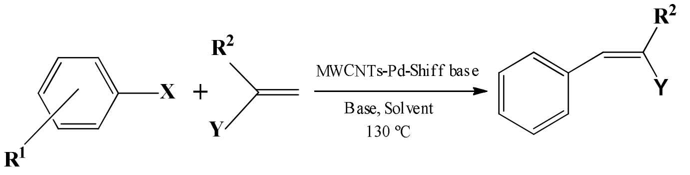
Palladium-catalyzed Csp^2-Csp^2 coupling reactions are widely used for organic synthesis. For instance, vinyl substitution (The Heck reaction) is one of the most important, reliable, and general reactions for C-C bond formation with applications in the areas of bioactive compounds, natural products, and high-performance materials. The Heck reaction is usually carried out in the presence of bulky phosphine ligands, which give Pd(0) species and accelerate the reaction rate. However, many phosphines can be sensitive to air and moisture with conversion to, for example, phosphine oxide species [1].On the basis of these considerations, it is important to developrewarding catalytic systems that meets the goals of high selectivity and high activity to aryl halides [2].The air- and moisture-stable, phosphine-free and reusable multi-walled carbon nanotubes (MWCNTs) functionalized with a palladium(II)-Schiff base complex is reported in this work as efficient catalyst for the Heck coupling of various aryl halides with alkenes. Activated and non-activated aryl halides provide the good to excellent yields of the corresponding styrenes. The catalyst could be recovered and reused for four reaction cycles. The results of Heck reaction exhibited a high selectivity favoring the *trans* product.



R^1= H, Alkyl, Aryl, -OR, -NO$_2$, -CN, Aldehyde
R^2= Aryl, -CO$_2$R, -CN
X= Br, Cl, I
Y=H, Alkyl

Scheme 1

References:

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Magnetic MCM-41 as an efficient reusable heterogeneous catalyst for one-pot three-component synthesis of bioactive derivatives of pyridopyrimidine-2-thiones & biological evaluation for their antitubercular activity

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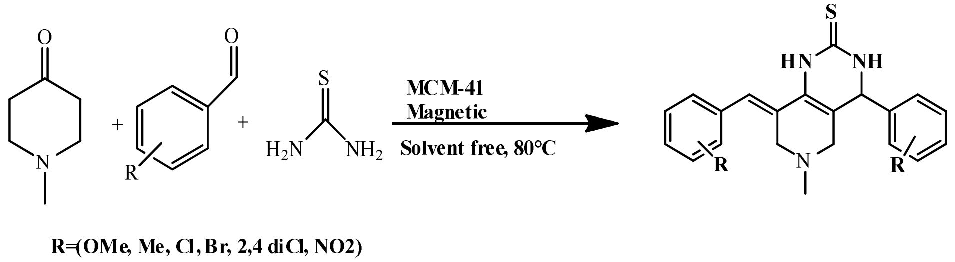
Increasing multidrug resistance in Mycobacterium tuberculosis continues to diminish the number of effective drugs available for treatment of active tuberculosis. Although there are a few novel products in clinical development, an active, robust pipeline of new chemical entities is critical to discovery of medicines to dramatically improve or shorten length of therapy via new mechanisms of action.

The pseudo four-component domino reactions of N-metyl-4-piperidones, substituted aromatic aldehydes and thiourea in the presence of Magnetic MCM-41 under solvent-free conditions afforded pyridopyrimidine-2-thiones in almost quantitative yields; an efficient and clean method with simple workup. The synthesized compounds were screened for their in-vitro activity against Mycobacterium tuberculosis H37Rv [1]. They are more active than the first line antitubercular drugs like ethambutol and ciprofloxacin, but still less active than rifampicin and isoniazid. In this project it is attempted to design new derivatives with more activity in comparison with first line drugs by using new nano-catalyst (Scheme 1).



Scheme 1

References:

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Preparation and characterization of phenol-formaldehyde resin using nano-silica sulfuric acid as an eco-friendly catalyst

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Phenol-formaldehyde resin is one of the versatile commercial polymers from the beginning of polymer invention and due to such a history and wide variety of applications and because of biocompatible production processes, great efforts have been made optimize a more secure and environmental friendly production method for this resin [1]. A catalyst (acidic or basic) is required in order to produce the mentioned resin. Since the liquid acid catalysts are hard to work under high pressure and high temperatures, with toxic vapors, corrosion on devices and process line, difficulty in transportation, difficulty in catalyst recycling and low purity of products, thus these catalysts are not appropriate [2-5].

In this study, we tried to produce phenol-formaldehyde resin in the presence of nano-silica sulfuric acid which is a proper solid catalyst and has able to completely segregate the products causes significant effects on corrosion less in production devices, minimizing friction and costs, higher security, biocompatibility and ease of recycling. We wish report a new methodology for synthesis of mentioned resin in the presence of nano-silica sulfuric acid as an eco-friendly catalyst. The product is achieved in good yield under mild condition and identified by FT-IR, TGA and DSC techniques.

$$\text{ArOH} + \text{HCHO} \xrightarrow[70\ ^{\circ}\text{C},\ \text{CH}_3\text{COCH}_3,\ \text{reflux}]{\text{Nano-silica sulfuric acid}} \text{Phenol-formaldehyde Resin}$$

Scheme 1

References:

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Melamine-formaldehyde supported H^+ catalysed two consecutive aminomethylation at the α-position of the β-dicarbonyl compounds: an easy access to hexahydropyrimidines and its spiro analogues

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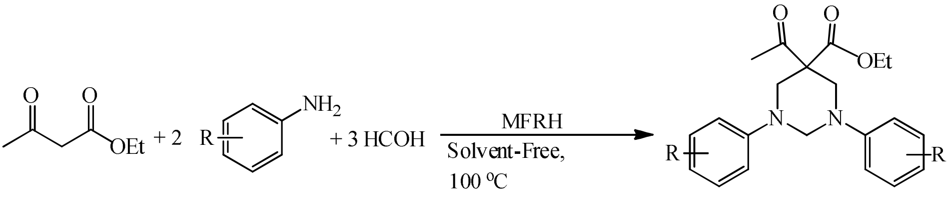
In recent years, multicomponent reactions (MCRs) have received substantial consideration from the organic community for their innumerable advantages over conventional multistep synthesis. These reactions provide instantaneous access to large compound libraries with diverse functionalities [1].

Hexahydropyrimidines containing various natural products and pharmaceutical agents show immense biological activities [2]. Different N-substituted hexahydropyrimidines are synthetic intermediates for spermidine-nitroimidazole drugs. Some suitably substituted derivatives have metal-complexing properties [3]. Classically, hexahydropyrimidines are prepared by condensation between substituted propane-1,3-diamines and aldehydes or ketones [4]. There are also a few reports in literature describing the synthesis of hexahydropyrimidine derivatives either by using α, β-unsaturated nitriles or by the reaction of substituted alanine and carbamide [5].

In this methodology, 1,3-dicarbonyl compounds, amines and formaldehyde react in one step in the presence of melamine-formaldehyde supported H^+ [MFRH] under solvent-free conditions at 100 °C temperature (Scheme 1).



Scheme 1

References:

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Lemon juice as a real green catalyst for condensation of cyanoacetamide and ethylcyanoacetate with aromatic aldehyde

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Concern for the environment demands the development of ecofriendly and economical processes wherein even slightly hazardous by-products are not desirable.

In the development of new syntheses, ecological points of view must be taken into account. A number of organic reactions employing natural catalysts such as clay [1,2] and phosphates [3] are reported in literature. In accordance with this, we report the Knoevenagel condensation of active methylene compound with aromatic aldehydes in the presence of lemon juice, a natural catalyst, without any solvent (Scheme 1).

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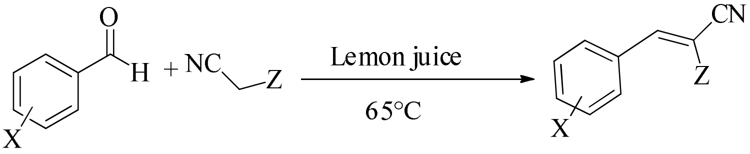

$Z: CO_2Et, CONH_2$

Scheme 1

References:

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Melamine-formaldehyde supported H^+ catalyzed N-formylation of amines under solvent-free conditions

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The formyl group is an important amino protecting group in peptide synthesis [1]. Formamides are important intermediates in organic synthesis that have been used in the synthesis of biological active compounds [2] and nitrogen-bridged heterocycles. They are also widely used as precursors for the preparation of isocyanates, formamidines, and nitriles [3].The most common methods for the synthesis of formamides are the reaction of amines with formic acid, in the presence of many catalysts [4]. These methods are suitable for certain synthetic conditions; however, many of these procedures are associated with one or more disadvantages such as expensive reagents, longer reaction times, tedious work-upprocedure, low selectivity, and large amounts of catalysts which would eventually result in the generation of large amounts of toxic waste.

Recently, melamine-formaldehyde supported H^+ (MFRH) has emerged as a promising solid acid catalyst for some acid-catalyzed reactions. This catalyst is safe, easy to handle, and environmentally benign, and presents fewer disposal problems. MFRH as a solid acid catalyst is prepared from the reaction of melamine-formaldehyde with hydrochloricacid at roomtemperature.Herein, we present a novel, mild, and efficient method for the N-formylation of amines using amines and formic acid in the presence of MFRH as a catalyst (Scheme 1).

$$RNH_2 + HCOH \xrightarrow[\text{Solvent-free, } 100\,^{0}C]{\text{MFRH}} RNHCOH$$

Scheme 1

References:

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Chiral oxo-vanadium (+)-pseudoephedrine complex supported on magnetic nanoparticles: an efficient, recyclable novel catalyst for eco-friendly oxidation of sulfides and cyanosilylation of carbonyl compounds

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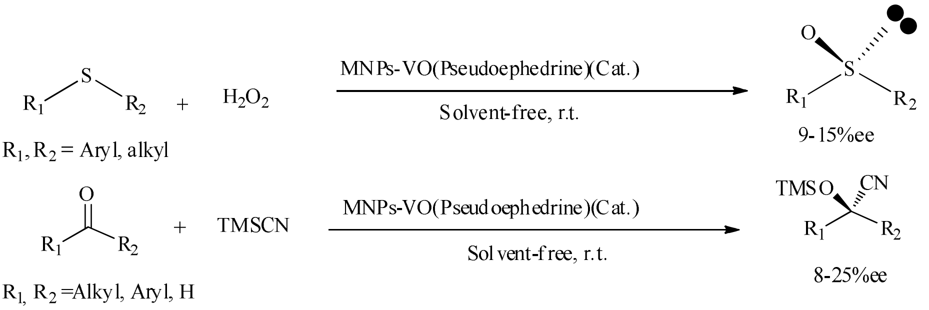
Email: b_atashkar@yahoo.com

Magnetic nanoparticles (MNPs) are considered as ideal supports for the heterogenization of homogeneous catalysts, since they can be recollected by using an external magnet [1].

The chemoselective preparation of chiral and achiral sulfoxidesis extremely important in organic chemistry, because sulfoxides are useful synthetic intermediates for the construction of various chemically and biologically significant molecules [2].

asymmetric addition of a cyanidesource to carbonyl compounds with a chiral catalyst representsone of the most appealing approaches to enantiomericallyenriched cyanohydrins, which can be readily transformed into number of key functional groups [3].Although a wide variety systems are available for sulfoxidation and cyanosilylation reactions however separable and reusable of catalysts or reagents are difficult.

In continuation of our studies on magnetic nanocatalysts [4], herein, we prepared a new chiral oxo-vanadium (V) (+)-Pseudoephedrine complex supported on magnetic nanoparticle Fe_3O_4, and examined its catalytic properties in the oxidation of sulfides to sulfoxides and cyanosilylation of carbonyl compounds (Scheme 1).



Scheme 1

In summary, we have synthesized MNPs-VO (Pseudoephedrine) as a novel catalyst for the oxidation of sulfides to sulfoxides and cyanosilylation of carbonyl compounds for the first time. The significant advantages of these procedures are (a) the use of the eco-friendly, cost-effective, highly reusable and chemically stable catalyst, (b) mild reaction conditions and very easy work-up.

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An efficient, one-pot and solvent-free synthesis of 2-aryl/alkyl-4(3H)-quinazolinones

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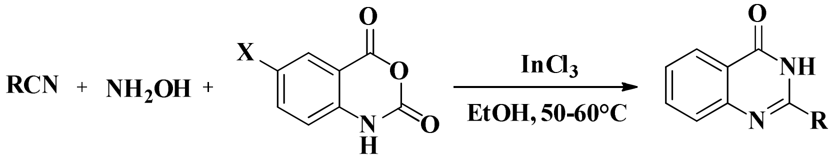
4(3H)-Quinazolinones, an important class of fused heterocyclic compounds, have attracted much synthetic attention because of their wide range of pharmacological and therapeutic activities such as anticancer,3 antiinflammatory anticonvulsant, antiulcer, and hypolipidemic. Some quinazolinones have been reported as potent chemotherapeutic agents in the treatment of tuberculosis [1-2].

Herein we have developed a novel and one-pot reaction of nitriles, hydroxylamine, and anthranilic acids for the preparation of 4(3H)-quinazolinones of potential synthetic and pharmacological interest. The simplicity of the starting materials, excellent yields of the products, neutral reaction conditions as well as solvent-free condition is the advantages of this method. We believe that this experimentally simple approach could be a useful addition to reported methods [3]. (Scheme 1).



Scheme 1

References:.

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Efficient acylation of alcohols by acetic acid in the presence of benzyl triphenyl phosphonium tribromide

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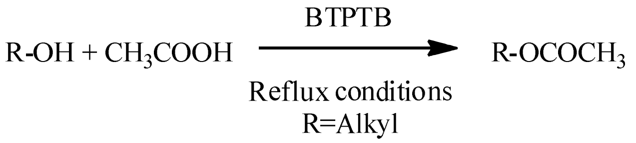
The acylation of alcohols is one of the most frequently used transformations in organic synthesis as it provides an efficient and inexpensive means for protecting hydroxyl group in a multistep synthetic process [1]. Acylation is usually performed employing acid anhydrides or acid chlorides in the presence of stoichiometric amounts of bases [2]. Some procedures have been developed wherein Lewis acid catalysts. However, most of these methods either suffer from problem in recovery of the large amount of soluble bases or acids or from the excessive use of acetic anhydride or acid chloride as acylating agent.

In continuation of our work to develop new synthetic methodologies [3], we wish to herein report an efficient and facile procedure for the direct acetylation of alcohols catalyzed by Benzyl triphenylphosphonium tribromide (BTPTB) under reflux conditions (Scheme 1).



$$\text{R-OH} + \text{CH}_3\text{COOH} \xrightarrow[\substack{\text{Reflux conditions} \\ \text{R=Alkyl}}]{\text{BTPTB}} \text{R-OCOCH}_3$$

Scheme 1

In conclusion, we have developed a simple phosphonium tribromide catalyst for acetylation of alcohols using inexpensive and readily available acetic acid as acetylating agent in base free conditions.

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The application of $La(NO_3)_3 .6H_2O$ and $Ce(NO_3)_3 .6H_2O$ catalysts on nitration of phenolic compounds

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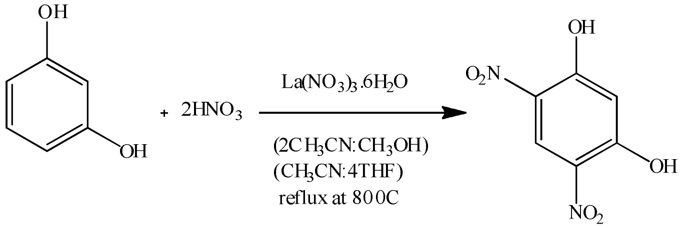
Nitration of organic compounds has long been a very active and rewarding area of research and is the subject of a large body of literature [1]. Nitro-aromatic compounds are extensively utilized and act as chemical feed stocks for a wide range of useful materials such as dyes, pharmaceuticals, perfumes and plastics [2]. Nitration of phenols using the traditional procedure of nitric acid in sulfuric acid, generally gives complex mixtures containing o- and p-nitro phenols, dinitrated phenols, along with inextractable tars of phenolic oxidation products [3].

In this project, a new method has been developed for nitration of phenolic compounds with increasing the selectivity of the reaction and detection of catalytic properties of Ce(Ш) and La(Ш) nitrate. Phenolic compounds have reacted with nitric acid in the presence of catalytic amounts $La(NO_3)_3.6H_2O$ or $Ce(NO_3)_3.6H_2O$ and acetonitrile:methanol as solvent system via reflux at 80 ^{0}C. 2,4-Dinitrophenol, 4,6-dinitroresorcinol (Scheme 1) and 2,4,6-trinitroresorcinol have been synthesized.



Scheme 1

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$CuFe_2O_4$ nanoparticles as a highly efficient and magnetically recoverable catalyst for the synthesis of 2H-indazolo[2,1-b]phthalazine-triones under solvent-free conditions.

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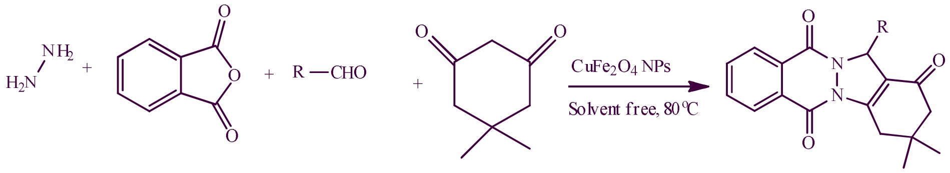
Among a large diversity of heterocyclic compounds, heterocycles containing phthalazine moiety are of interest because they show some pharmacological properties and biological activities [1-2]. Therefore the development of simple methods for the synthesis of 2H-indazolo[2,1-b]phthalazine-triones is considered very important. In recent years, nanoparticles have attracted considerable attraction with the aim of finding meaningful applications in organic reactions [3].

Herein, we report the use of $CuFe_2O_4$ nanoparticles as an efficient catalyst for the preparation of 2H-indazolo[2,1-b]phthalazine-1,6,11(13H)-trione derivatives by the four-component condensation reactions of phthalic anhydride, hydrazine monohydrate, aldehydes and dimedone under solvent-free conditions in good to excellent yields (Scheme 1).



Scheme 1

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Single-step synthesis of hydantion derivatives as precursors for α- amino acids

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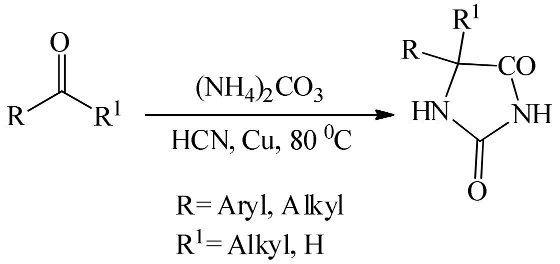
The imidazolidine-2,4-dione ring or hydantoin has been extensively studied. This five-membered heterocyclic ring containing a reactive cyclic urea core is present in a wide range of biologically active compounds [1]. Some hydantoin compounds are potent inhibitors of muscle and liver glycogen phosphorylase, metalloproteinase and HIV protease enzymes. Hydantoins are also used as herbicides, antibiotics and as DNA binding compounds [2]. The observed activities arise from the hydantoin heterocycle, but the different ligands attached to it are determinant in these properties [3]

In this work, a new strategy has been introduced for the preparation of hydantion derivatives. A variety of hydantoins have been prepared via combination of aldehydes or ketones with ammonium carbonate and hydrogen cyanide in the presence of a catalytic amounts of Cu at 80 ^{0}C (Scheme 1).



Scheme 1

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Synthesis of imidazo[1,2-*a*]pyridines using recyclable acidic solid catalyst under solvent-free condition

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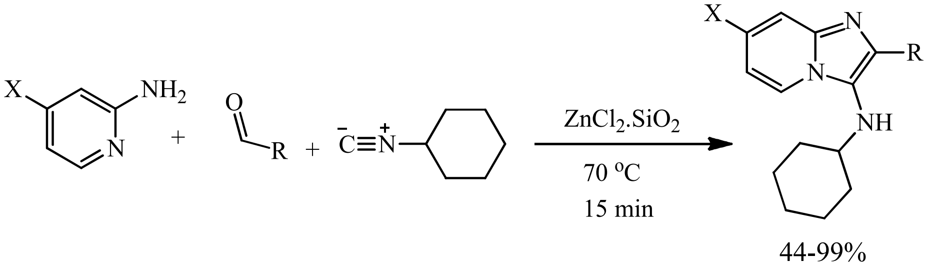
Imidazo[1,2-*a*]pyridine compoundshave received much attention toward to their diverse range of biological activities [1]. Recently more than a few synthetic methods for preparing these compounds based on multicomponent reactions have been reported [2-4]. Although, many of these methodshavecertain disadvantages suchaslong reaction time, complicated work-up, harsh reaction conditions, using of solvent and low yields [2-4].

Heterogeneous catalysts have gained significant attraction dueto economic and environmental considerations [5]. Immobilization ofcatalyst on porous solidsupports has some advantages such asgood dispersion of active reagentsites, cleaner reactions, easier work up and reducing in reaction times. The products were prepared under solvent-free conditions without any additives (Scheme 1). This simple method has many advantages, such as short reaction time, low cost catalyst, excellent yields, solvent-free conditions, and reusabilityof catalyst.



Scheme 1

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The oxadiazole-based azo-azomethine dyes; synthesis, biological properties and solvatochromism

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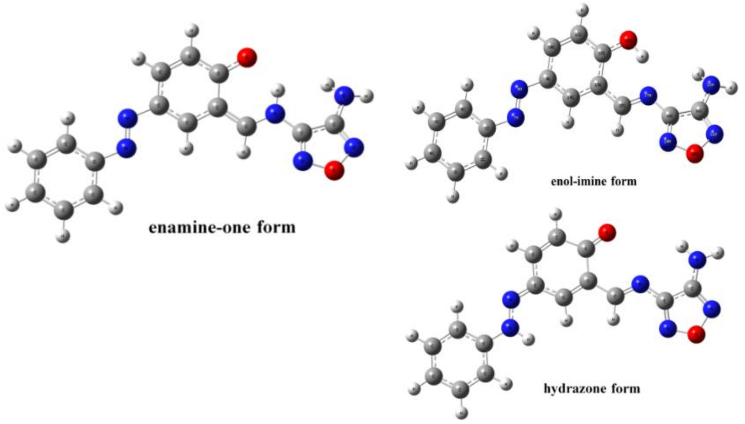
New air stable Schiff base compounds 2-[(4-amino-1, 2, 5-oxadiazol-3-ylimino) methyl) -4-(phenyldiazenyl] phenol (**2a-e**) dyes were prepared via condensation of 2-hydroxy-5-[(E)-(aryldiazenyl)]benzaldehyde with 3,4-diamino-1,2,5-oxadiazole. UV–Vis absorption spectra indicated positive solvatochromism in compound **2a-e** which is dependent on the substitution, nature of solvent, pH and environment temperature. The results indicated that the $\pi \rightarrow \pi^*$ band of these compounds, at 340–383 nm, shows red shift as the polarity of solvent was increased. The Quantum chemical calculations and UV-vis absorption spectra data show that positive solvatochromism of synthesized compounds behavior, which could be due to intramolecular hydrogen bond in enol–keto tautomeric and dipole moment changes



Scheme 1

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A novel modified basic nanocatalyst for the efficient synthesis of trisubstituted pyrimidine derivatives under solvent-free conditions

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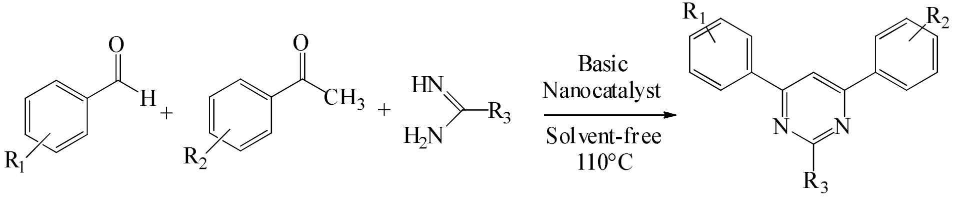
The application of modified mesoporous nanocatalysts in organic synthesis has gained much attention in recent years as an active and highly blossoming area of research. For example, this type of catalysts was applied in the Ullman-type coupling [1], clean O_2 oxidation of alcohols [2] and Heck and Knovenagel reactions [3]. 2,4,6-Triaryl pyrimidine derivatives have attracted considerable interest due to their remarkable pharmacological properties. These compounds were designed and synthesized as potent esterogen receptor binder [4], and antimalarial agents [2]. Therefore, the search for more environmentally benign and versatile synthetic methods for the preparation of this class of heterocycles is still an active area of research in organic chemistry. With a view of the above mentioned points, we wish to report a novel green condition for the preparation of pyrimidine-5-carbonitrile derivative using novel modified and efficient mesoporous nanocatalyst under solvent-free conditions.



Scheme 1

After completion of the reactions, the products were dissolved in ethanol and separated from the catalyst by vacuum filtration with a Buchi funnel. In summary, this methodology appears to be a good alternative to the present methodologies because of using solvent-free conditions, short reaction times, good to excellent yields of products and easy work-up of the products.

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Oxidation of sulfides with UHP catalyzed by (salen) copper (II) complexe heterogenised on mesoporous MCM-41

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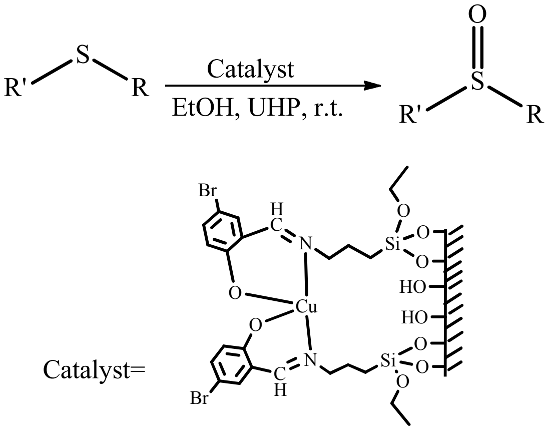
MCM-41 silica spheres were synthesized and functionalized with 3-aminopropyltriethoxysilane (3-APTES). The Schiff-base has been derived from amino groups and 5-boromo salicylaldehyde, then a tetra dentate Cu (II)–schiff base complexes was prepared. This compound was characterized by X-ray diffraction, nitrogen physisorption, UV–Vis spectrometer, transmission electron micrographys (TEM), IR-spectra and TGA/DTA. The prepared grafting Cu-salen-MCM-41 over mesoporous surface was found to be an efficient and selective catalyst for the oxidation of different sulfides into sulfoxides with urea hydrogen peroxide (UHP) with excellent yields at room temperature. The results showed that Cu-salen-MCM-41 is an effective catalyst for the oxidation of sulfides and can be repeatedly used and regenerated without any significant decrease in its catalytic ability.The results shown that the prepared material retained good mesoporous structure and the best catalytic properties (Scheme1).



Cu-Salen-MCM-41

Scheme 1

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Convenient and eco-friendly synthesis of 2,3-dihydroquinazoline-4(1H)-ones using heteropolyacid as a recyclable catalyst

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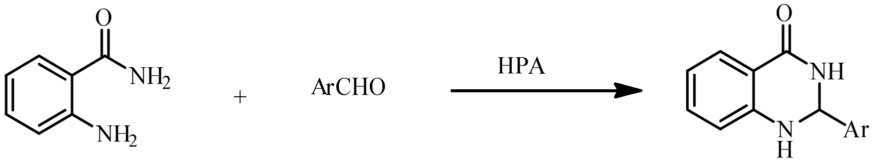
various procedures are reported for synthesis of 4(3H)-quinazolinones [1,2], some drawbacks such as low yields, prolonged reaction time, use of costly reagents or catalysts and use of toxic organic solvents, exist. Thus, the development of an environmentally benign methodology for the synthesis of 4(3H)- quinazolinones is in great demand. In this method after reaction, the catalyst can be recovered and can be and can be recycled at least three times without distinct loss in its catalytic activity.

Melting points were determined on an Electrothermal type 9100 melting point apparatus. IR spectra were recorded using a 4300 Shimadzu spectrophotometer with KBr plates. ^{1}H NMR spectra were recorded on a Bruker DRX500 spectrometer. The products were isolated and characterized by comparison of physical and spectral data with those of known samples.

It should be noted that, this method is effective for the preparation of 2,3-dihydro quinazolinone-4(1H)-ones by the condensation of 2-aminobenzamid with aromatic aldehydes using heteropoly acid (Scheme 1).



Scheme 1

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Regioselective ring opening of epoxides using $(NH_2)_2CS/Na_2SO_4$: An efficient approach for the synthesis of thiiranes under reflux conditions

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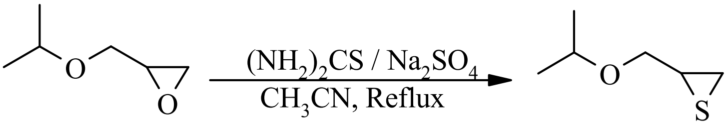
Thiiranes are probably the most interesting class of cyclic sulfides both from a theoretical and synthetically point of view [1]. They serve as useful precursors for the synthesis of olefins [2] and other functional group moieties [3] and so their synthesis is of fundamental interest. The most efficient route reported so far is based on the conversion of oxiranes into the corresponding thiiranes by an oxygen-sulfur exchange reaction. Sulfur introducing agents such as inorganic thiocyanates, thiourea [4-5].

Na_2SO_4 is certainly one of the most interesting reagents for the ring opening of epoxides, because it performs lewis acid catalyst role strongly. Sodium sulfate is chemically very stable, being unreactive toward most oxidising or reducing agents at normal temperatures.

Herein, we wish to introduce a simple and efficient method for Conversion of epoxides to corresponding thiiranes with Thiourea supported on Na_2SO_4 under reflux conditions. Thecapability of this synthetic protocol was investigated by the reaction of activated, deactivated, and cyclic epoxides with Thiourea/Na_2SO_4system under the optimized conditions. The epoxides were converted to the corresponding thiiranes in exellent yields within short times (Scheme 1).



Scheme 1

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Synthesis of 2-arylbenzimidazoles using of Fe(3)-Ce(8)-Zr(12)-SBA-15 as nanocatalyst

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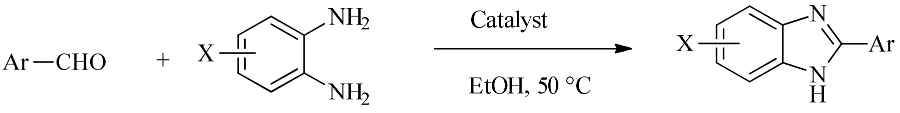
Pure zirconia, ceria and ferric oxide present one great disadvantage: they generally have relatively small surface area and non-uniform pore size. One possibility to achieve the high surface area is to combine a support with appropriate textural properties with these oxides.

In the present work, with the aim of obtaining solid heterogeneous catalysts with uniform mesoporous structure and high surface area, we prepared a multi-component Fe(3)-Ce(8)-Zr(12)-SBA-15 *via* impregnation of pure SBA-15 in appropriate concentrations of aqueous parent salts.

Iron-substituted mesoporous materials have redox properties and unusual activity in alkylation reactions [1]. Cerium, has great potential application for its excellent oxygen restoration and release ability. Mesoporous materials containing zirconium have received considerable attention in heterogeneous catalysis because of their high special surface areas and potential acid properties.

Benzimidazole structural motifs are found in numerous pharmaceutical agents [2] and in materials application [3]. Current clinical examples of benzimidazoles include antihistamines, antiulceratives and topoisomerase inhibitors.

In order to testing of catalyst activity, this nanocatalyst was tested in reaction of 2-arylbenzimidazoles from aryl aldehydes and 1,2-phenylenediamine and respective benzimidazoles obtained in the short reaction times and high yields in the absence of other oxidant.



Catalyst= Fe(3)-Ce(8)-Zr(12) SBA-15

R= H or 4-CH_3

Scheme 1

In summary, Fe(3)-Ce(8)-Zr(12)-SBA-15 is an extremely efficient nanocatalyst for the thesynthesis of 2-arylbenzimidazoles. The advantages are the excellent yields, inexpensive nature and availability of the reagents, easy and clean workup process.

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Propylsulfonic acid functionalized Boehmite nanoparticle for one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones

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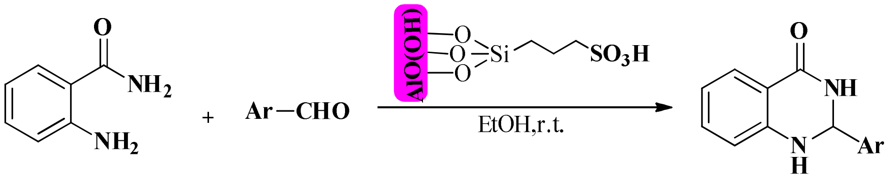
2,3-Dihydroquinazolin-4(1*H*)-ones have been synthesized in high to excellent yields through direct cyclocondensation of anthranilamides and aldehydes in the presence of sulfonic acid functionalized boehmite nanoparticle as a catalyst. Quinazolinone derivatives are a class of fused heterocycles that have drawn much attention due to their potential biological and pharmaceutical activities [1]. A number of classical methods for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones have been reported in the literature [2,3].

Nanoparticles as heterogeneous catalysts have attracted a great deal attention in recent years because of their interesting structure and high catalytic activities [4]. In this context, a new catalyst has been introduced for the preparation of 2,3-Dihydroquinazolin-4(1*H*)-ones (Scheme 1). A variety of 2,3-Dihydroquinazolin-4(1*H*)-ones have been prepared via combination of anthranilamides with arylaldhydes in the presence of a catalytic amounts propylsulfonic acid functionalized boehmite nanoparticle at room temperature.



Scheme 1

In conclusion, we have described a simple and efficient method for the synthesis of 2-substituted 2,3-dihydroquinazolin-4(1*H*)-ones using Bohemite-PrSO_3H as a reusable catalyst. Excellent yields, environmentally friendly procedure, short reaction times, simple work-up procedure, and easy isolation and recycling of the catalyst are some advantages of this method. Hence, it is a useful addition to the existing methods.

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Synthesis of spiro-pyrazole derivatives *via* a three-component reaction from ninhydrin, malononitrile and hydrazonyl chlorides

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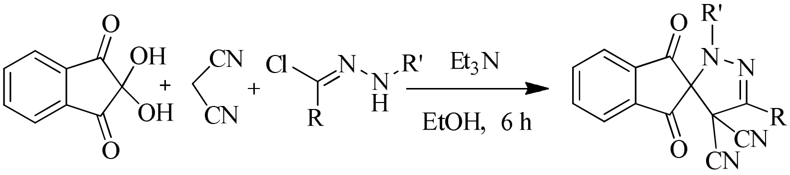
Email: yavarisa@modares.ac.ir

Spiroheterocycles are of considerable interest because the conformational restriction associated to the structural rigidity affects considerably their biological activity such as progesterone receptor modulators, anti-HIV, anticancer, antitubercular, antimalarial, and MDM2 inhibitor [1-3]. Among them, spiropyrazoles are the central structural frame works which are present in numerous bioactive natural products and alkaloids with biological and clinical activities. The biological and synthetic significance places this scaffold at a prestigious position in medicinal chemistry research.

As an extension of these studies [4,5], we report the preparation of highly functionalized spiro-pyrazole derivatives *via* the one-pot domino reactions of hydrazonyl chlorides, ninhydrin and malononitrile (Scheme 1).



Scheme 1

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An efficient and one-pot synthesis of 3,5-disubstituted 1,2,4-oxadiazoles: using polyurethane at room temperature

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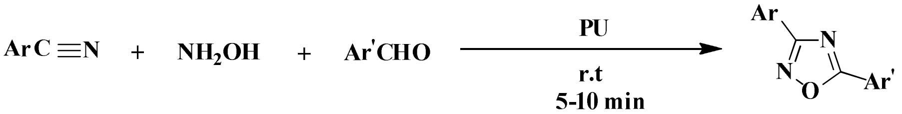
Heterocyclic compounds are valuable natural and synthetic materials that have been used as intermediates and solvents in pharmaceutical, chemical, textile, dye-stuff, petroleum, and photography photography industries [1]. 1,2,4- oxadiazoles are a class of important heterocycles which have been welldocumented throughout the literature due to their biological importance [2].

Polyurethanes (PUs) have been gaining importance in a widerange of applications such as paints, textile, adhesives, glovesand wood finishing because of their good physical and mechanical properties [3].

In this work we report an efficient procedure for the synthesis of 3,5-disubstituted 1,2,4-oxadiazoles via a one-pot reaction between nitriles, hydroxylamine, and aldehydes using of polyurethane (PU) as a catalyst at room temperature (Scheme 1).



Scheme 1

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Catalytic performance of vanadium Schiff base complex - MCM-41 for the oxidative coupling of thiols to disulfides

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Zeolitic molecular sieves decorated with transition metals, mainly by the isomorphous substitution, had attracted great interest in redox catalysis because of their exceptional catalytic activity over various organic compounds [1–3]. Among them, because of the unique one-dimensional channel walls and better stability, synthesis and modifications in MCM-41 materials flourish more than in the other MCM-48 (cubic) and MCM-50 (lamellar) materials, as the former can enhance the reaction of sterically bulkier molecules by the suitable choice of surfactants/organic modifiers. Indeed, the greater flexibility of silica networkenables the incorporation of various higher transition metals into the framework of MCM-41.

In this work we have grafted 3,4-dihydroxybenzaldehyde ligand with vanadium salt onto MCM-41 successfully. Oxidative coupling of different types of mercaptans was investigated. Therefore a disulfides have been prepared in the presence of a catalytic amount (V(IV)-MCM-41) and UHP as oxidant at room temperature (Scheme1).Under these conditions, a various types of mercaptans were selectively and efficiently oxidized to the corresponding disulfides. The V(IV)-MCM-41 catalyst has been recovered from the reaction mixture and has been reused successively several times under the same r conditions.

$$\mathrm{RSH} \xrightarrow[\text{Acetonitril, r.t}]{\text{V-MCM-41/UHP}} \mathrm{RSSR}$$

Scheme1

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One-pot synthesis of 2-amino-3-cyano-4-aryl-5,10-dioxo-5,10-dihydro-4H-benzo[g]chromene derivatives using *O*-benzendisulfunimide as green and recyclable catalyst

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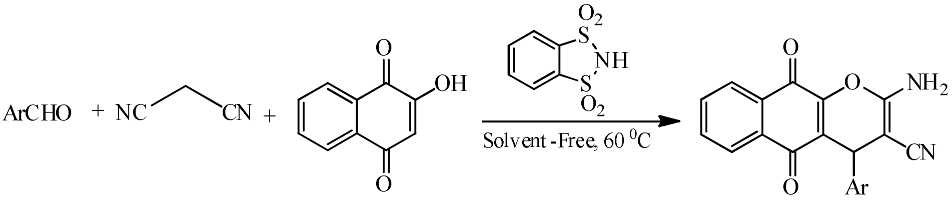
Naturally occurring naphthoquinones comprise an important class of natural products with a wide range of biological activity arising from their capability to cause DNA modification. Among the structurally diverse naphthoquinone natural products, lapachol and several 1,4- and 1,2-naphthoquinones are ass ociate with diverse biological activities and are components of antibacterial, fungicidal, antimalarial, trypanocidal, antiparasitic, and antitumoral agents [1-2].

In continuation of our interest in the application of solid acids in organic synthesis [3], we herein present efficient and environmentally benign protocols for the synthesis of 2-amino-3-cyano-4-aryl-5,10-dioxo-5,10-dihydro-4H-benzo[g]chromene derivatives using *O*-benzendisulfunimide under solvent-free conditions at 60 °C [4-5] (Scheme 1).



Scheme 1

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Sulfonated graphene oxide: an a highly efficient solid acid catalyst for the one-pot synthesis of 3,4-dihydropyrimidin-2(1H)-ones

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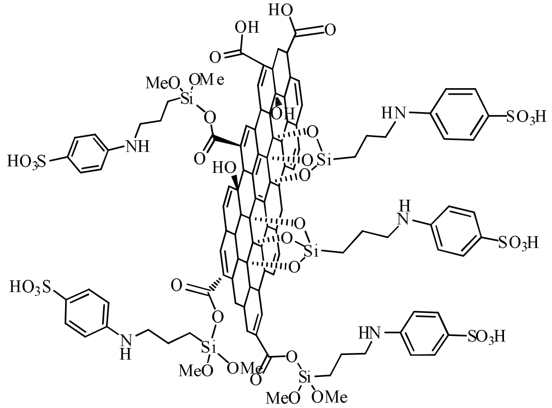
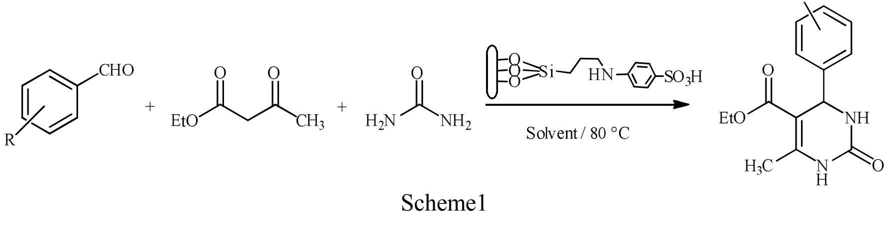
Multi-component reactions (MCRs) are of increasing importance in organic and medicinal chemistry [1]. The Biginelli reaction is one of the most useful examples of MCRs, gaining increasing importance in organic and medicinal chemistry due to their capacity to generate multi-functionalized products including 3,4-dihydropyrimidin-2-(1H)-ones (DPMs) [2-3].

In this paper, Sulfonated organosilane functionalized graphene oxides (SSi-GO) synthesized through thegrafting of graphene oxide (GO) with 3-(chloropropyl) trimethoxysilane and subsequentimmobilized sulfanilicacid (Scheme 1), have been used as acidic solid catalyst in Preparation 3,4-Dihdropyridine-ones (thiones).





Scheme1

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Catalytic oxidative coupling of thiols to disulfide using manganese(II) complex with bidentate O,N-donor Schiff base anchored on MCM-41 ligand and UHP oxidizing agent

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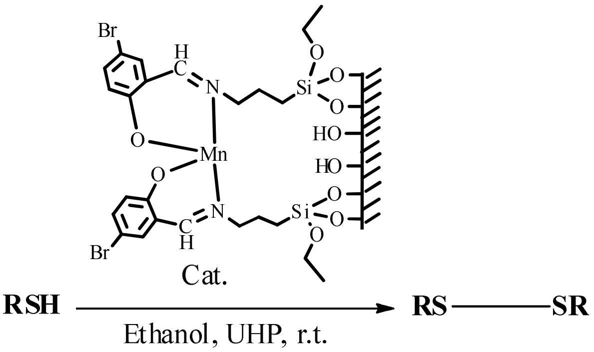
In recent years ordered mesoporous silica, for example, MCM-41 has been receiving much attention as solid support [1]. Properties like high surface area, large pore volume and well-defined hexagonal arrays of channels and cavities [2] of mesoporous silica made it suitable support for anchoring of metal. Complex Mn(II)–Schiff base complex was modified over mesoporous silica through the reaction of mesoporous silica functionalized 3-aminopropyltriethoxysilane (3-APTES) and 5-boromosalicylic aldehyde via schiff base condensation [3, 4]. The surface properties of the functionalized catalyst was analyzed by a series of characterization techniques like elemental analysis, XRD, IR-spectra, N_2 adsorption–desorption,TG-DTG and DR UV–vis. PXRD Adsorption–desorption analysis shows that the meso structure of silica remains intact after modification, while spectral technique show the successful anchoring of the neat complexes inside the porous silica support. The catalytic activity of the functionalized metal-salen complex was examined in the coupling of thiols. Further, the catalyst (Mn-Salen-MCM-41) was recycled three times in the oxidation of thiol and no major change in the conversion and selectivity is observed, which shows that the post-grafted metal-salen complex is stable under the present reaction conditions.



Scheme 1

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A novel three component synthesis of 2-amino-4*H*chromene derivatives using nano $CuInS_2$ catalyst

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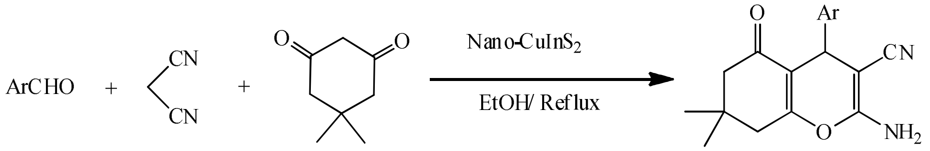
2-Amino-4H-chromenes and their derivatives are of considerable interest as they possess a wide range of biological properties, such as spasmolytic, diuretic, anticoagulant, anticancer and antianaphylactic activity. In addition, they can be used as cognitive enhancers for the treatment of neurodegenerative diseases, including Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, Parkinson's disease, AIDS associated dementia and Down's syndrome as well as for the treatment of schizophrenia and myoclonus. The increasing attention during recent decades for environmental protection has led modern academic and industrial groups to develop chemical processes with maximum yield and minimum cost whilst using nontoxic reagents, solvents and catalysts.

One of the tools used to combine economic aspects with the environmental ones is the multicomponent reaction (MCR) strategy; this process consists of two or more synthetic steps which are carried out without the isolation of any intermediate, thus reducing time and saving money, energy and raw materials.

We performed the synthesis of 2-amino- 4H-chromenes through a multicomponent reaction employing $CuInS_2$ as a nontoxic catalyst in ethanol as a greener solvent (Scheme 1).



Scheme 1

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Catalytic synthesis of spiroacenaphthylene derivatives with using of DABCO as a green catalyst in aqueous media

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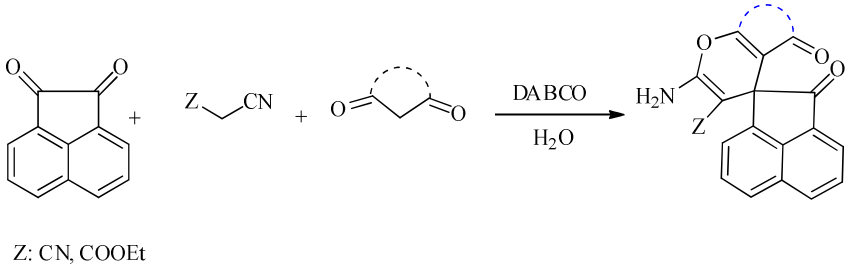
Multicomponent reactions (MCRs) are counted as one of the main synthetic strategies in organic, combinatorial, and medicinal chemistry mainly the synthesis of complicated molecules, in which three or more different starting materials come together in a single reaction vessel to give a final product containing substantial elements of all the reactants [1]. Pyran derivatives, a great part of many natural products [2], are identified for its wide array of biological activities such as antiviral, antitumor, antibacterial, spasmolytic. Also, recent discovery have propose that the compounds having 4H-pyran core are useful for the treatment of Alzheimer, Schizophrenia, and Mycolonous diseases [3].

In this work, we report an efficient method for three component reaction of acenaphthequinone, malononitrile or ethylcyanoacetate and variety of CH-acid compounds in water as green solvent and using the 1,4-diazabicyclo[2,2,2]octane (DABCO) as a catalyst. This procedure offers several advantages including high yields, an environmentally friendly procedure, short reaction times, cost effective and a simple work-up procedure. The ^{1}H NMR, ^{13}C NMR and FT IR spectra confirm the structure of compounds.



Scheme 1

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Zeolite: an efficient and reusable catalyst for one-pot synthesis of pyrazolo[1,2-a][1,2,4]triazole-1,3-diones

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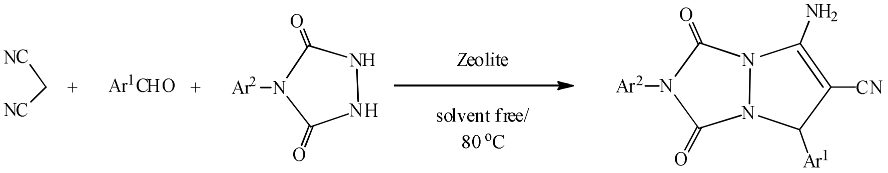
Pyrazoles are an important class of *N*-heterocyclic compounds of diverse structures with a wide range of interesting biological properties, such as analgesic, anti-pyretic, anti-bacterial, anti-inflammatory, anti-diabetic and psycho-analeptic activities.

Catalysts are attractive in green technology because of their importance in petrochemicals and fine chemicals synthesis. Heterogeneous catalysts have emerged as superior to conventional homogeneous catalysts since they can be easily recovered from the reaction mixture by simple filtration and reused after activation, thereby causing economical viability in the processes involved. The potential use of microporous catalysts in fine chemical production is enormous. These heterogeneous catalysts are known to suppress side reactions, which include self-condensation and oligomerization, resulting in better selectivity and product yield. Nanoporous silica seems a good candidate as a support for catalysts.

In this work and for the first time, the application of zeolite as an efficient and recyclable catalyst for the synthesis of pyrazolo[1,2-*a*][1,2,4]triazole-1,3-diones was investigated.



Scheme 1

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Efficient and selective oxidation of alcohols catalyzed by a molybdenumthiosemicarbazid schiff base complex

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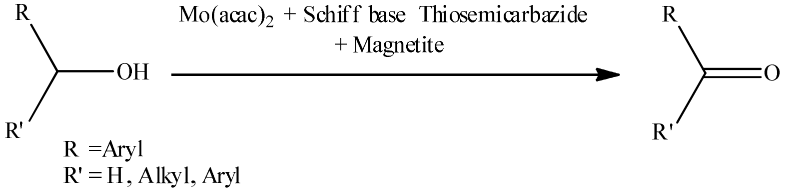
[b]*Faculty of Chemistry, Kharazmi University, Tehran, Iran*

In recent years considerable effort has been directed towards the transition metal complex catalyzed oxidation of organic compounds. Among these, oxidation of alcohols to aldehydes and ketones has specially been attended a lot, since carbonyl compounds are important intermediates in organic synthesis. Here in, We used a high- yield (70-90%) and selective oxidation procedure for the conversion of benzylic alcohols with various electron releasing and electron withdrawing substitutions, to corresponding aldehydes and ketones at 60°Cwith TBHP and H_2O_2 as oxidant, in the presence of Molybdenum complex with Schiff Base Ligand ThiosemicarbazidSupported on Magnetite as catalyst with short reaction times and high yields. The Presence of electron releasing and electron withdrawing substituents in ortho or para positions shows that the importance of steric and electronic effects due to high activity of the catalytic system are lower than expected. The presence of the catalyst seriously affects the oxidation of alcohols by TBHP and H_2O_2.



Scheme 1

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Zn Nanoparticle as promoter in benzene hydrogenation using Ni/MWCNTs

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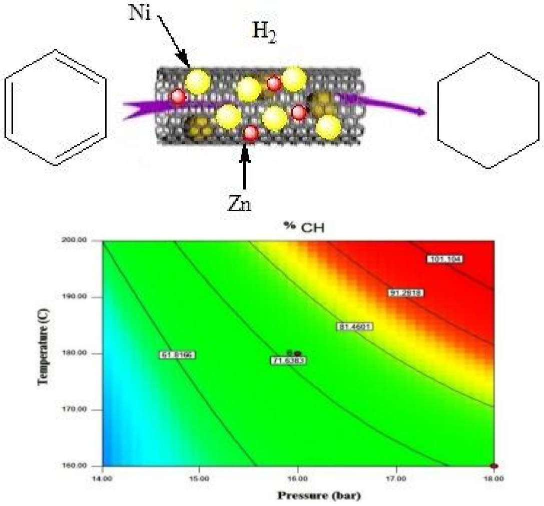
Cyclohexane due industrial application as precursor in production of adipic acid and as solvent has been attractive research. Benzene is known as carcinogen substance and as main pollutant of air and due limitations about amount of benzene in fuel; several investigations were carried out for reducing of benzene in gasoline [1-3].

The objectives of this work are evaluating the influence of Zn as promoter in catalytic activity of Ni supported on mesoporous multiwalled carbon nanotubes (MWCNTs). Modeling of benzene hydrogenation conducted on results by response surface methodology (RSM).



Scheme1

References:

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An efficient and rapid one-pot synthesis of highly functionalized stable phosphorus ylides containing the sulfur atoms

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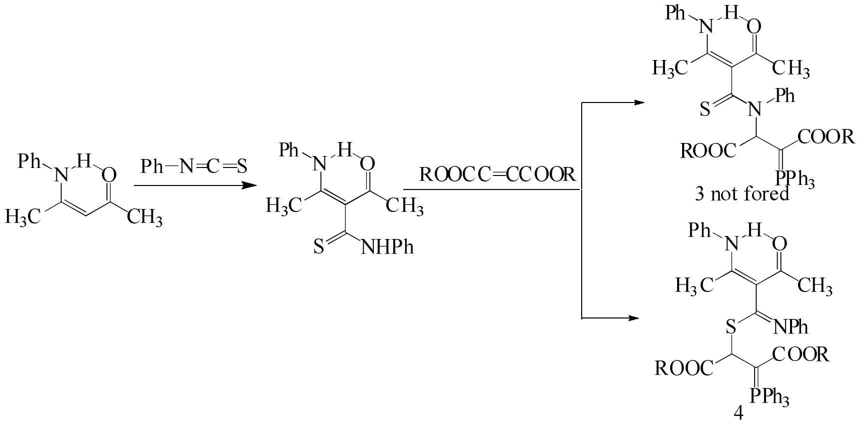
Phosphorus ylides are reactive intermediates and have important application in chemical, biological, and industrial uses [1-2]. These ylides are usually prepared by treatment of phosphonium Salts with a base [3]. β-enaminocarbonyl derivatives have been of considerable interest owing to their potential use as 1,3-dielectrophile synthons in organic synthesis [4].

In this investigation we report the reaction of ß-enamino ketone 1 with phenylthioisocyanate yielding corresponding compounds 2 in excellent yields via a sequence of C-thioacylidation of enamino tautomer 1 in the presence of montmorillonite K_{10} clay (Scheme1) [5].Compound 2 was further treated with dialkyl acetylenedicarboxylate at r.t in the presence of triphenylphosphine, and the corresponding phosphorus ylides 4 formed in high yields. In conclusion, we have developed a simple and an efficent method for the synthesis of phosphorus ylides via tree-compone reactions containing ph_3, acetylenic esters, N-H acid in good to excellent yields. This process shows that the sulfur anion acts as a stronger nucleophilic than the nitrogen anion (Scheme1).



Scheme 1

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One-pot synthesis of tetrahyrobenzo[b]pyran and dihydropyrano[c]chromene derivatives using aluminum ammonium sulfate in green media

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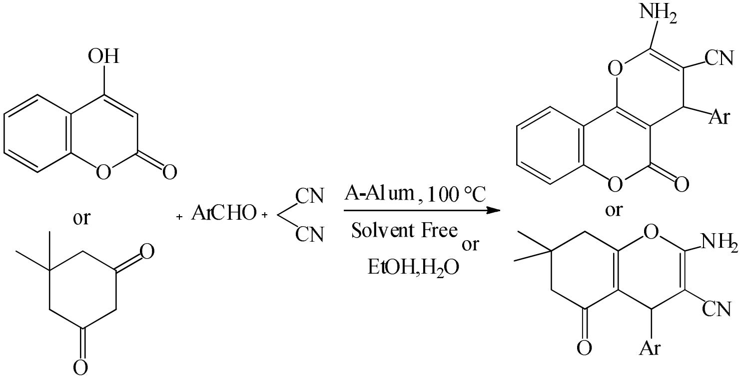
Tertrahydrobenzo[b]pyrans and dihydropyrano[c]chromenes have recently attracted much attention as an important class of heterocycles due to their useful biological and pharmacological properties [1-2]. In continuation of our works in green synthesis of heterocyclic compounds [3], we wish to report efficient one-pot and multicomponent synthesis of dihydropyrano[c]chromene and tetrahydrobenzo[b]pyran derivatives in the presence of aluminum ammonium sulfate as a catalyst. Green reaction media, good yields and simple work up, inexpensive and commercially available catalyst are advantages of this procedure.



Scheme 1

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Urea- 1,1-dihydroperoxycyclohexane/NH_4Br system as a new and mild reagent for efficient synthesis of 2-aryl-1H-benzothiazoles

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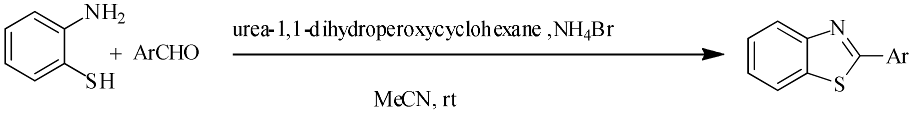
2-Substituted benzothiazoles are an important class of compounds in medicinal and industrial chemistry [1]. The compounds with benzothiazole cores have been known as antitumor drugs, antibacterial, antiglutamate/antiparkinson, broad spectrum Ca^{+2} channel antagonist, inhibition of enzymes such as aldose reductas, monoamineoxidase , lipoxyenase, cycloxygenase, acetyalcholoine esterase, thrombine, proteases, H^+-K^+ ATPase, carbonic anhydrase, HCV helicase, plant growth regulation [2].

As the importance of benzothiazoles, for synthesis of these compounds several methodologies have been reported [3]. Unfortunately, most of these procedures have many defects and limitations such as harsh reaction conditions, high reaction temperature, prolonged reaction times, requirement of excess of reagents, tedious work up procedures, low yields, using of costly, toxic or air sensitive catalysts, etc. Consequently, still, there is an important need to develop simple, mild, rapid and inexpensive procedures and/or further work on technical important.

Recently, *gem*-dihydroperoxides have been interested as new, effective and strong oxygen transfer oxidants [4]. So, in continuous of our interest in application of gem-dihydroperoxides [5], we used of urea-1,1-dihydroperoxycyclohexane/NH_4Br for catalysis of synthesis of 2-aryl-1*H*-benzothiazoles in mild condition and excellent yields.



Scheme 1

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Four-component ugi reaction of rhodanine-N-acetic acid with aniline and aromatic aldehydes in the presence of isocyanides

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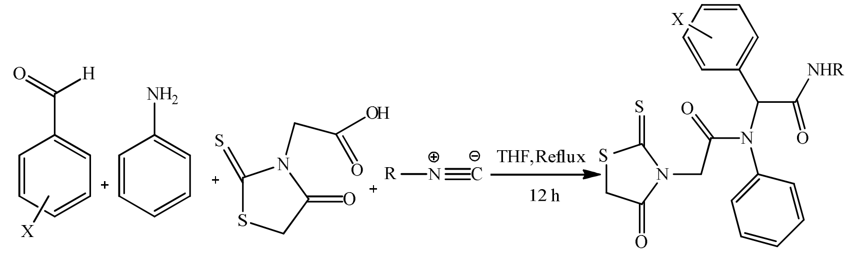
A major challenge of modern chemistry is the design of new chemical reaction sequences that provide novel compounds in high yields. Undoubtedly, one-pot multicomponent reactions (MCRs) from low-cost materials are convergent reactions with high atom efficiency, and higher yields in comparison to a similar multistep reaction. A large and important class of MCRs is constituted by the isocyanide-based Passerini and Ugi four-component reactions [1–3]. These reactions have become one of the most investigated transformations during the past decade, in conjunction with the enabling technologies, such as high-throughput screening, combinatorial and assembling complex pharmacologically important structures.

herein we report the four-component reaction of aromatic aldehydes **1**, aromatic amines **2**, rhodanine-*N*-acetic acid **3** and isocyanides **4** as a suitable procedure affords rhodanine-based amides **5** in good yields (Scheme 1).



1 2 3 4 5

X= H, Cl, Br, F, CN, OMe

R= ^{t}Bu , Cyclohexyl

Scheme 1

References:

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Modified magnetic polymer particles by diethyl amino ethyl methacrylate

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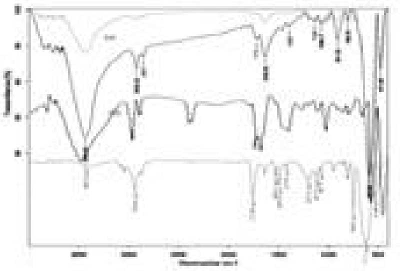
In recent years, inorganic polymer composite particles in different core-shell morphologies have been studied extensively. Polymeric phase of these particles can be an ion exchange resin and due to their application in separations processes, nowadays they have taken into consideration. Therefore, by designing appropriate functional groups on the surface of polymer magnetic particles, one can use these particles in separation of many chemical compounds such as heavy metals [1, 2]. In this work modification of magnetic particles by a polymer matrix containing ion exchange resins was carried out. Firstly, iron oxide particles became hydrophobic when they were coated by oleic acid and encapsulated with poly (styrene-divinyl benzene- HEMA), which called magnetic polymer particles (MPP) or core particle. In the second stage, MPP was encapsulated with poly (2-diethylamino ethylmethacrylate) (poly DEAEMA) using suspension polymerization technique to create amine groups on the MPP surfaces (MPP- DEAEMA). FTIR spectra and powder XRD pattern were shown in Figures 1 and 2 respectively. FTIR spectra and XRD spectrum of synthesized particles show characteristic peaks of maghemite and DEAEMA. So it is confirmed the embedment of magnetic particles in the polymer matrix.



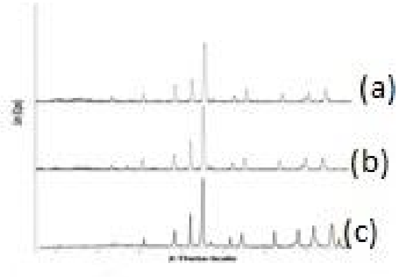


Fig. 1: IR spectra of (a) m-Fe3O4 Fig.2: XRD (a)Iron Oxide(b)Iron Oxide +St+HEMA(c) poly(MPP- co-DEAEMA) (b)MPP (c) MPP-MAH (d)MPP-MAH-co-DEAEMA

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Preparation of thiran from the raction epoxide with ammonium tiocyantae in poly ethylene glycol

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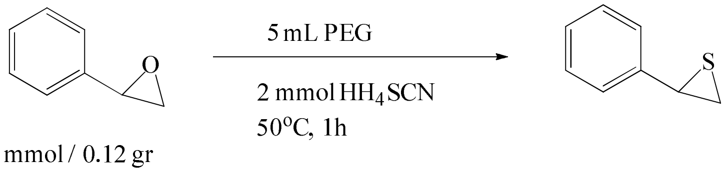
Heterocycles have many diverse structures and they significantly contribute in many kinds of pharmaceutical, veterinary and chemovegetative compounds and many other factors [1]. Epoxides often are considered as the most important materials for producing thirans by reacting them with thiocyanate or thiouria in water or aqueous solvents [2-4]. In this work, a new strategy has been introduced for the preparation of thrians.

In this project, ammonium thiocyanate was used for producing thirans and the reaction was carried out under the polyethylene glycol condition. In the absence of polyethylene glycol solvent , the reaction for converting epoxide to thiran is slowly and has a low efficiency, for example (Scheme1).



Scheme 1

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Zirconium(IV)-modified-MCM-41 as knoevenagel condensation catalyst

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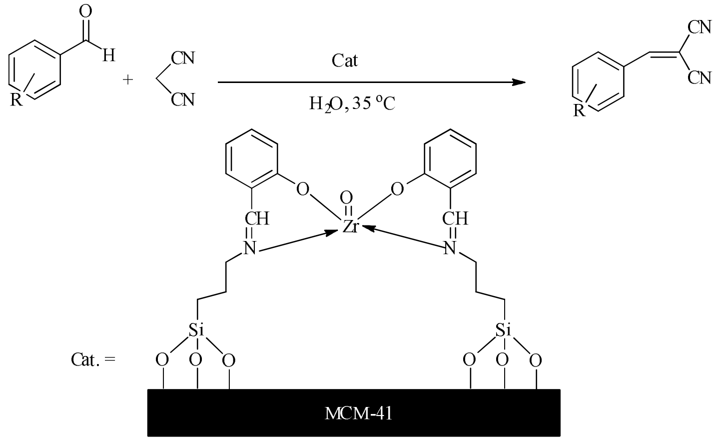
Mesoporous silica containing specific functional groups having a high specific surface areas and porosities that opened a wide field of applications in removal of toxic metal ions from waste-water and natural-waters [1]. Thus they provide a suitable approach to the development of green chemistry principles.

The importance of zirconium as a homogeneous catalyst has already been cited in the number of biologically and pharmaceutically significant organic transformations [2, 3]. Herein we have reported the importance of zirconium modified MCM-41 as a heterogeneous catalyst for the Knoevenagle condensation reaction of various aldehydes with malononitrile in water at 35 °C.



Scheme 1

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The spectroscopic (IR, and UV) and NBO analysis of iridatropylium, $C_6H_6Ir(PF_3)_3$, by density functional method

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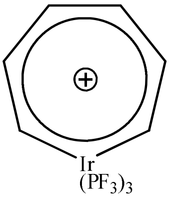
In this work, we report a theoretical study on molecular structure, vibrational spectra, NBO and UV-spectral analysis of iridatropylium (Scheme 1). The molecular geometry, harmonic vibrational frequencies and bonding features in the ground-state have been calculated by using the density functional method (mpw1pw91). Stability of the molecule, and charge delocalization has been analyzed using natural bond orbital (NBO) analysis. Energy and oscillator strength of electronic transitions in UV spectrum calculated by Time-Dependent Density Functional Theory (TD-DFT). The calculated HOMO and LUMO energies show that charge transfer occurs within the molecule.



Scheme 1

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An efficient method for amidoallkylation of electron-rich arenes dithiocarbamates catalyzed by $AlCl_3$

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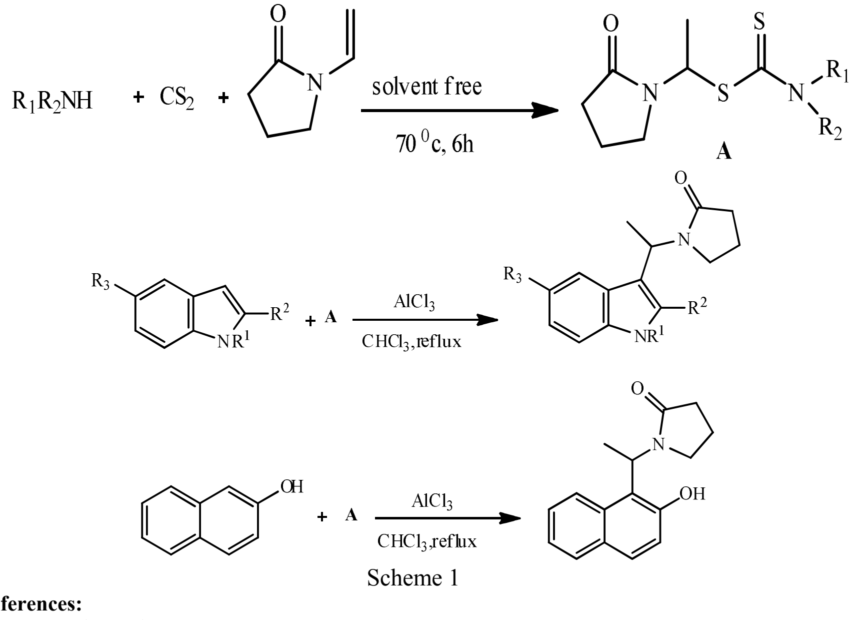
The Friedel–Crafts alkylation is an interesting reaction for C–C bond formation in organic chemistry. Arene derivatives such as phenols, naphthols and heteroarenes such as indole, and pyrrole derivatives have been successfully used as nucleophiles in Friedel–Crafts reaction in order to obtain arene's derivatives. The indole ring system exists ubiquitously in nature-occurring products, and many indole-containing compounds exhibit important biological activities and synthetic applications [1]. 3-Alkyl substituted indoles have potentially high biological activities [2]. They have also been used to synthesis complex indole derivatives that can be used as pharmaceuticals and agrochemicals [3]. In this paper an efficient procedure for amido-allkylation of electron-rich arenes with dithiocarbamats A (simply prepared via one-pot three component of amine, CS_2 and N-vinyl pyrolidone) [4] is reported. Indoles and naphtols have been used succsessfully in this procedure. The reaction is catalyzed by a Lewis acid such as $AlCl_3$. Good to excellent yield of products were obtained with excellent regio selectivity.



Scheme 1

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Synthesis of biscoumarins using silica gel-supported $AlCl_3$ as an environmentally friendly heterogeneous catalyst

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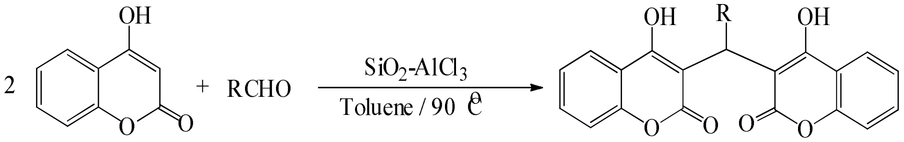
Coumarin and its derivatives are known to possess a wide range of biological activities including anti-HIV, anti-biotic, anti-fungal, anti-bacterial, anti-oxidant, anti-cancer, and anti-coagulant [1–4]. Among various derivatives of coumarin, biscoumarins have aroused considerable interest. They are usually prepared from the reaction of aldehydes with two equivalents of 4-hydroxycoumarin in the presence of a catalyst.

The use of catalysts on insoluble inorganic supports in organic synthesis is increasingly popular. Such heterogeneous catalysts compared with their homogeneous counterparts, often have the advantage of being easily separable from the reaction media, recyclability and improved selectivity in various organic reactions [5].

In continuation of our recent work on the use of solid supported catalysts, we found that silica gel-supported aluminium chloride (SiO_2-$AlCl_3$) was a good catalyst for Friedel-Crafts sulfonylation of aromatic compounds [6]. Along this line, we now wish

to report that SiO_2-$AlCl_3$ is also an environmentally friendly heterogeneous catalyst for the synthesis of biscoumarins by two-component one-pot domino Knoevenagel-type condensation/Michael reaction between various aliphatic and aromatic aldehydes with 4-hydroxycoumarin. This solid acid catalyst is stable (as bench top catalysts) and can be easily recovered and reused without appreciable change in its efficiency.



Scheme 1

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One pot and efficient synthesis of 2,4,6-triarylpyridines under solvent-free condition

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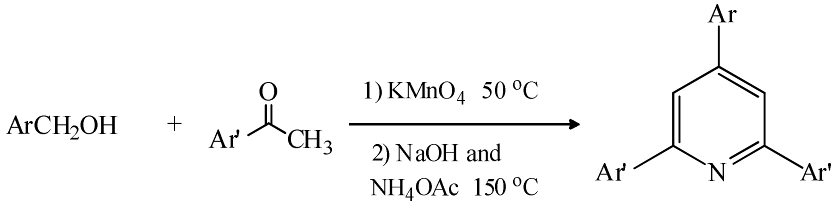
Pyridines are of interest because of the occurrence of their saturated and partially saturated derivatives in biologically active compounds and natural products such as NAD nucleotides, pyridoxol (vitamin B_6), and pyridine alkaloids [1]. Some examples are used as pharmaceuticals (as antimalarial, vasodilator and antiepileptic), dyes, additives (as antioxidant), agrochemicals (as fungicidal, pesticidal, and herbicidal) [2].

This work described a new strategy for the synthesis of 2,4,6-triarylpyridins via a reaction between benzylalcoholes, acetophenone derivatives and ammoniumeacetate in the presence of potassium permanganate. In this reaction, $KMnO_4$ used as an oxidant agent for oxidizing benzylalcohole to condense with acetophenone and then reaction with NH_4OAc will produce appropriate 2,4,6-triarylpyridins in good to excellent yields [3].

The structures of the isolated products were assigned on the basis of IR, ^1H and ^{13}C NMR, mass spectrometry and elemental analysis (Scheme 1).



Scheme 1

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Simple one-pot synthesis of 2-oxo-1,9a-dihydro-2H-pyrido-[1,2-a]pyrimidine derivatives catalyzed by polyurethane

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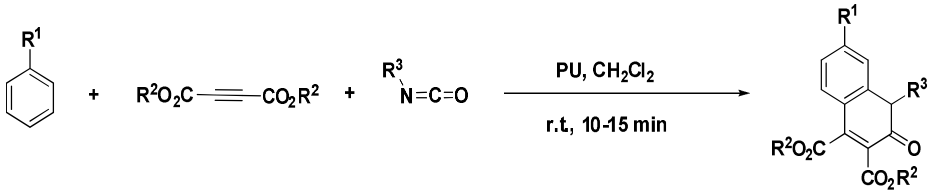
Email: helia_noos@yahoo.com

Pyrimidines are of chemical and pharmacological interest. Compounds containing a pyrimidine ring system have been shown to possess antitumor, antibacterial, antifungal, antimalarial, and anticonvulsant activities. Some examples are valuable drugs in the treatment of hyperthyroidism, acute leukemia in children and adult granulocytic leukemia [1-2]. Due to the unique properties of pyrimidine derivatives, the development of synthetic methods which enable a facile access to this heterocycle are desirable.

In this work, we report that pyridines undergo a smooth reaction with dialkyl acetylenedicarboxylates in the presence of isocyanatesand Polyurethane as catalystin dry dichloromethane at ambient temperature to produce functionalized 2-oxo-1,9a-dihydro-2H-pyrido[1,2-a]pyrimidines in good yields (Scheme 1).



Scheme 1

References:

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Reaction of vinylbenzylchloride copolymers with 5-chloro-8-hydroxy quinoline

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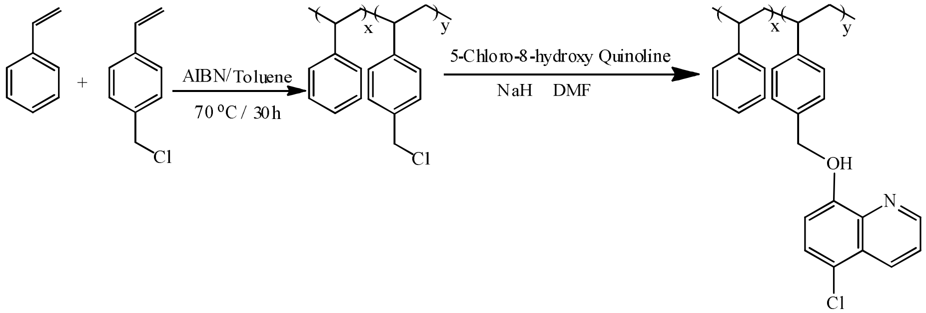
Vinylbenzylchlorid (VBC) can be easily polymerized with radical or cationic initiators [1]. Copolymerization reactions of VBC were performed with styrene and methyl metacrylat, in toluene at 70±1°C using α,ά-azobis(isobutyronitrile) (AIBN) az the radicalpolymerization initiator and the copolymers I,II collected respectively in good yields. Polymerswith chloromethyl group in the side chains are useful starting materials for the synthesis ofvarious functional polymers [2].The etherification reaction of polymers with salt of 5-chloro-8-hydroxy quinoline proceeded very smoothly to give the corresponding polymers with pendant eter residues. Characterizations of all the obtained polymers were performed with FT-IR and ^{1}HNMR spectroscopic techniques. The glass transition temperature (Tg) of the copolymers (I,II) was determined by dynamic mechanical thermal analysis (DMTA). The study of the DMTA curves for modified copolymers indicated that glass transition temperature values of the copolymers increase with incorporation of 5-chloro-8-hydroxy quinoline groups as side chains. The resulted copolymers are white solid and soluble in chloroform, dimethylsulphoxide and insoluble in nhexane, methanol, ethanol and water.



Scheme 1

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Synthesis of 3,4-dihydropyrimidin- 2(1H)-thiones using benzyltriphenylphosphonium chloride as a catalyst

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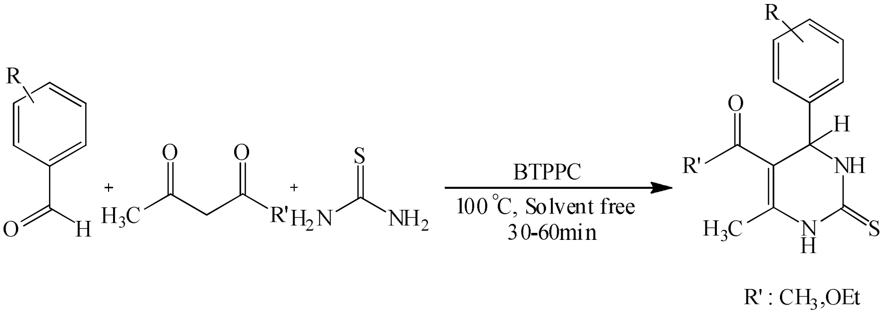
Multi-component reactions are very attractive tools to obtain the complex molecules from one-pot procedures. Among these reactions, the Biginelli multi-component reaction [1] is a well-known, simple and straightforward procedure for the synthesis of dihydropyrimidindiones/thiones by the three-component condensation of aldehyde, acetoacetate ester and urea/ thiourea.

Dihydropyrimidindiones/thiones represent heterocyclic systems of remarkable pharmacological efficacy and many exhibit antiviral, antitumor, antibacterial, anti-inflammatory activity [2]. Recently, much work on improving the yields and reaction conditions has been actively pursued. For example, modification and improvements include using Lewis acids as well as Br0nsted acids/bases, primary amine, chlorotrimethylsilane and hexaaquaaluminium tetrafluoroborate as promoters [3].

Due to the importance of these compounds, in this work, a simple and efficient procedure has been developed for the synthesis of 3,4-dihydropyrimidin- 2(1H)-thiones by a one-pot three component cyclocondensation reaction of β-dicarbonyl compound, arylaldehyde, and thiourea using benzyltriphenylphosphonium chloride (BTPPC) as the catalyst under solvent-free conditions at 100 ^{0}C (Scheme 1).



Scheme 1

High yields of the products, short reaction times, mild reaction conditions and simple experimental procedure make this protocol complementary to the existing methods.

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Formic acid: an efficient, inexpensive and environmentally friendly catalyst for three-component Strecker synthesis of α-aminonitriles with excellent yields

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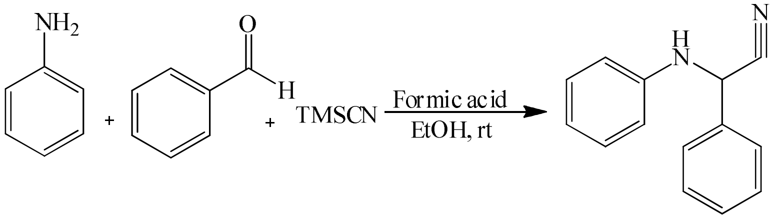
Multi-component Condensation Reactions (MCRs) have recently received great interest, due to the formation of multibonds in a one pot reaction, high atom efficiency, mild and simplified conditions and environmentally benign friendlines [1]. The Strecker reaction is the oldest known MCR and the most straightforward route for the synthesis of α- amino acids on both lab and technical scales [2].

In this work Formic acid that is an inexpensive and highly efficient catalyst was used in three component strecker reaction under mild conditions at room temperature with excellent yields. A remarkable advantage of formic acid is solubility in water. Reaction was complete in very short time and separation of catalyst from product is very simple. (Scheme 1).



Scheme 1

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Synthesis of 2,6-dicyanoaniline derivatives using water dispersed magnetic nanoparticles (H_2O-DMNPs) of α-Fe_2O_3

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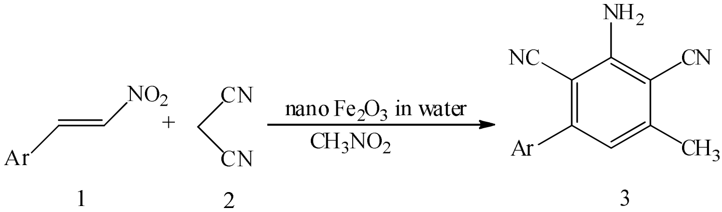
In nanochemistry, dispersed heterogeneous catalysts due to special reduced size and diffused particles are prepared and used satisfactorily due to the large surface areas and high densities of active sites [1]. Separation of magnetic nanoparticles is simple, economical, and useful for industrial applications. Carrying out reactions in water and using recoverable catalysts have economic and environmental advantages; because of these benefits this method is being attractive in recent years [2, 3].

A mixture of nitrostyrene **1** (1mmol) and malononitrile **2** (4 mmol) in the water dispersed magnetic nanoparticles (H_2O-DMNPs) of α-Fe_2O_3 will produece 2,6-Dicyanoanilines **3** . This method created a simple and environment friendly condition for the synthesis of the titled compounds in good to excellent yields (Scheme 1).



1 2 3

Scheme 1

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Synthesis and spectral characterization of a new diamine drivative of 4-flourophenol and its acyclic Schiff base ligand

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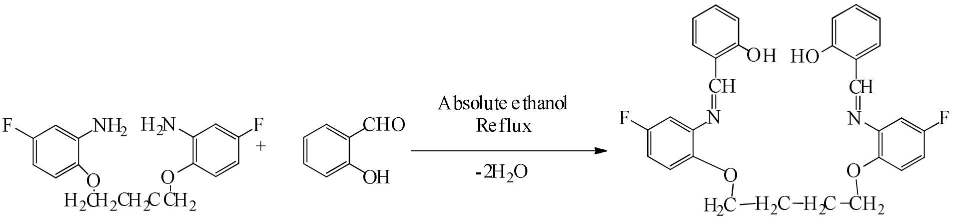
[b]*Department of Chemistry, Faculty of Science, Ilam University, P.O. Box, 69315516, Ilam, Iran*
Email:Hamid_gafshar@yahoo.com

The chemistry of Schiff base ligands and their metal complexes have attracted a lot of interest due to their facile synthesis and wide range of applications including antifungal, antibacterial, anticancer and catalytic fields [1]. The design, synthesis and structural characterization of salicylaldimine Schiff base ligands and complexes are a subject of current interest. Due to their interesting and versatile structural, magnetic, spectral, and catalytic and redox properties, they are used as models for metalloenzymes and various theoretical problems of chemistry [2].

In this work, a new diamine [6, 6'-(butane-1, 4-diylbis (oxy)) bis(3-fluorobenzenamine)] has been synthesized by modified previous procedure [3]. Then, we prepared its Schiff base ligand by condensation of this new amine with salicylaldehyde in absolute ethanol under reflux conditions (Scheme 1). The structure of the diamine and its free Schiff base ligand were determined by IR, ^{1}H- and ^{13}C-NMR and Mass spectra.



Scheme 1

References:

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Nuclephilic ring opening of epoxides promoted by $NaHSO_4$ catalyst: An efficient and eco-friendly route to synthesis of thiirane

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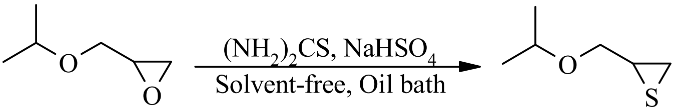
Epoxides are important and versatile synthetic intermediates in organic synthesis [1]. Epoxides can be opened under a variety of conditions, although the most practical and widely employed strategy for the synthesis of 1,2-bifunctional compounds is via nucleophilic ring-opening using a Lewis acid or a strong base [2].

Thiirane is found in naturally occurring compounds, herbicides, pesticides, polymeric compounds, pharmaceuticals, and in many other manmade chemicals [3] Transformation of epoxides to thiiranes by an oxygen–sulfur exchange reaction is a useful reaction [4].

$NaHSO_4$ is inexpensive, efficient, readily available, and mild catalyst, which has surface properties, and suggests very rich organic chemistry. solid acids as environmentally friendly and economically viable catalyst, are increasing continuously owing to their ease of handling, low cost, high catalytic activity, process simplicity and comparably easy work-up [5]. Finally, supported solid acid provides more effective catalytic reactivity by their much extended surface area [6].

As a part of our research program to the synthesis of thiiranes, herein, we wish to report a green and practical method for solvent-free conversion of epoxides to the corresponding thiiranes by $NaHSO_4$ under oil bath conditions (60 ˚C–70 ˚C). The epoxides were converted to the corresponding thiiranes in excellent yields within short times (Scheme 1).



Scheme 1

References:

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Reaction of poly[(chloromethyl) styrene] with salts of P-cresol

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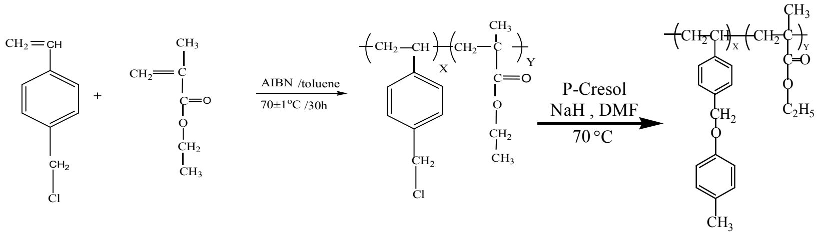
4-Chloromethyl styrene(CMS) and its copolymers with different monomers such as ethyl methacrylat and ethyl acrylat (in 1:3 molaration) were synthesized by free radical polymerization method in toluene solution at the temperature range 68- 70 using – azobis (isobutyronitrile) (AIBN) as an inititator and the copolymers I, II collected respectively in good yields. The obtained polymers are able to react with various nucleophilic reagents.The CMS units provide the handles for functionality attachment through nucleophilic substitution, which was employed in numerous studies [1-2]. The polymers, obtained in quantitative yield. All the resulted polymers were characterized by FT-IR and HNMR spectroscopic techinques and dynamic mechanical thermal analysis (DMTA). The solubility of all the copolymers was examined in various polar and nonpolar solvents. All the polymers containing eter group showed a high glass transition temperature in comparison with copolymers I, II. The increase of the glass transition temperature reflects the substantial increase in rigidity of new polymers bearing substituents inside chains [3].



Scheme 1

References:

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Synthesis of β-acetamido ketones using silica gel-supported $Ce(SO_4)_2$ as an efficient and reusable catalyst

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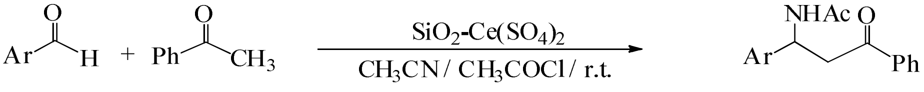
In recent years, the use of solid supported catalysts has received considerable attention in different areas of organic synthesis. The activity and selectivity of a catalyst dispersed on the surface of a support is improved as the effective surface area of the catalyst is increased manifold, and hence they are expected to perform more effectively than the individual catalysts [1,2].

β-Acetamido ketones are important synthons for a variety of biologically or pharmacologically important compounds [3-6]. These are precursors of 1,3-amino alcohols present in antibiotic nikkomycins or neopolyoxines. One-pot condensation of an aldehyde with an enolisable ketone, acetyl chloride, and acetonitrile is the most convenient method for the preparation of β-acetamido ketones.

In a continuation of our recent work on the use of heterogeneous catalysts, we now wish to introduce silica gel-supported $Ce(SO_4)_2$ (SiO_2-$Ce(SO_4)_2$) as a recyclable and environmental friendly heterogeneous catalyst for the synthesis of β-acetamido ketones from coupling of an aromatic aldehyde with acetophenone, acetyl chloride, and acetonitrile (Scheme 1).



Scheme 1

References:

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The synthesis of some new benzoyl thioureas and investigation of pesticide activity

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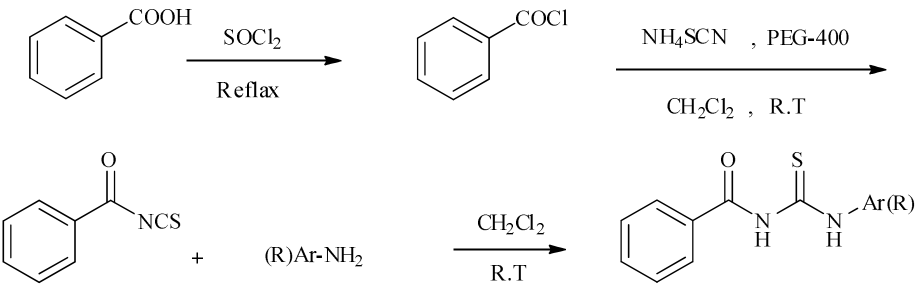
Benzoyl thioureas insecticides act as powerful insect growth regulators (IGRs) which interfere with chitin synthesis in target pests and cause death. These coumpounds insecticides have many attractive properties such as high selectivity, high biological activity, rapid degradation in soil and water and the acute low toxicity for animals, which make them suitable for inclusion in integrated pest management programs for crops [1]. On the other hand, interest in the safety of food products has increased, and pesticide residues in food crops have been the subject of increasingly strict regulations [2].

In this investigation, some new benzoyl thioureas were synthesized from adding various amines to benzoyl isothiocyanate (Scheme 1).



Scheme 1

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An efficient green access to α-keto aryl thioamides from readily available arylglyoxals using S_8 and Na_2S under solvent-free conditions

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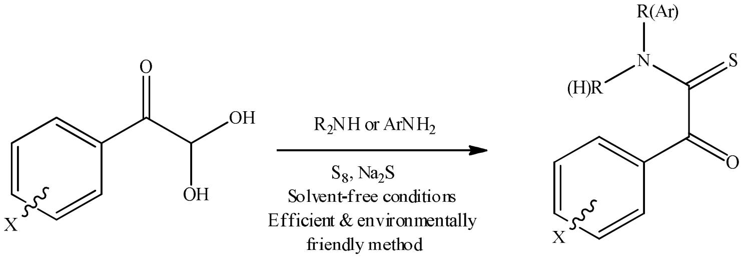
α-Keto aryl thioamides are a versatile and valuable building block for a number of biologically and pharmaceutically active compounds [1]. Limited attention has been given to the synthesis of this framework [2]. Addition of H_2S on to acylcyanides gave corresponding *N*-unsubstituted α-keto aryl thioamides. However, the synthesis of 2-oxothioamides is restricted to the *N*-unsubstituted derivatives. The reaction of (*N*,*N*-dimethylthiocarbomyl) lithium with methyl benzoate, afforded α-keto aryl thioamides. This reagent has been generated by Seebach at –100 °C by deprotonation of dimethylthioformamide with LDA. It is evident that the need for the development of new and flexible protocols is required to access α-keto aryl thioamides without using toxic reagents and avoiding extreme conditions. The development of environmentally benign technologies is the most challenging goal of contemporary chemistry. Herein we report a convenient preparation of α-keto aryl thioamides from readily available arylglyoxals using S_8 and Na_2S under solvent-free conditions (Scheme 1).



Scheme 1

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Polystyrene-supported $AlCl_3$ as a highly chemoselective heterogeneous Lewis acid catalyst for the synthesis of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols)

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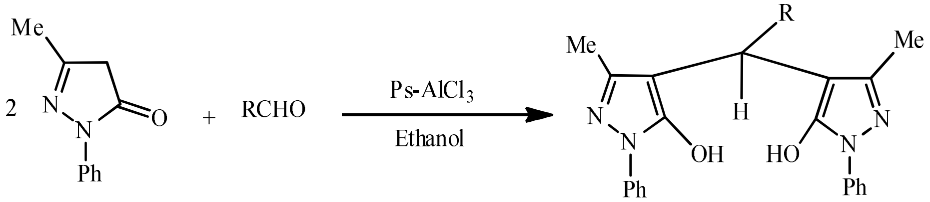
The utilization of polymer-supported Lewis acids offers several advantages in preparative procedures. Of these, enhanced stability, higher selectivity, easier handling, simple workup procedures, non-toxicity, non-corrosiveness, mildness of the reaction conditions, and the ease of recovery and reuse of the catalyst are most important [1].

Pyrazoles and their derivatives are known to possess a wide range of biological activities and are used as gastric secretion stimulatory, antidepressant, antibacterial, and antitumor [2-5]. One-pot tandem Knoevenagel-type condensation/Michael reaction between aromatic aldehydes with 2 equivalents of 3-methyl-l-phenyl-5-pyrazolone is one of the most pivotal preparation methods of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols).

In a continuation of our ongoing program to develop environmentally benign methods using heterogeneous catalysts [6], herein we now wish to report that cross-linked polystyrene-supported $AlCl_3$ (Ps-$AlCl_3$, 8% DVB) is an effective and highly chemoselective heterogeneous catalyst for the synthesis of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5ols) from the condensation reaction between aldehydes and 3-methyl-5-phenyl-pyrazolone (Scheme 1). The catalyst is reusable.



Scheme 1

References:

1. S.V. Ley, I.R. Baxendale, R.N. Bream, P.S. Jackson, A.G. Leach, D.A. Longbottom, M. Nesi, J.S. Scott, R.I. Storer, S.J. Taylor, *J. Chem. Soc., Perkin Trans.* 1 **(2000)** 3815.
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Natural biopolymers as a green catalyst for the synthesis of isoindolin-1-imine

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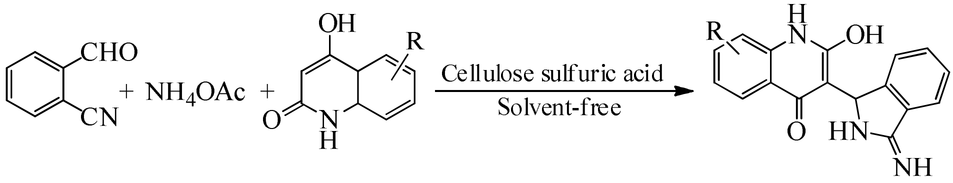
Cellulose sulfuric acid (CSA) has emerged as a promising biopolymeric solid-support acid catalyst for acid-catalyzed reactions, such as the synthesis of α-amino nitriles, aryl-14H-dibenzo[a.j]xanthenes, 1,4-dihydropyridines, Pechmann condensation, thiadiazolo benzimidazoles, imidazoazines, quinolines and 3,4-dihydropyrimidine-2(1H)-ones [1, 2]. Isoindole and its derivatives are one of the most important classes of N-heterocyclic biological active compounds. They have been received considerable attention from synthetic pharmacists and chemists due to their potent therapeutic and pharmacological activities. Isoindolin-1-imine series are an important class of isoindoles, and have exhibited typical pharmacological activities, including as NR2B-selective NMDA receptor antagonists [3] the thrombin receptor (PAR-1) inhibitors [3, 4] and antiproliferative effect.

Herein we report a simple one-pot method for the synthesis of isoindolin-1-imine derivatives via a three-component condensation of 2-cyanobenzaldehyde, ammonium acetate, and 4-hydrocoumarin derivatives or 1,3-dicarbonyl compounds, or 4-hydroxyquinolin-2(1H)-one derivatives in the presence of a catalytic amounts Cellulose sulfuric acid at room temperature (Scheme 1)



Scheme 1

References:

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Synthesis of esters from corresponding alcohols under ultrasonic irradiation using graphite oxide

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Direct method of conversion of alcohols to carboxylic esters holds promise in organic synthesis because it minimizes the number of steps [1]. Such transformation of alcohols into esters has been achieved using oxone/NaCl, $Ca(OCl)_2$, $NaBrO_3/NaHSO_3$, $NaBrO_2/AcOH$, $PhI(OAc)_2$, and H_2O_2/Br_2. Unfortunately, many of these procedures often require a large excess of reagents, expensive catalysts, transition metals, dry solvents, stringent reaction conditions, photochemical methods, and etc. [2].

Recent studies shown that carbon-based catalysts are very important in organic reactions [3]. Structure of graphite oxide (GO) indicates the reactive oxygen groups such as epoxide groups, alcohol and acid and it can be used as the oxidant agent in many organic reactions [4].

In continuation of our investigations [5] herein we report the use of GO, a readily available and inexpensive material, as a mild and efficient reagent for the direct conversion of alcohols to corresponding esters under ultrasonic irradiation. GO was demonstrated to catalyze direct conversion of alcohols to corresponding esters. These reactions were found to proceed under relatively mild conditions and afforded the desired esters in good to excellent yields. The present method has many obvious advantages as compared to many previous reports, including the simplicity and the generality of the methodology.

$$\mathrm{RCH_2OH} \quad + \quad \mathrm{R'OH} \xrightarrow[)))\text{, solvent}]{\text{GO}} \mathrm{RCOOR'}$$

References:

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Synthesis of modified carboxy methyl cellulose by glycidyl methacrylate as (CMC-g-GMA)

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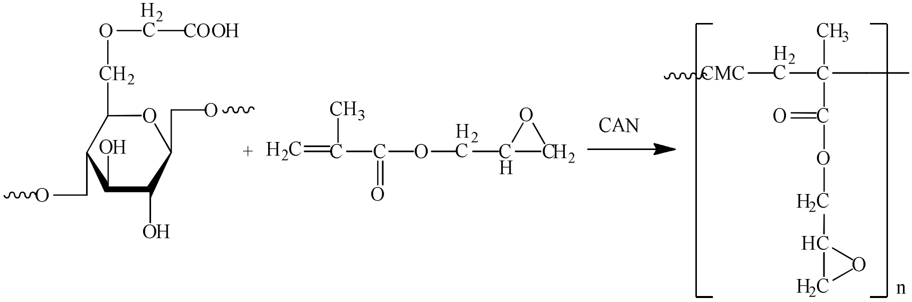
Email: am_rahgozar@yahoo.com

The poor physicochemical properties such as higher water and moisture absorption;
Lower chemical resistance and poor compatibility with most of the polymer matrices restrict their applications [1]. In order to overcome the disadvantages of different kinds of natural polymers, various kinds of surface modification techniques are employed to change their specific properties [2]. Among these techniques, graft copolymerization is one of the most promising methods to improve the physicochemical properties of polymers [3].

In this work, carboxy methyl cellulose, one of the well-known cellulose derivatives, has been modified by graft copolymerization. Glycidyl methacrylate (GMA) was chosen and grafted onto the carboxy methyl cellulose (CMC) polymer chain using ceric ammonium nitrate (CAN) as initiator. Acrylate groups were involved in the grafting reaction while the glycidyl groups remained as pendant groups for a subsequent reaction.

The principle of such a development is to introduce pendant reactive groups into cellulose to produce derivatives which can undergo cross-linking reactions.
In this regards, the modified CMC has been synthesized and ready to take place in subsequent reactions (Scheme 1).



Scheme 1

References:
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Synthesis and spectroscopic properties of new azo- dyes from derivatives aniline in reaction with acetylacetone

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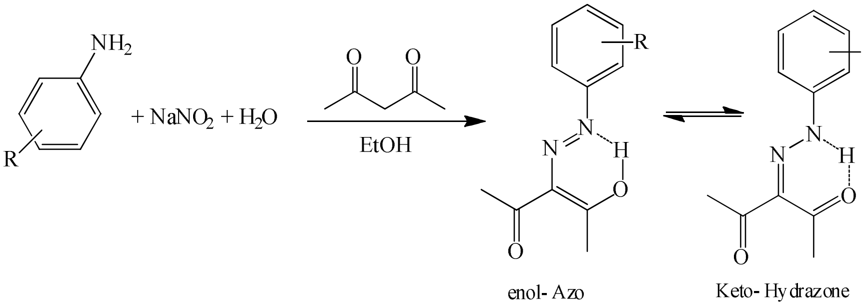
Azo compounds have been receiving much attention and have been widely used in many practical applications such as coloring fibers [1], photoelectronic applications, printing systems [2], optical storage technology, etc. Recently, metal complex dyes have also attracted increasing attention due to their interesting electronic and geometrical features in connection with their application for molecular memory storages, nonlinear optical elements, etc. [3].

In this work, four new azo-dye, 3- phenyl azo - pentane-2 ,4 dion (**LA**) , 3- (4 - nitro - phenyl azo) - pentane-2 , 4 dion (**LP**) and 3 - (2 - nitro - phenyl azo) - pentane 2, 4 dion (**LO**) and 4 - (1 - acetyle 2 - oxo - propyl azo) - benzene sulfanat sodium (**LS**) were synthesized from, aniline, 4-nitro aniline, 2- nitro aniline and sulfanilic acid with acetyl acetone respectively. The chemical structure of azo-dyes were characterized using FT-IR; ^{1}H-NMR; ^{13}C-NMR and UV-Vis. In the reaction with metal(II) cations (such as: Ni, Co, Cu and Fe) and formation complex, azo-dye can acts as a ligand with two or three teeth, N, O. Absorption maximum azo-dyes were also studied.



R= *O*- NO$_2$: $\mathbf{L_O}$, *P*- NO$_2$: $\mathbf{L_P}$
P- SO$_3$Na : $\mathbf{L_S}$, H : $\mathbf{L_A}$

Scheme 1

References:

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Novel one-pot process for synthesis of *N*-phenylbenzenamine from 2-chloro-*N*-aryl acetamide

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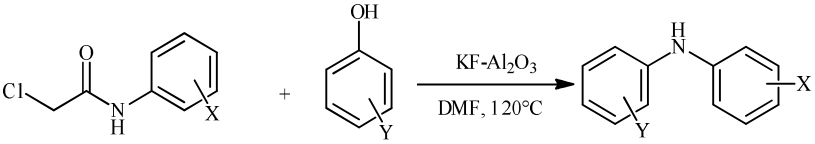
[b]*Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran Email: h_porkaleh@yahoo.com*

N-phenylbenzenamine derivatives are valuable building block for a number of biologically and pharmaceutically active compounds [1]. The title compounds are difficult to synthesize. To the best of our knowledge, there are a few methods for synthesis of this skeleton in the literature [2]. It is evident that a novel and flexible protocol with wide substituent tolerance and mild reaction conditions is desirable in the preparation of *N*-phenylbenzenamine. *N*-phenylbenzenamine derivatives could easily be produced by reacting phenol **2** derivatives of high commercial availability with 2-chloro-*N*-aryl acetamide **1**. The present paper has been completed based on the above finding (Scheme 1). The reaction proceeds well and *N*-phenylbenzenamines **3** are formed with moderate yields. This process is simple and clean. The molecular structure of products has been determined by ^{1}HNMR, ^{13}CNMR and MS techniques [3].



1 **2** **3**

Scheme 1

References:

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Synthesis and characterization of a new diamine containing 4-flourophenol and its potentially hexadentate N_2O_4 Schiff base ligand

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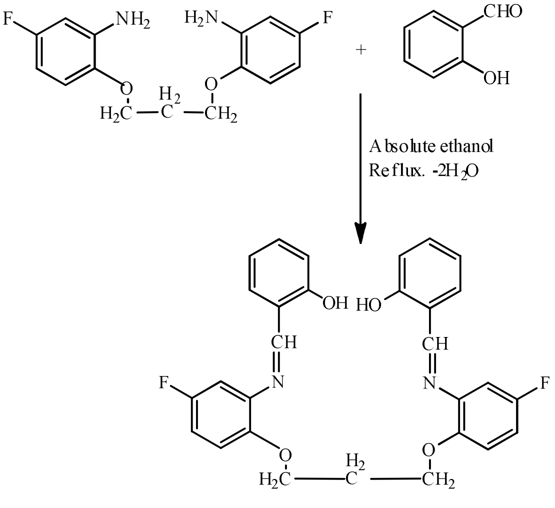
Schiff bases are known to be very important class of organic compounds because of their ability to form stable complexes with many different metal ions in various oxidation states and have the potential to be used in different areas such as catalysis, metallic deactivators, separation processes, electrochemistry, bioinorganic and environmental chemistry. Moreover they have increasingly importance in the pharmacological, dye, and plastic industries as well as in the field of liquid crystal technology [1, 2].

In this work, a new diamine [6, 6'-(propane-1, 3-diylbis (oxy)) bis (3-fluorobenzenamine)] has been synthesized by modified previous procedure [3]. Then, we prepared its acyclic Schiff base ligand by condensation of this new amine with salicylaldehyde in absolute ethanol under reflux conditions (Scheme 1). All compounds have been studied with IR, ^1H, ^{13}C NMR and Mass spectroscopy.



Scheme 1

References:

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Synthesis of novel cupper nanocatalyst based on dithiocarbamate for green synthesis of alpha- hydroxy amines in water and PEG400

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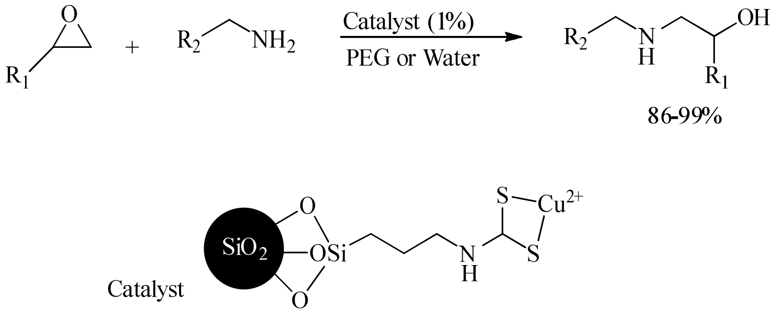
Alpha-hydroxyl amines are hazardous molecules because of their wide applications in synthesis of drugs [1]. Large number methods and catalysts are reported for synthesis of alpha-hydroxy amines [2]. Furthermore, cupper and its derivatives are used widely in several organic reactions in recent years [3].

In this research, amorphous silica NPs was functionalized with dithiocarbamate, then cupper cations were loaded on dithiocarbamate function group. Characterization of catalyst was done via SEM/EDAX, FT-IR, TGA and XRD. Synthetic catalyst was used in opening rings of epoxides by amines in green solvents such as PEG and water in room temperature (Scheme1). Regioselectivity, high efficient and short reaction time are characteristics of the reaction which is catalyzed by this catalyst.



Scheme 1

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One-pot Synthesis of polyhydroquinoline derivatives in the presence of copper oxide under ultra sound irradiation

Elham Ali Zadeh Houlasou, Mohammad Hossein Akhbari Shad, Salah Khan Ahmad Zade*
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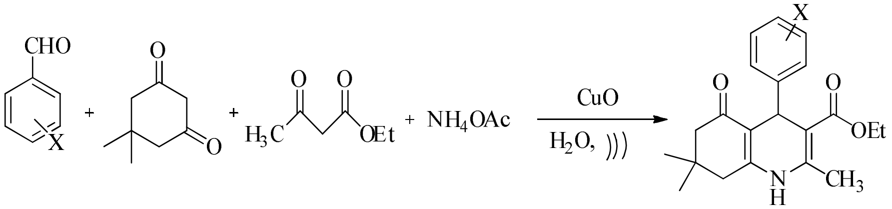
An efficient synthesis of polyhydroquinolines is achieved via a four-component reaction of aldehydes, dimedone, active methylene compounds, and ammonium acetate in one-pot under solvent-free conditions at room temperature on grinding [1,2]. In this method, polyhydroquinoline derivatives have been successfully prepared via four component condensation reactions of an aldehyde, dimedone, ethylacetoacetate and ammonium acetate in the presence of cupper (II) oxide (CuO) and under ultra sound irradiation. The reactions were performed in water as a green solvent. Simple work up procedure, high yield, short reaction time, easy available chemicals are among the important features of this work, and the procedure could be added to the present methods for the preparation of polyhydroquinoline derivatives (Scheme 1).



Scheme 1

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Convenient synthesis of pyrido[2,3-d]pyrimidine derivatives catalyzed by $CuFe_2O_4$ nanoparticles under ultrasonic assistance

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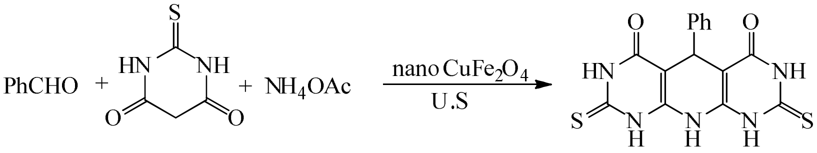
The use of ultrasonic waves in organic synthesis has been boosted in recent year [1]. Ultrasound is known to accelerate diverse types of organic reactions and it is established as an important technique in organic synthesis. Sonication also increases the reaction rate and avoids the use of high reaction temperatures [2]. Pyrido pyrimidine and its derivatives have been studied due to a variety of chemical and biological significance. The importance of pyrido pyrimidines as biologically active compounds includes their use as antibacterial, antiallergic, antitumor, antifolate, tyrosine kinase, calcium channel antagonists, anti-inflammatory, analgesic, antihypertensive, tuber-culostatic, anticonvulsants, diuretic, antileishmanial and antiaggressive activities [3].

In this work, we hope to develop a simple, efficient method for synthesis of pyrido [2,3-d] pyrimidines by treatment of aromatic aldehydes, 2-thiobarbituric acid, ammonium acetate in the presence of $CuFe_2O_4$ nanoparticles as catalyst under ultrasonic assistance (Scheme 1). The structure of pure products was confirmed by IR, ^1H NMR and ^{13}C NMR.



Scheme 1

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Simple and green synthesis of N-pyrroles catalyzed by Fe_3O_4 nanoparticles in water

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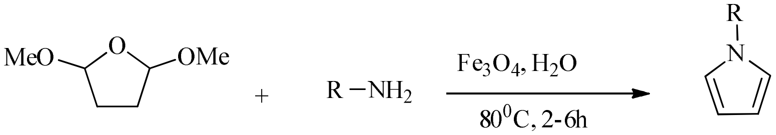
Pyrrole and its derivatives are kinds of the hazardous molecules in organic synthesis and biological systems. There are many reports and methods for synthesis of pyrroles in literatures [1]. Likewise, in recent years Magnetic Iron Oxide Nanoparticles (MNPs) are applied in different catalytic procedures as Lewis acid catalyst due to their characteristic such as simple magnetic separation, high surface area and reusability of catalyst [2].

In this research, a method is reported for synthesis of N-pyrroles catalyzed by Fe_3O_4 nanoparticles in water as a green solvent based on Lewis acid property of Fe atoms in Fe_3O_4 structure. In this attempt, Fe_3O_4 NPs were synthesized and characterized via XRD, SEM, FT-IR techniques then applied as catalyst in synthesis of N-Pyrroles in water (Scheme1). Short reaction time, moderate to good yield, simple magnetic separation of reaction mixture are characteristics of this methodology. ^{1}H-NMR, ^{13}C-NMR and FT-IR data confirm purity and formation of products.



Scheme 1

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Melamine-formaldehyde supported nucleophiles catalysedring opening of epoxides with nucleophiles

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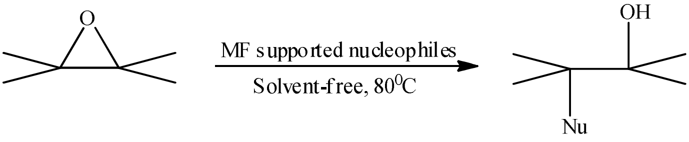
Epoxides are versatile intermediates in organic synthesis and their reactions with variety of reagents such as, electrophiles, nucleophiles, acids, bases, reducing agents, and some oxidizing agents are widely studied [1].Ring opening reactions of epoxidewith nucleophiles are considered as an interesting approach in organic synthesis of many functionalized oxygenated compounds. The reaction with nucleophiles such as oxygen compounds (water, alcohols, phenols) [2], nitrogen compounds (amine and derivatives of amines, azide, nitrate, isocyanate) [3], halides [4], and various carbon nucleophiles [5] have been performed in both organic and aqueous solvents. Polymeric reagents have proven useful for many chemical transformations in organic synthesis. The advantage of polymer supported reagents chiefly lie in the fact that they require no specialized polymer synthesis and purification techniques, thus rendering them simple to use. This coupled with their insolubility, physical stability, compatibility with a wide range of solvents including, in some cases water, and their toleration of a great number of reaction conditions, make them ideal as platforms on which to perform organic synthesis [6].

Herein, in continuation of our work on the synthesis and application of polymer supported nucleophiles in organic synthesis, we report the preparationand use of melamine-formaldehyde supported nucleophiles as efficient polymers for ring opening of different epoxidesunder solvent-free conditions at 80 °Ctemperature (Scheme 1).



MFR: Melamine-formaldehyde Resin

Scheme 1

References:

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Conducting polypyrrole/WO_3 nanocomposites: synthesis, characterization and study of their physical properties

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Nanocomposites are a special class of materials having unique physical properties and wide application potential in diverse areas. Encapsulation of inorganic nanoparticles inside the shell of conducting polymers such as polypyrrole (PPy) is the most popular and interesting aspect of nanocomposites synthesis. These materials differ from both the pure polymers and the inorganic nanoparticles in some of the physical and chemical properties [1-3]. WO_3, an *n*-type semiconductor metal oxide, has received considerable attention for use as chemical sensor because of its unique sensing properties for a series of target gases [4].

In the present research work, nanosized WO_3 was first synthesized as a light yellow powder by a colloidal chemical method from reaction of sodium tungstate and aqueous solution HCl. Then, a serious of PPy/WO_3 nanocomposites was fabricated by one-step *in situ* deposition oxidative polymerization of pyrrole hydrochloride with various amounts of WO_3 nanoparticles in the presence of $FeCl_3$ as an oxidant at 0°C. The obtained nanocomposites were characterized by Fourier-transform infrared (FTIR), thermogravimetric analysis (TGA), X-ray diffraction (XRD), and scanning electron microscope (SEM) techniques. The obtained results showed that WO_3 nanoparticles have been encapsulated by PPy with a strong effect on the morphology of PPy/WO_3 nanocomposites. Also, the synthesized PPy/WO_3 nanocomposites had higher thermal stability than that of pure PPy. The investigation of electrical conductivity of nanocomposites by four-point probe instrument showed that the conductivity of nanocomposite at low WO_3 content is much higher than of neat PPy, while with the increasing contents of WO_3, the conductivity decreases.

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A new method for sulfonation of multiwall carbon nanotubes with high percentage

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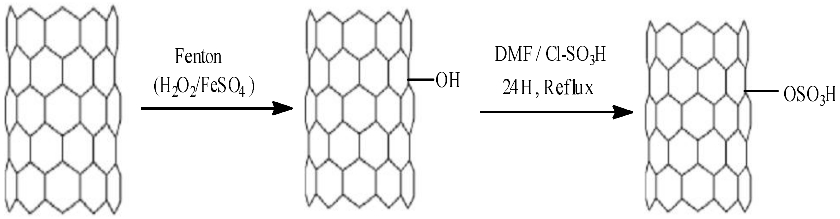
The discovery of carbon nanotubes (CNTs) has excited worldwide research interest for the prospect of developing novel carbobon-based nanomaterials due to their unidue structure-depdndent electronic and mechanical properties [1]. Recently, there has been great interest in developing the potential of carbon nanotubes for use as a catalyst support that can offer unparalleled flexibility in tailoring catalyst properties [2]. Chemical modification is a common method and is essential for the deposition of catalysts and other species onto nanotubes surfaces for nanocatalytic and sensor applications [3].

In this study, MWCNTs have been covalently Functionalized with chemical group ($-SO_3H$) using a tow step procedure. Initially, hydroxyl groups with a radical addition were covalently added to the surface of multi-walled carbon nanotubes (MWNTs) by Fenton reagents. And last step included Sulfonation of carbon nanotubes by chlorosulfonic acid. The result of Sulfonation of MWNTs was characterized by FTIR spectrometry, Raman spectroscopy and X-ray diffraction (XRD).



Scheme 1

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Experimental investigation, preparation and electromagnetic properties of polyaniline/ferrite composites

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Conducting polymers have attracted significant attention due to their potential applications in various fields, such as rechargeable battery, catalysts, electrodes and sensors, electromagnetic interference (EMI) shielding and microwave absorption [1–5]. Among the conducting polymers, PANI has received much attention in last two decades for its good environment stability, unique electrochemical and physicochemical behavior and relatively easy preparation [6,7]. Inorganic nanomaterials composited with PANI could enhance the mechanic property and other properties depending on the additives used. In this research, we have prepared ferrite/PANI magnetic composite particles by hydrothermal method, and the ferrite nanoparticles cover on their surface of PANI. The composites were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared (FTIR), and UV–vis spectra. The ferrite/PANI nanocomposites exhibit ferromagnetic behavior with high saturation magnetization (Ms=50 emu/g) and coercivity (Hc=119 Oe) at room temperature. The ferrite/PANI nanocomposites exhibit ferromagnetic behavior with high saturation magnetization and coercivity at room temperature. The composites also own good microwave absorption properties, and the absorption bandwidth with reflection loss below 27 dB is up to 3.8 GHz in the 2–18 GHz frequency range.

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Electron transfer, free activated energies and kinetics process study of [Zn[Pc(S–$C_6H_{13}OH)_4$]].[Cn] nano-structure complexes

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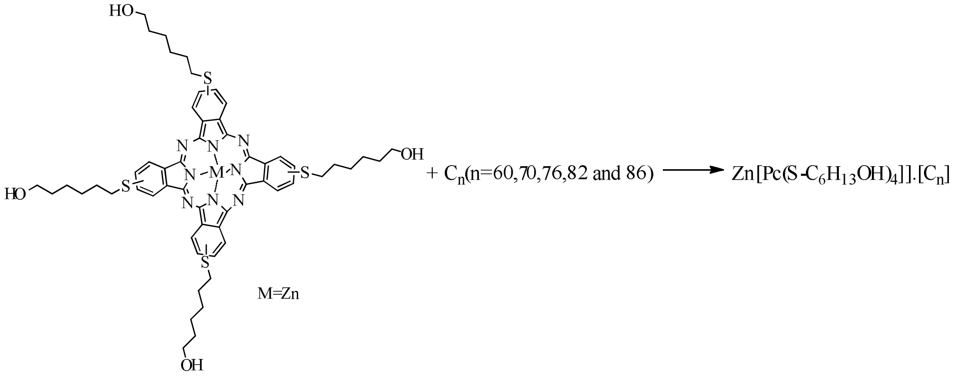
Phthalocyanine is an intensely colored macro cyclic compound that is widely used in dyeing. Phthalocyanines form coordination complexes with the most elements of the periodic table. Molecular structure of metallo-phthalocyanine zinc, 2,9,16,23-tetrakis(6-hydroxyhexylsulfanyl) phthalocyanine (Zn[Pc(S–$C_6H_{13}OH)_4$]) were studied before [1] . Metal phthalocyanine derivatives (MPcs) have attracted the attentions due to the prospects of application as electro-catalysts. Since the discovery of fullerenes (C_n), one of the main classes of carbon compounds, the unusual structures and physiochemical properties of these molecules have been discovered, and many potential applications and physicochemical properties have been introduced. Up to now, various empty carbon fullerenes with different numbers, such as C_{60}, C_{70}, C_{76}, C_{82} and C_{86}, have been obtained. The relationship between the number of carbon atoms and the free activation energies of electron transfer ($\Delta G^{\#}_{et(1)}$ to$\Delta G^{\#}_{et(4)}$), as assessed using the *electron transfer* (ET) equation on the basis of the oxidation potentials (^{ox}E) of (Zn[Pc(S–$C_6H_{13}OH)_4$]) for the predicted the complexes, between fullerenes(C_n) (n=60, 70, 76, 82 and 86), with (Zn[Pc(S–$C_6H_{13}OH)_4$]) as [Zn[Pc(S–$C_6H_{13}OH)_4$]]. [C_n], are presented here(Schem1). The calculations are presented for the four reduction potentials ($^{Red}E_1$ to $^{Red}E_4$) of fullerenes C_n. The results were extended for supramolecular complexes [Zn[Pc(S–$C_6H_{13}OH)_4$]].[C_n] for fullerenes C_{60} to C_{300}. The kinetic rate constants of the electron transfer (k_{et}, n=1-4)and maximum wave length ($\lambda_{max(et)}$) of the photoelectron transfer, were also calculated in this study.



Scheme 1

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Novel heat and corrosion resistant nanocomposite of DGEBA/functionalized magnetic Fe_3O_4 cured with 2,7-diaminoxanthone

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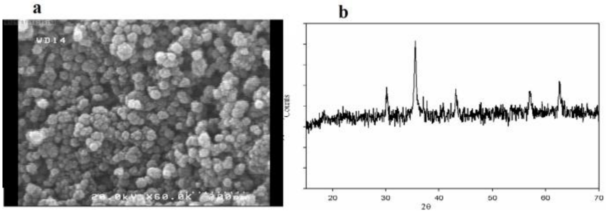
Xanthone derivatives are of naturally and synthetically important analogues that possessing admirable thermo-oxidative and hydrolytic stability with several biological and pharmacological properties [1, 2]. Magnetic supplies are one of the motivations in production of superior materials in the new technology area. Fe_3O_4 because of having versatile characteristics such as small size, supermagnetism and low toxicity are widely developed in various fields such as physics, medicine, biology and material sciences [3].

Polyxanthones are a class of high polymers with excellent thermal and chemical resistanc. In continuation of our ongoing work on polyxanthones [4] and also in order to access to epoxy resins with anticorrosion activity and high thermal stability, in the present study, we have used 2,7-aminoxanthone as curing agent for epoxy systems to acquire new types of functional polyxanthones. For this purpose, at first 2,7-diaminoxanthone were prepared and then used in thermally curing process of neat DGEBA and nanocomposite of DGEBA with magnetic functionalized Fe_3O_4 nanoparticle. The curing and thermal degradation kinetics of cured systems were studied by using DSC and TGA, respectively. The water sorption and anticorrosion activity of the fully cured epoxy systems were investigated. The epoxy resin and its nanocomposite were evaluated in 1.0M HCl by a series of electrochemical measurements such as corrosion potential (E_{corr}), polarization resistance (R_p) and corrosion current (I_{corr}).



Scheme 1**:** (a) SEM image of epoxy nanocomposite, (b) XRD pattern of Fe_3O_4

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Oxidative coupling of thiols into disulfides catalyzed by Cu(II) salen complex immobilized on Fe_3O_4 nanoparticles

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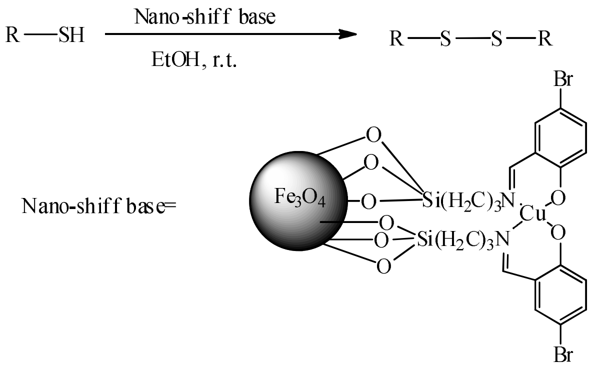
Selective oxidation of thiols to the corresponding disulfides is of interest from the point of view of biological and chemical process [1–2]. Thiols are among functional groups which can be easily over-oxidized and, therefore, extensive studies have been carried out to elaborate controlled conditions like iodine/hydrogen iodide, bromine, potassium dichromate, potassium permanganate/ copper(II) sulfate. Nevertheless, most if not all of reported methods produce the desired disulfides with concomitant formation of solid waste by-products requiring time and solvent consuming purification procedures prior to isolation of the pure product. Thus, there still exists a need for simple, mild, clean and efficient oxidative methods that would produce the target disulfides in high yields without complicated work-up procedures.

In this work we report a very efficient and simple method for oxidative coupling of thiols to the corresponding disulfides using H_2O_2 catalyzed by functionalized magnetic nanoparticles Fe_3O_4 with Schiff base complex of Cu(II) under mild conditions as shown in Scheme 1.



Scheme 1

References:

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Design, synthesis and applications of nanoparticles

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Nanotechnology, a rapidly growing science, is focused on the integration of fields such as physics, biology, engineering, chemistry, computer science and others. Over a few years the use of nanoparticles has brought a new era to the field of industry based on their unique optical, electronic, photonics, magnetic, biologic, catalytic properties. Many of the nanomaterials developed have already had a high impact on health care. Nanoparticles have shown an ability to improve pharmacokinetics, pharmacodynamics and to reduce the toxicity of associated drugs [1].

In our studies, due to potential applications of nanoparticles in medical diagnostics, imaging, and therapeutic treatments, in optoelectronics and data storage, designing and synthesizing of nanoparticles was studied and a variety of nanoparticles of different structural and chemical formulations have been tested for their target specificity such as drug carrier systems [2-8].

Also, we introduced new efficient and environmentally friendly reagents in the synthesis of nanoparticles. In these methods, the relative rates between nucleation and growth of nanoparticles are well controlled by choosing an efficient reducing as well as a capping agent and nanoparticles are formed with various interesting chemical and physical properties [9, 10].

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Rh/MWCNTs as effective catalyst in benzene hydrogenation and comparison its activity with Rh/AC

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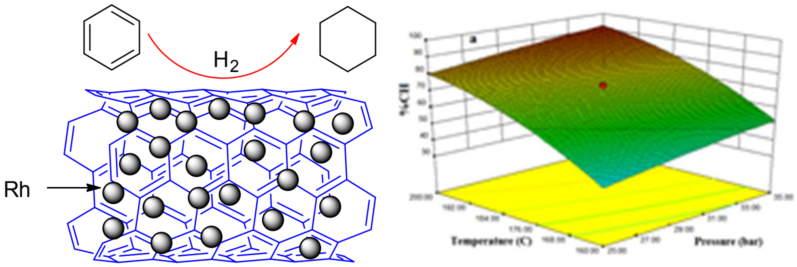
Hydrogenation of benzene to cyclohexane has been known to be an important industrial process due it application in production of nylon 66 and as solvent[1]. Benzene is known as carcinogen substance and as main pollutant of air in BTX group. According to MSAT (Mobile source air toxicity) limitations and Euro 4 and Euro v specifications for fuels, the amount of total aromatic compounds in gasoline is allowed at max 35% v and benzene is at max 1% v. many of countries such as European Community, USA, Japan and others reduce the amount of benzene in gasoline and have established in 1% (v/v) the maximum tolerated level of benzene in automotive gasoline [2–4].

The objectives of this work are evaluating the catalytic activity of Rh supported on mesoporous multiwalled carbon nanotubes (MWCNTs) and activated carbon (AC) on benzene hydrogenation (Scheme 1) and modeling of results by response surface methodology (RSM).



Scheme 1

References:

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Magnetic nanoparticles supported sulfonic acid, recoverable catalyst for mannich reaction

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[b] *Department of Chemistry, Islamic Azad University, Qaemshahr Branch Qaemshahr, Iran, Email: zareyee@Gmail.com*
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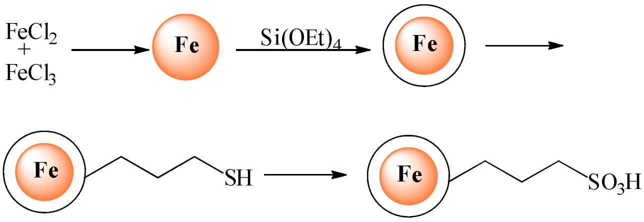
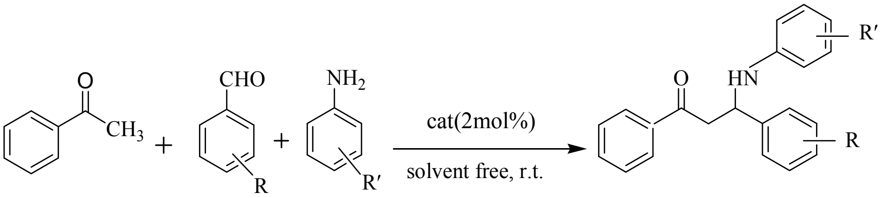
Mannich reaction produces β-amino carbonyl compounds from three components such as an amine, aldehyde and ketone. The products of the Mannich reaction are used for the synthesis of amino alcohols, peptides and lactams and as precursors to synthesize amino acids [1].

In recent years, magnetic nanoparticles are of more attention for researchers from a wide range of disciplines, including biotechnology/biomedicine, catalysis, magnetic resonance imaging, magnetic fluids and environmental remediation [2-4]. Functionalized magnetic nanoparticles are very promising for applications in catalysis, particularly in liquid-phase catalytic reactions. Along this line, we prepared magnetic nanoparticles supported sulfonic acid according to Scheme 1. The resulting material characterized with TEM, TGA, XRD, DLS, ZP and FT-IR.



Scheme 1

The catalyst was then tested as a solid acid catalyst for the mannich reaction of various types of aniline, acetophenone and benzaldehyde under solvent free reaction conditions at room temperature (Scheme 2).



Scheme 2

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Synthesis, characterization and investigation of physical properties of hybrid nanocomposite of polyaniline with $Fe_{0.01}Ni_{0.01}Zn_{0.98}O$ nanoparticles

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In the recent years, the synthesis and engineering of inorganic/organic hybrid materials in nano-scale have received great attention due to wide range of applications. Organic/inorganic composites may combine the advantages of both components and may offer special properties through reinforcing or modifying each other [1]. In the recent years, some of conducting polymers nanocomposites with inorganic nanoparticles such as TiO_2, SnO_2, SiO_2, ZnO and etc were synthesized and their properties were studied [2-4]. Polyaniline (PANI) is one of the best known conducting polymers due to its high conductivity, ease of preparation and good environmental stability, which make it suitable for variety applications

In this research work, $Fe_{0.01}Ni_{0.01}Zn_{0.98}O$ nanoparticles (FNZPs) as iron/nickel co-doped zinc oxide nanoparticles were first synthesized by sol-gel technique with mixing $Fe_2(NO_3)_3$, $Ni(NO_3)_2$ and $Zn(NO_3)_2$ in the presence of citric acid at pH 7 (by adding liquid NH_3 solution). Then, the novel conducting FNZP/PANI nanocomposite was synthesized by *in situ* free radical polymerization of aniline monomer in HCl aqueous solution, using ammonium peroxysulphate as an oxidant. The obtained nanocomposite was characterized by Fourier-transform infrared (FTIR), X-ray diffraction (XRD), scanning electron microscope (SEM) and UV-Vis absorption techniques. The obtained results showed that FNZPs have been encapsulated by PANI. The electrical conductivity measurements by four probe method showed that the synthesized nanocomposite exhibits high electrical conductivity at room temperature thus enhancing the property of semiconductor metal oxides.

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Grafting of dye Disperse Red 60 to the surface of carbon nanotubes

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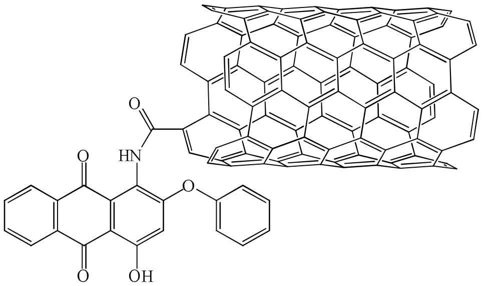
Carbon nanotubes (CNTs) are one-dimensional structures which are cylindrical in appearance and have unique properties that these structures for use in many applications of nano-technology, electronics, optics and other fields of materials science makes perfect. But the carbon nanotubes not having active groups, is chemically inert to the addition of chemical functional groups on the surface of the nanotubes, leading to the production of materials with new properties.The purpose of this study was to increase compatibility of CNTs through covalent bonding functional groups by Disperse Red 60. Overcome the effect of compressibility of the material in various solvents, resulting in separation and filtration of the nanotubes is facilitated. For evaluating the end product synthesis, solubility tests, scanning electron microscopy (SEM) and Raman spectra, 1HNMR, FT-IR, TGA, UV-VIS are used.



Scheme 1

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The aminopyridine based azo-azomethine dyes; spectroscopy, solvatochromism and biological properties of 4-((4-R-phenyldiazenyl-2-(pyridin-2-ylimino) methyl)phenol

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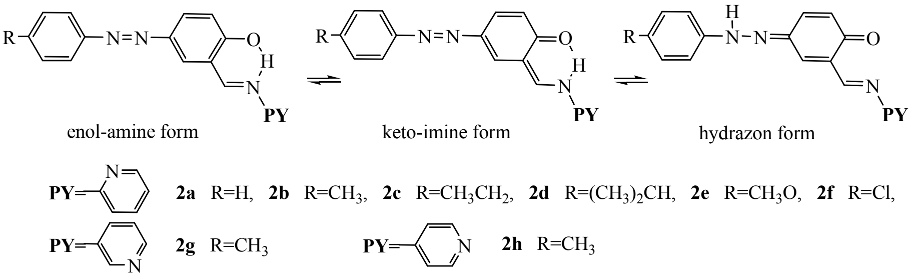
A series of azo-azomethine dyes based on pyridine rings were synthesized by condensation reaction of *n*-aminopyridine with 5-((4-R-phenyl)diazenyl)-2-hydroxybenzaldehyde [1-2]. Substitution, solvent environment, temperature and acid-base influence on the wavelength of electronic absorption have been studied. The absorption maxima of synthesized dyes show bathochromic shift (positive solvatochromism) in DMF and DMSO solvent. The nature of substitutions, solvent environment, hydrogen bonds, temperature, pH and changes in the dipole moment of the molecules are the key factors in deciding the solvatochromism of azo-azomethine dyes [4-6]. The compound **2h** showed higher antibacterial and antioxidant activity compared to others. The obtained results suggest the importance of the amino group in the 4- position of the pyridine ring for antioxidant and antibacterial activity.



Scheme 1

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Synthesis of functional graphene oxide by ionic liquids and its microwave absorbing properties as a nanofiller in nanocomposits

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Applications that involve specific requirements in microwave reflection suppression may require the development of new radar absorbing materials (RAM) [1,2]. RAM is used to cover the surface of targets, which include different types of equipment, land vehicles, aircraft and ships. Several parameters have to be taken into account in developing RAM. Among these, weight, thickness, microwave absorption, environmental resistance and mechanical strength are of particular importance [1,3].

In this work first graphene oxide prepared by modified Hummers and Offeman's method [4, 5] then the Ionic Liquid (ILs) used as a reagent and absorbing agent for the fabrication of functional graphene oxide nanostructures. The effect of the functional graphene oxideas as nanofillers in nanocomposit on the electromagnetic properties was investigated. The electromagnetic properties and absorption performance were evaluated by performing wave guide measurements in the 5.0–12.0 GHz range. Functional graphen oxide nanofillers were found to be suitable candidates for use as a lossy medium due to their peculiar electromagnetic properties**.**

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Synthesis and characterization of green polyvinylpyrrolidone/diacid modified-TiO_2 nanocomposites

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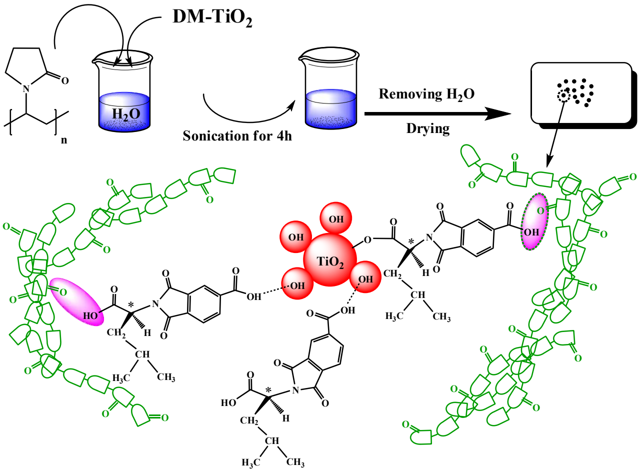
Polyvinylpyrrolidone (PVP) was selected as an organic component for the preparation of nanocomposites (NC)s due to its unique characteristics. This macromolecule is highly soluble in polar solvents therefore it is necessary to avoid phase separation in the reaction. Another advantage of use of PVP is that this material can be thermally cross-linked, and cause to the composites has exceptional thermal stability and high mechanical strength [1-3]. The goal of this study is to focus on preparation, investigation of the morphology and properties of new NCs loaded with 5, 10, and 15 wt.% of diacid modified-TiO_2 (DM-TiO_2) (Scheme 1). The data from analysis presented that the obtained PVP/DM-TiO_2 NCs have improved properties. Incorporation of TiO_2 NPs into the PVP system was seen to have a clear effect on the shape and size of PVP matrix. According to the thermogravimetric analysis results, the presence of DM-TiO_2 stabilizes thermal degradation of PVP.



Scheme 1

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Application of Fe_3O_4 nanoparticles decorated multi-walled carbon nanotubes for the removal of modafinil amide sulfide from aqueous solution

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This paper reports a simple and efficient chemical method to decorate multi-walled carbon nanotubes (MWCNTs) with iron oxide nanoparticles. The results of TEM and FTIR analysis of prepared nanocomposite shown that iron oxide nanoparticles were well deposited on the outer walls of MWCNTs. The size of the nanoparticles ranges from 30 to 50 nm. The sorption property of MWCNTs/Fe_3O_4 composites for the removal of Modafinil Amide sulfide from aqueous solution was explored. The results shown that MWCNTs/Fe_3O_4 composite possesses high sorption capability for removal of Modafinil Amide sulfide. This method has a high potential to remove pollutants from water samples.

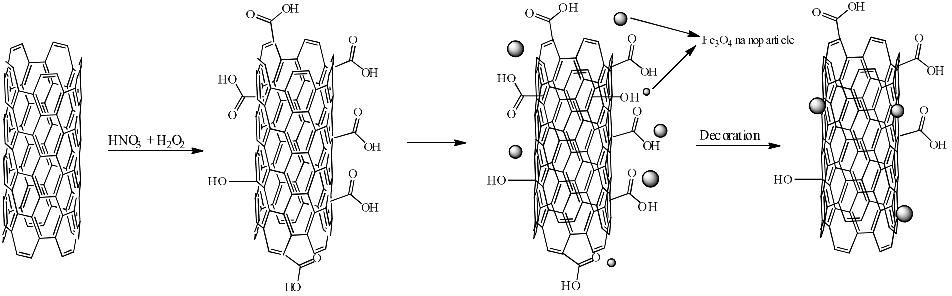
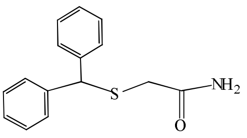


Illustration of the coating of iron oxide nano particles on MWCNTs



Modified Amid Sulfide

Scheme 1

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Sorption of cadmium from industrial wastewater treatment using magnetic nanoparticles

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The toxic heavy metals present in wastewater, effluents and soils are becoming a major environmental concern and multi-metal pollution is the usual situation in environmental media [1, 2]. Recently, more and more efforts have been made on remediation of soils and wastewater polluted by toxic metals, several approaches for remediation of aqueous systems contaminated with heavy metals have been reported [3, 4].Among these, adsorption is considered as an effective and economical method for the removal of pollutants from waste-water due to easy handling [1]. In this reasearch, effect of the Fe_3O_4 magnetic nanoparticles as a cadmium (Cd) adsorbent was studied. In the other hand, pH of solutions, contact time and adsorbent amounts as effective parameters were investigated. To this end, pH values were set at 2,4,6,8 and 10; also, contact times were set at 10,30,50,70 and 90 minutes. Amount of the cadmium in the solution was measured by atomic adsorption system (AAS). Results show that, best deletion was happened at the alkaline pH and 10 minutes as a contact time. Also, the results shown that, the efficient and operant amount of the Fe_3O_4 magnetic nanoparticles as a cadmium (Cd) adsorbent was 0.5 gr. In addition, reducing the pH value from 10 to 8 caused to increasing the contact time from 10 to 50 minutes, to saving the same yield in the elimination of the cadmium from the solutions.

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CdTe quantum dots as novel and highly efficient nonmaterials for removal of new fuchsine dye under visible light

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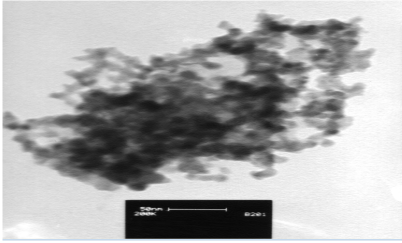
The industrial wastewater usually contains a variety of hazardous compounds and toxic substances, and water pollution has become a serious environmental problem facing humans. Currently, synthetic dyes are the main pollutant groups of wastewater. The presence of even very small amounts of dyes in water can cause serious environmental problems, for instance, growth of aquatic bacteria can be reduced light penetration into water by organic dye molecules [1]. Thus, there is a considerable need to treat these colored effluents before discharging them to various water bodies. The degradation of pollutants in water has attracted much interest in the last several decades due to the large-scale production of synthetic dyes, slow biodegradation, low decoloration and high toxicity [2]. The annual more than 10,000 different synthetic dyes are produced worldwide production of dyes is more than 7 $\times 10^5$ tons, and it has been estimated that nearly 5–15% of these lost dyes are continuously entering the water systems from various industries [3].

In this paper, the use of CdTe quantom dot has been investigated to degradation the new fuchsine dye. The QDs size was controlled by adding TGA as a capping agent. The CdTe quantom dot was characteized by using X-ray diffraction (XRD) and Transmission Electron Microscopy (TEM), PL and UV-Vis. The average size of CdTe quantom dot was found to be 3 nm. The effect of dosage of QDs, pH, time and initial dye concentration on the degradation effeciency of dyes were studied. A modified Langmuir- Hinshelwood model with a pseudo-steady state approachis used for kinetic analysis.



Scheme1: TEM Image CdTe quantom dot

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Polymer grafting of magnetic nanoparticles as a carrier in drug delivery

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Magnetic nanoparticles (MNPs) are a major class of nanoscale materials with the potential to revolutionize current clinical diagnostic and therapeutic techniques. Due to their unique physical properties and ability to function at the cellular and molecular level of biological interactions, MNPs are being actively as carriers for targeted drug delivery [1,2].Nano carriers are generally less than 100 nm in size and have theability to transport and release drugs to a target site with high efficiency and limited side effects[3,4]. Application of magnetic nano-particles depends largely on the preparation processes to select optimal conditions and type of modification. In this study iron oxide nano-particles (Fe_3O_4) were prepared by the co-precipitation method and then modified with 3-mercaptopropyltri methoxysilane in dioxane. Then functionalized sorbent was provided by coupling of Brilliant Cresyl blue. The obtained nano-adsorbent was characterized by Fourier transform infra-red spectroscopy, scanning electron microscopy and X-ray Diffraction. Then the effect of various parameters such as pH, and contact time were studied. Also, the adsorption isotherms kinetics and capacity at optimum conditions were investigated. The nano-adsorbent was used to measure for drug release in human biologic fluid. The concentration of drug was measured by conductometry technique.

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The interaction of anticancer drugs and nanotubes: an approach to drug delivery systems

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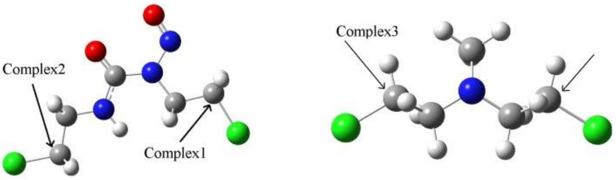
Carmustine is used to treat various types of cancer. It prevents DNA replication and DNA transcription that have chemotherapeutic activity and to release drugs in cell without damaging healthy cells, nanotubes can be used [1,2]. Mechlorethamine is a group of anticancer chemotherapeutic drugs. It works by binding to DNA, crosslinking two strands and preventing cell duplication. Complex1 that is formed between Nanotube and Carmustine has the lowest energy. So this composite is more stable than the other agents and NBO analysis was performed by B3LYP/6-31G(d) method , too Hyperconjugation may be given as a stabilizing effect that arises from an overlap between an occupied orbital when these orbitals properly oriented. This noncovalent bonding-antibonding interaction can be quantitatively described in term of the NBO approach that is expressed by means of the second – order perturbation interaction energy (E2) the composite between Nanotube-drug is more stable than drug only. All composites are shown in Scheme1 [3,4].



Scheme1

Because of the difference between of two head of carbon in carmustine two complexes are formed. Complex1 and 2 are related to carmustine but complex3 is related to Mechlorethamine. In all complexes Thermodynamic functions were calculated by frequency investigation. These results show that all of these reactions are exothermic and in all of them, the entropy decreases. So Entropies of reactions are thermodynamically unfavorable factor but Enthalpy is a favorable factor in the review. The obtained formation ΔG^0 of all complexes becomes negative in 298K. So all complexes could be formed according to thermodynamic laws.

Agent	ΔS^0/kcalmol^{-1}	ΔH^0/kcalmol^{-1}	ΔE^0/kcalmol^{-1}	ΔG^0/kcalmol^{-1}	Stability constant
Complex1	-0.0029	-15.0103	-15.0125	-14.1421	2.36×10^{10}
Complex2	-0.0927	-143.4444	-142.8507	-115.8076	8.69×10^{84}
Complex3	-.00211	-16.0043	-16.0212	-15.2341	2.12×10^{10}

Refrence:

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Produced nano-sized plants elements needed to increase the efficiency of nanofertilizer

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Nanotechnology offers an important role in improving the existing crop management techniques. Nano-encapsulated agrochemicals should be designed in such a way that they possess all necessary properties such as effective concentration (with high solubility, stability and effectiveness), time controlled release in response to certain stimuli,enhanced targeted activity and less eco-toxicity with safe and easy mode of delivery thus avoiding repeated application [1-5].

In this work,elements oxide nanoparticles were synthesized by a modified co-precipitation method. Sulfate or phosphate desired elements were dissolved in 50 mL 0.1 M HCl, which was then stirred then 100 mL of 1.5 M NaOH solution was injected and the reaction to be continued.

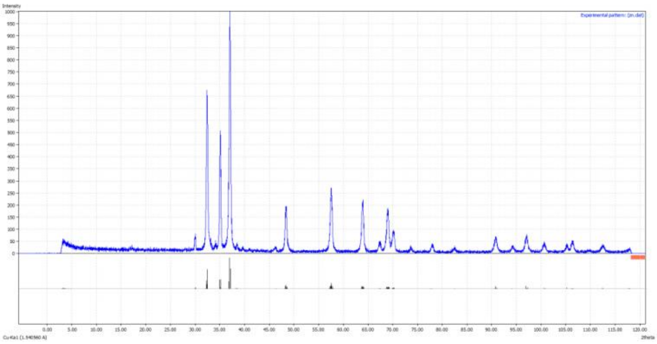

Figure 1. XRD spectrum of ZnO.

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Preparation of MWCNT/TiO$_2$-Co nanocomposite electrode by electrophoretic deposition

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A multi-walled carbon nanotube (MWCNT)/decorated by TiO$_2$-Co nanoparticlescomposite coating with excellent microstructural homogeneity was produced on copper substrate from aqueous suspensions using electrophoretic deposition (EPD) method. Electrophoretic deposition (EPD) has been used to combine multi-walled carbon nanotubes of diameter in the range 20–30 nm and commercially available TiO$_2$ nanoparticles (23 nm particle size) in composite films[1]. The TiO$_2$-Co NPs have been synthesized by sol-gel method, using PVP polymer[2].In the EPD the concentrations of different additives were optimized to obtain stable suspensions of MWCNT. The suspensionused for EPD was prepared using 25 mLacetylacetonel, 0.0075 g CNTs, 12.5 mLacetone,12.5 mLetanol,0.04g Iodine, 0.3 g Tio$_2$-Co and 0.04 g Mg(NO$_3$)$_2$. The mixture was ultrasonicated for 1 h.In addition, optimization of different parametersthat was effective in the EPD, including electrode materials type, deposition time, electrode separation, deposition voltage and electric field, were studied. The optimum EPD conditions were obtained at voltage of 80 V and deposition time of 5 minand electrode separation of 2 cm with well With a homogeneous layer of MWCNT/TiO$_2$-Co on the copper substrate.The electrodes were made with dimensions of $10\times10\times0.02$ mm^3. The copper substrates were cleaned with acetone and distilled water in an ultrasonic bath and Nitric acid for 5 min before the deposition process. After EPD, samples were dried upright in a desiccator. For the laminate coatings the deposited layers were dried for at least 30 min before deposition of the next layer (up to 4 layer). Structural and morphological characterizations have been carried out using XRD, SEM.

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The influence of Ga doping on the physical property in the zigzag BN nanotube to phenol adsorption

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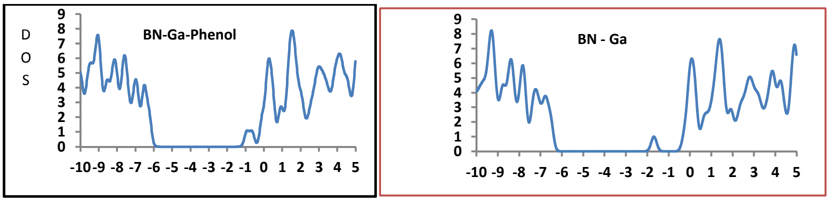
In this investigation, we have considered the physical properties and electronice structures in the pure BN nanotube and impured by Ga atom in order to phenol adsorbtion by using density functional theory method.
In the impure sample one B atom replaced by Ga atom.
In the both models, in both mouthes are saturated by H atoms.

We have computed, Density of states, nuclear magnetic resonance by using B3LYP - 6-31G* on the optimized forms [1]. Information energy shows that impure structure is more stable than pure structure. Density of states shows that there is a sharp peak near to Feremi level and conductivite to be increased (scheme1). Mean while, Phenol adsorbtion in the impure form is more than pure form. NMR parameters are changed for B and N atoms that are directly connected to Gallium atom. But for other atoms the those parameters remain unchanged.



Scheme 1

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Investigation of the last solution pH role on the growth mechanism and configuration of NiSe nanostructure layers

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NiSe semiconductor nanostructure thin films have been synthesized through a simple chemical bath deposition approach. X-ray diffraction characterization suggested that the product consists of hexagonal phase pure NiSe. The samples were also characterized by absorbance spectra for energy band gap determination and scanning electron microscopy (SEM). The results showed that pH plays a crucial role in the process. Other parameters preparations such as the deposition time and pH also have influence on the morphology and the energy band gap of the final products to some extent. In comparison to other similar works, our method is simple, low cost and can be easily controlled. The ultimate goal is to create high quality thin films that have been engineered by tailoring the configuration and thickness.

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A novel one-pot approach to the synthesis of symmetric trithiocarbonates from carbon disulfide and alkyl halides using imidazole

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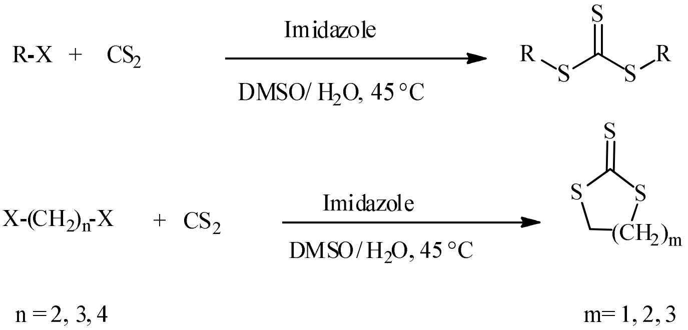
Dialkyl trithiocarbonates are of importance in organic synthetic[1]. medicinal application [2] agrochemicals[3]. RAFT agent in the free radical polymerization reactions [4]. Pharmaceuticals [5]. In froth flotation[6]. The most convenient method for the synthesis of symmetrical trithiocarbonates arylation) of CS_3^{2} with alkyl (aryl) halides. The is alkylation(trithiocarbonate anion is generally prepared by *in situ* one-pot reaction of carbon disulfide with the catalysts inorganic. A novel method is reported for the synthesis of symmetric dialkyl and cyclic (5, 6 and 7 member) trithiocarbonates from alkyl halides and carbon disulfide in the presence of imidazole and water in DMSO under mild reaction conditions. Imidazole is used as an inexpensive, non-toxic and readily available catalyst in this procedure. (Scheme1)



Scheme 1

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Enhanced antibacterial activities of ZnO thin films: a comparative study of hybrid semiconductor nanomaterials

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To improve optical, catalytic, photocatalytic, antibacterial properties, many researchers have beenfocused on modified semiconductor oxides includingdoped, heterojunctionlayers and inorganic hybrid. Among these, the multilayer heterojunction structureshave increasingly attracted attention mostly due totheir excellent properties which aredifferent from the conventional monolayer thin films [1].In this paper, Nanostructure single ZnO, NiO and multilayered ZnO/NiO/ZnO films were prepared using sol–gel method. The two sols were prepared separately using $Zn(CH_3COO)_2 \cdot 2H_2O$and $Ni(NO_3)_2.6H_2O$ as precursors. Then, the glass substrateswere dipped alternatively in each sol, six coating cycles were repeated for each layer and finally thermal annealingwere performed at 500 °C. XRD pattern correspond to ZnO hexagonal wurtzite structure forall samples, Fig. 1.The photobiocideactivities of samples against a Gram-negative bacterium Escherichia coli and a Gram-positive bacterium Staphylococcus aureuswere investigated applyingthe so-called "antibacterial drop test"under UV illumination and in the dark condition. Antibacterial activity of multilayered ZnO/NiO/ZnOfilm was higher compared with single film, Fig. 2. In addition, Escherichia coli inactivated more efficiently compared to Staphylococcus aureus.The compatibilities of multi-layer oxide films and the choiceof substrate material for latticematching and preferential growth along certain crystallographicdirectionare the important factors for improved ZnO/NiO/ZnO film.

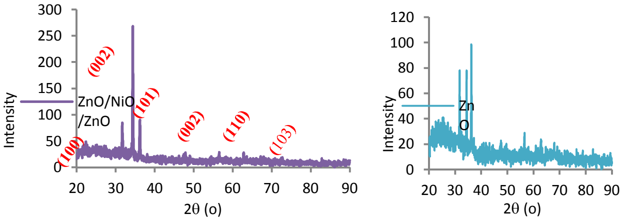

Fig. 1. XRD patterns of samples

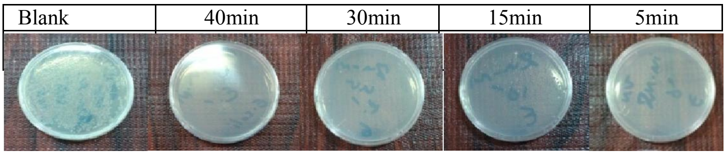

Fig. 2. Images of the petriplates showing growth of bacterial colonies of E. coli using ZnO/NiO/ZnO as catalyst after 40,30,15 and 5 min UV illumination

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Inrestigation of the effects of three isopropilat aluminum nano particles increasing on value of viscosity changes and Ethilenglicole thermal conductivity

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In this research the effects of three isopropilate Aluminium nano particles increasing on thermal conductivity and viscosity changes of EthilenGolicole as a base fluid in 25, 30, 35, 40 , 45 °C temperatures And %1, %2, %3, %4 and %5 Mol denses Have been investigated. In this investigation the optimal concentration for Ethilen Golicol fluid nano has been determined and the heart for identical distribution of nano particles in fluid has been used. The results of thermal conductivity and viscosity indicate their increasing along with the adition of the concentration and also increasing of thermal conductivity along with temperature increase and viscosity decreasing along with temperature increasing.

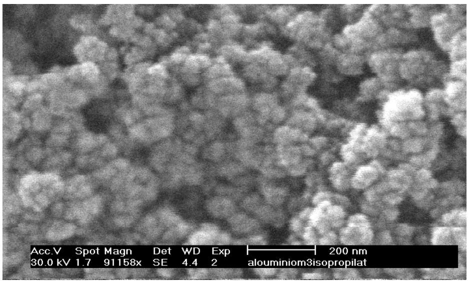

Image 1: Sem nano particles Aluminum three isopropilat

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Study of photocatalytic activity of CdTe quantum dots as efficient nanoparticles for removal of Aniline Bule

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CdT**e** quantum dots (QDs), were prepared for photodecolorization of Aniline Bule, as a model dye, under UV light irradiation. The syntheses of QDs were carried out using a simple chemical co-precipitation method. The prepared samples were characterized by various techniques including X-ray diffraction, transmission electron microscopy, photoluminescence and UV-Vis spectrophotometry. The average size of QD CdTe was found to be 3 nm. The effect of dosage of QD, pH, temperature, time and initial dye concentration on the degradation effeciency of dyes were studied. The efficiency of dye degradation for Aniline Blue were nearly 98%. The optimum conditions were obtained in pH=7, T=65 ^{0}C and 100 min for Aniline Blue. Finally, the reproducibility and kinetic model of the dye degradation were discussed [1-3].

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Biosynthesis of silver nanoparticles using *Scrophularia striata* flower

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Silver nanoparticles are reported to possess anti-fungal, anti-inflammatory,anti-viral anti-angiogenesis, antiplatelet activity and an effective antimicrobial agent against various pathogenic microorganisms [1]. There have been numerous study on the synthesis of silver nanoparticles using hazardous chemicals, low material, conversions, high energy requirements, difficult and wasteful purifications [2]. Use of fungi, bacteria and plant extracts for the synthesis of nanoparticles is quite n-ovel leading to green chemistry which provides advantages over chemical and physicalmethods as it is cost effective and environment-friendly, and can be scaled up for large scale preparation [3].

In this work, an eco-friendly process for synthesis of silver nanoparticles has been carried out using aqueous extract of *Scrophularia striata* flower. The synthesized nanoparticles were characterized using UV–Vis spectroscopy, fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM). To optimize the biosynthesis of silver nanoparticles, the effect of process variables such as extract concentrations, mixing ratio of the reactants and time were also investigated. The results of XRD and SEM showed the size of nanoparticles is below 100 nm. The antibacterial activity of the synthesized silver nanoparticles was confirmed against *Staphylococcus aureus* and *Escherichia coli.*

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Green synthesis of silver nanoparticles using *Rosa Canina* fruit

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Nanotechnology is a most promising field for generating new applications in all areas. The process of development of reliable and eco-friendly metallic nanoparticles is an important step in the field of nanotechnology [1]. Metallic nanoparticles have received great attention from chemists, physicists, biologists and engineers who wish to use them for the development of a new generation of nanodevices [2].

In the present study, silver nanoparticles (AgNPs) were synthesized from aqueous $AgNO_3$ through a simple and eco-friendly route using *Rosa Canina* fruit extract as a reductant and stabilizer. AgNPs were then characterized by UV–Vis spectrophotometer, X-Ray Diffractometer (XRD), Scanning electron microscope (SEM), and Fourier transform infrared (FTIR) spectroscopy. UV–visible spectrum of the aqueous medium containing silver ion showed a peak around 432 nm due to the plasmon absorbance of AgNPs. The morphology of the AgNPs was determined by SEM and the average diameter of the particles was determined below 100 nm with nearly spherical in shape. To optimize the synthesis of silver nanoparticles, the effect of process variables such as extract concentrations, mixing ratio of the reactants and time were also studied. Finally, the antibacterial activity of the obtained AgNPs was performed against *Staphylococcus aureus* and *Escherichia coli.*

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Adsorption of lead ions from aqueous solution using dendritic modified CNTs

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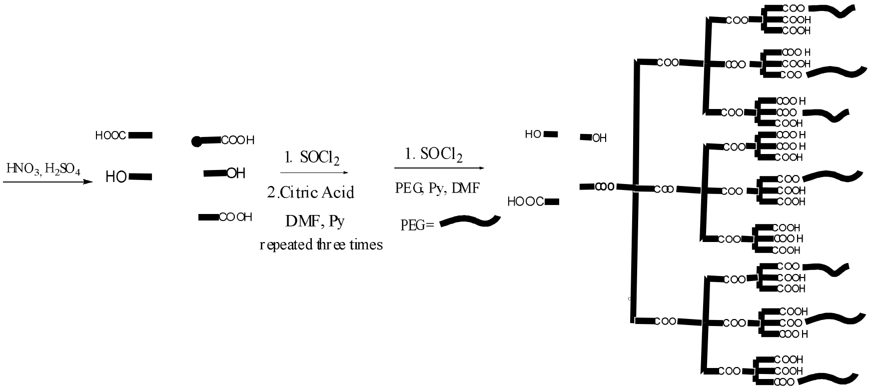
Water contaminated by heavy metal ions had become much more serious with a rapid development of industries and competitive use of fresh water in many parts of words [1,2]. It is necessary to remove these ions from the waste waters before releasing them into the environment. Carbon materials are a class of significant and widely used engineering adsorbent. As a new member of the carbon family, carbon nanotubes (CNTs) have exhibited great potentials as an attractive adsorbent in waste water treatment [3].

The objective of this work, capability of the dendritic modified CNT for lead ion (Pb^{2+}) removal from water was investigated. Also, Langmuir and Freundlich isotherms and three kinetic models were applied to fit the experimental data.



Scheme 1

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Synthesis of α-aminophosphonate immobilized on nanosilicate substrate for selective extraction of metal ions

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Toxic heavy metal ions, that are mostly toxic even at very low concentration, in groundwater and wastewater is a rising environmental problem worldwide. Removal of these pollutants from aqueous solution plays an important role in wastewater treatments. Therefore in recent years extensive studies have been undertaken to find more effective and cheaper methods for removal of heavy metal ions from aqueous effluents [1]. A wide range of techniques have been developed for the removal of these metal ions from wastewater such as ion exchange, reverse osmosis, adsorption, precipitation, co-precipitation, filtration, and coagulation. The adsorption technique is very popular and efficient due to simplicity and low cost [2,3].

In this work, we were synthesized the silica nanoparticles with size distribution less than 100 nm using the sol – gel method. For functionalizing this support we were used a one-step (based on Kabachnik- Fields reaction) and three-component approach consists of aldehyde, diethylphosphite and immobilized 3-(triethoxysilyl)propan-1-amine on silica support. The fabricated adsorbent materials were characterized by Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), X-ray diffraction (XRD), BET specific surface area, thermo gravimetric analysis (TGA), elemental analysis(CHN) and Fourier transform infrared spectroscopy (FT-IR) analysis. In the present work, we were studied heavy metal adsorption process for solutions including Zn2+, Ni^{2+}, Fe^{3+}, Co^{2+}, Cr^{3+}, Cu^{2+}, Cd^{2+}, the pH dependency of sorption, adsorption isotherms and adsorption kinetics at 25°C.

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A novel mixed organic fuels for synthesis of zinc aluminum oxide nanoparticles

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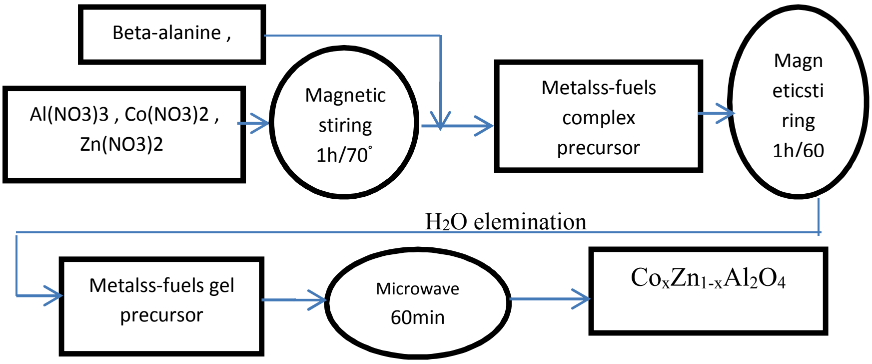
Thernard's Blue namely, cobalt (II) aluminate spinel, CoAl2O4,is one of the most popular of inorganic pigments and its physicochemical features, such as high thermal and chemical stability, high resistance to acids, alkalis, light and various atmospheric agents make it suitable for various industrial applications, such as ceramics, glass, plastics, paint, paper, rubber, and color TV tubes. unfortunately less attention has been paid to more environ-mentally aware synthesis of oxide-based pigments. Usually, a non-polluting method is associated with non-toxic raw materials and reaction intermediates as well as minimal energy usage. This paper concerns a novel, less-toxic, flexible and reproducible, organic fuels based synthesis of cobalt aluminate oxide spinels, CoxZn1-xAl2O4 (x = 0, 0.1, 0.2, 0.4, 0.6, 0.8 and 1), which comprise the gradual insertion of Co(II) cations within a gahnite (ZnAl2O4) host lattice. The carbohydrate has a triple role during the synthesis as complexing,template and gelation agent.[1,2]

Combustion synthesis or self-propagating high-temperature synthesis is an effective, low-cost method for production of various industrially useful materials.[3]by using a microwave oven instead of kiln we reach the cost-effective method without need to reach the high temperature above 800$^{\circ c}$.

The reaction process are compeletly explained in the following Scheme. the resultant powders were characterized by means of XRD, XRF, SEM, TEM, BET surface area, diffuse reflectance spectrometry and CIEL*a*b* color measurement.



Scheme 1

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Synthesis and characterization of novel dye from multi-walled carbon nanotubes and anthraquinone through diazotization reaction

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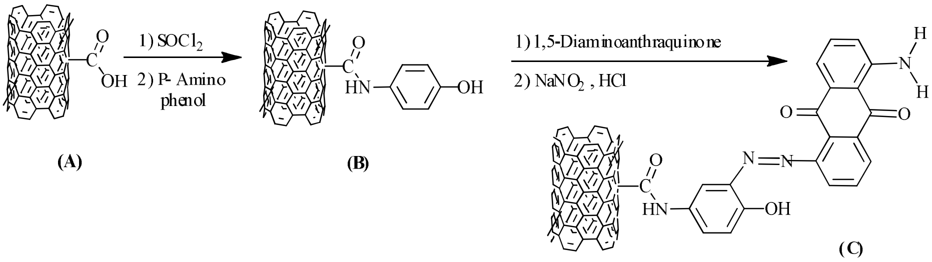
Carbon nanotubes have many properties such as Young's modulus, high tensile strength, high thermal conductivity, electrical conductivity and optical properties. But one of the main problems is the lack of solubility in aqueous and organic solvents, so it case all levels of reactivity and efficiency greatly will reduce. The main solution to this problem was functionalization of the CNTs [1]. Anthraquinone to form the main structure of the disperse dyes which have luminance and good stability [2] and can make a covalent bond with the nanotube.

In this project we first functionalize MWCNT with 4-Aminophenol and continue with 1,5-Diaminoanthraquinone through diazotization reaction coupled to the phenolic ring. Synthesis of phenolic Intermediate compound and final product by conventional spectroscopic methods such as IR, ^{1}HNMR, Raman, TGA and SEM images confirmed.

Comparison results of dye made of MWCNT show that the thermal resistance and very good solubility in organic solvents and water, which makes taking advantage of the unique properties of carbon nanotubes as a high-performance color in industries such as composites, paints and resins, textiles and ... [2,3].



Scheme 1

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Synthesis of some new 1,5-benzodiazepines fused with different heterocyclic moieties

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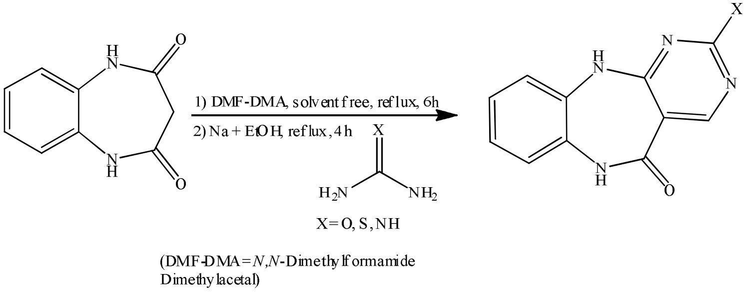
Benzodiazepines have been widely employed in clinical practices as anxiolytics, sedative-hypnotics, anticonvulsant vasopressin antagonists, and anticipated CNS-depressants [1]. Benzodiazepines and their polycyclic derivatives are used in pharmaceutical and biological chemistry, where they are used as antitumor agents, nevirapine analogues and anti–HIV-1 (Human Immunodeficiency Virus) agents. They also are screened for in vitro cytotoxicity against a number of cancer cell lines, such as colon cancer, breast cancer, lung cancer, and bladder cancer [2].

2-Amino pyrimidine is the most important member of all the diazines as this ring system occurs widely in living organisms. Further, these derivatives represent one of the most active classes of compounds possessing a wide spectrum of biological activities such as antimicrobial, cytokinin, pesticide, fungicide and anticancer activities[3]. Fragments of 2-Amino pyrimidine exist in structure compounds Inhibitors of Dihydrofolate Reductase (DHFR). The inhibition of DHFR leads to partial depletion of intracellular reduced folates with subsequent limitation of cell growth[4]. DHFR inhibition has long been an attractive goal for the development of chemotherapeutic agents against bacterial and parasitic infections as well as cancer [5].

In this work we report a simple and highly efficient approach for the synthesis of fused benzodiazepines with 2-aminopyrimidine ring and similar rings. 1,5-benzodiazepine-2,4-dione react with DMF-DMA and then produce was treated with nucleophiles such as guanidine, urea and thiourea to give the corresponding products. The FT-IR, ^{1}H-NMR and ^{13}C-NMR spectra confirms the structure of products. Currently, the biological properties such as antimicrobial activity of benzodiazepine derivatives and other synthetic derivatives are examining.



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Synthesis and characterization of one new copoly(amideimide) and this corresponding copoly(amideimide) /organoclay nanocomposite based on metaphenylenediamine, parapheylenediamine and trimellitimide units in the main chain

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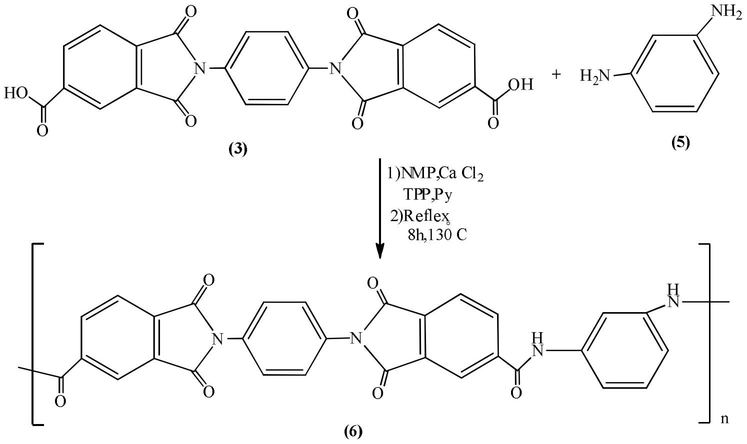
In this study poly (amide - imide) was synthesized by direct polycondensation reaction of trimellitimide with Para- phenylenediamine and Meta- phenylenediamine in the presence of triphenyl phosphite (TPP) , $CaCl_2$, pyridine and N-methyl-2- pyrolidon(NMP) (scheme1). In this work one new poly (amide - imide) nanocomposite reinforced by 5 % of organoclay particles was prepared .The structure and morphology of the were determined by X-ray diffraction (XRD) , scanning electron microscopy (SEM) , FT- IR spectroscopy. The thermal and optical behaviors of poly (amide – imide) nanocomposite studied by UV-vis spectroscopy and TGA.



Scheme 1

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Corticosteroids-loaded nanocapsules: preparation and characterization

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Now adays to treat the disease usually a high dose drug are used that has a wide side effects in tissues and cells. One of the most common solution for this problem is drug delivery system. In this study, corticosteroids-loaded nanocapsules were prepared by interfacial deposition of poly (ε -caprolactone) PCL. Major activity in this area has entered on aliphatic polyesters, principally due to the favorable toxicology of their degradation product. Polymeric nanoparticles have been extensively studied as drug carriers because they have the ability to control the release of a variety of drugs, to increase the drug stability and to reduce their toxicity [1]. In the last years, several researchers have shown the potential of the poly(ε-caprolactone) PCL nanocapsules as drug delivery systems [2]. In this investigation, the lipid-core nanocapsules were prepared by interfacial deposition of preformed polymer. PCL, sunflower seed oil, sorbitan monooleat, and cortisone were dissolved at ambient temperature in acetone. The organic phase was injected, under stirring, into the aqueous phase consisting of polysorbate 80 and water. The suspension was kept under stirring and then, the acetone was evaporated and the final volume (10 mL) of the suspension was adjusted using reduced pressure. The nanoparticle size distribution were measured by photon correlation spectroscopy then, we can saw nanotechnological properties such as nanometric mean size (194.3 nm) and negative zeta potential(-30.3 mv). The structure and morphology of nanocapsules were studied by UV, FT-IR and SEM techniques and cortisone was assayed by high-performance liquid chromatography (HPLC). Corticosteroids-loaded PCL nanoparticles have been characterized in terms of the mean size, morphology, and size distribution and SEM images of them (Fig 1)

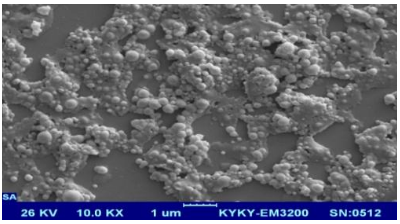

Fig1. SEM image of the main product

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Nanocapsules of oil soluble drug in biodegradable polymers

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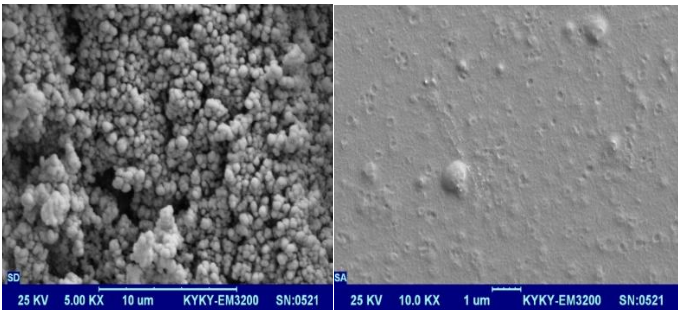
In this study, corticosteroids-loaded nanocapsules were prepared by interfacial deposition of polycaprolactone. Major activity in this area has centered on aliphatic polyesters, principally due to the toxicology of their degradation product by UV, FT-IR and SEM techniques and their supernatant were used for the spectroscopic scan analysis from 190 to 800 nm. Scanning electron micrographs was used for surface characterisation of both PCL nanoparticles and cortisone loaded PCL nanoparticles. SEM characterization of cortisone loaded PCL nanoparticles (Fig. a) and PCL nanoparticles (Fig. b). The particle size and poly dispersity indices were measured by photon correlation spectroscopy. Cortisone loaded PCL nanoparticles have minus zeta potential. Consequently, the information obtained allows establishing criteria for selecting a method for preparation of nanocapsules according to its advantages, limitations as a drug carrier [1-2].



a b

Scheme 1

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Efficient route for synthesis of 2*H*-spiro[acenaphthylene-1,4'-pyran]-2-one derivatives in the presence of morpholine as catalyst

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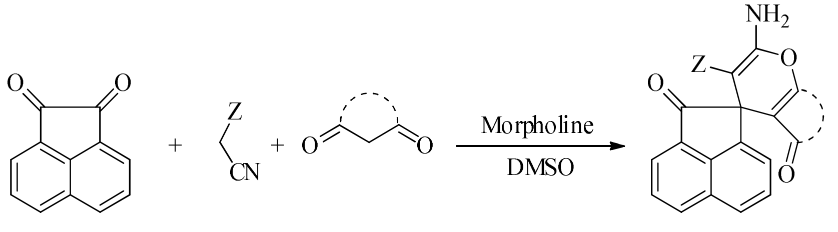
In multicomponent reactions (MCRs), three or more reactants come together in a single reaction vessel to form new products that contain structural units of all the components. This type of reaction becomes increasingly important in organic and medicinal chemistry because it allows obtaining highly sophisticated polyfunctional molecules through simple one-pot procedures.

Spiro compounds are important pharmacophores with analgesic, fungicidal, antidepressant, antitumor, and antibiotic activities [1,2]. Also, heterocyclic compounds containing pyran ring possess a wide spectrum of biological activities such as spasmolytic, anticoagulant, diuretic, anticancer, etc [3-5].

We now report an efficient method for the preparation of spiropyran fused heterocycles by reaction of acenaphthenequinone, malononitrile (or ethylcyanoacetate) and variety of active methylene componds in the presence of morpholine as catalyst. This reaction proceed smoothly in DMSO at room temparature and completed within 3 h (Scheme 1).^{1}H and ^{13}C NMR spectra of the crude product clearly indicate the formation of 2H spiro[acenaphthylene -1,4'-pyran]-2-one derivatives and does not appeared any by-product.



Z=CN,COOEt

12 Samples

Scheme 1

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Solvent-free coumarin synthesis via von pechmann reaction using magnetic nanoparticles supported sulfonic acid catalyst

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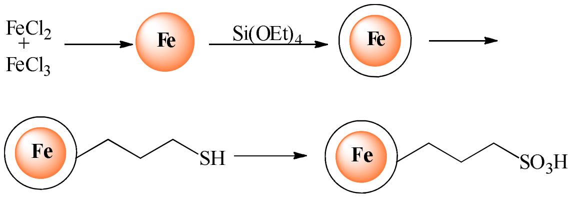
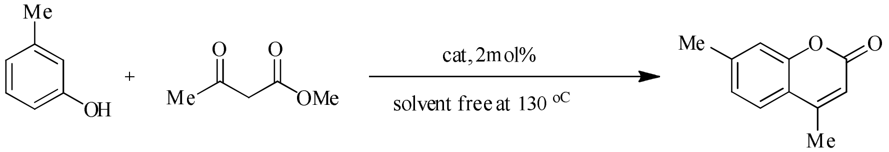
A valuable and simple protocol for coumarin ring synthesis is coupling of two components (phenol and *β*-Keto ester) (von Pechmann reaction) using acid catalysts [1]. In the conventional production of coumarins by the Pechmann reaction, concentrated sulfuric acid is used as the catalyst [2]. Several other acid catalysts, including Lewis acids, are known to affect this condensation [3]. However, moisture sensitivity of the majority of Lewis acids to the water produced in the Pechmann reaction renders them unsuitable for use in large scale applications. To address the above mentioned problems, a number of heterogeneous alternatives such as Nafion-H [4], Amberlyst-15 [5] and Montmorillonite clay [6] have been employed for this purpose in the Pechmann condensation. Although, these methods are suitable for certain synthetic conditions, in many of these methods the yields of products were not always satisfactory and the catalytic activities were lower than homogeneous catalysts in most cases.

Based on green chemistry protocols, we prepared magnetic nanoparticles supported sulfonic acid (Scheme 1). The resulting material was used successfully in Pechmann reaction under solvent-free reaction conditions at 130 °C (Scheme 2).



Scheme1



Scheme 2

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Synthesized hydrogel-silver nanocomposites poly(acrylic acid) modification with cysteine

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Silver nanoparticles are the most widely used antibacterial agents with a number of advantages. the higher degree of biocompatibility and long-term antibacterial activity can be achieved with hydrogel-silver nanoparticles.The design of hydrogel network which are begin empolyed az templates for nanoparticles synthesis is very much crucial,the present work involves the evaluation of few hydrogesl which are different in their nature to act as effective templates for synthesis of silver nanoparticles. upon the addition of hydrogels to the aqueous solution of silver salt,the silver ions get absorbed or anchored by the polymer network by ion exchange process of hydrogel functional groups or just by entrapment of silver ions in the free space existing between the gel network, when these silver salt-loaded hydrogels were added to naBH4 solution, an immediate color change was observed in the hydrogel from colorless to brown or dark brown, which is due to the excitation of surface plasmon vibrations of nanosized silver particles.

Purpose To improve the mucoadhesive properties of poly(acrylic acid) by the introduction of sulfhydryl groups. Mediated by cysteine was covalently bound to poly(acrylic acid) forming amide bonds between the primary amino group of the amino acid and the carboxylic acid moieties of the polymer. Polymers with thiol groups might represent a new generation of mucoadhesive polymers displaying comparatively stronger adhesive properties. the presence of $AgNO_3$, ammonium persulphate and polystyrene sulphonic acid. The resulted nanocomposites were characterized by scanning electron microscopy (SEM), x-ray diffraction (XRD), ultraviolet visible spectra (UV-vis) and fourier transform infrared spectroscopy (FT-IR).

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Effect of pressure on growth cubic boron carbide nano and micro structure by HFCVD

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Among various boron to carbon stoichiometry, the ratio higher than 2, are known as boron carbides. This is the case in the B-C system in which several compounds which do not appear in the phase diagrams were observed. Ploog and Amberger [1,2] There is several tetragonal compounds $B_{51}C$, $B_{50}C_2$, $B_{49}C_3$. The most stable B-C structure is rhombohedral with a stoichiometry of $B_{13}C_2$, $B_{12}C_3$, or B_4C, and some other phases close to $B_{12}C_3$ [3].

In this research, cubic boron carbide(c-BC) nano and microstructures were synthesize using hot filament chemical vapor deposition (HFCVD) regime in the five pressures such as: a) 1.5torr b) 4torr,c)8torr d)12torr and e)16torr for study pressure effect on growth c-BC structures. FESEM Fig (1), Raman, and XRD revealed that by increasing pressure: roughness was increased and Grin size from 38nm to 14nm and Crystal size from 14nm to 80nm was decreased respectively. Because increase pressure caused Probability of collapsing ions together was increased, so make a new sites as catalyst. In result of that numerous crystals growth on surface and roughness was increased.

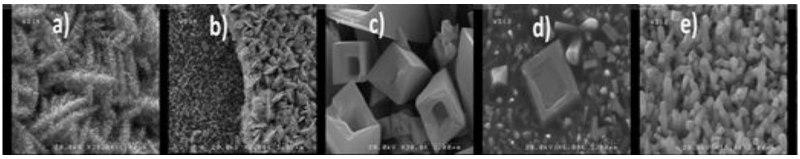

Fig 1: FE-SEM showed that increasing pressure growth from 1.5 torr to 16 torr caused complete cubic and was reduced dimensions of the c-BC.

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Ultrasonic activated efficient synthesis of chromenes using amino-silane modified Fe_3O_4 nanoparticles

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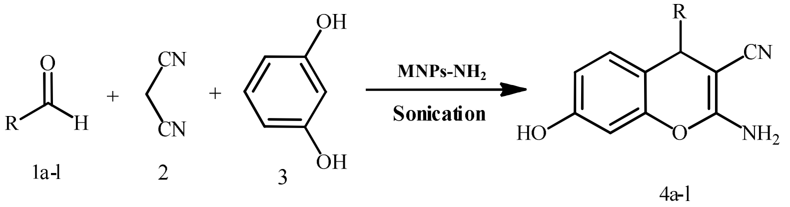
Multicomponent coupling reaction (MCR) is a powerful synthetic tool for the synthesis of biologically active compounds. Heterocycles containing the chromene moiety show interesting features that make them attractive targets for MCRs. The 2-amino-chromenes are widely employed as pigments, cosmetics, potential agrochemicals, and represent an important class of chemical entities being the main constituents of many natural products [1-3].

An efficient synthesis of 2-amino-4*H*-chromenes is achieved by one pot three component coupling reaction of aldehyde, malononitrile, and resorcinol using amino-silane modified Fe_3O_4 nanoparticles ($MNPs\text{-}NH_2$) heterogeneous nanocatalyst under sonic condition. The attractive advantages of the present process are mild reaction conditions, short reaction times, easy isolation of products, good yields and simple operational procedures (Scheme 1).



Scheme 1

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Synthesis and characterization of high purity metallic nanoparticles in ionic liquids via electrodeposition method

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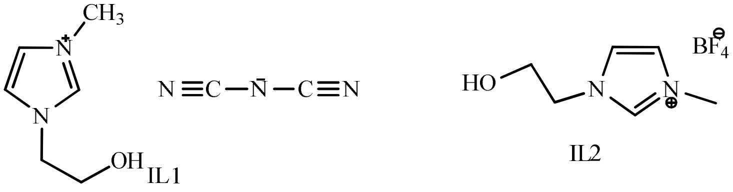
Synthesis method of nanoparticls has great effect on their physicochemical properties. At present, a variety of methods have been reported for the synthesis of nanoparticles such as microemulsion, sol-gel, sonochemistry and hydrothermal techniques [1]. Some of these methods suffer from complexicity of procedures and using toxic chemical solvents. Besides some procedures are time-consuming and lead to impure final products so that it is required to further purification [2].

Room temperature ionic liquids (RTILs) have also been known as green solvents with many unique properties, such as wide electrochemical window, high electrical conductivity and low surface tension [3]. In this study, electroreduction of Ni, Mo and Pd nanoparticles were carried out using imidazolium-based ionic liquids, 1-(-2-Hydroxyethyl)-3-methylimidazolium dicyanamide [C_2OHMim] [DCA] and 1-(-2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate [C_2OHMim] [BF_4]. The electrochemical reduction of Ni, Mo and Pd were studied with staircase cyclic voltammetry in different conditions such as scan rate, deposition potential and time, current density, Type of ILs and concentration of purposed metal salts. The synthesized products were characterized with powerful techniques such as SEM and DLS that confirmed their particle size distribution and morphology.

From viewpoint of application aspects, the results showed that the tested ILs containing metal nanoparticles exhibited the most affinity toward organosulfur species in comparison with the pure ILs. .



Scheme 1

References:

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Preparation of new poly(amide-imide) nanocomposites reinforced silicate nanoparticles based on trimellitice acid 1,3-propane diamine, and 4, 4'-diamino diphenyl ether

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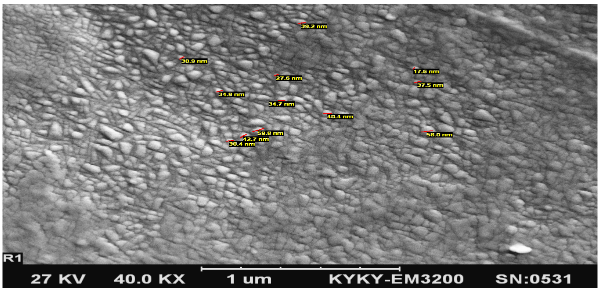
Synthesis and development of the high-performance polymers in the past thirty years have particularly drawn the attention of many polymer scientists and investigators. In general, these polymers possess excellent deformation resistance (physics) and deterioration resistance (chemistry) at high temperatures over a long period of time [1].

Polymer Nanocomposites - Clay composite types Powder are considered .The nanocomposites due to favorable properties such as high strength, wear resistance, corrosion resistance, high heat resistance, low gas permeability and flammability and ability to break down in the environment, have attracted the attention of industry and academia [2-3].

In this work two new poly (amide - imide) nanocomposites reinforced by 5 % of organoclay particles were prepared .The structure and morphology of them were determined by X-ray diffraction (XRD), scanning electron microscopy (SEM) and FT- IR spectroscopy.The neat poly (amide - imide) were synthesized by direct polycondensation reaction of Trimellitice acid (**1**) with 1,3-Propane Diamine (**2**) and 4, 4'-diamino diphenyl ether (**3**) in the presence of triphenyl phosphite (TPP), $CaCl_2$, pyridine and N-methyl-2-pyrolidon (NMP).The thermal behaviors of poly (amide – imide) nanocomposites studied by TGA spectroscopy (Scheme 1).



Scheme 1

References:

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Study on antioxidant activity of *Stevia rebaudiana Bertoni* extract from Guilan and its effect on the synthesis of gold nanoparticles

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Various methods invented and developed for the synthesis of gold nanoparticles that increases daily consumed. According to this method, including potential environmental pollution problems and the complexity of the synthesis, in this study, the feasibility of using the extract leaves of *Stevia* for the reduction of gold ions to nanoparticles form have been studied [1-2].

The aim of this study was to investigate the antioxidant properties of this plant and its ability to synthesize gold nanoparticles.*Stevia* leaves were used to prepare the aqueous extract for this study. The antioxidant activity of the methanloic leaves extract of *S.rebaudiana* was measured using DPPH free radical, Measurement of total phenolic content was achieved using Folin–Ciocalteau reagent, flavonoid content was measured by colorimetric method of aluminum chloride [3]. Fourier transform infrared (FT-IR) analysis and spectroscopic child as well as the UV-VIS confirmed the formation of gold nanoparticles, Transmission electron microscopy (TEM) images show that the nanoparticles are spherical and uniformly distributed, and its size is from 5 to 15 nm. The scanning electron microscopy (SEM) and X-ray diffraction (XRD) spectra imply the right of forming gold nanoparticles.

Results: The average of total phenolic and flavonoid contents were found to be 570.48±12.23 mg gallic acid and 416.72±1.39 mg quercetin, the average precent inhibition of DPPH radical of extract was obtained to be 51.97±0.8 mg/ml and these result shows that this plant has good antioxidant activity. The results of TEM, SEM, FT-IR, UV-VIS and XRD confirm that the leaves extract of *Stevia* can synthesis gold nanoparticles.

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Synthesis and characterization of functionalized graphene oxide- based magnetic nanoparticles for thiocyanate ion removal

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Magnetic separation due to the high surface area and ease of separation using external magnetic fields has received considerable attention in recent years rather than other used methods. Thiocyanate (SCN−) is widely used in a variety of industrial processes such as manufacturing of thiourea, photo finishing, metal separation, and electroplating [1]. Among various methods used for treat thiocyanate-contaminated water, adsorption is an efficient and economically feasible alternatives [2].In the present work, we combined the advantages of magnetic nanoparticles with the selectivity of iron porphyrins for SCN- ions and high surface to volume ratio of GO to design and fabricate a novel nano-adsorbent based on GO for SCN- removal from aqueous solution. The magnetic iron porphyrin-functionalized GO nanoparticles (MIGNs) and GO were characterized by XRD, SEM, TEM, FTIR and TGA. The effect of different parameters such as pH, sorbent dosage and contact time on SCN- removal was investigated and optimized. In this research optimal conditions are achieved for thiocyanate concentration of 50 mg/L as follows, contact time: 20 min, pH: 5.5, and nanosorbents dosage: 10 mg .FTIR and TGA results confirmed successful synthesis of GO and MIGNs. In SEM Images of synthesized MIGNs spherical nanoparticles with homogenous size distribution of about 12 nm were observed. Results obtained from TEM revealed that iron porphyrin had been assembled on the surface of graphene oxide layers.

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Synthesis and characterization of nano-FeO using metal organic framework

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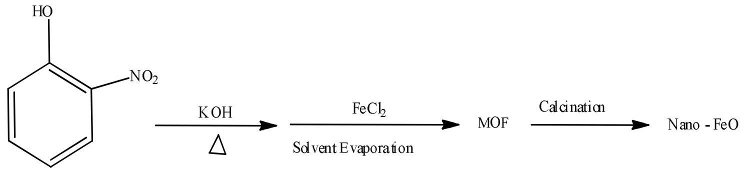
Metal-Organic frameworks (MOFs) are compounds consisting of metal ions or clusters coordinated to often rigid organic molecules to form one-, two-, or three-dimensional structures that can be porous. In some cases, the pores are stable during elimination of the guest molecules (often solvents) and could be used for the storage of gases such as hydrogen and carbon dioxide. Other possible applications of MOFs are in gas purification, in gas separation, in catalysis and as sensors. MOFs and zeolites are produced almost exclusively by hydro thermal or solvothermal techniques, where crystals are slowly grown from a hot solution.

In this work, a new Iron-organic framework was synthesized successfully by using 2_nitrophenol and $FeCl_2$ in aqueous solution. 2-nitrophenol solved in KOH solution and added to $FeCl_2$ aqueous solution at room temperature. After the reaction, the product is classified as needle crystals. Functional groups of MOF were determined by FT-IR and UV-Vis spectroscopy and the structure and morphology of that was determined by X-ray diffraction (XRD) and scanning electron microscopy (SEM).

Finally, nano-particles of FeO can be prepared by calcinations of mentioned MOF using of programmable electric grills.



Scheme 1

References:

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More efficient poly-esterification in poly propylene fumarate (PPF) synthesis by a new method

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Recently, biodegradable polymer's applications have increased in medical science [1]. One potentially important area is using as part of cements for surgical bone repair [2-3].

One particularly promising material for this application is poly (propy1ene fumarate) (PPF), a linear unsaturated polyester which consists of alternating propylene glycol and fumaric acid derivation units.

Many different methods for synthesizing PPF have been reported [5,6], but none of them give a clear method. There are some difficulties with control of polymer molecular and problems with consistency.

The present paper describes a new method which overcomes most of the problems in PPF synthesis compare to other reported techniques. ''Mixed reflux-distillation'' system (see in Figure.1), which has several important merits compared to other systems, is one of the best PPF synthesis systems. This method is a mixed reflux system coupled with simple distillation system that it is very efficient for PPF synthesis. HNMR of the best product has been shown in Figure 2.

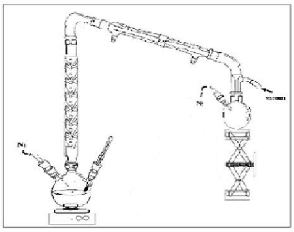

Fig.1. Mixed reflux-distillation system.

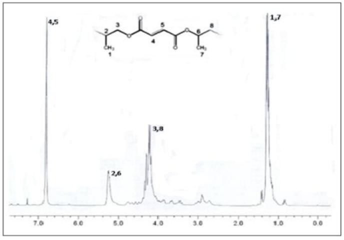

Fig 2. ^{1}H NMR spectrum of purified PPF

As a result, this novel system is very suitable and efficient for PPF and other polyesters synthesis with high repeatability of the reaction.

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Synthesis of a novel dimethyl amino propyl amin carbamat-chitosan derivative for fixed facilitated transport of CO_2 through a PVA/PS Thin Film Composite (TFC) membrane

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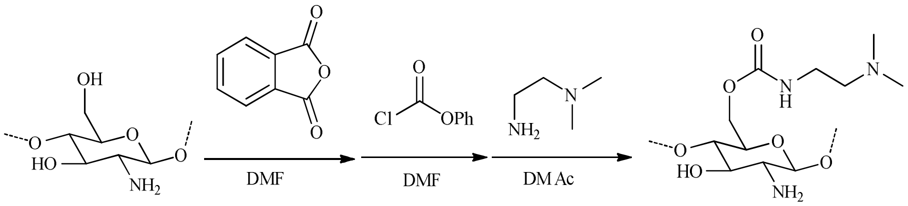
Gas separation based on membrane has an advantage over the conventional separation methods because of low capital cost and high-energy efficiency. Facilitated transport membranes show fairly high selectivity as well as high permeability [1-3].

In this work, for natural gas sweetening a novel water soluble amino derivative of chitosan was synthesized in a several step process (scheme1) and employed as CO_2 carrier in a Thin Film Composite (TFC) membrane. The membranes provided the facilitated transport in addition to the solution-diffusion mechanism in PVA/PS TFC membranes and the effect of polyamine content on the performance of PVA/PS membrane for the separation of CO_2 from CH_4 was investigated.



Scheme 1

References:
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The aminothiophenole-based azo-azomethine dyes; synthesis, computational study, solvatochromism and biological properties

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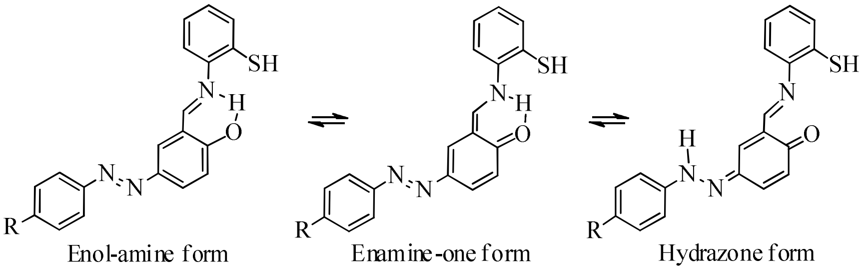
The condensation reaction of 2-hydroxy-5-(aryldiazenyl)benzaldehyde (**1a-d**) with 2-aminothiophenole affored Schiff base compounds 2-((2-mercaptophenylimino)methyl-4-(-aryldiazenyl)phenol (**2a-d**). The **2a-d** shows enol–keto tautomeric and positive solvatochromism. The antibacterial activities of **2a-d** were also evaluated by disc diffusion method. Compound **2b** displayed activity against *S. aureus* and *B. cereus*, **2a** and **2c** were active against *B. cereus* but **2d** did not exhibit activity against the tested organisms. Among the tested compounds, **2b** showed the best antioxidant properties as evaluated by free radical scavenging activity on 1,1-diphenyl-2-picryl-hydrazyl and ferric reducing power determination. The prepared compounds are potentially an –N=N-, -C=N and O multidentate chelating ligand which could form stable complexes with metal ions.



Scheme 1

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Synthesis of 1-aryl-1,2-dihydronaphtho[1,2-e][1,3]oxazine-3-ones in the presence of ascorbic acid as a catalyst

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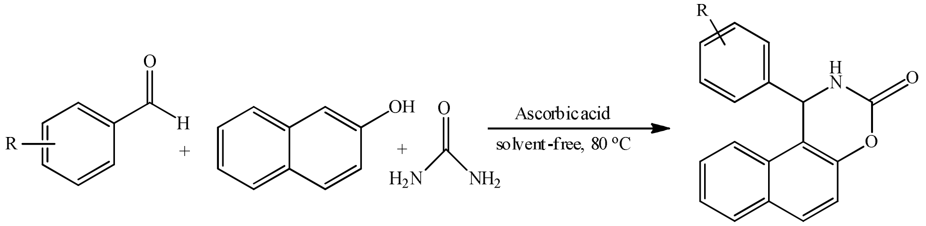
1,3-Oxazin-2-ones derivatives exhibit a variety of biological activities and medicinal properties.

To our best knowledge, there are only few methods available for the synthesis of substituted 1-aryl-1,2-dihydronaphtho[1,2-e][1,3]oxazin-3-ones, which involves either toxic chemicals or long reaction time[2,3]. Hence, there is still scope for the development of milder, safer, economical, and more efficient synthetic protocols for the preparation of aromatic-fused oxazinones.

The catalytic potential of ascorbic acid in the synthesis of aromatic-fused 1-aryl-1,2-dihydronaphtho[1,2-e][1,3]oxazine-3-one derivatives (Scheme1) has been investigated.



Scheme 1

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Poly(o-phenylenediamine)/MWCNTs nanocomposite: Preparation, characterization and its application as an anti-corrosion coating

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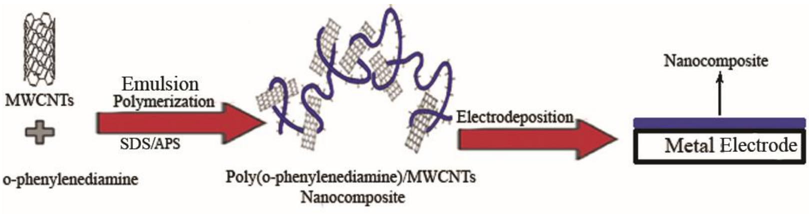
The corrosion of metals is an enormous economic problem. Thus, efforts to develop more efficient and environmentally compliant methods to prevent corrosion have beenongoing throughout this century [1]. Recently the use of conducting polymers for the protection ofmetals against corrosion has investigated [2]. Among these polymers,aniline andits derivatives have beenof particular interest because of their environmental stability, controllable electrical conductivity andinteresting redox properties associated with the nitrogens in the backbone of the polymer [3].

In this study poly (o-phenylenediamine)/MWCNTsnanocomposite was prepared by emulsion polymerizationmethod using ammonium peroxydisulfate (APS) as an oxidant and sodium dodecyl sulfate (SDS) as a surfactantin presence of o-phenelendiamine and MWCNTs using various feed ratios under sonication. The prepared nanocomposites were characterized by FT-IR, XRD, SEM and TGA analyses. The corrosion protective performance of nanocomposite coatings on different metals such as copper and steel in various corrosive media was evaluated by potentiodynamic polarization. The corrosion data including corrosion current density (Icorr) andcorrosion potential (Ecorr) were determined from Tafel plots. Considering the results synthesized nanocomposites showed good characteristics for the corrosion protection on copper and steel.



Scheme 1

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A practical and eco-friendly method for conversion of epoxides to corresponding thiiranes with thiourea and NH_4Cl supported on Al_2O_3 under solvent-free conditions

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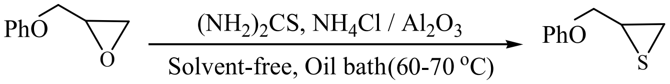
Thiiranes, the simplest sulfur heterocycles, play an increasing pivotal role in organic synthesis as versatile building blocks in asymmetric reactions. Moreover, they are used as intermediates in the pharmaceutical, polymer, pesticide, and herbicide industries. Although there are many methods reported in the literature for the preparation of thiiranes, the most general route is the conversion of oxiranes to thiiranes by an oxygen– sulfur exchange reaction [1-4].

Ammonium chloride, an inorganic compound with the formula NH_4Cl, is a white crystalline salt, highly soluble in water. Aluminium oxide catalyses a variety of reactions that are useful industrially. Aluminium oxide serves as a catalyst support for many industrial catalysts, such as those used in hydrodesulfurization and some Ziegler-Natta polymerizations.

Herein, we wish to introduce a simple and efficient method for Conversion of epoxides to corresponding thiiranes with Thiourea and NH_4Cl supported on Al_2O_3 under solvent-free conditions. The capability of this synthetic protocol was investigated by the reaction of activated, deactivated, and cyclic epoxides with NH_4Cl/Al_2O_3 system under the optimized conditions. The epoxides were converted to the corresponding thiiranes in exellent yields within short times. Epoxides were readily converted to the corresponding thiiranes by NH_4Cl/Al_2O_3 system under solvent-free conditions. The reactions were completed within 1–8 min at 60–70°C. The thiiranes were obtained in 88–97% yields (Scheme 1).



Scheme 1

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Superparamagnetic poly(aniline-co-m-phenylenediamine)/Fe_3O_4 nanocomposite as an adsorbent for sorption of metal ions

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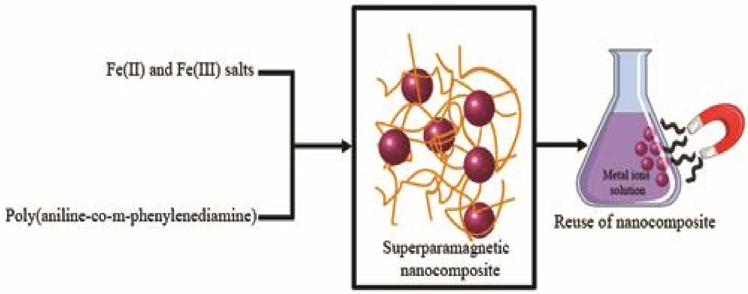
Pollution of water by heavy-metal ions in supplies has steadily increased over the recent years as a result of over population and growth of industrial activities [1]. Metal pollution has a harmful effect on biological systems and does not undergo biodegradation [2]. The removal of toxic metal ions from water is an important and extensively studied research area [3]. The main goal of this research is to introduce the preparation of nanocomposite based on aniline copolymers and Fe_3O_4 magnetic nanoparticles as efficient nanoadsorbent for sorption of metal ions.

The magnetic nanocomposite was prepared by in-situ coprecipitation method in presence of poly (aniline-co-m-phenelendiamine), Fe (II) and Fe (III) salts. The prepared nanocomposite was characterized by FT-IR, XRD, SEM, and VSM analysis and used as a nanoadsorbant for removal of risky heavy metal ions such as, Pb(II), Cu(II), Cd(II), Zn(II) and Fe(II). Results showed that the nanocomposite had good potential for sorption of metal ions from water. Scheme 1 shows preparation and reuse of nanocomposite.



Scheme 1

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Synthesis of a new amino-chitosan derivative as a carrier for fixed facilitated transport of carbon dioxide through a polysulfone membrane

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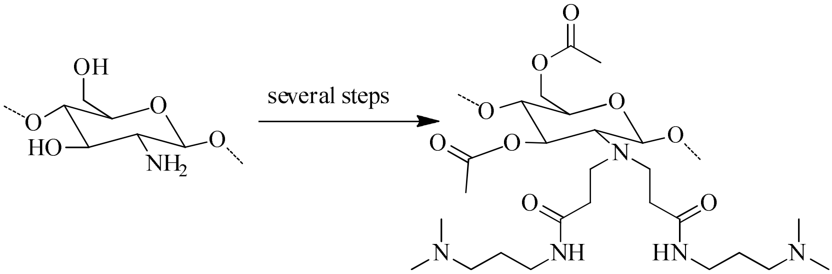
Nowadays natural gas sweetening processes is an important process because CO_2 and H_2S lead to pipeline corrosion and waste the capacity of the pipeline. Membrane separation process because of their low capital cost and low energy consumption are competitive processes. Fixed facilitated transport of CO_2 through polymeric membranes can improve their performance [1-3].

In this work a new water and organo soluble amino derivative of chitosan was prepared successfully (scheme 1) and identified using of H-NMR and FT-IR techniques. This novel chitosan derivative was used as a CO_2 carrier in thin film composite membrane and performance of prepared membrane were investigated in different conditions.



Scheme 1

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Effect of side chain modification with benzoic acid on chloromethyl styrene polymers structure and glass transition temperature of polymers

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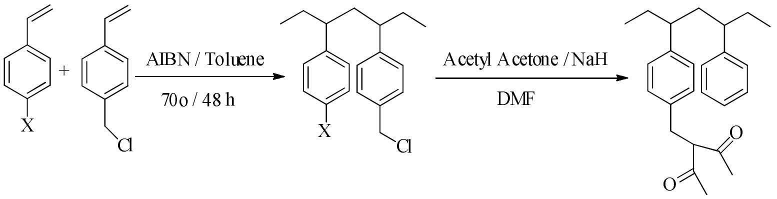
p-Vinylbenzyl chloride (VBC), or 4-chloromethyl styrene (CMS), is one of the most important monomers which is produced industrially in pure form. Many nucleophilic substitutions are possible at the benzylic chlorine, leaving the double bond unchanged and providing new functionalized monomers under appropriate conditions [1,2]. In this research, 4-Chloromethyl styrene (CMS) and its copolymers with different monomers such as styrene and methyl metacrylate (in 1:3 molaration) were synthesized by free radical polymerization method in toluene solution at the temperature range 70-75 using α,α′- - azobis(isobutyronitrile) (AIBN) as an inititator and the copolymers I, II collected respectively in good yields [3,4]. Poly (CMS) or related copolymers must have the best possible accessibility of the reactants to the chloromethyl group, which gives the process of copolymerization its full importance. The acetyl acetone substituents were attached to the obtained copolymers with replacement of all the chlorine atoms in CMS units [5]. All the resulted polymers were characterized by FT-IR and HNMR spectroscopic techinques and dynamic mechanical thermal analysis (DMTA). All the polymers containing acetyl acetone group showed a high glass transition temperature in comparison with copolymers I, II. The increase of the glass transition temperature reflects the substantial increase in rigidity of new polymers bearing substituents in side chains [6].



Scheme 1

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Synthesis of a new amino cellulose as a novel polymeric derivative for fixed facilitated transport of CO_2 through aPVA/PS Thin Film Composite (TFC) membrane

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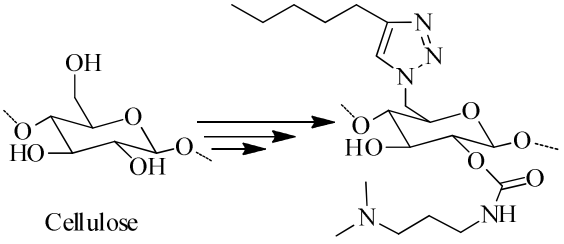
CO_2 Is a corrosive gas and reduces the heating value of natural gas, it must be separated from the natural gas stream to improve the quality of the product before transfer using pipeline. Membrane based gas separation methods have low cost and occupy small place [1-2].

In this work a new amino derivative ofcellulose was synthesized in a several step process (scheme 1) and employed as CO_2 carrier in a Thin Film Composite (TFC) membrane. The membranes provided the facilitated transport in addition to the solution-diffusion mechanism in PVA/PS TFC membranesfor the separation of CO_2/CH_4 gas mixture.The effect of polyamine content and operating parameters on performance of PVA/PS membrane were investigated.



Scheme 1

References:

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Polyurethane foam glycolysis

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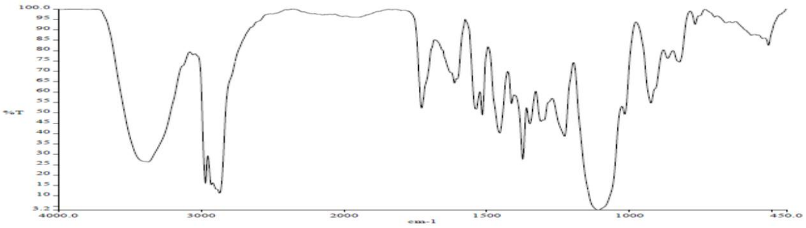
Polyurethanes (PU) have been used in diverse areas and are one of the most important groups of plastics because of their versatility. Flexible PU foams are the most important group among PU specialties. The goal of chemical recycling of flexible foams is to regain the polyols suitable for manufacturing new PUR foam. Hydrolysis, treatment with esters of phosphoric acid, aminolysis with low weight alkanolamines and glycolysis have been described as suitable procedures to break down the PU chain [1-6] by transesterification. The most important method is glycolysis of PU that the polyurethane chain is degraded by successive transesterification reactions of the urethane bond with low molecular weight glycols with the aid of a catalyst. The important factor affecting properties of the recovered products is the choice of catalyst. The activity of stannous octoate in comparison with the other catalysts assayed was so high that a new study for the optimization of the conditions for using stannous octoate in the polyol reclaim process is necessary (Scheme 1).



Scheme 1

References:

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Synthesis and characterization of new magnetic poly(amide-imide) nanocomposites containing pendent dibenzoxanthene groups

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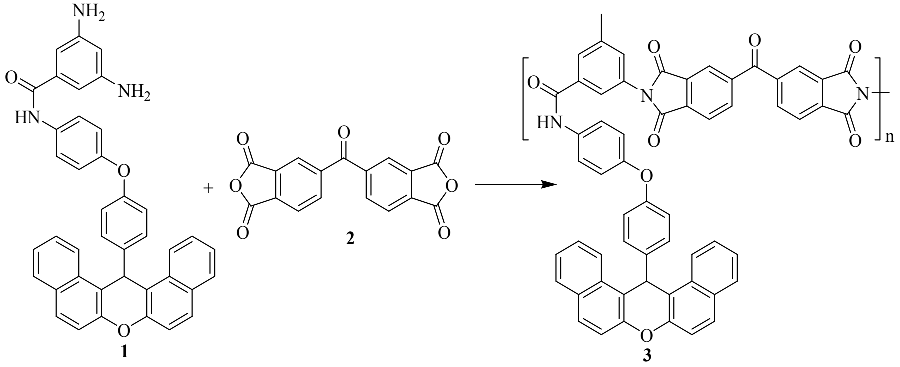
Nanocomposites have been extensively studied, since just a small amount of nanomaterials as an additive leads to production of new high-performance materials with good physicochemical properties [1,2]. Fe_3O_4 (magnetite) particles have exhibited unique electric and magnetic properties based on the electrons transfer between Fe^{2+} and Fe^{3+} in the octahedral sites. For their good biocompatibility, tunable magnetic properties and low toxicity, magnetite nanocomposites have received considerable attention in many areas [3].

In this work, we report synthesis of new magnetic poly(amide-imide) nanocomposites containing pendent dibenzoxanthene groups via in situ-polymerization (scheme 1). Fe_3O_4 nanoparticles were synthesized using sonochemical reaction. The new diamine monomer 1 containing xanthene moiety was synthesized by using the five-step reaction. The influence of nanoparticles to the thermal properties of polymer matrix was studied. Magnetic properties of Fe_3O_4 nanoparticles and poly (amide-imide)/Fe_3O_4 nanocomposites were also compared.



Scheme 1

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Synthesis, characterization and investigation of eleactivity studies of Ag/Polyaniline/Polystyrene sulphonic acid nanocomposites

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Nanocomposites of conducting polymers and inorganic particles have concerned significant academic because they have interesting physical properties and potential applications [1]. Polyaniline (PANI) is known among conducting polymers due to its high conductivity, ease of preparation, good environmental stability, and a large variety of technological applications in rechargeable batteries, chemical sensors, corrosion protection coatings, and etc. [2]. On the other hand, metal nanoparticles such as silver (Ag) have attracted much attention due to their unique physical high electrical and thermal conductivity, antibacterial activity, electrocatalytic ability and superior performance in technological fields [3]. Incorporation of Ag NPs between the PANI chains could yield functional materials having unique properties and wide varieties of potential applications in various areas including electronic, optics, biotechnology, electrocatalytic and sensors. Hence the synthesis of polyaniline/Ag nanocomposites is receiving wide attention. Here, we have developed a simple method to prepare of Ag/polyaniline nanocomposites with polystyrene sulphonic acid to get better and some new synergistic properties which could not be attained from individual materials. The procedure involves oxidative polymerization of aniline in the presence of $AgNO_3$, ammonium persulphate and polystyrenesulphonic acid. The resulted nanocomposites were characterized by x-ray diffraction (XRD) (Fig.1), scanning electron microscopy (SEM)(Fig. 2), energy-dispersive X-ray spectroscopy (EDX), ultraviolet visible spectra (UV-vis) and fourier transform infrared spectroscopy (FT-IR). Furthermore, Ag/PANI nanocomposites were immobilized on the surface of a glassy carbon electrode (GCE) and was investigated electroactivity behavior by cyclic voltammetry (CV).

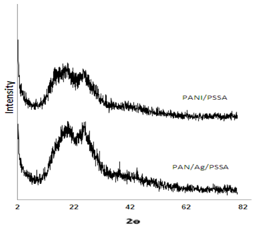

Fig. 1

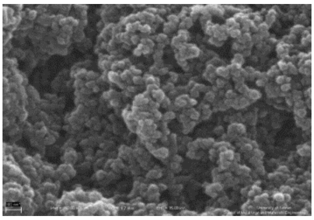

Fig. 2

References:

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Synthesis and application of modern functional poly(ionic liquid) electrolyte for Dye-sensitized solar cell

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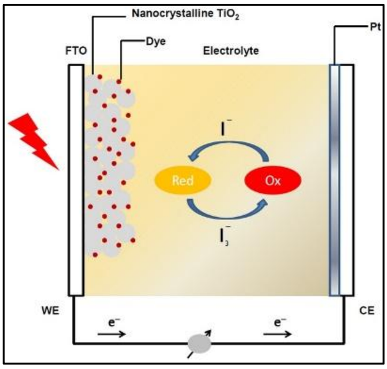
In recent years, poly(ionic liquid)s (PILs) were found to take an enabling role in some fields of polymer chemistry and material science [1]. PILs combine the uniqueproperties of ionic liquids with the macromolecular architectures andprovide novel properties and functions that is of huge importance in multitude applications. Mixtures between ionic liquids and molecular solvents exhibit interest in gphysical and chemical properties [2] such as very low vapor pressure, high ionic conductivity etc, which make them promising for future applications in dye-sensitized solar cells (DSSCs) [3-4] as electrolyte components.

In this research we focus on novel functional Poly(ionic liquid) as electrolyte, iodine as redox mediator and acetonitrile as solvent in electrolyte concentrationand light harvesting efficiency. It can be explained by the reduced (I^-/I^-_3) pair-formation as shown in following Scheme 1:



Scheme 1

References:

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Electrochemical polymerization of pyrrol in aqueous micellar solution containing sodium dodecyl sulfate and investigation morphology of pyrrol films

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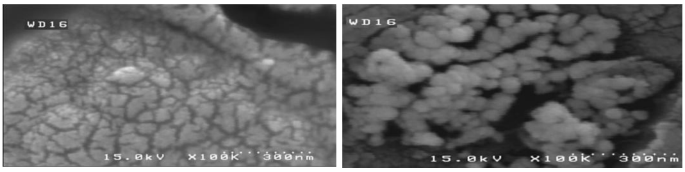
The chemical and electrochemical synthesis of conducting polymers continues to receive great attention in fundamental as well as in applied studies [1]. In particular, micro-and nanostructures of polypyrrol are under active investigation because of the many existing and new possibilities for applications in optical, electrical and sensing device [2].

In this work, electropolymerization of pyrrole has been studied in the presence of anionic surfactant (SDS) in aqueous media. The rate of polymer growth and its properties depended to electropolymerization conditions such as electrosynthesis techniques, substrates, electrolyses, monomer concentration and also the presence of material stabilizers.

The results show that the rate of electropolymerization increases in presence of SDS and then yields the electroactive, adhesive and unit polymer films. Also, we find that the optimized concentration of monomer decreases in presence of SDS. Anodic peak and activation energy polymerization, approach to low qualities in presence of SDS.

Scanning electron microscopy images show that PPy films take a small size and extended surface particles with better diffusitywich affected by stabilizers. Models of polymer growth is flowers-like in absence of SDS and it is string-like in SDS media.



Scheme 1

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The effect of polarity of the media on color changes in photochromic nanoparticles containing spiropyran under UV irradiation

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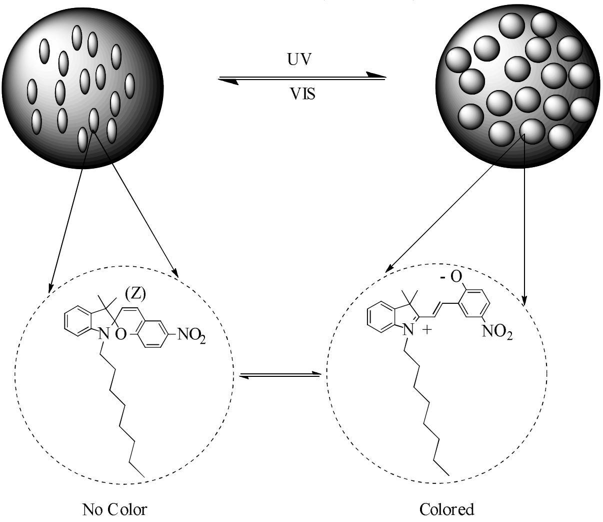
Photochromic compounds based on spiropyran can show a variety of colors with the changes in polarity of the environment due to their isomerization. The presence of a transition state of the isomer is the main reason for such color changes. The hydroxyl group involving in resonance with the aromatic ring is responsible for these changes and quite dependent on the polarity of the media and this color changes is reversible too [1].

In this work, functionalized spiropyran with acrylic group was synthesized [2, 3] and the effect of polarity was studied by UV-Vis irradiation. Then it was copolymerized with methyl methacrylate through emulsion polymerization [4]. Some piece of papers was contaminated with the above latex by impregnation and drying. Afterward, these papers were soaked in several solvents with different polarities and irradiated by UV light. The results reveal that the protic solvents favor the open isomers and stabilize it more (Scheme1).



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Synthesis of poly(styrene-co-maleic anhydride) and poly(styrene-co-maleic acid)

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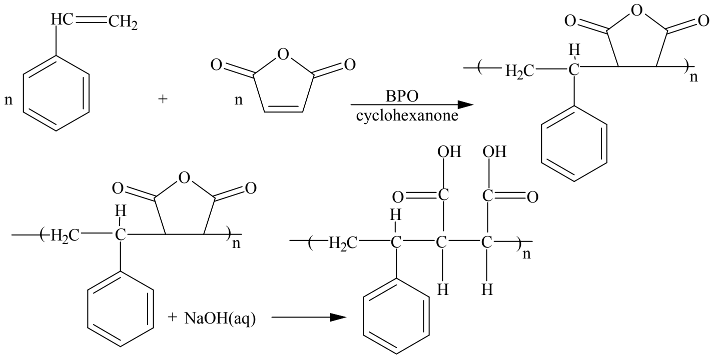
The synthetisized copolymers have given some interesting characteristics to the polymers, that is why in the last decades synthesis *of copolymers (especially copolymers based on styrene) have been drastically increased* [1]. Copolymerization of styrene and maleic anhydride has been studied from many aspects [2-3].

In this work, at first we have synthesized poly(styrene-co-maleic anhydride) in different solvents and different conditions, then we have purified it and have taken FT-IR spectra. After that, with saponification reaction in aqueous and organic solutions, we have converted them to poly(styrene-co-maleic acid) (Scheme 1).This copolymers show some interesting properties, for example they can be used as a adhesive.

The synthetisized copolymers' properties such as their changes of stability and viscosity with respect to changes of temperature in different times, and the effects of the ratio of the monomers in the feed on the adhesive forces have studied.



Scheme 1

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Synthesis and characterization QSAR of new copoly(amide-imide)based on 1,3-Propane Diamine and 4, 4'-diamino diphenyl ether and 1,2,4-benzene-tricarboxylic-1,2-anhydride

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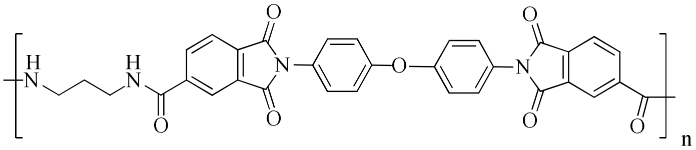
Polymers have become major synthetic materials of the 21st century. The intractable characteristic of aromatic polyimides is major problem as a result of high melting points and insolubility. To overcome this drawback, copolymerization is an effective approach and various copolyimides have been developed. Recently, poly(amide-imide)s have been developed as an alternative material offering a compromise between excellent thermal stability and process ability [1-6].

In this study, two novel monomers were synthesized successfully by the condensation reactions between 1,2,4-benzene-tricarboxylic-1,2-anhydride (**1**) and 1,3-Propane Diamine (**2**) or 4, 4'-diamino diphenyl ether (**3**) in glacial acetic acid as solvent. Functional groups of monomers were determined by FT-IR spectroscopy.

Two new copoly (amide- imide)s were synthesized due to the condensation reactions between monoers and compound (**2**) or compound (**3**) in the presence of triphenylphosphite (TPP), $CaCl_2$ and pyridine in N-methyl-2-pyrolidon (NMP) as solvent.

The structures and spectroscopic properties of the synthesized copolymers were investigated by means of FT-IR spectroscopy, elemental analysis and inherent viscosity. Also, thermal stabilities of mentioned copolymers were studied by using thermal gravimetric analysis (TGA) and differential thermal gravimetry (DTG). Experimental data showed that second copolymer is more stable than the first one (Scheme 1).



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Chemical synthesis of polypyrrole via $CHCl_3/CH_3CN$ binary organic solvents

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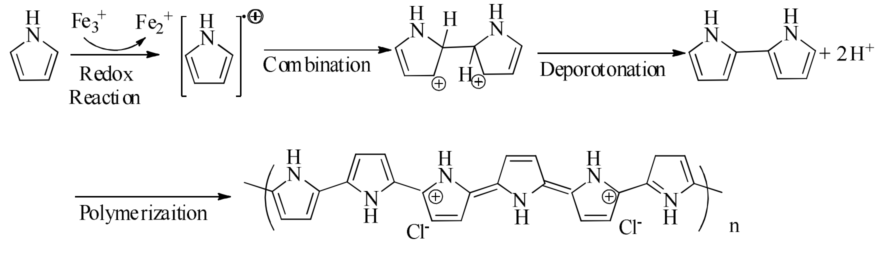
Polypyrrole (PPy) is a technologically important, environmentally stableconducting polymer exhibiting high electronic conductivity atphysiological PH [1].Chemical polymerization of PPyhas a significant preference forprocessing purposes compared to electrochemical polymerization because it may be easier to scale up this batch process and itresults in the formation of powders or colloidal dispersions. Furthermore, it is possibleto use chemical deposition to coat other nonconducting materials [2-4].

In the present study,a facile and efficient method to achieve PPy polymer has been introduced(Scheme 1). The polymer was prepared in $CHCl_3/CH_3CN$ binary organic solvents with 2/1 volume ratio at 0 °C using iron (III) chloride ($FeCl_3$) as the polymerization oxidant.This strategy allowed the oxidant to be adequately dissolved in the reaction medium. FT-IR and XRD analyses thoroughly confirmed the success of the method used. Further characterizations were carried out by scanning electron microscopy (SEM) and thermal analyses (TGA/DTG and DTA).



Scheme 1

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Fabrication of water-soluble magnetic nanoparticles by amphiphilic copolymer: A novel vehicle for entrapment of poorly water-soluble drugs

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Magnetic nanoparticles (MNPs) have many potential biomedical applications such as magnetic separation, cell labeling, targeted drug delivery, hyperthermia treatment of solid tumors and contrast agents for magnetic resonance imaging (MRI) [1]. In these applications, the MNPs need to be stable in aqueous solution, which can be achieved by the macromolecules on the surface of the MNPs such as peptides [2] and hydrophilic polymers [3].

In this work, we report a synthetic method of water dispersible magnetite nanoparticles having oleic acid and poly(ethylene glycol)- poly(2-ethyl-2-oxazoline)- poly(3-caprolactone), (PEG-POX-PCL) amphiphilic copolymer as polymeric stabilizers. The particles were prepared by coprecipitation of Fe(II) and Fe(III) in NH_4OH and had bilayer surface with hydrophobic inner layer and hydrophilic corona. PEG-POX-PCL copolymer was synthesized by a ring-opening polymerization of 3-caprolactone using PEG-POX-OH as a macroinitiator in the presence of stannous octoate catalyst.

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Relationship between the flash point of some binary base oils with flash point of their constituent oils

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[b] *Barzin Sepand Sepahan Company, Dehagh Industrial City, Isfahan, Iran.*
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Miscellaneous binary blends containing solvent neutral-150 (SN-150), solvent neutral-500(SN-500), Bright Stock-150 (BS-150), polyalphaolephin-6 (PAO-6), PAO-100, a processed low sulfur waxy material, and polyisobutene-600 (PIB-600) have been made. Thereafter; the corresponding flash point (FP) of each blend has been measured. By using the measured data, the plots of FP vs. weight percentage of minor component have been drawn. Then, the equations due to each plot have been derived. Except PIB-600 containing mixtures, linear relation between FP of blends and weight percentage of constituents has been observed. Also the obtained data indicate that except PIB-600 containing blends the FP of such mixtures can be calculated from the summation of "FP × weight ratio" of each component. In the case of PIB-600 containing blends: nonlinear and decreasing; nonlinear and increasing; as well as constant trends of FP vs, weight percentage of minor component is observed. The observations have been interpreted based on the composition, molecular weight, and interactions of the constituents of the base oils.

The flash point is the lowest temperature at which an ignition source causes the vapors of the specimen (lubricant) to ignite under specified conditions [1].
The flash points of binary base oil mixture scan be predicted from the following equation: $FP_{blend} = [(FP)_1 \times (\text{weight ratio})_1] + [(FP)_2 \times (\text{weight ratio})_2]$. The blends of PIB-600 do not obey from the above equation.

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Synthesis and preparation of magnetic nanoparticles imprinted polymer for azithromycin and its application in controlled release

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Molecular imprinting technology has an enormous potential for creating satisfactory drug dosage forms [1]. Molecularly imprinted nanoparticle polymers (MIPs) are design to have a memory for their molecular templates [2].

Magnetic iron oxide nanoparticles with super paramagnetic property have shown potential as multifunctional nanoparticles for drug delivery [3].

In this way, for synthesis (MIPs), in pre-polymerization step functional monomers making around of molecular template in order to making interactions between template and functional monomers, then in next step, polymerization reaction with cross linking agent occurs between template and functional monomers to remain structure of template in their memories and the imprinted molecules (template) are subsequently removed from the polymer. In step of synthesis magnetic nanoparticles, iron oxide (Fe_3O_4) synthesized from Fe^{3+} and Fe^{2+} ions then a silica shell encapsulated (Fe_3O_4) and trapped in MIPs. The aim of the present study is to use novel synthetic conditions of precipitation polymerization to obtain magnetic nanosized azithromycin molecularly imprinted polymers for application in new drug delivery, that was carried out in presence of functional monomer (Methacrylic acid (MAA)),cross linking agent (Trimethylolpropane trimethacrylate (TRIM)) and initiator (2,2-azobis-isobutyronitrile (AIBN)).

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Thermal reversion mechanism of urethane cured natural rubber

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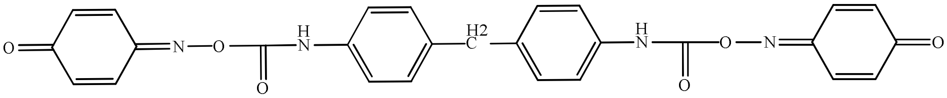
Rubber product properties are related to vulcanized structure and influenced by curing system. Vulcanization system based on curing agent give vulcanizates with tailored properties. Optimum curing system present thermal resistance natural rubber with well aging behavior. Non sulfur vulcanization give carbon carbon crosslink bond with good aging properties. Diisocyanate (Scheme 1) as a rubber curing agent give thermal stable an especial type crosslink bond. The urea type bond produced according urethane basic chemistry. Mechanism of adding urea bond on natural rubber macromolecule controlled by nature of crosslink agent and vulcanization condition such as reaction temperature and time. Isocyanate group adding need a reactive side on macromolecule, that producing is possible by prior reactive mixing.



Scheme 1

In this paper, mechanism of isocyanate crosslink adding on the rubber molecules after reactive mixing with peroxide was studied. The attempted has been made for increasing thermal reversion resistance of natural rubber by the new crosslinking mechanism.

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Nano Boehmite-H_2PO_3 a new catalyst for the preparation of triazolo[1,2-a]indazole-triones

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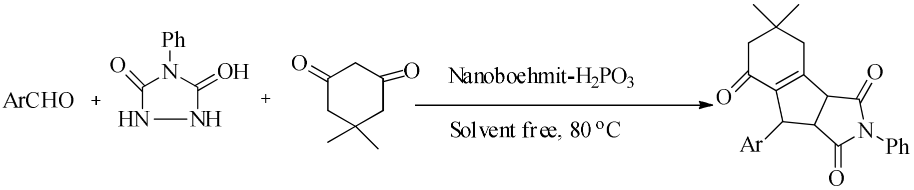
Among a large variety of N-containing heterocyclic compounds, those containing hydrazine moiety as 'fusion site' have received considerable attention because of their pharmacological properties and clinical applications [1].

An efficient practical approach to triazolo[1,2-*a*]indazole-1,3,8-triones from urazole, dimedone, and aldehydes was developed that uses nanoboehmite phosphoric acid as a green catalyst in a solvent-free one-pot three-component cyclocondensation reaction. This method should provide good yields, a shorter reaction time, an easy work-up, purification of products by the non-chromatographic method, and a cleaner reaction [2-4] (Scheme.1).



Scheme 1

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Efficient synthesis of *N*-substituted topiramate (anticonvulsant drug) derivatives: Investigation of their proton and sodium affinity

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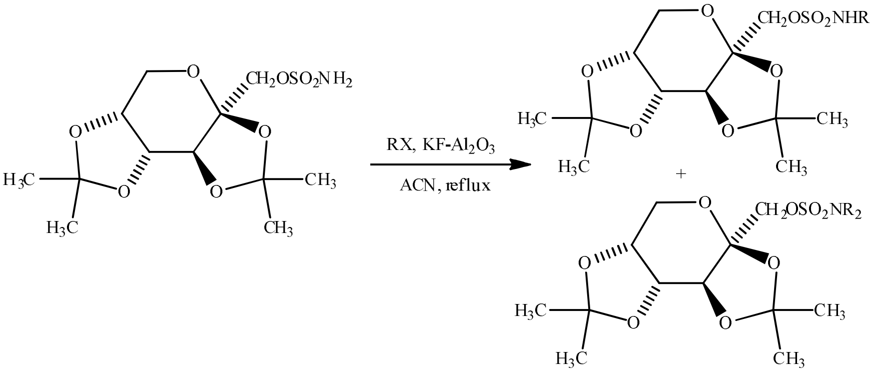
Email: h_porkaleh@yahoo.com

Epilepsy has been recognized as a neurological disorder, affecting a large section of people. Every year, approximately 0.25 million new cases are added to this population [1]. Anticonvulsant drugs are estimated to be useful in treating 90% of the epileptic patients. Newer drug topiramate, 2,3:4,5-bis-O-(1-methylethylidene)-beta-D-fructopyranose sulfamate, has emerged as promising anticonvulsant drug marketed worldwide for the treatment of epilepsy and the prophylaxis of migraine [2]. Bruce E. Maryanoff *et al* reported the synthesis and biological activity studies of topiramate as antiepilepsy drug in 1979. Because of the multiple etiologies of epilepsy, the limited understanding of the biological molecular mechanism of topiramate and the adverse effects of it, the search for structural improvement of topiramate and other compounds as less toxic and more efficient agents for the treatment of seizure disorders is an ongoing struggle [3]. In this context, and as part of our continuing effort on the design of new routes for the preparation of biologically active organic compounds, herein, we report synthesis of *N*- substituted topiramete by reacting topiramate with alkyl halides in presence of KF-Al_2O_3 [4] as an efficient solid base (Scheme 1).



Scheme 1

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Synthesis of 1-amido or aminoalkyl-2-naphtholes in the presence of reusable sulfanilic acid-functionalized Fe_3O_4/SiO_2 magnetic nanoparticles

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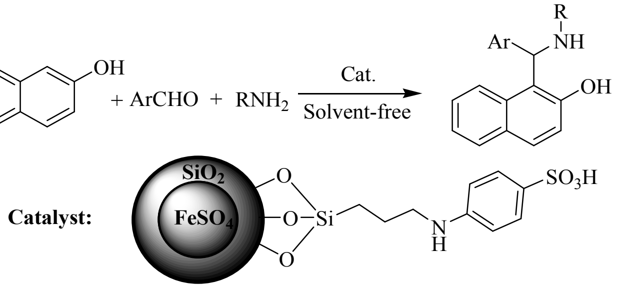
Multi-component reactions (MCRs) are a promising and vital field of chemistry because the synthesis of complicated molecules can be achieved in a very fast, efficient and time saving manner without the isolation of any intermediate [1]. Therefore, researchers have made great efforts to find and develop new MCRs. Amidoalkyl naphthols are important synthetic building blocks and are used as precursors for the synthesis of 1-aminomethyl-2-naphthol derivatives, which exhibit important cardiovascular activity [2]. Heterogenation of important organic ligands including important homogeneous catalysts onto suitable supports has seen increased interest due to the demand for green chemistry and environmentally friendly technologies [3,4].

In the present work, the sulfanilic acid was immobilized onto Fe_3O_4/SiO_2 magnetite nanoparticles via 3-(chloropropyl)triethoxysilane (CPTES) to form an acidic solid catalyst. The catalyst was used successfully for the solvent-free synthesis of 1-amido or aminoalkyl-2-naphtoles from condensation reaction of 2-naphthol, aldehydes and amides or amines (Scheme 1). The structural, surface, and magnetic characteristics of the nanosized catalyst were investigated by various techniques such as transmission electron microscopy (TEM), powder X-ray diffraction (XRD), vibrating sample magnetometry (VSM), thermogravimetric analysis (TGA) and FT-IR.



Scheme 1

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Preparation of chlorohydrins from epoxides using hexachloroacetone/ triphenyl system phosphine

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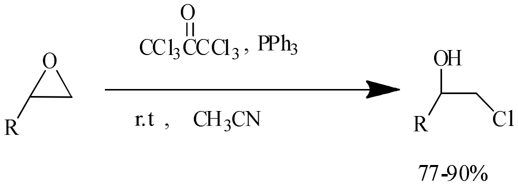
Hexachloroacetone (HCA) is versatile electrophilic reagent that may act as a source of chloronium ions or as acylating agent. These reagent have been used for the trichloroacetylation of alcohols and amines, and conversion of alcohols in to alkyl halides and carboxylic acids in to amides [1-2].

Chlorohydrins are an important class of organic compounds and versatiles intermediates in the synthesis of a vast range of biologically active natural and synthetics products, unnatural amino acids, and chiral auxiliaries for asymmetric synthesis. Due to the importance of vicinal halo alcohols in organic synthesis diverse reagents have been used for their preparation from epoxides. For example: halogen and triphenylphosphine [3], PPh_3/ DDQ/ R_4NX (X= Cl, Br, I), and PPh_3/ NXS [4].

In continuation of our work on the ring opening of epoxide [5], we report here, a mild, new and regioselective procedure for the direct conversion of epoxides in to their corresponding chlorohydrins using triphenylphosphine/ HCA system, in good to excellent yields (Scheme 1).



Scheme 1

References:

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A new Schiff base system bearing two naphthalene groups as fluorescent chemosensor for Al^{3+} ion

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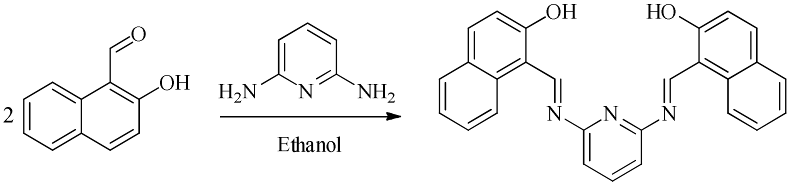
A new Schiff base system (H_2L) was synthesized using 2-hydroxy-1-naphthaldehyde and 2,6-diaminopyridine (Scheme 1). The influence of metal cations Cr^{3+}, Mn^{2+}, Co^{2+}, Cs^{+}, Al^{3+}, K^{+}, Zn^{2+}, Ni^{2+}, Hg^{2+}, Ba^{2+}, Cu^{2+}, Mg^{2+}, Na^{+}, Ag^{+}, Cd^{2+}, Pb^{2+}, Fe^{2+} and Fe^{3+} on the spectroscopic properties of the Schiff base (H_2L) in ethanol were investigated by means of absorption and emissions spectrophotometry. When increasing concentrations of Al^{3+} ions were introduced, the fluorescent emission of (H_2L) was drastically increased. This special change was not observed when other metal ions were used (Fig. 1a). As the concentration of Al^{3+} was increased, the fluorescence gradually increased (Fig. 1b). The Schiff base (H_2L) was found to be as an effective fluorescence sensor for Al^{3+} ions.



Scheme 1. The synthetic Schiff base (H_2L)

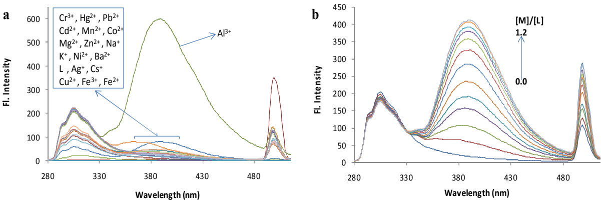


Fig 1. Fluorescence spectra of H_2L (a) and Changes in the fluorescence spectra of H_2L (b)

References:

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Reaction of ethyl 2-(1,2-dihydro-(4*H*)-3,1-benzoxazin-4-one)-2-oxoacetate with HOCN

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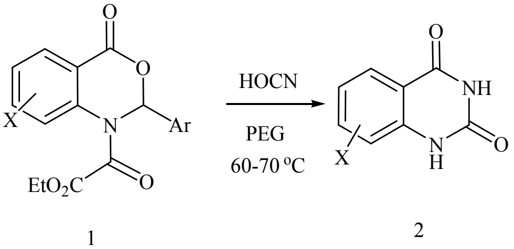
N-Substituted-1,2-dihydro-(4*H*)-3,1-benzoxazin-4-ones are potential starting material for synthesis of biologically important heterocycles [1-3] such as 1,4-benzodiazepine-2,5-diones and indoxyls. Quinazoline-2,4-diones are considered as an important chemical synthesis of various physiological significance and pharmacological applications [4,5].

In this study, the synthesis of 2,4(1*H*,3*H*)-quinazolinedione **2** bearing quinazolinone moiety has been carried using ethyl 2-(1,2-dihydro-(4*H*)-3,1-benzoxazin-4-one)-2-oxoacetate derivatives **1** with acidic solution of KOCN in PEG as an excellent green solvent. The developed synthetic route is simple and high yielding (Scheme 1).



X = H, Br, Cl, NO_2, OH, Me, OMe

Scheme 1

References:

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Investigation of the one-pot reaction of 1,3-cyclohexanedion with cyanogen bromide and various aldehydes in the presence of sodium methoxide and/or ethoxide

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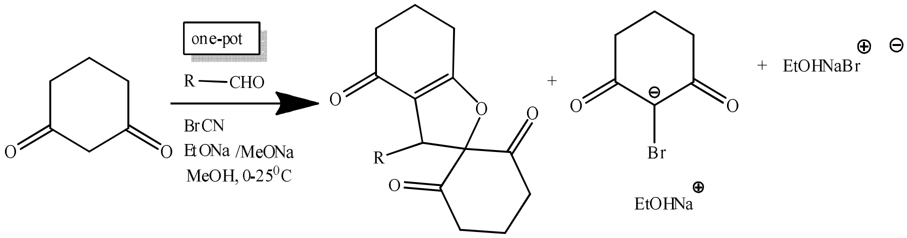
The one-pot reaction of 1,3-cyclohexanedione with cyanogen bromide and various aldehydes in the presence of sodium methoxide and/or ethoxide led to selective formation of spirodihydrofuranes in methanol in excellent yield. The mechanism of the formation were discussed.

In this one-pot reaction with a ratio of 1,3-cyclohexanedion with various aldehydes in the presence of sodium methoxide and cyanogen bromide in methanol at a temperature of 0-25 °C for 48 h with a mixture of the new compounds were obtained spirodihydrofurans, Which are important in terms of biological and pharmaceutical.



Scheme 1

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Silica tungstic acid as an efficient and reusable catalyst for the one-pot synthesis of benzofuran derivatives

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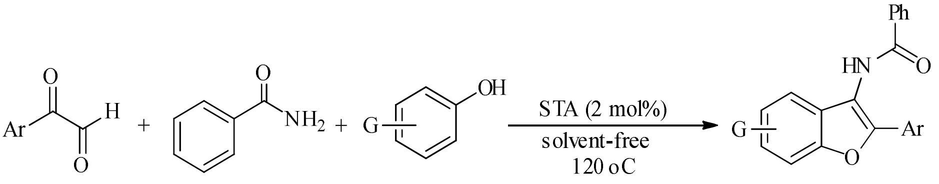
Benzo[*b*]furan derivatives are important group among naturally occurring systems. They have shown biological properties, such as anti-bacterial, anti-fungal, anti-inflammatory, anti-depressant, and anti-convulsant activities [1-3]. In continuation of our interest in use of heterogeneous catalysts [4-5], in this work we describe a new and green strategy for the preparation of novel benzofuran derivativesvia the one-pot three-component reaction of arylglyoxals, benzamide, and phenolic substrates using silica tungstic acid (STA) as a superior solid acid catalyst.



Scheme 1

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Copper-catalyzed *n*-arylation of nitrogen heterocycles inethylene glycol media under microwave irradiation

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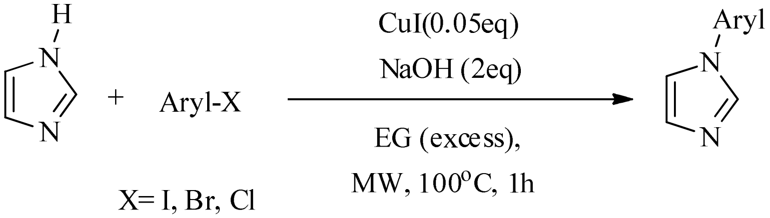
Nitrogen-containing heterocycles such as *N*-arylamines, *N*-arylpyrroles, *N*-arylindoles, *N*-arylimidazoles and N-arylpyrazoles are subunits found in numerous natural products and in many biologically active pharmaceuticals and recently, in the area of N-heterocyclic carbene chemistry. One route to these compounds is the cross-coupling of NH-containing heterocycles with different aryl halides to form the respective N-arylatedheterocycle (Ullmann coupling) [1].

To date, there have been numerous copper-catalyzed methods published to allow for such a transformation.However, these reports generally suffer from important limitations such as high reaction temperatures (often 140°C or higher), long reaction times,poor substrate generality, high cost of ligand or base and use of high boiling point polar solvents [2].

Ethylene glycol (EG) has been used as a ligand in several copper-catalyzed cross couplings of different N-nucleophiles with aryl halides [3]. Here we report *N*-arylation of N-heterocyclic compounds in EG and under microwave irradiation. Ethylene glycol acts both as a ligand for copper and a solvent for the reaction. Low amounts of copper source (5mol%), use of NaOH as a low cost, efficient, inorganic base, recyclability of catalyst and short reaction times are benefits of this protocol. Also, the reaction proceeds with aryl bromides and chlorides as well as iodides.



Scheme 1

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Microsynthesis and fragmentation mechanisms in electron ionization mass spectrometry of spiroalkylphosphonates

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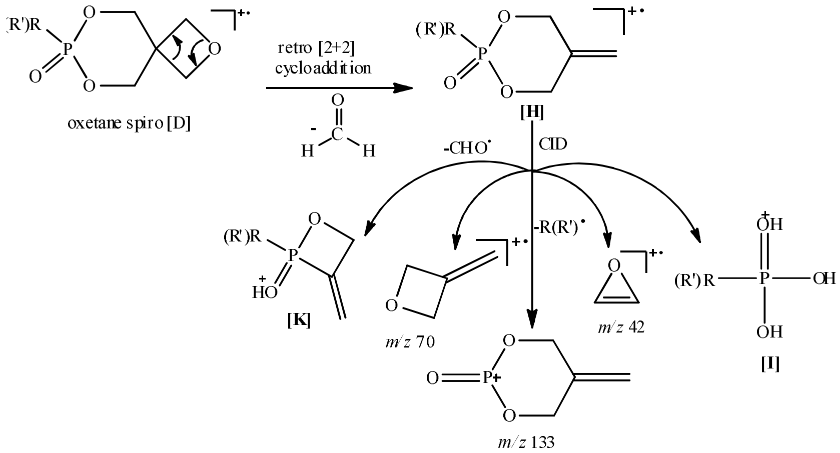
The availability of mass spectra and interpretation skills are essential for unambiguous identification of the Chemical Weapons Convention (CWC)-related chemicals [1-2]. This paper examines electron ionization (EI) and electrospray ionization (ESI) mass spectral fragmentation routes of spiroalkylphoshonate as *schedule chemicals*. Structures of fragments were confirmed using analysis of fragment ions of deuterated analogs and tandem mass spectrometry. Mass spectrometric studies revealed some interesting fragmentation pathways during the ionization process, such as elimination of alkoxy with 1,2 P-O alkyl shift, alkene, HCl and aldehyde elimination and McLafferty-type rearrangements. The results will make a substantial contribution to the Organization for the OPCW Central Analytical Database (OCAD) which may be used for detection and identification of CWC-related chemicals during on-site inspection and/or off-site analysis such as OPCW proficiency tests.



Scheme 1

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Synthesis of 2*H*-Indazolo[2,1-*b*]phthalazine-1,6,11(13*H*)-trione using nanoboehmite-H_2PO_3 as heterogeneous acid catalyst under solvent-free condition

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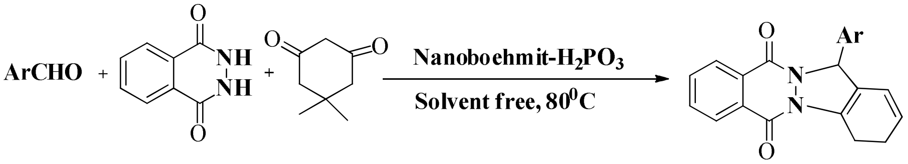
Phthalazine derivatives constituting a bridgehead hydrazine have been reported to possess a multiplicity of pharmacological properties including anti-convulsant [4] vasorelaxant, [5] and cardiotonic [6] activities.

we devised a simple and efficient one-pot approach to 2*H*-indazolo[2,1-b]phthalazine-1,6,11(13*H*)-trione derivatives*via* the three-component reaction of phthalhydrazide, dimedone, and aldehydes under solvent-free conditions at 100 ºC catalyzed by nano boehmite-H_2PO_3 through the domino Michael addition/intramolecular cyclization sequence. Short reaction times, high yields, simple operation, reusability of the catalyst, and easy work-up are some advantages of this method [1-3] (Scheme 1).



Scheme 1

References:

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Synthesis of new benzylidenethiobarbiturate derivatives containing ether groups

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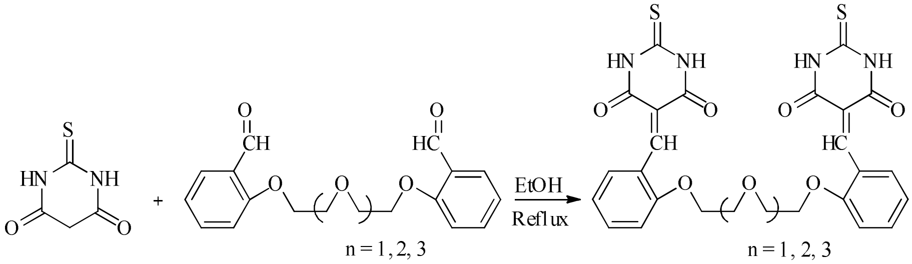
Benzylidenebarbituric acids which are potential organic oxidizers [1] are used in preparation of oxadeazaflavines, unsymmetrical synthesis ofdisulphides, synthesis of Merocyanine dyes and as antibacterial agents [2]. Benzylidenebarbiturate derivatives such asbenzylidene(thio)barbiturate-β-D-glycosides act as mushroomtyrosinase inhibitors [3]. Furthermore, benzylidenebarbituric acids are important building blocks in the synthesis of pyrazolo[3,4-d]pyrimidines and pyrido[2,3-d]pyrimidines, which show a broad spectrum of biological activities [4]. Some of these compounds have also been studied as nonlinear optical materials [5].

In the present investigation, a series of novel benzylidenethiobarbiturate derivatives containing hydrophobic ethylene glycol spacers were designed and synthesized by the condensation of ethylene glycol-substituted benzaldehydes with thiobarbituric acid. The structures of products were deduced from their spectroscopic data (The FT-IR, ^{1}H-NMR, ^{13}C-NMR spectra and elemental analysis) (Scheme 1).



Scheme 1

References:

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Highly selective base catalyzed ring closing Ugi-adducts from the reaction of 2-formylindole, 2-bromoacetic acid, amines and isocyanides

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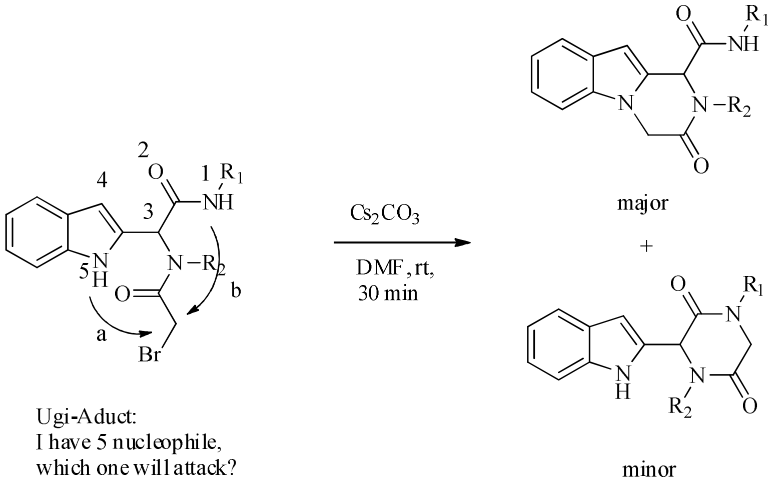
Multicomponent reaction (MCR) techniques not only make the rapid construction of diverse and complex molecules possible, but also saves time and costs, and reduces waste, in alignment with the principles of green chemistry [1-6]. A subtle change in the design of MCRs, followed by an efficient post-MCR transformation, can improve the diversity and complexity of organic compounds.

The intermediate products of the Ugi reaction between indole-2-carboxaldehyde, 2-bromoacetic acid, amines and isocyanides were treated with Cs_2CO_3 in DMF to form a series of novel cyclised 1,2-dihydropyrazino[1,2-*a*]indol-3(4*H*)-ones (indole -NH cyclization) as major and piperazin-2-ones (amide -NH cyclization) as minor products.



Ugi-Aduct:
I have 5 nucleophile,
which one will attack?

Scheme 1

References:

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Synthesis, characterization and study of catalyst activity of nanoparticles of cobalt(II) new macrocyclic complex immobilized on zeolite-Y

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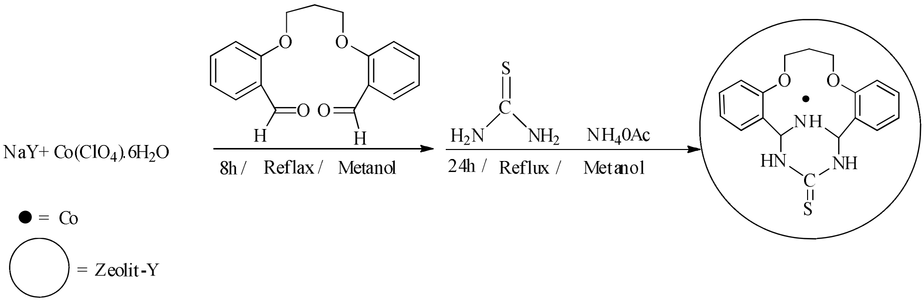
Nanopores encapsulated metal complexes are mostly used as heterogeneous and redox catalysts in the production of chemicals for various types of shape-selective conversion and separation reaction. They represent the basis of new environment-friendly technologies, involving cheaper, more efficient and more environment-friendly ways for carrying out chemical reactions [1-3].

This work reports the synthesis and characterization of macrocyclic cobalt(II) complex encapsulated within the nanopores of zeolite-Y(scheme 1). The obtained new complex nanoparticles entrapped in the nanopores of zeolite have been characterized by FT-IR, XRD, TGA and DRS spectroscopic techniques. This complexe (neat and encapsulated) were used for oxidation of cyclooctene with tert-butyl hydroperoxide (TBHP) as oxidant in different solvents.



Scheme 1

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Synthesis of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols) using poly[styrene-*co*-(1-((4-vinylphenyl)methyl)-3-methylimidazolium) chloroaluminate] as a heterogeneous catalyst

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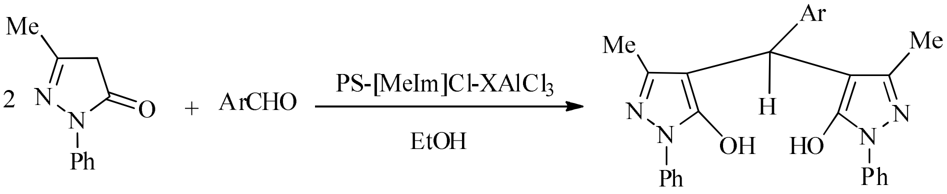
One of the primary groups of ionic liquids is based on mixture of aluminium chloride and 1,3-dialkyl-imidazolium or 1-alkyl-pyridinium chlorides [1,2]. The acidity of the resulting ionic liquid can be controlled by varying the relative amounts of $AlCl_3$ and organic chloride. An acidic chloroaluminate melt is one in which the $AlCl_3$ mole fraction is larger than 0.5. In such acidic melts, the anions $Al_2Cl_7^-$ and $Al_3Cl_{10}^-$ exist, which act as very strong Lewis acids.

2,4-Dihydro-3*H*-pyrazol-3-one derivatives including 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols) are known to possess a wide range of biological activities and are used as gastric secretion stimulatory, anti-inflammatory, antidepressant, antibacterial, antifilarial, antitumor, and antiviral agents [3-5]. Two-component one-pot domino Knoevenagel-type condensation/Michael reaction between aromatic aldehydes with 2 equivalents of 3-methyl-l-phenyl-5-pyrazolone is one of the most pivotal preparation methods of 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ols).

In this pursuit, and during the course of our ongoing interest in the application of heterogeneous catalysts in organic reactions, we now wish to introduce poly[styrene-*co*-(1-((4-vinylphenyl)methyl)-3-methylimidazolium) chloroaluminate] (PS-[MeIm]Cl-XAlCl$_3$) as a heterogeneous catalyst for the condensation reaction between aromatic aldehydes and 3-methyl-l-phenyl-5-pyrazolone (Scheme 1). The catalyst is reusable.



Scheme 1

References:

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Synthesis and characterization of silica nanoparticles via sonochemical method assisted by organic ligand

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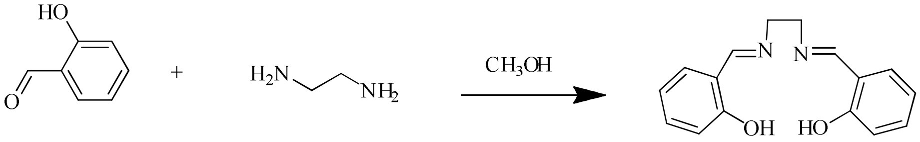
In recent years, sonochemical methods have been extensively explored to synthesize various nanostructures, including rods, wires, tubes and particle [1–2].

In this work, Silica nanostructures were synthesized via a sonochemical method and the reaction between tetraethyl orthosilicate, ethylenediamine and methanol in water, in the attendance of organic Schiff base ligand (H_2Salen) as capping agent. The effects of synthesis parameters such as: sonochemical irradiation time, sonochemical power and molar aspect ratio of Schiff-base ligand to TEOS were considered. The symmetrical Schiff-base ligand N,N′-bis(salicylaldehyde) ethylenediamine, (H_2Salen), was prepared by refluxing salicylaldehyde and ethylenediamine in dried ethanol, and cooling the reaction mixture (Scheme 1). The compound has been characterize by FT-IR and ^{1}HNMR spectroscopy.



Scheme 1

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Sonochemical synthesis of two new nano-sized Schiff base complex for preparation of two metal oxides as nanoparticles

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Imines compounds as Schiff bases, named after Hugo Schiff [1] are formed when any primary amine reacts with an aldehyde or a ketone under specific conditions. Structurally, is a nitrogen analogue of an aldehyde or ketone in which the carbonyl group (-C=O) has been replaced by an imine or azomethine group (-HC=N-). Many Schiff-base complex have been investigated as models for active sites of enzymes [2, 3], including DNA-cleavage systems [4, 5], Nanoparticles of four new Fe (III) and V (V) have been synthesized by the reaction between a three dentate Schiff base ligand E-2-(((2-hydroxypropyl)imino)methyl)-6-methoxyphenol and a tetradentate Schiff base ligand 2-((E)-(E)-2-hydroxybenzilideneamino) methylamino) methyl)phenol with metal ions in MeOH as a solvent in an ultrasonic bath for 10 min, and their structures were characterized by scanning electron microscopy (SEM), X-ray powder diffraction (XRPD), FT-IR spectroscopy and elemental analyses.

In the other part of this work the nano-sized Fe_2O_3 and V_2O_5 were prepared by heating of nano-sized metal Schiff base complex in an electrical furnace (THERMOLYNE 1500) at 450 ^oC for about 2 h. The crystalline structure of nano-sized metal oxides characterized by X-ray diffraction (XRD) system, FT-IR spectra were recorded in the 400-4000 cm^{-1} range and KBr pellet technique. The morphology and average particle size of nono-sized metal oxides were further investigated by scanning electron microscopy (SEM).

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Synthsis of CdS nanoparticles via a sonochemical method and pH dependent size of particles

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Semiconductor nanoparticles are synthesized by different chemical, physical and physiochemical methods.Varying temperature, pressure, concentration and many other factors provide a unique environment for reactions and then result in producing nanoparticles with different size, shape, and crystal structure[1-2].

In this work, CdS nanoparticles are produced via a sonochemical route in a solvent including water and ethylendiamine and CS_2 and $CdCl_2$ are employed as reactant. It is demonstrated that by reducing the pH of the initial solution, the size of nanoparticles and also their final density are reduced through decrease in the release rate of S^{2-}(Figure 1). The size of particles can be investigated from the blue-shift in the UV-Vis spectrum as a consequence of quantum confinement effect.

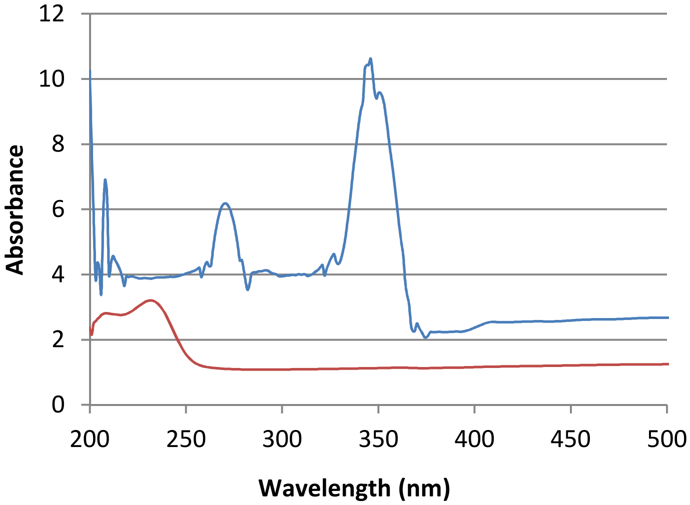

Figure 1: Blue line: pH=11, red line: pH=8

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Optimization of electrocoagulation process for removing copper, as an algaecide poison, from urbane drinking water by Taguchi method

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Cyanobacteria (blue-green algae) caused the following problems in water treatment plants such as *Microcystis* were responsible for taste and odor problems, *Anabena* had been implicated in chloroform production, and *Microcystins* were cyanobacterial hepatoxines [1]. The optimum concentration of copper sulphate, a blue crystalline solid, for killing cyanobacteria was 1 mg/l. The presence of copper in drinking water had led to several environmental effects such as taste and odor [2]. Removal technologies of copper from water included adsorption, ion exchange, and electrocoagulation [3].

The aim of this applied-analytical study was to investigate copper removal from urban drinking water by batch reactor electrocoagulation with aluminum electrodes. Copper removal efficiency was examined in different operating cases of the variables current density (0.8-2.4 mA/cm^2), initial concentration (1-100 mg/l), pH (3.5-10.5), and time (20-60 min). The results indicated that increasing the current density from 0.8 to 2.4 mA/cm^2 and reaction time from 20 to 60 min had a positive effect on the Cu^{+2} removal efficiency. The findings of our study indicated that Cu^{+2} removal rate enhanced with increasing the initial concentration of copper. Results showed that, at a batch mode with an initial concentration of 100 mg/l, a pH of 7.5, a reaction time of 60 min, and a current density of the anode of 2.4 mA/cm^2, Cu^{+2} reduction was 99.5%. The results of copper removal efficiency by Taguchi method showed that reaction time was the most important variable. Thus, experiments indicated that the electrocoagulation reactor could be efficient in removing copper from drinking water.

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Study of extraction and identification of antifungal compounds from medicinal plants by Gas Chromatography-Mass Spectrometry method (GC-MS)

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Nowadays, the use of compatible with environment technologies to prevent of damage and environmental pollution is a necessity. In order to investigate the extraction and identification antifungal compounds from medicinal plants for Reduction of pesticide residues was performed in the Tirtash Research & Education Center in 2012. In this study, nine species of medicinal plants were selected from of mountainous areas of northern iran. The plants were dried in a greenhouse, then were ground. The plant compounds were extracted with water, acetone, normal hexane, ethanol and methanol. The minimum inhibitory concentration of each extracts was determined by agar diffusion method in the department of pathology. Results indicated that crude extracts of Tobacco, Catmint, Thyme, Fennel, Hyssop and badrashbi have remarkable antifungal activity. Methanol was the best solvent to extract antifungal compounds. minimum inhibitory concentration of methanol extract of Tobacco, Catmint and Thyme were equal to 1.5, 1.5 and mg/ml, respectively when tested tobacco fungal pathogens. The chemical composition of plant extracts were determined by Gas Chromatography-Mass Spectrometry method (GC-MS). The major components were identified in the Catmint was Thymol, Menthol, Menthanol, Flavone, Anthracene, Nonenal, Phethalazine, Silane, Phenanthrene, Isoquinoline, Methl piperazin, Tobacco extract was composed by Nicotine, Lemonen, Silane, Thunbergol, Pyridine, Phenanthrene, Phytol, Globulol, Thyme extract was composed by Thymol, Silane, Anethole trans, Naphthalenole, Nonenal, Phenanthrene, Anisole and Carvacrol.

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Production and characterization of activated carbon form oak cap by chemical activation

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The present work comprises study of oak cap activated carbon (ASAC) impregnated by (HNO_3, H_3PO_4, H_2SO_4) used as adsorbent. The objective of this work was to determine the ability of activated carbon in Aromatic compound removal. Prepared activated carbon was characterized by determining BET and SEM image to examine the extent and nature of porosity. The higher sorbent number demonstrates that fairly mesoporous carbon has been developed by the process which can facilitate its applicability as potential aromatic compound removal adsorbent. The FTIR results strongly support significant spectral and chemical changes occurring with the activation of the oak cap for phosphoric acid treatment. The physical morphology clearly shows that the data obtained is consistent to the structural surface as determined by analyzing the SEM micrographs.

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The evaluation of toxicity of amitraz with PBO on the common pistachio psyllid, *Agonoscena Pistaciae*

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The using of pesticides more than common application for controlling of the common pistachio psyllid, *Agonoscena Pistaciae* makes them be resistant to most of pesticides specially amitraz. In some cases, using of synergists is useful in the pesticide resistance management programs [1]. One of the synergists is piperonyl butoxide that has ability to increasing the toxicity of some pesticides.

In this research the synergistic effect of piperonyl butoxide (PBO) on the toxicity of amitraz to adults of summer and winter forms of common pistachio psyllid was evaluated by residual contact vial (RCV) bioassay in laboratory conditions [2].

Bioassay results indicated that LC_{50} values of amitraz when use alone and by PBO together in the summer form of *A. pistaciae* were 213.7 and 151.8 mg L^{-1}, and in the winter forms were 351.6 and 123.6 mg L^{-1}, respectively. Synergistic ratio in the summer and winter forms were 1.3 and 2.8-fold, respectively.

Therefore, PBO had additive effect in the summer form and synergistic effect in the winter form. According to this research, it seems that piperonyl butoxide can apply for increasing the toxicity of amitraz against the winter form of common pistachio psyllid in chemical control.

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DFT Studies of conformational properties of thio-semicarbazone derivatives

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Thiosemicarbazone and its derivatives is the sulfur–containing class of organic substances which is similar to the structure of semicarbazones, but it contains a sulfur atom instead of oxygen. These compounds have various pharmaceutical features with beneficial biological activity [1-2], that they have been developed and they have also attracted considerable interest in recent years. The structural representation of medicines plays an important role in determining their mechanism of medicinal actions between medicine and the receptors. In the present structural study, with the help of DFT-MO (One of the selected methods is B3LYP/6-31+G*) and theoretical UV-spectrometry, the most stable tautomer and conformer of the simplest thiosemicarbazone have been revealed and using PES (potential energy surface) scan the change of potential energy with dihedral angel for the most stable tautomer were also calculated. This conformational study shows the relative energy of conformers for each of the tautomers **1-5** in thiosemicarbazone.

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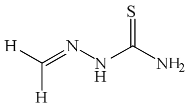

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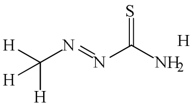

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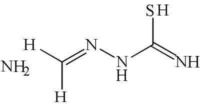

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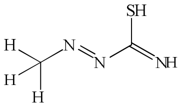

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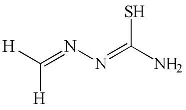

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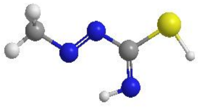

Most Stable Tautomer (1) Most Unstable Tautomer (4)

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An investigation on the thione-thiol tautomerization of 1,2,4-triazole derivatives: a DFT study

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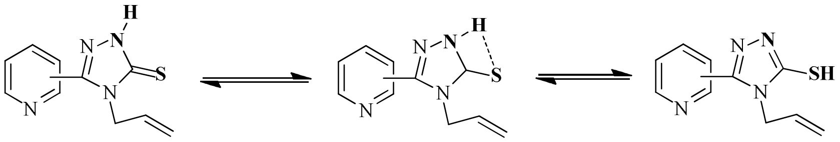
1,2,4-Triazole and its thione derivatives represent one of the most biologically activeclasses of compounds, possessing a wide spectrum of medicinal activities, as wellas specific magnetic properties [1,2]. These compounds can exist in two major tautomeric forms that exhibit different reactivity [3]. The thione-thioltautomerism of thesecompounds remains as a matter of controversy because it is not straightforward to determine which of the two forms is present. The present study focuses on the gasphase tautomerization of 4-allyl-5-(*o*, *m*, *p*-pyridyl)-1,2,4-triazole-3-thiones, 1-3, at B3LYP/6−31G(d,p) level,using GAUSSIAN 03 program package (Scheme 1).



1-3

1: 2-Pyridyl, **2**: 3-pyridyl, **3**: 4-pyridyl
Scheme 1

The calculated data (Table 1) show that all the thione forms are predominant tautomers.The predicted energy difference between thione and thioltautomers is within the rangeof ca 13–15 kcalmol^{-1}, while the activation energy of the process is within the range ofca 52–58 kcalmol^{-1} for thionetothiol reaction, and within the range of ca 43–45kcalmol^{-1} for the reverse reaction. This finding confirms that the aromaticity of 1,2,4-triazole ring cannot compensate the stability gained from the proton transfer of S to N.

Table 1. Energies (a.u) along with the energy differences and activation energies (kcalmol^{-1}) for **1-3** in thione/thioltautomerization.

Structure	Thione	Thiol	ΔE	E_a(f)	E_a(r)
1	-999.566464	-999.545838	-13.0	57.5	44.5
2	-999.566926	-999.554724	-7.7	52.5	44.8
3	-999.568629	-999.544946	-14.9	58.5	43.6

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Synthesis of 1*H*-pyrano[2,3-*d*]pyrimidin-2(8a*H*)-one derivatives via three-component reaction using poly(4-vinylpyridine)-supported ionic liquid as a heterogeneous catalyst

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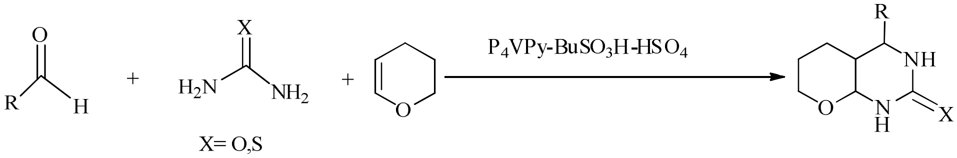
Brønsted acidic ionic liquids are of special important because they possess simultaneously proton acidity and the characteristic properties of an ionic liquid. Among them -SO_3H functionalized ionic liquids are of particular value, because of their negligible vapor pressure and outstanding acidity. Thus, they are designed to replace traditional mineral liquid acids such as sulfuric acid and hydrochloric acid in chemical procedures [1-3].

Pyranopyrimidinones and related fused ring pyrimidinones are known to possess a wide range of biological properties, such as antitumor, antibacterial, antihypertensive, vasodilator, bronchiodilator, hepatoprotective, cardiotonic, and antiallergic activities [4-6]. One-pot, three-component reaction of aromatic aldehydes, urea or thiourea, and 3,4-dihydro-2*H*-pyran is one of the most pivotal preparation methods of 1*H*-pyrano[2,3-*d*]pyrimidin-2(8a*H*)-one derivatives.

In this pursuit, and during the course of our ongoing interest in the application of heterogeneous catalysts in organic reactions, we now wish to introduce poly(4- vinylpyridine-*co*-1-sulfonic acid butyl-4-vinylpyridinium)hydrogen sulfate ($P_4VPy\text{-}BuSO_3H\text{-}HSO_4$) as a heterogeneous catalyst for the preparation of 1*H*-pyrano[2,3-*d*]pyrimidin-2(8a*H*)-one derivatives via one-pot three-component reaction of aromatic aldehydes, urea or thiourea, and 3,4-dihydro-2*H*-pyran under solvent-free conditions (Scheme 1). The catalyst is reusable.



Scheme 1

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Synthesis, characterization and study of catalyst activity of nanoparticles of copper(II) new macrocyclic schiff-base complex immobilized on zeolit-Y

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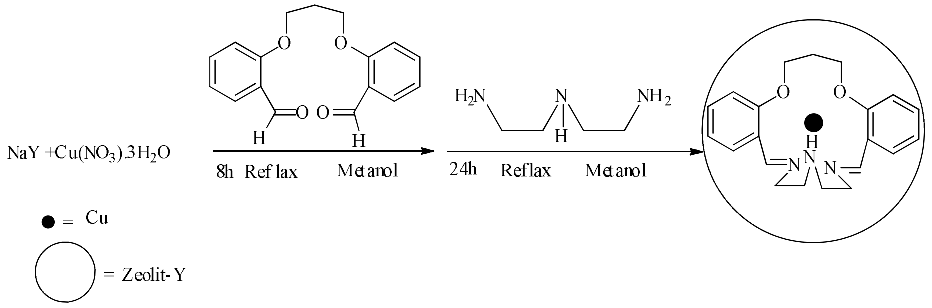
Complex nanoparticles entrapped in the nanopores of zeolite Y are fascinating class of materials, which have attracted wide spread attention in basic science as well as technology development. Some of the prominent physical characteristics of zeolites are their ruggedness to temperature and pressure and their ability to recognize, discriminate and organize molecules with less than 0.1 nm levels precision at the active site. more- over, non corrosive, environment friendly and economically viable nature of the zeolite catalyzed reactions have provided the opportunity for the development of various industrial processes such as hydrocracking and oxidation [1-3].

This work reports the synthesis and characterization of macrocyclic copper(II) complex encapsulated within the nanopores of zeolite-Y(scheme 1). The obtained new complex nanoparticles entrapped in the nanopores of zeolite have been characterized by CHN, (AAS), FT-IR, UV-VIS and DRS spectroscopic techniques. This complex (neat and encapsulated) were used for oxidation of cyclooctene With tert-butyl hydroperoxide (TBHP) as oxidant in different solvents.



Scheme 1

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Ultrasound mediated green synthesis of alkylaminophenols via Petasis Boronic Mannich reaction in deep eutectic solvent

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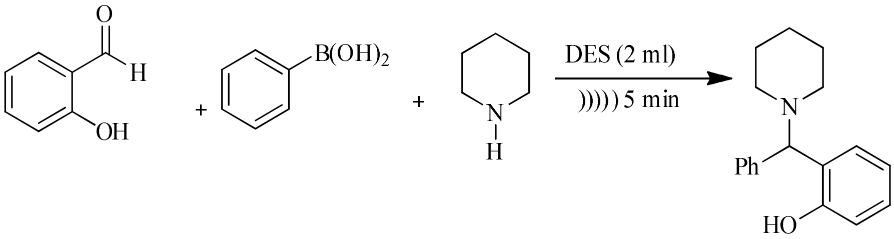
Development of green methodologies with high yields is pioneer and in this context, ionic liquid (IL) has attracted much attention and utilized in many organic reactions. But despite all valuable properties of ionic liquids, such as low vapor pressure, exceptional chemical and thermal stability and recyclability, they are not as green as expected. But despite all valuable properties of ionic liquids, such as low vapor pressure, exceptional chemical and thermal stability and recyclability, they are not as green as expected. At the beginning of this century a new generation of solvents named deep eutectic solvent was introduced by Abbott group. DES has many advantages than IL such as simple preparation, low price, chemical inertness with water, high atom economy, passing purification problems and waste disposal encountered with common ILs while their physico-chemical properties are very close. So far many organic reactions have performed in choline chloride based DES. In all reports short reaction time and easy isolation process makes DES worthy to be considered as solvent and catalyst in other valuable organic reactions [1-2].

During the course of our study aimed for improving the ecocompatibility of certain organic processesherein, we wish to report an efficient and fast one-pot preparation of Synthesis of alkylaminophenols via Petasis Boronic Mannich Reaction in deep eutectic solvent under ultrasound irradiation



Scheme 1

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Deep eutectic solvent as new green media with promising applications

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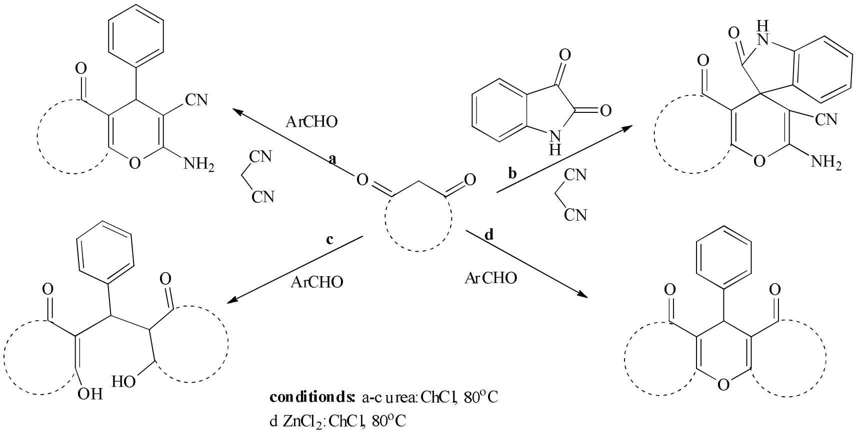
Environmental concerns have made scientists to find greener alternatives for some toxic organic solvents which are safer both for human beings and environment with safer manufacture [1-2]. Recently ionic liquid (IL) and especially their new generation named deep eutectic solvent (DES) are subject of interest owing to their pioneer properties compared to traditional organic solvents. Due to their promising properties they have many valuable applications such as their potential as green media including separation process, organic reactions, nano chemistry, electrochemistry, solar cell and etc [3].

Herein some efficient and green condensations reactions in DES as green solvent and chemo selective catalyst is reported [4-5].

In summery some applications and valuable properties of DES based on choline chloride as a novel media in industry and research laboratory will be considered.



conditionds: a-c urea:ChCl, 80°C
d $ZnCl_2$:ChCl, 80°C

Scheme 1

References:

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Dye stuff removal of wastewater by novel modified bentonite-based polyurethane foams

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Nowadays, the pollutions of non-biodegradable and hazardous wastes and the procedures of their handling are serious challenges [1]. Malachite Green (MG), one of the highly toxic colours in textile industries, is a widely used cationic dye in developing societies [2]. The tremendous impacts of MG on environment have been necessitated the removing or remediation of this compound. Here, novel polyurethane foams containing lignosulfonate-based bentonites were synthesized through the mixing of modified bentonite particles and the polyol and next curing by the polyisocyanate hardener. After the chemical characterization of prepared foams, their capability for removing of MG from aqueous solutions was evaluated. The chemical structure of synthesized polyurethane foam was confirmed by disappearing the NCO band at 2270 cm^{-1} [3]. The adsorption experiments confirmed that more than 50% MG is removed from dye solution at the first 10 minutes.

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Determination of organic pollutant of water and modeling with GMDH-type neural network during the different environmental conditions

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In this research, the physico-chemical water quality parameters and the effect of climate changes on water quality were evaluated. During the observation period (6 months) environmental conditions such as water temperature, turbidity, saturated oxygen (Os), dissolved oxygen (Od), pH, chlorophyll-a, salinity, conductivity, total nitrogen (TN) and total phosphorus (TP)(nutrient level) were determined, which has effected on the amount of organic pollutant, from July to December 2012 in the Karaj dam area.

Nowadays new agricultural policies and environmental regulations have been developed in several countries for decreasing the different source of pollution, and help to improving the quality of water [1]. Organic compounds and their related substances are much more important than before and several analytical methods have developed for evaluation of these parameters [2]. On the other hand, the concentration of nitrogen and phosphorous as nutrient parameters are considered as main source of pollution ,so determination of different anions are recognized as the key parameters to characterize the quality of water [3]. Therefore the purpose of this research is determination of different physico- chemical parameters, nutrient level and organic pollutant in different depth of Karaj dam and also using another powerful approach based on the GMDH network for modeling these parameters. 750 experimental data points of water parameter quality in different environmental conditions is used.

Mean absolute error percent (MAE %) of hybrid GMDH model for training and testing were obtained 0.1275 and 0.1347 and RSME were 0.1720 and 0.1750 respectively. The results indicated that the hybrid GMDH systems as a polynomial neural network type can accurate estimatethe importance of pollution in environment.

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Amino acid-assisted super paramagnetic $CoFe_2O_4$ nanostructures as a green and reversible adsorbent for removal of Cr(VI) from water

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Facile synthesis of super paramagnetic $CoFe_2O_4$ nanostructures with the assistance of an amino acid is employed for efficient removal of Cr(VI) from wastewater. The obtained novel adsorbent is characterized by XRD, SEM, FTIR and VSM, TGA. The pseudo- second-order kinetic model is used to describe the kinetic data and the rate constant. The adsorption isotherm is well fitted to Langmuir adsorption model. Desorption studies confirm that the adsorbent can be effectively regenerated and reused.

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Synthesis and characterization of a new asymmetric potentially pentadentae Schiff base (N_3S_2)

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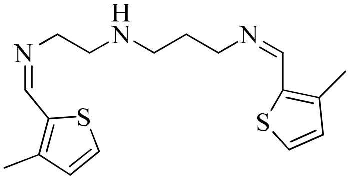
Schiff base ligands are considered as a very important class of organic compounds which have wide applications in many biological aspects such as anticancer [1], antibacterial [2], antifungal [3], antioxidant and antitumor activities [4]. These wide applications of Schiff bases have generated a great deal of interest in metal complexes. Schiff base. Transition metal complexes are one of the most adaptable and thoroughly studied systems These complexes have also applications in clinical and analytical fields [3]. Some of Schiff base complexes are used as model molecules for biological oxygen carrier systems. Certain Schiff bases play an important role in active biological systems, for example Salicylaldehyde amino acid Schiff base complexes are used as non enzymatic models for the metal-pyridoxal (Vitamin B6) amino acid Schiff base systems which are key intermediates in many metabolic reactions of amino acids catalyzed by enzymes which require pyridoxal as a cofactor (transamination, decarboxylation, and elimination, racemization, etc.) [5]. In this work we report the synthesis of an asymmetrical potentially pentadentate (N_3S_2) Schiff base ligand derived from condensation reaction of 3-(2-aminoethylamino)-propylamin with 3-methyl-2-thiophenecarbaldehyde in 1:2 molar ratio (Scheme1). The Schiff base ligand and was characterized by FT-IR, ^{1}H NMR, ^{13}C NMR and elemental analysis methods.



Scheme 1

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Persistent organic pollutants (polychlorinated dibenzo-p-dioxins) associated in water of Karun River

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The distribution of polychlorinated dibenzo-p-dioxins measured in suburban farmland, vegetable, and orchard collected associated to water of the Karun River was obtained with gas chromatography-mass spectrometer analysis in 2013.

Persistent organic pollutants (POPs) targeted by the Stockholm Convention are suspected of causing cancer and teratismushermpahroditicus or known to damage nervous system and endanger growth of normal infant and child [1, 2]. As a result, an objective assessment of the current state of water pollution by POPs in China is needed to provide baseline information for further regulatory efforts to include organic pollutants in the assessment of drinking water safety.

The Kārun is Iran's most effluent, and the only navigable, river. It is 450 miles (720 km) long. It rises in the ZardKuh mountains of the Bakhtiari district in the Zagros Range, receiving many tributaries, such as the Dez and the Kuhrang, before passing through the capital of the Khuzestan Province of Iran, the city of Ahwaz. The Karun continues toward the Persian Gulf, forking into two primary branches on its delta: the Bahmanshir and the Haffar that joins the Shatt al-Arab (ArvandRud in Persian), emptying into the Persian Gulf. Downstream 25 kilometres (16 mi), the Karun widens into the reservoir formed by the Karun-3 Dam.The Karun then turns north into the reservoir of ShahidAbbaspour Dam (Karun-1). The Karun flows southwest into the impoundment of MasjedSoleyman Dam (Karun-2). Gotvand Dam, MasjedSoleyman Dam, Karun-1 (ShahidAbbaspour Dam), Karun-3, and Karun-4, all are on the main stem. Results showed that total polychlorinated dibenzo-p-dioxins varied from 0.01 to 3.04 $\mu g.g^{-1}$ with the median value of1.07 $\mu g.g^{-1}$.

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Preparation and characterization of cellulose acetate /organically modified montmorillonite (OMMT) nanocomposite membrane for separation of humic acid from water

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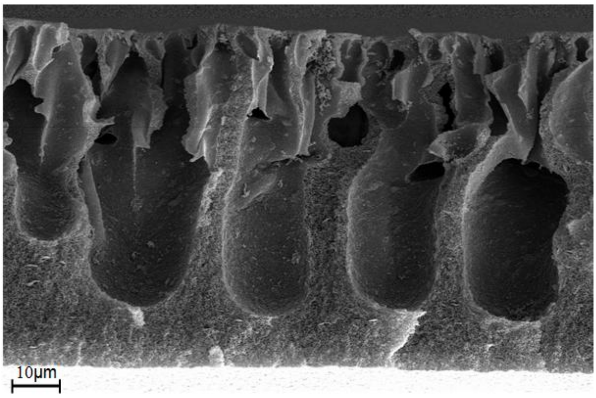
In this paper, asymmetric nanocomposite membranes based on cellulose acetate and organically modified montmorillonite (OMMT) were prepared by combination of solution dispersion and wet-phase inversion methods. The Effects of OMMT on theproperties and performance of prepared nanocomposite membranes were investigated. The prepared nanocomposite membranes were characterized by scanning electron microscopy (SEM), contact angle measurement and tensile strength techniques. Pure water flux and rejection of humic acid as organic Fertilizer from waterwere studied using an ultrafiltration experimental setup. The results showed that the addition of OMMT has improved the hydrophilicity of membranes and permeate flux while rejection decreases by OMMT loading into the polymer matrix.



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Synthesis of 1-[aryl-(pyrimidin-2-ylamino)-methyl]-naphthalen-2-oles by humic acid catalyzed reaction between 2-naphthol, aldehydes and 2-aminopyrimidine

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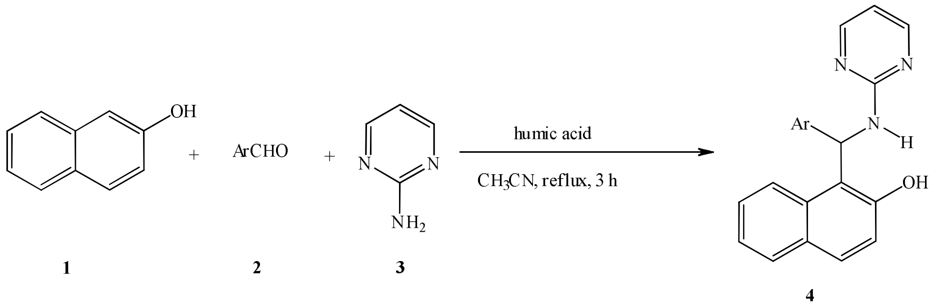
Multi-component reactions (MCRs) have emerged as an important tool for building of diverse and complex organic molecules through carbon–carbon and carbon–heteroatom bond formations taking place in tandem manner [1]. Particularly, in the last three decades a number of three and four-component MCRs have been developed [2-3].

In continuation of our previous works on three-component reactions between an aldehyde, an enolic system, such as substituted 2-naphthols, 4-hydroxycoumarine or acetophenone derivatives and a nucleophile [4-6], here we wish to report that three-component reaction between 2-naphthol, aromatic aldehydes and 2-aminopyrimidine in the presence of catalytic amounts of humic acid (HA).



Scheme 1

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A facile and eco-friendly synthesis of imidazo[1,2-*a*]pyridines using nano-sized $LaMnO_3$ perovskite-type oxide as an efficient catalyst under solvent-free conditions

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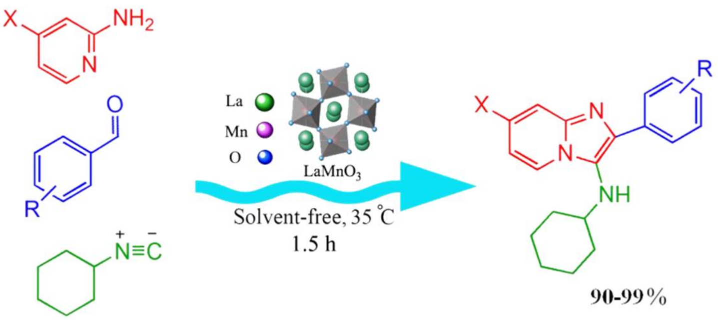
Imidazo [1,2-*a*]pyridine derivatives display a diverse range of biological activities [1]. A new three-component condensation to approach such fused imidazoles was developed in 1998 [2-4]. Since the first reports were published, various methods have been performed to improve this powerful multi component reaction synthetic methodology. However, these methods possess several disadvantages such as long reaction time, complicated work-up procedure and harsh reaction conditions, requirement of excess amount of catalysts and low yields [4, 5].

$LaMnO_3$perovskite nanoparticles were prepared using a sol-gel method [6].This perovskite-type oxide as a green and reusable catalyst showed excellent catalytic activity for the synthesis of imidazo[1,2-*a*]pyridines.$LaMnO_3$ catalyst could be recovered and reused in five reaction cycles, giving a total TON = 2790 and TOF = $372 hr^{-1}$. The products were prepared under solvent-free conditions without any additives (Scheme 1). Principal features of this simple method include non-hazardous reaction conditions, low catalyst loading and excellent yields.



Scheme 1

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Theoretical with combined practical investigations of Zn (II), Cu (II) and Pb(II) ions study on the selectivity of a nanoanalcime zeolite loaded bya multi dentate Schiff base ligand by flame atomic absorption spectroscopy

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In recent years, density functional theory (DFT) calculations have been used extensively for calculating a wide variety of molecular properties such as equilibrium structure, charge distribution and clarifying the mechanism of selective capture and transportation of metal ions by ligands and provided reliable results which are in agreement with experimental data [1-4].

The aim of this work is to develop a rapid and efficient method for the selective extraction and preconcentration of μg/l levels of Cu (II), Zn(II) or Pb(II) ions in aqueous solution using a nonporouszeolite modified by bis-(2-hydroxy-1-naphtaldimine)-N-diethylentriamineSchiff base ligand prior to their flame atomic absorption spectrometric determination. In addition, in this study, DFT theory with B3LYP functional is employed to compute the binding energies of the bivalent cations to the title Schiff base compound. The present calculations could make a step towards the prediction of the applicability of an extractant for different metal ions in many related analytical techniques. All calculations were carried out with the Gaussian 03 package [5].

However, the present chemical modeling cannot take into account all facts of the present complex chemical system. Although the present DFT calculations do not predict the exact trend observed in the extraction power of the Schiff-base ligand, but they enable us to say which cations are more susceptible for extraction by the ligand or may act as interferences.

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Phytochemical analysis of anisosciadium orientale

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GC-MS one of the best methods for chemical composition analyzes of the plants essential oil and volatile extracts.Thymus species are well known as medicinal plants because of their biological and pharmacological properties.The genus Thymus L., known as ‘‘Avishan” in Persian, is a well-known aromatic perennial herb originated from Mediterranean region.Among 215 species of this genus grown in the world, 14 speciesare distributed in Iranian flora [1,2].The aim of this research was to studythe essential oil composition of Anisosciadium orientale specie of the genus Umbelliferae by GC-Mass analyze.

20 grams of air dried and grinded plant materials were subjected to hydrodistillation by an all-glass Clevenger type apparatus for 2 hrs.Extracted yellow colored essential oils were dried over anhydrous Na2So4 and kept at refrigerator in sealed dark glass vials until analysisGC–MS analysis was carried out by use of Thermoquest-Finnigangas chromatograph equipped with fused silica capillary DB-1column (60 m×0.25 mm i.d.; film thickness 0.25 lm) coupledwith a TRACE mass (Manchester, UK). Helium was used as carriergas with ionization voltage of 70 eV. Ion source and interface temperatureswere 200 ºC and 250 ºC, respectively. Mass range wasfrom 35 to 456 amu.oven temperatureprogram was 60–250 ºC at the rate of 4 ºC/min and finally held isothermallyfor 10 min; split ratio was 1:50.

Hydrodistillation of the aerial parts of the plant yielded 0.37 v/w of oil. The oil was subjected to GC–MS analysis. The composition of the oil was determined by comparison of their mass spectra and the calculated GC retention indices to those reported in the literature for the standard compounds[3].Fourteenconstituents, have been identified in the essential oil extracted from the aerial parts of this plant. Limonene (40/93), Careene<delta-3-> (21/02), α-Pinene (6/58) were the major components.

	Compound Name	KI	Area		Compound Name	KI	Area
1	α-Pinene	939	6.58	**8**	Elemene<beta->	1391	0.19
2	β-Pinene	979	0.24	**9**	Caryophyllene<(E)->	1419	0.41
3	Careene<delta-3->	1031	21.02	**10**	Farenesene<(E)>-beta	1457	0.2
4	Phelandrene<alpha->	1003	4.26	**11**	Germacrene D	1485	2.19
5	Limonene	1029	40.93	**12**	Selinene<beta->	1490	0.16
6	Ocimene<(E)-beta->	1050	0.67	**13**	Germacrene B	1561	1.03
7	Terpinene<gamma->	1060	1.00	**14**	Caryophyllene oxide	1583	1.52

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Chemical analysis the essential oil of *Teucriumpolium* L. From Iran, obtained by hydrodisttilation and HS-SPME instrument and comparison results

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Teucrium has been used since ancient time for a variety of medicinal purposes as anti bacterial, sedative, antipyretic and gastric lesions [1- 3].

The Flora of Iran comprises 12 species of *Teucrium* of which 3 are endemic [4]. In this investigation no polar compound of leaves with young branches of *Teucriumpolium* from shahrood, Iran, obtained by hydrodistillation and head space-solid phase microextraction (HS-SPME) and comparison result. The composition of the volatile oils was investigated by GC-FID and GC-MS [5]. The main component in the oil obtained with Clevenger instrument were β-pinene (14.14%), sabinene (13.87%), α-pinene (9.88%), germacrene D (5.91%) and muurolol (5.89%). The major constituent of the oil identified by HS-SPME coupled with GC-MS, were α-pinene (39.24%) and sabinene (47.16%). The isolated oils from leaves of *Teucriumpolium* observed with HS-SPME characterized by monoterpenes and in isolated oil with Clevenger observed sesquiterpenes (31.53%) and monoterpenes (55.13%) of representing of the total components were identified (87.07%).

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Preparation, characterization and antioxidant activity of di- and tri-hydroxy benzoyl chitosan nanoparticles

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Chitosan is a linear copolymer of β(1→4) linked 2-amino-2-deoxy-β-D-glucopyranose (GlcN) and 2-acetamido-2-deoxy-β-D-glucopyranose (GlcNAc) units. Recently, degradation by radiation processing of polysaccharides has gained much attention due to its technological effectiveness in producing low molecular weight [1]. The antioxidant activity of chitosan was studied in *vitro* and in *vivo* systems and the hydrogen-donating ability of chitosan is a major antioxidant mechanism [2]. Modified chitosans with 3,4-dihydroxy benzoyl groups (CS-DHBA) and 3,4,5-trihydroxy benzoyl groups (CS-THBA) were synthesized and their nanoparticles were prepared via ionic cross linking by tripolyphosphate (TPP) [3]. The chemical structure and morphology of particles were studied using the X-ray diffraction (XRD) patterns and scaning electron microscopy (SEM), respectively. The antioxidant activity of the CS, CS-DHBA, CS-THBA and their nanoparticles were investigated by the radical scavenging activity method using 1,1-diphenyl-2-picrylhydrazyl (DPPH). Fig. 1 shows DPPH free radical scavenging activity (%) of CS, DHBA, THBA, CS-DHBA, CS-THBA, CSNp, CS-DHBANp and CS-THBANp in different concentrations. The results indicated that the DPPH scavenging free radical capacity of CS-THBA and CS-DHBA nanoparticles increased up to 89% and 74%, respectively, when the concentration reached 6 µg/mL.

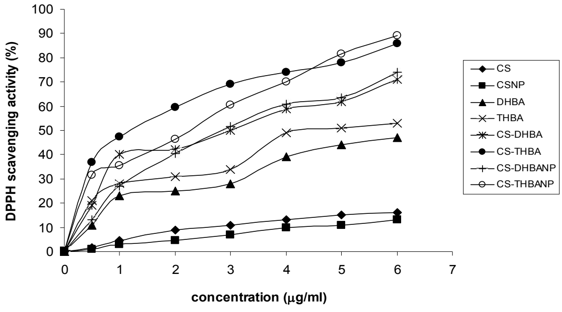

Fig. 1. DPPH free radical scavenging activity (%) of CS, DHBA, THBA, CS-DHBA, CS-THBA, CSNp CS-DHBANp and CS-THBANp in different concentration

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Chemical composition of the essential oil from aerial parts of *Anthemis rhodocentra* compositae (Asteraceae) using the head space solid phase microextraction method prior to gas chromatography-mass spectrometry

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The genus Anthemis (Compositae) comprises about 37 species in the Iran. The present report deals with the analysis and comparison of composition of the volatiles component obtained by head space-solid phase microextraction (HS-SPME) procedures from the aerial parts of *Anthemis rhodocentra* compositae (Asteraceae). The plant material was collected from of south Khorasan Province, Iran [1-2]. The SPME headspace volatiles were collected using a fiber coated with polydimethylsiloxane (PDMS).

The composition of the volatile essential oil from aerial parts of *Anthemis rhodocentra* compositae (Asteraceae) was investigated by GC-FID and GC-MS. β-pinene (29.02%) was the main constituent in the aerial parts of *Anthemis rhodocentra*. The other main components in the aerial parts oil were camphene (18.72%), 1,8-cineole (18.16%), α-pinene (8.71%), borneol (6.8%) and limonene (3.38%) [3].

References:

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The synthesis of some new oxime ethers and investigation of pesticide activity

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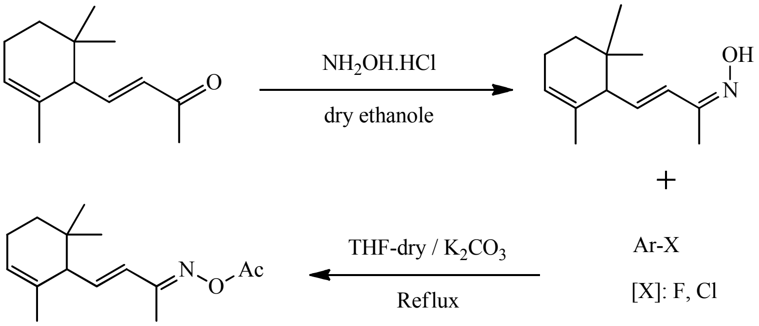
Oxime ethers are important bioactive compounds. The study of their derivatives has become of much interest in recent years on account of their antiprotozoan, antibacterial activity, antienteroviral, antifungal, anti-neoplastic,anticonvulsant, and antimicrobial activities. also different oxime ether derivatives have also been reported to possess anticholinergic, insecticidal and acaricidal activities[1-4].

In this investigation, some new oxime ethers were synthesized from O-Arylation of corresponding oxime by various aryl halides during aromatic nucleophilic substitution mechanism (SNAr) (Scheme 1).



Scheme 1

References:
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Studying of chemical constituents of Tobacco Leaf Oriental by changes of temperature and relative humidity

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Several thousand compounds could be identified in tobacco, many of which contribute to the flavor; aroma and physiological effects [2]. The changes in oriental tobacco chemical compositions during the curing and aging process are not widely studied. There are lacks of the knowledge on the difference of chemical changes in oriental tobacco in different conditions. The relationships between chemical compositions and sensory quality, and the possibility to use chemical changing index for predicting the quality of this tobacco in tobacco industry [4]. This changes include hydrolysis of starch to free sugars and partial respiration of those sugars to carbon dioxide, hydrolysis of proteins into free amino acids and the conversion of nitrate into nitrite and its subsequent reaction with tobacco alkaloids to form tobacco specific nitrosamines [1,3]. This study carried out in Tirtash Research and Education center in 2010-2011, (1) to find out the change in regularity of chemical composition (pH, nicotine, volatile alkali, total organic acids, volatile acids, total water-solubility sugar, and reducing sugar, nitrite, total nitrogen, protein, total ash) and others substances in different process; (2) to test the possibility to predict the quality of oriental tobacco in the curing and aging process by using the forecast models. For this study the tobacco leaves were at temperature of (35, 40, 45, and 50^{oc}), relative humidity (90%-15%) and Time (3 and 6 hours). The results showed that the changes of chemical compositions were between 5% - 40%. The protein and acidy number were determined in percentage of 40 and 25 that had the highest changes to other constituents. The lowest changes were pH and total N (8%-10%). But nicotine had not changes. In conclusion the studies showed that the temperature and relative humidity and Times, changes the chemistry and quality of the leaf tobacco.

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Investigations of the effects of novel peptides on amyloid Abetafibril formation

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Proteins are one of the most important biological polymers that can perform a number of roles including catalysis, structural, and regulatory in organisms. Proteins are made of amino acids building blocks, which define their primary structures. In order for proteins to be functional, they need to undergo folding processes to create their secondary and tertiary structures. Under certain conditions such as adverse temperature and pH, a protein can misfold to a nonnative structure. One of the major forms of misfolding is amyloid formation which has been known as a causative agent in more than 40 diseases in humans. In Alzheimer, a neurodegenerative disease, a small peptide (Abeta), made of 42 amino acids, has been shown to misfold into insoluble fibrils [1-2].

Our approach has been using small novel peptides to inhibit or slow down Abeta fibril formation. In designing novel peptides, charge density, sequence variability, different morphology of peptides have been considered. For synthesis of small peptides, solid phase methodology or solid support are used. The inhibitory role of the novel peptides on the Abeta amyloid fibril formation is monitored by CD (or FTIR), SDS-PAGE and fibril specific fluorescence dyes [3-4].

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Layer effects on quinolizidinyl derivatives of anti-Alzheimer's AChE inhibitors with GA-ANN

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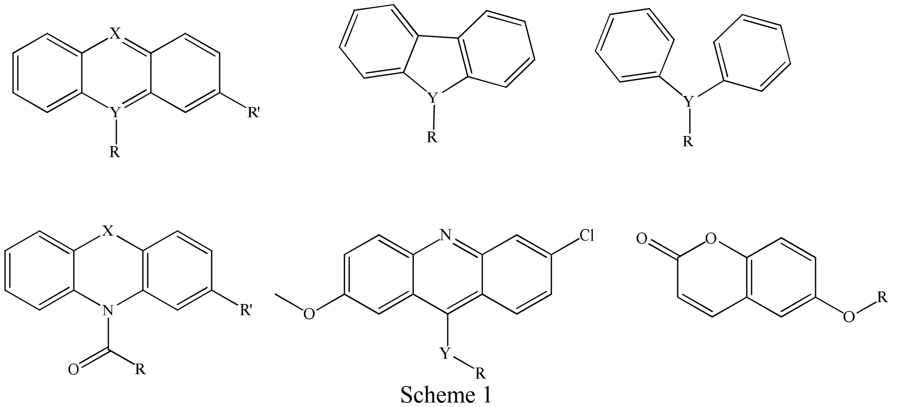
Alzheimer's disease (AD) is an age-related neurodegenerative process characterized by a progressive memory loss; decline in language skills and other cognitive impairments [1]. Quantitative structure–activity relationships (QSARs), an important area of chemometrics have been widely utilized to study the relationship between chemical structures and biological or other functional activities. QSAR has become increasingly helpful in understanding many aspects of chemical-biological interactions in drug and pesticide research as well as in many other areas [2].

In this work, layer effects study has been done on quinolizidinyl derivatives of anti-Alzheimer's Acetylcholinesterase(AChE) inhibitors. Genetic algorithm (GA), artificial neural network (ANN) and stepwise multiple linear regression (stepwise-MLR) were used to create then on non-linear and linear QSAR models. In the gas phase the best root-mean square errors of the training set and the test set for GA–ANN model using jack-knife method, were 0.1409 for layers [10,1] and [11,1], 0.2093 for layer [3,1] and $R^2$for layer [3,1] was 0.88. Also, the R and R^2 values in the gas phase were obtained 0.86, 0.75 from GA-stepwise-MLR model. The structures of the quinolizidinyl derivatives used in this study are shown in Scheme 1 [3].



Scheme 1

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Chemical composition and antimicrobial activities of essential oil and methanolic extraction of *Stachys lavandoliplia* from Ramsar – Iran

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Microwave assisted hydro distillation (MAHD) is an advanced hydrodistillation (HD) technique utilizing a microwave oven in the extraction process [1]. In this research the essential oils and methanolic extraction of aerial parts of *Stachys lavandoliplia* were studied. Chemical analysis using GC and GC-MS has resulted in identification of 32 constituents, comprising about 96% of the total constituents in oils of aerial parts. The antioxidant activities of methanolic extraction were studied by determination of inhibitory effect of them against DPPH. *In vitro* antimicrobial and antifungal activities of extraction were investigated by disk diffusion method and the MIC and MBC determination against four strains of bacteria (gram +/-) and a test yeast strain, Candida albicans. The oil exhibited a stronger effect against tested gram positive than gram negative bacteria.

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Volatile constituents, antioxidant and antimicrobial activities of (*Bunium persicum* Boiss.) from Ramsar–Iran

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The aerial parts seeds of (*Bunium persicum* Boiss.*)* growing wild in highest of Ramsar in Iran after collected were air-dried for 4 days before isolation of essential oil [1]. The essential oil obtained by solid phase micro extraction (SPME). The methanolic extraction was obtained by maceration method after 24h. The yield of the essential oil was 0.38% (w/w) and extract was 8.6% (w/w) based on the dry weight of the plant [2]. The oil analyzed by GC and identified by GC-MS twenty two components representing 98.4% of the total oil. The antimicrobial activities of the extract of (*Bunium persicum* Boiss.) were determined by measuring the growth inhibitory zones (MIC) against effective antioxidant. Six gram-positive and gram-negative bacteria. The evaluation of antibacterial activity of the extract indicated significant activity against all of the bacteria. The antioxidant activities of the extract were determined by measuring the power of trapping of DPPH. The results showed that methanolic extract of (*Bunium persicum* Boiss.*)*, act as effective antioxidant.

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Extraction and identification of fatty acids composition of some salvia species

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Fatty Acids are aliphatic monocarboxylic acids which act as the building lipids blocks. The importance of fatty acids in human diet due to the positive effects in the prevention of diseases such as heart disease, cardiovascular, skin inflammation, blood pressure and blood clotting. It also helps immune function and promotes health brain and prevents cancer [1]. Omega-3 and Omega-6 fatty acids for fetal growth and development are important, especially to the Central Nervous System (CNS) [2]. You should always enter the body through dietary fatty acids is needed and this will require new sources of these acids. Thereby, this work is trying to introduce new sources of plant fatty acids [3]. Firstly, extraction and derivatization methods were optimized on several species of plants of the genus Salvia. Then, methylated fatty acids were analyzed qualitatively and quantitatively respectively by GC and GC-MS. Finally, the profile of fatty acids in some species of Salvia was determined.

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Identification of combination forming the essence and anti-microbe of alcoholic and hydro-alcoholic extract of Euphorbia helioscopia plant of Qom region

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Since, some of herbal extracts including Euphorbia helioscopia have anti-bacterial effects, they can be used as anti-microbial factors in treating infections [1-2]. The assessment of the essence combination and the anti-microbial quality of stem's extract of this plant is the purpose of this study.

In this empirical study, the plant's essence was extracted by the distillation method and the combination of this essence was separated and identified by the chromatography/mass spectrometer GC/MS and the column DB-5, and extract-making on the Euphorbia helioscopia plant was performed by different solvents and use of Soxhlet system and the soaking method. Extract–making was performed by solvents such as methanol, ethanol, hexane, distilled water and water-ethanol. Anti-microbial activity of this plant identified by measuring the diameter of controlling haloand the minimal density of controller of the growth (MIC) for levels: Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Salmonellatyphi, Candida albicans and by method of Plait sump and diluting in cultivate liquid environment, respectively.

Finding showed that the all extracts did not react toward the Salmonellatyphi, and the extracts of stem showed more effect on Pseudomonas aeruginosa Bactria that there was a significant difference with standard antibiotics. According to performed study, it can be concluded that extracts of the stem of Euphorbia helioscopia plant has the high anti-bacterial activity.

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Phytochemical investigation and antibacterial activity of the leaves extract of *Rhazyastricta* L. from Bam

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Antioxidant activity of leaves in methanol, Ethanol, Aqueous, Acetone and Chloroform extracts and the Total phenol, Protein and Flavonoid content were studied. The Total phenol, Protein and Flavonoids content were determined using FolinCiocalteu, Bradford, Woisky methods while antioxidant activity were determined using 2,2-diphenyl-1-picryl hydrazine (DPPH) method and Ferric reducing antioxidant power (FRAP) assay [1,2].

The Aqueous extract was showed highest antioxidant activity in both methods. In DPPH method, IC_{50} was 57.64 µg/mland in FRAP assay it was 42.37 mMFe2+/mg sample. The amount of Phenolic compounds, Protein and flavonoid were founed to be 13.32 mg GAE/gD.W, 129.86mgAlbu/ D.w and 68.26 mg Quer/g Extract respectively.

The Ethanol and Aqueous extracts have been significant antibacterial effect on *Salmonella*, *Acinetobacter*, *Micrococcus* and *Yersinia* pathogens.The Aqueous extract has been highest effect. Therefore, due to the high amount of natural component, antioxidantand antibacterial activity, *Rhazyastricta L*. can be used fortreating diseases that were caused by oxidative stresses and pathogenic bacteria.

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Phytochemical investigation and antibactrial activity of the fruit extracts of the *Ribeskhorasanicumassadi and saghafi. endemic species* from Razavikhorasan province

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Antioxidant activities of this plant were received by means of DPPHand FRAP methods [1]. For this purpose, plant was extracted by six different solvent (Methanol, Ethanol, Acetone, Water, Ethyl acetate,Chloroform) .in DPPH method, methanolic extract with IC_{50}= 85 µg/ml and FRAP method 34.17 mM Fe^{2+}/mg sample had the highest antioxidant effects and Chloroformic extract in DPPHmethod with IC_{50}= 755.96 and FRAP method 2.85 Mm Fe^{2+}/mg sample.

Antibacterial activity was carry out for two extract (Ethanol and Aqueous) on four (*Salmonella*, *Acinetobacter*, *Micrococcus* and *Yersinia*) pathogens.In all cases Ethanolic extract showed strong antibacterial activity rather than aqueous extract. Furthermore chemical composition were measured by using of total phenol, Protein and Flavonoids testes. The amount of Total phenol was estimated using Folin-Ciocalteu photometric method. The result was showed 7.24 mg GAE /g D.W.In addition, the content of, Proteinand Flavonoids were obtained 92.289 mg Albumen/gr D.W, 65.029mg Quercetin/gr Extract, respectively [2].

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The first benign synthesis of *N*-aryl 1,2-dihydroquinoline derivatives via ZnO nanoparticles-catalyzed one-pot Knoevenagel condensation/ enamination reaction of 2-(*N*-arylamino)benzaldehydes and dimedone

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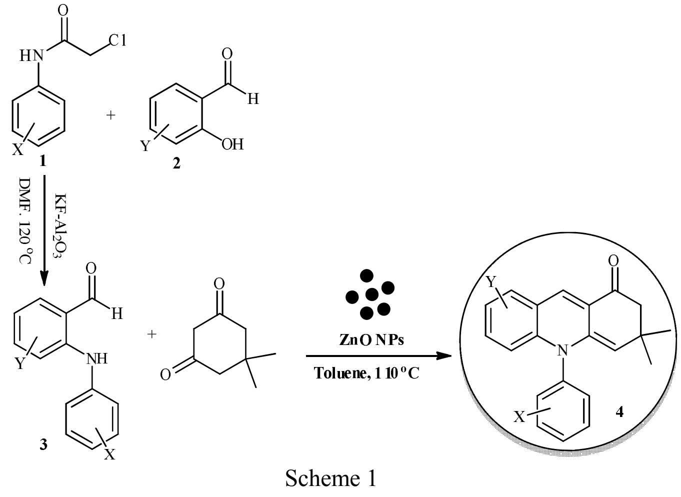
1,2-Dihydroquinoline derivatives are versatile and valuable building blocks and intermediates in the synthesis of biologically and pharmaceutically active compounds and natural products [1]. A good number of methods have been already reported in the literature for the synthesis of various 1,2-dihydroquinoline derivatives which show the high importance of this class of compounds. In our earlier work, we reported the synthesis of 2-(*N*-arylamino)benzaldehydes **3** from 2-hydroxybenzaldehydes via Smiles rearrangement, as a useful intermediate in organic synthesis [2]. These fine compounds can be used as useful synthones in the substrates of *N*-aryl 1,2-dihydroquinoline derivatives. On the other hand, during our studies on the preparation of ZnO nanoparticles by controlled microwave heating and its promising application in *O*-acylation of alcohol and synthesis of β-acetamido ketones/ esters *via* a multicomponent reaction [3], we became interested in the synthesis of highly substituted *N*-aryl 1,2-dihydroquinoline derivatives using nano ZnO as a nanocatalyst. Herein, we wish to report an efficient one-pot reaction of Knoevenagel condensation/ enamination reaction of 2-(*N*-arylamino)benzaldehydes **3** and dimedone in the presence of ZnO nanoparticles, which leads to *N*-aryl 1,2-dihydroquinoline derivatives **4** in moderate to high yields (Scheme 1).



Scheme 1

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Phytochemical investigation and antibacterial activity of the fruit extract of *Sambucusebulus* L.

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Sambucusebulus L. is a perennial herbaceous plant native to southern and central Europe and Southwest Asia [1].

In this present study some phytochemical parameters such as the amount of total Phenol content (using Folin-ciocalteu method), total Flavonoids (using Woisky method), total Protein (using Bradford method) were measured and they were 13.32 mg GAE/gD.W, 129.86 mg Albu/gD.w and 68.26 mg Quer/gExtract respectively. After that the antioxidant activity of six extracts (Methanol, Ethanol, Aqueous, Chloroform, Ethylacetate and 2-propanol) were evaluated by 2,2-diphenyl-1-picryl hydrazine (DPPH) method and Ferric reducing antioxidant power (FRAP) assay. The Aqueous extract showed highest antioxidant activity in both DPPH and FRAPmethod (IC_{50}=153.43 µg/ml, 60.77 mMFe^{2+}/mg sample).

Finally the antibacterial activity of two extracts (Ethanol and Aqueous) were investingated against fourpathogenic bacteria such as *Salmonella*, *Acinetobacter*, *Micrococcus* and *Yersinia* pathogens. The result showed that *S.ebulus* has been significant antibacterial effect and the aqueous extract has been highest effect compare ethanol extract. Because of antibacterial and antioxidant activites, this plant can be usefull.

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Phytochemical investigation and antibacterial activity of Seed, Fruit and Leaves extract of *Carica papaya* L.

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Papaya, botanical name *Carica papaya*, is an lozenge tropical fruit, often seen in orange-red, yellow-green and, with a rich orange pulp.

Antioxidant activity of Seed, Fruit and leaves in Methanol, Ethanol, Aqueous extracts were determined by 2-diphenyl-1-picryl hydrazine (DPPH) method and FRAP assay. Then the Total Phenol, Protein and Flavonoidscontent were studied [1].

For antioxidant activity The methanol extracts for Seed and Fruit showed highest antioxidant activity in DPPH (IC_{50}= 194,563.52μg/mland) and FRAP (21.97, 14.97 mMFe2+/mg sample) assays but for leaves, ethanol extracts showed highest antioxidant activity in DPPH (IC_{50}=46.64μg/mland) and FRAP (42.43 mMFe2+/mg sample) assays.

The amount of Phenolic compounds, Protein and Flavonoid in seed was founed to be 3.156 mg GAE/gD.W, 99.07 mg Albu/gD.w and 65.59 mg quer/g extract and in Fruit was founed to be 3.255 mg GAE/gD.W, 105.39 mg Albu/gD.w and16.72 mg quer/g extract and in Leaves was founed to be 4.828 mg GAE/gD.W, 67.81 mg Albu/gD.w and90.25 mg quer/g extract. The Ethanol and Aqueous extracts have been significant antibacterial effect on *Salmonella*, *Acinetobacter*, *Micrococcus* and *Yersinia* pathogens. The Aqueous extract has been highest effect.

References:

1. S. Sahoo, G. Ghosh, D. Das, S. Nayak, *Asia. Pac. J. Trop Biomed.* 3 (**2013**) 871.

Antimicrobial, antioxidant activities and phytochemical screening of the *Periploca aphylla* L., *Lavandula angustifolia L., Juglans regia L., Eucalyptus L.* and *Nerium oleander*

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The present study was carried out to investigate of some phytochemical parameters on aqueous and ethanolic extracts of the *Periploca aphylla, Lavandula angustifolia, Juglans regia, Eucalyptus* and *Nerium oleander*. The ethanolic extracts showed higher antioxidant activity than the aqueous extracts in both 2,2-diphenyl-2-picryl hydrazyl (DPPH) [1] and Ferric reducing antioxidant power (FRAP) methods [2]. The amount of phenolic, protein and flavonoid compounds in *P.aphylla, L.angustifolia, J.regia, Eucalyptus* and N.oleander were found to be (22.92, 15.62, 24.31), (3.33, 25.82, 13.64), (54.77, 18.74, 95.051), (41.95, 25.29, 27.64) and (4.194, 34.52, 43.49) mg/g D.w, respectively. The obtained extracts were assayed in different concentration for their antimicrobial activity against two Gram-positive and three Gram-negative bacteria, by agar diffusion method. Results show that all extracts were active against all tested antimicrobial experiments. However, the ethanolic extracts were more active than aqueous extracts.

Therefore, because of the high amount of natural component, antioxidant and antibacterial activities, these plants can be used for treating diseases that were caused by oxidative stresses and pathogenic bacteria.

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An overview from synthetic methodology to medicinal chemistry: applications of various functional groups as biologically active compounds

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Cancer is a disease characterized by the uncontrolled growth of abnormal cells. Many studies suggested that once a tumor grows beyond a critical size, which is of approximately 1 mm^3, it has an ability to develop its own blood supply system for the gain off sufficient nutrients and oxygen and the removal of toxic wastes by angiogenesis. Angiogenesis, the formation of new blood capillaries from existing vessels, is an important mechanism for supplying nutrients to cells that are distant from existing blood vessels. Angiogenesis is essential in physiological processes (such as growth and development, wound healing and reproduction) and is also involved in pathological conditions such as tumor growth, metastases, and certain chronic diseases. This multi-step process is tightly controlled by a balance of angiogenesis inducers and inhibitors. In pathological conditions (such as tumors), the regulatory mechanisms which "turn off" neovascularization in healthy tissue do not function normally, and a shift in the balance of positive and negative angiogenesis regulators towards the positive molecules is observed. Additionally, angiogenesis is not only responsible for the critical growth of a tumor but also for the metastasis of a tumor. Because of these reasons, the effective inhibition of tumor angiogenesis can block tumor progression and growth beyond a critical size or metastasis to other organs.

The purpose of this lecture focuses on the following topics:

1. Synthesis of various functional groups under solvent-free/aprotic conditions
2. Synthesis of various functional groups as cytotoxic and antiangiogenesis agents
3. Synthesis of metal-based drugs (Biometals) as cytotoxic agents
4. Synthesis of biologically active compounds as antimicrobial, antioxidant, antileishmania, antiproliferative, anti-*Mycobacterium tuberculosis*, neuroprotective agents
5. Synthesis of DNA intercalators
6. Synthesis of enzyme inhibition agents (carbonic anhydrase, aldose reductase, topoisomerase II, tyrosinase, aldose reductase, metallo-β-lactamase, acid phosphatase, tyrosine kinase)
7. Molecular Modeling.

References:

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Synthesis of some novel β-hydroxytriazole derivatives having carbazole core as potential chemotherapeutic agents

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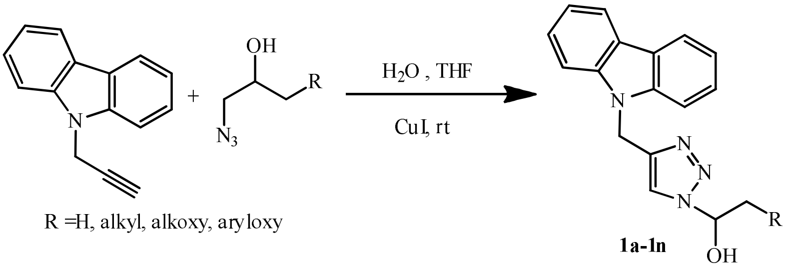
Carbazole has attracted considerable attention in organic and medicinal chemistry. Carbazole is a key structural motif found in many famous drugs and bioactive compounds exhibiting diverse biological activities including antifungal, anticonvulsant, antimicrobial, antiviral, anti-inflammatory, and analgesic activity [1]. In addition, some carbazoles are useful in optoelectronic materials, conducting polymers, and synthetic dyes [2].

The 1*H*-1,2,3-triazolyl group encompasses the remarkablebiological activities as well as the recognition by enzymes and receptors in the cell [3]. 1,2,3-Triazolescan readily associate with biologically targets through thehydrogen bonding and dipole interactions [4]. Therefore, the incorporation of the 1*H*-1,2,3-triazolyl group into a molecular structure is an important strategy in drug design. Having encouraged by the remarkable biological activities of carbazole and 1,2,3-triazole derivatives, herein we describe the design and synthesis of new structure**1** having carbazoleand 1,2,3-triazole residues. In this research, a variety of compound**1** analogues were efficiently synthesized viaHuisgen 1,3-dipolar cycloaddition reaction between *N*-propargylcarbazole and structurally diverse *β*-azido alcoholsin the presence of CuI (Scheme 1).



Scheme 1

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Nanotechnology study of anti-cancer and anti-stress properties compounds of nutmeg plants by ab initio calculation methods

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In this study, ab initio calculation methods carry out for solvent effects and NMR studies of eight anti-stress effective compounds of nutmeg plants. These effective nutmeg compounds were included terpional (α, β, γ) and 4-terpional enantiomers and gerional and three its derivatives format, butiran, acetate. The calculation have done in different basis sets such as 6-311G, 6-311G* and 6-311+G. Onsager reaction field method which is branched of self-consisted reaction field (SCRF) has employed to determinate stability of the products in different solvents. Water, ethanol and heptane solvents have chosen for modeling these nutmeg anti-stress compounds. The NMR parameters including isotropic and anisotropic parameters and chemical shifts of atoms of these molecules have investigated with same method and basis sets. The results of molecules calculation show that all four terpional enantiomers have a same behavior NMR and physiochemical properties but gerional derivatives illuminate a little different behavior compare terpional.

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Methotroxate loaded PVA coated iron oxide nanoparticles for targeted drug delivery

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In the past few decades, Magnetite (Fe_3O_4) nanoparticles have attracted growing research interest that this material has many applications in medicine and drug delivery. Drug targeting to specific organs and tissues has become one of the critical endeavors of the century since the use of free drugs in conventional dosage forms generally involves difficulties in achieving the target site at the appropriate dose after or during a proper time period [1]. Magnetic drug targeting is a drug delivery system that can be used in locoregional cancer treatment. Coated magnetic particles, called carriers, are very useful for delivering chemotherapeutic drugs [2].

In this work, our goal is to conjugate the Methotrexate (MET) with various polyvinyl alcohol (PVA) coated iron oxide nanoparticle carriers and study the drug loading from these carriers. Iron oxide nanoparticles were synthesized by co-precipitation technique PVA solution. XRD, SEM, FTIR, and VSM were used to characterize the synthesized nanoparticles. These magnetic carriers were loaded with the anti-cancer drug MET and its in vitro loading were studied. The novelty of this work is the binding of MET to the PVA coated iron oxide nanoparticles, the study of drug loading and subsequent in vitro drug release in order toevaluate the suitability of MET loaded PVA coated iron oxide nanoparticlesas magnetic carriers for drug delivery.

$$Fe^{+2} + 2Fe^{+3} + 8OH^- \longrightarrow Fe_3O_4 + 4H_2O$$

Scheme 1

Magnetite (Fe_3O_4) nanoparticles have been successfully synthesized by three methods viz chemical co-precipitation, oxidative hydrolysis and composite fluid methods [3]. We have developed a simple precipitation route to synthesize magnetite (Fe_3O_4) nano-particles with controlled size without any requirement of calcination step at high temperatures.prepared polyvinyl alcohol phosphate (PVP) coated magnetite nanoparticleshaving a broad size distribution (13–55nm) which were superparamagnetic at room temperature.

Magnetic carriers consisting of PVA coated superparamagnetic iron oxide (magnetite) nanoparticles were synthesized by precipitation of iron oxide and subsequently coated with PVA. The magnetic carriers were characterized by XRD, SEM, FTIR and VSM techniques. XRD showed a magnetic core of average size of 10 nm, a decrease in the saturation magnetization of the carriers was observed with increase in PVA concentration.

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Nano hydroxyapatite synthesis with Sol-Gel procedure, its modification with Ionic Iiquid and increasing its resistance by using Ostrich egg crystal layer

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Hydroxyapatite (HA) is of high relevance in material science, biology and medicine as they constitute the major inorganic phase of human hard tissues like bone and teeth [1]. The properties of HAP including bioactivity, biocompatibility, solubility, sinterability, castability, fracture toughness and absorption can be tailored over wide ranges by controlling the particle size and morphology [1].

Various techniques have been developed for the synthesis of HAP due to its growing importance and applications [2]. Among the alternative methods, sol–gel synthesis of HA ceramics has recently attracted much attention, due to its many advantages, which include high product purity, homogeneous composition, and low synthesis temperature [3].

In this work, we produce HA powder from the nature sources and then use the ionic liquid for its modification. In order to enhancing the resistance of producing powder, we use the Ostrich egg crystal layer. In the last step, the clinical test will done on the product and then we will checked its biocompatibility and suitability for bone substitution and correction of dental defects.

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Synthesis and antimicrobial effects of a novel nano composite: NaOCl@nano chitosan

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Dentistry and endodentistry are taking a great advantage of NaOCl bactericidal ability. What's more, nano chitosan (CS) is also known as an attractive antimicrobial bio-compatible compound with implications in medicine, biology, pharmacy, dentistry, *etc*. We wondered if we could multiply the bactericidal effects by dispersing NaOCl on the surface of CS. In doing so a positive synergic effect is demonstrated by our novel NaOCl@CS. The latter composite is fully characterized by IR, NMR, UV, XRD, SEM, and TEM.

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Proton and sodium ion affinities calculation of Topiramate derivatives (anticonvulsant drugs) by DFT

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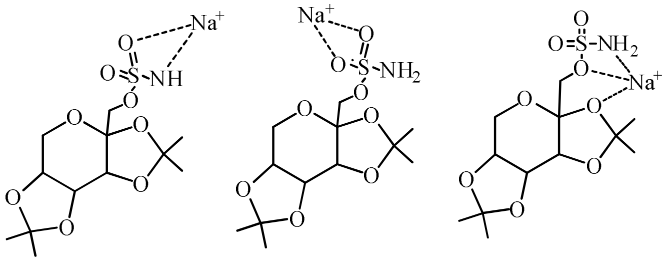
Epilepsy has been recognized as a neurological disorder, affecting a large section of people. Every year, approximately 0.25 million new cases are added to this population [1]. Bruce E. Maryanoff *et al.* reported the synthesis and biological activity studies of Topiramate as antiepilepsy drug in 1979 [2]. Despite the fact that Topiramate is structurally unrelated to other antiepileptic drugs and its biological molecular mechanism of action is still unknown, this drug acts by multiple neurostabilizing mechanisms. Blockade of voltage-dependent sodium channels is one of them. Sodium ion, biologically the most important electrolyte, is one of the most abundant metal ions in biological systems, where it is involved in a variety of processes, including osmotic balance, the stabilization of biomolecular conformations and information transfer via ion pumps and ion channels. For a better understanding of interactions of Topiramate with Na^+ and H^+, information about the intrinsic binding modes of these ions to Topiramate, is necessary. The present study addresses this subject by using DFT calculations (Scheme 1). To the best of our knowledge, the proton and sodium ion affinities of topiramate have never been taken into consideration in DFT calculations.



$$\text{Topiramate} + H^+ \longrightarrow [\text{TopiramateH}]^+$$
$$\text{Topiramate} + Na^+ \longrightarrow [\text{TopiramateNa}]^+$$

Scheme 1

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Synthesis of 8-amino heptaacetyl lactoside as precursor for the synthesis of biotin-appended ganglioside analogues

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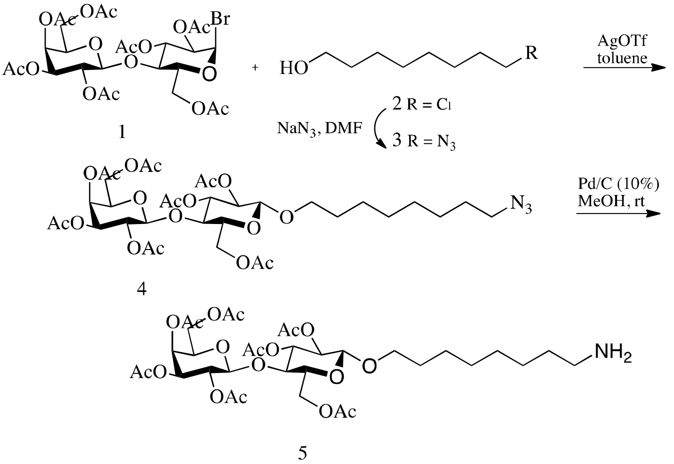
Ganglioside are primary targets for auto-antibodies that cause immune-mediated forms of polyneuropathy including Guillain-Barré Syndrome [1], in which apart from anti-GM1 antibodies, antibodies against other gangliosides are relevant [2-3]. Thus, the synthesis of structurally analogous mimics of gangliosides containing biotin-appended aglycone would thus bring advantages to the field of detection and diagnostics, as well as to other (bio)medical applications that involve biotin-streptavidin interactions. For the use as a starting compound in this study, the 8-aminooctyl heptaacetyl lactoside **5** was synthesized (Scheme 1). Peracetylated lactosyl bromide **1** was glycosidated with 8-azidooctanol **3**, prepared by a substitution reaction from 8-chlorooctanol **2**, to give 8-azidooctyl heptaacetyl lactoside **4** in a moderate yield. The azido group in **4** was reduced by hydrogenation, to give the amino terminated lactoside **5** in a nearly quantitative yield.



Scheme 1

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Synthesis of some novel hydroxyl alkyl 1,2,3-triazolyl *N*-heterocycle derivatives as potential chemotherapeutic agents

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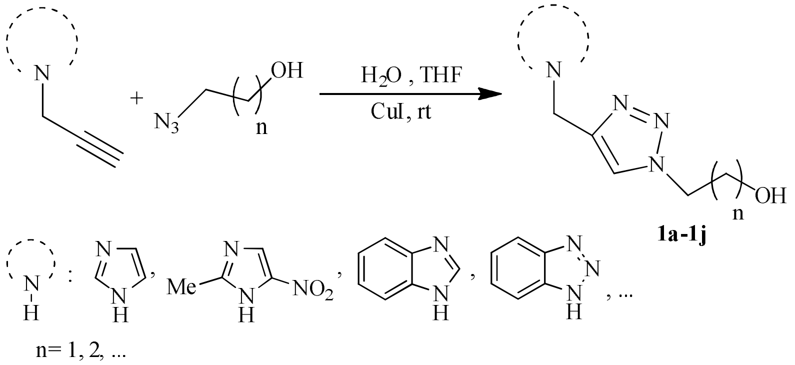
1,2,3-Triazole derivatives are important compounds in medicinalchemistry owing to their wide applications in drug discovery. They can readily associate with biologically targets through thehydrogen bonding and dipole interactions [1]. The 1,2,3-triazole coreis a key structural motif in many bioactive compounds, exhibitinga broad spectrum of biological activities, such as antiviral, anticancer, anti-HIV, antibiotic, antibacterial, and antimicrobial [2,3]. Additionally, they have found significant industrial applications asdyes, agrochemicals, corrosion inhibitors, photo stabilizers, andphotographic materials [4].

As a prototype of 'click chemistry', the recent advance of Cu(I)-catalyzed Huisgen'sazide-alkyne cycloaddition (CuAAC) hasemerged the powerful tool for introducing a 1,2,3-triazolyl residue into the molecule [3]. Inspired by the remarkable biological activities of 1,2,3-triazole derivatives, we have designed and synthesized some novel hydroxyl alkyl 1,2,3-triazolyl *N*-heterocycles**1a-1j**. Initially, the reaction of various bioactive *N*-heterocycles with propargyl bromide afforded the prerequisite terminal alkynes which subsequently converted to title compounds viaHuisgen'sazide-alkyne cycloaddition reaction with preformed azido alcohols in the presence of catalytic amount of CuI (Scheme 1).



Scheme 1

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Synthesis and study of the properties of drug carrier nano particles based on cyclodextrin and their applied in targeted drug delivery

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Magnetic nanoparticles (MNPs) are being of great interest due to their unique purposes. Especially in medicine, application of MNPs is much promising. The importance of targeted drug delivery and targeted drug therapy is to transport a drug directly to the center of the disease under various conditions and thereby treat it deliberately, with no effects on the body [1].

The excellent biocompatibility and unique inclusion capability as well as powerful functionalization capacity of cyclodextrins and their derivatives make them especially attractive for engineering novel functional materials for biomedical applications [2].

In this work, Pure magnetic nanoparticles were prepared by co-precipitating of iron salts in the presence of aqueous ammonia solution under nitrogen atmosphere. Magnetic nanoparticle Fe_3O_4 is encapsulated within a shell of SiO_2 that ensures biocompatibility of the nanocomposite. Hydrophilic β-cyclodextrin derivative, carboxymethyl β-cyclodextrin were synthesized. MNPs grafted on β-cyclodextrin derivative then anti cancer drug, 5-flurouracil loaded in carrier's cavity. At last the properties of novel magnetic carriers were studied.

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Synthesis of 2-[chloro(phenyl)methyl]-4*H*-benzo[*d*][1,3]oxazin-4-one derivatives under mild conditions

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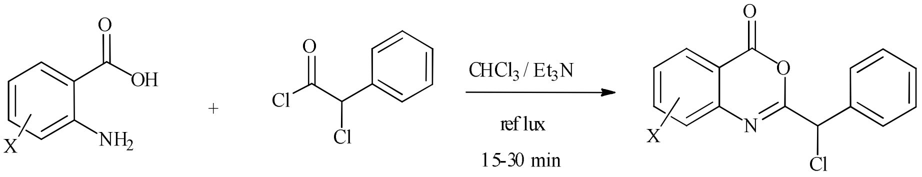
4*H*-1,3-Benzoxazin-4-ones as an important class of fused heterocyclic compounds have considerable interest owing to their industrial and wide biological applications. They are found in nature and have been used as key intermediates in the synthesis of a wide variety of biologically important heterocyclics such as quinazolinones and quinolines.

Herein, an easy strategy is described for the one-pot synthesis of 2-[chloro(phenyl)methyl]-4*H*-benzo[*d*][1,3]oxazin-4-one derivatives **2** using condensation and cyclization reaction of anthranilic acid derivatives **1** with α-chlorophenyl acethyl chloride in the presence of triethylamine under mild reaction conditions (Scheme 1). Good to high yields of some new of the title compounds obtained in short reaction times with simple work-up.



1

2

80-95%

Scheme 1

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Synthesis and purification of fluvoxamine maleate in green solvents with high yield

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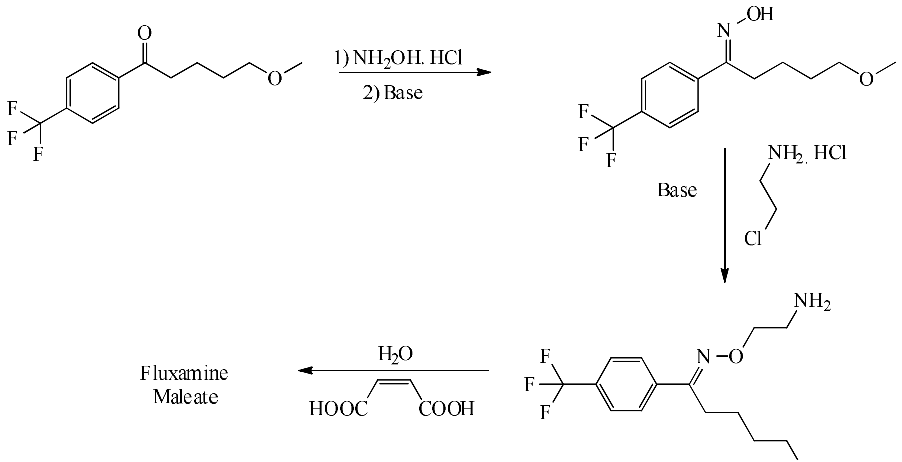
Fluvoxamine maleate is a medication which functions as a selective serotonin reuptake inhibitor and σ1 receptor agonist. Fluvoxamine is used primarily for the treatment of obsessive-compulsive disorder and is also used to treat major depressive and anxiety disorders, such as panic and posttraumatic stress disorders. Fluvoxamine is approved to treat social anxiety symptoms [1-2].

In this work, a new strategy has been introduced for the synthesis of fluvoxamine maleate in two steps. The first step is a reaction between 5-methoxy-1-[4-(trifluoromethyl)phenyl]-1-pentanone and hydroxyl amine and a base in an environmentally safe solvent under reflux conditions which leads to high yields of the expected product. The second step occurs between oxime and 2-choloroethylamine and a base. This step is also gives high yields of the target compound which in reaction witrh maleic acid produces the final fluvoxamine maleate salt.



Scheme 1

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Synthesis of 2-(1-(3-mercaptopropanoyl)-2-oxoindolin-3-ylidene)-N-phenyl/alkylhydrazinecarbothioamide derivatives as metallo-β-lactamase inhibitors and study of drug-enzyme interactions using molecular modeling

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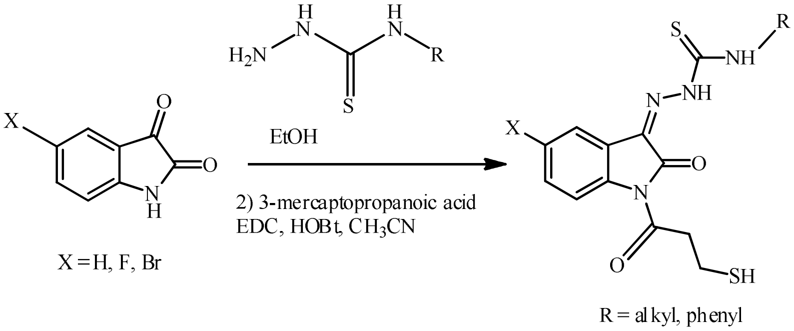
The β-lactam antibiotics are crucial chemotherapeutics for the treatment of bacterial infections. In bacteria, the production of enzymes such as the serine-β-lactamases (SBLs) and metallo-β-lactamases (MBLs) increasingly confers resistance to an ever broader range of common β-lactam antibiotics such as penams, carbapenems and cephalosporins. Thus, the development of an inhibitor for SBLs and MBLs is an attractive approach to maintain the usefulness of existing antibiotics.The aim of this work was to develop candidate MBL lead inhibitors through the synthesis, testing and in silico docking of compounds based on isatin. An IMP-1 MBL which occurs in both *Pseudomonas aeroginosa* and *Klebsiellapneumoniae* was selected as a target since these pathogens are well known for recorded outbreaks of antibiotics-resistant bacterial infections in medical settings, and since this enzyme is relatively well studied (e.g. crystal structures have been reported) (Scheme 1) [1-3].



Scheme 1

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Synthesis of Flunixin in high-temperature water

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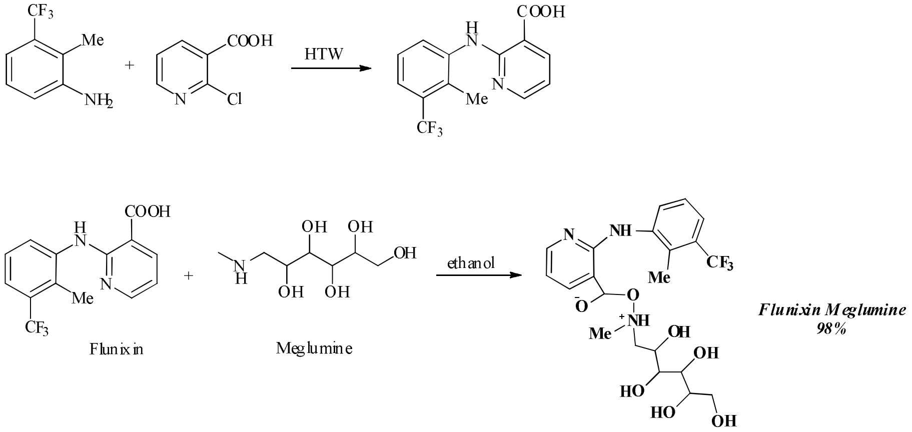
Organic reactions in high-temperature water (HTW) were introduced because of a desire for cleaner, safer, and more environmentally benign chemical processes. High-temperature water has properties very different from those of ambient liquid water such as relatively high solubility of organic compounds, lower dielectricconstant, and fewer and less persistent hydrogen bonds.

Flunixin, known as 2[[2'-methyl-3'-(trifluoromethyl)phenyl]amino]-3-pyridinecarboxylic acid, is a non-steroidal anti-inflammatory drug (NSAID), analgesic, and antipyretic used in veterinary medicine. It is often formulated as the meglumine salt. This study focused on a green synthesis of flunixin through the reaction of 3-(trifluoromethyl)-2-methylbenzenamine and 2-chloropyridine-3-carboxylic acid in HTW condition followed by the preparation of flunixinmeglumine salt using N-methyl-D-glucamine (meglumine) in ethanol.This reaction protocol finally can drive improvement of the yield and reaction conditions compared to existing methods.



Scheme 1

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Schiff base complex of cupper (II) supported on magnetic Fe_3O_4 nanoparticles: green and efficient nano catalyst for oxidation of sulfides into the corresponding sulfoxides

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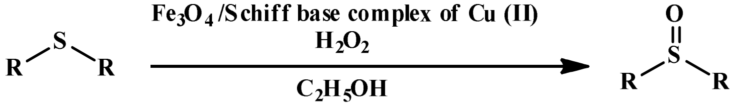
Nanoscale materials have been a subject of particular interest due to properties, which differ from their bulk counterparts [1]. In contrast to the difficulty observed in recovering and reusing most solid catalysts, core–shell nanostructure magnetic catalysts can be easily retrieved under the influence of a magnetic field and used in subsequent reactions. Therefore, using magnetic core–shell structure composites as catalysts has been recommended in literature [2]. Schiff base complexes have key role in catalysis of a variety of organic reactions [3].

In this work, a new Schiff base complex of cupper (II) was synthesized from the reaction between Schiff base and $Cu(NO_3)_2$ salt on Fe_3O_4 surface. Then, catalytic ability of Fe_3O_4/Schiff base complex was found to be an efficient nano catalyst for the oxidation of sulfides into their corresponding sulfoxides compounds with H_2O_2 as oxidation agent in ethanol solvent.



Scheme 1

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The one-pot synthesis of spiro[4H-pyran-3,3-oxindole] catalyzed by 1,3-dibromo-5,5-dimethyl hydantoin (DBDMH) under mild reaction condition

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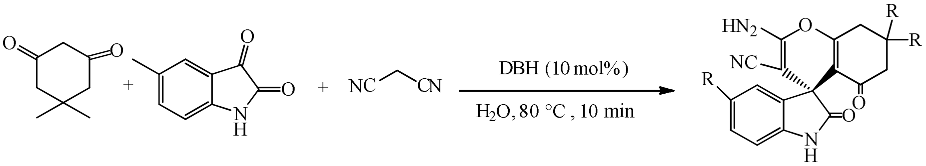
Spirooxindole derivatives are important class of heterocyclic compounds. The spirooxindole system is a widely distributed structural framework that is present in a number of pharmaceuticals and natural products including cytostatic alkaloids like spirotryprostatins and strychnophylline [1-3].

Despite the importance of these biological active compounds, a few reports have been found for the synthesis of them which must of the previous methods suffer from several disadvantages including long reaction times, low yields of product, harsh reaction conditions, hard and time-consuming work-up procedure, and the use of expensive and toxic reagent and solvent. Herein, we wish to report a highly efficient method for the synthesis of unsymmetrical spiro[4H-pyran-3,3-oxindole] by three-component condensation of isatin, malonitrile and dimedone in the presence of catalytic amount of DBDMH; High yields of products, short reaction times the use of non-toxic solvent and easy work-up in combination with commercial availability, low cost and non-toxicity of the catalyst make this work eco-friendly and commercially acceptable (Scheme 1).



Scheme 1

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Synergetic effect of ionic liquid based heteropoly acid and magnetic nanoparticles on hydroamination reaction

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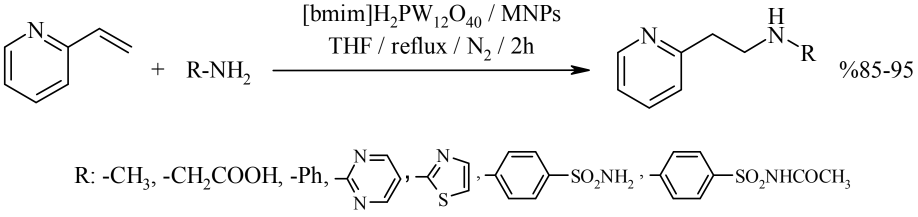
Hydroamination reaction, addition of an amine to an unsaturated carbon–carbon bond, resulted in direct formation of a carbon–nitrogen bond [1,2]. Ionic liquids (ILs) appear particularly favorable for catalytic systems [3]. Polytungstic acid ($H_3PW_{12}O_{40}$) as a heteropoly acid (HPA) is more active catalyst for various organic reactions and is the most widely used catalyst owing to its high acid strengths, thermal stabilities, and low reducibilities [4]. A supported IL strategy has been applied for the immobilization of a heteropoly acid. Magnetically recoverable nanoparticles (MNPs) have synergetic effects on organic reactions and can be easily separated from the reaction mixture using an external magnetic field [5]. In the present paper, an efficient and simple procedure for hydroamination reaction using IL/MNPs as catalyst are disclosed.

In this study, among various nanoparticles as heterogeneous solid supports, NPs-Fe_3O_4@DE (Diatomaceous Earth) acts as a good catalyst for C-N bond formation via Michael addition type reaction (Scheme 1). Because of dual catalytic action in HPAs (Brønsted & Lewis acid), best results was obtained by use of these compounds as catalyst. Higher reaction rates are observed in ILs with high dielectric constant. In conclusion, the method for C-N bond formation via Michael addition type reaction as reported in this paper, is a simple and mild procedure with clean workup. Product isolation involves simple separation of MNPs with magnet at the end of the reaction followed by purification of residue.



Scheme 1

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Exploring new approach for synthesis of pyrazolo[3,4-d]pyrimidine derivatives containing piperazine and piperidine moiety

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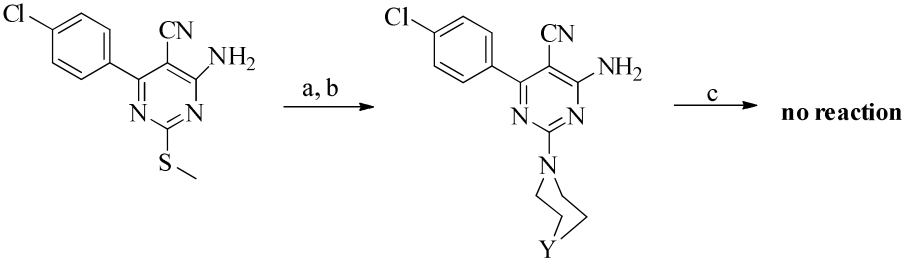
In this research, we are attempting to expand our previous work [1] to synthesis of other heterocyclic building blocks. Furthermore, with a view of piperidine and piperazine as important structural motifs in a number of bioactive compounds, the potential of atwo-stepmethod in our previous report [2] for the synthesis of pyrazolo[3,4-*d*]pyrimidine derivatives possessing such motifs was studied using two other pyrimidine derivatives substituted with piperidine and piperazine at C(2) of the pyrimidine ring (**2m** and **2n**), under the optimized reaction conditions (Scheme 1). For this purpose (**2m**) and (**2n**), were prepared through a differentsynthetic pathway from (**1**) (Scheme 1) [3].To our surprise, no reaction was observed between these two pyrimidine derivatives and hydrazine hydrate in EtOH under reflux conditions (Scheme 1).



1

Y = NH (**2m**)
CH_2 (**2n**)

Reagents and conditions:
(a) 1mmol of **1**, 3 mmol of oxone, acetone/ water, r.t, over night (quant.).
(b) Piperazine or piperidine (2eq.), dioxane, r.t, over night.
(c) 1mmol of **2m** or **2n**,NH_2NH_2 (0.5 mL), EtOH, reflux.

Scheme 1

In order to find out why fused pyrimidine derivatives were not formed from the reaction between these pyrimidine derivatives and hydrazine hydrate, we investigated the effect of pyrimidine ring substituents on C(2) computationally [3].

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Melamine-formaldehyde resin supported H^+catalyzed synthesis of 1,4-dihydropyridines

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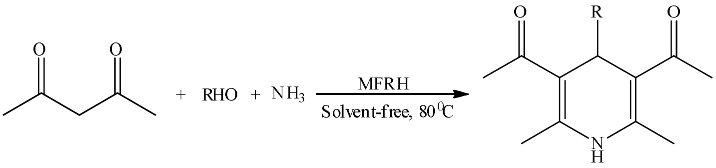
In recent years economic and environmental concerns encourage the application of heterogeneous catalyst to carry out various organic transformations. These catalysts make the processes clean, safe, high-yielding and inexpensive [1]. Melamine-formaldehyde works under heterogeneous conditions. It is an inexpensive and non-hazardous solid acid catalyst. It can easily be handled and removed from the reaction mixtures by simple filteration. 1,4-Dihydropyridines (1,4-DHPs) have received much attention because of their wide range of pharmaceutical and biological properties such as antiviral, antibacterial, antihypertensive and antitumor effects [2]. Synthesis of 1,4-DHPs is usually completed via one-pot Hantzsch condensation of aldehydes with ethyl acetoacetate, and ammonia either in acetic acid, alcohol [3]. However, this method involves long reaction time, harsh reaction conditions, and gives products in low yields. Recently, much effort has been devoted to developing more efficient methods for the synthesis of 1,4-DHPs [4].

Now, we report an efficient and convenient procedure for the one-pot reaction of β-dicarbonyl compounds, aldehydes and ammonia, by using heterogeneous catalyst melamine-formaldehyde resin supported H^+ under solvent-free conditions to produce the 1,4- dihydropyridine derivatives in excellent yields. As a consequence, an eco-friendly method was developed for the preparation of DHPs derivatives, which is important for pharmaceuticals industries (Scheme 1).



MFRH: Melamine-formaldehyde resin supported H^+

Scheme 1

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Investigation of the possibility of inclusion complex formation between β-cyclodextrin nano cavity with chlorpheniramine

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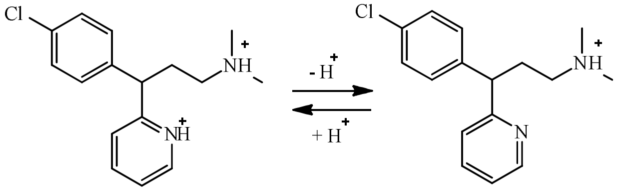
The acid–base equilibria of chlorpheniramine was studied in the absence and presence of β-cyclodextrin (β-CD) [1]. The conditional acidity constants of Chlorpheniramine is obtained by spectrophotometric methods as a function of various concentrations of β-CD and different pH values. Also the stability constants for inclusion complexes of β-CD with both acidic and basic forms (chlorpheniramine) were calculated [2-3].

The conditional acidity constant increases by increasing β-CD concentration for chlorpheniramine. The calculated stability constants show that the basic form of chlorpheniramine (615 M^{-1}) forms more stable inclusion complex than its acidic (162 M^{-1}) forms (Scheme 1).



Scheme 1

References:
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Understanding the structure, substituent effect, natural bond analysis and aromaticity of borepine: A DFT study

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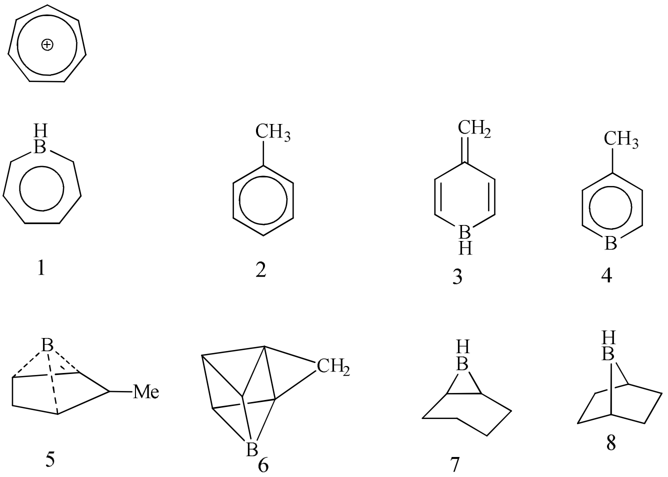
The structure and properties of borepine have been studied theoretically at the B3LYP/6-311++G (d,p) level. The calculations include the optimized geometries of isomers (Scheme 1), the frontier orbitals, vibrational analysis, electronic spectrum analysis, aromaticity and thermodynamic. The most stable of these on the C_6H_7B surface is isomer **2**. Natural bond orbital (NBO) analysis has been performed on isomer **1**. The energy and oscillator strength calculated by Time-Dependent Density Functional Theory (TD-DFT) results, and indicates indicate that, in all the molecules HOMO-1 LUMO transition has the major contribution in the most intensity electronic transition.



Scheme 1

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Substituent effects on regioselectivity of the hetero-Diels-Alder reaction of 2-aza-1,3-butadiene with styrenes using the HSAB principle

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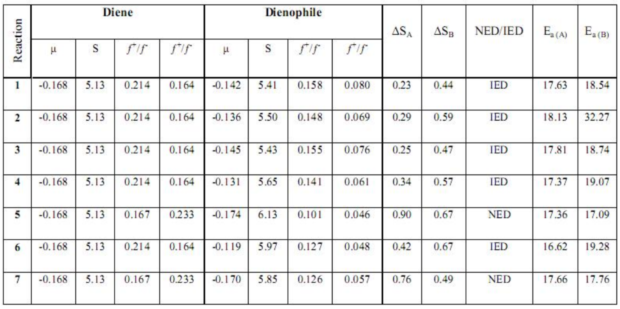
The qualitative frontier molecular orbital theory (FMO), as first expressed by Fukui [1], continues to be utilized extensively by organic chemists to predict cycloadduct regiochemistry and Diels–Alder (DA) reaction stereoselectivity. If one considers frontier orbital relative energies for diene and dienophile systems, the DA reactions can be divided into two limiting categories: (1) the normal electron demand (NED) DA reaction, $HOMO_{diene}$-$LUMO_{dienophile}$ controlled, and (2) the inverse electron demand (IED) type, in which the energy gap between $HOMO_{dienophile}$ and $LUMO_{diene}$ governs the reaction rate [2]. Moreover, the regioselectivity in the cycloaddition reactions has been described in terms of a local hard and soft acid and base (HSAB) principle, and some empirical rules have been proposed to rationalize the experimental regioselectivity pattern observed in some DA reactions. In this paper, regioselectivity of DA reaction of para substituted styrenes (X= H (**1**), CH_3 (**2**), F (**3**), OH (**4**), NO_2 (**5**), NH_2 (**6**) and CN (**7**)) with 2-aza-1,3-butadiene investigated by Fukui parameters. All of calculations were performed at DFT/B3LYP/6-311++G** level using the Gaussian 09 program. It is worth to mention that these reactions produce two regioisomeric products (4-phenylaza-1-cyclohexenes (**A**) and 5-phenylaza-1-cyclohexenes (**B**)). Calculated chemical potentials (μ), Fukui functions (f^+/f^-), total softnesses and softness differences (S, ΔS_A, ΔS_B), NED/IED characters and activation energies (E_a in kcal/mol) for these reactions are given in the following Table. As shown in this Table, the major product of reactions **1-4** and **6** is **A** regioisomer while in reaction **5** the major product is **B** regioisomer. In general, these results indicate that the major product for each reaction (product with the lower softness difference value, ΔS) has the lower value of activation energy. Moreover, most of investigated reactions proceed via IED character.



Reaction	Diene				Dienophile				ΔS_A	ΔS_B	NED/IED	$E_{a(A)}$	$E_{a(B)}$
	μ	S	f^+/f^-	f^+/f^-	μ	S	f^+/f^-	f^+/f^-					
1	-0.168	5.13	0.214	0.164	-0.142	5.41	0.158	0.080	0.23	0.44	IED	17.63	18.54
2	-0.168	5.13	0.214	0.164	-0.136	5.50	0.148	0.069	0.29	0.59	IED	18.13	32.27
3	-0.168	5.13	0.214	0.164	-0.145	5.43	0.155	0.076	0.25	0.47	IED	17.81	18.74
4	-0.168	5.13	0.214	0.164	-0.131	5.65	0.141	0.061	0.34	0.57	IED	17.37	19.07
5	-0.168	5.13	0.167	0.233	-0.174	6.13	0.101	0.046	0.90	0.67	NED	17.36	17.09
6	-0.168	5.13	0.214	0.164	-0.119	5.97	0.127	0.048	0.42	0.67	IED	16.62	19.28
7	-0.168	5.13	0.167	0.233	-0.170	5.85	0.126	0.057	0.76	0.49	NED	17.66	17.76

Figure 1

References:

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A theoretical approach toward structural features and properties of C_{20}, and its complex with $Fe(CO)_4$

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The structural and electronic properties of $C_{20}...Fe(CO)_4$ complex is studied using the hybrid density functional mpw1pw91 theory with the 6-311G (d,p) basis for non metal elements and LANL2DZ for Fe and Fe described by effective core potential (ECP) of Wadt and Hay pseudo potential. The negative nucleus-independent chemical shift (NICS) confirms that $C_{20}...Fe(CO)_4$ cage exhibit aromatic characteristics. On the basis of vibrational analyses, the thermodynamic properties of the title compounds at different temperatures have been calculated. Finally, the UV-vis spectrum and electronic absorption properties was explained and illustrated from the frontier molecular orbitals.

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Theoretical study of structure and properties of tautomers of sila-isoindole

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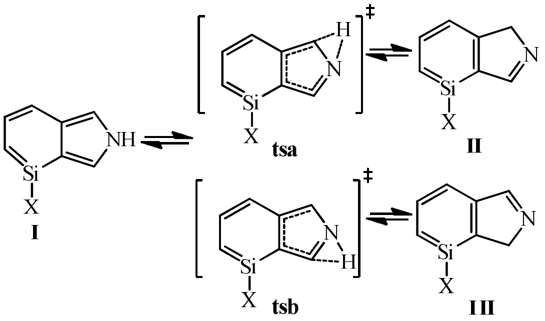
Density functional theory (B3LYP) calculations were performed on the sila-isoindole tautomers and its transition state (Scheme 1). The calculations revealed that sila-isoindole isomers are the less energy rather than sila-1H-isoindole. Aromaticity of rings analyzed in the light of the nucleus-independent chemical shift (NICS). The UV-vis spectra and electronic absorption properties were explained and illustrated from the frontier molecular orbitals. Also, changes in ^{14}N NQR parameters of molecules are studied.



Scheme 1

References:

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Theoretical study of a set of benzenoid hydrocarbons

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In the present investigation, a set of benzenoid hydrocarbons having 6n π-electrons were evaluated by different aromaticity indexes (Figure 1). According to Clar's sextet rule [1], the compounds are considerably stable. The structures of all compounds were optimized at the *B3LYP/6-311+G***level of density functional theory (DFT) and their properties were evaluated by geometrical and magnetic indexes of aromaticity, such as Nucleus-independent chemical shifts (NICS), magnetic susceptibility (χ) and HOMO-LUMO energy gaps at the same level of theory. The study reveals the dependence of aromaticity on the molecular geometry.

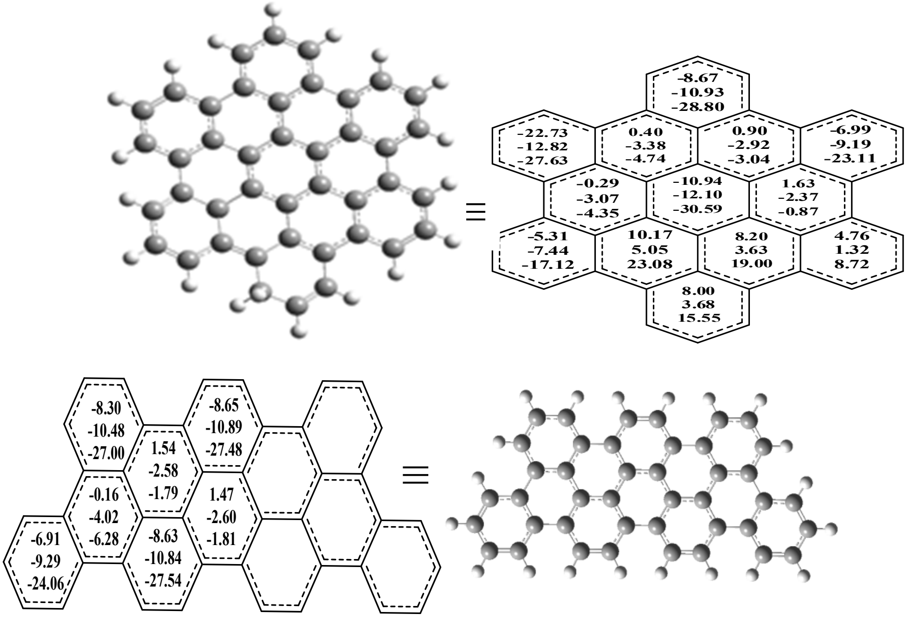

Figure 1. NICS-based indexes calculated inside the rings (in top to bottom order): NICS(0), NICS(1) , NICS(1)zz .

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The triazine-based azo-azomethine dyes; spectroscopy, solvatochromism and biological properties

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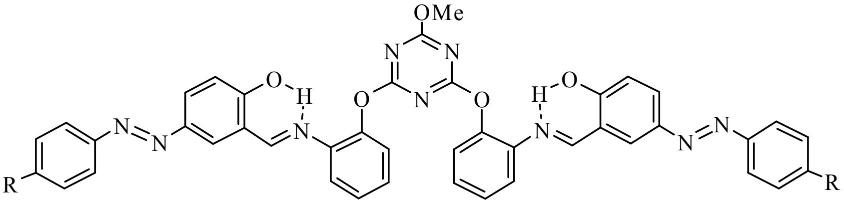
The synthesized compounds were obtained from condensation reactions of azo-azomethine Schiff bases 2-((2-hydroxyphenylimino)methyl)-4-(phenyldiazenyl)phenol and 2,4-Dichloro-6-methoxy-1,3,5-triazine. The solvatochromism of dyes was evaluated in various solvents. The effects of substitution, pH as well as environment temperature on the electronic absorption spectra are also reported. The newly synthesized compounds are explained on a basis of positive solvatochromism behavior of compounds due to intramolecular hydrogen bond in enol–keto tautomeric and dipole moment changes. The nature of substitutions, solvent environment, hydrogen bonds, temperature, pH and dipole moment of the molecules are the key factors in deciding the solvatochromism of azo-azomethine dyes. The synthesized compounds did not exhibit any remarkable antibacterial activity. But, they are having electron donating group showed moderate antioxidant activities.



Scheme 1

References:

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Ab Initio molecular orbital (MO) study and natural bond orbital (NBO) interpretation of the aromatic character of expanded octaphosphacubanes

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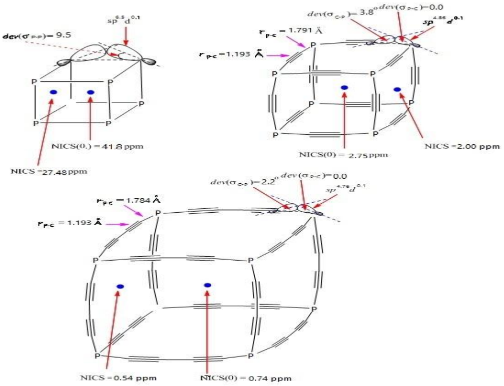
In pericycline macrocyclic structures, the saturated corner atoms are connected by ethynyl linkages [1]. The 'exploded' cubane is as an example of pericyclines in which acetylenic scaffolding is extended in three-dimensional space [2]. In order to estimate the aromatic characters of chemical compounds, we may use nucleus-independent chemical shift (NICS) values [3]. In this work, the structures and aromatic character of three differently sized P/C rings and cages using Phosphorus containing building blocks (compounds 1-3, octaphosphacubane and Phosphapericyclines) are investigated be means of ab initio molecular orbital (MO) study and natural bond orbital (NBO) interpretation.

Ab initio molecular orbital (MO) based method (HF/6-31G*), NBO and NMR interpretations were used to study the correlations between the stabilities, aromatic characters, structural parameters, hybridized orbitals and angle strains of compounds 1-3. The results obtained showed that, contrary to compound 1, compounds 2 and 3 are antiaromatic and the antiaromatic character decreases from compound 1 to compound 3 (see Figure).



Figure

References:

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Aromaticity of a group of aromatic hydrocarbons incorporating the BN moiety

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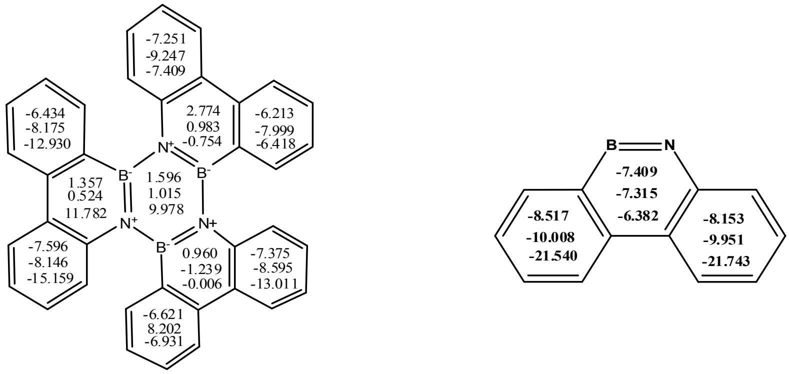
The incorporation of BN moiety at different positions of the PAHs significantly alters the electronic properties of the molecules without great structural perturbation [1]. In this study, the chemistry of a group of BN substituted polycyclic aromatic compounds has been studied at *B3LYP* level of density functional theory (DFT) (**Figure 1**).

All of the structures were optimized at the *B3LYP/6-311+G*** level, and the magnetic susceptibility (χ, *CSGT-B3LYP/6-311+G***), Nucleus-independent chemical shifts (NICS, GIAO-*B*$_3$*LYP/6-311+G***), have been calculated using the *B3LYP* optimized geometries. The study shows that the stability of compounds can change dramatically, depending on the BN substitution in the molecular structures.



1 **2**

Figure 1. NICS aromaticity indexes computed at *B3LYP/6-311+G**,* for a prototype BN-containing PAH(1) in comparison to its substructure(2).The numbers inside the rings are, from top to bottom, NICS(0), NICS(1)and NICS(1)zz.

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DFT study of 1,3-dipolar cycloaddition reactions of pyrazole derivatives

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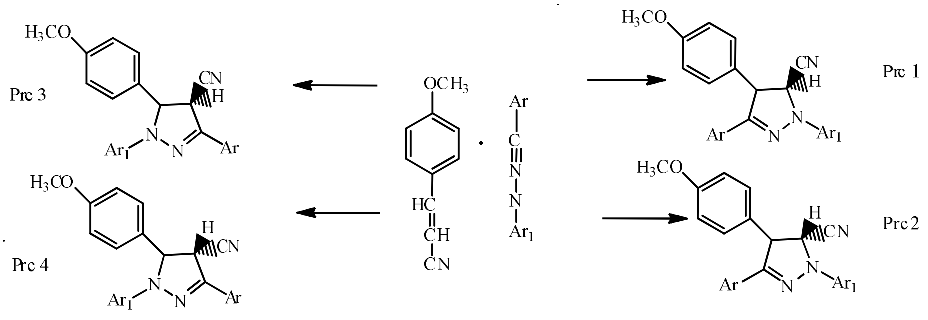
The pyrazoles constitute an interesting class of heterocyclic compounds as important building blocks in organic synthesis and more potent biologically active molecules in pharmaceutical and medicinal chemistry. These compounds have done via 1,3-dipolar cycloaddition reactions of alkenes a with nitrile imines [1-2].

In view of the enormous applications associated with pyrazole systems, here in, as a part of our ongoing theoretical research program in the area of 1,3-dipolar cycloaddition reactions, we report a DFT study on the all possible region-and stereo cycloaddition channels for the syensis of 3,4-diaryl-1-phenyl-4,5-dihydro-1 H-pyrazole-5-carbonitriles derivatives. The comparative analysis will be made on the basis of the relative energies of products and the global and local reactivity indices [3] and FMO analysis. The results of relative energies showed that the energy of compound 4 is more stable then another.

Then, it can be predicted that region isomers will be formed preferentially, in good agreement with the FMO analysis and local electrophilicity indices and Fukui functions.



Scheme 1

References:

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The mechanism investigation of halocycloalkenones as Diels-Alder dienophiles by computational method

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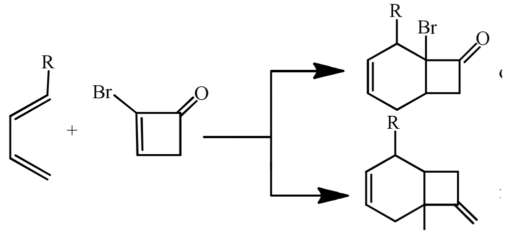
The Diels-Alder reaction serves as a benchmark for efficiency and selectivity for the generation of molecular complexity [1]. Despite the impressive advances in the development of the Diels-Alder reaction, there is a less investigate [4+2] cycloaddition reactions of cyclobutenones [2].

In continues of our research, in this work we have investigated the mechanism of 2-hallocyclobutenone and 1,3-butadiene derivatives DA cycloaddition reaction. The geometrical, energetic properties and electronic indexes were analyzed for the stationary points. Herein, by computational methods we show that 2-halocyclobutenones dienophiles are highly *endo* selective and significantly more reactive than their non hallogenated parent compounds. The potential energy surface estimated for all of channels and the results showed ortho regioisome is more stable than others.

Also, the FMO analysis and DFT-based reactivity indices confirmed the experimental *ortho* regioisomeric pathway [3].



Scheme 1

References:

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Anthracene, phenanthrene and acridine: a computational study

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[b]*Department of Chemistry, School of Sciences, Payame Noor University (PNU), Iran*
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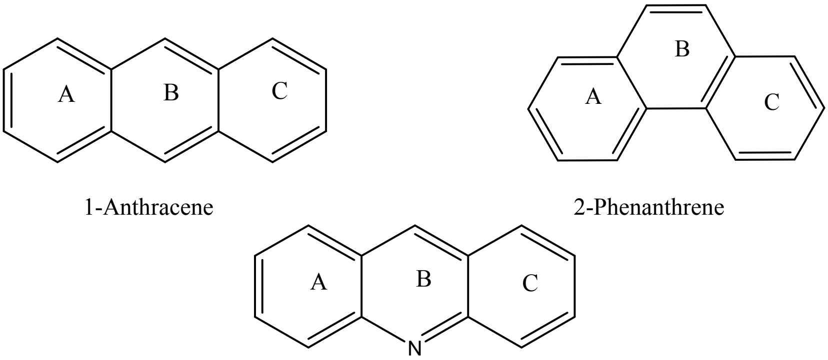
Aromaticity is one of the cornerstones of modern organic chemistry, aromaticity is a manifestation of electron delocalization in closed circuits,either in two or in three dimensions[1–2], The molecular geometries of aromatic rings in (Scheme 1) have been fully optimized and their wave functions have been used to characterize topological properties of the electronic charge density. The AIM 2000 program [3] was used for topological analysis of electron density,the properties derived from topological analysis of electron density at the ring critical point, RCP[4], have been used to model four different aromaticity indices. The intercorrelations between various aromaticity indices and some properties extracted from the RCPs of 9 aromatic rings have been investigated. It was found that individual RCP properties can not be considered as reliable quantitative characteristics of ***π*** electron delocalization in heterocyclic compounds (Scheme 1).



1-Anthracene

2-Phenanthrene

3-Acridine

Scheme 1

References:

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DFT Study on mechanism of Diels-Alder cycloaddition reaction between disymmetrical 2,4-cyclihexadienone derivatives and methyl vinyl ketone

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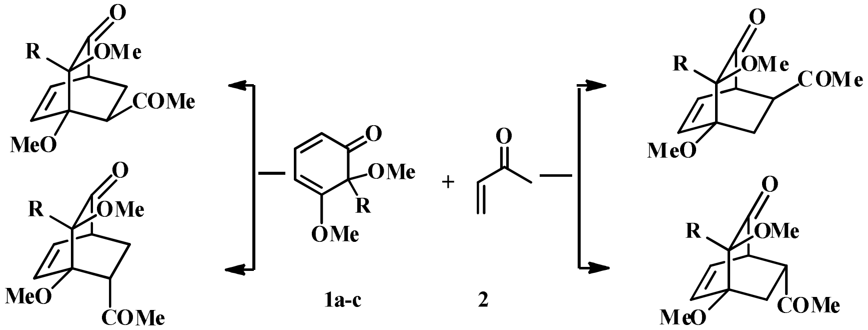
In recent years, several readily accessible plane nonsymmetric cyclopentadienes have been extensively probed for the diastereoselection. Considerable attention has also been focused on unsymmetrical 1,3-cyclohexadienes [1-2].

However, in this research, we report our results on π-facial selectivity in the Deils-Alder reactions of simple dissymmetric 2,4-cyclohexadienones by theoretical method.

The DFT study have done on the Deils-Alder reaction of dissymmetric cyclohexadienones (**1a-c**) and methyl vinyl ketone [3]. The results showed that all dienones displayed complete syn preference, to methyl vinyl ketone.

A theoretical study of the regio and stereoselectivities of the Diels-Alder cycloaddition of 2,4-cyclohexadienones with methyl vinyl ketone is carried out using DFT method. Potential energy surface analysis showed that these Diels–Alder reactions favor the formation of the ortho-endo cycloadduct in all of cases. The analysis of the electronic factors of the reactants explains the behavior of methyl vinyl ketone as strong nucleophile in an Asymmetric Diels–Alder cycloadditions.



Scheme 1

References:

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Theoretical analysis of mechanisms of the hetero Diels-Alder reaction of chromans

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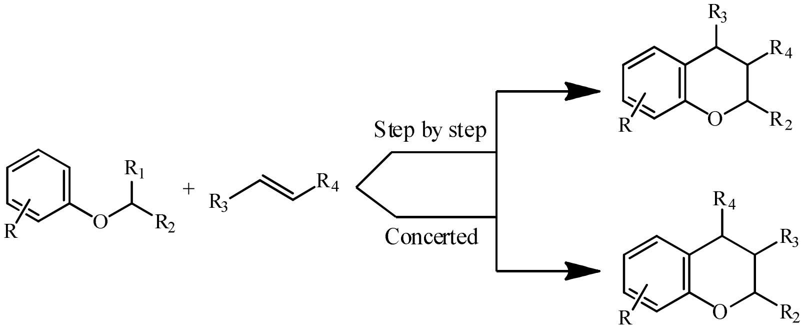
Hetero Diels-Alder reaction and their formal equivalents provide a powerful means the rapid construction of heterocyclic scaffolds. Oxa- and aza-hetero Diels-Alder variants have been developed in which the dienophile and/or dienes can incorporate the heterocomponents [1]. One such aza-variant is the povarov reaction [2-3], originally developed 50 years ago.

Given the considerable utility of the povarov reaction we were interested to establish whether the mechanism of O-aril oxonium species with dienophiles can take place via stepwise or concerted mechanism? The results of calculations revealed that the concerted transition states have higher energy than diradical intermediates by a B3lvyp density functional method. The energy barriers and electronic factors confirmed the step wise mechanism is favorable than concerted mechanism.



Scheme 1

References:

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Aromatic stabilization energies of oxadiazoles and thiadiazoles. A hybrid-density functional theory study

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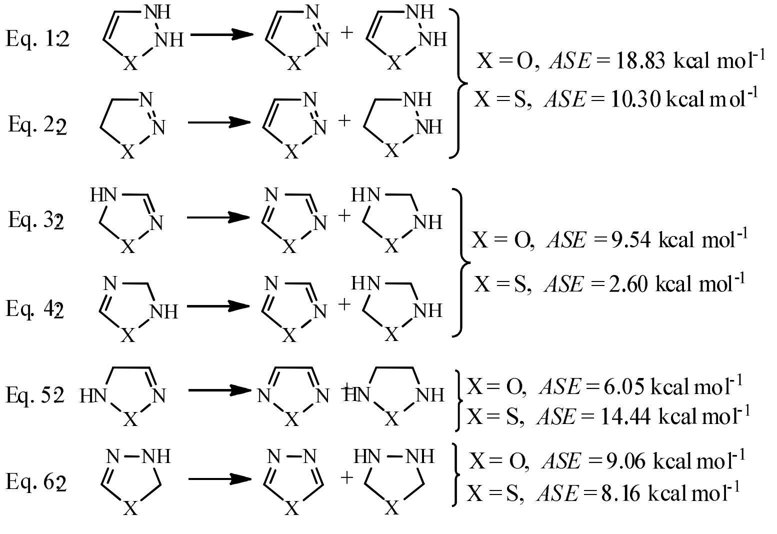
Oxadiazoles and thiadiazole are five-membered heterocyclic aromatic compounds consisting of one oxygen or sulphur atom, two nitrogen and two carbon atoms [1]. In this work, the aromatic stabilization energies (*ASE*) in the various isomers oxadiazoles and thiadiazoles have been investigated by means of B3LYP/6-311+G** level of theory [3]. Similar to the equation argued as a measure of the *ASE* for benzene [3], we also used the homodesmotic and strain-balanced[3]Eqs. (1-6) to evaluate the *ASE* in the the1,2,3-, 1,2,4-, 1,2,5-, 1,3,4-oxadiazole and -thiazole isomers (see Scheme 1). In the isodesmic reactions [Eqs. (1-6)], almost everything except the electron delocalization of the σ- and π-electrons are conserved, and the energy of each reaction would mainly provide the stabilization energy due to the σ-π electron conjugation of the corresponding molecule.Based on Eq. (5) results showed that the *ASE* calculated for the 1,2,5-isomer of thiadiazole is greater than the corresponding value in oxadiazole.



Scheme 1

References:

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(E)-2-(5,5-Dimethylhexahydropyrimidin-2-yl)-4-(phenyldiazenyl)synthesis, X-ray crystallography and density functional theory calculations

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The title compound was prepared via condensation of (E)-5-(2-phenyldiazenyl)-2-hydroxybenzaldehyde and 2,2-dimethylpropane-1,3-diamine in 20 ml EtOH:CHCl3. The mixture solution was stirred and refluxed for 3 h. Colorless prismatic shape crystals were obtained after evaporation of the excess solvent. The structure was solved by direct methods (SHELXSK97 [1] and refined by full-matrix least-squares techniques against F2 (SHELXL-97 [2]. Hexahydropyrimidine has a chair conformation. Intramolecular hydrogen bonds are formed between the phenol hydroxyl groups and the nearest N atom in the hexahydropyimidine groups [O—H···N = 2.584 (2) Å]. The packing of the structure is stabilized by relatively strong N—H···O & N—H···N hydrogen bonds (see Tab. 1), and C—H···π contacts [C—H-cetroid = 2.70 Å] between neighboring molecules. No significant π-π interactions are found in the crystal structure.

In the other part of this work some quantum mechanics study were done on the structure and its geometries were completely optimized. All density functional theory (Becke's hybrid HF-DFT procedure [3] with the Lee-Yang-Parr [4] correlation functional [B3LYP/6-31G(d)]) calculations were done with GAUSSIAN03[5]. To assess the appropriateness of the chosen model chemistry, selected structural parameters calculated by the B3LYP/6-31G(d) procedure for compound 2 are compared with the corresponding experimental data. Agreement is generally very good between X-ray and theoretical data.

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Anomeric effect associated with the electron delocalization, electrostatic model associated with the dipole-dipole interactions and steric effect impacts on the configurational properties of 2,3-dichloro-1,4-dioxane, -oxathiane and –oxaselenane. A hybrid density functional study and natural bond orbital interpretation

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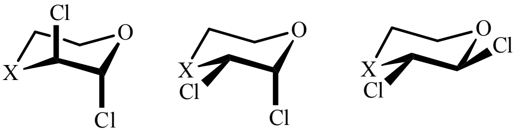
In this work, the impacts of the anomeric effect associated with the electron delocalization, electrostatic model associated with the dipole-dipole interactions and steric hindrances on the configurational properties of 2,3-dichloro-1,4-dioxane(**1**), 2,3-dichloro-1,4-oxathiane(**2**) and 2,3-dichloro-1,4-oxaselenane(**3**) have been investigated using the hybrid-DFT based method (B3LYP/6-31G*) and natural bond orbital(NBO) interpretations (see Scheme) [1,2].



X = O (**1**), S (**2**), Se (**3**)

Scheme 1

Based on the calculated, the decrease of the calculated Gibbs free energy differences between the equatorial-axial and axial-axial configurations [i.e. $\Delta(G_{\mathrm{eq,ax}}\text{-}G_{\mathrm{ax\text{-}ax}})$] from compound 1 to compound 3 can be justified by the decrease of the $AE = AE_{\mathrm{eq\text{-}ax}}\text{-}AE_{\mathrm{ax\text{-}ax}}$ the calculated total dipole moment value differences between the equatorial-axial and axial-axial configurations [i.e. $\Delta(\mu_{\mathrm{eq,ax}}\text{-}\mu_{\mathrm{ax\text{-}ax}})$] increase from compounds **1→3**. the calculated total dipole moment value [i.e. $\Delta(\mu_{\mathrm{eq,ax}}\text{-}\mu_{\mathrm{ax\text{-}ax}})$] increase from compounds **1→3**. Consequently, the rationalization of the conformational preference solely in terms of the electrostatic model associated with the dipole-dipole interactions fails to account for compounds **1-3**.

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More sustainable synthesis of diphenylsulfone derivatives catalyzed by Pd(II) in deep eutectic solvent

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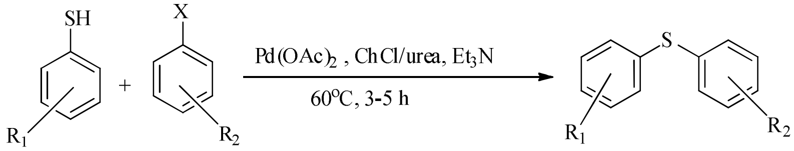
Thiol containing organic compounds play important roles in biological processes due to properties of the thiol function. They found various applications as enzyme inhibitors, biological active calcium antagonist; and abnormal level of these species culminate in certain diseases [1]. Deep Eutectic Solvents (DESs) have many eligible solvent properties compared to common organic solvents. In fact, they have physiochemical properties of room temperature ionic liquids (RTILs) [2]. In recent years, many reports are published for Heck-Suzuki coupling reaction for synthesis of phenyl containing molecules [3].

In this study, we report an efficient protocol for synthesis of diphenylsulfone derivatives catalyzed by Pd (II) in deep euthectic solvent (Scheme1). Green reaction media, short reaction time, high efficient are characteristic of this protocol. Ultimately, formation and purity of aimed diphenylsulfone derivatives confirmed by ^{1}H-NMR, ^{13}C-NMR, IR and MS spectroscopy.



Scheme 1

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Synthesis of multi-substituted imidazoles *via* multi components condensation promoted by MCM-41-nPr-$NHSO_3H$

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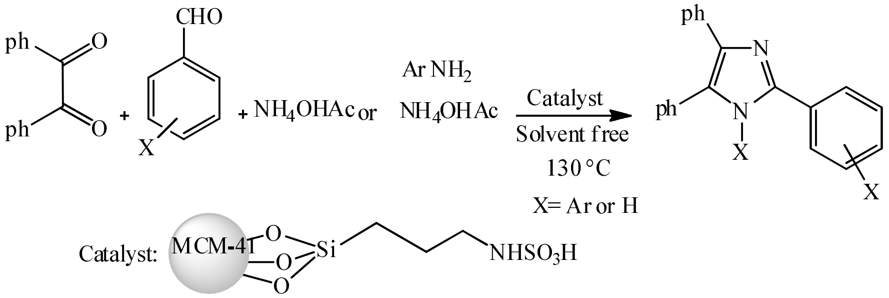
The application of silica and silica-based materials to life-science technologies is attracting attention from numerous research fields, including biotechnology, and nanomaterial science. Imidazoles are a class of heterocyclic compounds that contain nitrogen and are currently under intensive focus due to their wide range of applications, because they have many pharmacological properties and play important roles in biochemical processes [1,2]. Owing to the wide range of pharmacological and biological activities, the synthesis of imidazoles has become an important target in the resent years. In continuation of our investigation into the application of solid acids in organic synthesis [3,4]. Herein we describe the preparation of a new heterogenised catalyst by functionalising MCM-41 with 3-aminopropyltriethoxysilane and subsequent immobilization of sulfonic acid group on the synthesized MCM-41-$(CH_2)_3NH_2$. Resulting MCM-41-nPr-$NHSO_3H$ was applied as a new heterogeneous catalyst for the one-pot synthesis of multisubstituted imidazoles by combination of a vaiety of aldehydes, benzil, and ammonium acetate or primary amines/ammonium acetate under solvent-free conditions at 130 °C (Scheme1).



Scheme1

References:

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First report on graphene quantum dots as novel and highly efficient nonmaterials for removal of Celestine Bluedye under visible light

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The industrial wastewater usually contains a variety of hazardous compounds and toxic substances, and water pollution has become a serious environmental problem facing humans. Dyes are an abundant class of colored organic compounds that represent and increasing environmental danger. The release of those colored wastewaters in the environment is a considerable source of nonesthetic pollution and eutrophication and can originate dangerous byproducts through oxidation, hydrolysis or other chemical reactions taking place in the wastewater phase [1]. Synthetic dyes are toxic refractory chemicals that can generate intensive color and are hazardous to the environment. Most dyes are resistant to biodegradation and direct photolysis [2]. In recent decades, heterogeneous photocatalytic detoxification of environmental pollutants such as water and wastewater contaminants has become a popular technique. Photocatalysis technology can lead to the complete degradation of various organic, inorganic and biologically hazardous compounds [3–5].

In this paper, a novel and efficient method for decolorization of Celestine Blue (CB) dye based on the synthesized graphene quantum dot (GQD) was reported. Preparation of GQD was carried out by pyrolyzing method. Decolorization ability of the prepared GQD samples were investigated for removal of organic dye (i.e., CB) as model molecule. Effect of the experimental parameters such as pH of dye solution, contacting time, concentration of CB dye and amount of GQD on the decolorization efficiency of GQD were studied. Finally, the kinetic model for decolorization of CB in the presence of GQD was fitted and discussed.

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Application of organic surfactants for hydrolysis of cellulose in bioethanol production process

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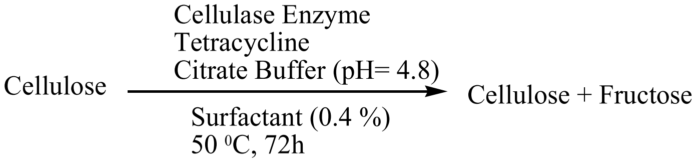
According to limitations of fossil fuel resources, the green fuel application of plant resources is considered. Bioethanol which is a suitable fuel resource is produced from the plant wastes such as sugarcane, beet, cotton, etc. The most important step in bioethanol production is the conversion of cellulose to monosaccharide and reducible sugars like glucose and fructose which is performed via enzymatic reaction in the presence of different additives [1-4].

In this research, different organic surfactants (Dulaplex, Etyleneglycol, Polyethyleneglycol and Tween-20) are used and compared for increasing the yield of cellulose conversion of sugarcane bagasse [5-6]. The reaction is performed in pH=4.8 (citrate buffer) at alkaline pretreatment in 50°C for 72h. The produced sugar in the presence of Teween-20 is about 3.5 times higher than in the case of surfactant absence. The Dulaplex, Etyleneglycol, Polyethyleneglycol have increased the reaction yield 0.98, 1.98 and 1.65 times respectively.



$$\text{Cellulose} \xrightarrow[\substack{\text{Surfactant (0.4 \%)} \\ 50\ ^0\text{C, 72h}}]{\substack{\text{Cellulase Enzyme} \\ \text{Tetracycline} \\ \text{Citrate Buffer (pH= 4.8)}}} \text{Cellulose + Fructose}$$

Scheme 1

References:

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An efficient and green procedure for the synthesis of 2-aryl benzimidazoles

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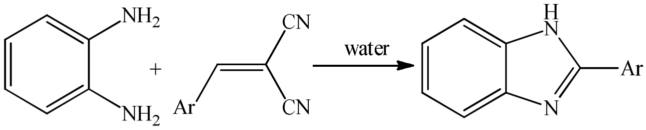
In recent years considerable attentions have been given carry out organic reactions under aqueous media, particularly from the view point of green chemistry. Due to using water, in contrast to common organic solvent offers many advantages, such as simplicity of reaction conditions, ease of work-up and product isolation, increasing the selectivity of a wide variety of organic reactions and accelerating reaction rates [1].

Benzimidazoles are important scaffolds in medicinal chemistry due to their biological and pharmacological activities [2]. Two general approaches have been used for the synthesis of 2-substituted benzimidazoles. One of them, is the condensation of 1,2-phenylenediamines with carboxylic acids or their derivatives such as acid chlorides, nitriles, imidates and orthoesters under strong acidic conditions at high temperature. Another route is the oxidative cyclodehydrogenation of 1,2-phenylenediamine and aldehydes in the presence of different oxidants [3-4].

Accordingly, in order to further development of synthetic protocol of benzimidazoles, herein we have devoted our effort towards the development of an efficient method for the synthesis of 2-aryl benzimidazole derivatives through reaction of 1,2-phenylenediamines and arylidene malononitriles under catalyst-free condition in water as green solvent.



Scheme 1

References:

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Characterization, physical, electrochemical properties of 1-(-2-Hydroxyethyl)-3-methylimidazolium dicyanamide [C_2OHMim] [DCA]

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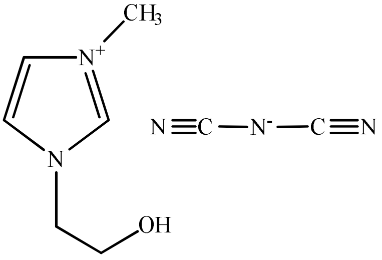
In this research, Characterization and physical and electrochemical properties of a novel task specific Ionic Liquids (TSILs) was investigated. In survey on the literature [1-3], no report was found about temperature dependence of some volumetric, thermal and transpose properties especially in a wide range of 0 to 100 °C 1-(-2-Hydroxyethyl)-3-methylimidazolium dicyanamide [C_2OHMim] [DCA] was carried out.

Several properties including viscosities, thermal stability, surface tension, refractive index, pH and density were investigated as function of temperature.The electrochemical stability of ionic liquids, as electrolytes for voltammetric aspects, was studied at platinium electrode.

Besides characterization of the studied TSIL was studied by using ^{1}HNMR, IR, Mass, TGA, DSC and elemental analysis. The results revealed a wide voltage range of the electrochemical window. This wide window allows studies on compounds such as organosulfur compounds especially mercaptans and hydrogen sulfide.



TSIL1
Scheme 1

References:

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Green chemistry tools to influence a characterization azacrown compound and research chemistry based organization

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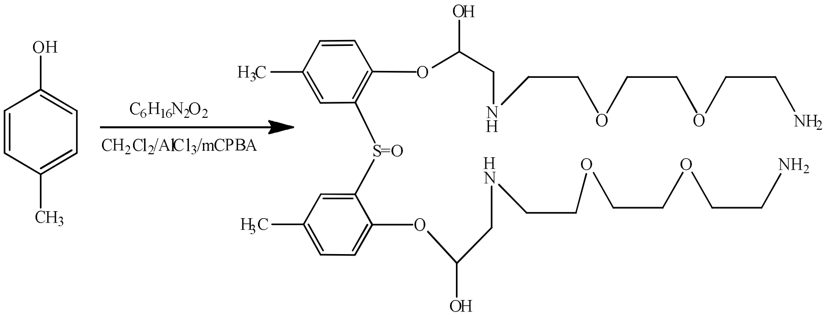
Green chemistry is difussing throughout the chemical industry, and icludes use and development of new substances and processes that impact other sectors such as agricultuer, healthcare, energy, electronic, and azacrown compound. The role green chemistry is intimately related to broad emerging trend in policy [1-2].

For this reason perpose sulfoxid was prepared by reaction of p-cresol and thionylcholoride and dicholoromethane as solvent then compound react with allyl bromide give bisallyl and bisallyl oxidized with mCPBA give bisepoxide at last compound with diamine (diethyleneteriamine) reaction give azacrown compound. The main products were identified by spectral such studies such as C NMR, H NMR and spot test.



Scheme 1

References:

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An efficient one-pot, four-component synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-diones

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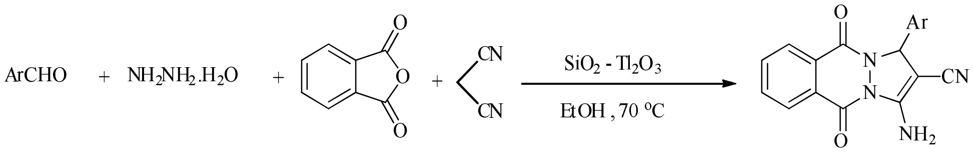
Multicomponent reactions (MCRs) have been proven to be a very elegant and rapid way to access organic compounds in a single synthetic operation. These reactions are characterized by their convergence, ease of execution, high yields, efficiency, and atom economy [1]. 1H-pyrazolo[1,2-b]phthalazine-5,10-diones are one of the interesting clean of organic compounds and the developing of new MCRs for their synthesis under mild reaction conditions is currently interest. These compounds have been widely used as medicinal intermediates because of their useful biological and pharmacological properties [2-3].

In view of these properties and in continuation of our research program on the synthesis of organic compounds [4], we report herein a green approach for the synthesis of 1H pyrazolo[1,2-b]phthalazine-5,10-diones by the reaction of aromatic aldehyde, hydrazine monohydrate, phthalic anhydride, and malononitrile in the presence of the catalytic amount of silica Tl_2O_3 in ethanol at 70 °C (Scheme 1).



Scheme 1

References:

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Synthesis of benzothiazoles using nano silica phosphoric acid as an efficient catalyst under solvent-free conditions

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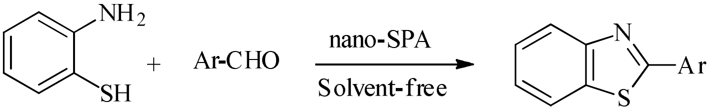
Benzothiazole and their derivatives are often found in heterocyclic compounds, which exhibit a variety of biological activities, such as a cathepsin S inhibitoran HIV reverse transcriptase inhibitor an anticancer agent and anorexin-1 receptor antagonist .They can also be used in industry as antioxidants, vulcanization accelerators, and as a dopant in light-emitting organic electroluminescent devices [1]. Numerous synthetic methods are available for the preparation of 2-arylbenzothiazole. The most important ones include the reaction of *o*-aminothiophenole with aromatic aldyhydes in a wide set of conditions [2]. In recent years, more attention has been directed toward the application of solid acids in organic synthesis because such reagents not only simplify purification processes but they also help prevent release of reaction residues into the environment [3].

Nano silica phosphoric acid (nano-SPA) as an efficient and eco-friendly catalyst was prepared by the reaction of nano silica chloride (nano-SC) with dry phosphoric acid. [4].Herein, an efficient and simple protocol has been developed for the synthesis of benzothiazole derivatives from the reaction of aromatic aldehydes with *o*-aminothiophenole in the presence of catalytic amounts of nano-silica phosphoric acid under solvent-free conditions (Scheme 1). Short reaction times, simple work-up procedure, high yields, easy availability and use of an eco-friendly catalyst are some of the striking features of the present protocol. Final products were characterized by FT-IR, ^{1}H NMR and comparison of their physical properties with those reported in the literature.



Scheme 1

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A versatile, efficient and regioselective synthesis of *β*-nitratohydrines using cross-linked poly (4-vinylpyridine) supported nitric acid under solvent-free conditions

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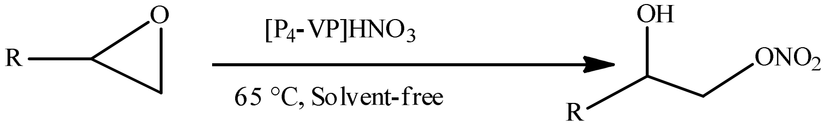
Ring-opening reactions of epoxides have extensively been studied with a large number of nucleophiles. However, there are few applications of thenitrate ion as the nucleophile for these reactions [1-3]. *β*-Nitratoalcohols have been previously prepared from epoxides by treatment with concentratedHNO$_3$ [1], CAN [2], or NO in air [3]. However, thefirst method suffered from low yields and strongly acidic conditions, the reaction of CAN with epoxides was generallycarried out at high temperatures (80 °C) and with styrene oxide and the reaction afforded benzaldehyde as the major product. The reactionof NO with epoxides [3] was found to requirelong reaction times (12–32 h).

In continuation of our work [4,5], on the development of useful synthetic methodologies, we have found that poly (4-vinylpyridine) supported nitric acid can be utilized efficiently for the ring opening of epoxides to form the corresponding *β*-nitratoalcohols (Scheme 1).



Scheme 1

The advantages of this method over conventional classical methods are mild reaction conditions, safe handling, rapid, and very simple work-up.

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A rapid and high efficient microwave promoted multicomponent domino reaction for the synthesis of spirooxindole derivatives

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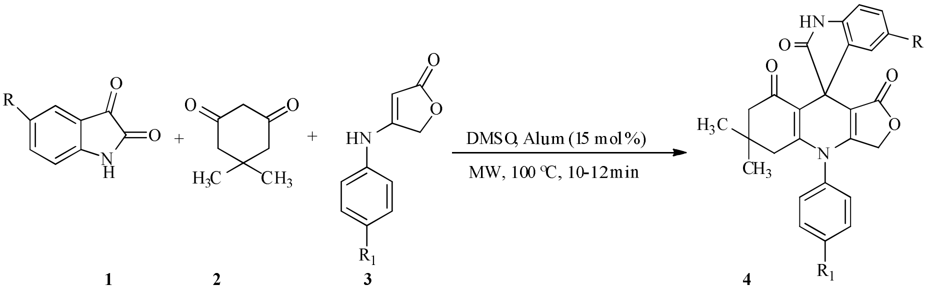
The development of efficient formation of multifunctionalized complex products such as natural products and analogs, drugs, diagnostics and etc. by using simple reactants has been an important issue in organic synthesis [1]. In this regard, multi-component domino reactions have become increasingly attractive and the best tools in modern organic synthesis and medicinal chemistry, because of their green characteristics of atom-economy, bond-forming economy, and structural economy [2]. The use of microwaves as a valuable and powerful technology has become a major motivation for both industry and academia. Replacing the oil bath with a microwave reactor, opens a new window to perform reactions in dramatically shortened time as well as increasing yields and the involved reactions are often very cleaner [3]. Oxindole derivatives for decades have drown great attention because these compounds are characterized by extensive applications in biology and pharmacology as well as the presence of this framework in a number of natural products [4, 5].

In this research, we report herein a simple, efficient and high speed method for the preparation of spirooxindoles through domino one-pot and multicomponent condensation reactions of isatins, dimedone, and anilinolactones using Alum as an inexpensive, nontoxic, and available Lewis acid catalyst under microwave irradiation (Scheme 1)



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

Scheme 1

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One-pot facile synthesis of stabilized phosphorus ylides via multicomponent reactions

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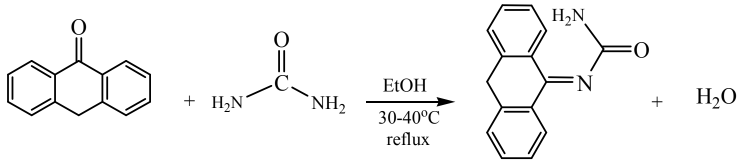
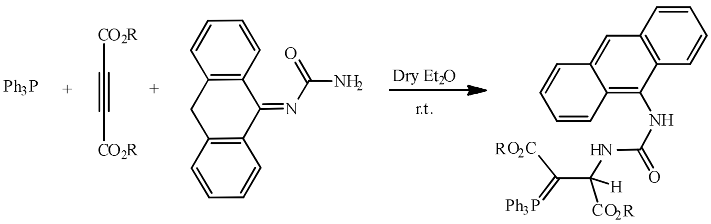
Organophosphorus compounds have many applications in variety of industrial, biological, pharmacological activities and chemical synthetic uses [1]. Among them, phosphorus ylides are reactive intermediates which have been used in many synthesis of natural products and compounds of biological and medicinal properties [2-3].

We have described a simple and efficient one-pot three-component reaction between triphenylphosphine (TPP), dialkyl acetylenedicarboxylates (DAAD) in the presence of NH-acid which has been prepared from a reaction between Urea and Anthrone (Scheme 1), to produce high stabilized phosphorus ylides in excellent yield at ambient temperature (Scheme 2).



Scheme 1

The reactions take place easily by the Michael addition of TPP to DAAD and concomitant protonation of the intermediate by NH-acid leads to the salts which are unstable intermediates and undergo a subsequent Michael addition leads to stabilized phosphorus ylides. Comparison of UV spectra of the initial compounds and ylides make confirmed conjugated circles and anthracene pattern.



Scheme 2

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Green and facile approach towards the one-pot organocatalyzed multicomponent synthesis of 2-amino-5,6,7,8 tetrahydrospirooxindole-3-carbonitrile derivatives

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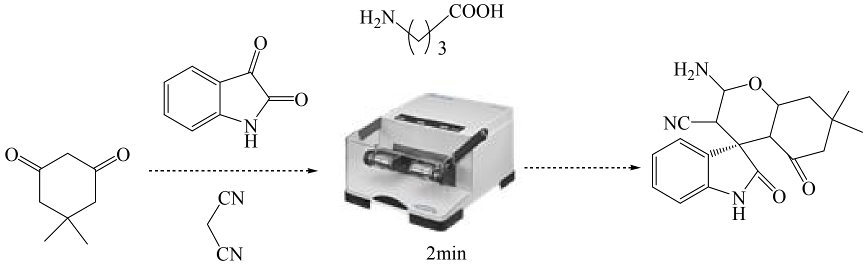
Polyfunctionalized heterocyclic compounds play important roles in the drug discovery process. Among these heterocycles, compounds carrying the indole moiety exhibit antibacterial and antifungal activities and spirooxindoles nucleus consequently increase these properties. The heterocyclic spirooxindole ring system is a widely distributed structural framework that is present in a number of pharmaceuticals and natural products including cytostatic alkaloids like spirotryprostatins and strychnophylline. The unique structural array and the highly pronounced pharmacological activity displayed by this class of spirooxindole compounds have made them attractive synthetic targets.

Considering the recent reports, and as a continuation of our work studying the synthesis of heterocyclic compounds, we are currently investigating the use of □-amino butyric acid (GABA) as bifunctional organocatalyst for the synthesis of various 2-amino-5,6,7,8 tetrahydrospirooxindole-3-carbonitrile. This reaction proceeds *via* a facile one-pot three-component condensation reaction of isatin, active methylene compounds and 1,3-diketones under solvent-free conditions at ambient temperature using ball milling technique to afford desired products in high yields, short time and ease of handling.



Scheme 1

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Ultrasound-promoted synthesis of phthalazinone catalysed by heterogeneous sulfonic acid functionalized MCM-41

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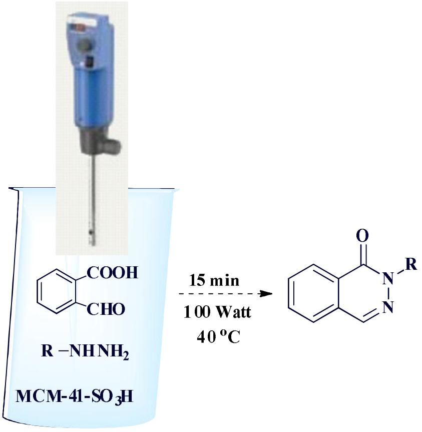
Iran University of Science and Technology, Tehran 16846-13114, Iran. E-mail: shjavan@iust.ac.ir

Phthalazinones constitute an interesting family of bioactive N-heterocycles. Due to their diverse pharmacological activities, selected derivatives are used in the treatment of asthma, diabetes, hepatitis B, arrhythmia, and vascular hypertension. There is a continuing interest in the development of novel synthetic methodologies for the preparation of phthalazinones. Despite these advances, there is still a need for original methodologies that avoid strongly basic or acidic reaction conditions and allow for an efficient assembly of the phthalazinone core from readily available starting materials [1-2].

Ultrasonic-assisted organic synthesis has been considered a powerful technique to accelerate reactions using a green chemistry approach, since it affords maximum yield by minimizing the amount of waste by-products [3]. Although this technique has been employed in many organic reactions, this is the first ever attempt to synthesize Phthalazinones under ultrasonic irradiation.

Hence, a green method for the synthesis of different phthalazinone derivatives has been described by the reaction of phthalaldehydic acid and various hydrazine derivatives in the presence of catalytic amounts of MCM-41-SO_3H nanoparticle in ethanol under ultrasonic irradiation.



Scheme 1

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Facile synthesis of 1,2-diacetates catalyzed by ZnO under reflux condition

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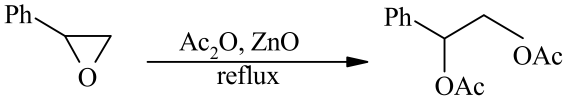
1,2-Diacetates are valuable synthones and being extensively used as key intermediates in the synthesis of various biologically active natural and synthetic products[1]. The easiest and straight forward approach for their synthesis involves the ring opening of epoxides with appropriate nucleophile under acidic or basic conditions [2].

ZnO Is inexpensive, efficient, readily available, and mild catalyst, which has surface properties, and suggests very rich organic chemistry. The surface of ZnO exhibits both Lewis acid and base characters, and it is excellent adsorbent for a wide variety of organic compounds and it also increase the reactivity of the reactants [3-4].

Herein, we have described an efficient, simple and convenient protocol for the ring opening of certain epoxides using ZnO as a catalytic system. In addition to its efficiency, simplicity and mild reaction conditions, this procedure provides high yields of 1,2-diacetates in short reaction times with high selectivity(Scheme 1).



Scheme 1

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1,3-Dihalo-5,5-dimethylhydantoin as a new reagent for the synthesis of alkyl halides

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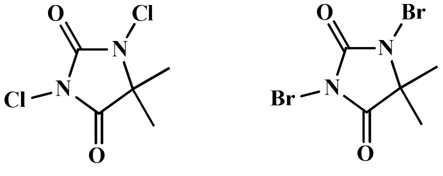
1,3-Dihalohydantoin is an *N*-halo reagent which has found wide spread applications in industrial processes due to its economic advantages [1]. The transformation of alcohols into the corresponding alkyl halides is one of the most studied reactions in organic synthesis, and many reagents can be usually used [2].

In this work, 1,3-dichloro and 1,3-dibromo-5,5-dimethylhydantoin have been introduced for the preparation of alkyl halides. The reaction proceeded in the presence of triphenylphosphine (PPh_3). Therefore a variety of alkyl halides have been prepared *via* reaction of triphenylphosphine and 1, 3-dihalo-5,5-dimethylhydantoin with alcohols at room temperature under mild conditions (Scheme 1).

$$\mathbf{RCH_2OH \xrightarrow[\text{Solvent/r.t}]{\text{DCDMH or DBDMH/PPh}_3} RCH_2X}$$

R=Aryl,Alkyl
X=Br, Cl



DCDMH **DBDMH**

Scheme 1

References:

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Synthesis of some [1,2-b] pyrrole derivatives by using Ba(ClO$_4$)$_2$ as a catalyst

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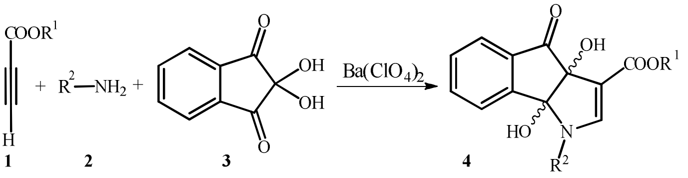
Pyrroles important classes of compounds with many medicinal activities [1-2]. For these reasons, many ways for the synthesis of substituted pyrroles are known [3]. In research prompted by our interest in multiple component reactions and as part of programmers in the area of heterocyclic compounds containing nitrogen [4]. and due to the resultant pharmacological interest in compounds which belong to the Polyhydroxylated alkaloids, Although this reaction done previously in other conditions, [5].

But, herein we report in free solvent, one pot reaction, with high yields ,easy separation of product and three-component method for the construction of some new tetrahydrodihydroxy-oxoindeno[1,2-b] pyrroles ,via condensation of amines, alkyl propiolates and ninhydrin by using Ba(ClO4)$_2$ as a catalyst.



Scheme 1

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Solvent-free improved protocol for synthesis of modified chitosan

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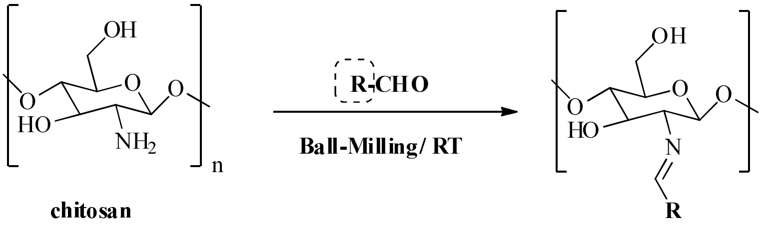
Among those nitrogen-containing compounds, imines or secondary amines are of particular importance. Imines are important intermediates that widely used in the manufacturing of pharmaceuticals, dyestuffs, synthetic rubbers, herbicides, insecticides and agrochemicals [1]. They are common ligands in coordination chemistry. For example, the condensation of salicylaldehyde and chitosan in presence of different solvents give families of imine-containing chelating compounds [2].

Herein, we present for the first time the effective condensation of aldehydes and chitosan in ball mill. So, a mixture of an aldehyde (1 mmol) and chitosan (0.1 g) was milled vigorously at 27-28 Hz, under ambient condition. The corresponding imines were obtained in good yields after 1 h (Scheme 1).

We believe that the present method can serve also for imination of other polysaccharides. Further reactions are under consideration.



Scheme 1

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One-pot synthesis of 2-arylpyrrolo[2,3,4-*kl*]acridine-1(2*H*)-one derivatives using *N*-halo catalysts

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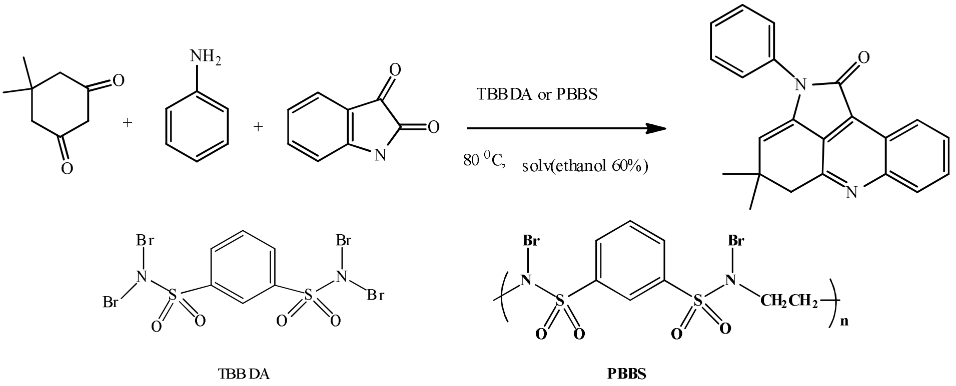
2-Arylpyrrolo[2,3,4-*kl*]acridine-1(2*H*)-one derivatives are an important class of fused heterocycle that display a wide spectrum of such as anthelmintic, antifungal, biological, and medicinal properties. Some of these compounds inhibit the growth of cancerous cells *via* binding to DNA, whereupon they offer potential lead frameworks for developing novel anticancer drugs [1].

One-pot three-copmonent condensation of dimedonewith aniline and isatin, using solvent conditions in the peresence of a catalyst such as TBBDA or PBBS[2-3] provides high yields of the 2-arylpyrrolo[2,3,4-*kl*]acridine-1(2*H*)-one derivatives (Scheme1).



Scheme 1

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Synthesis of tryptanthrin derivatives using DABCO as an efficient reusable catalyst

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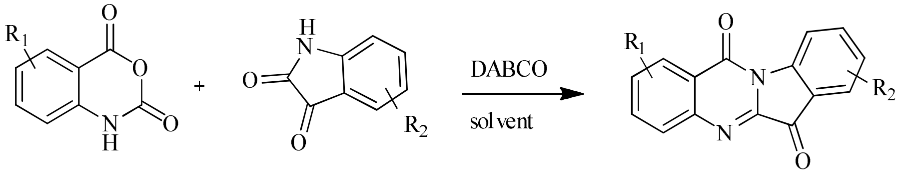
Tryptanthrin is a natural product, which shows significant biological activity such as antibacterial [1], antiparasitic [2], and antineoplastic [3] properties. The most common approach for the synthesis of these compounds involves the condensation of isatoic anhydride and isatin to give tryptanthrin in moderate to high yields. The driving force for this reaction is the development of carbon dioxide and water. Some catalysts such as triethylamine, morpholine, oxone and sodium hydride were used for this transformation [4]. 1,4-Diazabicyclo[2.2.2] octane (DABCO), a cage-like compound, is an inexpensive, eco-friendly, high reactive and non-toxic base catalyst that were used for various organic transformations [5].

As part of our research program to develop selective, efficientand green methods and catalysts in organic synthesis [6], we report here the application of DABCO, as a novel recyclable catalyst, for the synthesis of tryptanthrin derivatives (Scheme 1).



Scheme 1

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The synthesis of substituted imidazoles by using functionalized ferrate(ш) catalyst under green chemistry conditions

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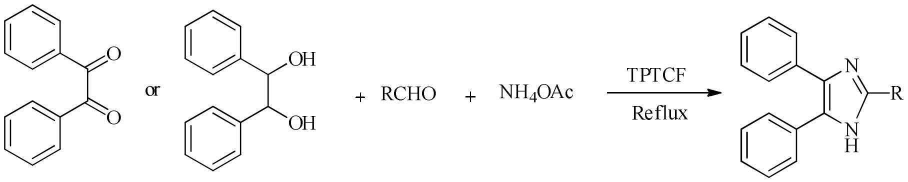
Recently, the design and applications of new methods in organic synthesis based on the multicomponent reactions (MCRs) is attracted researchers of academy and industry. Because, they allow the assembly of complex molecules in one-pot and show a facile execution, high atom-economy, high selectivity, high yields and are fundamentally different from two-component and stepwise reactions [1].

Imidazoles are very useful building blocks for the development of molecules that are important in medicinal chemistry. Substituted imidazole derivatives have found applications as diverse biologic activities such as angiotensin inhibitors, anti-inflammatory, glucagon antagonist, antiviral, antimicrobial, fungicidal and high cytotoxicity, which has indicated them as new candidates in cancer therapy [2,3].

In continuation of our interest in the application of new catalysts in organic synthesis via MCRs [4,5], herein, an efficient and highly selective synthesis of highly substituted imidazoles has been developed by the condensation of benzil or benzoin with various substituted aldehydes and ammonium acetate by using tetraphenylphosphonium tetrachloroferrate (TPTCF) as a catalyst in refluxing ethanol under mild reaction conditions in excellent yields.



Scheme 1

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Three component reaction between arylidenemalononitrile and carbon disulfide in the presence of CH-acids

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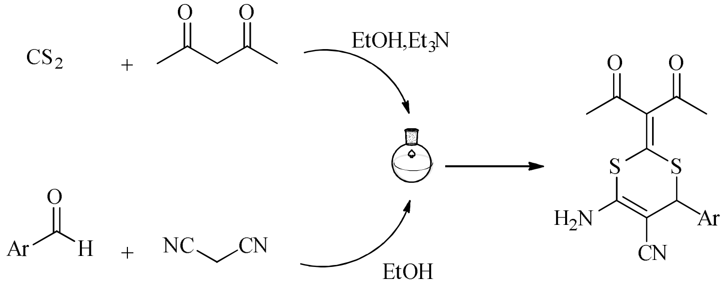
A multi-component reaction (MCR) is a process in which three or more easily accessible components are combined together to produce a final product displaying features of all inputs and thus offers greater possibilities for molecular diversity per step with a minimum of synthetic time [1].

In spite of the significant useful attributes of MCRs for modern organic chemistry and their suitability for building up large compound libraries these reactions were of limited interest in the past fifty years. However, in the last decade, with the introduction of high-throughput biological screening, the importance of MCRs for drug discovery has been recognized and considerable efforts from both academic and industrial researchers have been focussed especially on the design and development of multi-component procedures for the generation of libraries of heterocyclic compounds. This growing interest is stimulated by the significant therapeutic [2-3].

This investigation we report an efficient synthesis of 6--amino-2-(2,4dioxopentan-3-ylidene)-4- phenyl-4H-1,3-dithiine-5-carbonitrile derivatives by reaction of arylidenemalono-nitrile and variety of active methylene compounds in the presence of carbon disulfide proceeded smoothly in EtOH at room temperature and completed within 12 h (Scheme 1). The 1H NMR, 13C NMR and FT IR spectra confirm the structure of compound.



Scheme 1

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One-pot synthesis of novel pyrrolo[1,2-*a*]quinoxaline-4(5*H*)-ones and pyrrolo[1,2-*a*]pyrazines using o-phenylenediamine/ethylenediamine, acetylenic esters and nitrostyrene derivatives

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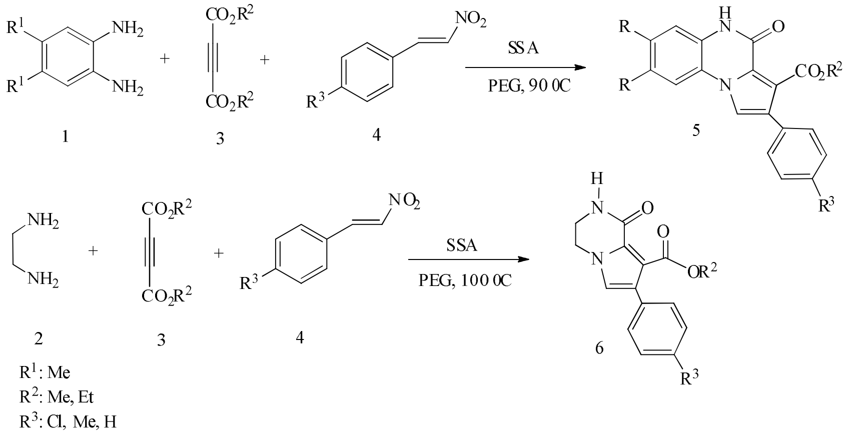
Up to now, MCR is one of the most interesting subclasses of modern chemistry and a vital tool for the preparation of multifunctional molecules from simple materials [1]. Due to the importance of pyrroles as pharmaceuticals, agrochemicals and in biological processes, an extensive amount of research has been conducted toward their synthesis [2]. In recent years, pharmacological evaluation and structure-activity relationships of some of pyrrolo[1,2-a]pyrazines [3-4] and pyrroloquinoxalines [5] have been reported.

Herein, we report a simple and convenient process for the one-pot synthesis of title compoundes. The reaction of *o*-phenylenediamines **1**/ethylendiamine **2**, acetylenic esters **3** and □-nitrostyrenes **4** derivatives in the presence of silica sulfuric acid (SSA) leads to the corresponding functionalized pyrrolo[1,2-*a*]quinoxalines **5** or pyrrolo[1,2-*a*]pyrazines **6** in good yields (Scheme1).



Scheme 1

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Three component synthesis of 3-aminoalkylindoles using Iron(Ш) phosphate

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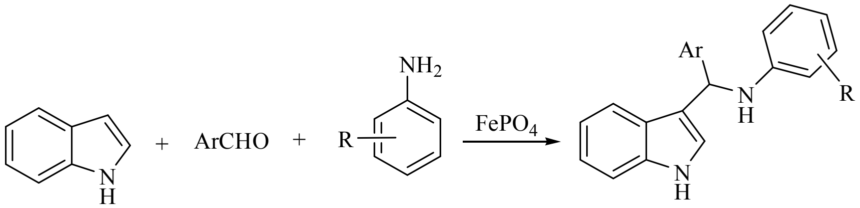
Multi component reactions (MCRs) are of increasing importance in organic and medicinal chemistry[1], as they offer important advantages over conventional linear-type synthesis such as high atom economy, low cost, reduction in overall reaction time and operational simplicity[2].The immense potential of indole nucleus as drug candidates prompted among the synthetic chemists to explore different methods suitable for the synthesis of 3-substituted indoles [1].They have a variety of biological activities such as antibacterial, anticonvulsant and anti hypertension activity antiviral [2].

There are only a few methods for the synthesis of 3-aminoalkylated indoles which have been found in various natural products. Recently, a one-pot method was developed for the synthesis of 3-aminoalkylated indoles by the reaction of aldehyde; amine and indole .The reaction requires a long reaction time, high temperature and is generally accompanied by formation of bis-indolyl compounds. Thus, there is still need for the development of an efficient method for the synthesis of 3-aminoalkylated indoles.[2]

In this regards, iron (Ш) phosphate has been synthesized and new applications of this catalyst explored. Therefore a variety of 3-aminoalkylated indoles have been prepared via combination of aromatic and aliphatic aldehydes, anilines and indole in the presence of a catalytic amounts iron (Ш) phosphate. (Scheme1).



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Synthesis of four membered cyclic ketene dithioacetals

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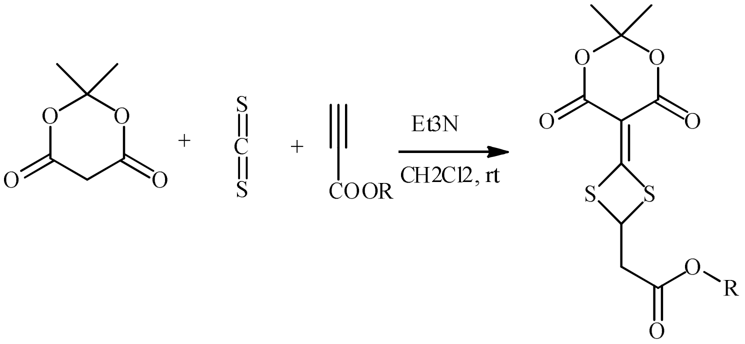
Since the reports by kelber et al., Ketene dithioacetals have received considerable attention as organic synthetic intermediates for the synthesis of a wide variety of aromatic and heterocyclic compounds [1-2]. Ketene dithioacetals, which consist of push-pull ethylene systems with one or two electron-withdrawing groups at the α-carbon and two electron donating groups and also a good leaving groups (alkylsulfanyl) at the β-carbon atom. Consequently alkylsulfanyl groups can be substituted sequentially by a variety of nucleophiles. These compounds have been considered to be highly versatile starting materials for the preparation of several aromatic and heterocyclic compounds, such as pyridines, pyrimidines, thiophenes, pyrazoles [3-4].

A general method for the synthesis of functionalized ketene dithioacetals involves the condensation of an active methylene compound with carbon disulfide in the presence of a suitable base followed by alkylation. In this investigation we report an efficient synthesis of novel ketene dithioacetals by the reaction of active methylene compounds and carbon disulfide in the presence of propiolate derivatives based on double Michael addition reaction. The FT-IR, ^{1}H-NMR, ^{13}CNMR spectra confirms the structure of products.



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Enantioselective synthesis of modafinil drug using titanium catalyst and chiral dioles of tartaric acid derivatives

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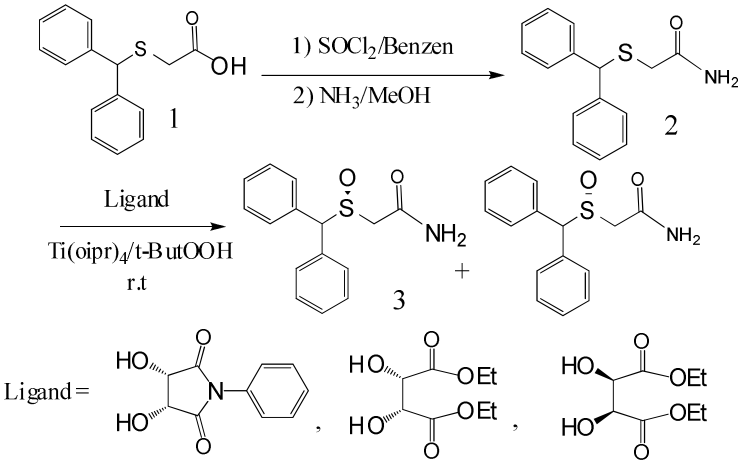
Modafinil [Provigil] is a psychostimulant used in the treatment of narcolepsy [1]. However, its mechanism of action appears different from that of other CNS stimulants such as d amphetamine [2]. Given their unique pharmacological properties, clinical work has begun to explore the utility of these agents as pharmacological treatments for stimulant dependence [3]. The synthesis of R-modafinil, begins with the reaction of benzhydrol and thioglycolic acid in trifluoroacetic acid to afford benzhydrylsulfanylacetic acid 1 in 99% yield. The reaction of modafinic acid 1 with thionyl chloride in benzene followed by treatment of the corresponding acid chloride with concentrated ammonium hydroxide gave acetamide 2 in 87% yield. After we focused on the preparation of R-modafinil. We synthesized these enantiomer using an enantioselective oxidation. Attempts to oxidize 2 using diethyl tartrate derivatives, Ti(O-i-Pr)4, and cumene hydroperoxide proved successful and with high enantioselectivity. (Scheme 1).



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A facile synthesis of α-hydroxy 1,4-dicarbonyl compounds from aromatic 1, 2-diketones

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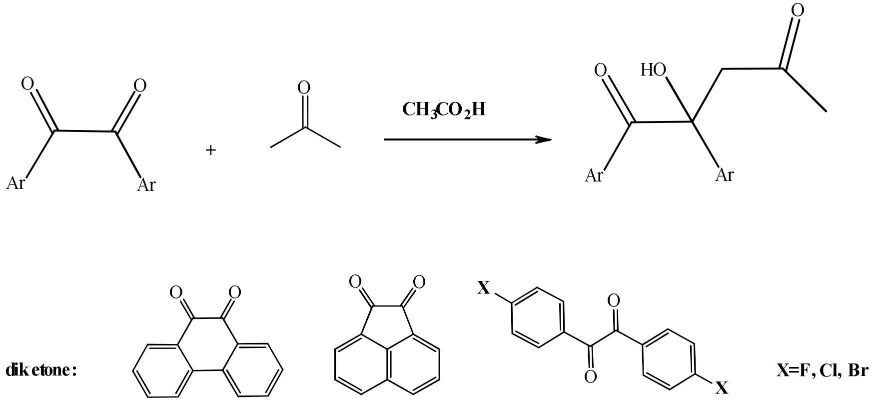
α-Hydroxy carbonyl is perceived in many biologically active natural products such as sugars and antibiotics [1-2]. Also, α -Hydroxy carbonyls are profitable synthones in organic synthesis [3]. Many methods have been presented for the synthesis of α –hydroxy carbonyls in literature. For examples reduction of 1, 2-diketones, oxidation of enol phosphates [1], selective oxidation of vicinal diols [2], oxidation of diarylalkynes [4] and else.

Herein, we report an efficient, inexpensive, and mild synthetic route to α-hydroxy 1, 4-dicarbonyl compounds in moderate yield. We carried out the reaction of an aromatic 1, 2-diketone and acetone in acetic acid at room temperature and the condensation product was obtained in moderate yield (scheme1). The structure of compounds is supported with spectral data (^{1}HNMR, ^{13}CNMR, IR) and elemental analysis.



Scheme 1

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Synthesis, characterization and catalytic activity of Co(II)-salen complex anchored on mesoporous silica

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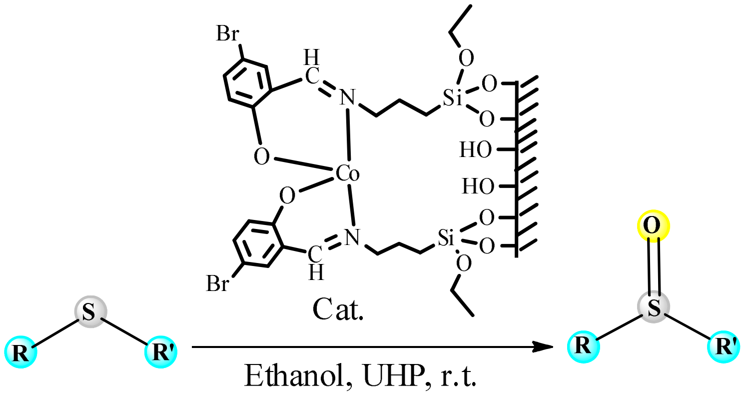
Recently much attention has been focused on developing eco-friendly catalytic processes based on efficient catalysts with easy recoverability. Schiff base transition metal complexes are considered as promising candidates because of their excellent catalytic performances in a wide range of oxidation reactions [1]. A new hybrid catalyst has been prepared by tethering a cobalt(II) Schiff-base complex via post-synthesis modification of mesoporous silica, MCM-41. The Schiff-base has been derived from 5-boromo salicylaldehyde and 3-aminopropyltriethoxysilane (3-APTES) which is chemically anchored on MCM-41 via silicon alkoxide route [2-3]. The catalyst has been characterized by X-ray diffraction, nitrogen physisorption, UV–Vis spectrometer, IR-spectra and TGA/DTA studies. The activity of the catalyst has been assessed the oxidation of sulfides using with urea hydrogen peroxide (UHP) as oxidant in heterogeneous condition (scheme 1). The catalyst can be recycled and reused several times without significant loss of activity.



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A novel catalyst for the synthesis of 1H-pyrazolo[1,2 b]phthalazine-5,10-dione derivatives

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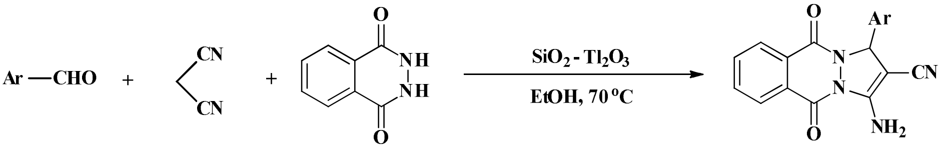
1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivatives are important classes of nitrogen containing heterocycles which exhibit significant pharmacological and biological activities such as anti-bacterial, anti-viral, anti-hypoxic, antiinflammatory, analgesic, and anti-pyretic agent [1,2]. Due to their pronounced applications, many classic methods have been reported for their synthesis [3,4]. But, generally, many of these methods, use expensive reagents, suffer from long reaction times and lower yields. Therefore new synthetic methods are still required.

In the light of the above mentioned findings, we decided to the synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivatives by a three-component reaction of aromatic aldehydes, malononitrile and phthalhydrazide in the presence of a catalytic amount of silica Tl_2O_3, as an efficient and rusable catalyst in ethanol at 70 °C (Scheme 1). The method developed has allowed us to obtain quantitative yields of the required products in reduced reaction times.



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Highly diastereoselective synthesis of 5-substituted 1H-tetrazolesvia a multi-component domino Knoevenagelcondensation/1,3 dipolar cycloaddition reaction catalyzed by reusable nano NiO

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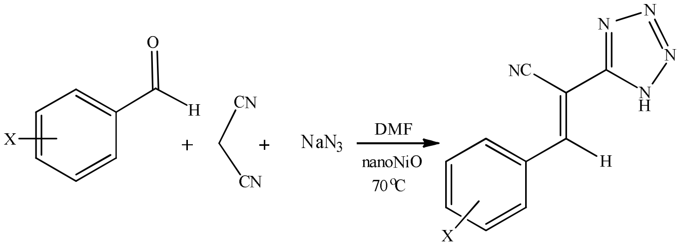
The growth of tetrazole chemistry over the last years hasbeen significant, mainly as a result of the roles played by tetrazolesin coordination chemistry as ligands, in medicinal chemistry asstable surrogates for carboxylic acids and in materials applications,including explosives, rocket propellants, and agriculture [1-3]. Generally, multicomponent reactions are performed without need to isolate any intermediate during the reaction, which *reduce* the used*time*and*energy* [4]. There has been tremendous development in three or four component reactions.Herein, wewould like to reporta novel andone-pot process for the synthesis of 5-substituted 1H-tetrazoles viaa domino Knoevenagel condensation and 1,3 dipolar cycloadditionreaction using nano NiO catalyst.

An approach for the synthesis of 5-substituted-tetrazoles via multi-component reaction of carbonyl compounds, malononitrile and sodium azide in DMF with nanoparticlesNiO is an effective and reuseable heterogeneous catalyst has been reported. This general protocol provides a wide variety of 5-substituted 1H-tetrazoles in good yields under mild reaction conditions (Scheme 1).



Scheme 1

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An efficient, clean synthesis of 4,4'-(arylmethylene)bis(1*H*-pyrazol-5ol) derivatives

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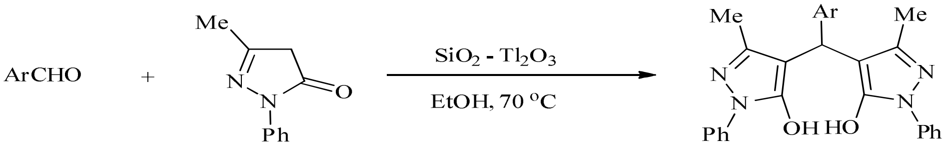
2,4-Dihydro-3H-pyrazol-3-one derivatives including 4,4'-(arylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ols) are known to possess a wide range of biological activities and have been used as antibacterial and antiviral agents [1,2]. A number of synthetic approaches have been made for the synthesis of 4,4'-(arylmethylene)bis(1*H*-pyrazol-5-ol) derivatives [3,4]. Although some of these methods afford moderate to high yields of the corresponding products, the majority suffer from one or more of the following disadvantages, including (1) the use of a costly catalyst; (2) the requirement for a tedious work-up procedure; (3) the need for high temperatures; and (4) long reaction times.

Herein, we report the development of a mild, efficient, and environmentally benign procedure for the synthesis of 4,4'-(arylmethylene)bis(1*H*-pyrazol-5-ol) derivatives by the condensation reactions of 1-phenyl-3-methylpyrazol-5-one with several different aromatic aldehydes in ethanol at 70 °C in the presence of silica Tl_2O_3 as a solid heterogeneous catalyst (Scheme 1).



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A three-component reaction approach to the preparation of substituted pyrano[2,3-c]pyrazoles

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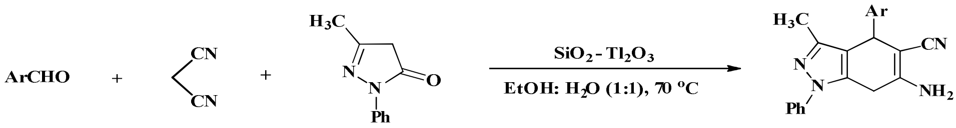
Silica Tl_2O_3 is found to catalyze the three component condensation of an aromatic aldehyde, malononitrile, and 1-phenyl-3-methylpyrazol-5-one to afford the substituted pyrano[2,3-c]pyrazoles in high yields. Substituted pyrano[2,3-c] pyrazoles are attractive heterocyclic compounds for drug discovery since many of these scaffolds exhibit wide range of biological, medicinal and pharmaceutical activities [1,2]. They have found uses, for example, as anticancer, anti-inflammatory, antimicrobial, and also as biodegradable agrochemicals [3].

As part of our current studies on the development of new routes to heterocyclic systems, in this letter we describe a convenient, mild, and environmentally friendly synthesis of substituted pyrano[2,3-c]pyrazoles (scheme1). This new methodology is of interest due to high yields, relatively short reaction time, simple work-up and reusability of catalyst. Structures of the products were confirmed by IR and NMR spectroscopic methods.



Scheme 1

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An efficient, one-pot, three-component synthesis of 4H-pyrido[1,2-a]pyrimidines: using polyurethane at room temperature

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Multicomponent reactions (MCRs) have attracted much attention during recent years. These one-pot high-yielding proceduresare interesting synthetic methods for attaining new and usefulproducts [1]. The development of simple synthetic routes for widelyused organic compounds from readily available reagents is one of the major tasks in organic synthesis. Bridgehead nitrogen heterocycles are of interest because they constitute an important class of natural and unnatural products, many of which exhibit useful biological activity [2].Polyurethane (PU)ionomers are well-known and user-friendly polymers [3].

In this work we report a one-pot, versatile and simple route to functionalized 4H-pyrido[1,2-a]pyrimidines from [1+2+3] atom fragments using simple starting materials and involving the formation of three bonds. Thus, a mixture of an isocyanide, a dialkyl acetylenedicarboxylate and an N-(2-pyridyl)amideundergoes a smooth 1:1:1 addition reaction in dry CH_2Cl_2 at ambient temperature to produce 2-amino-4H-pyrido[1,2-a]pyrimidine-3,4-dicarboxylatesin 80–91% yields (Scheme 1).

Scheme 1

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A facile route to synthesis bis (3-phenylaziridin-2-yl)methanone

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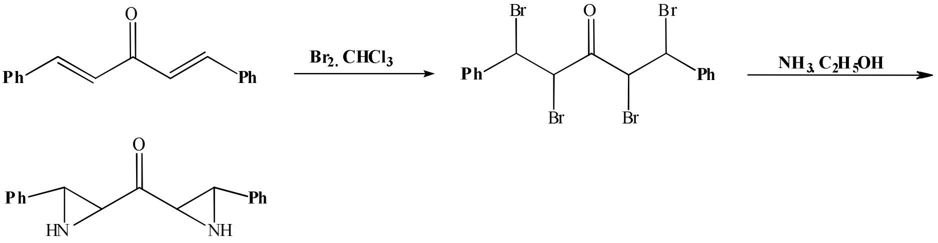
Aziridines have been synthetic targets as well as useful building blocks in synthesis since Gabriel's 1888 discovery of the smallest nitrogen containing heterocycle [1-2]. Attracted by the increased strain and unique reactivity of the three-membered ring, synthetic chemists have extensively exploredthe various manipulations of aziridine-containing compounds [3]. Many of these advances have been overlooked in organic chemistry textbooks, as discussion of aziridines is often limited to heterocyclic nomenclature. Nonetheless, aziridines exhibit a wide range of useful reactivities including nucleophilic ring opening, which harnesses the release of ring strain. In recent years, many other transformations have been described, such as cycloadditions [4], but the limited application of aziridines in organic synthesis is due in large measure to the paucity of general methods for their preparation.

Herein, we report an efficient, inexpensive, and mild synthetic route to bis (3-phenylaziridin-2-yl)methanone in good yield(scheme1). The structure of compounds is supported with spectral data (^{1}HNMR, ^{13}CNMR, IR) and elemental analysis.



Scheme 1

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Application of Ag-TiO₂ nanocomposite as a green and recyclable catalyst for the one-pot three component synthesis of 12-aryl xanthene derivatives under ambient temperature

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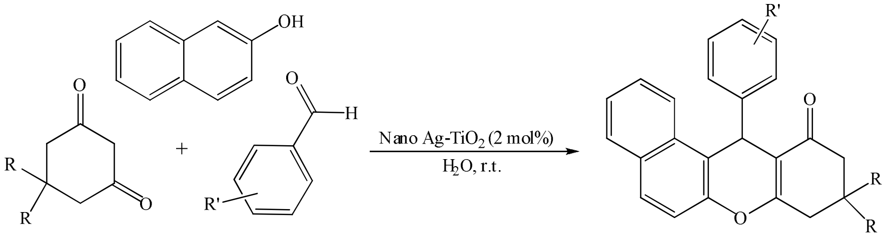
Nanoscience and nanotechnology in the past decade, has turn into an admired field for research and development [1]. Nanomaterials, due to their reduced size and dimension, possess remarkable properties not seen in their bulk form [2]. Nanomaterials have attracted extensive interest for their unique properties in various fields such as catalytic, electronic, and magnetic in comparison with their bulk counterparts [3]. Among the different application field, the heterogeneous catalysis was cited as a thriving application that has great benefits for humanity [4, 5].

Application of nanoAg-TiO_2 as an efficient and benign catalyst has been explored in the synthesis of 12-aryl xanthene derivatives via condensation reaction of *β*-naphthol, aryl aldehydes and dimedone. The reactions proceed under heterogeneous and mild conditions in water at room temperature to provide 12-aryl xanthene in high yields. The described novel synthesis method propose several advantages of safety, mild condition, short reaction times, high yields, simplicity and easy workup compared to the traditional synthesis method (Scheme 1).



Scheme 1

References:

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One-pot multicomponent synthesis of 2-amino-4*H*-chromene derivatives using UHP as a mild and highly efficient catalyst

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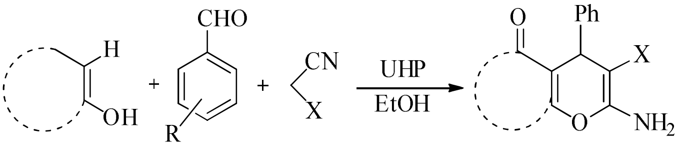
Multicomponent reactions (MCRs) allow the assembly of complex molecules in one-pot and show a facile execution, high atom-economy and high selectivity, as afford good yields and are fundamentally different from two-component and stepwise reactions in several aspects [1]. Highly functionalized 4*H*-chromenes occur commonly in numerous natural compounds [2], showing a wide range of biological activities [3,4].

In continuation of our interest in the application of new catalysts in organic synthesis via MCRs [5-7], herein, an efficient and highly selective synthesis of 2-amino-4*H*-chromene derivatives has been developed by the condensation of CH-acids (dimedone, 1,3-cyclohexadiene, barbituric acid, 4-hydroxycoumarin), aldehydes and active methylene nitriles (malononitrile, ethyl cyanoacetate) using urea/hydrogen peroxide (UHP) as a supported green catalyst in ethanol in short reaction times under mild reaction conditions and excellent yields.



Scheme 1

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$Ca(ClO_4)_2$: An effiecent catalyst for synthesis of tetrahydro-dihydroxy oxoindeno[1,2-b]pyrroles

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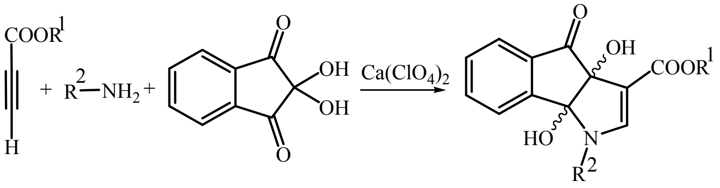
The development of efficient and mild methods for heterocyclic compound synthesis and application drugs represents a broad area of organic chemistry [1]. Pyrroles important classes of compounds with many medicinal activities. For these reasons, many ways for the synthesis of substituted pyrroles are known [2]. It is known that dihydroxy-oxoindeno[1,2-b] pyrroles exhibit a wide range of biological activities [3-5].

Although this reaction done previously in other conditions, [6]. herein we report in one pot reaction, with high yields, easy separation of product and three-component method for the construction of some new tetrahydrodihydroxy-oxoindeno[1,2-*b*] pyrroles ,via condensation of amines, alkyl propiolates and ninhydrin by using $Ca(ClO4)_2$ as a catalyst.



1 2 3 4

Scheme1

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A facile synthesis of highly functionalized spiro compound

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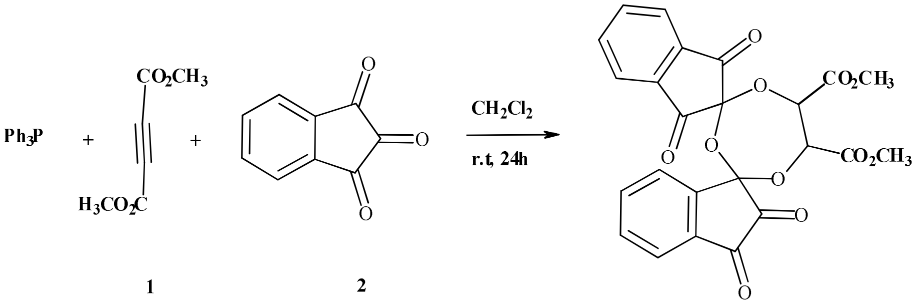
Many different products were obtained from the reaction between activated alkynes and trivalent phosphorus nucleophiles in the presence of other compounds [1-3]. There are some reports which trivalent phosphorus treats to link the other components of the reaction as a catalyst [4].

We here report the reaction of ninhydrine **2** and dimethylacetylenedicarboxylates **1** in the presence of triphenylphosphine so that trivalent phosphorus links two ninhydrine molecules to acetylenic ester and an interesting spiro compound is isolated (Scheme1). The structure of product is supported with spectral data (^{1}HNMR, ^{13}CNMR, IR) and elemental analysis.



Scheme 1

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Construction of new spiro[indene-2,2'-pyrido[2,1-a] isoquinoline]-3',4'-dicarboxylate derivatives via 1,4-dipolar cycloaddition of isoquinoline-*acetylenicesters* zwitterions with 2-(1,3-dioxo-1H-inden-2(3H)-ylidene)malononitrile

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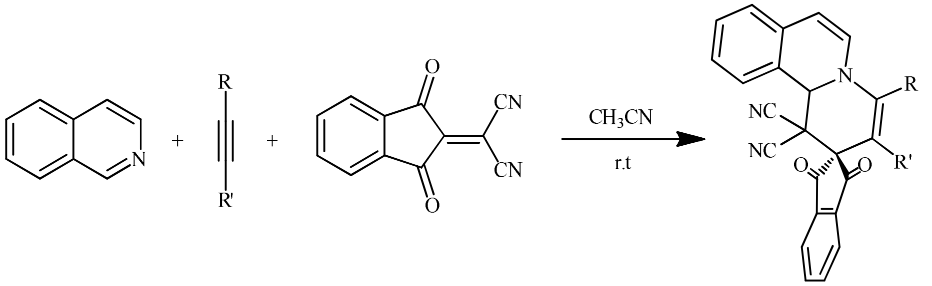
The reaction of pyridine or isoquinolines with activated acetylenes has been the subject of considerable research over the last several decades [1]. The earliest work in this area appears to be that of Diels and Alder, who in 1932 showed that pyridine reacts smoothly with dimethyl acetylenedicarboxylate (DMAD) to form an adduct of unknown structure. Decades later, the structure of the adduct was established as the 4*H*-quinolizine by the systematic investigations of Acheson and co-workers. Huisgen recognized this reaction as the 1,4-dipolar variant of the classical Dielse Alder reaction. [2-3].

In this paper we report the synthesis of some spiro[indene-2,2'-pyrido[2,1-a]isoquinoline]-3',4'-dicarboxylates. These reactions between isoquinoline, acetylenic esters and 2-(1,3-dioxo-1*H*-inden-2(3*H*)-ylidene)malononitrile proceeds in CH_3CN at room temperature in good to excellent yields. (Scheme 1).



Scheme 1

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Efficient synthesis of polyhydroquinolines by the reaction of dimedone, 1,3-diaryl-2-propen-1-ones and ammonium acetate

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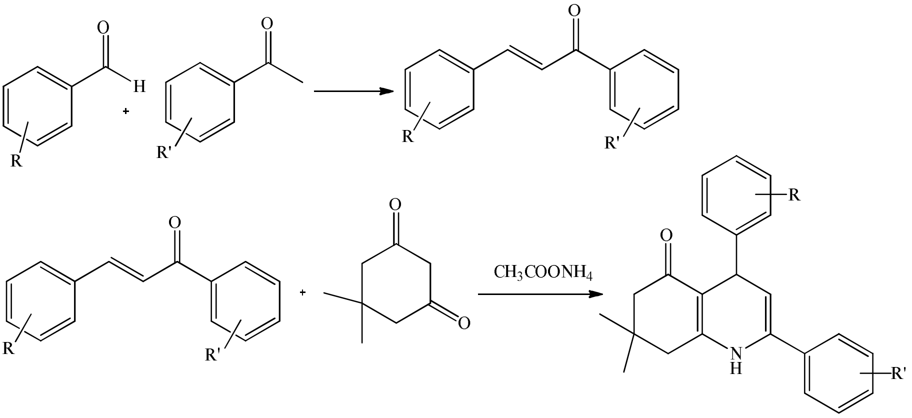
Polyhydroquinolines are an important group of nitrogen containingheterocycles that have attracted much attention becauseof their diverse therapeutic and pharmacological properties, suchas calcium channel blockers, vasodilator, hepatoprotective,anti-atherosclerotic,bronchodilator, antitumor, geroprotective, antidiabeticactivity [1]. Therefore, several methods have been developed for the preparationof polyhydro-quinoline derivatives by using various catalysts [2].

In continuation of our research work in the development ofhighly expedient methodologiesby multicomponent reactions [3], we developed theapplicability of triethyl amine for efficient, convenient and facile synthesis of polyhydroquinolines derivativesthroughthe reaction of dimedone, 1,3-diaryl-2-propen-1-one derivatives andammonium acetate under solvent-free condition at 80 °C (Scheme 1).



Scheme 1

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Ion recognition by lower rim 1,3-di-conjugates ofcalix[4]arene derivative as receptors

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[b]*Chemistry and Chemical Engineering Research Center of Iran (CCERCI),Tehran, Iran*
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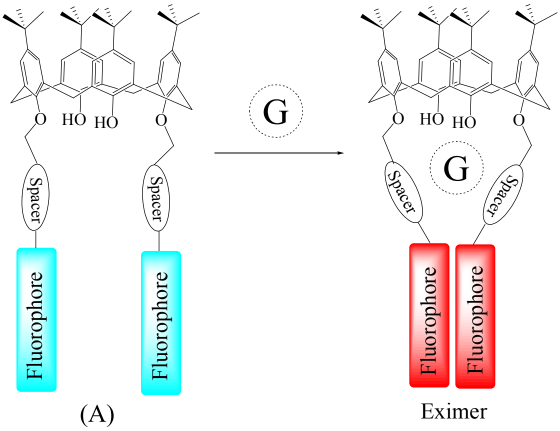
Calixarenes are one of the most studied macrocyclic receptors besides crown ethers, cyclodextrins, cryptands, andcucurbiturils [1-3].These compounds can be synthesized from the base-catalyzedcondensation reaction of *p*-substituted phenols with formaldehyde [4].Calixarenes have several advantages over other molecular systems, such as: the presence of a hydrophobic cavity, easy organic modifiability both at lower and upper rims, and it can be adorned by aflexiblebut well-defined binding core. The direct involvement of calixarene moiety in the recognition ofmetal ions is established in the literature as a result of the metal complexation [5,6].

In this work, the synthesis and evaluation of a novel calix[4]arene-based fluorescent chemosensor A containing fluorene derivatives for the detectionof $Pd^{2+}$and $Hg^{2+}$is described. The fluorescent spectra changes observed upon addition of various metalions show that A is highly selective for $Pd^{2+}$and Hg^{2+}over other metal ions. Addition of $Pd^{2+}$and $Hg^{2+}$to the solution of A results in ratiometric measurement of these cations.



Scheme 1

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Natural biopolymers as a green catalyst for the synthesis of piperazine-1-carboxylate

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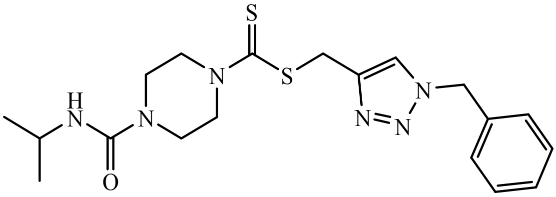
Cellulose sulfuric acid (CSA) has emerged as a promising biopolymeric solid support acid catalyst for acid-catalyzed reactions, such as the synthesis of α-amino nitriles, aryl-14H-dibenzo[a.j]xanthenes, 1,4-dihydropyridines, Pechmann condensation, thiadiazolo benzimidazoles, imidazoazines, quinolines and 3,4- dihydropyrimidine-2(1H)-ones [1-2].

1,2,3-Triazoles have been a fruitful source of inspiration for medicinal chemists for many years due to their synthetic accessibility by click chemistry as well as their numerous biological activities [3]. 1,2,3-Triazole is a versatile moiety found in a large variety of bioactive molecules, such as anti-fungal, anti-bacterial, anti-allergic, anti-HIV, anti-tubercular and anti-inflammatory agents [4-6].



Scheme 1

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Bismuth vanadate as an efficient and reusable catalyst for the synthesis of bis-coumrines

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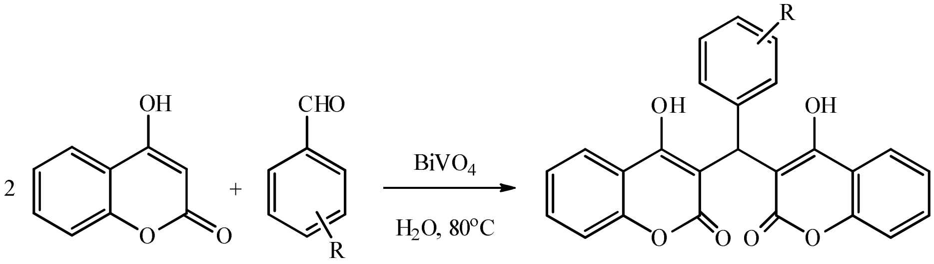
An efficient, mild, and environmental friendly method has been developed for the synthesis of dicoumarols in water over Lewis acid catalyst bismuth vanadate ($BiVO_4$). The method involves the condensation of various aromatic aldehydes with 4-hydroxycoumarin.

It affords the corresponding product in high yield with short reaction times employing a very low loading of catalyst. The catalyst was reused several times without significant change in activity.



Scheme 1

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Poly (4-vinylpyridinium tribromide): an efficient catalyst for the synthesisof 1,1-diacetates from aldehydes

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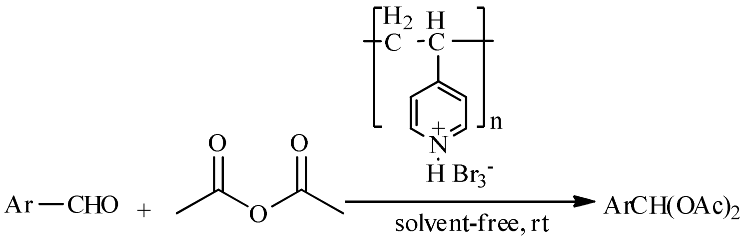
1,1-Diacetates are one of the essential carbonyl protecting groups because of their stability under neutral and basic media [1]. Diacetates of α,β-unsaturated aldehydes are important starting materials for synthesis of dienes in Diels–Alder reactions [2,3], and they are also useful intermediates in various transformations [4]. Moreover, acylals can be converted into other functional groups by reaction with suitable nucleophiles [5,6].

Herein we report a mild and efficient polymeric catalyst for the preparation of 1,1-diacetates from aldehydes in the presence of acetic anhydride under solvent-free conditions at room temperature. This method has some advantages such as general, rapid, inexpensive, and having a low environmental impact.



Scheme 1

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Coupling chamazulene with 3-methoxy-2-cyclohexen-1-one and the study of its effect on tubuline polymerization in the mouse brain

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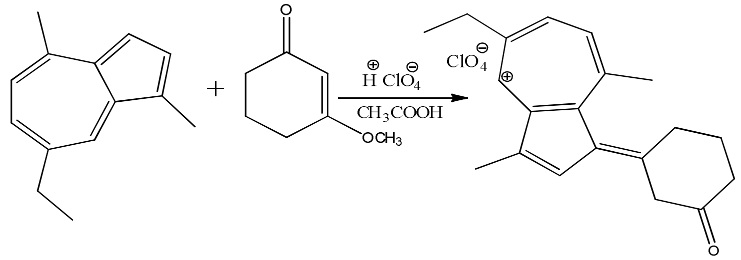
[b]*Department of Biochemistry, University of Tehran, Tehran, Iran*
Email: samaahmadi64@yahoo.com

Chamazulene as an artifact of matricine by distillation, is a degradation produc of chamazulene carboxylic acid [1-2]. It has been examined and its antiphlogistic action has been proved in a variety of experimental inflammatory reaction . It is a natural agent which presents interesting properties concerning radical processes. These processes are implicated in numerous pathophysiological condidion like arthrosclerosis, inflammation, gastric ulceration, neuronal degeneration and tumor promotion [3-4].

In the present study the reaction of chamazulene with a cyclic ketone was preformed. Chamazulene was reacted with 3-methoxy-2-cyclohexene, 1-one in optimum acidic condition and pH. Then the reaction mixture was cooled, washed with water and dried over suitable absorbent. Experimental data related to in vivo investigations showed that the new product was able to increase tobuline polymerization .The molecular structure of product was characterized and confirmed by Analytical and spectroscopic methods (IR, ^{1}H-NMR).



Scheme 1

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A green, facile and highly efficient approach to synthesis of biscoumarin derivaties in water using tetraethylammonium 2-(carbamoyl)benzoate (TEACB) as a bifunctional organocatalyst

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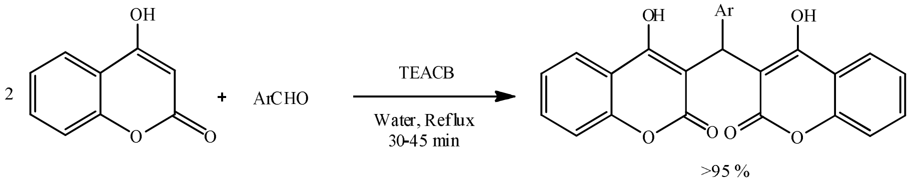
4-Hydroxycoumarin derivatives are compounds of great interest because of their anticoagulant, spasmolytic, and rodenticidal activities. Some coumarin derivatives are known for their antifungal and anti-HIV activities They are also extensively used as analyticalreagents. The most widely used antithrombotic in the USA and Canada is the racemic sodium Warfarin [1].

Bifunctional organocatalysts have received great attention for chemical synthesis, traditional catalytic approaches rely on the activation of only one of the reacting species, so attention has recently turned to the development of bi-and poly-functional catalytic systems that can activate different sites of the reaction simultaneously. Organocatalysts are free of toxic transition metals, they can easily be separated from the reaction products and recovered after the completion of the reaction, therefore, they provide a promising green route for chemical processes [2].

In this work, Tetraethylammonium 2-(carbamoyl)benzoate(TEACB) produced from phthalimide and tetraethylammoniumhydroxide has been used as a highly efficient organocatalyst for synthesis of biscoumarin derivatives from the reaction of 4-hydroxycoumarin and different aldehydes, the reaction proceeds very well in water under reflux conditions and leads to excellent yields in short times. No toxic organic solvent has been used neither as the solvent nor in the work-up process to obtain the pure products. (Scheme 1).



Scheme 1

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Synthesis and characterization of trisubstituted imidazoles using nano silica phosphoric acid under thermal conditions

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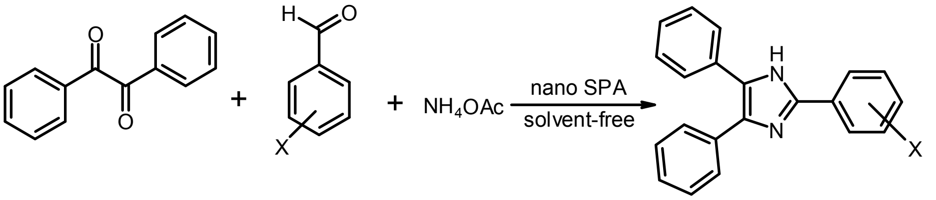
Many of organic solvents such as chlorinated hydrocarbons have toxic nature that threaten the environment. Because of this, the use of heterogeneous catalysts were more concerned in the area of green chemistry [1]. Processes which those are solvent- free and low wasted [2]. Recently, organic chemists are trying to use multicomponent reactions (MCRs) in solvent-free conditions [3].

Trisubstituted imidazoles are an important class of compounds in the field of pharmaceutical and exhibit a wide range of biological activities [4]. Nano silica phosphoric acid as an efficiant catalyst have been used to one pot synthesis of trisubstituted imidazoles. Simple and highly efficient synthesis of 2,4,5- trisubstituted imidazoles are achieved by three component cyclocondensation of benzil, various aromatic aldehydes and ammonium acetate in the presence of solid catalyst (Scheme 1). The structure of products have been characterized by spectroscopic techniques such as IR, ^{1}HNMR and ^{13}CNMR.



Scheme 1

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Microsynthesis and mass spectral analysis of chemical weapons convention-related compounds

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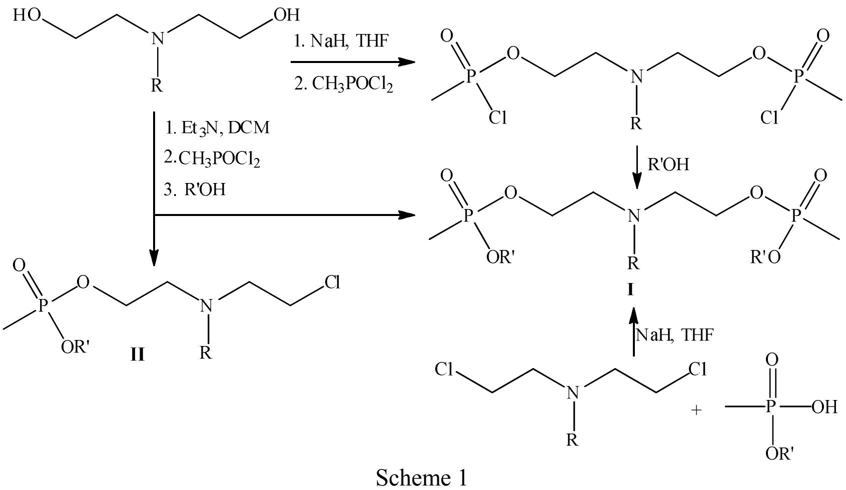
Email: h_porkaleh@yahoo.com

Chemical warfare agents (CWAs), mainly mustard gas, were used on a large scale in the World War I. In addition to mustard gas, neurotoxic agents, which are also known as nerve agents, such as sarin and tabun were employed for the first time in the Iran–Iraq war then were used in some terrorist attacks in Japan [1]. The Chemical Weapons Convention (CWC) which came into force on 29 April 1997, prohibits the production, development, storage and use of CWAs. Chemicals regard to potential risk and toxicity are listed in an annex to CWC in three distinct schedules and therefore called *scheduled chemicals*.The availability of mass spectra and interpretation skills are essential for unambiguous identification of the Chemical Weapons Convention (CWC)-related chemicals [2].

Herein, we wish to report a general microsynthesis protocol for the *N*-alkyl bis(2-(alkoxy-methylphosphoryloxy)amine(Scheme 1). Electron ionization (EI) mass spectra of these chemicals with possible fragmentation routes are also investigated through the analysis of fragment ions of deuterated analogs, MS/MS experiments and energy calculations. Density functional theory (DFT) calculations were done in order to find relative preference formation of fragment ions.



Scheme 1

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Facil and efficient synthesis of xanthenes derivatives using W-ZnO as a nano catalyst

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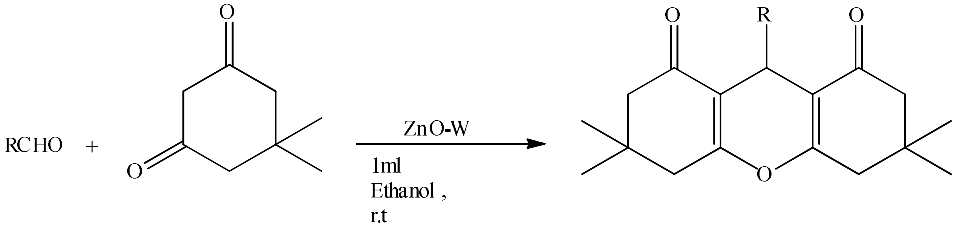
In the past decade, synthesis of xanthenes derivatives has been of considerable interest to organic chemists because they posses various biological and pharmaceutical activities such as antiviral, antibacterial, and anti-inflammatory properties. These are being utilized as antagonists for paralyzing action of zoxazolamineand in photodynamic therapy. Furthermore, these compounds can be used as leuco-dyes, in laser technology and pH-sensitive fluorescent materials for the visualization of biomolecular assemblies. Among this class of molecules, xanthone is a prominent structural moiety found in numerous natural products and synthetic compounds with important biological activity.

Consequently, the development of novel methods for the synthesis of these heterocyclic compounds has been receiving considerable interest in both organic and medicinal field [1-3].



Scheme 1

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An efficient synthesis of pyrido [2,3-d]pyrimidine derivatives using catalytic amount of $CuFe_2O_4$ nanoparticles as catalyst under microwave irradiation

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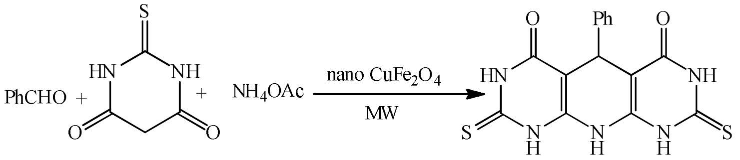
In modern synthetic organic chemistry, development of a novel and efficient method for the construction of several mono as well as poly heterocyclic scaffolds is one of the current areas of research interest. [1]. Pyrido pyrimidine and its derivatives have been studied for over a century because of a variety of chemical and biological significance [2]. Pyrido[2,3-d] pyrimidines are known to be pharmacophoric elements in numerous active compounds such as anti-cancer, anti-viral and anti-inflammatory agents [3]. In this research, a new method has been introduced for the preparation of pyrido[2,3-d] pyrimidines.

In this work, we were synthesis of pyrido[3,2-d]-pyrimidines from aromatic aldehydes, 2-thiobarbituric acid, ammonium acetate in the presence of $CuFe_2O_4$ nanoparticles as catalyst (Scheme 1). The present approach offers the advantages of simple methodology, clean and mild reaction, short reaction time, high yield, and excellent purity. The structure of products was confirmed by IR, ^1H NMR and ^{13}C NMR.



Scheme 1

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Ce-ZnO as a nano catalyst for the synthesis of biscoumarins

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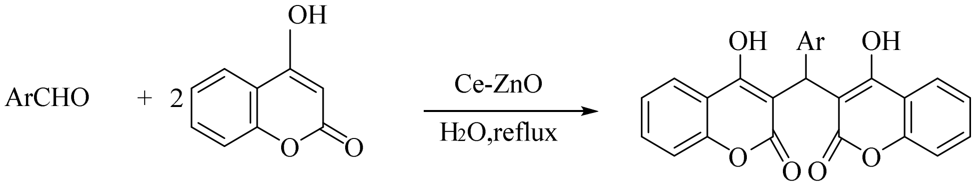
Multicomponent reactions are performed without need to isolate any intermediate during the reaction, which *reduce* the amount of *time* and *energy* used [1]. There has been tremendous development in three or four component reactions. Biscoumarin derivatives have been attracted considerable interest because of their biological and pharmacological activities [2-3].

In this work, a new strategy has been introduced for the preparation of biscoumarins. In this regards, Ce-ZnO has been synthesized and new applications of this catalyst explored. Therefore a variety of biscoumarin have been prepared via combination of aromatic aldehydes and 4-hydroxycoumarin in the presence of a catalytic amounts of Ce-ZnO under reflux condition in water as solvent. (Scheme 1).



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Synthesis and characterization of modified silica gel with the new method and study of properties

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The modification of adsorbents with organic functional groups has been shown to improve the selectivity of the adsorbents for binding desired metal ions and has recently drawn much attention. In this work, silica gel was activated by hydrochloric acid [1-2]. Activated silica gel were covalent grafted with 3-aminopropyl trimethoxysilane to give functionalized silica gel. Dialdehyde was added to functionalized silica gel for preparation of modified silica gel. This product prepared with two methods: normal method, vice versa method. The vice versa method is new manner in synthesis of modified silica gel with dialdehyde. All products were characterized with different physicochemical techniques such as FT-IR, XRD, SEM, TGA/DTA and UV-Vis.

The modified silica gel with dialdehyde have been used in the extraction of Cu(II), Cd(II), Ag(I), Ni(II), Zn(II) and Pb(II) ions from aqueous solution. The percentage of extracted metal ion determined by atomic absorption spectroscopy. This compound exhibits a good extractive affinity for Ag(I). HNO_3 and HCl was used for desorption of Ag. Best desorption was achieved using HCl.

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Synthesis and characterization of a new Schiff base ligand as a fluorescent chemosensor for aluminium ion

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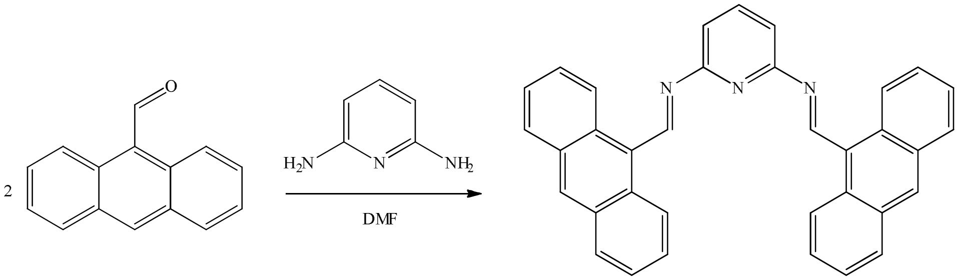
A new Schiff base system (L) chemosensor containing two anthracene fluorophores has been synthesized (Scheme 1). Upon treatment with aluminum ions, the fluorescence of the Schiff base (L) was enhanced due to the formation of a complex between the ligand and aluminum ions at room temperature. Other metal ions, such as Zn^{2+}, Ni^{2+}, Na^{+}, Cs^{+}, Fe^{3+}, K^{+}, Mn^{2+}, Co^{2+}, Hg^{2+}, Cr^{3+}, Cu^{2+}, Mg^{2+}, Ba^{2+}, Fe^{2+}, Cd^{2+}, Ag^{+} and Pb^{2+}, had no significant effect on the fluorescence (Fig. 1a). To further investigate the chemosensing properties of Schiff base (L), fluorescence titration of Schiff base (L) with Al^{3+} was performed (Fig. 1b).

A Schiff base (L) was synthesized for selective detection of Al^{3+}. Upon complexation with Al^{3+}, Schiff base (L) exhibited a pronounced enhancement in the fluorescence emission spectrum. Schiff base (L) could be used as a fluorescent chemosensor for the detection of aluminium ions.



Scheme 1. The synthetic Schiff base (L)

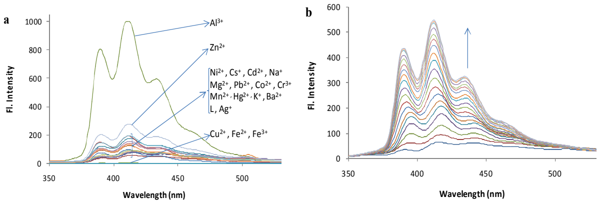


Fig 1. Fluorescence spectra of L (a) and changes in the fluorescence spectra of L (b)

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Alginic acid: a highly efficient renewable and recoverable bio-polymer catalyst for one-pot 4-component synthesis of polyhydroquinoline derivatives via Hantzch condensation reaction

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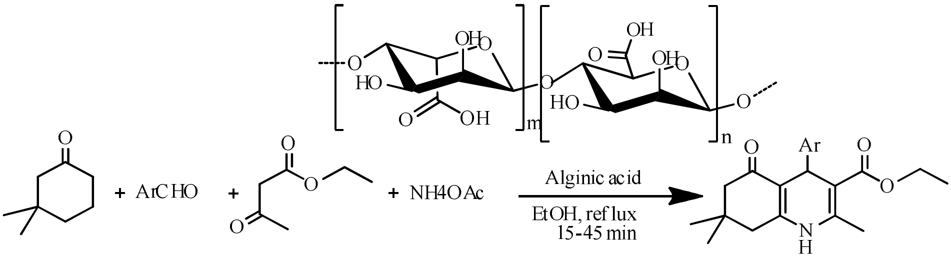
Multicomponent processes, considering the fundamental principles of synthetic efficiency and reaction design have proven to be a very remarkable and advantageous tool for the synthesis of a wide range of useful compounds, including pharmaceuticals [1]. Polyhydroquinoline derivatives are hetrocycles of immense importance due to their diverse therapeutic and pharmacological properties, such as calcium channel blockers, vasodilator, hepatoprotective, anti-atherosclerotic, antitumor, etc [2-3].

In this work, Alginic acid, a natural biodegradable polysaccharide generated by brown algae, in it's commercial form without any post-modification has been used as a green and highly efficient renewable and easily recoverable bio-polymer catalyst for the rapid and convenient synthesis of polyhydroquinoline derivatives from one-pot reaction of dimedone, ethyl acetoacetate, different aldehydes and ammonium acetate under mild conditions in excellent yields. An extensive progress in designing more sustainable chemical process takes place if biopolymers themselves and without any post-modification can be used as heterogeneous catalyst [4]. The polyhydroquinoline derivatives have been prepared through Hantzch condensation reaction catalyzed by alginic acid as a natural heterogeneous bifunctional organocatalyst. (Scheme 1).



Scheme 1

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An efficient method for chemoselective reduction of nitro compounds using bimetallic Fe-Ni NPs/$H_3PW_{12}O_{40}.xH_2O$ system

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Reduction of the nitro compounds to amines which find applicability in diverse fields including dyes, pharmaceuticals, agrochemicals, photographic, antioxidants, and conducting polymers, is a very useful synthetic transformation [1].To date, there are a vast array of reagents which can be used to convert nitro compounds to their corresponding amines. Conventional methods of reduction of nitro compounds use hydrogenation, electron-transfer, electrochemical and hydride transfer conditions [2].

Nanomaterials are more effective than conventional reagents because of their extremely small size and tremendous surface area-to-volume ratio. In continuation of our interest in exploring the utility of nanoparticles in organic synthesis [3],in the present work we would like to report an efficient and chemoselective method for the reduction of various nitro compounds to the corresponding amines by treatment with bimetallic Fe-Ni NPs/$H_3PW_{12}O_{40}.xH_2O$, system (Scheme 1).

$$\mathrm{R-NO_2} \xrightarrow[\mathrm{H_2O,\ 50\ ^\circ C}]{\mathrm{Fe\text{-}Ni\ NPs\ /\ H_3PW_{12}O_{40}.xH_2O}} \mathrm{R-NH_2}$$

R= 4-CNC_6H_4, 3-$NO_2C_6H_4$, 1-Cl 4-$NO_2C_6H_3$, 4-$CO_2HC_6H_4$, 2-$CO_2HC_6H_4$, 4-$CHOC_6H_4$, 4-$AcNHC_6H_4$, 4-$AcOC_6H_4$, 3-Cl 4-$NH_2C_6H_3$, 2,4-dichloro-6-methylpyrimidin, C_6H_5, 4-OHC_6H_4, 4-$OHCH_2C_6H_4$, 4-$NH_2C_6H_4$, 2-$NH_2C_6H_4$, 4-MeC_6H_4, cyclohexyl

Scheme 1

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Sensing of cyanide using highly selective thiazole-based Cu^{2+}chemosenso

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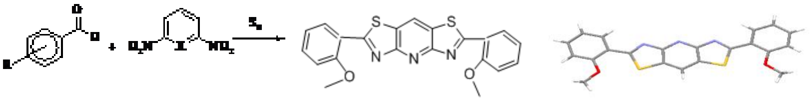
The recognition and detection of anions is a field that has attracted increasing interest in recent years due to the fundamental importance of these species in many chemical and biological processes. Cyanide (CN^{-}) is a hazardous chemical that occurs naturally, both in the geologic and biologic world.

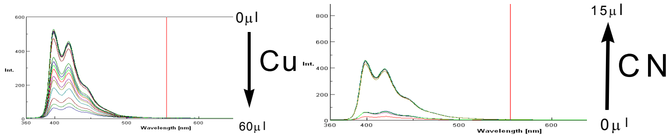
Herein, we report the synthesis, characterization and properties of a new fluorescent chemosensor [1]. The chemosensor 1 was obtained in a 20% yield by theWillgerodt-Kindler reaction of the 2-methoxybenzaldehydewith 2,6-diaminopyridine and sulfurin refluxing DMF.

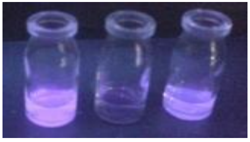
The planar structure of 1 is confirmed by X-ray analysis crystallography(Fig 1).



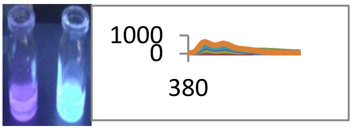
(Fig 1)

Once combinedwith Cu(II) in methanol solution, ligand 1 displays a fluorescence quenching effect to form an complex between Cu and ligand 1, which could befast dissociated by the addition of cyanide in this system so that "ON–OFF–ON" type fluorescence change can be achieved.





The system of"ON–OFF–ON" can be also used for the specific detection of millimolar concentrations of acid in water.



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Tungsten-doped ZnO nanocomposite: An efficient catalyst for the aqueous phase synthesis of Bis-(4-hydroxycoumarin-3-yl)methanes

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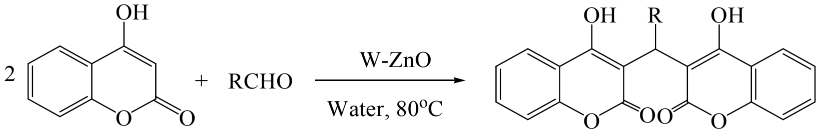
MCRs leading to interesting heterocyclic compounds are particularly important for the preparation of diverse chemical libraries of 'drug-like' molecules [1]. Coumarin derivatives have received considerable attention because of their biological importance and numerous pharmacological activities. Some coumarin derivatives, in general, and biscoumarins, in particular, are known for their antifungal,anti-HIV, anticancer, antithrombotic, anticoagulant, antimicrobial and antioxidant, cytotoxicity and enzyme inhibitory activities [2].

In this work,a new strategy has been introduced for the preparation of biscoumarins. In this regards, W-ZnO has been synthesized and new applications of this catalyst explored With the optimized conditions in hand, The catalytic process was performed in a liquid phase. In a typical reaction, 4-hydroxycoumarin (2.0 mmol), the corresponding aldehyde (1.0 mmol), H_2O (6.0 ml) and W-ZnO (20mg) were taken in a 50 mL round-bottom flask at 80 °C (Scheme 1).



Scheme 1

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Regio- and stereo selective synthesis of trans-imidazolidine-2-ones from trans-ketoaziridines

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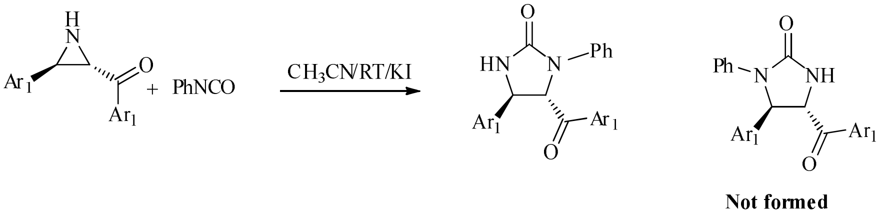
Aziridines are well known as useful reagents for the synthesis of many categories of nitrogen-containing compounds [1]. The coupling of an isocyanate and aziridine is an effective way to access heterocyclic ring systems [2].

Throughout our earlier studies [3], we motivated to imidazolidines via a regio- and stereo-controlled ring expansion of N-H ketoaziridines from aziridines and isocyanates (Scheme 1).



Scheme 1

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Fabrication of non-doped red organic light emitting diode using naturally occurring curcumin as a donor-acceptor-donor (D-A-D) emitting layer with very low turn-on voltage

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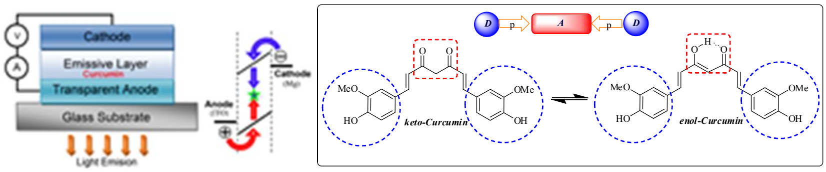
Curcumin is a naturally occurring yellow pigment used in spices, cosmetics and the traditional medicine treating wounds, infections, and other skin problems [1]. Curcumin has been used extensively for the construction of various compounds exhibiting a wide spectrum of biological activities [2]. However, there is no report for use of curcumin toward other applications especially in electrical devices.

The doping level in the fabrication of dopant-based red organic light-emitting diodes (OLEDs) is often low and confined in a narrow range which is not convenient for the rapid and mass production of OLEDs [3]. Nowadays, non-doped OLEDs have attracted increasing interest because they are the alternative method to the current fabrication process of red OLEDs [3]. Among many low band gap organic compounds, the donor-acceptor type of chromophores are particularly of interest as potential NIR chromophores because their band gap levels and other properties can be readily tuned through a variety of donors and acceptors. Π-conjugated donor-acceptor-donor (D-A-D) oligomer and polymers have been extensively investigated for their controlled optoelectronic properties that include linear and nonlinear optical effects [4]. Herein, we report the fabrication of redOLEDsusing naturally occurring curcuminas a donor-acceptor-donor (D-A-D)chromophore. The electroluminescent (EL) spectrum has the EL peak at 612 nm and the maximum external quantum efficiencies (EQE) for this device found to be 0.029 %.



Scheme 1

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Chemical composition of the essential oil teucrium polium L. from Iran

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Teucrium has been used since ancient time for a variety of medicinal purposes as anti bacterial, sedative, antipyretic and gastric lesions [1-3].

The Flora of Iran comprises 12 species of Teucrium of which 3 are endemic. Teucrium Polium L. [4].collected from sbzewar Province of ghorasan razavi and dryed in the shed and suitable air condition. The water- distilled essential oils of Teucrium Polium L. were analyzed by using GC and GC/MS instruments. Forty components, representing of the total components were identified 86.22%. The oil was characterized by larger amounts of monoterpenes (61.8%) and smaller amounts of sesquiterpenes (24.42%). The major monoterpenes in the oil were α- pinene (19.54٪) and β-pinene (10.71٪) limonene (8.22%) and myrcene (6.87). The major sesquiterpenes in the essential oil were Germacrene and transcaryophyllene (6.16% and 6.02% respectively) [5].

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Cu(II) Schiff base complex immobilized on magnetic nanoparticles as efficient catalyst for the oxidation of sulfides into sulfoxids

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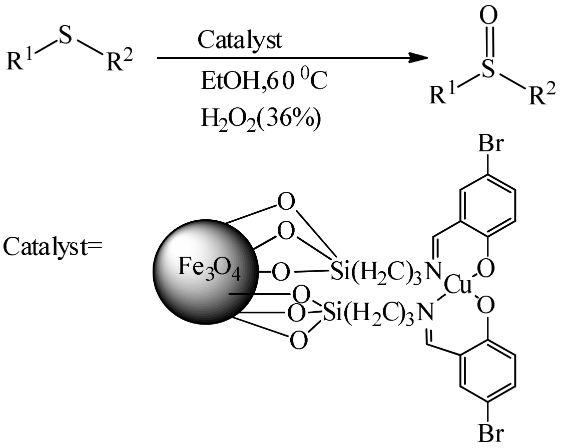
Catalytic oxidation processes play a key role in the manufacture of bulk and fine chemicals. Sulfides may be considered as important intermediates in organic chemistry owing to their versatile usage in fundamental research; especially the chiral sulfoxides serve as important intermediates in the synthesis of biologicallyand medicinally important compounds [1-2]. Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts in a wide range of reactions. These complexes have been extensively used for the hydrogenation of organic substrates, epoxidation of olefins, asymmetric ring opening of terminal epoxides and oxidation reactions [3].

In continuing our studies about investigation of new catalysts or catalytic methods in organic synthesis [4-5] we became interested to report preparation of functionalized magnetic nanoparticles Fe_3O_4 with Cu(II) Schiff base complex and its application as catalyst for the oxidation of sulfides to sulfoxidesusing hydrogen peroxide under mild cconditions (Scheme 1).



Scheme 1

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Computational studies of the proton affinity, theoretical spectroscopy (IR, Raman and NMR) and electronic investigations of thio-semicarbazone molecule

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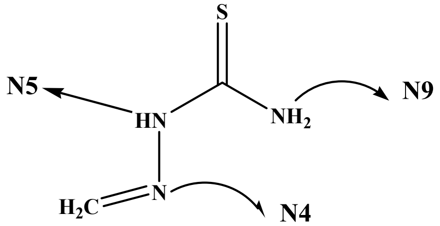
Thiosemicarbazone derivatives are widely used in the vast variety of complexes as a ligand [1-2], which have extensive medical effects [3-4]. Structural and electronic analysis can be used to comprehenddrug-receptor interactions. As the drug action correspond to electronic surface of the drug and the active site. The purpose of this research is to investigate the proton affinity, Electronic analysis using MEP(Molecular Electrostatic Potentials) and theoretical study of IR, Raman and NMR spectrum of the simplest form of the most stable tautomer of thiosemicarbazone (we previously reported). We have used four different methods (HF, B3LYP, MP2 and G2MP2) and different basis sets based on the accuracy of property that we need.



Protonation on N4, N5, N9
Scheme 1

References:

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Microsynthesis and mass spectral analysis of chemical weapons convention-related organophosphorus compounds

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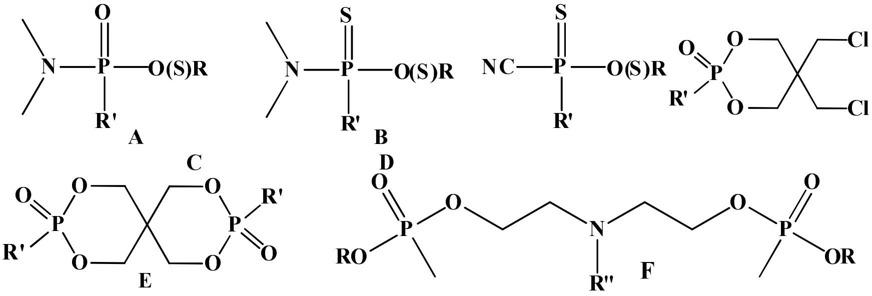
All activities related to the production, development, stockpiling and use of chemical weapons are forbidden by the chemical weapons convention (CWC), which came into force on 29 April 1997. The state parties to CWC have established the Organization for the Prohibition of Chemical Weapons (OPCW) to achieve the object and purpose of CWC. It is interesting to note that the Nobel peace prize for 2013 is to be awarded to OPCW for its extensive efforts to eliminate chemical weapons by the Norwegian Nobel committee. The availability of mass spectra and interpretation skills are essential for unambiguous identification of the CWC-related chemicals [1-4].

This paper describes a study on a general microsynthesis procedure for organophosphorus compounds (Scheme 1). Subsequently, electron ionization (EI) mass spectra of these chemicals, with possible fragmentation routes, were investigated via analysis of fragment ions of deuterated analogs and MS-MS experiments and DFT calculations. The results will make a substantial contribution to OPCW Central Analytical Database (OCAD) which may be used for detection and identification of CWC-related chemicals during on-site inspection and/or off-site analysis such as OPCW proficiency.



$R = CH_3, {}^{13}CH_3, CD_3, C_2H_5, C_2D_5, i\text{-}C_3H_7, i\text{-}C_3HD_6, \ldots$ $R'(R'') = CH_3, C_2H_5,$

Scheme 1

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A multi-component electro-organic assembling of aldehydes, phthalhydrazide and malononitrile to synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-diones

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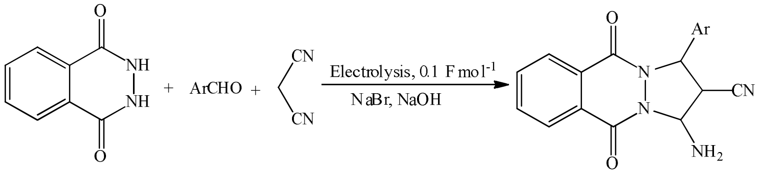
Multi-component reactions (MCRs) constitute an especially attractive synthetic strategy for rapid and efficient library generation due to the fact that the diversity can be achieved simply by varying the reacting components. Recently, the development and application of electrodes as catalyst in organic chemistry, have received considerable attention. This unique electrochemical procedure is valuable for large-scale processes because of its catalytic nature and the use of a cheap and environmentally responsible chemical reagent, namely electricity. They can be conducted at ambient temperature and pressure [1-3].

Due to our interest in the synthesis of heterocyclic compounds [4], we have developed a convenient and efficient method for the electrosynthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivatives through the reaction of aromatic aldehyde against malononitrile and phthalhydrazide inside an undivided cell where sodium bromide was present as electrolyte in ethanol medium. This procedure resulted in efficient and selective formation of the products in good yields and short reaction time.



Scheme 1

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Electrochemical synthesis of 2, 3-diaminophenazine

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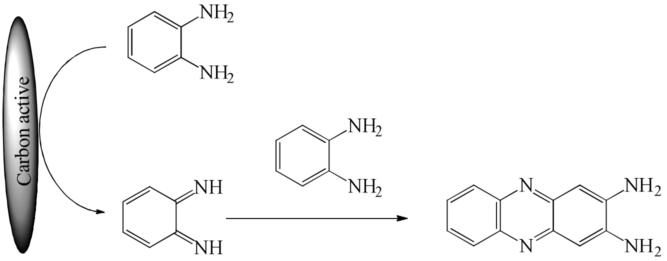
2, 3-Diaminophenazine (DAP) is important for its chemical and physical properties. Due to the importance of DAP in fluorescence sensitive assays and in the manufacture of conductive polymers, a great deal of effort has been devoted to the chemical synthesis of this compound [1, 2].

In this work, a simple and efficient method for the synthesis of DAP in aqueous solution using the electrochemical oxidation of *o*-phenylenediamine has been developed. The electrochemical synthesis of DAP has been performed at carbon rod electrodes in a divided cell using a constant potential. The results indicate that the quinone-diimine [3] obtained from electro-oxidation of *o*-phenylenediamine reacts with another molecule of o-phenylenediamine to form DAP (Scheme1). The electrochemical synthesis of DAP was also performed by means of constant current electrolysis to improve the applicability of the procedure.



Scheme 1

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Investigation of physicochemical properties of Lewisites using DFT calculations in support of the chemical weapons convention

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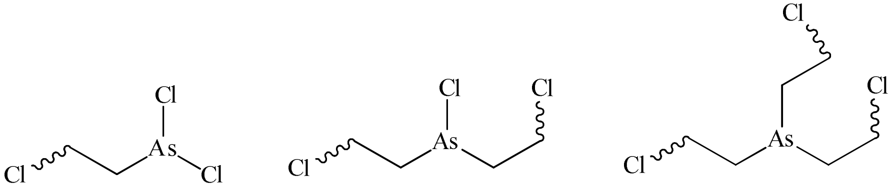
Chemical Weapons Convention (CWC) prohibits the production, storage and use of chemical weapons (CWs), and stated that all member states must destroy all the CWs over a fixed period of time [1]. Millions of chemicals are listed in CWC annex of chemicals in three distinct schedules. On the other hand, the CWC verification also includes identification of degradation products of CWC chemicals. Such large number of CWC-related chemicals puts more complexity to the analytical activities under CWC verification requirements which need unambiguous identification of chemicals in complex environmental samples. The compound 2-chlorovinyldichloroarsine (Lewisite I, Scheme 1), a powerful blistering agent first produced near the end of World War I, is capable of inflicting severe chemical burns of the eyes, skin and lungs [2]. The determination of the chemical properties of the various isomers of lewisite can aid in understanding data from the screening of possible lewisite antidotes. Also, this information can potentially lead to identifying whether a specific isomer of lewisite causes the vesicant injury. In this paper, DFT calculations were used for investigation of physicochemical properties of all isomers of Lewisite such as NMR data, electrophilicity index, structural data and the relative stability of the isomers. There is an obvious advantage to the application of computational methods to this highly toxic system.



Lewisite I
Lewisite II
Lewisite III

Scheme 1

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Morphology-controlled synthesis and electromagnetic properties of $PbFe_{12}O_{19}$ nanostructures

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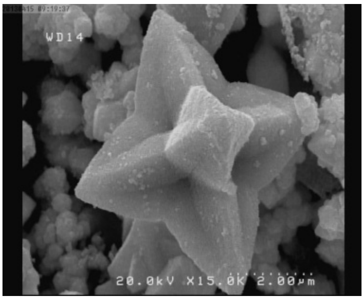
The development of Radar absorbing materials has been reviewed in several paper [1-2]. Exploitation of radar absorbing materials started in the 1930's shortly after the advent of radar. Absorber design has incorporated materials with different loss mechanisms and has made use of physical optics to optimise absorption over wide bandwidths. Absorbers therefore come with many different shapes and structures, ranging from thick pyramidal structures, to multilayers and single coatings.

Microwave absorbing materials have been used in commercial settings, for anechoic chambers and for reducing the reflected signals from buildings and superstructures around radar installations. Current communication technologies at microwave frequencies are driving the development of absorbers and frequency selective surfaces [3].In This Research Various morphologies of $PbFe_{12}O_{19}$ nanostructures were synthesized via a simple hydrothermal reaction. The effect of different parameters such as mol ratio, temperature and precursor on the morphology of the products was investigated. Result show that the as-obtained $PbFe_{12}O_{19}$ nanostructures show a strong photoluminescence peak at 400 nm at room temperature. The magnetic properties of the samples were also investigated using an alternating gradient force magnetometer (AGFM). We found that the $PbFe_{12}O_{19}$ nanoparticles exhibit a ferromagnetic behaviour with a saturation magnetization of 64 emu/g and a coercivity of 1640 Oe at room temperature.



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Boric acid as a new, effective and reusable catalyst for conversion of aldehydes and ketones to corresponding gem-dihydroperoxides

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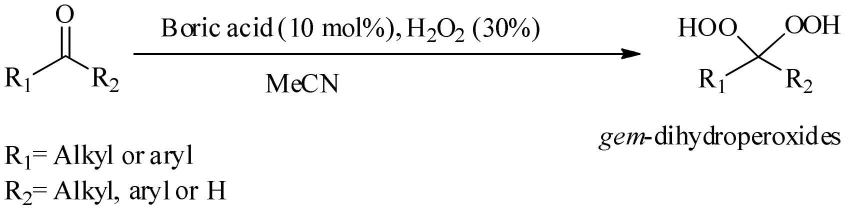
Gem-dihydroperoxides (DHPs) are considered as stable derivatives of ketones and aldehydes [1], which have been of considerable interest because of their relevance to peroxidic antimalarial drugs [2]. Also, these compounds are important intermediates in synthesis of a number of classes of peroxides including tetraoxanes, silateraoxans, spirobisperoxyketals, bisperoxyketals, and 1,2,4,5- tetraoxacycloalkanes [3]. *Gem*-dihydroperoxides have also been employed as reagents for oxidation reactions such epoxidation of α,β-unsaturated ketones, enantioselective oxidation of 2-substituted 1,4-naphtoquinones and oxidation of sulfides [4]. However, some methods have been reported to synthesis of *gem*-dihydroperoxides, many of these methods have certain drawbacks including the use of concentrated H_2O_2 and excess acid, low yield, limited substrate range and production of mixtures of peroxidic products. Also, poor selectivity and the presence of ozone sensitive groups in the substrates are further limitations in ozonolysis reaction.

Due to the importance of *gem*-dihydroperoxides, in this work, we wish to introduce the Boric acid as a low-cost, green and effective recoverable solid catalyst in the synthesis of gem-dihydroperoxides from ketones and aldehydes with 30% aqueous H_2O_2 at room temperature (Scheme 1). A variety of aldehydes and ketones have been converted to corresponding *gem*-dihydroperoxides by this method in excellent yields.



Scheme 1

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Synthesis of GAP base polyurethane/triazole network using isocyanate terminated hyperbranch prepolymer

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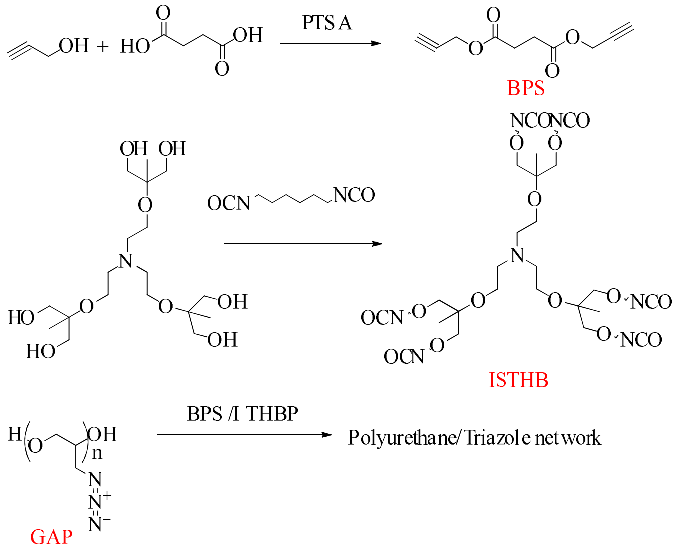
Glycidyl azide polymer (GAP) is one of the new types of polymers developed for advanced solid propellant application [1 – 3]. The main benefits of GAP are higher heat of formation and its compatibility with high energy oxidizers like AND and HNF, which results in higher specific impulses when it is used in propellant formulations. The chemical structure of GAP has two functional groups: hydroxyl and azide. So GAP can be cross-linked by diisocyanates, dipolarophiles or by dual curing method[9, 10].The present work focuses on obtaining a new type of dual curing agent by using BPS (bis propargyl sucsinate) and isocyanate terminated hyper branch prepolymer that can give a polyurethane/triazole network that have good and acceptable tensile strength and strain to new polymer network. The new polymeric network has synthesized via following routes:



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Optimizing of the production process of DPT explosive from hexamine dinitrate using central composite design of experiments

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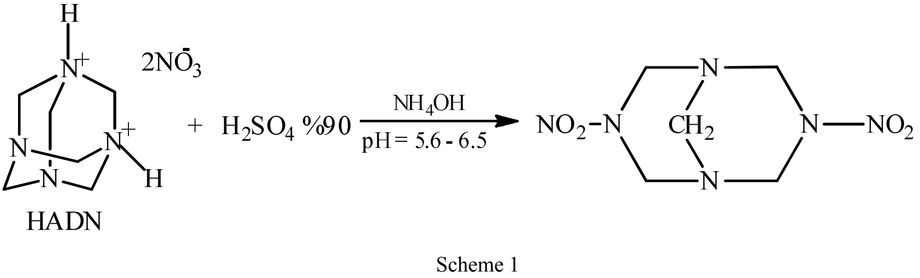
Dinitrosopentamethylenetetramine (*DPT*) bearing the IUPAC name of 3,7-dinitro-1,3,5,7-tetraazabicyclo[3,3,1]nonane and also 1,5-endomethylene-3,7-dinitro-1,3,5,7-tetrazacyclooctane, is a stable intermediate in the production of renowned explosives of HMX and RDX. This white-colored crystal solid has two polymorphs with melting points of 222-223 ºC and 204-205 ºC, the 'chair-chair' conformation of which is more stable. DPT contains two nitroamine groups with explosive properties [1]. HMX, DPT, and RDX are three nitroamines with similar chemical structures, among which DPT is the intermediate for producing the powerful explosive, hexamethylenetetranitramine (HMX), bearing particular importance in the production industry of energetic materials, and being considered a powerful explosive. DPT is a desirable and high efficiency substitute for RDX and HMX in weapon and rocket propellants. Various methods have been proposed for the production of this material, including hexamine in the presence of acetic acid [2], synthesis using nitrourea, synthesis using urea and nitroamide. All of which require a rather wide variety of raw materials, causing considerable increase in DPT production cost.

The present study proposed a desirable alternative for selective, inexpensive, and single-stage synthesis of dinitrosopentamethylenetetramine (*DPT*) form commercial raw materials by nitrating Hexamin Dinitrate (HADN), using commercial concentrated sulfuric acid solution, commercial concentrated nitric acid solution, and ammonia, resulting in a much cheaper and safer synthesis method compared to the existing methods. The required qualitative and quantitative analyses, including, ^{13}CNMR, and ^{1}HNMR, melting point analysis, were subsequently conducted to measure and approve the quality of the product. Furthermore, to optimize the production process, and evaluate the effects of different factors on the yield, a number of experiments were designed adopting central composite design (CCD) and using Minitab, the results of which were modeled and analyzed. Practical assessments and statistical analyses showed desirable consistency between the proposed model and the actual results, allowing for the possibility of the selective and inexpensive production of HMX explosive, at a % 46 yield and with high purity. The results furthermore indicated that the four major factors influential on reaction efficiency, namely, reaction temperature, the length of time of adding reagents, and the amounts of added sulfuric acid and nitric acid solutions, had considerable impacts on the yield and purity of the product, independently. Results obtained in this study are significantly helpful in determining the optimized production process of two-stage nitration of hexamine dinitrate into HMX explosive as well as in investigating the determining factors on its production process efficiency.



Scheme 1

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Assessment the practical impact of the controlled crystallization of HMX polymorphs

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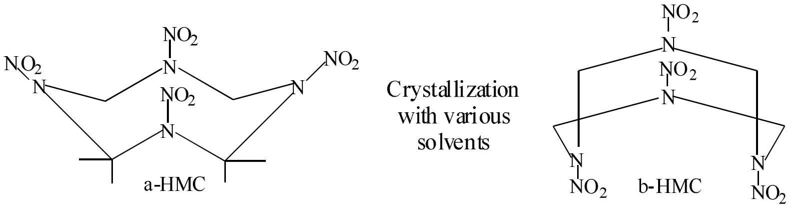
The solvent has a large effect on the crystal morphology of the organic explosive compound octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX, $C_4H_8N_8O_8$).It is a very important explosive of great power and brisance. HMX exists in four solid polymorphs, labeled α-, β-, γ-, and δ-HMX; reportedly each can be prepared by applying a specific cooling rate to the reaction solution. The β phase of HMX has the highest density and is the most stable at room temperature; it is also the form in which HMX is normally produced and used. The control of crystal morphology during the crystallization steps constitutes an important industrial challenge since the shape of a crystal affects solid–liquid separation characteristics, packaging, handling, drying, storage behavior and end-use properties of the crystallized material [1].

For the explosive compounds, an important product performance parameter is the packing density. A high packing density is needed to obtain a high explosive power in a small volume. The particle shape largely determines the packing density. Needles and plate-like crystal have a low density and thus are unwanted shapes. Higher packing densities can be obtained with isometric crystals. Besides, the sensitivity of the explosive compound is dependent on the crystal morphology to a great extent. Therefore, investigations on crystal morphology control are very important for the energetic materials [2].

At This study has been paid examines the role of various solvents at the conversion from polymorph α-HMX to β-HMX. That means has been converted from polymorph α-HMX to β-HMX with cheap price and the organic industry solvents in the country and with imposed digestion or dissolution conditions.

Then quantitative and qualitative analysis required, including X-ray diffraction (XRD) and optical microscopy photography has been done to identification and confirmation the quality of the product.



Scheme 1

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Synthesis, magnetic and electromagnetic properties of flower-like Fe_3O_4 with performance of microwave absorption

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In recent years, there is an intense interest in the hierarchical assembly of one-dimensional nanoscale building blocks into ordered superstructures because of their widespread potential applications in catalysis, drug delivery,acoustic insulation, photonic crystals, and other areas [1]. Moreover, the particular structural features of the hierarchical nanostructures have large surface areas and allow for heterostructures,which can be applied in photovoltaics and multifunctional nanoelectronics [2]. A dendrite is a kind of material that has a main stem from which many side branches grow out and a hierarchical structure with primary, secondary, tertiary, and even higher-order branches [3]. Flower-like microstructures were achieved with the phase transformation from dendritic α-Fe_2O_3 to Fe_3O_4 , Fe by partial and full reduction, and γ-Fe_2O_3 by a reduction - oxidation process..The Radar absorber materials were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared (FTIR), and UV–vis spectra. This Radar Absorbers exhibit ferromagnetic behavior with high saturation magnetization (Ms = 95 emu/g) and coercivity (Hc =112 Oe) at room temperature. The composites also own good microwave absorption properties, and the absorption bandwidth with reflection loss below 30 dB is up to 16.7 GHz in the 2–18 GHz frequency range.

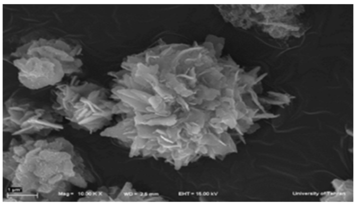

Fig. 1

References:

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Use of acidic ionic liquids for synthesis of HMX via nitrolysis of DPT

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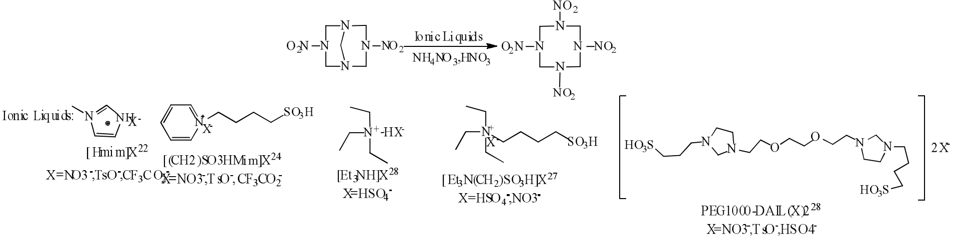
1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane (HMX) is one of the most powerful military explosives [1-2-3]. The conventional methods to synthesize HMX involve the nitrolysis of hexamine [3], DPT [4], TAT [5], DADN [5-6-7]. DPT can be obtained with high yield from broadly available and inexpensiveurea via nitrourea and/or dinitrourea [4-6]. of $HNO_3$was used. Some other HNO_3–NH_4NO_3-base systems were also investigated to afford HMX in moderate or low yields of 60%, 62% and 39% when MgO[9], P_2O_5[10] were added, respectively. ionic liquids (ILs) have attracted much attention as environmentally benign media or catalysts thanks to many interesting properties such as wide liquid range, negligible vapor pressure, high thermal stability, andgood solvating ability for a wide range of substrates and catalysts. Qiao et al. developed a silica gel-immobilized Brønsted ionic liquid and used it as recyclable solid catalyst in the nitration of aromatic compounds, which offered practical convenience for the separation of product from catalyst [8]. Qian et al reported the ultrasonic assisted nitrolysis of DAPT in [BMIM]$PF_6$to achieve HMX in a high yield of 66.8% [5]. Little attention has been paid to the nitrolysis of DPT in an acidic ionic liquid based system. Zhi et al reported a new method to synthesize HMX from DPT via nitrolysis using N_2O_5/HNO_3catalyzed with a new dicationic acidic ionic liquid PEG200-DAIL with 64% yield. In this paper, we investigated the application of a series of acidic ILs in the synthesis of HMX by nitrolysis of DPT with HNO_3 (see Scheme 1).The results showed that [Et_3NH] $HSO_4$was the best catalyst among 18 ILs used and the yield of HMX was up to 61% against 45% without IL.



Scheme 1

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Diimidazulium hypergolic ionic liquid synthesizes based on anion dicyanamide

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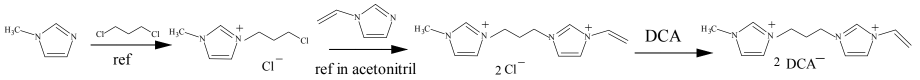
The design and synthesis of ionic liquids based on energetic materials provide a powerful methodology in the development of a new type of hypergolic fuel simply by the combination of different ions for a specific purpose [1]. This liquids tend to have low volatilities, high thermal and chemical stabilities, and often exhibit long liquid ranges which could allow utilization of these substances as replacements for the current bipropellant fuels which contain toxic hydrazine [2,3].

In this study, the synthesis of several new unsymmetrical diimidazolium ionic liquid with based on anion dicyanamide are as followed. for instance; initially, the monocation intermediate is synthesized by reacting with 1-methylimidazol by the 1,3-dichloropropane which is in excess during the reaction to decrease the symmetric dicationic byproduct; Then, the unsymmetrical dicationic compounds with the dicyanamide anion is synthesized by the metathesis reaction from the dichloride compound which is obtained; that shown in scheme 1.



Scheme 1

References:

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Solvent-free one-pot synthesis of 2,3-dihydroquinazolin-4(1H)-ones derivatives using *N*-halo catalysts

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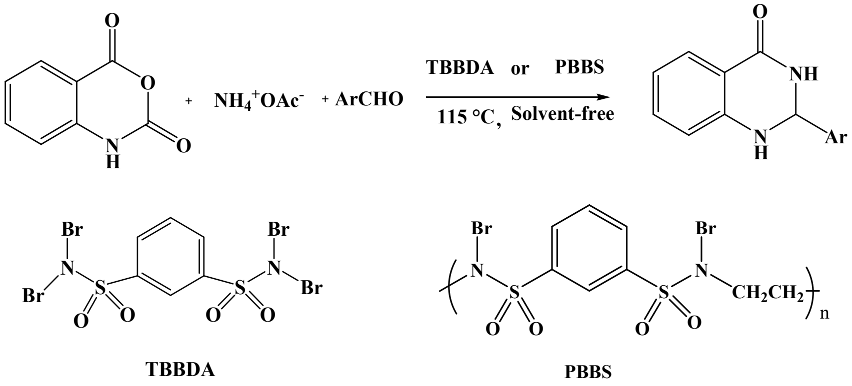
2,3-Dihydroquinazolinone-4-(1H)-one derivatives are an important class of fused heterocycle that display a wide range of biological, pharmacological, and medicinal properties involving antitumor, antibiotic, antipyretic, analgesic, antihypertonic, diuretic, antihistamin, antidepressant, and vasodilating activities [1].

One-pot three-copmonent condensation of isatoic anhydride with ammonium acetate and aromatic, aliphatic and heterocyclic aldehydes under solvent-free conditions in the peresence of a catalyst such as TBBDA or PBBS [2-3] provides high yields of the 2,3-dihydroquinazolin-4-(1H)-one derivatives (Scheme1).



Scheme 1

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Ultrasonic-assisted synthesis of tetrahydropyrimidine derivatives using functionalized core-shell nano-catalyst

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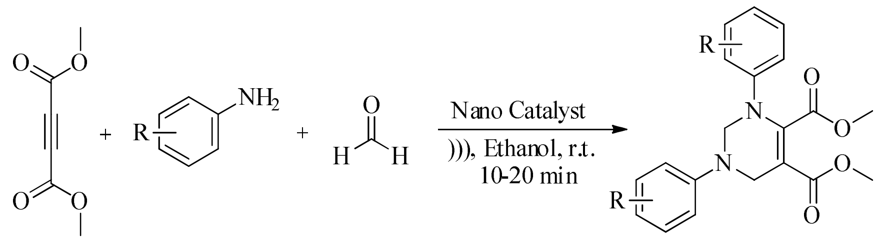
Pyrimidines and their analogues hold a special place among pharmaceutically significant natural products and synthetic compounds [1]. Tetrahydropyrimidine scaffold has displayed a fascinating array of pharmacological and biological activities such as antihistaminic, antibacterial activity and is the core unit in several biologically active HIV protease inhibitors, mycobacterium tuberculosis inhibitors and have served as muscarinic receptor agonists for treatment of Alzheimer's disease [2,3]. Hence, the synthesis of this class of compounds has gained great importance in organic and medicinal chemistry.

A survey of literature revealed that very few synthetic methods are reported for the synthesis of polysubstituted 1,2,3,6-tetrahydropyrimidines, which were also associated with drawbacks like low yields, high temperature, toxic catalysts, long reaction time, tedious work up and purification. Herein, we wish to report the sonically enhanced method for the synthesis of different 1,2,3,6-tetrahydropyrimidine derivatives via the one-pot reaction of dimethyl acetylenedicarboxylate (DMAD), aniline derivatives and formaldehyde in the presence of functionalized core-shell nano-catalyst under green chemistry conditions.



Scheme 1

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Efficient synthesis of dihydro[2,3-*c*]chromones contained chromonyl moiety in aqueous media

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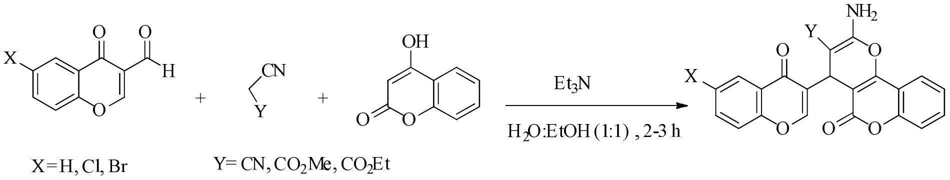
Chromone derivatives exhibited extended biological activities. Pyrano[3,2-c]chromones are valuable systems for the synthesis of pharmacological agents. Due to the wide applications of the pyranochromenes, there are considerable eforts for finding mild reaction conditions and also synthesis of functionalized pyranochromones. Recently, 3-formyl chromone with three electrophilic centers was used as a suitable substrate for the synthesis of various heterocyclic skeletons in our research group. Considering the bioactivities of the pyranochromone skeleton and also chromonyl moiety, we hypothesize that the integration of chromene scaffold with pyranochromene may result in the discovery of new bioactive compounds through synergism effect. In this work, we report a three-component reaction of 3-formyl chromone, 4-hydroxy coumarin and active methylene compounds such as malononitrile, alkyl cyanoacetates in aqueous media in the presence of catalytic amount of triethylamine as a base catalyst.

The structure of products was confirmed based on spectroscopic data. A characteristic signal for all these compounds appeared at δ 4.50-5.10 ppm as a singlet which is due to H-C(sp^3)-4. The investigation of the progress of reaction showed that the reaction could proceed through domino Knoevenagel/ Michael reaction.

Easy work-up, atom economy, convevenience, and the formation of no by-products are other attractive feature of this method. Investigation of the synthesized compounds is in progress in our group.



Scheme 1

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Spectroscopy and solvatochromism studies along with antioxidant and antibacterial activities investigation of aminothiophenoles based-azo-azomethine

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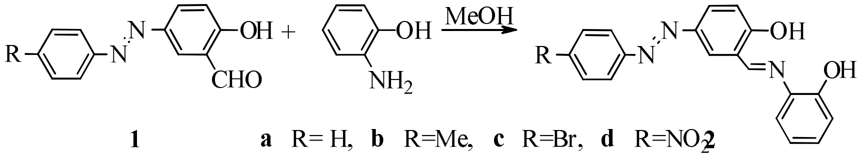
The azo-azomethine compounds 2-(2-hydroxyphenylimino)methyl)-4-phenyldi azenyl)phenol (**2a-d**) were prepared from the reaction of 2-aminophenol with 2-hydroxy-5-(aryldiazenyl)benzaldehyde(**1a-d**). The electronic absorption spectra indicated enol–keto tautomeric and positive solvatochromism in compounds (**2a-d),** which is dependent on the substitution, nature of solvent, pH and environment temperature. The prepared dyes show antibacterial and antioxidant activity. The prepared compounds are potentially an –N=N-, -C=N and O multidentate chelating ligand which could form stable complexes with metal ions.



1 **a** R= H, **b** R=Me, **c** R=Br, **d** $R=NO_2$

Scheme 1

References:

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Synthesis and characterization of Ni(II) Schiff base complex supported on nanomesoprous silica MCM-41 and its catalytic performance in the oxidation of thiols to disulfide using UHP as oxidant

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[b]*Department of chemistry, Faculty of science, Sayyed jamaleddin Asadabadi University, P.O. Box 6541835583 Asdabad, Iran; Email: e_nikoorazm@yahoo.com*

MCM-41 is a promising support, developed in the Central Research Laboratory of Mobil Research and Development Cooperation [1], in 1992. These materials have unique properties, such as high specific surface area and tunable and narrow pore size distribution. These features can be useful in many applications such as catalysis, photo catalysis, adsorption, gas separation and ion exchange [2,3].The Ni-grafted meso porous catalyst was prepared using 5-boromosalycylaldehyde as ligands. The compound was characterized by FT-IR, XRD, N_2 adsorption/desorption and TGA/DTA. In the other hand the conversion of thiols to the corresponding disulfides under mild condition plays an important role in synthetic chemistry and biochemistry. In this work the wide range of thioles were subjected to oxidation using UHP as oxidant in the presence of prepared catalystin acetonitrile. The high yields of disulfide products were obtained by this catalytic system indicate the high efficiency of Ni-salen-MCM-41 catalyst. It was also found the catalyst is active, stable and reusable (Scheme1).

$$\mathrm{RSH} \xrightarrow[\text{Ethanol, r.t}]{\text{Ni-Salen-MCM-41/UHP}} \mathrm{RSSR}$$

Scheme1

References:

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New bidentate Schiff base ligands derived from aniline derivatives: synthesis, characterization and crystal structure determination

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The *ortho*-hydroxy Schiff bases show thermochromism and photochromism via the intramolecular proton transfer. Photochromic compounds are used in optical switches and optical memories, variable electrical currents, and ion transport through membranes. In addition, they are widely used as ligands in the field of coordination chemistry as well as in diverse fields of chemistry and biochemistry owing to their biological activities [1-2].

In this research,we report the synthesis of new bidentate Schiff base ligands using reaction of 5-bromosalicylaldehyde with aniline derivatives in ethanol at room temperature. These ligands were characterized by ^{1}H NMR, IR, UV-Vis and their solid state structures were determined using single crystal X-ray diffraction.

The asymmetric unit of the *Para*-chloro aniline Schiff base ligand, Fig. 1, comprises a potentially bidentate Schiff base ligand. In the crystal structure, intramolecular O–H···N hydrogen bond makes *S*(6) ring motif. The crystal structure is further stabilized by intermolecular π···π interactions.

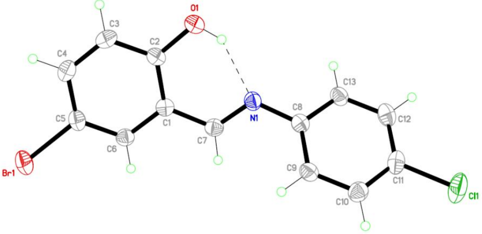

Fig 1

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Synthesis of 14-aryl-14H-dibenzo[a,j]xanthenes over sulfonic acid functionalized pyridinium chloride

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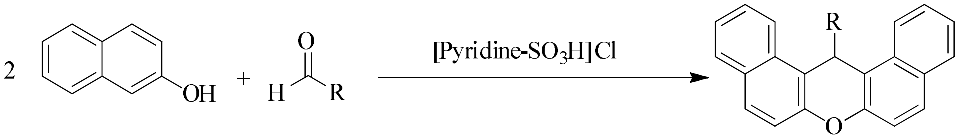
14-Aryl-14H-dibenzo[a,j]xanthene functionality is a key structural element of many biologically active compounds, such as antibacterials [1], antivirals [2] and anti-inflammatory agents [3], and in photodynamic therapy [4]. Xanthene-based compounds have also been investigated for agricultural bactericide activity and some other benzoxanthenes find applications in industry as dyes in laser technology [5] and fluorescent materials for visualization of biomolecules [6]. Xanthene dyes are extracted naturally from soil and plants such as Indigofera Longeracemosa [7,8].

In this work, we would like to introduce sulfonic acid functionalized pyridinium chloride as a highly efficient and heterogeneous catalyst for the preparation of 14-aryl-14H-dibenzo [a,j]xanthene derivatives by the reaction of 2-naphthol with aromatic aldehydes under solvent-free conditions (Scheme 1).



Scheme 1

References:

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Catalyst-free, solvent-free one-pot, four-component synthesis of 4*H*-pyrano[2,3-*c*]pyrazoles

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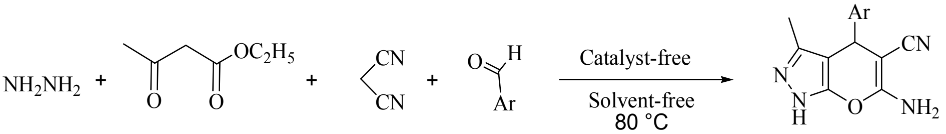
In recent years, focus on green chemistry by using environmentally benign reaction conditions is one of the most fascinating developments in synthesis of widely used organic compounds [1].

Pyrazoles and their derivatives are an important class of bioactive drug targets in the pharmaceutical industry, as they are the core structure of numerous biologically active compounds [2]. Morovere, the pyran pharmacophore is an important core structure of many natural products showing antibacterial, antitumor, antiallergic, antibiotic, hypolipidemic, and immunomodulating activities [3]. On the basis of biological studies, the existence of two or more different heterocyclic moieties in a single molecule often enhances the biological activity remarkably [4].

In continuation of our research based on green chemistry protocols [5], herein we would like to report a solvent-free, catalyst-free, four-component synthesis of 4*H*-pyrano[2,3-*c*]pyrazole derivatives under thermal conditions (Scheme 1).



Scheme 1

References:

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$FeNH_4(SO_4)_2.12H_2O$ as a heterogeneous catalyzed for one-pot synthesis of dihydroquinazolinon-4(1*H*)-one derivatives

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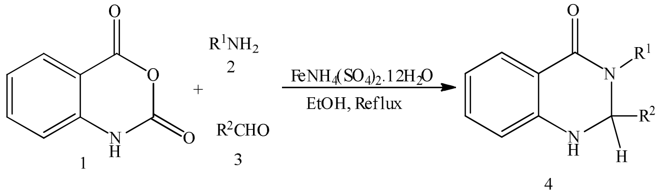
2,3-Dihydroquinazolinone derivatives have drawnmuch attention due to their broad range of pharmacologicalactivities such as antibiotic [1], antidefibrillatory [2], antispermatogenic [3], vasodilatory [4], and analgesic [5] ability.

Several methods have been reported for the synthesis of 2,3-dihydroquinazolinones.[6] In this work, we designed the synthesis of 2,3-disubstituted 2,3-dihydroquinazoline-4(1H)-ones **4** from isatoic anhydride **1**, primary amine **2**, and aldehyde **3** in the presence of catalytic amount of $FeNH_4(SO_4)_2.12H_2O$in ethanol.



Scheme 1

Refrences:

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One-pot three-component synthesis of tetrahydrobenzo[*b*]pyran derivatives using trichloroisocyanuric acid (TCCA)

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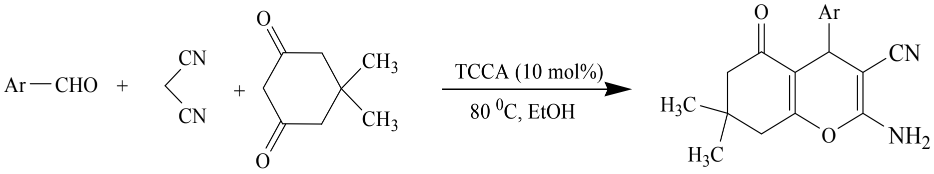
Compounds having dihydropyran structural motif exhibit a wide range of biological and pharmacological activities [1] which include spamolytic, diuretic, anti-coagulant, anti-cancer, and anti-anaphylactic properties. In addition, 4H-pyran derivatives have also been applied for the treatment of several neurodegenerative disorders, such as Alzheimer's disease, amyotrophic lateral sclerosis, Huntington's disease, and Parkinson's disease [2]. Furthermore, these compounds can be employed as pigments, photoactive materials and utilized as potential biodegradable agrochemicals [3].

Considering the importance of these compounds, numerous methods for the synthesis of 5-oxo-5,6,7,8-tetrahydro-4H-benzo[*b*]pyran derivatives have been reported. However, some of the reported methods have their own merits but at least one of the limitations such as poor yields, long reaction times, effluent pollution, harsh reaction conditions, and the use of complex, inaccessible, toxic or expensive reagents [4].

Herein, we wish to report an efficient method for the synthesis of 5-oxo-5,6,7,8-tetrahydro-4H-benzo[*b*]pyran derivatives from one-pot three-component condensation of aromatic aldehydes 1, malononitrile 2 and dimedone 3 in the presence of catalytic amounts of TCCA as a safe, stable, and cheap commercially available reagent in very short times (Scheme 1).



Scheme 1

References:

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Computational study on Diels-Alder reaction of chiral cyclopropenyleketones

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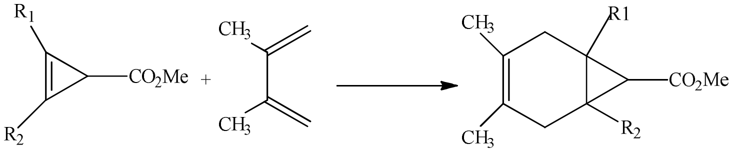
For many years, cyclopropenes have been recognized as reactive dienophiles in the Diels-Alder reaction [1], and high diastereoselectivity has been observed in the Diels- Alder reactions of cyclopropenes with alkadienes [2].

Then in this research a theoretical study for the Diels-Alder reactions between cyclopropenyle ketones derivatives and 2, 3-dimethylbutadiene has been carried out by density functional theory (DFT) method. The results of calculations showed four possible reaction channels.

The reaction and relative energies were investigated for all of the Channels, which the channel with *exo*-trans transition state was lower than others.Also the local and global electronic factors Calculated at DFT method for stationary points to investigate the regio selectivity of products of cyclopropene with C-3 hydrogen.



Scheme1

Refrences:

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A novel three-component, one-pot synthesis of 10,10-dimethyl-7-phenyl7,10.11.12-tetrahydro-9H-benzo[*c*]acridin-8- one derivatives.

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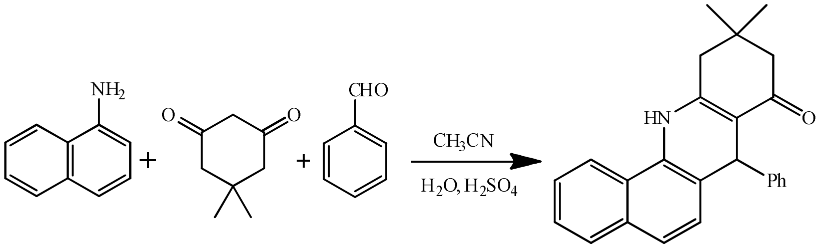
The concept of privileged medicinal structures or scaffolds [1] has emerged as one of the guiding principles of the drug discovery process. These privileged scaffolds, such as substituted benzoxanthenes, dihydroquinoline and naphthoquinones, commonly consist of a rigid heterocyclic system with well-defined orientation of appended functionalities for target recognition [2]. Multicomponent reactions (MCRs) constitute an especially attractive synthetic strategy due to the fact that the products are formed in a single step and diversity can be achieved simply by varying the reacting components [3]. In continuation of our previous work on the synthesis of heterocyclic compounds and MCRs, we wish to report a Facile and convenient one-pot syntheses of 10,10-dimethyl-7-phenyl7,10.11.12-tetrahydro-9H-benzo[*c*]acridin-8-one

derivatives, have been reported under extremely mild reaction conditions using a catalytic amount of H_2SO_4 in water, which could be recycled.



Scheme 1

References:

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Synthesis of 4,4′-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s using $Fe_3O_4@SiO_2@C_3H_6NH_2$

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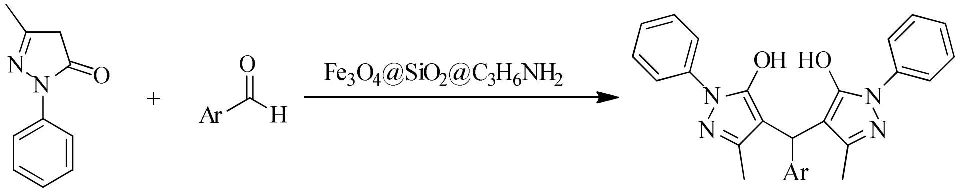
Pyrazolone derivatives are of importance as they have various biological activities; these compounds are essential scaffold of many commercialized drugs for brain ischemia [1], and myocardial ischemia [2]. Moreover, 4,4-(arylmethylene)-bis(3- methyl-1-phenyl-1H-pyrazol-5-ol)s, as an important class of pyrazolones, have been used as anti-inflammatory [3], antipyretic[4], gastric secretion stimulatory [5], antidepressant [6], antibacterial and antifilarial agents. These compounds have been also applied as fungicides, pesticides, insecticides, dyestuffs, and chelating as well as extracting reagents for different metal ions [7].

In this work in continuation of our previous projects involving applications of heterogeneous catalysts in organic transformations, we have used $Fe_3O_4@SiO_2@C_3H_7NH_2$ for the synthesis of 4,4′-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s by the condensation of 1-phenyl-3-methylpyrazol-5-one with various aromatic aldehydes under mild conditions, which exhibits many interesting properties (Scheme 1). Moreover, some theoretical studies have been carried out on the products.



Scheme 1

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A mild and efficient one-step synthesis of flavanones

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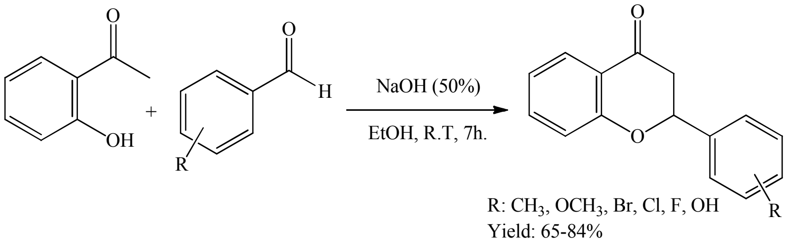
Flavanones, which exhibited broad spectra of biological activities, have attracted the interest of chemists from earlier stages to the present [1].

Flavanones have broad range of biological activities [2]. These compounds are known to exhibit several useful biological properties including anti-inflammatory, antibacterial, and anti-AIDS drugs [3].

Flavanones are commonly synthesized via condensation between 2′-hydroxyacetophenone and a benzaldehyde [4].

In this work, A simple, mild and practical procedure has been developed for the synthesis of flavanones. In this regards, a variety of flavanones have been prepared via combination of aromatic aldehydes, 2′-hydroxyacetophenone and Ethanol in the presence of 50% NaOH aqueous solution at room temperature (Scheme 1).



R: CH_3, OCH_3, Br, Cl, F, OH
Yield: 65-84%

Scheme 1

References:

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Reaction of aziridine and thioglycolic acid

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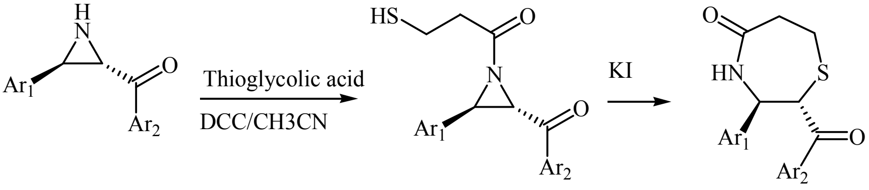
Aziridine functionality represents a valuable three-membered ring system in modern synthetic chemistry. It is well recognized as a significant building block for synthes of many useful compounds [1]. which are biologically important [2].

Our study in the transformation of the aziridine ring to regio-isomers of oxazoline (*via* C-N bond cleavage), oxazoles (*via* C-C bond cleavage), or alkenes lead us to synthesis of some new Heterocycles.

Treatment of aziridine with thioglycolic acid in present of DCC (N,N'-dicyclohexylcarbodiimide) in acetonitrl under refluxingcondition give N-acyl aziridines(scheme 1).



Scheme 1

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Clean and efficient synthesis of tetrahydrobenzo[b]pyrans using nano-magnetite titanium dioxide under solvent free condition

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[a]*Faculty of Chemistry, Bu-Ali Sina University, Hamedan, 6517838683, Iran.*
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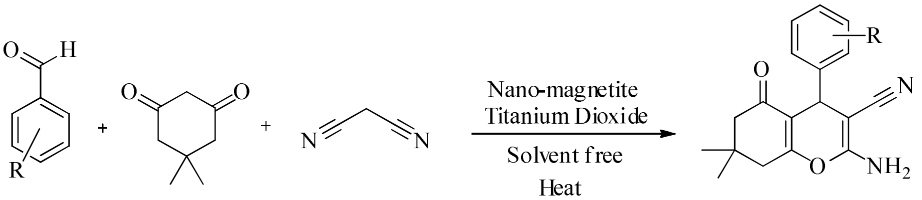
The preparation of tetrahydrobenzo[b]pyran derivatives is important because of their significant anti-coagulant, diuretic, spasmolytic, anti-cancer, and anti-anaphylactic properties [1]. 2-amino-4H-pyran derivatives can be widely applied as photoactive materials [2]. Moreover, substituted 4H-pyrans are observed as units in the structure of some natural products [3, 4]. Several methods have been introduced for the synthesis of tetrahydro4H-benzopyran derivatives [5-7]. However, some of them suffer from one or more drawbacks such as the use of toxic metals, the use of volatile organic solvents, high cost and low yields.

Having the above facts, we would like to introduce Nano-magnetite titanium dioxide as a highly efficient and reusable catalyst for the synthesis of tetrahydrobenzo[b]pyrans via the one-pot three component reaction of various aldehydes, dimedone and malononitrile under solvent-free condition (Scheme 1).



Scheme 1

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A novel three-component, one-pot synthesis of [(1H-Indol-3-yl)-phenyl-methyl]-phenyl-amine derivatives.

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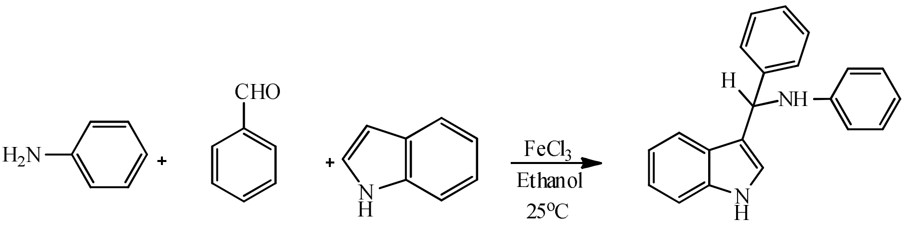
Multicomponent reactions (MCRs) constitute an especially attractive synthetic strategy due to the fact that the products are formed in a single step and diversity can be achieved simply by varying the reacting components.[1] Multicomponent reactions are performed without need to isolate any intermediate during the reaction, which *reduce* the amount of *time* and *energy* Used.[2] In continuation of our previous work on the synthesis of heterocyclic compounds and MCRs, we wish to report a new strategy, novel, efficient, one-pot method for the preparation of [(1H-Indol-3-yl)-phenyl-methyl]-phenyl-amine Derivatives. In the presence of $FeCl_3$ as catalyst the one-pot reactions of aniline, aromatic aldehydes and indole in ethanol at room temperature proceeded smoothly to give [(1H-Indol-3-yl)-phenyl-methyl]-phenyl-amine in good yields.



Scheme 1

References:

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Alkylation of anilines derivatives with arylmethanols in presence of $Fe(ClO_4)_3/SiO_2$

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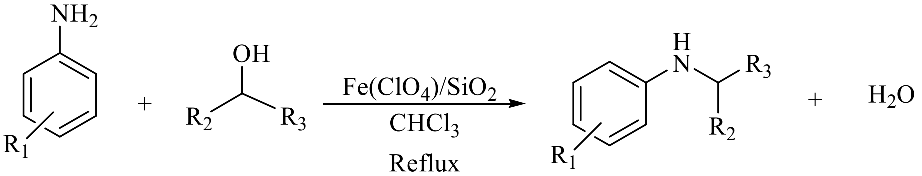
Aromatic secondary amines have broad applications in pharmaceutical, polymer, photographic, pigment, and electronic industries [1]. One of the best-known examples is their utility as antioxidant additives in polymer and rubber products [2].There are two aniline-based methods to prepare aromatic secondry amines: N-alkylation with halides in the presence of a base [3,4],and reductive amination with carbonyl compounds [5]. In recent years, transition metal-catalyzed hydroamination of alkenes or alkynes, amination of aryl halides, and N-alkylation of arylamines have been developed. This article introduces $Fe(ClO_4)_3/SiO_2$-promoted alkylation of anilines with arylmethanols in $CHCl_3$ under reflux conditions (Scheme 1).



Scheme 1

References:

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A new approach for C-substitution of 5-bromo-2,4-dichloro-6-methyl pyrimidine

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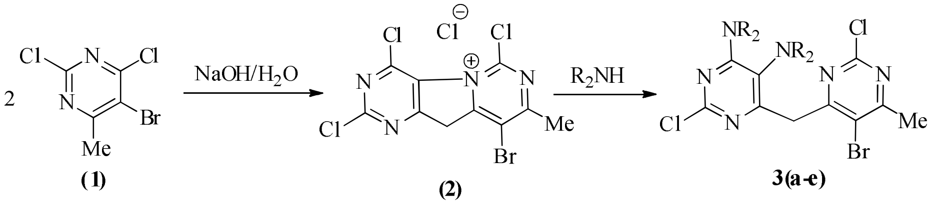
Heterocyclic compounds are present in a lot of bioactive compounds like DNA and RNA as pyrimidines and purines heterocyclic ring system. The biological significance of pyrimidine derivatives and structural similarities of these compounds with bioactive ones gave a prosperous scope to these compounds [1-4].

In this study, initially, 5-bromo-2,4-dichloro-6-methyl pyrimidine (1) was synthesized according to our previous procedure [5]. The treatment of this compound with aqueous solution of NaOH gave quantitatively the novel an unexpected heterocyclic compound (2) which its structure was confirmed by its spectral and micro analytical data. The reaction of various secondary amines with this compound was also evaluated.



Scheme 1

References:

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Efficient and selective oxidation of alcohols catalyzed by a tungsten based nanocatalyst

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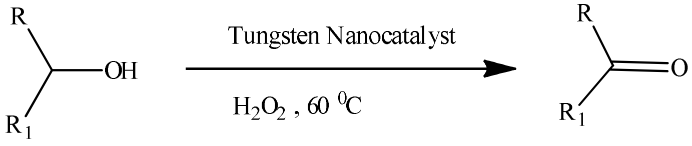
In recent years considerable efforts has been directed towards the transition metal catalyzed oxidation of organic compounds .Among them, oxidation of alcohols to aldehydes and ketones has specially been attended a lot, since carbonyl compounds are important intermediates in organic synthesis. Herein, we used a high- yield (70-90%) and selective oxidation procedure for the conversion of benzylic alcohols with various electron releasing and electron withdrawing substitutions, to corresponding aldehydes and ketones at 60℃ with H_2O_2 as oxidant, in the presence of tungsten nanocatalyst, and green solvent DMF with short reaction times and high yields. The presence of electron releasing and electron withdrawing substituents in ortho or para positions shows that the importance of steric and electronic effects due to high activity of the catalytic system are lower than expected. The presence of the catalyst seriously affects the oxidation of alcohols by O_2 and H_2O_2.



R = Aryl
R_1 = H, Alkyl, Aryl

Scheme 1

References:
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Synthesis of modafinil drug using ultrasonic

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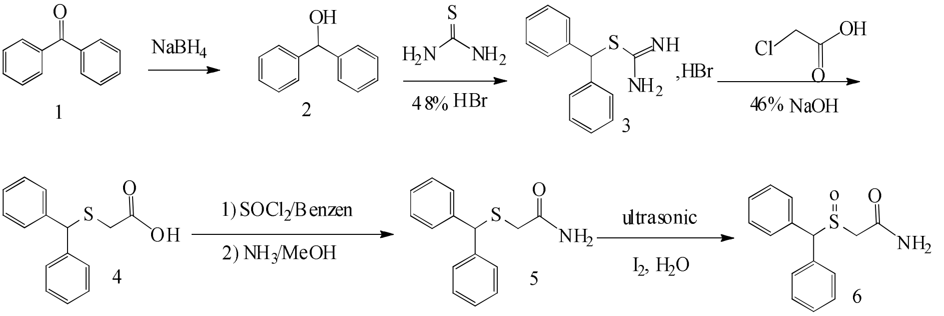
Narcolepsy is a sleep disorder that affects approximately 0.06% of the population in North America and Western Europe.[1] It is a disabling, neurological disorder that is characterized by chronic sleepiness and a marked disorganization of sleep/awake behavior. Psychostimulants, such as modafinil, are used clinically for treatment of narcolepsy, as well as attention deficit/hyperactivity disorder (ADHD) [2,3]. The synthesis of modafinil, begins with the reaction of benzophenone with sodiumborohydride. Then, the reaction of benzhydrol and thiourea in HBr to afford benzhydrylthioureniume 3 in 80% yield. Then producing diphenylmethylthioaceticacid by chloroaceticacid. The reaction of modafinic acid 4 with thionyl chloride in benzene followed by treatment of the corresponding acid chloride with concentrated ammonium hydroxide gave acetamide 5 in 87% yield. Finally, oxidation of sulfide group by mixture of H_2O/I_2 in ultrasonic, the target molecule was synthesis after 4 hours with 59.5% yield. The stractures of products was assigned by^1 HNMR,^{13} CNMR and IR (Scheme 1).



Scheme 1

References:

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Efficient methods for the synthesis of functionalized fluorenes containing spirooxindole moiety

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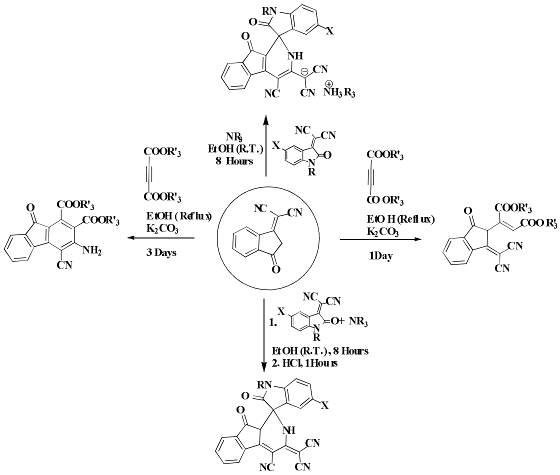
Fluorene and fluorene derivatives are important compounds and have different types of biological activities, such as anti-inflammatory and antitumor activites [1]. These compounds also have gained much attention due to their potential application in electronic devices such as light-emitting diodes [2].

Indole and indoline are important fragments of a large number of natural products and medicinal agents [3], and several indolines, spiro-annulated with heterocycles at the 3-position, have shown good biological activity [4]. The spirooxindole system is the core structure of many pharmacological agents and natural alkaloids [5].

In continuation of our interest on the synthesis of new heterocyclic compounds, herein, novel methods for the synthesis of highly functionalized fluorenes and spirooxindole-fused fluorenes are reported.



Scheme 1

Prominent among the advantages of this method are operational simplicity, good yields, mild reaction conditions and easy work-up procedures employed.

Refrences:

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Synthesis of coumarin and biscoumarin derivatives using $AgTiO_2$ nanocomposite as a reusable catalyst under ambient temperature

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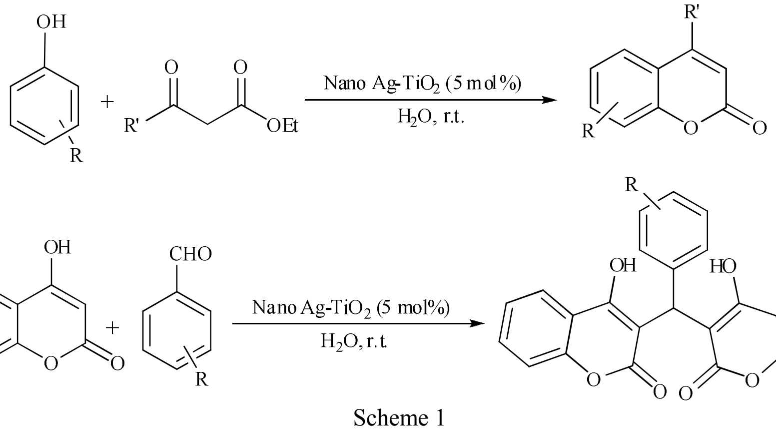
Nanomaterials, due to their reduced size and dimension, possess remarkable properties not seen in their bulk form [1]. Nanomaterials have attracted extensive interest for their unique properties in various fields such as catalytic, electronic, and magnetic in comparison with their bulk counterparts [2]. The synthesis of coumarin and biscoumarin derivatives has attracted considerable notice of many organic and medicinal chemists for several years. This interest arises from the fact that a variety of natural and synthetic compounds which contain the coumarin substructure and biscoumarins, exhibit significant biological activities such as urease inhibitory [3], cytotoxicity, enzyme inhibitory activities [4], antifungal, anti-HIV, anticoagulant, antithrombotic, anticancer, antioxidant and antimicrobial [5].

Herein, we report an efficient process for the preparation of coumarin derivatives using the nano $Ag-TiO_2$ as a catalyst in the Pechmann reaction. In proportion to Scheme 1, the synthesis was prepared through a mixture of phenol derivatives with a *β*- ketoester in water solvent under ambient temperature. Furthermore, we statement a well-organized method for the preparation of biscoumarin derivatives using 5 mol% nano $Ag-TiO_2$ as a catalyst in the condensation reaction of 4-hydroxycoumarin with aromatic aldehyde in water solvent at room temperature (Scheme 1).



Scheme 1

References:
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A novel and efficient one-pot three-component procedure for the synthesis of 4H-benzo-[b]-pyrans

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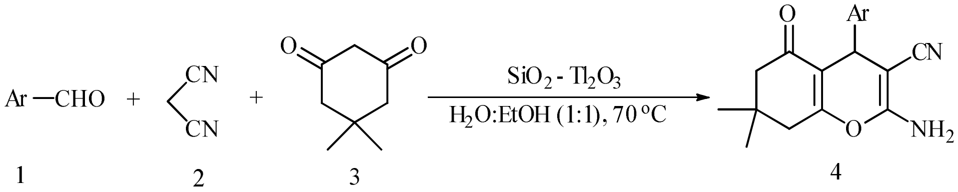
4H-Benzo-[b]-pyrans are an important class of heterocyclic compounds, which are employed in the area of pharmaceuticals and therapeutic such as antiallergic, antibacterial [1,2], anticoagulant, and anticancer activities [3]. Furthermore, 4H-benzo-[b]-pyrans have been used as pigments, cosmetics, and potential biodegradable agrochemicals [4]. For these reasons, the syntheses of 4H-benzo-[b]-pyrans have become an interesting field in synthetic organic chemistry.

Herein we wish to report a fundamentally new procedure to the synthesis of 4H-benzo-[b]-pyrans by the multicomponent reaction between aromatic aldehyde, malononitrile and dimedone in the presence of catalytic amounts of silica Tl_2O_3 under mild condition (Scheme 1).



Scheme 1

This method has advantages such as available starting material, the use of the clean, and recoverable catalyst, simple procedure, good to excellent yield of the products, the avoid of any toxic and expensive solvent.

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A facile, one-pot and direct synthesis of lauryl polyglucoside

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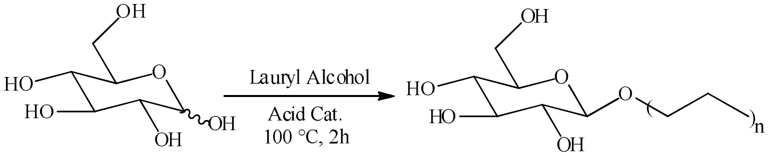
Alkyl polyglycosides (APGs) represent a nonionic surfactant class produced on a large scale. They are being used in a wide range of technical and consumer products, such as detergents, cleaning agents, cosmetic products and pesticide formulations, because of their excellent behavior at interfaces [1]. Previous works represented an indirect synthesis of APGs also known as transglucosidation [2].

In the present work, a direct synthesis for the preparation of alkyl polyglucosides has been introduced. A mild acidic catalyst, namely *p*-toluene sulfonic acid or preferably linear alkyl benzene sulfonate was employed. The product could be characterized by its surface properties, IR spectroscopy, C-NMR and H-NMR spectra [3].



Scheme 1

References:
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One-pot clean and efficient synthesis of 1,8-dioxo-decahydroacridine derivatives using nano zinc oxide via Hantzsch condensation

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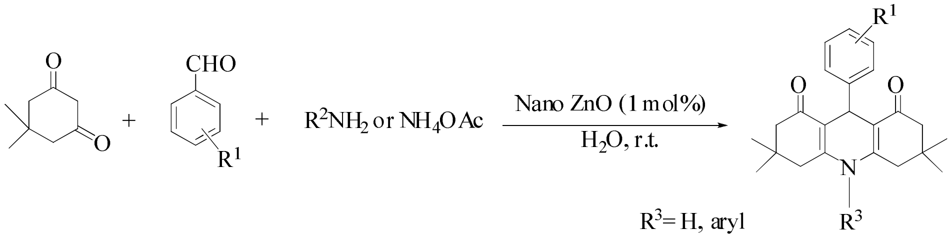
Nanomaterials are drawn in a number of fields such as chemistry, electronics, sensors, and catalysts [1]. Because of NMs dimensions, which differ from the isolated atoms and the bulk phase, the NMs properties are special [2]. Therefore the design and synthesis of novel materials with modified properties are targeted by different researchers [3]. The heterogeneous catalyst shows the great application and benefits in different industries [4].

In this study, the catalytic property of zinc oxide in the synthesis of 1,8-dioxo-decahydroacridines was investigated. The one-pot three component reaction of dimedone, aromatic aldehydes and aromatic amines and ammonium acetate in water afforded the subsequent 1,8-dioxo-decahydroacridine derivatives in excellent yields. This reaction has been carried out in the presence of 1 mol% of catalyst at room temperature. Also, this catalyst possesses several advantages including lower catalytic loading, mild reaction condition, high yield of the products, shorter reaction times, and also including the economically and cleanly of the reaction (Scheme 1).



Scheme 1

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Cu(I)-catalyzed synthesis of 1,2,3- triazole compounds in pure water

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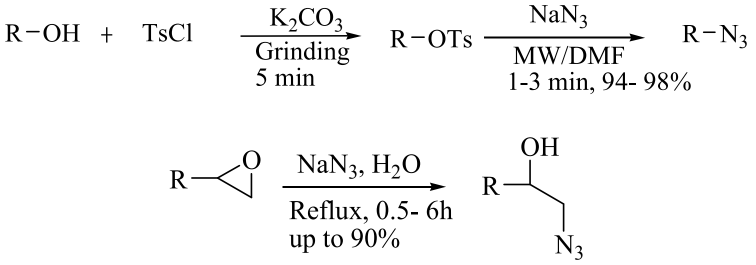
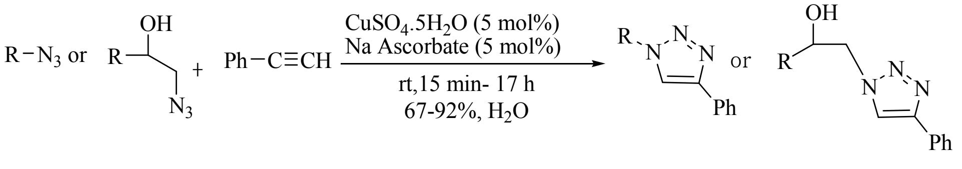
The Cu(I)-catalyzed azide alkyne cycloaddition (CuAAC), one of the most reliable click reactions, has enabled practical and efficient preparation of 1,4-disubstituted 1,2,3-triazoles from a wide range of substrates with excellent selectivity [1]. The CuAAC has found wide spread application in drug discovery, material science and bioconjugation [2]. In the recent past, water has become the solvent of choice to perform many organic transformations, this being one of the most abundant, cheapest and greener solvents [3].

In this work, at first the alkyl azides have been prepared from alcohols and epoxides used as starting materials under green chemistry conditions. Then, the prepared organic azides were reacted with phenyl acetylene in the presence of catalytic amounts of Cu(I) ions in pure water. In this method, the corresponding 1,2,3- triazols were synthesized in the short reaction times and very good yields according to green chemistry principles.



Scheme 1



Scheme 2

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Synthesis of thiazol-2-imine derivatives via a one-pot reaction of primary amines, α-chloroacetaldehyde, and phenylisothiocyanate

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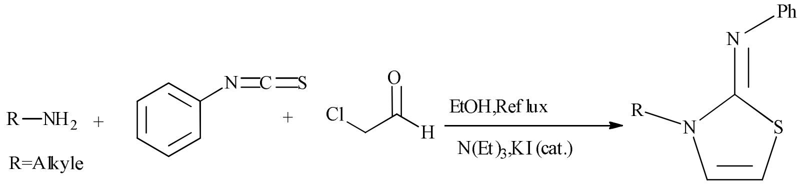
The design of one-pot reactions is an important field of research in organic synthesis. These reactions afford good yields and ready operations. The thiazol-2-imine ring system has attracted considerable attention due to its presence in several drug candidates with different biological activities [1] such as anti-inflammatory, analgesic and kinase (CDK1, CDK5, and GSK3) inhibition [2], antifungal [3], and melanin-reducing activity.

In this work we wish to report a simple one-pot procedure for the synthesis of thiazol-2-imine derivatives via the reaction of primary amines, α-chloroacetaldehyde, and phenylisothiocyanate in the presence of a catalytic amount of triethylamine and potassium iodide in ethanol (Scheme 1).



Scheme 1

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A simple and clean procedure for synthesis of spirooxindoles

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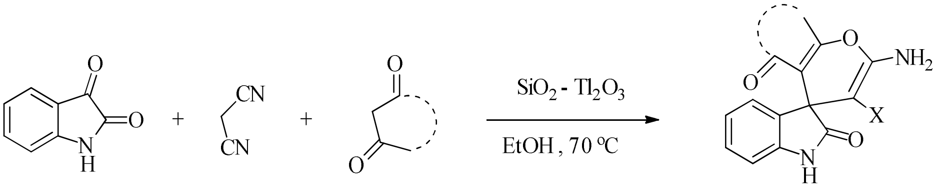
Spirooxindoles are core structures, in numbers of natural, pharmacological, and biological compounds, including cytostatic alkaloids such as spirotryprostatins A, B, and strychnophylline. In addition, the unique structural array and the highly pronounced pharmacological activity displayed by the class of spirooxindole compounds have made them attractive synthetic targets [1,2]. The application of heterogeneous catalysts to carry out various organic transformations has great importance in organic synthesis. These catalysts can conveniently be handled and removed from the reaction mixture, making the experimental procedure simple and ecofriendly [3].

In this work we used silica Tl_2O_3 as an efficient heterogeneous catalyst for the synthesis of spirooxindoles via condensation of isatin, malononitrile, and 1,3-dicarbonyl compounds in ethanol at 70 °C (scheme 1). This one-pot procedure is very simple and affording good to excellent yields. Structures of spirooxindoles identified by spectroscopic methods such as FT-IR and ^{1}H-NMR.



Scheme 1

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Cationic polyurethane as an eco-friendly polymeric catalyst for Cannizzaro reaction

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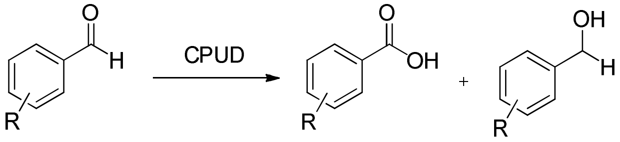
Green chemistry is a rapidly developing and an interesting area in the chemical science. Among the purposes of green chemistry, using efficient and eco-friendly catalysts have been in focus [1]. Cationic polyurethane dispersions (CPUDs) are important eco-friendly polar polymers. Polyurethanes are commodity synthetic polymers and have a broad range of well-known applications, nevertheless their possible use as a green catalyst or solvent is yet unknown [2]. To the best of our knowledge, there is no report in open literature concerning the using PUD as a green catalyst for synthesize of organic chemicals.

Herein, we report the first example of the CPUD application as a novel, green, expeditious, very mild, recyclable, biocompatible and very remarkable polymer solvent and catalyst for Cannizzaro reaction. The redox disproportionation reaction of non-enolizable aldehydes was performed under very mild conditions and room temperature in the presence of the CPUD. (Scheme 1).



Scheme 1

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An efficient and one-pot synthesis of 6-aryl-8H- dibenzo [d,h][1,3,7,2] dioxazaborecin-8-ones: using polyurethane at room temperature

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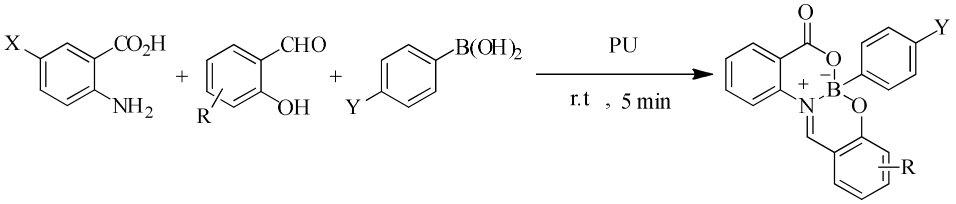
Multi-component reactions (MCRs) have emerged as an efficient and powerful tool in modern synthetic organic chemistry due to their valued features, such as atom economy, straightforward reaction design, and the opportunity to construct target compounds by the introduction of several diversity elements in a single chemical event [1].

In this work, we report a new and efficient strategy for the synthesis of 6-aryl-8H dibenzo[d,h][1,3,7,2]dioxazaborecin-8-ones, which are of potential chemical, synthetic, and pharmacological interest [2]. We have established a new method for the one-pot assembly of boron heterocycles based on 2-aminobenzoic acids, 2-hydroxybenz aldehydes, and arylboronic acids, in the presence of polyurethane (PU) at room temperature (Scheme 1).



Scheme 1

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Theoretical studies on structure, conjugation, resonance and stability in pyridine–derived and pyranylidene carbenes

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All calculations were performed using Gaussian 03. All structures were optimized using hybrid functional B3LYP9 and 6-31G** basis set without any symmetry constraints.[1,2]

Singlet–triplet energy splittings, relative energies and LUMO–HOMO energy gaps of various electron-deficient pyridine-Derived and pyranylidene carbenes are investigated using DFT calculations. Three diverse quantitative aromaticity indices: the nucleus independent chemical shifts (NICS) [3, 4], the aromatic stabilization energies (ASE) [5], harmonic oscillator measure of aromaticity (HOMA) are employed to investigate aromaticity of this molecule. [6, 7]

The results show that in all of these coumponds singlet carbenes are more stable than triplet carbenes. In general, singlet- triplet energy solittings, aromaticity in N-carbenes are more than O-carbenes.

The nucleophilicity O-carbenes are lawer than N-carbenes and based on $\Delta E_{\text{Homo-Lumo}}$, N-carbenes are harder than O-carbenes.

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Synthesis and the interaction of new water-soluble metal Schiff base complex with DNA

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Uranyl ion (UO_2^{+2}) having favorable photophysical properties and high bond affinity toward phosphate backbone across the minor groove of DNA, is worth pursuing as a possible photonuclease. Beside this ion was found to be potentially important in many biochemical applications such as probing local DNA structure and metal ion-bonding sites in a DNA [1,2].

In earlier investigations, $UO_2(CH_3COO)_2.2H_2O$ and $UO_2(NO_3)_2.6H_2O$ salts have been used in photoinduced DNA scission and other biochemical applications. However, one of the major disadvantages of working with simple UO_2^{+2} salts for a wide range of biochemical applications is that, the PH must be maintained as neutral or highly acidic to prevent the uranyl ion from forming insoluble aggregate [3].

Here, to circumvent this problem, we synthesized a new UO_2^{+2}- Schiff base complex, $[UO_2(\text{Schiff base})(H_2O)]$, Schiff base = $pn(acac)_2$ with good solubility in water within the physiological PH range (PH= 6-8).

And n (independent binding site based on our result, K_{bind}) have been reported.

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Theoretical study in to the gold(I)-catalyzed reaction of furan with cyclopropene

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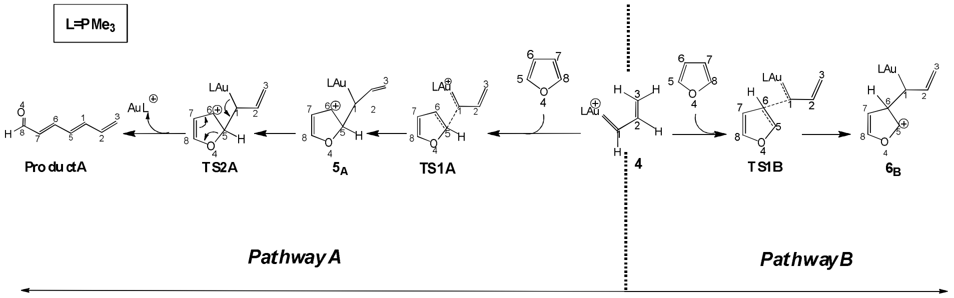
Conjugated trienes are important structural units in many biologically important polyene natural products such as antifungal macrolides and anticancer retinoids, as well as p-extended materials.

Recently, the reaction of indoles with cyclopropenes in the presence of a Au^I catalyst was studied by Li and coworkers. They showed that the reaction leads to the formation of **3.** To rationalize the mechanism of the formation of cyclopropenes, the following mechanism is proposed(Pathways A and B). In pathway **A**, Furan attacks from its C_5 position to the ring-opened intermediate while in pathway **B**, Furan attacks from its C_6 position to the ring-opened intermediate. Our preliminary calculations show that the energy barrier for the addition of furan from its C_5 position is calculated to be 6.5 $kcal.mol^{-1}$ while the addition from C_6 position is calculated to be 7.9 k $cal.mol^{-1}$. These results suggest that the addition from pathway **A** is kinetically more favored than pathway **B**. Analysis of HOMO of furan that the contribution of HOMO orbitals at the C5 position is higher than C6 by 22%. This suggests that a higher HOMO contribution at C5 position leads to a stable transition structure. Another interesting result is the considerable stability of **5A** to **6B**. As it can be clearly seen in the Figure **1**, **5B** is thermodynamically less stable than **6B**. This suggests, due to the high instability of **6B**, the reaction could proceed reversely toward the formation of **5A**.



Scheme 1

References:

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Synthesis and characterization of Schiff base complexes with N_2O_4 potential ligand contining 2,2′-methylen bis (4-chloro phenol)

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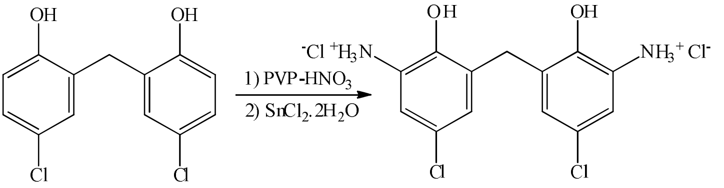
Schiff bases derived from an amino and carbonyl compound are an important class of ligands that coordinate to metal ions via azomethine nitrogen and have been studied extensively [1]. In azomethine derivatives, the C=N linkage is essential for biological activity, several azomethine has been reported to possess remarkable antibacterial, antifungal, anticancer and antimalarial activities [2-3]. Also Schiff-base complexes are considered to be among the most important stereo chemical models in main group and transition metal coordination chemistry due to their preparative accessibility and structural variety [4]. For example complexes of copper with Schiff bases have wide applications in food industry, dye industry, analytical chemistry, catalysis, fungicidal, agrochemical, anti-inflammable activity, antiradical activities and biological activities [5].

In this research ,in the first nitration of 2,2′- methylen bis (4-chloro phenol) by PVP-HNO_3 under mild conditions. Then nitro compound obtained was reduced by Tin(II) chloride (Scheme). Finally synthesized ligand and was formed complex in presence number of transition metals. Then structure of the synthesized compounds by spectroscopic techniques such as FT-IR,^{1}H-NMR , ^{13}C-NMR and CHN was identified.



Scheme1

References:

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A versatile procedure for the oxidation of sulfides to the sulfoxides using DBDMH

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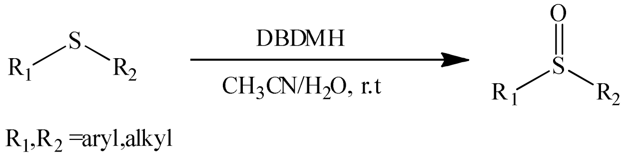
Sulfoxides are important intermediates in the synthesis of various natural products [1,2]. The oxidation of sulfides into the corresponding sulfoxides is one of the most important functional group transformations in organic synthesis [3]. Sulfoxides as a class of important compounds are generally used as synthetic intermediates for the construction of various chemically and biologicall significant molecules, as well as for the synthesis of drugs and natural products [4]. Therefore, many efficient methods have been developed for the oxidation of sulfides to sulfoxides. In continuation of our studies, we became interested to report a new strategy for the oxidation of sulfides to the sulfoxides using 1,3-dibromo-5,5-dimethylhydantoin in the mixture of acetonitril and water at room temperature (Scheme). The use of these reagents significantly reduced reaction time, and increase products yields.



Scheme 1

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Synthesis of a carbon-14 analogue of 2-hydroxy-4-methyl pentanoic acid

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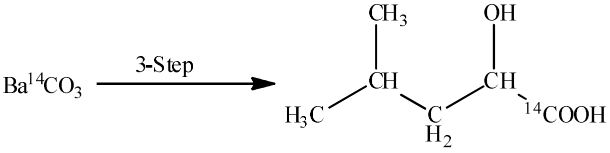
α-Hydroxy acids have been a rich source of biologically active molecular entities and are related to a wide family of compounds with well known pharmacological properties. Among this chemical compound category, 2-hydroxy-4-methyl pentanoic acid is an important α-Hydroxy acid. To further elucidate the mechanism of action and for studies of pharmacokinetics and drug metabolism of this compound, the version with a metabolically suitable carbon-14 label was required. This paper reports the Synthesis of Carbon-14 analogue aforementioned compound [1,2].

In this investigation, after conversion of Barium^{14}C-carbonate to potassium [14C]-cyanide via treatment with potassium azide under furnace condition. In the next step 2-hydroxy-4-methylpentanenitrile-[cyano-^{14}C] was obtained from reaction between potassium [14C]-cyanide and Isovaleraldehyde in the presence of $NaHSO_3$. In the final step the latter product was then be converted to 2-hydroxy-4-methyl pentanoic acid-[carboxy-^{14}C] via hydrolysis under acidic condition [3,4]. The FT-IR, ^{1}H-NMR spectra confirm the structure of compounds and radioactivity was determined by liquid scintillation instrument.



Scheme 1

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Three-component synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones in glycerol

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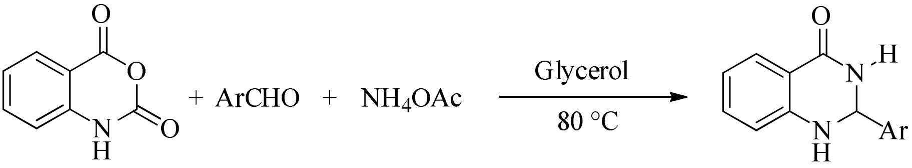
One of the most important synthetic strategies interested by organic chemists is the multi-component reactions (MCRs), which they allow the creation of several bonds in a single operation [1]. 2,3-dihydroquinazolin-4(1H)-one derivatives are an important class of quinazolinones, with a wide range of pharmacological and biological activities [2]. 2,3- Dihydroquinazolin-4(1H)-ones mainly, have been synthesized *via* condensation of amines and aldehydes with isatoic anhydride or anthranilide, in the presence of an appropriate catalyzed [3,4].

Consequently, we decided to design a new procedure for the one-pot synthesis of 2,3-Dihydroquinazolin-4(1H)-Ones by combination of isatoic anhydride, aldehydes and ammonium acetate, which in the presence of glycerol acts as solvent and catalyst at 80°C (scheme1).



Scheme 1

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Copper-catalyzed synthesis of tetrasubstituted pyrimidines from alkynes, sulfonyl azides, trichloroacetonitrile and tetramethylguanidine

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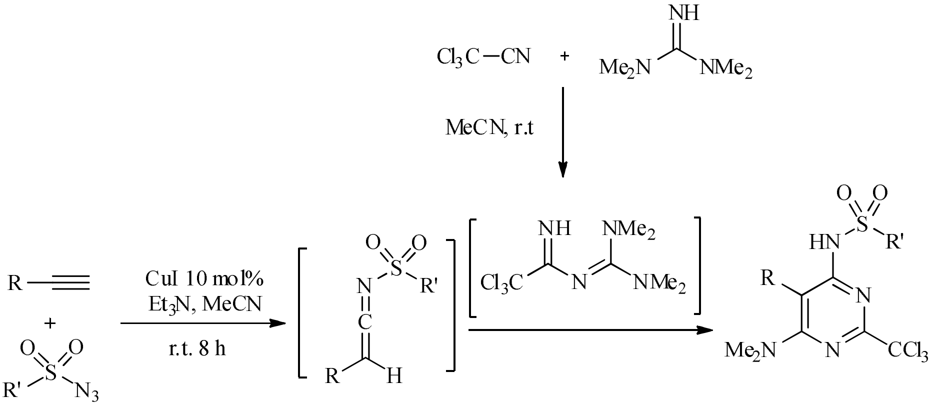
Pyrimidine derivatives exhibit important biological activities and are widely used as key building blocks for pharmaceutical agents [1,2]. The pyrimidine skeleton has also been found in several marine natural products with interesting bioactivities [3].

Ketenimines, have attracted much attention due to their diverse chemical reactivity [4]. One of the attractive methods for generation of ketenimines is the copper-catalyzed azide-alkyne cycloaddition. Herein, we report a simple and efficient procedures for the synthesis of *N*-(6-(dimethylamino)-5-aryl(alkyl)-2-(trichloromethyl)pyrimidin-4-yl)-4-aryl(alkyl)sulfonamide *via* the Cu-catalyzed four-component coupling reaction of terminal alkynes, sulfonyl azides, trichloroacetonitrile, and 1,1,3,3-tetramethylguanidine (Scheme 1).



Scheme 1

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Synthesis, characterization and antibacterial activity of new acyclic pentadentate N_2O_3 Schiff base ligand

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[b]*Department of Chemistry, Faculty of Science, Ilam University, P.O. Box, 69315516, Ilam, Iran;*
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Schiff bases are studied widely due to their synthetic flexibility, selectivity and sensitivity towards the central metal atom; structural similarities with natural biological compounds [1], Schiff base compounds are found to have various characteristics, which result in their applications in biology, analysis and material industry, in addition to their important roles in catalysis and organic synthesis. Schiff bases having chelation with oxygen, nitrogen etc. donors and their complexes have been used as drugs and reported to possess a wide variety of biological activities against bacteria, fungi, and certain type of tumors and also, they have many biochemical, clinical and pharmacological properties [2,3].

In this work, An acyclic Schiff base ligand containing N_2O_3 donor atoms was synthesized by the condensation reaction of 2,6-diformyl-4-methoxyphenol and 4-aminoantipyrine. The synthesized ligand was characterized by ^{1}HNMR, ^{13}CNMR, mass spectrometry, UV/visible, FT-IR and elemental analysis measurements. Also, this new ligand was tested for their in-vitro antibacterial activity.

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Cellulose sulfuric acid (CSA) as an efficient catalyst for the synthesis of tetrahydropyridines.

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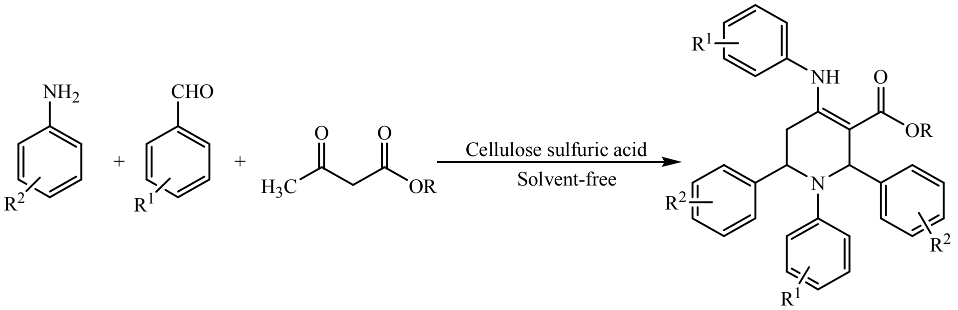
Cellulose sulfuric acid (CSA) has emerged as a promising biopolymeric solid support acid catalyst for acid-catalyzed reactions, such as the synthesis of α-amino nitriles, aryl-14H-dibenzo[a.j]xanthenes, 1,4-dihydropyridines, Pechmann condensation, thiadiazolo benzimidazoles, imidazoazines, quinolines and 3,4-dihydropyrimidine-2(1H)-ones [1,2].

Tetrahydropyridine (THP) derivatives are useful against several metabolic disorders and human ailments. The prominent biological activities associated with this pharmacophore are antiparasitic, antimicrobial, anticancer, antiviral etc [3,4].

We report a simple method for the synthesis of Tetrahydropyridine by one pot three component reaction of aromatic aldehydes, anilines, and a β-keto ester in the presence of a catalytic amounts Cellulose sulfuric acid at room temperature (Scheme 1).



Scheme 1

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Glycerosulfonic acid as a green catalyst for the synthesis of 1-amidoalkyl-2-naphtols

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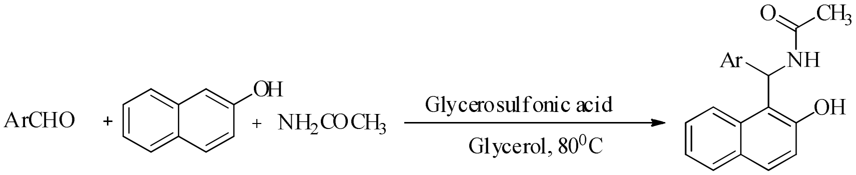
Multicomponent reactions are performed without need to isolate any intermediate during the reaction, which reduce the amount of time and energy used [1]. There has been tremendous development in three or four component reactions. 1-amidoalkyl-2-naphthol derivatives have been attracted considerable interest because of their biological and pharmacological activities [2,3].

In this work, a new strategy has been introduced for the preparation of 1-amidoalkyl-2-naphtoles. In this regards, glycerosulfonic acid has been synthesized and new applications of this catalyst explored. Therefore a variety of 1-amidoalkyl-2-naphtoles have been prepared via combination of aromatic aldehydes, acetamide and 2-naphtol in the presence of a catalytic amounts glycerosulfonic acid at 80 ^{0}C (Scheme 1).



Scheme 1

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Synthesis of 3,4-dihydropyrimidin-2-one-5-carboxylates as cardiotonic agents

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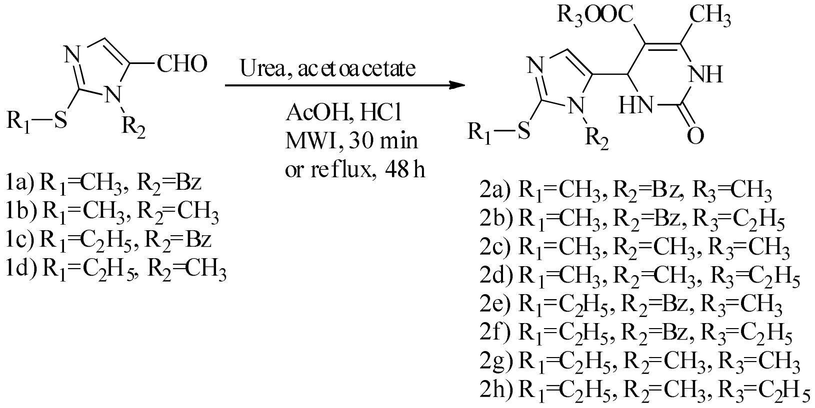
Dihydropyrimidinones (DHPMs), also called Biginelli compounds have interesting biological properties such as cardiotonics [1]. In this study, a series of imidazolyl dihydropyrimidines were synthesized in two ways: classical method and microwave method (scheme 1). All compounds were purified by chromatography and characterized by H-NMR and FTIR.



Scheme 1

We used rat isolated perfused right atria method. According to the achieved results, compound 2d increased the number of rates (in concentration of 0.01M) as the increase was in positive control limit (theophylline), even a bit more but there was no significant difference between them. Compound C decreased the number of the atrium rates imperceptible and compounds 2a and 2b did not have much effect but in concentration of 0.01M decreased the number of rate a little. In terms of the effect of contractile power, none of them have a significant effect. These negative results can be related to the type of method we used

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Nano-silica phosphoric acid as an eqo-friendly catalyst for synthesis of nitro and nitroso aromatic compounds under solvent free conditions

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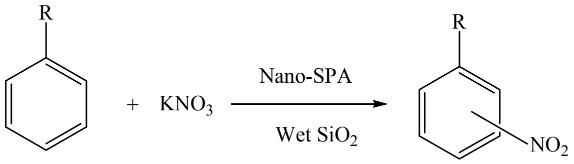
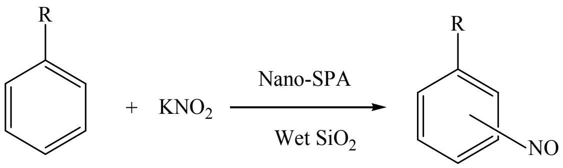
[b]*Department of Chemistry, College of Science, Yazd University, Yazd, Iran*

Nitration and nitrosation of aromatic compounds is an important process in both industrial and academic research and is the subject of a large body of literature. Also nitro and nitroso aromatic compounds are extensively utilized as a chemical feedstock for a wide range of useful materials such as dyes, pharmaceuticals, perfumes, and plastics [1,2].

Recently, nanosilica Phosphoric Acid, as a solid acid has been widely used in chemical reactions [3,4]. Nitro aromatic and nitroso aromatic derivatives have large structural varieties and extensive uses. In addition, these reactions, in presence of nano-SPA and without any solution, can fulfill a large number of green chemistry principles; hence, the present study sought to obtain these derivatives in a reaction without using any solvent and in presence of nanosilica phosphoric acid, which is a solid acid catalyst with several advantages over common liquid acids. (Scheme 1, Scheme 2). Short reaction time duration, high yield, easy availability and eco-friendliness are some of the striking features of the present protocol



Scheme 1



Scheme 2

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A green approach for the synthesis of some asymmetrical cyclic acetals using nano-$TiCl_4/SiO_2$ as an eco-friendly heterogeneous catalyst under solvent-free conditions

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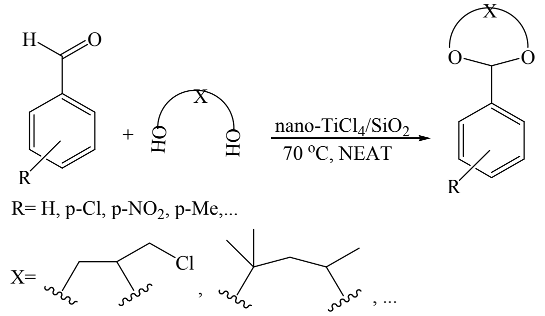
Functional group interconversion (protection/deprotection) is an unavoidable protocol in the synthesis of many designed target molecules such as drugs and multifunctional natural products [1]. In this regard, acetals have widely used as protecting groups in organic synthesis and, are an important class of compounds that have found their direct applications in diverse areas in the chemical industry such as perfumes, flavours, pharmaceuticals, solvents, and polymer chemistry [2]. Recently, the application of solid acids has been extensively considered in organic synthesis [3].

Silica supported $TiCl_4$ is a mild solid Lewis acid that promotes acidic catalyzed organic reactions [4]. In this work, a new strategy has been introduced for the preparation of acetals from the various aromatic aldehydes with diverse diols in the presence of catalytic amounts of $TiCl_4$ supporting on nano SiO_2 as an efficient solid acid catalyst under thermal and solvent-free conditions in good to excellent yields (Scheme 1). Mild and heterogeneous reaction conditions, clean synthesis, easy work-up, high yields are important advantages of this protocol.



Scheme 1

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Studies on the synthesis of new polycyclic fused pyrimidines using [DMBSI]HSO_4 as ionic liquid catalyst

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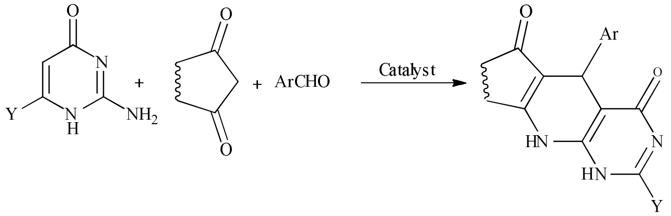
Multi-component reaction (MCRs) have emeraged as an efficient and powerful tool in modern synthetic organic chemistry due to their valued features, such as atom economy, straightforward reaction design and the opportunity to construct target compound by the introduction of several diversity elements in a single chemical event [1]. Pyrido[2,3-d]pyrimidine are known to exhibit pharmacological activities such as neuroleptic [2] and turberculostatic [3].

In continuation of our recent interest in the synthesis and chemistry of hetrocyclic compounds [4], we have devised an efficient one-pot three-component reaction for the regioselective synthesis of novel fused derivatives of pyrido[2,3-*d*]pyrimidine in high yields and lower reaction times (Scheme 1). The details of this protocol will be discussed in this presentation.



Scheme 1

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One-pot synthesis of novel substituted pyrazoles using sulfonic acid supported on HAp-encapsulated-γ-Fe_2O_3 as nano catalyst

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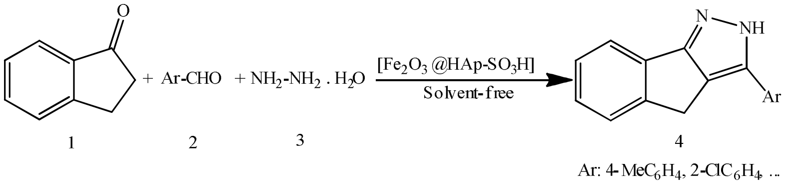
Recently, magnetic nanoparticles have gained recognition as potential environmentally benign replacement of the conventional Lewis acid and base catalysts in various organic synthetic processes [1]. Also, the magnetic nature of these particles allows for easy recovery and recycling of the catalysts by an external magnetic field [2].

On the other hand, The construction of pyrazoles has gained significant interest among the azole family due to their important role in the agrochemical and pharmaceutical industries, as they are the core structure of numerous biologically active compounds, including blockbuster drugs such as Celebrex2, SC-558 and Via- gra [3].

Following our continued research program for the synthesis of heterocycles of medicinal value [4], at the outset of this study HAp-encapsulated-γ-Fe_2O_3 [γ-Fe_2O_3 @HAp-SO_3H] were prepared and their nano-structure was established by spectroscopic analyses [2]. Then we devised an efficient one-pot three-component protocol for the synthesis of novel substituted pyrazoles (**4**), by the reaction of 1-indanone (1), arylaldehydes (**2**), hydrazine hydrate (**3**) in the presence of [γ-Fe_2O_3 @HAp-SO_3H] as catalyst. The advantages of this method are high to excellent yields, easy work up and short reaction times.



Scheme 1

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Application of microwave as a green procedure for the synthesis of fulleropyrazolines/fulleroisoxazolines

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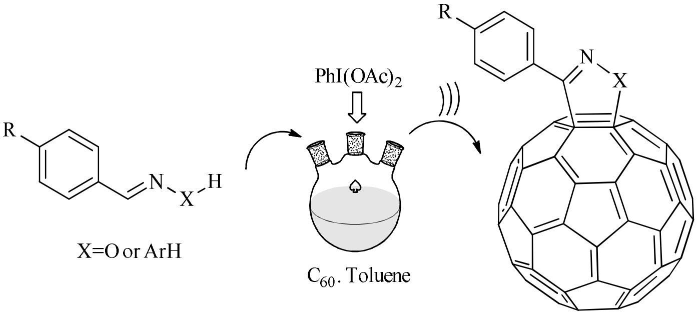
Fullerenes as the third allotrope of carbon were discovered by Kroto et al. [1] in 1985. The chemistry of fullerenes began to develop greatly after W. Kratschmer and D. Huffman [2]. Surface modification of fullerenes is an attractive approach in materials science and pharmaceutical applications [3-5]. The use of microwave irradiation in organic synthesis has interestingly been used in recent years [6].

In this context, a green strategy has been introduced for the synthesis of fulleropyrazolines/ fulleroisoxazolines. The 1,3-dipolar cycloaddition reaction of C_{60} with substituted phenylhydrazones/oximes, and $PhI(OAc)_2$ at room temperature were promoted by microwave irradiation as a green and sustainable synthetic method in very short reaction times, good yields and high purity (Scheme 1).



Scheme 1

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Green and efficient one-pot synthesis of pyranopyrazole derivatives by recyclable nano-Mn(bpdo)$_2$Cl$_2$/MCM-41-catalyzed reactions in water media

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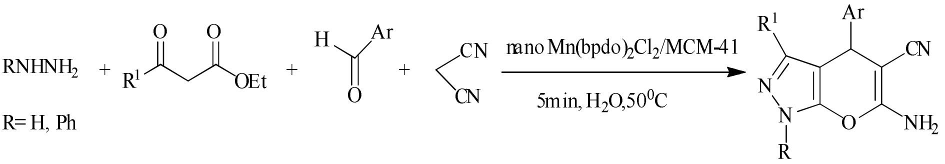
A clean, simple, one-pot, four-component synthesis of some important pyranopyrazole derivatives with aromatic aldehydes, ethylacetoacetate, malononitril and hydrazine hydride in the presence of nano- Mn(bpdo)$_2$Cl$_2$/MCM-41 as catalyst was carried out under green and environmentally benign conditions because of water media [1].

Nano-Mn(bpdo)$_2$Cl$_2$/MCM-41 is inexpensive, reusable, easy to handle, non-corrosive and environmentally benign solid catalyst. Using of these catalysts, offer advantages including simplicity of operation due to the heterogeneous nature of reaction, easy work-up, high yields of products and the recyclability of the catalysts [2].

Pyranopyrazoles are an important class of heterocyclic compounds. They find applications as pharmaceutical ingredients and biodegradable agrochemicals. They have useful biological and pharmacological properties, such as antimicrobial, insecticidal, and anti-inflammatory.

In this project we report the synthesis of pyrano pyrazole derivatives with some advantages: mild condition, short reaction time, high yield, using nanocatalysis as a nontoxic and recyclable catalysis and using water as a clean solvent [3].



Scheme 1

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Synthesis of five- and six-membered heterocyclic nitrogen compounds using 22% Co/CeO_2-ZrO_2

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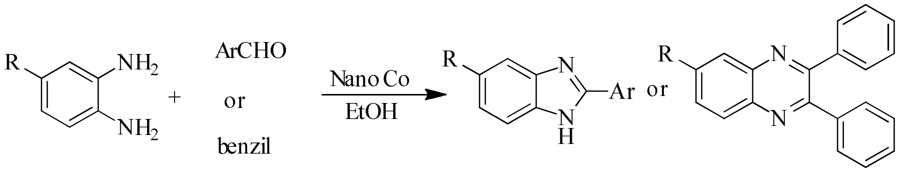
The chemistry of heterocyclic compounds is one of the most complex branches of organic chemistry. It is equally interesting for its theorctical implications, for the diversity of its synthetic procedures, and for the physiological and industrial significance of heterocyclic compounds. Among various classes of heterocyclic compounds, quinoxalines and benzimidazole derivatives [1,2] constitute an important component of pharmacologically active compounds such as, echinomycin, levomycin and actinoleucin, which inhibit the growth of Gram positive bacteria and are active against various tumours. Many synthetic routes have been developed for the synthesis of quinoxaline and benzimidazole derivatives. Most common method is the condensation of aromatic 1,2-diamine with 1,2-dicarbonyl compound in refluxing ethanol or acetic acid.

In this study, we report synthesis of benzimidazole and quinoxaline derivatives as five- and six-memberd heterocyclic nitrogen compounds using 22% Co/CeO_2-ZrO_2 as a nano catalyst (Scheme 1).



Scheme 1

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A novel approach for the synthesis of rhodanine-based amide

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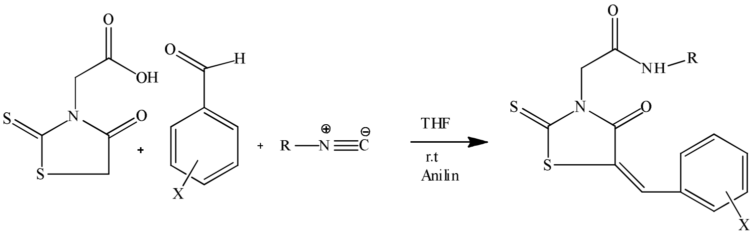
Amides are a very important class of organic compounds with a wide range of applications. Some derivatives of amides exhibit biological properties such as anthelmintic, antihistamine, antifungal and antibacterial [1]. The classical method for the synthesis of amides is the reaction of carboxylic acids with amines at high temperature. Due to the low activity of carboxylic acids, various methods for their activation have been reported in the literature [2]. Draw backs of these methods include modest yields, expensive coupling reagents and difficulty in removal of excess reagents and by-products.

Following our studies towards the development of new routes to the synthesis of new organic compounds and our interest in isocyanide-based reactions [3], we herein report a simple reaction, which starting from rhodanine-*N*-acetic acid (1), aromatic aldehydes (2) and alkyl isocynides (3) affords amide derivatives (4) in good yields (Scheme 1).



1 2 3 4

X=Cl, Br, F, Me, OMe R= ^{t}Bu, Cyclohexyl

Scheme 1

References:

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Synthesis and characterization of new ligand derived from -2-(3-hydroxybenzylideneamino)benzaldehyde and ethylenediamine

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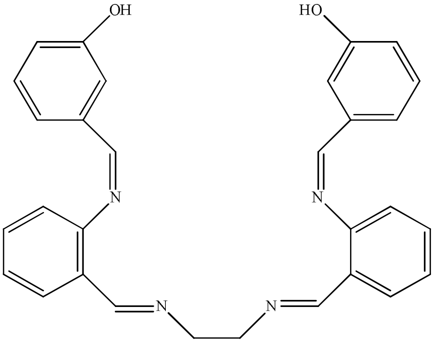
Ligands with a good selectivity in different chemical surrounding are very useful in chemistry as well as biological and environment sciences. Among them, considerable interest has been shown in the synthesis and applications of azo-Schiff base ligands containing both N=N and N=C functional groups [1,2].

In this work, new ligand hydroxybenzylideneamino)benzylidene)amino)ethylimino) methyl) phenylimino) methyl) phenol has been synthesized, this ligand was characterized by elemental analysis, Mass, IR and ^{1}H and ^{13}C NMR spectroscopy (Scheme 1). In the IR spectrum of ligand no peaks attributed to NH_2 and carbonyl groups implied that the condensation reaction have been completed.



Scheme 1

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Synthesis and characterization of new Schiff base ligand containing (2-aminoethoxy)ethoxy)ethanamine unit

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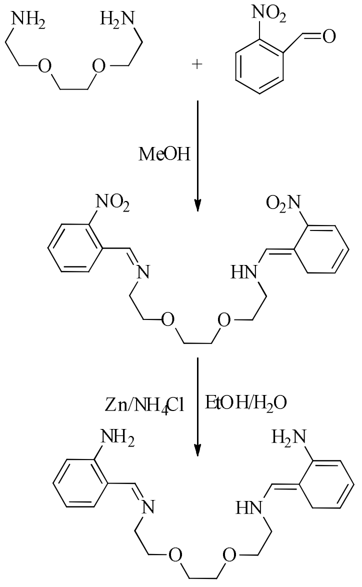
Interest in Polyamine Schiff base compounds is growing on account of their unique coordination and structural properties, their bioinorganic applications, their utility as contrast reagents in MRI, their use as tumor- directed radioisotope carriers, and their ability to carry out controlled molecular movements and translocations [1-2].

In this work, first we synthesized nitrobenzylideneamino)ethoxy)ethoxy)-(2-nitrocyclohexa-2,4-dienylidene)methyl)ethanamine by condensation reaction between 2-(2-(2-aminoethoxy)ethoxy)ethanamine and 2-nitrobenzaldehyde and then reduce NO_2 group to NH_2 (Scheme 1). This polyamine Schiff base was characterized by elemental analysis, Mass , IR spectroscopy.



Scheme 1

References:
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Synthesis and characterization of new ligand containing 3-hydroxybenzaldehyde unit

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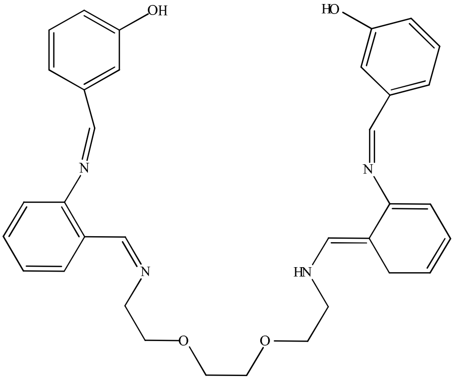
Polyamine ligands have remained an important and popular area of research due to their simple synthesis, versatility and divers range of applications [1]. Schiff base condensations have long been used to form macrocyclic and macroacyclic ligands from diamines and dicarbonyl compounds [2].

In this work, macroacyclic ligand (L) has been synthesized from (2-aminocyclohexa-2,4dienylidene) methylamino) ethoxy)ethoxy) ethylimino)methyl) benzenamine and 3-hydroxybenzaldehyde (Scheme 1). This ligand was characterized by elemental analysis, Mass , IR ,^{1}H and ^{13}C NMR spectroscopy.



Scheme 1

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Synthesis of 1,2,4-triazol-3-thione derivatives as antioxidant and radical scavenger

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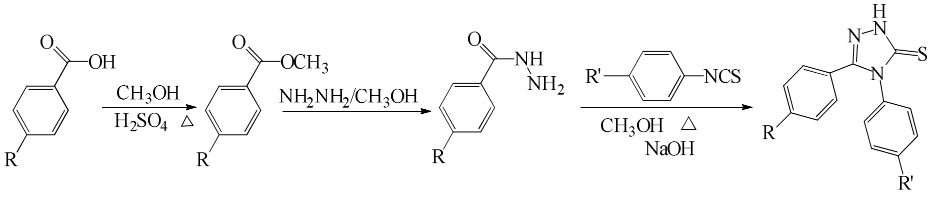
Reaction oxygen species are believed to play a very significant role in the pathogenesis of several diseases including Alzheimer's and Parkinson's disease, hyperlipidemia and cardiovascular disease [1,2].

Recent studies show that free-radical scavengers, both synthetic and natural can be effective for treatment or prophylaxis of disorders attributed to free-radical damage [3,4].

There is growing interest toward antioxidants of herbal resources such as vegetables, fruits, teas and grain product. There is a well known oxidation of aliphatic thiol compounds for formation of S-S bound. In the other hand, for imidazoline-2-thiones, a facile conversion to the corresponding bis (imidazol-2-yl) sulphids has been reported [5]. A group of 1,2,4-triazole-3-thions, in which triazole ring at position 4 and 5 was substituted by different substituted aryl, that 4 position aryl was taken from isothiocyanate and 5 position from aryl hydrazide was synthesis.



Scheme 1

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Synthesis and characterization of new Schiff base ligand with N_4O_2 donor atoms containing 2-Hydroxy banzaldehyde

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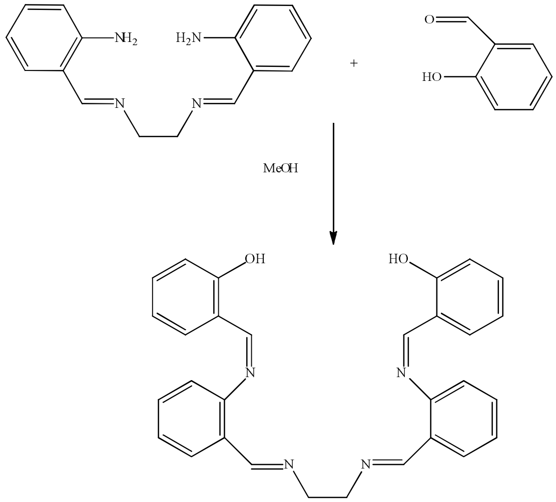
Considerable attention has focused on the synthesis of new hetroacyclic ligands containing azo groups because of their role in the development of coordination chemistry as well as optical materials , dyes and so on [1,2].

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 ligands (Scheme 1). Also this Schiff base was characterized by elemental analysis, Mass and IR spectroscopy.



Scheme 1

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Efficent synthesis of novel peptides and azapeptides contained coumarin skeleton

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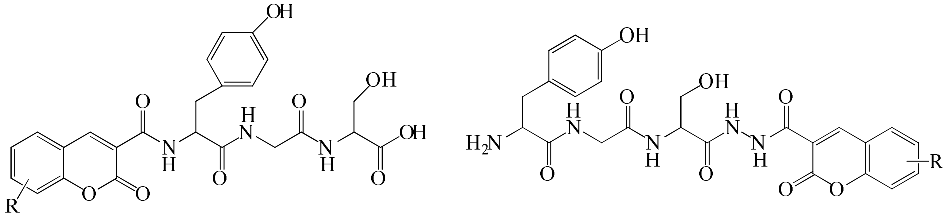
Some peptides derived from food proteins are potentially antioxidants, Zheng et al isolated tripeptide (Tyr-Gly-Ser) from Peanut meal that had strong activity against peroxidation but show negligible DPPH radical scavenging activity and no metal ion chelating activity [1].

Due to extanded biological activity of peptides, we wish to report herein the synthesis of peptides which contained the coumarin skeleton. The coumarin skeleton was selected due to its antioxidant activity designing of novel reaction to combine the heterocyclic skeleton to the peptides is an interesting subject in peptide chemistry [2].

For the synthesis of target molecules, at first the tripeptide was synthesized and then coupling to the coumarin-3-carboxylic acid and coumarin-3-carboxyhydrazide was done using TBTU as coupling reagent to access desired peptides and azapeptides (Scheme 1).

The structure of products were confirmed based on mass spectrometry data. The investigation for antioxidant activity of these compounds are in progress. The details about the synthesis will discuss in the conference.



Scheme 1

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One-pot synthesis of substituted benzimidazoles by air oxidation using Al-grafted MCM-41 as a microreactor and reusable catalyst

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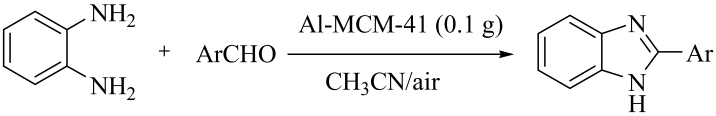
The synthesis of benzimidazoles has gained importance in recent years, because they exhibit illustrious biological and pharmacological activities and are used as antitumor, antiviral, and antimicrobial agents, and for HIV, influenza, and human cytomegalovirus. They are also used in diverse areas of chemistry and are very important intermediates in various organic reactions [1-2].

From green chemistry point of view there is an increasing demand for transformation of homogenous into heterogeneous catalyst in organic synthesis. Mesoporous alumina silicate Al-MCM-41 is well known to show remarkable catalyst activity [3-4].

We report here, convenient and efficient methodology for the synthesis of benimidazoles by air oxidation at room temperature without the use of any oxidative reagent in good to high yields, employing Al-MCM-41 as a lewis acid and microreactor.



Scheme 1

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An efficient tandem approach for the synthesis of functionalized 2-pyridone-3carboxylic acids using three-component reaction in aqueous media

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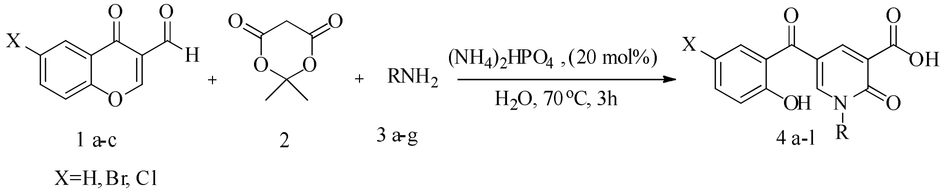
2-Pyridone ring represents an important structural motif with extended biological activities [1,2]. Moreover, in the recent years, 2-pyridone derivatives were utilized as versatile important synthons for the synthesis of different nitrogen containing heterocycles and other biologically active compounds. Existence of a carboxylic acid in the structure of 2-pyridone skeleton could add its biological activity. As part of our current studies on the development of multicomponent reactions, herein we wish to report an efficient three-component reaction for the synthesis of functionalized 2-pyridones through three-component reaction of 3-formyl chromone, Meldrum's acid and also primary amines in the presence of catalytic amount of diammonium hydrogen phosphate (DAHP) in water (Scheme 1).



Scheme 1

The desired products **4a-l** was formed in good yields and easy work-up.The broad scope, operational simplicity, practicability, high yields and environmentally friendly character render it an attractive approach for the generation of different 2-pyridone-3-carboxylic acid derivatives. Moreover, these products can be used for the synthesis of novel unusual peptides which contained biologically active pyridines.

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Palladium catalyzed sequential Ugi-4CR/C-H activation reactions for the synthesis of 3-(diarylmethylene)-2-oxindoles

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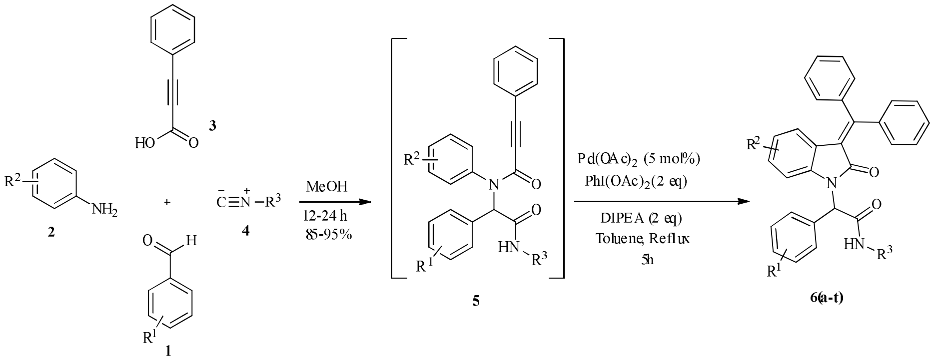
Palladium catalyzed cross-coupling of aryl halides with organometallic reagents is now recognized to be one of the most useful methods for the construction of C-C bond. In this way, the use of C-H bond as a functional group in cross-coupling reaction which we know it as C-H activation approach has more advantages including; efficiency of reactions and reducing the synthesis steps. Due to the biological activities of 2-oxindoles many approaches have been developed for the synthesis of these compounds. There are different methods for the synthesis of 2-oxindoles, but metal-catalyzed domino cyclization of *N*-substituted-2-alkynamides is known as the best way to construct 2-oxindole skeleton.Due to the importance of these compounds, and in continuation of our research work toward the synthesis of functionalized 2-oxindoles, we wish to report, herein a sequential Ugi-4CR/ C-H activation/C-C bond formation reaction of functionalized *N*-susbstituted 2-alkyneamides to construct 3-diarylmethylidene-2-oxindoles using palladium catalyst and diacetoxyiodobenzene in good to high yields and in shorter reaction times (Scheme 1).



Scheme 1

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An effective method for acetylation of alcohols and phenols catalyzed by tribromoisocyanuric acid (TBCA)

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The protection of hydroxyl groups of alcohols and phenols by the formation of esters is one of the most important and widely used transformations in organic chemistry [1]. The OH group acetylation provides an efficient route for the synthesis of compounds with industrial value, for the production of medicines, flavors, fragrances, solvents, food preservers, plasticizers, and cosmetics [2]. In this paper, we wish to report the acetylation of alcohols and phenols by employing acetic anhydride in the presence of TBCA as a catalyst under solvent-free conditions (Scheme1).

$$\mathrm{ROH} + \mathrm{Ac_2O} \xrightarrow[\text{Solvent-free, r.t.}]{\text{TBCA}} \mathrm{ROAc}$$

R: Alkyl, Aryl

Scheme 1

The reaction of the various alcohols and phenols with Ac_2O in the presence of TBCA afforded products in high yields. The special features of this methodology are using the low cost reagent, simple reaction conditions and easy work-up procedures.

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A green protocol for the easy synthesis of thiiranes from epoxides using thiourea/$CuSO_4.5H_2O$ in the reflux conditions

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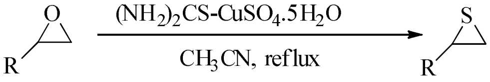
Thiiranes (episulfides) are the simplest sulfur heterocycles and occur in nature, mostly in the plants [1]. These three-member heterocyclic compounds have found wide application in pharmaceutical, pesticide, herbicide, and polymer industries [2]. Moreover, they played a pivotal role as versatile building blocks in asymmetric synthesis [3].

Copper(II) sulfate, also known as cupric sulfate or copper sulphate, is the chemical compound with the chemical formula $CuSO_4$. This salt exists as a series of compounds that differ in their degree of hydration. Copper(II) sulfate exothermically dissolves in water to give the aquo complex $[Cu(H_2O)_6]^{2+}$, which has octahedral molecular geometry and is paramagnetic. Other names for copper (II) sulfate are blue vitriol and bluestone. Copper sulfate is employed in organic synthesis. The anhydrous salt catalyses the trans acetylation in organic synthesis.

Herein, we wish to introduce a simple and efficient method for Conversion of epoxides to corresponding thiiranes with Thiourea supported on $CuSO_4.5H_2O$ under reflux conditions. The capability of this synthetic protocol was investigated by the reaction of activated, deactivated, and cyclic epoxides with Thiourea/$CuSO_4.5H_2O$ system under the optimized conditions. The epoxides were converted to the corresponding thiiranes in excellent yields within short times (Scheme 1).



R=Aryl, Allyl, Alkyl, H

Scheme 1

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Nano-CeO_2 catalyzed synthesis of xanthene derivatives in aqueous media

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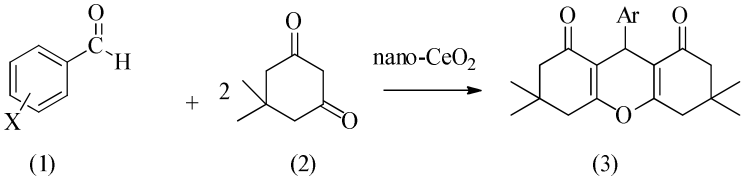
Xanthene derivatives are very important heterocyclic compounds and have been widely used as dyes fluorescent materials for visualization of bio-molecules and laser technologies due to their useful spectroscopic properties [1]. They have also been reported for their agricultural bactericide activity [2], photodynamic therapy [3], antiflammatory effect and antiviral activity [4].

In our continued interest in the development of highly expedient methods for the synthesis of heterocyclic compounds and in continuation of our investigation on the use of water as solvent for chemical preparation, we report here a facile and improved protocol for preparation of xanthene derivatives, from benzaldehydes, dimedon and nano-CeO_2 as a catalyst in water at ambient conditions (Scheme 1).



Scheme 1

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Application of thermodynamic equations to surface tension prediction of ionic liquids solutions

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Ionic liquids (ILs) have attracted large amount of interest due to their unique properties. Large effort has been focused on the investigation of their potential application, characterization of properties and structure–property relationships. In this paper corresponding-state group-contribution method (CSGC) has been used to prediction the surface tensions of Ionic liquids+organic solvent solution based on the thermodynamic definition of surface tension and critical parameters is used, which is different from existing ones with respect to theoretical background and formulation. The model parameters obtained by correlating binary surface tension at one temperature can be used to predict surface tension at other temperatures with good accuracy. The average relative error obtained from the comparison of experimental and calculated surface tension values for binary systems are less than 10%. Therefore, the model has good accuracy in comparison with other predictive equations.

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One-pot three component synthesis of pyrimidine 5-carbonitrile derivatives in aqueous glucose solution as medium and promoter

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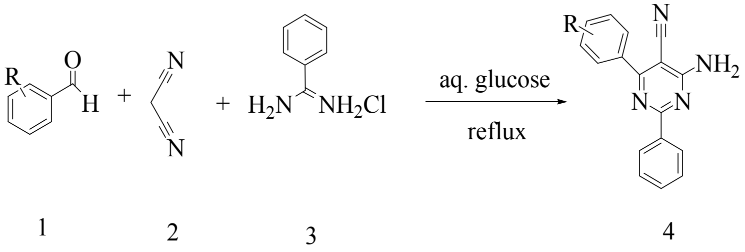
Pyrimidine derivatives have attracted considerable interest due to their remarkable pharmacological properties. These compound were designed and synthesized as potent and selective antiviral [1], anti HIV [2] and anticancer [3] agents. Therefore, the search for more environmentally benign and versatile synthetic methods for the preparation of this class of heterocycles is still an active area of research in organic chemistry.

With a view of the fact that the idea of green chemistry has shifted somehow toward employing biobased materials with diverse structures, such as sugars, for the purposes of synthesis and catalysis [4], we have already reported the synthesis of benzimidazole derivatives in aqueous glucose solution [5]. Herein, we wish to report a novel green condition for the preparation of pyrimidine-5-carbonitrile derivative using aqueous glucose solution as media and promoter.



Scheme 1

The products were precipitated completely after formation and can be isolated easily and washed by stirring in water. This reaction did not proceed well in pure water inferring to the role of glucose in the process. In summary, this methodology seems to be a good alternative to the present methodologies because of using an ecofriendly carbohydrate aqueous solution as medium and catalyst.

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One-pot, green and convenient synthesis of 3,4-dihydropyrimidin-2(1H)-ones catalyzed by citric acid

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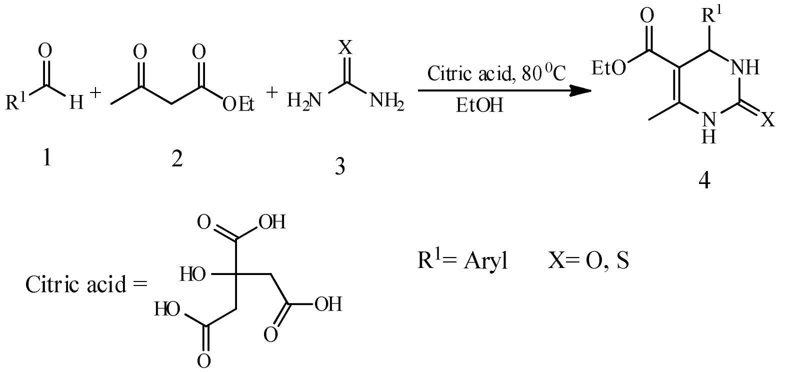
Compounds with biological activity are often derived from heterocyclic structures. 3,4-Dihydropyrimidin-2(1H)-ones and their sulfur analogs (DHPMs) are an important class of heterocycles with a wide range of pharmacological and biological activities including antiviral, antibacterial and antihypertensive activity [1,2], as well as efficacy as calcium channel modulators and α_{1a}-antagonists [3]. Recently, because of the simplicity of the synthesis of DHPMs, the Biginelli reaction has received renewed interest.

In this work, we report one-pot three-component condensation of ethyl acetoacetate, aldehyde and urea/thiourea in refluxing ethanol in the presence of catalytic amounts of citric acid for the synthesis of corresponding 3,4-Dihydropyrimidin-2(1H)-ones/thiones in high yields. The catalyst is reusable and can be applied several times without any decrease in product yield.



Scheme 1

References:

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Synthesis of new derivatives of tetra aza[12]annulene using vinamidinium salts

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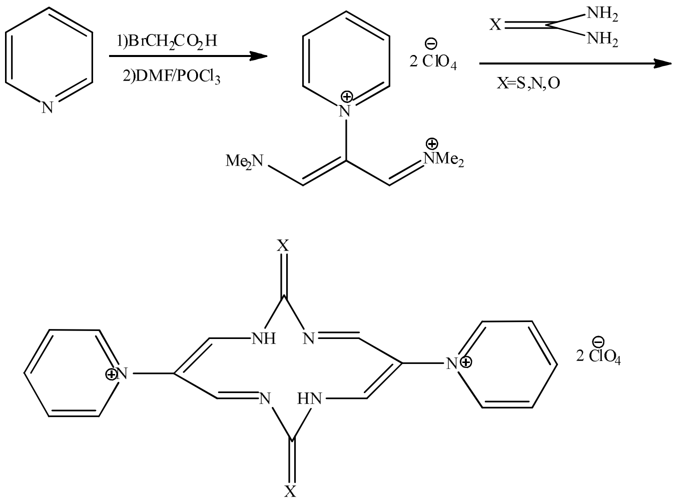
Tetra aza[12]annulene derivatives have been attracted attention as important class of heterocyclic compounds for their biological and pharmaceutical applications. Also, these compounds can serve as a model for the study of porphyrins and Corinne rings in biological systems [1,2]. Because of their broad spectrum of applications in biology, and chemistry [3,4], the mentioned compounds have received a great deal of attention in connection with their synthesis. Therefore, this research project, aims to introduce a simple and efficient method for synthesis of some new derivatives of tetraaza[12]annulene using vinamidinium salts.

The reaction pathway to synthesize of the new tetraaza[12]annulene derivatives from corresponding vinamidinum salts are shown in Scheme 1.



Scheme 1

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One-pot, four-component synthesis of novel spiro [indeno] quinoxaline-pyranopyrazole

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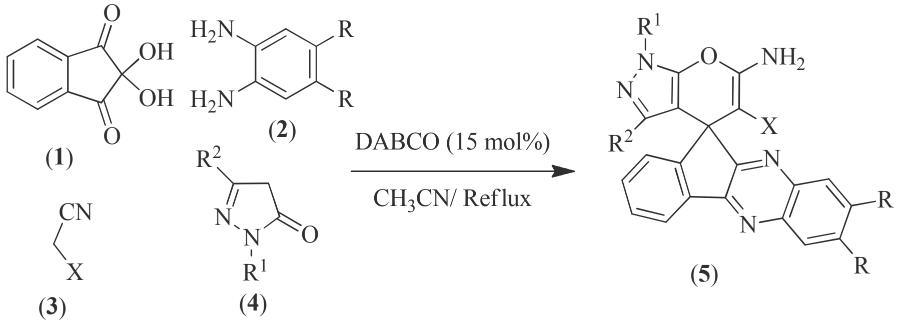
Functionalized nitrogen and oxygen containing heterocycles play a predominant role in medicinal chemistry and they have been intensively used as scaffolds for drug development [1]. Multi-component reactions (MCR's) have emerged as a powerful tool for delivering the molecular diversity needed in the combinatorial approaches for the preparation of bioactive compounds [2].

In continuation of our recent studies on green protocols, multi-component reactions and synthesis of quinoxalines and spiro compounds [3], herein we report a one-pot, four-component method for the synthesis of novel spiro[indeno[2,1-*b*] quinoxaline-11,4′-pyran]-2′-amines from ninhydrin (**1**), 1,2-diaminobenzenes (**2**), alkylmalonates (**3**) and α-methylencarbonyl compounds (**4**) in the presence of DABCO as a non-toxic and effective solid base catalyst (Scheme 1).



Scheme 1

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Investigation into the bis-Diels-Alder reactivity in the 3-(2-(furan-2-yl)vinyl)-5,5-dimethylcyclohex-2-enone system

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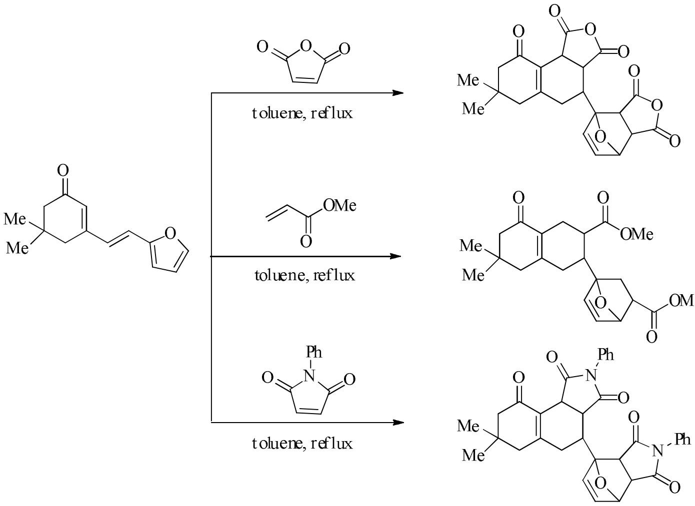
Among various types of cycloadditions, the Diels-Alder reaction is the most important and frequently practiced process due to the ability it has to construct six-membered rings with upto four contiguous stereogenc centers in a predictable fashion in one step operation.

We have recently reported the synthesis of various styrocyclohex-2-enone dienes [1] and revealed their Diels-Alder reactions with different dienophiles [2,3]. Among various dienes we synthesized, the furan-2-yl substituted diene can display an interesting bis Diels-Alder reactivity where both the central diene and the furan diene systems can sequentially enter into the cycloaddition processes. Reactions of the system with maleic anhydride, methyl acrylate and *N*–phenylmaleimide under thermal and Lewis acidic conditions are being studied (Scheme 1).



Scheme 1

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Efficient synthesis of functionalized quinazolinones through novel multicomponent reaction

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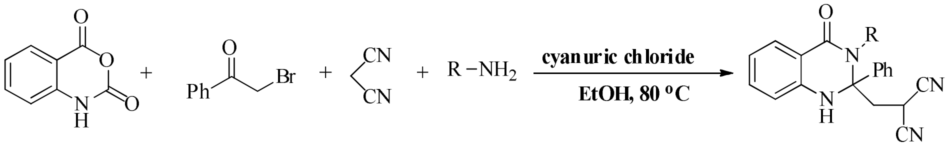
Designing of novel multicomponent reaction to access the molecules with high bond forming and more active functional group is one of the main object in organic synthesis. To access this goal using of suitable starting materials has an important role in this approach. To ensure efficient molecular diversity and complexity, there is a continous need for novel reactions with high selectivity.

More active biologically active compounds contain quinazolinone skeleton. In continuation of our research to find novel reactions, herein we wish to report four-component reaction for the synthesis of functionalized quinazolinones reaction was carried out using isatoic anhydride, primary amine, malononitrile, phenacyl bromide in the presence of cyanuric chloride in EtOH.

The structure of products were assigned based on spectroscopic data. The products have more functional groups which could be used for further transformations.



Scheme 1

In our recent research, we would like to design novel sequential reaction for the cyclization of these products.

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One pot synthesis of ordered mesoporous silica containing platinum nanoprticles within their nanochannels

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Since the discovery of MCM-41 in 1992, ordered mesoporous silicas were widely studied as supports for catalysts or as a matrix for the preparation of nanosized, high surface area materials. Synthesis and application of modified mesoporous MCM-41 materials 1,2 that have an active species attached to the framework via host–guest interactions, creating discrete and uniform catalyst sites on the inner walls of the porous systems [1-3].

In the present work, platinum nanoparticles were incorporated within the nanochannels of ordered mesoporous silica using an in situ approach. At first a hydrophobic platinum precursor was added to the surfactant solution of synthesis. Then, after enough stirring of this solution, the hydrophobic platinum precursor was diffused in to the hydrophobic core of micelles. After that, TEOS was added to the synthesis solution and silicate spices were arranged around the platinum containing template (micelle).

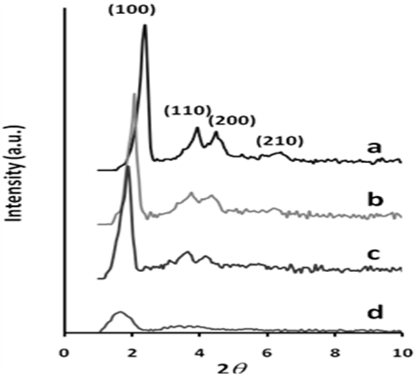

Fig. 1 Low angle PXRD patterns of a: parent MCM-41, b: Pt1/MCM, c: Pt2/MCM, d: Pt3/MCM.

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Efficient and selective oxidation of organic functional groups in the presence of molybdenum complex with Schiff base ligand of alanine supported on nanolayers of montmorillonite-k10

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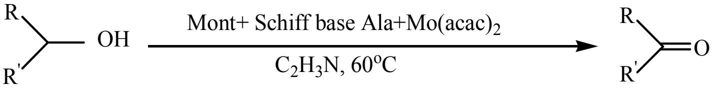
The selective oxidation of benzyl alcohols to the corresponding aldehydes and ketones, respecttively, is a ubiquitous and pivotal reaction in organic synthesis and the chemical industry [1,2].we interested to perform the safe oxidation of benzyl alcohols with high- yield (70-90%) with t-butyl hydroperoxide (TBHP) and (H_2O_2) as oxidant in acetonitrile in the presence of molybdenum alanine Schiff base complex supported on the montmorillonite_k10. This work is performed with the aim to find a way to control the oxidation of various organic compounds and their conversion to the corresponding aldehydes and ketones. To achieve this goal, first a heterogeneous molybdenum catalyst was prepared and then its catalytic activity was investigated in oxidation of alcohols with (TBHP) in acetonitrile as solvent. The reaction shows good results in the case of benzyl alcohols. It is noticeable that the reaction was proceded selectively for all the alcohol to the corresponding aldehydes and ketones. All of the products were characterized with gas chromatography. Advantages of this method are the high performance, process as well as the relatively short time and good yield of the reaction. Finally, this work resulted in the introduction of a new method for controlled oxidation of organic compounds.



R = Aryl
R' = H, Alkyl, Aryl

Scheme 1

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Biodegradable polyester and biological characterization

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Issues related to the development of production and consumption of plastics has led to particular attention to the issue of disposal methods and return plastic to nature. Many methods developed in this field among which the use of biopolymers and chemical agents in accelerating polymer degradation reactions are the most important. Control of polymer degradation process with respect to the required conditions to initiate the reaction, such as temperature, humidity, time and etc. is the most important factor for the optimization of polymer degradation to predict the polymer performance and design of polymers with specific degradation time. The goal of the project is to investigate and optimize the degradation kinetics control methods to design biodegradable polyesters with controlled and predictable properties [1].

In this project, the biodegradable plastic films were produced. Hydrolytic degradation at different PHs, tensile test, DSC test, and biodegradation in soil environment were studied on the produced films.

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Theoretical study of halogen bonded complexes of heterocyclic (C_2H_4M) with (CH_3-X) and (NH_2-X) (M=Ge, Si and X= F, Cl, Br, I)

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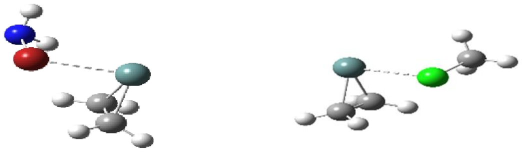
Halogen bonding is of considerable interest in many fields within chemistry and material science because these noncovalent interactions play roles in a wide variety of chemical phenomena [1]. Halogen bonds are of particular interest in biochemistry and medicinal chemistry because they are often involved in proteinligand interactions that are either biologically detrimental, as in the case of interactions involving organohalogens found in the environment, or beneficial, because of their potential usefulness in the design of novel ligands that interact with proteins in a very specific way[2,3]. In this work Ab initio calculations are used to analyze the interaction between heterocyclic (C_2H_4Si) silylene and heterocyclic (C_2H_4Ge) germylene with methyl halides (CH_3-X) and mono-substituted amines (NH_2X) (X= F, Cl, Br, I). Calculations were carried out at the second-order Moller-Plesset perturbation theory (MP2) with the 6-311++G(2d,2p) basis setfor all atoms, except iodine, for which the def 2-TZVPP (default-2 triple-zeta valence with the large polarization) basis set was used. The contraction scheme of this basis set is [6s5p3d2f] for I atom. The electron densities of all complexes have been analyzed using the Atoms in Molecules (AIM) method with the AIMAll program. According to our results strength of interactions M….X (M=Si, Ge and X= F, Cl, Br, I) decreased as follows:

1) Ge…ICH_3 > Ge…$BrCH_3$> Ge…$ClCH_3$> Ge…FCH_3
2) Si… ICH_3 > Si…$BrCH_3$ > Si…$ClCH_3$ > Si…FCH_3
3) Ge…INH_2 > Ge…$BrNH_2$ >Ge…$ClNH_2$ > Ge…FNH_2
4) Si…INH_2> Si…$BrNH_2$ > Si…$ClNH_2$> Si…FNH_2



Scheme 1

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Synthesis and study of physical properties of nanocomposites based on polyaniline and ZnO nanorods in camphorsulfonic acid

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In recent years, developments of inorganic/organic hybrid materials on nanometer scale have received significant attention due to wide range of potential applications and high absorption in the visible part of the spectrum and high mobility of the charge carriers [1]. Polyaniline (PANI) is the most attractive conductive polymer because of the presence of the reactive -NH- groups in polymer chain, and used in wide applications such as batteries, sensors, electronic devices and etc [2,3]. Zinc oxid (ZnO) is a nontoxic material and n-type semiconductor with wide band gap (3.37 eV) [4].

This research work, describes preparation of PANI/ZnO nanocomposites by the chemical oxidative method of aniline monomer in champhorsulfonic acid medium with different amounts of ZnO nanorods, using ammonium peroxydisulphate (APS) as an oxidant. The composition, morphology and structure of the obtained nanocomposites were characterized by Fourier transform infrared (FTIR), X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), thermogravimetric analysis (TGA) and UV-Vis spectroscopy. The characteristic FTIR peaks of PANI were found to shift to higher or lower wave number in PANI-/ZnO nanocomposites due to formation of H-bonding. XRD patterns showed that the crystallinity of PANI is more pronounced after addition of ZnO, while the intensity of the peaks increased by addition of ZnO. The electrical conductivity measurements by four point probe instrument showed that PANI/ZnO nanocomposites have low electrical conductivity than that of the pure PANI. TGA results showed that the synthesized nanocomposites have high thermal stability than that of PANI in room temperature.

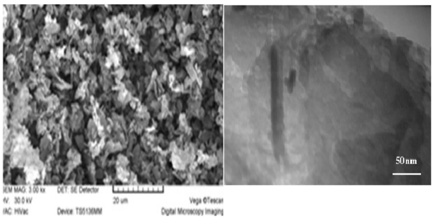

Fig. 1 Scanning electron micrograph of PANI–ZnO 2 wt% nanocomposites. TEM micrograph of PANI–ZnO 2 wt% nanocomposite.

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Synthesis and characterization of silica–4-chloro methyl polystyrene core–shell nano composite via RAFT polymerization

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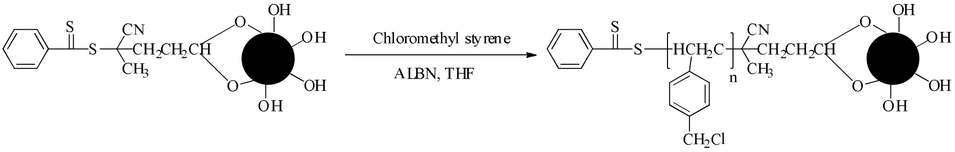
In recent decades, much attention has been paid to polymer/clay nanocomposites as advanced polymeric materials. Relatively low loading of clay has resulted in significant improvements in mechanical properties [1], thermal stability and flame retardancy [2], magnetic and electric properties [3], gas permeation [4], and enhanced modulus for the synergism between the components. On the contrary, the degree of dispersion of the clay platelets into the matrix determines the structure of nanocomposites and affects the aforementioned properties. This research work reports the synthesis of structurally well-defined silica–poly chloro methylstyrene (SiO_2-PCMS)hybrid nanoparticles using a RAFT agent carboxylic end group. Due to the strong tendency of nanoparticles such as metal oxides to agglomerate, homogeneous dispersion of these materials in a polymeric matrix is extremely challenging. In order to overcome this problem and to enhance the filler polymer interaction, this study focused on living polymerization that was initialized from the surface of silica nano fillers. A simple method for synthesizing SiO_2/polymer nano composites was found with a good dispersion of the nano fillers using this RAFT agent, 4-cyano-4-[(phenyl carbon thioyl) solfanyl valeric acid. This RAFT agent has an available carboxyl group to anchor onto SiO_2 nanoparticles and C=SPh moiety for subsequent RAFT polymerization of 4-chloro methyl polystyrene to form n-SiO_2/4CMS nanocomposites (Scheme 1).



Scheme 1

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Novel engineering polymers of alginate-based polyurethanes

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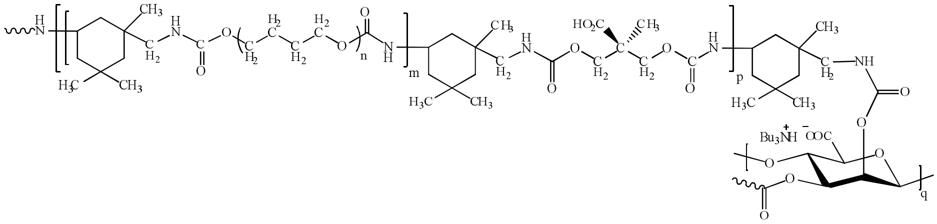
Recently, we have introduced two interesting procedures including the blending of sodium alginate (SA) with a new generation of polyurethanes (PUs) and dispersing the alginate nanoparticles on the cationic polyurethane matrix to overcome the obvious incompatibility between SA and PUs [1-2]. Nevertheless, the introduction of compatible alginate-based polyurethanes with desired properties is an open challenge.

Here, we describe the synthesis and characterization of the novel soluble alginate based polyurethanes in common aprotic organic solvents for the first time (Scheme 1). The novel soluble alginate based polyurethanes in organic solvents were synthesized by the reaction of NCO−terminated prepolymers and tributylammonium alginate (TBA−Alg). The chemical structures of synthesized polyurethanes were characterized using FTIR, ^{1}H NMR and TGA. The reaction completion was confirmed by disappearing of NCO band in FTIR spectra. Furthermore, a peak at 4.71 ppm and some small peaks at a range of 4.12−4.37 ppm in the ^{1}H NMR of alginate-based polyurethanes were assigned to the backbone of alginate.



Scheme 1

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Sublation method for the surfactant separation

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Surfactants enter waters and wastewaters mainly by discharge of aqueous wastes from household and industrial laundering and other cleansing operations [1-2].

The sublation method is specific for surfactants, because any substance preferentially adsorbed at the water-gas interface is by definition a surfactant. The surfactant is adsorbed at the water-gas interfaces of the bubbles and is carried into the ethyl acetate layer. The solvent is separated, dehydrated, and evaporated, leaving the surfactant as a residue suitable for analysis. [3-4].

Successive 5-min sublations were made from1 L of sample containing 5 g NaHCO3 and 100 g NaCl. Under the conditions specified, extensive transfer of surfactant occurs in the first sublation and is substantially complete in the second. We Selected a sample to contain not more than 1 to 2 mg surfactant. The sample was filtered through the medium-porosity qualitative filter paper. The nitrogen flow started, and the rate increased carefully to 1 L/min initially but did not exceed a rate at which the liquid phases begin vigorous intermixing at their interface. With various known surfactants at 0.2 to 2 mg/L and appropriate analytical methods, over 90% of added surfactant was recovered in one 5-min sublation from 10% NaCl. With regard to the recovered surfactant, the method is a satisfactory method.

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Synthesis of TiO_2/WO_3/functional graphen oxide nanophotocatalysts and photodegradation of air pollutants

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It is well-known that the poor air quality of indoor environments, such as buildings, houses, cars, and aircraft cabins, can promote transmissible respiratory illnesses, allergies and sick building syndrome. Indoor air pollution is a serious problem especially in urban cities. Pollutants such as NOx, SO_2 and CO cause adverse health impacts on occupants. Advanced oxidation process (AOP) such as photocatalysis is a promising technology for air purification. Photodegradation occurs at room temperature and pressure and actually oxidizes pollutants to H_2O and CO_2 [1-3].

The synthesis of inorganic materials in Room temperature ionic liquids (RTILs), is a rather new development and has attracted increasing interest in recent years. In this work, we present the control synthesis of TiO_2/WO_3 architectures in the presence of the imidazulim based ionic liquid, and used for the photocatalytic degradation of NOx,SO_2 and CO. The prepared photocatalysts were systematically characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) Photoluminescence spectroscopy (PL) and X-ray photoelectron spectroscopy (XPS).

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Synthesis of polyimide nanocomposite membranes based on silica

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Polymer electrolyte fuel cells (PEFCs) have been identified as promising power sources for vehicular transportation and for other applications requiring cleaning, quiet, and portable power [1-2].The most important component of a PEFC is polymer electrolyte membrane itself. It is well-known that aromatic polyimides have found wide applications in many industrial fields due to their excellent thermal stability, high mechanical strength, good film forming ability, and superior chemical resistance. It is well-known that aromatic polyimides have found wide applications in many industrial fields due to their excellent thermal stability, high mechanical strength, good film forming ability, and superior chemical resistance [3-4]. In this study asulfonateddiamine monomer, 4,4'-diaminodiphenyl ether-2,2'-disulfonic acid (ODADS), was successfully synthesized by direct sulfonation of a commercially available diamine, 4,4'-diaminodiphenyl ether (ODA). A series of sulfonated polyimides were prepared from 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTDA), ODADS, and diamine3,5-diamino benzoyl amino phenyl-14H-dibenzo[a,j]xanthene. Thermally stable sulfonatedpolyimide/silica hybrid nanocomposite films have been successfully synthesized through the in situ formation of silica within a polyimide matrix via sol-gel process. The chemical structure of the resulting polymers was characterized by FT-IRand ^{1}H NMR spectra.The obtained nanocomposites were characterized by FT-IR, powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM) and thermogravimetric analysis (TGA).

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Preparation and characterization of dendritic PEG-PAMAM and using of that as a polymeric material for CO_2/CH_4 separation via a PVA/PS membrane

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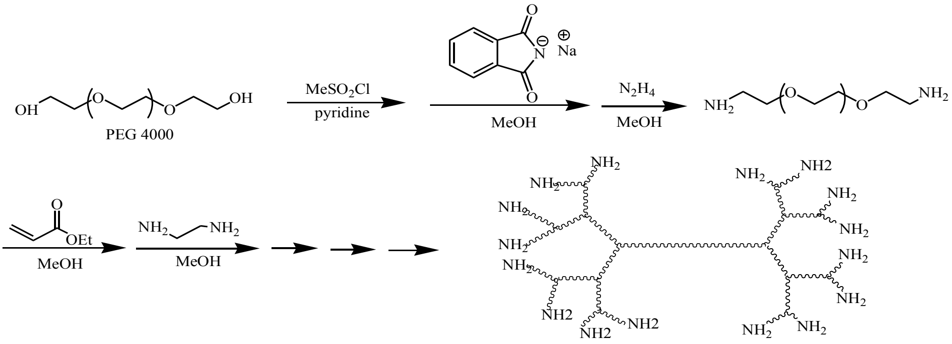
Removal of CO_2 from CH_4 and other gas streams by facilitated transport membranes has the benefit in contrast with conventional polymeric membranes because of high permeability and high selectivity [1-3].

A triblock dendritic copolymer PAMAM-b-PEG-b-PAMAM was synthesized (Scheml) and characterized by FT-IR and H-NMR methods. Subsequently, this copolymer was used as fixed carrier for CO_2 transportation in a thin film composite (TFC) membrane which was prepared using PVA as the skin layer and PS the support. The performance of prepared membranes at different PAMAM-b-PEG-b-PAMAM content was investigated.



Scheme 1

References:

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Studies on the synthesis of 5-aryl-2-thioxothiazolidin-4-ones as key intermediates in the synthesis of biologically important heterocycles

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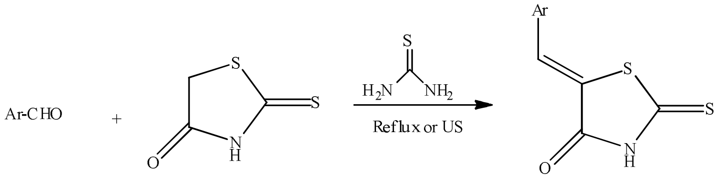
Thiazolidines particularly thiazolidine-2,4-dione and 2-thioxothiazolidin-4-one have attracted many interests because of their versatile pharmacological activities such as antidiabetic, antimicrobial, antimalarials, antiviral, anticonvulsant, antiinflammatory and also act as thyroid hormone receptor antagonists. Additionally, rhodanine-based molecules have been popular as small molecule inhibitors of numerous targets such as HCV NS3 protease, aldose reductase, b-lactamase, UDP-N-acetylmuramate/L-alanine ligase, antidiabetic agents, cathepsin D, and histidine decarboxylase [1-5].

In this study, in the course of our continuing interests in heterocycles of medicinal importance [3], the synthesis of (Z)-5-aryl-2-thioxothiazolidin-4-ones was carried out by the reaction of 2-thioxothiazolidin-4-ones and an appropriate aryl aldehyde in the presence of thiourea and acetic acid as catalyst under reflux or ultrasound conditions. The structure of the synthesized products were fully confirmed by spectroscopic (IR, ^{1}H NMR, ^{13}C NMR) analysis.

These valuable intermediates were employed in the synthesis of novel biologically important heterocyclic compounds. The details of this protocol will be discussed in the presentation.



(Z)-5-Arylidene-2-thioxothiazolidin-4-ones

Scheme 1

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One-pot, two-step synthesis of novel carbonylthioureas as antibacterial agents

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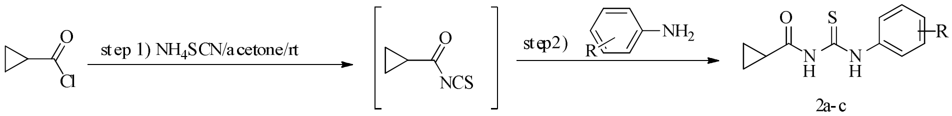
Acylthioureas exhibit very useful biological activities, such as antiviral, antifungal, herbicidal, and antibacterial activities; as well as cytotoxicity against cancer cells [1-2]. They also have extensive use in the synthesis of various heterocycles [3].

One-pot, two-step synthesis of several 1-cyclopropanecarbonyl-3-(substituted phenyl)-thioureas were carried out for the first time. In this way, we succeeded in achieving a simple procedure for the synthesis of 1-cyclopropanecarbonyl-3-(substituted phenyl)-thioureas derivatives via a one-pot, two-step process, without the need for work up and purification of intermediates. The structures of the synthesized compounds were confirmed by elemental analysis, FT-IR spectroscopy and ^{1}H-NMR, ^{13}C-NMR. All synthesized compounds were evaluated for antibacterial activity using S.enterica (SE), Micrococcusluteus (ML), Bacillus subtilis (BS) and Pseudomonas aeruginosa (PS).



2a-c

R= a) p-Me, b) p-Et, c) p-OMe

Scheme 1

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Demonstrating the ability of conducting polymers (polyaniline and polypyrrole) in attenuation of hard X-radiation.

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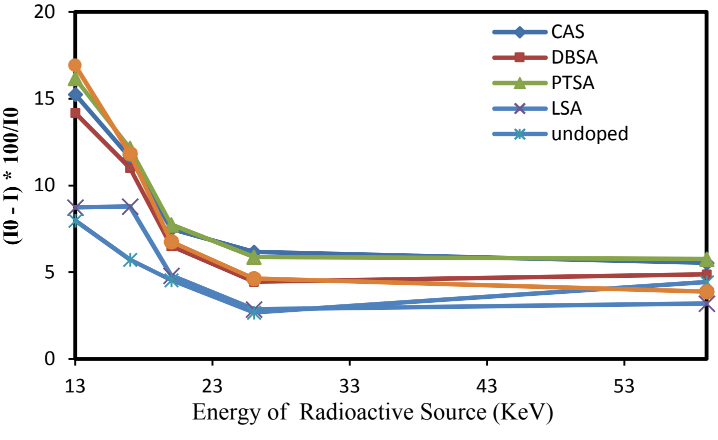
Conductive polymers have emerged as a new class of materials in last three decades. Because of their high conductivity, intriguing electrical properties and potential applications such as microwave absorbers were considered after the discovery of these materials. It is known that conducting polymers can effectively shield electromagnetic waves [1]. Moreover, With the development of nuclear weapon and spaceflight technology, great attention has been paid to low weight and flexible radiation shielding materials over the last twenty years [2].

In this study, polyaniline and polypyrrole were fabricated using different dopants; LSA, PTSA, DBSA, CSA and HCl. Also, undoped form of them was synthesized. The conductivity of prepared ICPs were measured using four probe method to compare how their electrical density could effect on their ability in absorption of X-radiation. Upon the obtained results, it was proven that increasing in conductivity, has an obvious impression on X-ray absorption.



Scheme 1:X-Ray absorption property of PANi prepared with different dopants

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Catalytic ozonation of phenol in wastewater with nano Fe_3O_4 coated on activated carbon: identification and toxicity of intermediates

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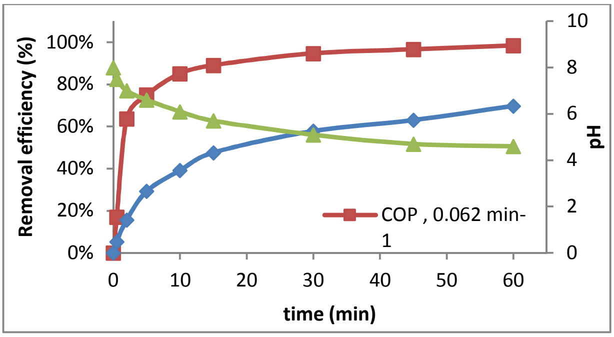
In this study, a new strategy in catalytic ozonation removal method for degradation and detoxification of phenol from industrial wastewater was investigated. Magnetic carbon nano-composite, as a novel catalyst was synthesized and then used in the catalytic ozonation process (COP) and the effects of operational conditions such as initial pH, reaction time and initial concentration of phenol on the degradation efficiency and the toxicity assay have been investigated. The results showed that the highest catalytic potential was achieved at optimal neutral pH and the removal efficiency of phenol and COD are 98.5% and 69.8%, respectively.

First order modeling demonstrated that the reactions were dependent on the initial concentration of phenol, with kinetic constants varying from 0.038 min^{-1}([phenol]$_0$= 1500 mg/L) to1.273 min^{-1}([phenol] $_0$ = 50 mg/L). Bioassay analysis showed that phenol was high toxic to *Daphnia magna* (LC_{50} 96h = 5.6 mg/L). Comparison of toxicity units (TU) of row wastewater (36.01) and the treated effluent showed that TU value, after slightly increasing in the first steps of ozonation for construction of more toxic intermediates, severely reduced at the end of reaction (2.23). Thus, COP was able to effectively remove the toxicity of intermediates which were formed during the chemical oxidation of phenolic wastewaters [1-4].



The degree of phenol degradation and COD removal in the COP, [phenol]o= 500 mg/L; Catalyst concentration of 2 g/L; initial pH of 8:0.

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Synthesis and characterization of novel poly(ether-imidazole-imide)/SiO_2 hybrid nanocomposite

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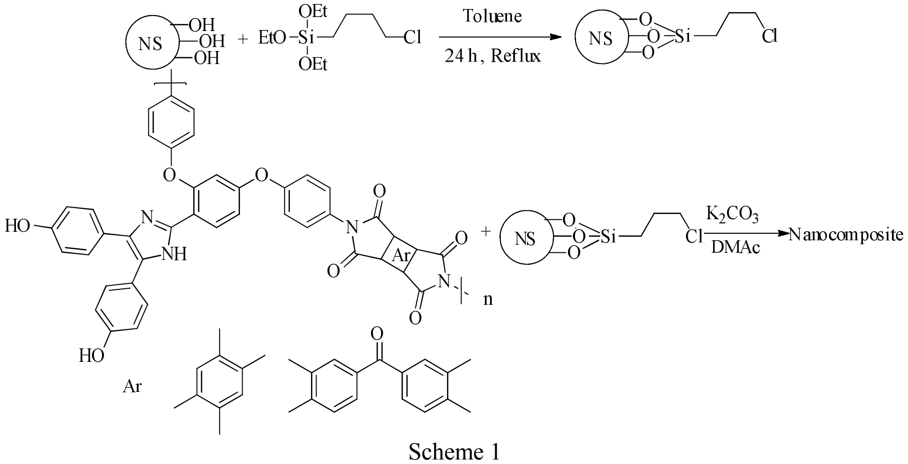
Organic-inorganic hybrid nanocomposites, which are the hybridization of organic polymer and inorganic material on a nano-scale, have attracted tremendous attention because of the combining totally different properties of them within a single molecular material. Polymer-inorganic materials are distinguished by their enhanced mechanical strength and thermal stability combined with optimal thermal properties [1].

In this study, a series of aromatic poly(imide-ether-imidazole) (PIEI)s containing derivatives of imidazole heterocyclic ring and flexible ether linkages was synthesized from polymerization reaction between 4,4'-(2-(2,4-bis(4-aminophenoxy)phenyl)-1H-imidazole-4,5-diyl)diphenol and various dianhydrides in a green media of ionic liquid (IL) without using NMP-pyridine-acetic anhydride [2] (Scheme 1).

Polymers having inherent viscosities of 0.55-0.67 dL/g were produced in high yield. All the PIEIs were noncrystalline and soluble in various organic solvents. The resulting nanocomposites were characterized using FTIR and ^{1}HNMR spectroscopy, and elemental analysis. The morphology of worn surfaces of films was examined by atomic force microscope (AFM). Thermal properties of the novel PIEIs and nanocomposites were also evaluated by thermogravimetric analysis and differential scanning calorimetry.



Scheme 1

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Recent advances of using PEBAX as polymer matrix in memebrane science

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Membrane performance is primarily limited by material properties, for which, polyether/amide block copolymers often referred as PEBAX, have recently been employed successfully as polymer matrix in membrane applications. PEBAX is a thermoplastic elastomer combining linear chains of rigid polyamide segments interspaced with flexible polyether segments [1]. Different methods were used by researchers for increasing membrane performance in separations. Generally, crosslinking is a way for modifying basic polymers in order to attain enhanced selectivities and render the polymer suitable for various applications. Some studies focused on crosslinking PEBAX membrane and achieved good results for that [2]. As an attractive material that demonstrates outstanding separation properties, mixed matrix membrane (MMM) has been the subject of worldwide academic studies conducted by many researchers especially those related to membrane technology. The recent advances have shifted towards the introduction of new and novel materials namely carbon nanotubes, metal organic framework, inorganic fillers such as silica, TiO_2, etc as potential fillers in the polymer matrix. On the other hand, preparing PEBAX composite membranes formed by laminating the PEBAX on a microporous substrate used as an efficient method. Here, effects of using various methods employed for modifying the structure and performance of PEBAX based membranes are explained and briefly discussed.

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Synthesis and characterization of a biopolymer based on CMC-Ch-*g*-poly(AcA-*co*-ECH) nanocomposite

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In this article, we synthesize of a novel CMC-based superabsorbent nanocomposite hydrogel via graft copolymerization of acrylic acid (AcA) monomer in the presence of Epicholorohydrine as a crosslinking agent and ammonium persulfate (APS) as an initiator. A novel superabsorbent hydrogel nanocomposite based on *Carboxymethylcelloluse* (CMC) and Chitosan(Ch) have been prepared via graft copolymerization of acrylic acid (AcA) monomer in the presence of Epicholorohydrine as a crosslinking agent and ammonium persulfate (APS) as an initiator. Evidence of grafting was obtained by comparison of FTIR and TGA spectra of initial substrates and superabsorbent composite. Moreover, morphology of the samples was examined by scanning electron microscopy (SEM). the swelling of superabsorbing hydrogels also, was examined in solutions with pH values ranging between 1.0 and 13.0.

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A new method for the synthesis of thieno[2,3-b]thiophene derivatives

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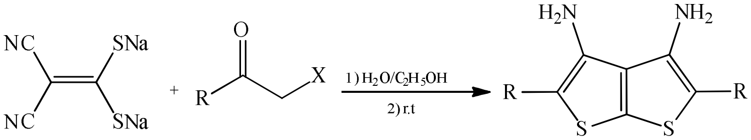
Thienothiopheneis a privileged structure because of its presence in a number of pharmacologically important compounds. These compounds have been reported as beinganti-tumor, anti-viral, antibiotic, anti-glaucoma and inhibitors of platelet aggregat ion activities [1-2]. Synthesis approaches to these compounds are varied and use basic catalysts such as MeONa, KF, NEt_3 and K_2CO_3. In this research we wish to report on the high efficiency synthesis of thieno[2,3-b]thiophene derivatives from treatment malononitriledithiolate sodium salt with the various α-halocarbonyls in a single-phase system of water/ethanol (Eco-friendly solvents), absence of catalyst and the room temperature.



Scheme 1

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Cu-catalyzed, direct synthesis of symmetric organic disulfides *via* domino reactions of sulfur transfer reagents with aryl (alkyl) halides

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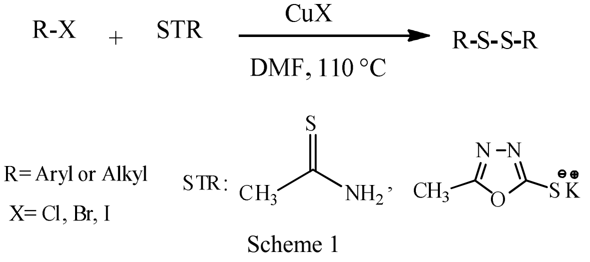
Organic disulfides are of importance in synthetic chemistry, biochemistry and industry [1]. They are commonly used to prepare many kinds of reactive intermediates, and participate in chemical substitution or addition reactions. Many biologically active compounds such as proteins, peptides and prodrugs, and industrial vulcanizing agents, have disulfide linkages. These compounds are typically prepared by oxidative coupling of thiols to disulfides in the presence of oxidants [2]. However, potential environmental and health risks as well as difficulty in working with thiols have persuaded organic chemists to provide new methods to reduce its disadvantages. In this regard, much attention has been directed to the use of sulfur-transfer reagents for the synthesis of organic disulfides from alkyl and aryl halides through coupling reactions. However, there are a limited number of methods for the direct synthesis of disulfides from aryl halides.

In continuation of our efforts on the synthesis of organosulfur compounds [3], we managed to provide new methods for the synthesis of symmetric disulfides from aryl and alkyl halides. Similarly, we became interested in providing other new methods for the synthesis of compounds in the presence of commercially available and inexpensive reagents. For these purposes thioacetamide and potassium 5-methyl-1,3,4-oxadiazole-2-thiolate were selected and used in the studies.



Scheme 1

So, a series of symmetric diaryl (dialkyl) disulfides were synthesized from related aryl and alkyl halides in the presence of some available copper salts such as CuI and CuCl.

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Cu(II) salen-MCM-41, as a versatile nano reactor, catalyzed oxidation of sulfides into sulfoxides

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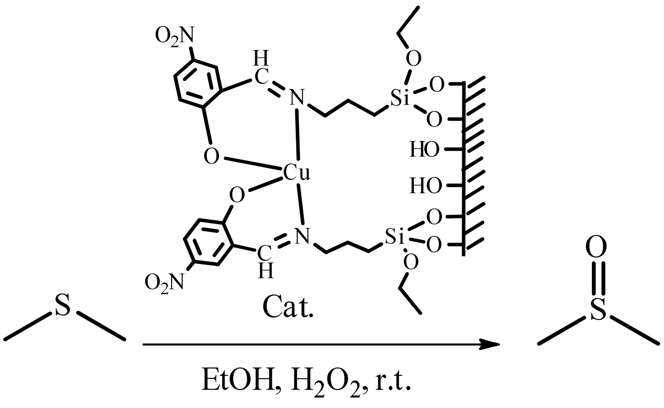
Schiff base which functionalized MCM-41 mesoporous materials were synthesized by post-grafting of 2-hydroxy-5-nitrobenzaldehyde onto silylated amino-modified MCM-41 and followed by the insertion of Cu(II) ions via a ligand exchange reaction. The surface properties of the functionalized meso porous were analyzed by a series of specified techniques like X-ray diffraction (XRD), N_2 adsorption–desorption, FT-IR, UV–vis spectroscopy, transmission electron micrography (TEM), IR-spectra and TGA/DTA. The prepared grafting Cu-salen-MCM-41 over mesoporous surface was found to be an efficient catalyst for the oxidation of different type of sulfides into sulfoxides with hydrogen peroxide (H_2O_2) with excellent yields at room temperature. The results shown that Cu-salen-MCM-41 is an effective catalyst for the oxidation of sulfides and can be repeatedly used and regenerated without any significant decrease in its catalytic ability. The results shown that thin complex is an active and selective catalyst for the oxidation of sulfides and complex is stable under present reaction conditions (Scheme 1).



Scheme 1

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The management of organic reactions in spite of all present limitations

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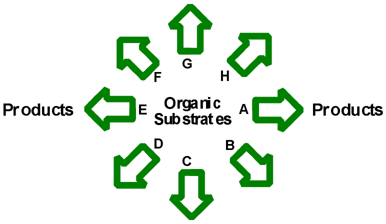
The development of simple, efficient and environmentally benign chemical processes or methodologies for widely used organic compounds from readily available reagents is one of the major challenges for chemists in organic synthesis [1].

Chemical transformations, as well as other industrial production processes, are experiencing a profound transformation to meet sustainability criteria, moving from old methods to new approaches that have been developed in accordance with green chemistry principles [2].

The aim of green chemistry is to reduce chemical related impact on human health and virtually eliminate contamination of the environment through dedicated, sustainable prevention programs. Green chemistry searches for alternative, environmentally friendly reaction media and at the same time strives to increase reaction rates and lower reaction temperatures.

This speech presents some scientific abilities of our research group in some green organic transformations [1-10] (Scheme 1).



A= Nanorector; B= Nanocatalyst; C= Nanocomposite; D= Polymeric Catalyst; E= Solvent-Free; F= SDS/H_2O; G= Electrosynthesis; H= Photochemical Synthesis

Scheme 1

In summary, we believe that the present methods open new possibilities for medicinal chemistry and material sciences and could be an important addition to the existing methodologies.

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Amino acid containing polymers: from nanostructure to bionanocomposites

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Amino acids as one type of the major building blocks of living systems are the main components of all naturally occurring proteins. The incorporation of amino acids in the polymer backbone not only increases the biocompatibility of peptide-based system, but also have been found to show nano-scale ordering into stable hierarchical superstructures administered by the formation of secondary structures in the peptide segments [1,2]. Important scientific and technological interest has focused on polymer inorganic nanocomposites (NC)s over the last two decades [3]. In this regards, we have synthesized a variety of NCs based on different fillers and matrixes. For example TiO_2 nanofiller was incorporated into the biodegradable poly(ester-imide)(PEI) containing L-tyrosine amino acid for the preparation of novel PEI/TiO_2 bionanocomposites (BNCs). Also, nano-ZnO surface-coupled by 3-aminopropyltriethoxylsilane as a coupling agent was employed for the preparation of poly(amide-imide) (PAI)/ZnO NCs through ultrasonic cavitations process [4-6]. Morphology study of all the resulting nanostructure polymers and NCs were characterized by field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM) analyses (Figure a).

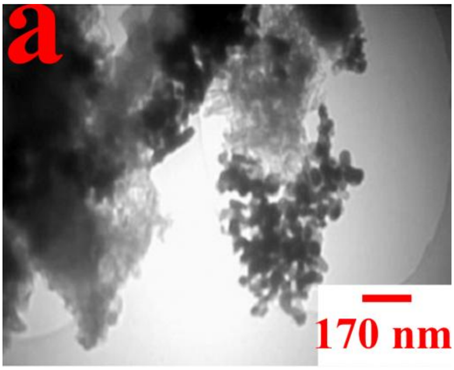

Fig. a. TEM image of PAI/ZnO NC (8 wt%)

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Preparation, characterization and catalytic application of heterogeneous palladium catalysts in C-C and C-heteroatom bond formation reactions

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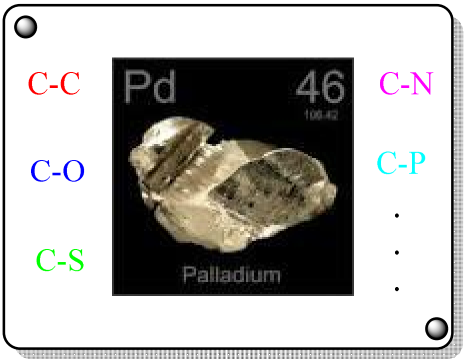
Silica surface is highly porous and can trap and stabilize the Pd nanoparticles; hence it has been used as a substrate for the immobilization of Pd nanoparticles. The main problem with this catalytic system is that the Pd nanoparticles are easily separated from the substrate surface and released into the reaction media. Thus, this is a challenging that improves the catalytic activity and heterogeneity of these catalytic systems using modification of silica by various organic compounds. We present some of our recently reported palladium catalyst systems based on modification of silica for fine immobilization of PNPs as heterogeneous catalyst system [1].

The efficient separation and subsequent recycling of homogeneous transition metal catalysts especially Pd continues to present a real scientific challenge. The development of magnetic nanoparticles supported Pd catalysts seems particularly suitable for C-C and C-heteroatom bond formation reactions due to the wide accessibility, simple separation from reaction mixture, and excellent stability of these solid supports. Thus herein, we would like to report our recent progress in magnetic recyclable palladium catalyst systems [2].



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Synthesis of multipart heterocycles based on active methylenes

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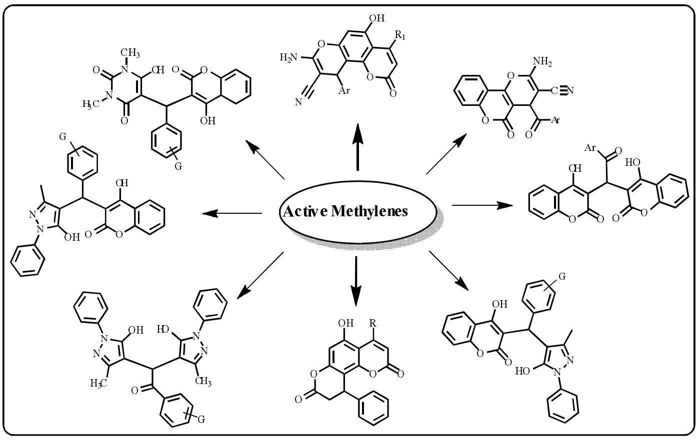
Methylene active compounds are one of the important substrates that play key role in heterocyclic syntheses. So far, numerous applications of them in synthesis of heterocycles have been reported. In the current research, by the use of new designed strategies, a number of novel multi-part heterocyclic compounds such as three substituted methanes, khelactones, pyrano[c]chromenes, biscoumarins, and bispyrazolones [1-8] have been synthesized by employing some novel methods based on methylene active compounds (Scheme 1). Modification and development of preliminary methods through changing the reaction conditions and using various acidic and basic catalysts and nanocatalysts have also been investigated. Some of the advantages of these methods are the compatibility with green chemistry principles, simple experimental conditions, and high productivity.



Scheme 1

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Theoretical study of 1,3-diolar cycloaddition reaction between methyl thiocyanate and cyclononyne

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The energy content in alkynes may be increased further by bending the normally linear triple bond, as in the small cycloalkynes. Cycloadditions of 1,3-dipoles may occur by concerted Huisgen mechanisms. Isothiazole is a member of a class of compounds known as azoles. In contrast to the isomeric thiazole, the two heteroatoms are in adjacent positions. The ring structure of isothiazole is incorporated into larger compounds with biological activity such as the pharmaceutical medicines. 1,3-Dipolar cycloaddition, also known as the Huisgen reaction, is the reaction belonging to the larger class of cycloaddition between a 1,3-dipole and dipolarophile to form a five membered ring. the reactivity and strain energy effect of cyclononyne with methyl thiocyanate will be discussed in light of computational studies using B3LYP/6-31G* method. The investigation of the structural properties, theoretical thermodynamic, kinetic data and rate constants of the reactions will be presented and discussed.

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Synthesis, characterization and application of environmentally–benign reagents and catalysts in chemical transformations

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In this research, different types of catalysts including:

- Lewis acids such as Bi(III) salts
- Solid acids such as nano-silica sulfuric acid, heteropoly acids and supported heteropoly acids
- Brønsted or Lewis acidic ionic liquids and supported ionic liquids
- Nanoparticles-based dendritic catalysts

Were prepared and used in some important organic transformations such as esterification reactions, protections and deprotections, synthesis of heteorocyclic compounds, and coupling reactions [1-6].

High product yields, operational simplicity, excellent selectivity, stability, and easy recovery and reuse are the remarkable features of these catalytic systems.

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The interaction energy calculations between glycoluril clip and benzoique acid derivatives using DFT calculations: comparison with glycoluril clip

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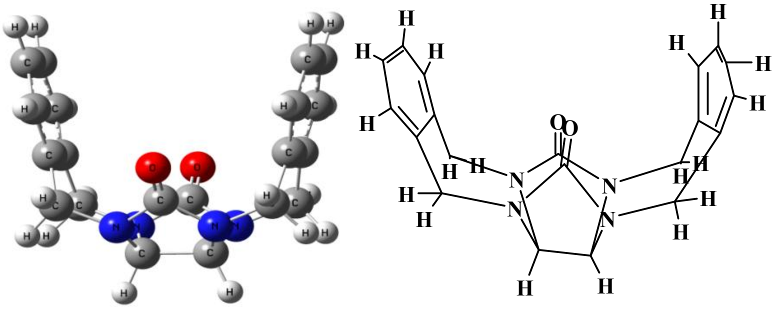
The glycolurils have been received a great deal of attention due to their practical applications, such as fertilizers, polymer crosslinking, explosives, stabilizers of organic compounds against photo-degradation, combinatorial chemistry, radioiodination agents for biomolecules, psychotropic agents, catalysts, bleaching activators, and they have also been applied for the monomer in supramolecular chemistry[1-3]. In this work, theoretical calculations were carried out to determine the interaction energy between a glycoluril, TGL, as a host molecular clip and Benzoique Acid derivatives as the guest molecules (host-guest complex, Meta tiyol benzoique Acid The theoretical calculations on TGL benzoique acid derivatives and Meta tiyol benzoique acid were done, using a hybrid functional closed-shell RB3LYP and the 6-31G* basis set, employing the Gaussian 03. The energetic and geometric parameters, especially the bond lengths were investigated for TGL, benzoique acid derivatives and Meta tiyol benzoique Acid and their parameters compared to glycoluril, GL molecule (host-guest complex Meta tiyol benzoique) (Scheme 1).



Scheme 1

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Synthesis and characterization of some new ligands from bis ((o-allyl)cresyl) sulfoxide and diamine with nano catalytic property

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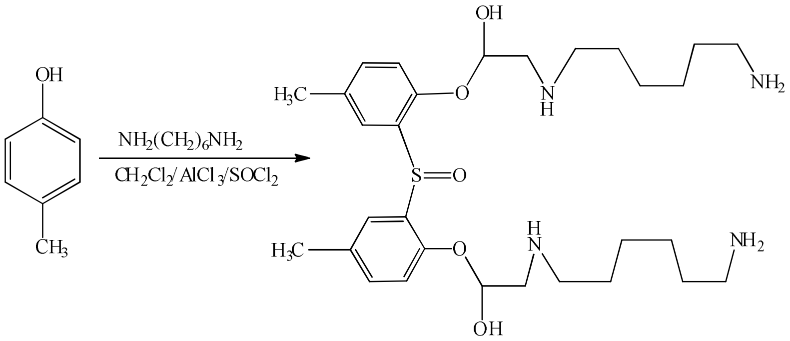
Podands now exist in a great many structural variations ranging from single-chained basic compounds to multiarmed dendrimers like inolecules and from highly flexible to rather rigidly preorgnized molecular architectures [1]. The applications of Podands which can be mentioned is ecology, biochemistry, nuclear power, nano-industry (nano-medicine, nano-catalysts), separation and purification of metals and cations, the separation of isotopes of heavy industry [2-3]. Our purpose in this research work was to prepare and to characterize a new podand and then pure it. The procedures are follows as: The p-cresol was converted into sulfoxide (1) in reaction with $SOCl_2$ compound (1) resulted to bis allyl (2) in reaction with allyl bromide. The compound (2) was oxidized to corresponding bis epoxide (3) compound (3) in reaction with proper diamine (hexandiamine) was yielded dihydroxy podand (4). The structures of all synthesized compound were recogenized by IR, ^{1}H NMR and ^{13}C NMR (Scheme 1).



Scheme 1

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Synthesis of bisthiazolin compounds from bisthiosemicarbazon derivatives and dialkyl acetylene dicarboxylates under ultrasonic conditions

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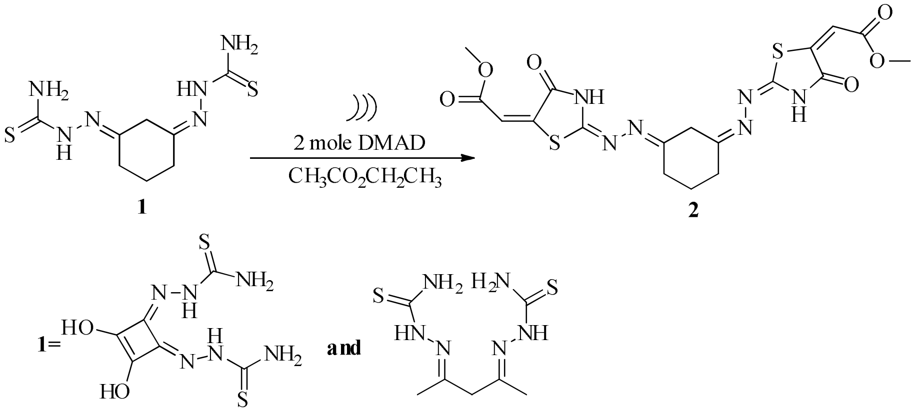
Thiazolin play very vital role in the manufacturing of various biologically active drugs as analgesic [1], anti-inflammatory, anti-depressant, anti-cancer, antimicrobia, anti-diabetic [2]. Some of the thiazolin have shown a wide range of pharmaceutical properties. Recently we have reported reaction of thiosemicarbazone derivatives with DMAD and DEAD [3].

Treatment of 1,3 and 1,2-dicarbonyl compounds with thiosemicarbazide afford the corresponding thiosemicarbazone derivatives.

In this work we synthesized [2-({3-[(5-methoxycarbonylmethylene-4-oxo-thiazolidin-2-ylidene)-hydrazono]cyclohexylidene}-hydrazono)-4-oxo-thiazolidin-5-ylidene] acetic acid by reaction of 1,3-bisthiosemicarbazone derivatives of 1,3-bicarbonyl with DMAD and DEAD under ultrasonic conditions. The structures of the products were identified by ^{1}HNMR, ^{13}CNMR, and IR spectroscopy and elemental analysis.



Scheme 1

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Facile, efficient and diastereoselective synthesis of α-hydrazine tetrazoles through a novel one-pot four-component reaction

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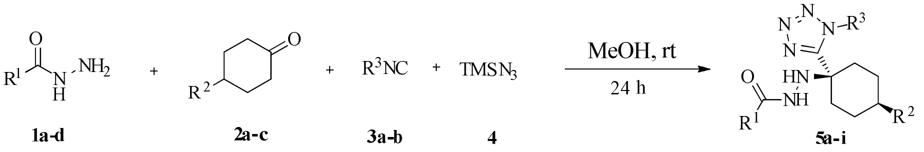
Tetrazoles are useful heterocyclic skeletons because there are in many important biological compounds and drugs. Among the pharmaceutically important tetrazoleslosartan and valsartan,two widely used angiotensin receptor blockers, deserve a special mention. Access to 1,5-disubstituted tetrazoles is of considerable interest, and numerous approaches to this scaffold have been disclosed in the literature. Major synthetic strategies utilized for the preparation of 1,5-disubstituted tetrazoles are *via* intermolecular cycloaddition reactions, and isocyanide-based reactions and conversion of substituted tetrazoles into 1,5-disubstituted tetrazoles [1]. Among the various pathways toward 1,5-disubstituted tetrazole derivatives, those based on the isocyanide multicomponent reactions are especially noteworthy.

As part of our continuing efforts on the development of new routes for the preparation of biologically active heterocyclic compounds by means of isocyanide-based multicomponent reactions, herein, we describe a novel diastereoselective synthesis of α-hydrazinotetrazoles*via* a facile azideUgi four-component reaction using various cyclic ketones, hydrazides, isocyanides and trimethylsilylazide as Ugi acidic partner (Scheme 1).

Good to high diastereoselectivity, good yields, easy work-up are advantages of this approach. The structures of the products were confirmed based on spectroscopic data and also X-ray crystallography data [2].



R^1 = Boc-phe-NHNH$_2$, phenyl, *p*-toluenesulfyl, thienyl
R^2 = *t*-butyl, ethyl, methyl
R^3 = *t*-butyl, cyclohexyl

Scheme 1

References:

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The oxidation of banzyl alcohol by the polypyridyl Cu(II) complex as catalyst

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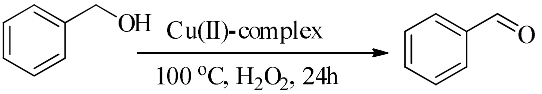
Oxidation reactions play an important role in synthetic chemistry and provide important methodology for the introduction and modification of functional groups. A large number of coordination complexes are able to undergo redox reactions and catalyse the homogeneous and heterogeneous reactions. Catalysts based on coordination complexes are very efficient for many chemical reactions due to their correct stability, variety of oxidation states, different geometries, coordination modes, and variety of ligands [1-3]. We reported here a novel environmentally friendly oxidation process for the oxidation of benzyl alcohol by using Two polypyridyl copper(II) complexes, [Cu(phen)(phen-dione)Cl]Cl **(1)** and [Cu(bpy) (phen-dione)Cl]Cl **(2)**, (where Phen =1,10-phenanthroline, bpy=2,2'-bipyridine and Phen-dione=1,10-phenanthroline-5,6-dione), and H_2O_2 as oxidant under solvent free conditions. The effects of various parameters such as reaction temperature, reaction time, etc, were studied. These complexes were able to catalyze the benzyl alcohol oxidation into benzaldehayde with good yields and conversion percentage for complex **(1)** was higher than complex **(2)**.



Scheme 1

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A facile approach for the synthesis of novel benzo[b]pyrazolo[5',1':2,3]pyrimido[4,5-e][1,4]thiazine derivatives

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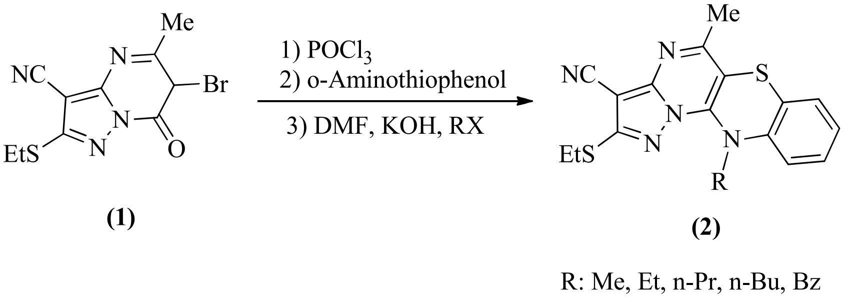
Pyrazolo[1,5-a]pyrimidines, which are synthetic analogs of purines, exhibit a wide variety of biological activity, such as enzymatic, antibacterial, antiphlogistic and antiparasitic activities [1]. They are also used as intermediates in the dyestuff industry [2]. Besides, thiazine and 1,4-benzothiazine derivatives possess a wide spectrum of biological and pharmacological activities, such as calcium channel blockers, phosphodiesterase 7 inhibitors, 5-HT3 antagonists, antipsychotics, sedatives and Na^+/H^+ exchange inhibitors [3].

Due to the widespread biological activities of fused heterocyclic systems, in this study, we synthesized a novel benzo[b]pyrazolo[5',1':2,3]pyrimido[4,5-e][1,4]thiazine heterocyclic system. In our protocol, the desired compound were obtained from the reaction of pyrazolo[1,5-a]pyrimidine (1) with $POCl_3$ and then with o-aminothiophenol. As shown in scheme 1, the resulting compound was alkylated with various alkylhalides to give the corresponding products (2) in good yields.



Scheme 1

References:

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One-pot synthesis of 2,4(1*H*,3*H*)-quinazolinediones from the reaction of 2-[chloro(phenyl)methyl]-4*H*-benzo[*d*][1,3]oxazin-4-one with urea

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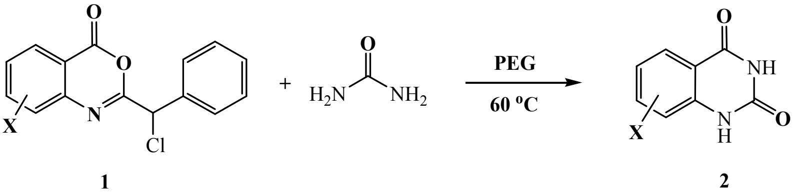
2-Functionalized (4*H*)-3,1-benzoxazin-4-one and its derivatives are used directly or indirectly in many clinical applications [1]. The susceptibility of the C-4 carbonyl to nucleophilic attack causes the (4*H*)-3,1-benzoxazinones are not satisfactorily stable rings. Thus, they are used as suitable starting materials in the synthesis of biologically active heterocycles [2,3].

With the aim of expanding the synthetic potential of the (4*H*)-3,1-benzoxazinones, we have studied the reaction of **1** with urea (Scheme 1). Quinazoline-2,4-diones **2** [4-6] are obtained with good to high yields under mild reaction conditions.



X = H, 5- Me, 6-Cl, 6-Cl, 6- Br, 6,7-di-MeO, 6-OH, 6-NO_2

70-90 %

Scheme 1

References:

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A new solid phase for efficient synthesis of azapeptides containing azaglycine moiety

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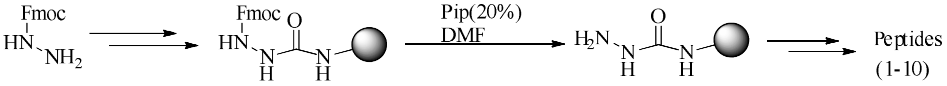
Peptide libraries constructed from naturally occurring amino acids have been widely used to screen for biological activity. However, increased activity, bioavailability and degradative resistance often require incorporation of unnatural residues in the peptide framework. Besides, the incorporation of aza-glycine in peptides has been performed to facilitate structure-activity relationship studies in the pursuit of mimics with improved activity and enhanced metabolic stability [1]. On the other hand, Solid-phase peptide synthesis (SPPS) has evolved into a powerful synthetic method since it was first reported in 1963. It is considered the method of choice for the automated preparation of peptides in numerous laboratories around the world. SPPS is now being used to rapidly synthesize peptides in a combinatorial fashion [2,3].



Scheme 1

In view of this report and also due to our attention in the synthesis of peptides, we herein has been described a new methodology for preparation of aza-glycine in peptides by Fmoc- hydrazine and *p*-nitrophenyl chloroformate as starting material on Rink amide as Solid-phase. This method has many advantages among them; avoid using dangerous compounds such as phosgene and potassium cyanides, high yield, clean and safer than previous procedures [4] (Scheme 1).

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Versatile synthesis of substituted imidazoles using nano tin(II) nitride as a source of ammonia

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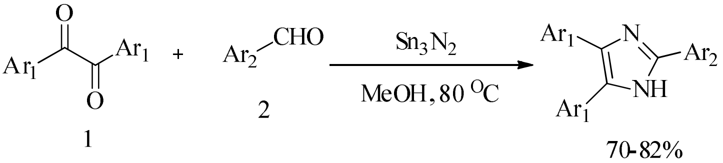
The study aims at evaluating the application of nano tin(II) nitride (Sn_3N_2) as a suitable source of ammonia for the synthesis of 2, 4, 5-trisubstituted imidazoles. The tests revealed that heating a mixture of a benzaldehyde, a benzyl, and nano tin(II) nitride in methanol leads to the formation of functionalized imidazoles in good to excellent yields. Regarding the atom economy, simple reaction design, and the ability to construct compounds of desire by the introduction of several elements in a single chemical event, multicomponent reactions (MCR) have changed to a significant part of the set of methods currently used in combinatorial chemistry [1]. The purification of the products of such reactions is also very easy due to the fact that all of the organic reagents used take part in the reaction and are incorporated into the target product. The application of MCR to construct interesting heterocyclic scaffolds is of specific use in the preparation of various chemical libraries of 'drug-like' molecules. Imidazoles constitute scaffolds in very important biomolecules, such as histamine, biotin, istidine, pilocarpine alkaloids and other alkaloids, with considerable biological activities like antimicrobial, anticryptococcal or inhibition of nitric oxide synthase, or cytotoxic activities. Highly substituted imidazoles are prepared through a variety of methods. Ammonia is a common source of nitrogen in organic chemistry, the small scale use of which is limited due to handling issues. Nano Sn_3N_2 was mentioned to be applicable as a source of ammonia that can be used in organic syntheses, based on the reactions below. Regarding the unrivaled pharmacological properties of imidazols, a convenient protocol, using nano tin(II) nitride as the ammonia source and different aldehydes and benzyls, for the synthesis of these heterocycles is described [2,3] (scheme1).



Scheme 1

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Synthesis of conjugated benzodiazepine with L-alanine amino acid

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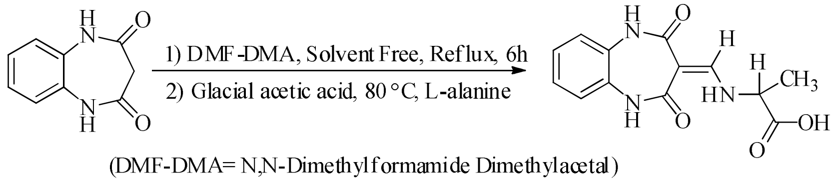
Benzodiazepines and their derivatives have attracted considerable attention from researchers due to their bioactive and pharmaceutical properties. Many members of this family are widely used as anticonvulsant, anti-anxiety, anti-seizures, analgesic, seditative, antidepressive and hypnotic or anti-inflammatory agents. They have also been used as antibacterial and antifungal agents and in the management of skeletomuscular spasticity, panic or as premedication prior to surgery. In addition, 1,5-benzodiazepines have found applications as readily available intermediates in the synthesis offused ring compounds such as triazolo-, oxazolo-, isoxazolo-, oxazino- or furano-benzodiazepine. Benzodiazepine derivatives also find commercial use as dyes for acrylic fibers. The search for new heterocyclic systems including the 1,5-benzodiazepine-2,4-dione moiety for biological activities therefore is of much current importance [1,2].

In this work we selected compound produced from reaction 1,5-benzodiazepine-2,4-dione with DMF-DMA for reaction with some amino acids [3]. Substitution of the dimethylamino group with the amino acid L-alanine proceeded smoothly in glacial acetic acid at 80˚C giving product (scheme1). The FT-IR, ^{1}H-NMR and ^{13}C-NMR spectra confirms the structure of product.



(DMF-DMA= N,N-Dimethylformamide Dimethylacetal)

Scheme 1

References:

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Synthesis of new derivatives of pyridazino[6,1-c]pyrimido[5,4-e][1,2,4]triazine

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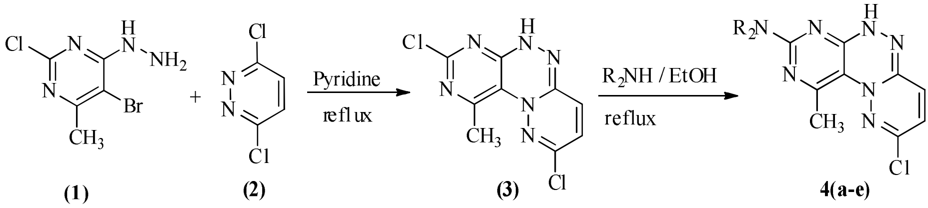
Pyrimidine derivatives and heterocyclic annulated pyrimidines continue to attract great interest due to the wide variety of interesting biological activities observed for these compounds, such as anticancer [1], antiviral [2], antitumor [3], and anti-inflammatory activities [4].

In this study, 5-bromo-2-chloro-4-hydrazino-6-methyl pyrimidine (1) was synthesized according to our previous method.[5] The treatment of this compound with 2,6-dicholoropyridazine (2) in pyridine gave quantitatively the desired heterocyclized pyridazino[6,1-c]pyrimido[5,4-e][1,2,4]triazine derivative as a novel heterocyclic system. Eventually, the reaction of it with various secondary amines obtained new derivatives of pyridazino[6,1-c]pyrimido[5,4-e][1,2,4]triazine 3(a-e).



Scheme 1

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A facile synthesis of an oxazolo[5,4-d]pyrimidine analogues

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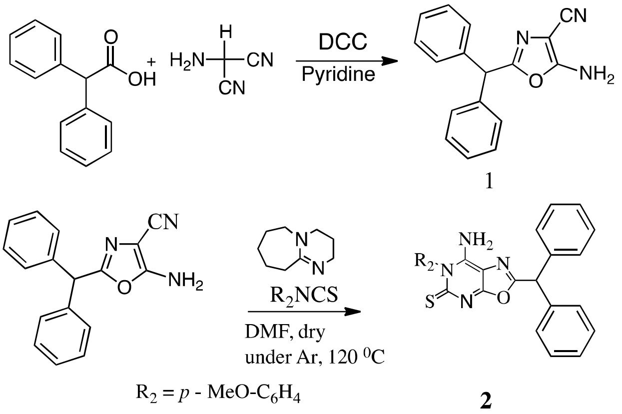
Receptor tyrosine kinases such as VEGFR2 (vascular endothelial growth factor receptor 2, KDR) or EGFR (epidermal growth factor receptor) play crucial roles in a variety of diseases, such as cancer [1-2]. Recently, some pyrrolopyrimidines were shown to be potent EGFR inhibitors [3]. Therefore, new types of oxazolo[5,4-d]pyrimidine **2** were synthesized via 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as base catalyzed heteroannulation of 5-amino-2-benzhydryl-4-cyano-1,3-oxazole **1**, (prepared by a solution of aminomalononitriletosylate (AMNT) in 1-methyl-2-pyrrolidinone with diphenylacetic acid and 1,3-dicyclohexylcarbodiimide, DCC), with p-methoxyphenylisocyanate (Scheme 1). In this communication, we were interested in finding new non-nucleosidic chemotypes and natural substrate, a virtual screening approach led to the proposal of 7-amino-2-benzhydryl-6-(4-methoxyphenyl)-oxazolo[5,4-d]pyrimidine-5(4H)-thione **2**.



Scheme 1

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Three component reaction for synthesis of spiro [indene-2, 4'-pyran]-1, 3-dione derivatives in water and using of DABCO as catalyst

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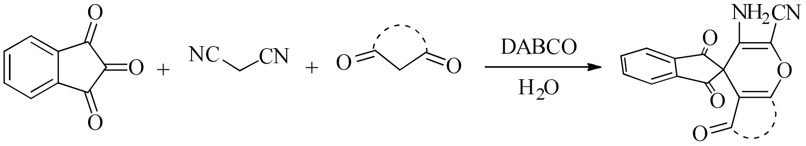
Development of environmentally benign and clean synthetic procedures has become the goal of present day organic synthesis. Water plays an essential role in life processes and is also an environmentally friendly medium for organic reactions [1]. Multicomponent reactions (MCRs), which can produce a diversity of compounds, provide one of the most efficient methods for the combinatorial synthesis of structurally diverse compounds [2].

Pyran derivatives, a great part of many natural products [3], are identified for its broad range of biological activities such as antiviral, antitumor, antibacterial, spasmolytic. Also, recent discovery have propose that the compounds having 4H-pyran core are useful for the treatment of Alzheimer, Schizophrenia, and Mycolonous diseases [4].

We now report a clean and efficient method for the preparation of spiropyran-fused heterocycles by reaction of Ninhydrin, malononitrile and variety of active methylene compounds in water and using the 1,4-diazabicyclo[2,2,2]octane (DABCO) as a catalyst.



Scheme 1

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Magnetic nano Fe_3O_4 particles as catalyst for the synthesis of 2-methylthio pyrimidine-5-carbonitrile derivatives

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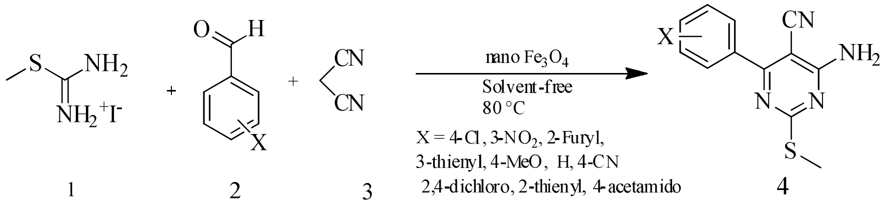
Magnetic metal nanoparticles have emerged as a new class of nano catalysts system for reactions needing alkaline promoters. So Fe_3O_4 nano particles have been used in some organic transformations such as acylation of phenols or alcohols [1], synthesis of α-aminophosphonates [2] and preparation of propargylamines from alkynes, amines and aldehydes [3].

The results showed that the magnetic nano Fe_3O_4 particles has good activity and high efficiency, when the reaction was performed without solvents under conventional thermal heating. Their high surface area of the magnetic nano Fe_3O_4 particles facilitates higher catalytic activity than conventional heterogeneous catalysts.

Structures containing pyrimidine heterocyclic moiety often play an essential role in medicinal chemistry as are analgesics, antihypertensives, antipyretics, and anti-inflammatory drugs as well as in some pesticides, herbicides, and plant growth regulators [4].

Herein, we wish to report the application of magnetic nano Fe_3O_4 particles as catalyst for the synthesis of 4-amino-6-aryl-2-methythio pyrimidine-5-carbonitrile derivatives via a one-pot cyclocondensation reaction under solvent-free conditions (Scheme1).



Scheme 1

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Copper(II) modified MCM-41 an efficient catalyst for the oxidation of sulfides to the sulfoxides using UHP as oxidant

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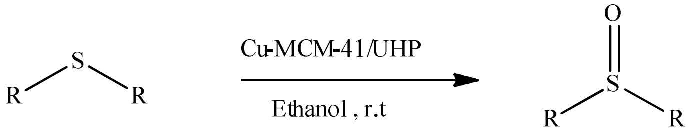
A general strategy for converting a homogeneous process into a heterogeneous one is to anchor the soluble catalyst onto large surface area of inorganic supports [1,2]. The main advantages of heterogenization are the easy separation of the catalyst from the reaction mixture, allowing the possibility to recover and reuse the catalyst, and the possibility of continuous-flow operation. common problem of this methodology is leaching of the active sites from the solid surface into the solutions, when applied to liquid-phase reactions. However, this can be avoided or minimized by covalently anchoring the active sites onto the inorganic solid supports [3].

We have successfully reported grafted 3,4-dihydroxybenzaldehyde ligand onto the inner walls of amino functionalized MCM-41, made the strong host for Copper (II).

This conversion of sulfides to the sulfoxides offerssimple reaction conditions, commercial availability reagents, excellent product yield.Therefore sulfoxides have been prepared in the presence of a nano reactor catalyst (Cu-MCM-41) and UHP as oxidant at room temperature (Scheme1).The Cu-MCM-41 has been recovered from reaction mixture and has been reused successively several times under the same reaction conditions.



Scheme1

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Cu Supported Fe_3O_4/polyethylene glycol nanocomposite for the synthesis of substituted imidazoles

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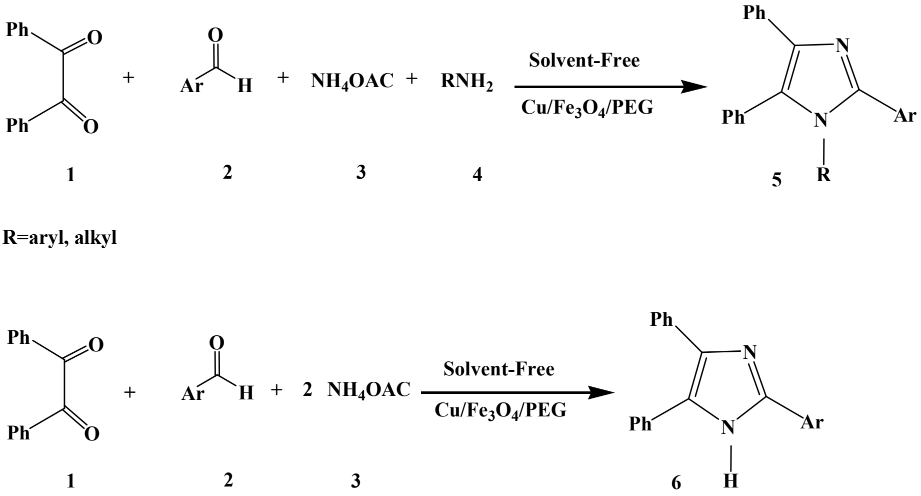
Naturally occurring substituted imidazoles, as well as synthetic derivatives thereof, exhibit wide ranges of biological activities, making them attractive compounds for organic chemists. Consequently, the development of a new catalytic system to overcome these shortcomings and fulfill the criteria of a mild, efficient, and environmentally benign protocol for the synthesis of substituted imidazoles is an important task for organic chemists [1-3].

In the present study, we carried out chemical synthesis and characterization for Fe_3O_4/polyethylene glycol nanocomposite. Copper (Cu) nanoparticles were deposited onto the surface of Fe_3O_4/PEG nanocomposite and the catalytic activity of the Cu/Fe_3O_4/PEG nanocomposites was proved for the synthesis of highly substituted imidazoles (Scheme 1).



Scheme 1

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Tribromo melamine as novel and versatile catalyst for the acetylation and formylation of alcohols

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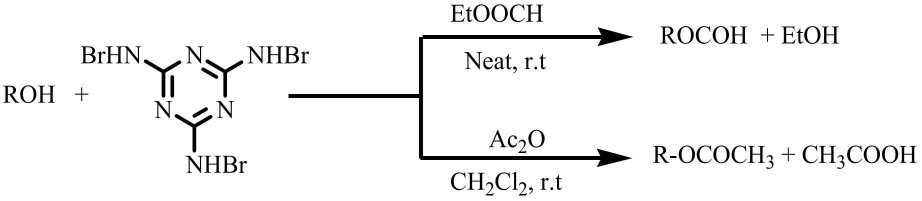
During the multistep synthesis of natural products, the efficiency of the synthetic protocol employed often depends largely on protection and deprotection of the functional groups involved. To this end, protecting groups have been playing a crucial role during the synthesis of complex natural products [1].

In this work, Tribromo melamine has been introduced as efficient and green organocatalyst for the acetylation and formylation reactions of alcohols with acetic anhydride and ethyl formate at room temperature and under mild reaction conditions. Following our previous works in development of new methods for the protection of the hydroxyl group [2-3], herein, we would report an effective procedure for the acetylation and formylation of alcohols with acetic anhydride and ethyl formate in the presence of catalytic amounts of tribromo melamine at room temperature (Scheme 1).



Scheme 1

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A new and regioselective method for ring opening of epoxides using 1,1'-(1,4-butanediyl) dipyridinium salts in presence cross-linked poly (4-vinylpyridine) supported sulfuric acid as a catalyst under solvent-free condition

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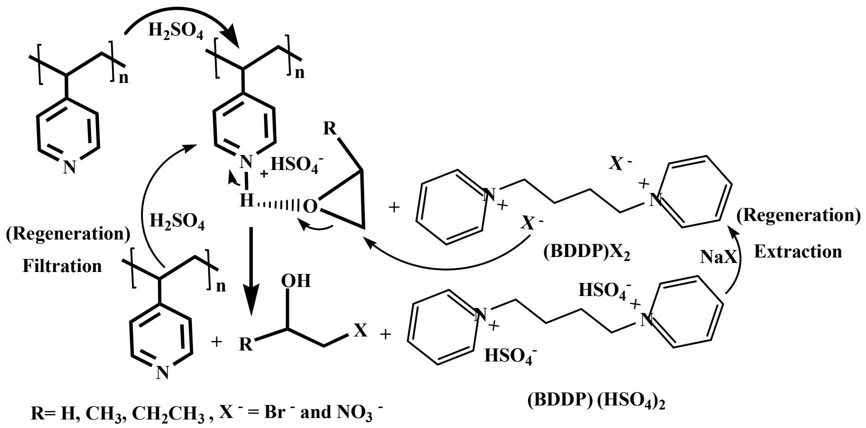
Nucleophilic addition to epoxides is an easy step reaction for preparation of several 1, 2-disubstituted products such as vicinal halohydrins and *β*-hydroxy nitrates. Bromohydrins and other halohydrins are also versatile intermediates in the synthesis of a vast range of biologically active, natural and synthetic products [1, 2]. Organic nitrates have useful applications in organic synthesis including as effective protecting groups for hydroxy groups [3].

In continuation of our work [4], on the development of useful synthetic methodologies, we have found that 1,1'-(1,4-butanediyl) dipyridinium dibromide, or dinitrate (BDDP)X_2 as an exchange reagent in the presence of cross-linked poly (4-vinylpyridine) supported sulfuric acid as a catalyst converted epoxides to vicinal halohydrins and *β*-hydroxy nitrates (Scheme 1). This method is efficient and very rapid under solvent-free conditions.



Scheme 1

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Synthesis of a new maleic anhydride derivative and study of its pharmaceutical effect on microtubules polymerization

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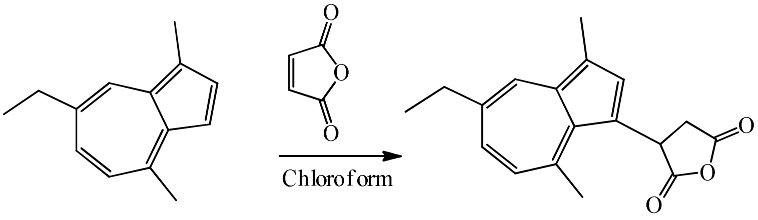
Chamomile (*Matricaria recutita* [L.] Rauschert, Asteraceae) is one of the oldest and agronomically most important medicinal plant species in Europe. It originates from southeastern Europe and western Asia, but is nowadays cultivated throughout the world. The essential oil of chamomile flowers has significant antimicrobial activity and is therefore used for several pharmaceutical, nutritional and cosmetic applications. The pharmaceutically active components of the flower oil are chamazulene, a degradation product spontaneously formed during steam distillation from the sesquiterpene lactone matricine, several bisabolol-type sesquiterpenes ((−)-α-bisabolol, bisabolol oxides), flavonoids and two en-in-dicycloethers [1,2] with chamazulene and the bisabolols being the main active constituents[3] .

In this study the coupling of Chamazulene with Maleic anhydride at room temperature was investigated. The residue was washed with petroleum ether to remove unreacted materials and sublimed at reduced pressure. After purification and recrystalization, the molecular structure of product was characterized and confirmed by analytical and spectroscopic methods (IR, ^{1}H-NMR, ^{13}C-NMR). Experimental data showed the new product has excellent ability for increasing of microtubules polymerization. The new synthesized material could play an important role in drug industries in future.



Scheme 1

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Pyrrolidine catalyzed synthesis of new 2-amino-4*H*-pyran-3-carbonitriles derivatives and related materials by the one-pot reaction conditions

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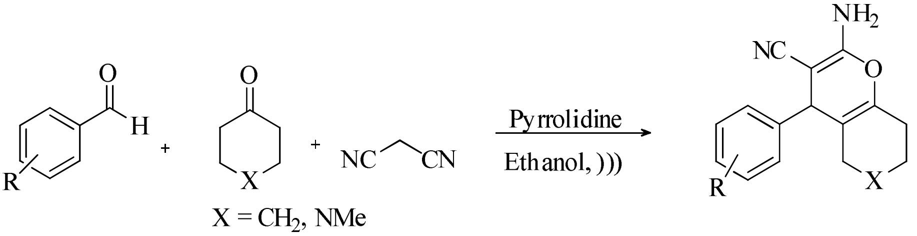
4*H*-Pyran and its derivatives are important class of organic and bioorganic compounds. They are often used in cosmetics, pigments and are utilized as potentially biodegradable agrochemicals [1]. Polyfunctionalized 4*H*-pyrans are a common structural unit in a number of natural products and biologically interesting compounds which possess various pharmacological activities, such as antiallergic, antitumor and antibacterial [1,2] which are well known for their antioxidant and anticarcinogenic activities [3].

In this work a one-pot reaction is reported in which a cyclization between malononitrile, an arylaldehyde and a cycloketone occurs under ultrasound waves and in the presence of pyrrolidine as an efficient organocatalyst. Products form in good to excellent yields (Scheme 1).



Scheme 1

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A highly efficient nano-Fe_3O_4 encapsulated-silica particles bearing sulfonic acid groups as a solid acid catalyst for synthesis of 1,8-dioxo-octahydroxanthene derivatives

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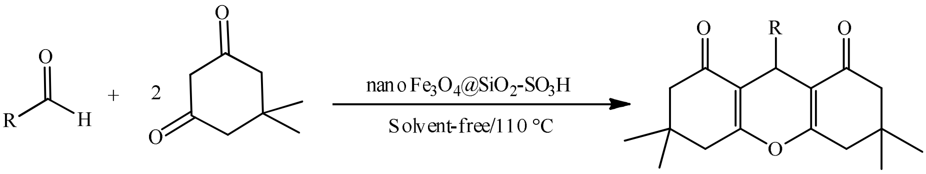
Recently, Fe_3O_4 magnetic nanoparticles (MNPs) have been intensively investigated because of their superparamagnety, high coercively and low Curie temperature [1]. In addition to these characters, MNPs are also non-toxic and biocompatible. MNPs have been used in various fields such as sealing, oscillation damping, information storage and electronic devices [2]. One of the rapidly developing applications of magnetic nanoparticles in recent years is in biomedical areas, including rapid biologic separation and drug delivery [3,4]. However, unmodified MNPs tend to aggregate because of their high specific area and strong inter particle interaction, which limit their utilization. Therefore, it is necessary to develop strategies for the chemical stabilization of the naked magnetic nanoparticles against aggregation over a long period.

In this context we were prepared Fe_3O_4 nanoparticles by chemical co-precipitation method and subsequently coated with tetraethoxysilane (TEOS) via silanization reaction. Grafting of chlorosulfonic acid on the $Fe_3O_4@SiO_2$ nanoparticles was afforded sulfamic acid-functionalized magnetic nanoparticles ($Fe_3O_4@SiO_2-SO_3H$). They were found to be a mild and efficient solid acid nano catalyst for the one-pot synthesis of 1,8-dioxo-octahydroxanthenes under solvent free conditions at 110 °C (Scheme 1).



Scheme 1

References:

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Synthesis of novel spiropyrano quinazoline *via* one-pot, three-component reaction

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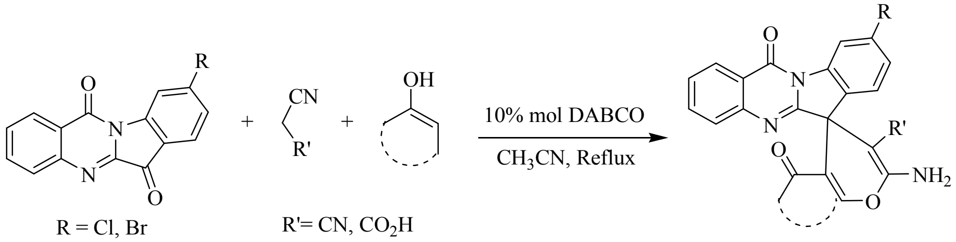
In last few years Synthesis of active biological molecules is one of the main challenges in pharmaceutical fields which attracted much attention. Spiropyran derivatives, specially have shown wide range properties, such as anticancer, antibacterial, antifungal, and antisterility agents [1,2]. They are also used as pigments, cosmetics and biodegradable agrochemicals. Due to their application, the synthesis of heterocyclic derivatives of these polyfuncthionalized spiropyrans has great importance in medicinal chemistry and organic synthesis [3].

The present work describe method for synthesis of various 2-amino-spiropyrano carbonitril (carboxylate) derivatives via one-pot three component condensation of malononitrile (ethyl cyanoacetate), tryptanthrin, and active methylene compounds in the presence DABCO as catalyst in acetonitrile under reflux condition. Short reaction times and high yields, simple work-up, no extra purification are the advantages of this method (Scheme 1).



Scheme 1

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Synthesis of tert-butyl-substituted 3-carboxy coumarinsin water in the presense of para toluene sulfonic acid (PTSA) as a catalyst

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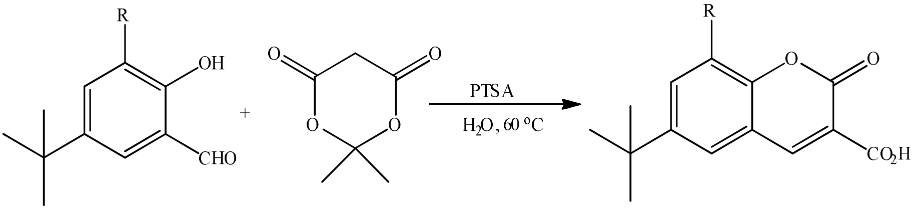
3-Carboxycoumarins are important initial compounds for the synthesis of coumarins. Coumarins are natural products and well known for their diverse biological activities. Substituted coumarin-3-carboxylic acid derivatives were potent and selective inhibitors of monoamineoxidases [1].

PTSA (para toluene sulfonic acid) has been used as a catalyst in the synthesis of tert-butyl-substituted 3-carboxy coumarins [2].

Here we describe a two-component condensation reaction between antert-butylsalicylaldehydes and meldrumacid efficiently provides tert-butyl-substituted 3-carboxy coumarins in a one-pot reaction in the presence of PTSA as catalyst (Scheme 1).



Scheme 1

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Regioselective ring opening of epoxides using NH_4SCN/ $NaHSO_4$: An efficient approach for the synthesis of β-hydroxy thiocyanate under solvent-free conditions

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Regioselective ring opening of epoxides with nucleophilic reagents is a useful tool for the preparation of several 1,2-disubstituted products and is an important reaction for synthetic organic and medicinal chemists [1]. The formation of thiiranes from oxiranes and thiocyanates has been explained by the intermediacy of the corresponding β-hydroxy thiocyanate. However, β-hydroxy thiocyanates have not been isolated due to rapid conversion into the corresponding thiiranes [2]. It has been reported that the presence of some hydroquinone or DDQ is required to stabilize the produced β-hydroxy thiocyanates, and to inhibit its conversion to thiirane [3].

Acid catalysts are of fundamental importance because of their ubiquity [4]. In view of green chemistry, the substitution of harmful liquid acids by reusable solid acids as catalysts in organic synthesis is the most promising application [5]. Recently, solid acids as environmentally friendly and economically viable catalyst, are increasing continuously owing to their ease of handling, low cost, high catalytic activity, process simplicity and comparably easy work-up [6].

Herein, we wish to report the facile and regioselective synthesis of various β-hydroxy thiocyanates by ring opening of corresponding epoxides with fresh $NH_4SCN/NaHSO_4$, as an active nucleophile producer and very efficient catalyst. To find optimal conditions, the ring opening of styrene oxide was investigated as a model substrate under different conditions in solvent-free. The epoxides were converted to the corresponding β-hydroxy thiocyanates in exellent yields within short times (Scheme 1).

Scheme 1

References:

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The synthesis of 2-(3,3,6,7-tetramethylindolin-2-ylidene) malonaldehyde and 2-oxo-5-(3,3,6,7-tetramethyl-3H-indol-2-yl)-1,2-dihydropyridine-3-carbonitrile and 3,3,6,7-tetramethyl-2-(2-methylpyrimidin-5-yl)-3H-indol

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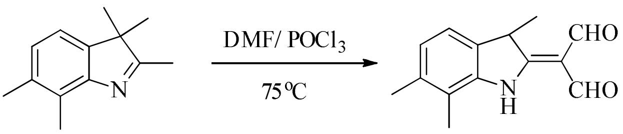
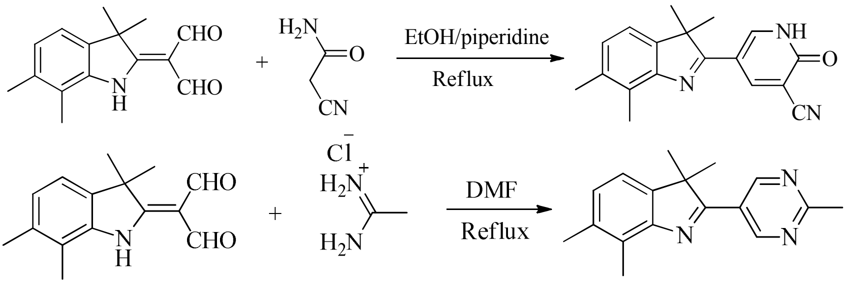
In 1959, Fritz [1] reported the N-formylation of the 3,3-disubstituted 3H-indole (indolenine) with using the Vilsmeier reagent DMF and $POCl_3$. No further studies of the formylation of these types of compound have been reported since.

In this research, we synthesized the novel diformyl compounds from 2,3,3,6,7-pentamethyl - 3H-indole by the action with Vilsmeier reagent at 75 °C in excellent yield [2].



Scheme 1

Condensation of corresponding diformyl with 2-cyanoacetoamide produced 2-oxo-5-(3,3,6,7-tetramethyl-3H-indol-2-yl)-1,2-dihydropyridine-3-carbonitril [3] and 3,3,6,7-tetramathyl-2-(2-methyl pyrimdin-5-yl) -3H-indol, respectively, in excellent yields.



Scheme 2

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Synthesis of a new derivative of 4-methoxybezylamine and the study of its pharmaceutical effects on serotonin

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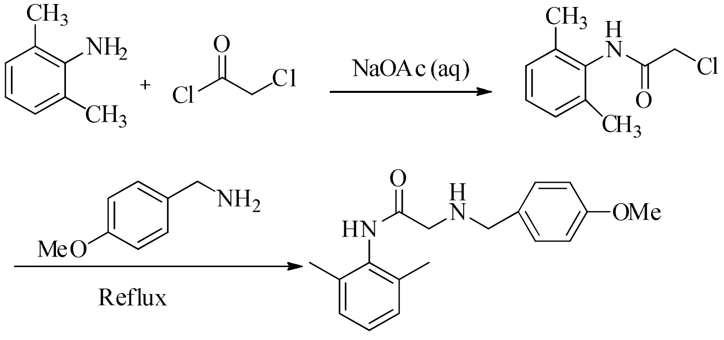
Neurotransmitters are extremely important. These substances carry impulses between nerve cells. Serotonin is a compound used in the chemical transfer of information from one cell to another. It also plays a role in the state of relaxation or constriction of blood vessels. All of the serotonin normally in the blood is stored in the platelets and is released by platelet aggregation [1]. Serotonin also plays a role in mood, sleep, and appetite [2]. Sometimes, a lower serotonin level might be beneficial, for example in the ultimatum game where players with normal serotonin levels are more prone to accept unfair offers than participants whose serotonin levels have been artificially lowered [3].

For this purpose a new serotonin inhibitor was prepared in two steps by the reaction of 2,6-xylidine with chloroacetyl chloride in acidic media followed by the reaction with4-methoxybenzylamine in toluene. Molecular structure of the new product was characterized and confirmed by spectroscopic methods (IR, ^{1}H-NMR, ^{13}C-NMR) and its effect on serotonin was investigated in vivo conditions. Experimental data showed that the new synthesized compound is a powerful serotonin inhibitor.



Scheme 1

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Silica sulfuric acid immobilized on magnetic nanoparticles as an efficient and recyclable nanocatalyst for the oxidation of sulfides onto sulfoxsides using H_2O_2 under metal- and solvent-free conditions

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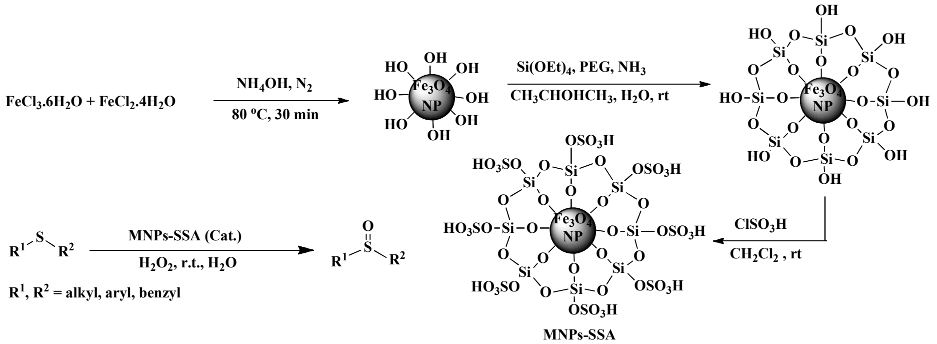
Nanoparticles have recently emerged as efficient alternatives for the immobilization of homogeneous catalysts. However, particles with diameters of less than 100 nm are difficult to separate by filtration techniques; this draw back can be overcome by using magnetic nanoparticles, which can be easy recovered by external magnet [1].

Sulfoxides are fine chemicals, pharmaceuticals and valuable intermediates in the synthesis of chemically useful and biologically active molecules [2]. Oxidation of sulfides is the most straightforward method for the synthesis of sulfoxides. Concerning the green oxidant, hydrogen peroxide is one ofthe most powerful candidates besides molecular oxygen, becauseit is inexpensive, readily availableand high atom efficiency.

In continuation of our studies [3], herein, we report the magnetic nanoparticle-supported sulfuric acid (MNPs-SSA) as a novel and reusable nanocatalyst for the oxidation of sulfides to sulfoxides using H_2O_2 in water at room temperature (Scheme 1). TheMNPs-SSA was prepared by the concise route outlined in Scheme 1.



Scheme 1

This method offers several advantages including high yield, short reaction time, simple work-up procedure, ease of separation, and recyclability of the magnetic nanocatalystwithout significant loss of their catalytic efficiency.

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Reaction of 2-(thiophen-2-yl)-4*H*-benzo[*d*][1,3]oxazin-4-ones with KOCN

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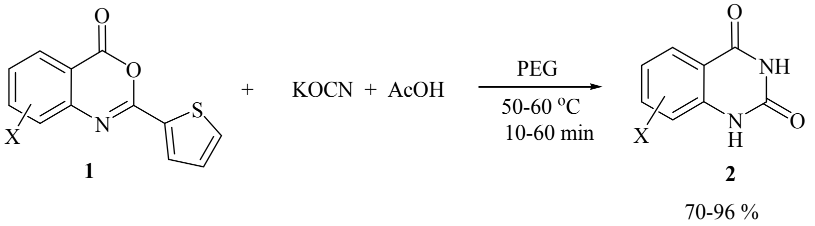
The 4*H*-1,3-benzoxazinones are key starting materials for further transformations in design and synthesis of biologically active compound [1,2]. 2,4(1*H*,3*H*)-Quinazolinediones and their derivatives are versatile intermediates in the synthesis of heterocycles with high pharmacological [3] and biological activities [4]; thus, considerable attention has been focused on their synthesis [5].

Herein, the reaction of 2-(thiophen-2-yl)-4*H*-benzo[*d*][1,3]oxazin-4-ones **1** with acidic solution of KOCN in PEG leads to the quinazolin-2,4-diones **2** (Scheme 1). Good to high yields of **2** are obtained under mild reaction conditions with easy work-up of the reaction mixture.



X = H, 6-OH, 5-Me, 6-Cl, 6-Br, 6-NO_2, 7- Cl, 6,7-diMeO, 8-Me

Scheme 1

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$ZrOCl_2 \cdot 8H_2O$ as an efficient catalytic system for the synthesis of highly functionalized 2-naphthol Betti bases under solvent free conditions

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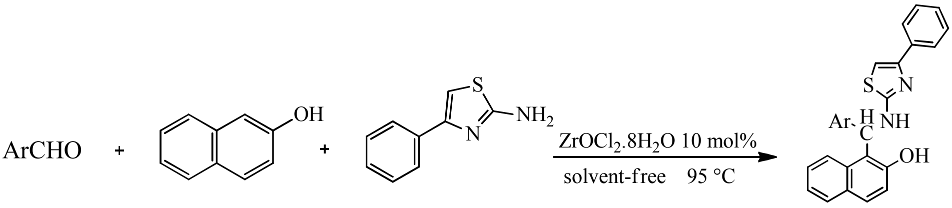
In recent years multicomponent reactions (MCR) have become a powerful tool for atom efficient and waste-free synthesis of complex building blocks of 'drug-like' motifs [1]. Generally MCR strategy affords time and cost advantageous, environmentally benign pathways leading to the synthesis of a library of compounds.

The Betti reaction is a convenient method with which to prepare aminobenzylnaphthol derivatives. Earlier, this three-component modified Mannich reaction with 2-naphthol, benzaldehyde and ammonia resulted in 1,3-diphenylnaph-thoxazine, which on subsequent hydrolysis, gave the desired1- a -aminobenzyl-2-naphthol (Betti base) [2,3].

Our present aim was to insert a new functional group (e.g., phenyl thiazole) into Betti base derivatives, and use efficient catalytic and solvent free approach for the synthesis.Reactions between 2-naphthol, aromatic aldehydes and 2-Amino-4-phenylthiazole resulted in the synthesis of 2-amino-4-phenylthiazolomethyl naphthols in the presence of $ZrOCl_2.8H_2O$ as catalyst (Scheme 1).



Scheme 1

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Solvent-free one-pot synthesis of tioamidoalkyl and bis-thioamidoalkyl naphthols catalyzed by 1,3-dibromo-5,5-dimethylhydantoin

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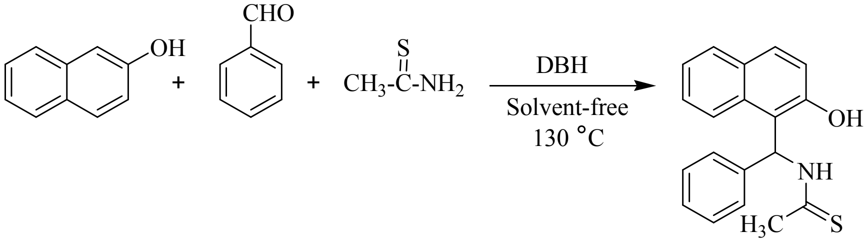
Multicomponent reactions (MCRs) have elicited increased interest since they are performed without the need to isolate any intermediate, thus reducing time and saving energy and raw materials [1]. One of these MCRs is the synthesis of amidoalkyl naphthols, which are ubiquitous to a variety of biologically important natural products and potent drugs, including a number of nucleoside antibiotics and HIV protease inhibitor, such as ritonavir and liponavir [2]. A straightforward method of synthesis of these compounds involves a three-component condensation of 2-naphthol, aromatic aldehyde and amid (thioamide) in the presence of a catalyst. In consequence of the lower reactivity of the thio analogous of acetamide and urea comparatively few publications have appeared on this field [3-4].

In this work, we report our results on the efficient and rapid synthesis of thioamidoalkyl naphthols and bis-thioamidoalkyl naphthol from 2-naphthol, aryl aldehydes and thioacetamide in the presence of catalytic amounts of 1,3-dibromo-5,5-dimethylhydantoin (DBH), at 130 °C under solvent-free conditions (Scheme 1). In summary, the present procedure provides an efficient and improved modification of the 1-thioamidoalkyl-2-naphthol synthesis.



Scheme1

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Synthesis of cyclic ketoximes using $NH_2OH.HCl$ in the presence of water-EtOH

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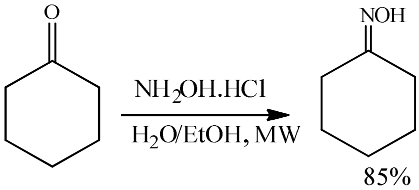
Microwave-assisted organic reactions have been applied as an effective technique in organic synthesis [1]. Microwave irradiation often leads to shorter reaction times, increased yields, easier workup, matches with green chemistry protocols, and can enhance the regio- and stereoselectivity of reactions [1]. Microwave irradiation can accelerate many reactions as well as condensateion of cyclic ketones with hydroxylamine hydrochloride. In conclusion, we have developed a simple and efficient method for the preparation of cyclic ketoximes using $NH_2OH.HCl$ under microwave irradiation (Scheme 1).



Scheme 1

References:

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Pectin as an efficient biocatalyst for the synthesis of spiroindoline-3,2′-quinazolines derivatives under ultrasound irradiation

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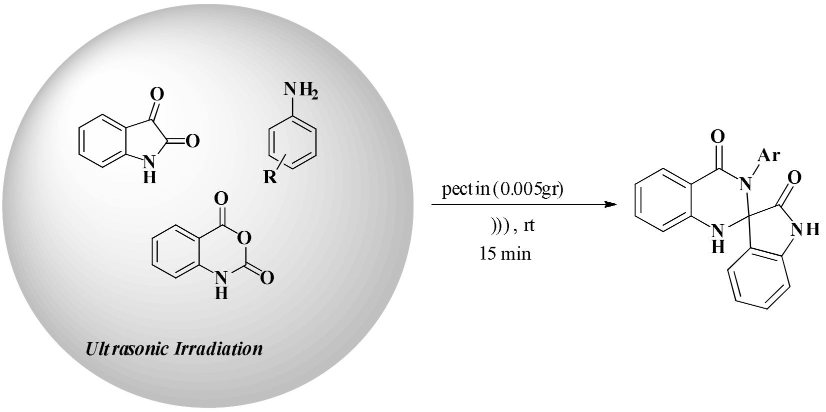
Pectin is a biocompatible and versatile polysaccharide recently used in pharmaceutical applications as drug delivery system and in biomedical field as coating of different biomaterials.

2,3-Dihydroquinazolinone derivatives are an important class of fused heterocycles that display a wide range of biological, pharmacological, and medicinal properties involving antitumor, antibiotic, antipyretic, analgesic, antihistamine, and vasodilating activities. Combinatorial chemistry is now routinely applied to find out novel biologically active compounds. In this perspective, multicomponent reactions (MCRs) are prevailing tools in the modern drug discovery process in terms of lead finding and lead optimization. Consequently, to develop efficient and robust methods for the preparation of biologically active dihydroquinazolinone ring bearing the spirooxindole scaffold from readily available building blocks, we have developed a facile, efficient one-pot method for the synthesis of the biologically important spiroindoline-3,2′-quinazolines by the reaction of isatoic anhydride, isatin and amines using pectin as catalyst under sonication irradiation.



Scheme 1

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Optimization of the synthesis of saccharin from oxidative ring closure of 2-methyl benzene solfonamide

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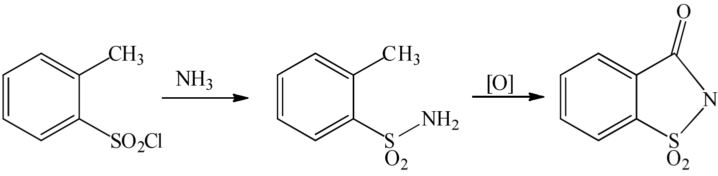
Sodium saccharin, which was discovered by Fahlberg & Remsen (1879), it became acommonly used artificial sweetener because it is 300–500 times sweeter than sucrose, and is slowly absorbed and not metabolized by the humans [1]. The saccharin moiety has been identified as animportant molecular component in various classes of 5HT1a antagonists, human leukocyte elastase (HLE) inhibitors, analgetics and human mast cell tryptase inhibitors [2]. Saccharinhave been synthesized by oxidative ring closure of 2-methylbenzenesulfonamide. In turn, 2-methylbenzenesulfonamide may be obtained from treatment of 2-methyl benzenesulfonylchloride with ammonia or ammonium carbonate. In this project, we have optimized a two step procedure for preparation of saccharin, synthesis. The first step includes the amination of o-toluene sulfonyl chloride using ammonium carbonate. At this step, we have altered ammonium carbonate with other ammonium releasing agents such as ammonium chloride, ammonium sulfate, ammonium sulfide and ammonium hydrogen phosphate. The best result was obtained using ammonium chloride.The second step is oxidation of resulting o-toluene sulfonamide with alkaline potassium permanganate. We have successfully replaced the oxidative reagent with hydrogen peroxide as an eco-friendly reagent. Furthermore, the two step procedure was reduced to a one-pot reaction using ammonium dichromate both as ammonium releasing and oxidative agent.



Scheme 1

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A green synthesis of ketothioamides via Willgerodt–Kindler reaction

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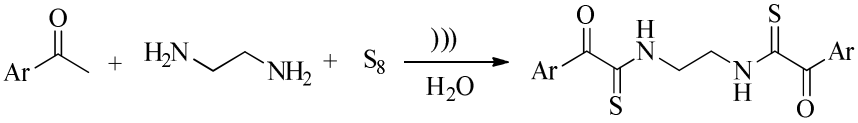
The Willgerodt-Kindler reaction has, in recent years, received limited attention and application in synthetic organic chemistry. With the advent of new technology such as microwave-assisted heating, several new, high-yielding, practical, and more environmentally friendly reaction protocols have been developed [1]. However, like the Willgerodt-Kindler reaction, these methodologies are not general for the synthesis of ketothioamides [2].

The role of ultrasonic irradiation in boosting the reactivity and selectivity of synthetic organic reactions is widely demonstrated in recent years [3]. Consequently, several protocols are developed to perform chemical reactions in shorter time periods and under more environmentally benign conditions. Based on our previous experiences on sonochemistry and in continuation of our attempts to develop green chemical methodologies, we recently reported a non-thermal Willgerodt-Kindler reactions using ultrasound irradiation [4]. We would like now to report a one-pot preparation of bis α-oxothioamide derivatives which form the in situ oxidation of the Willgerodt-Kindler products obtained from the reaction between acetophenone derivatives with ethylenediamine under ultrasound irradiation.



Scheme 1

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An efficient and one-pot method for synthesis of chromene derivatives using Fe[(*L*)-proline]$_2$ as catalyst

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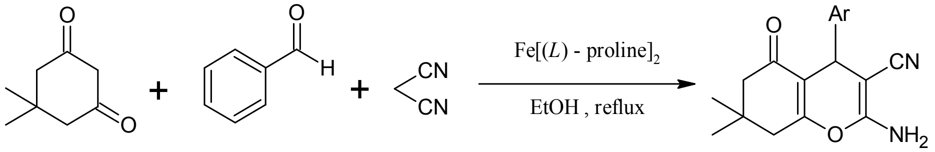
4*H*-Chromene derivatives are important scaffold in organic and medicinal chemistry. They belong to a class of naturally occurring benzopyran derivatives with a wide range of biological applications, such as antiallergic, anticancer, antibacterial, antiviral and potent apoptosis inducers. Such diverse biological activities have made chromene derivatives important for further development in medicina and organic synthesis studies. In particular, 2-amino-4*H*-chromenes are of recent interest for their cytotoxic activities [1-3].

In this study, we investigated a simple and one-pot method for preparation of chromenes using the condensation reaction between dimedon, aromatic aldehydes and malononitril in the presence Fe[(*L*)proline]$_2$ as an acidic catalyst at 80 ^{0}C (Scheme 1).



Scheme 1

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Use of anhydrous $FeCl_3$ as oxidant in synthesis of a new nanocomposite of poly(2-methylaniline) in the presence of silica-supported sulfuric acid in solvent-free condition

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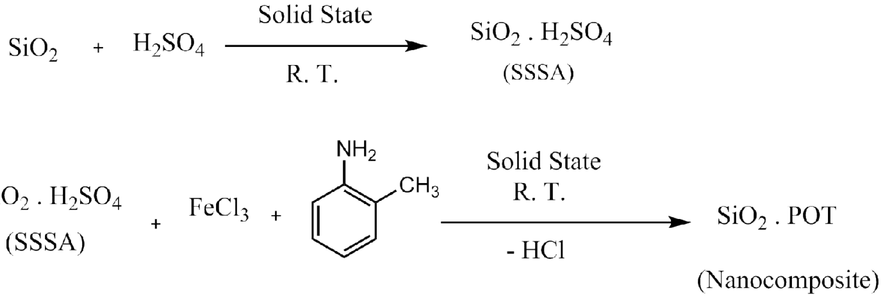
Among conducting polymers, Polyaniline (PANI) is widely studied because of its moderately high conductivity upon doping by protonation, good environmental stability and ease of synthesis [1]. Recently, Poly-ortho-toluidines have attracted considerable attention since they exhibit better solubilities and hence better processability than polyaniline [2]. Many different inorganic acids were used to doping polyaniline and its derivatives [3]. In this investigation H_2SO_4(98%) was added to silica to gain silica-supported sulfuric acid (SSSA) as dopant and then anhydrous $FeCl_3$ was added then 2-methylaniline was added to mortar and was grinded for 60 minutes to prepare silica-supported sulfuric acid-poly(2-methylaniline) in solid state condition at ambient temperature (Scheme 1). The composite which was prepared from silica gel (mesh 60, 0.2 to 0.063 mm), surprise, was converted to nanocomposite, that is, average size of particles were below 100 nm. Indeed, this nanocomposite was obtained without using any template and/or any nanostructure material such as nanosilica.



Scheme 1

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Synthesis of a new yellow polyurethane elastomer containing polyethylene glycol soft segment

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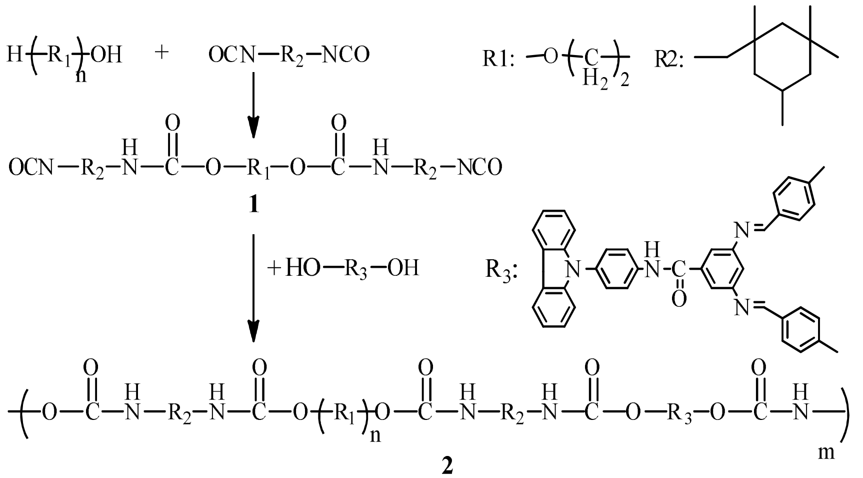
The yellow polyurethane was synthesized based on isophorone diisocyanate (IPDI), polyethylene glycol (PEG) and a yellow Schiff-base diol N-[4-(9H- carbazol-9-yl)-phenyl]-3,5-bis-[(4-hydroxy-benzylidene)-amino]-benzamide as a chain extender. The structure of PU was confirmed by means of FTIR and ^{1}H-NMR spectroscopy [1].

The synthesis process of PU is shown in Scheme 1. Isophorone diisocyanate (IPDI) and polyethylene glycol (PEG) were first added into the reactor to produce prepolymer 1 according to a suitable molar ratio. The prepolymerization of polyurethane was carried out at 80–90°C under N_2 atmosphere until the content of NCO group reached the theoretical value. Then diol and a bit of catalyst (stannous octoate) were added into the system and reacted with prepolymer 1 to formed polymer 2 at 90°C for 12 h. After 12 h, reaction mixture was poured into cold saturated aqueous solution of sodium chloride to precipitate out the polyurethanes and washed with deionized water for three times [1, 2].



Scheme 1

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Synthesis of benzimidazoles in presence of nano-silica phosphoric acid as an efficient catalyst under thermal conditions

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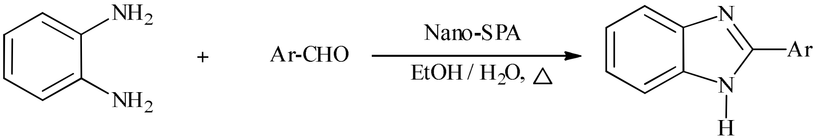
Benzimidazoles, have been widely used interest because of their clinical applications such as anti-fungal, anti-parasite, antimicrobial and etc [1]. Therefore, the widespread interest in benzimidazoles has prompted extensive studies for their synthesis [2]. The most common method for the synthesis of benzimidazoles is the coupling of *o*-phenylene diamine with carbonyl compounds like carboxylic acid, orthoesters and aldehydes which often requires strong acidic conditions and sometimes very high temperatures. All these protocols require excess amount of oxidants to be used and many of them produce toxic, often require laborious work-up and purifications that lead to low isolated yields [3,4].

Here, we introduce a simple and efficient method for the synthesis of benzimidazoles using a catalytic amount of nano-silica phosphoric acid (Nano-SPA). This method exhibits the mild and simple procedure for the preparation of benzimidazoles from the reaction of aldehydes with *o*-phenylene diamine in the presence of Nano- SPA as an efficient catalyst in ethanol and water in the same ratio as green solvents under thermal condition (Scheme1). Short reaction times, easy work-up and high yields are the main advantages of this process.



Scheme 1

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Synthesis of benzoxazoles based on orthoamino phenol in the presence of nano silica phosphoric acid as a solid acid catalyst under thermal and grinding conditions

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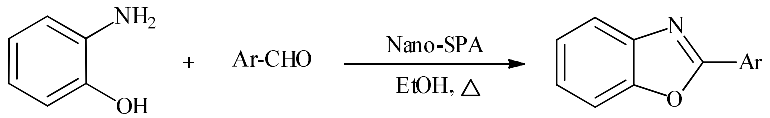
Nano silica phosphoric acid (nano-SPA) [1] as an efficient and reusable catalyst was prepared by reaction of nano-silica chloride [2] with dry phosphoric acid. Nano silica chloride was prepared by reaction of commercial nanosilicagel with thionyl chloride in reflux condition [3].

Benzoxazole derivatives are important compounds due to their biological activities and diverse medicinal uses such as gram-positive antibacterial agents, antibiotics, antiparasitic, anti-stress, anti-cancer agents and so on [4].

Here, we introduce a mild and efficient method for the synthesis of benzoxazole derivatives from the reaction of aldehydes with *o*-aminophenol in the presence of catalytic amounts of nano silica phosphoric acid under thermal and grinding conditions (scheme 1).

Short reaction times, simple work-up procedure, easy availability, high yields and use of an eco-friendly catalyst are some of the striking features of the present protocol.



Scheme 1

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A novel one-pot three component synthesis of bis-cinnoline derivatives by bis-glyoxal

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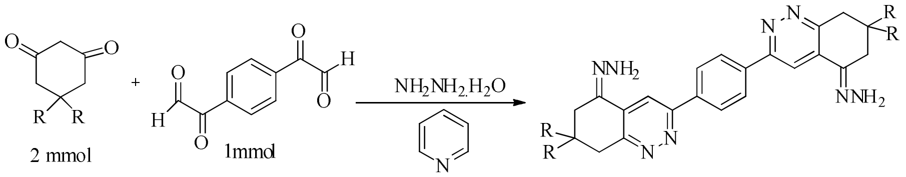
Cinnolines and their derivatives exhibit a broad range of biological activity, such as: anticancer, fungicidal, bactericidal, and anti-inflammatory properties [1]. Additionally, compounds containing a cinnoline fragment demonstrate a series of interesting physical characteristics, such as luminescent and nonlinear optical properties[2]. Hence, the synthesis of cinnoline has been studied for many years [3,4].

Therefore, we report the synthesis of new derivatives of bis-cinnoline based on MCR method in which bis-glyoxal (1mmol) reacted with 1,3-cyclo hexanedione or dimedone (2mmol), and hydrazine hydrate(excess) in presence of catalytic amount of pyridine in DMF under microwave conditions for 5 minutes or under reflux in THF for 1hr to give the corresponding product as cream crystals with good to high yields (Scheme 1). The structures of products were confirmed by their FT-IR and H-NMR spectral data.



R=H (MWI;62%, Reflux; 87%)
R=Me (MWI;68%, Reflux; 95%)

Scheme 1

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N-Alkylation of spiro[indoline-3,9'-xanthene]trione derivatives under solvent-free conditions

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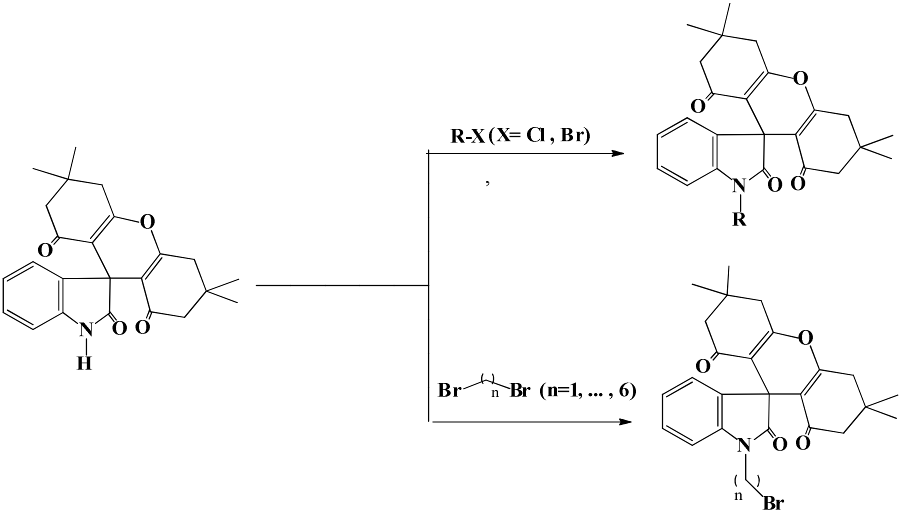
Xanthene core and its derivatives are the important biologically active heterocycles[1]. These compounds were shown a wide range of activities such as; antibacterial, anti-inflammatory, antiviral properties. These also were used in photodynamic therapy for destroying the tumor cells. Such compounds are also utilized for antagonism of the paralyzing action of zoxazolamine [2]. Some other derivatives of these compounds have found applications in industries such as dying, fluorescent materials for visualization of biomolecules, and in laser technology [3].

In present study we report the alkylation of spiro[indoline-3,9'-xanthene]trione with alkyl halides under solvent-free conditions (Scheme 1). The products were identified and confirmed by physical and spectroscopic data such as IR, ^{1}H NMR and ^{13}C NMR.



Scheme 1

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One-pot synthesis of spiroquinolines using boric acid through the aza Diels-Alder reaction

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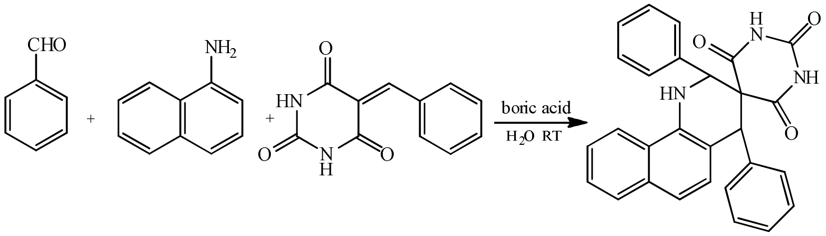
The aza-Diels–Alder reaction is one of the most important synthetic routes for the construction of six-membered heterocycles containing *N*-atom. Spiroquinolines constitute an important class of compounds with profound interest to medicinal chemist since the spiroquinoline moiety exhibits diverse biological properties. The classical methods that have been reported for the synthesis of spiroquinolines involve the reaction of imines (derived from aromatic amines and benzaldehydes) with dienophiles employing various catalysts [1-2].

Boric acid (H_3BO_3) is a useful and environmentally benign catalyst that has been successfully utilized in numerous reactions [3]. As part of our ongoing studies devoted to the development of practical, safe, and environmentally friendly procedures for several important organic transformations we now describe a simple and efficient protocol for the synthesis of spiroquinolines by one-pot coupling reactions of aldehydes, 1-naphthylamine and barbituric acid using boric acid at room temperature.



Scheme 1

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A highly efficient and recyclable Fe_3O_4 nanoparticle-supported Cu(II) catalyst for Synthesis 1,2,3-triazoles

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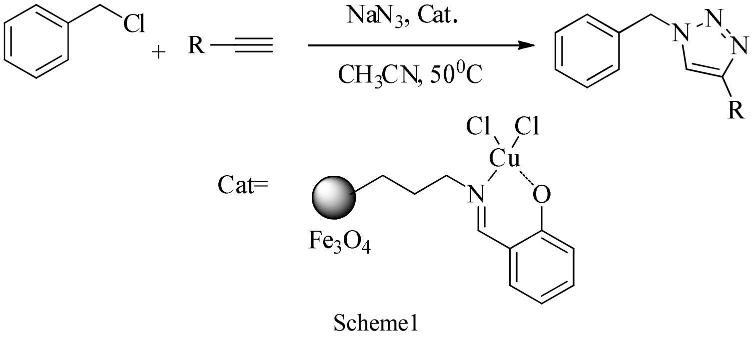
Organic shell/inorganic core composite particles have received a lot of attention in a wide range of industrial fields due to their functional properties, high dispersibility and stability after a certain thickness of polymer coating [1]. The core/shell nanostructure is an ideal composite system that combines the advantages of both the core and the shell to offer enhanced physical and chemical properties. In recent years,magnetic nanoparticles (MNPs) (e.g. Fe3O4) have been extensively investigated as inorganic cores for the synthesis of organic/inorganic core–shell composite particles, due to their potential applications in many industrial and biological fields [2]. Fe3O4 nanoparticles are naturally hydrophilic because of the existence of plentiful hydroxyl groups on the particle surface. Since, they are prone to aggregate and their dispersion in an organic media is difficult, the surface coating or modification of iron oxide nanoparticles is very important in many applications.

An important example of click chemistry [3] is the copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddition of azides and terminal alkynes (CuAAC)[4] for the regioselective synthesis of 1,4-disubstitiuted 1,2,3-triazole derivatives. These compounds have received significant attention because of their wide applications in chemical, material, and biological sciences.[5] Aromatic azides are versatile intermediates with various applications in organic and bioorganic chemistry. They are very useful starting materials for the click reaction and are commonly prepared by the reaction of diazonium salts with azides (Scheme1).



Scheme1

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Cross-aldol condensation reaction over sulfonic acid functionalized pyridinium chloride

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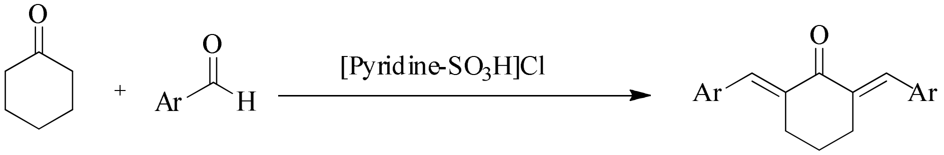
The aldol condensation reaction has been widely applied for carbon-carbon bond formation in organic synthesis [1]. Among them, the cross-aldol condensation of cycloalkanones with arylaldehydes leading to α,α′-bis(arylidene)cycloalkanones [2], which have attracted much attention due to their use as precursors for the synthesis of pyrimidine derivatives [3], and their intriguing biological activities such as antiangiogenic [4], quinine reductase inducer [5], and cholesterol-lowering properties [6].

In this work, we have reported sulfonic acid functionalized pyridinium chloride as a highly efficient catalyst and ionic liquid in the cross-aldol condensation reaction between cycloalkanones and arylaldehydes, under solvent-free conditions (Scheme 1).



Scheme 1

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Synthesis of 2-alkyl-1-selenocyanato-*N*-sulfonylethanimies from sulfonyl azides, alkynes and KSeCN

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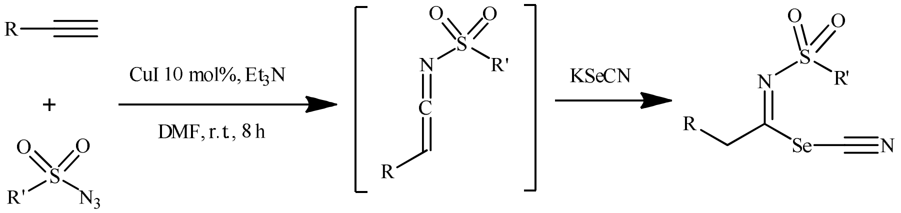
Selenium is a trace element, essential for normal human development, growth, metabolism, and function of the immune system. Originally, selenium was considered as one of the most toxic elements [1-3].

Ketenimines, have attracted much attention due to their diverse chemical reactivity [4,5]. One of the attractive methods for generation of ketenimines is the copper-catalyzed azide-alkyne cycloaddition. Herein, we report a simple and efficient procedures for the synthesis of cyanic-2-phenyl-*N*-tosylacetimidic selenoanhydride *via* the Cu-catalyzed three-component coupling reaction of terminal alkynes, sulfonyl azides, and KSeCN (Scheme 1).



Scheme 1

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Synthesis of *N*-(1*H*-benzo[*d*]imidazol-2-yl)-2-alkyl-*N′*-sulfonylacetamidines from sulfonylazides, alkynes and 2-aminobenzoimidazole

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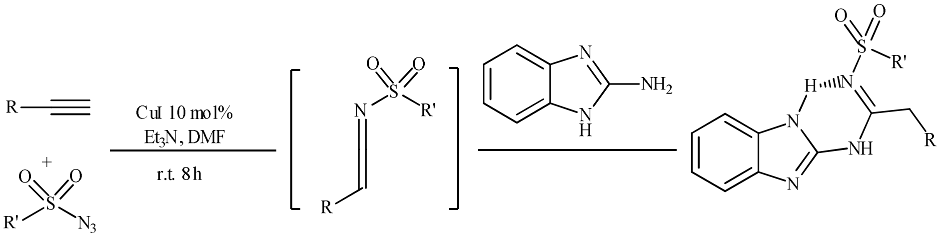
Amidines could be well-fitted for these criteria since they are prominent structural motifs in numerous bioactive natural products. Furthermore, they serve as pharmacophores, synthetic intermediates, and efficient coordinating ligands. The benzamidine variant is often employed as an excellent guanidine surrogate in medicinal chemistry [1,2].

Ketenimines, as useful intermediates, have attracted much attention due to their diverse chemistry and relative reactivity [3, 4]. Due to the activity of the central carbon atom of ketenimines towards various nucleophiles, they are applied in the construction of heterocycles. Perhaps, the most attractive method for generation of ketenimines is the copper-catalyzed azide-alkyne cycloaddition (Scheme 1).



Scheme 1

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Facile and direct synthesis of anhydrides using a powerful and efficient mixed reagent

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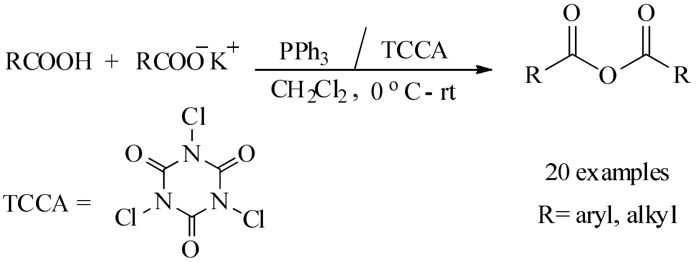
Carboxylic acid anhydrides are important intermediates which used as acylating agents and reactive intermediates for preparing many other functional groups in organic synthesis. They are preferred reactive acid derivatives for the preparation of amides, esters, and peptides. Direct preparation of carboxylic acid anhydrides from carboxylic acids are still in great demand. Although many reagents for the synthesis of carboxylic acid anhydrides have been developed, research in this field is still active. In continuation of our study to extend the scope of *N*-halo reagents in conjunction with PPh_3 [1-3], in this work, a useful method for the direct synthesis of symmetric carboxylic anhydrides from carboxylic acids by using triphenylphosphine (PPh_3)/ trichloroisocyanuric acid (TCCA) / potassium carboxylate system with excellent yields and high purity of products is presented (Scheme 1). The reaction has the generality for a wide range of carboxylic acids. Aromatic, aliphatic carboxylic acids with electron donating and electron withdrawing substituents were successfully converted into their corresponding carboxylic acid anhydrides.

This protocol has the following advantages: i) direct conversion of the carboxylic acids to carboxylic anhydrides in a short reaction time at room temperature, ii) mild reaction conditions, iii) low cost, safety, and availability of reagents, iv) simple experimental procedure, and v) easy work-up of the products.



Scheme 1

References:

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CS_2 as an effective reagent for conversion of aldoximes to nitriles

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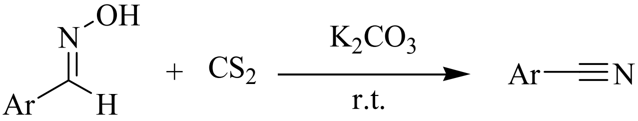
Nitriles are important synthetic intermediates and valuable chemicals in organic chemistry due to various applications [1]. One of the useful and convenient routes for the synthesis of nitriles is dehydration of aldoximes. There have been many reagents for dehydration of aldoximes, such as acid chlorides, acids, bases, transition metal catalyst, bromodimethylsulfonium bromide, etc [2,3].

In this study, we have been tried to introduce the CS_2 as an efficient reagent for conversion of aldoximes to nitriles. A series of nitriles have been prepared via aldoximes and CS_2 in the presence of K_2CO_3 as base at room temperature. High yields and straightforward work-up advantages of this protocol (Scheme 1).



Scheme 1

References:

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Synthesis of pure anatase TiO_2 nanoparticles by organic liagan as capping agent and its application in dye sensitized solar cells

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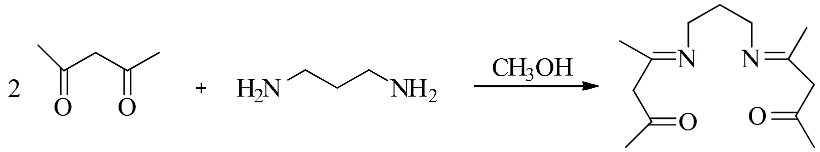
A Schiff base, is a compound with a functional group that contains a carbon-nitrogen double bond with the nitrogen atom connected to an aryl or alkyl group, not hydrogen. This compounds have the ability to bonding with metals, which this using for the capping as agent or surfactant.

The anatase phase of TiO_2 nanoparticles prepared with mixturing of tetraethyl ortho titanate, triethanolamine and a new ligand that plays role of surfactants in the reaction.

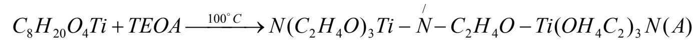
The effect of time, pH and the mole ratio of ligand on purity, size and morphology of product were investigated.

TiO_2 nanoparticles have photo catalytic properties that crystalized in three phases; includes anatase, rutile, and brookite.The band gap of anatase phase is 3.23 ev and this value for rutile phase is 3.06 ev according to these values, the anatase form is better than rutile form to use in photo catalytic application [1].

As-synthesized TiO_2 nanoparticles characterized with SEM, FT-IR, TEM, XRD analyses. Also characterized with FT-IR and ^{1}HNMR. As-product was used for preparation of paste via a optimal conditions [2].



Scheme 1



$$C_8H_{20}O_4Ti + TEOA \xrightarrow{100^\circ C} N(C_2H_4O)_3Ti - \overset{/}{N} - C_2H_4O - Ti(OH_4C_2)_3N(A)$$

$$A \xrightarrow{H_2O} Ti(OH)_4 + H_2acacpn \xrightarrow{140^\circ C} TiO_2$$

Scheme 2

References:

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Oxidation of benzylic alcohols to corresponding carbonyl compounds using bis(bipyridine)cobalt(II)perchlorate

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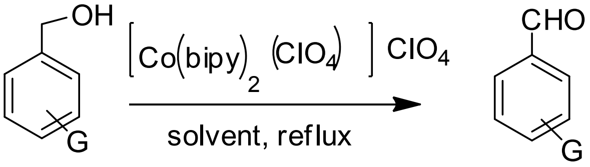
For economical and environmental reasons, the development of efficient and selective catalyst for oxidation of alcohols into their corresponding carbonyl compounds is a vital prerequisite in the chemical industry [1].

Transition metal–catalyzed oxidation of organic substrates is of current interest [2]. Various catalytic methods based on transition metals have been developed [3]. Consequently, elegant transition metal complexes have been synthesized and their catalytic properties in oxidation, epoxidation, carboxylation, hydrogenation and other functional group transformations have been reported [4].

In this work, bis(bipyridine)cobalt(II)perchlorate has been synthesized and new applications of this oxidant for selective oxidation of benzylic alcohols explored. Therefore a variety of benzylic alcohols have been oxidized to carbonyl compounds via combination of stochiometric amounts of alcohols and oxidant in acetonitrile as solvent under the reflux condition in good to high yields.



Scheme 1

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Reaction of vinylbenzylchloride copolymers with 5-chloro-8-hydroxy quinoline

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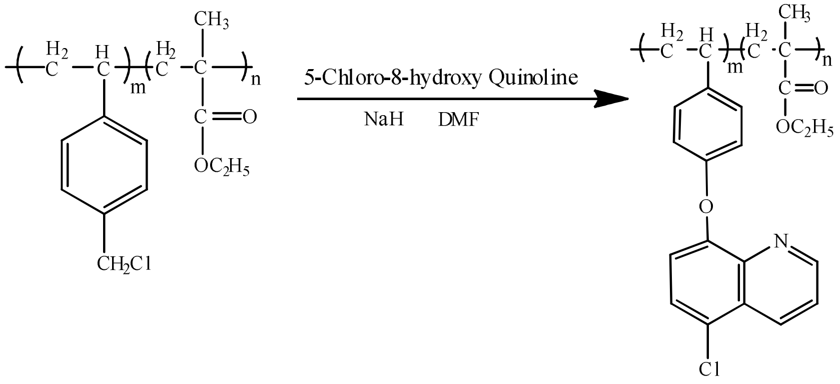
Vinylbenzylchlorid (VBC) can be easily polymerized with radical or cationic initiators [1]. Copolymerization reactions of VBC were performed with styrene and methyl metacrylat, in toluene at 70±1˚C using α,ά-azobis(isobutyronitrile) (AIBN) az the radicalpolymerization initiator and the copolymers I,II collected respectively in good yields. Polymers with chloromethyl group in the side chains are useful starting materials for the synthesis of various functional polymers [2]. The etherification reaction of polymers with salt of 5-chloro-8-hydroxy quinoline proceeded very smoothly to give the corresponding polymers with pendant ether residues. Characterizations of all the obtained polymers were performed with FT-IR and ^{1}HNMR spectroscopic techniques. The glass transition temperature (Tg) of the copolymers (I, II) was determined by dynamic mechanical thermal analysis (DMTA). The study of the DMTA curves for modified copolymers indicated that glass transition temperature values of the copolymers increase with incorporation of 5-chloro-8-hydroxy quinoline groups as side chains. The resulted copolymers are white solid and soluble in chloroform, dimethylsulphoxide and insoluble in nhexane/methanol, ethanol and water.



Scheme 1

Reference:

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Synthesis and characterization novel biodegradable polyurethane from novel diphenolic monomer derived tyrosine

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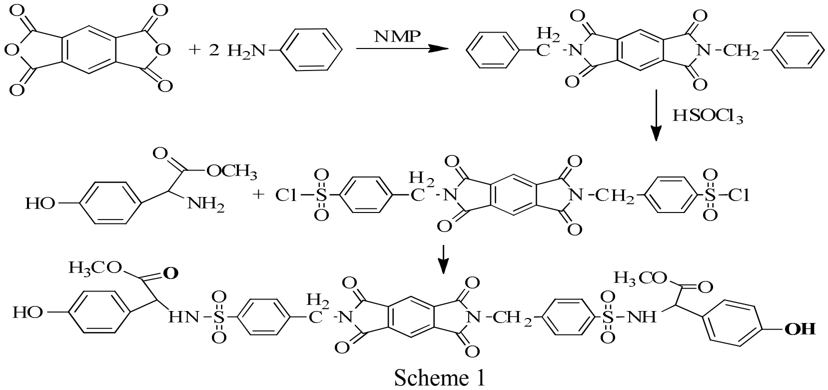
Bisphenols (BPs) such as bisphenol-A (BPA) are a group of chemical materials which consist of two phenolic rings joined together through a bridging carbon [1]. BPA is used as a material for the production of phenol resins, polyacrylates and polyesters. BPA is cytotoxic so may not be suitable candidate as monomers in medical implant and biodegradable materials. So, there is a significant need for a non-cytotoxic diphenolic monomer that could be used as a building block in the design of biodegradable materials. This need was addressed by the development of some tyrosine-based monomers. A novel diphenolic monomer containing sulfonamide group was synthesized from natural tyrosine in tree steps (Scheme 1). A new family of biodegradable polyurethanes (PUs) was prepared by the polycondensation reaction of new diol monomer with several different diisocyanates. The resulting new PUs were obtained in good yields with good inherent viscosities and are soluble in polar aprotic solvents. They showed good thermal stability and biodegradability. The synthetic compounds were characterized and studied by FT-IR, ^{1}H-NMR, ^{13}C-NMR elemental and thermogravimetric analysis (TGA) techniques. Soil enzymatic assay showed that the synthesized diol and its polymer are biologically active and probably biodegradable in soil environment.



Scheme 1

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Synthesis of tannic chitosan as new derivative and its application as a carrier for drug delivery

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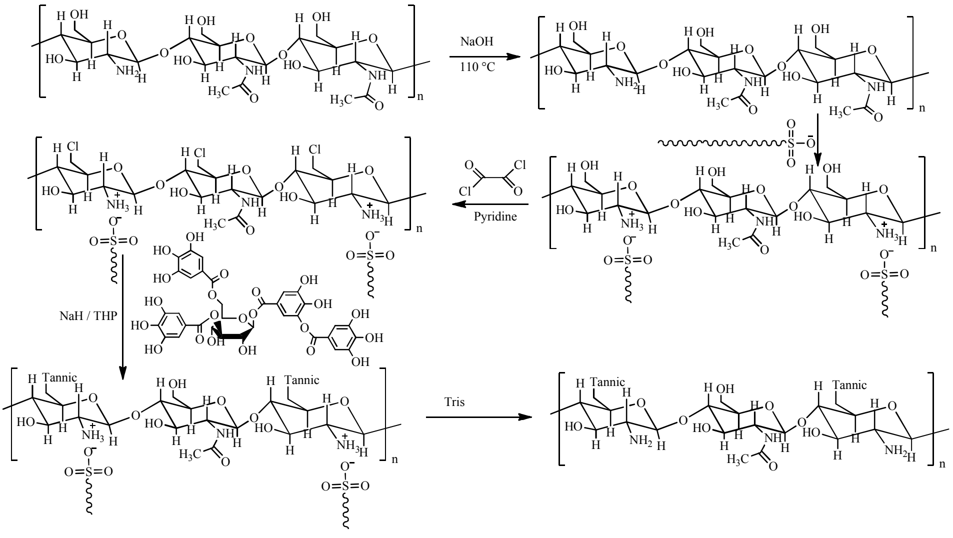
Chitosan is a cationic polysaccharide which has wide application in biotechnology, pharmaceutical, textile, food, cosmetics, and agriculture due to its abundant availability, inherent pharmacological properties polycationic, nontoxic, biodegradable and biocompatibility properties[1-3]. Unfortunately, chitosan is soluble only in aqueous at pH higher than its pKa (~pH 5.5-6.5). Tannic acid is a specific commercial form of tannin which have been reported to exert many physiological effects, such as to accelerate blood clotting, reduce blood pressure, decrease the serum lipid level, produce liver necrosis, and modulate immunoresponses. Present study introduced a new compound by conjugating tannic acid to C6 position of chitosan under mild condition to improve the biocompatibility and water solubility of chitosan. The chemical structure of prepared polymer was chrectrerized by FTIR and ^{1}HNMR spectroscopy. The TEM, SEM, AFM and DLS techniques were used to characterize prepared particles size. In vitro investigation of anticancer drug release from nanoparticles was carried out to evaluate nanopraticles potential as nano carrier for oral delivery of Ibuprofen as model drug of poorly water soluble drugs.



Scheme 1

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The synthesis and characterization of (3-(p-tolyl) isoxazole -5- yl) methyle acetate

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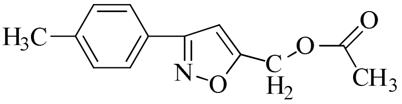
Isoxazole derivatives have been used a key intermediates in synthesis and have been investigated intensively for the last several years because of their biological activities and for the preparation of natural compounds and their derivatives have similar structures [1-2]. Isoxazole derivatives are widely used as drugs with hige potential have been studied, isoxazolel industrial applications in different industries can be found in semiconductors, paint, photographic applications, polymers as thermally resistant material cited [3]. This research work describes the synthesis of new compound of isoxazole family. In present research, two kinds of isoxazole and an oxime compound have been synthesized. 4-methylebenzaldehyde changed in to 4- methyl benzaldoxime (1) by increasing of sodium hypochlorite to hydroxylamine hydrochloride in pyridine as a solvent. The compound (1) changed to nitrile oxide and [3+2] cycloaddition happened by using propargyl alcohol. As a result 3-(4- methyl phenyl) -5- hydroxyl isoxazole (2) was prepared. In final step, (3-(p- tolyl) isoxazole -5- yl) methle acetate (3) was prepared by reaction of acetic and compound (2) in CH_2Cl_2. The structure of synthesized compound were confirmed by FT-IR,^{1}H NMR and ^{13}C NMR spectroscopies.



(3)

Scheme 1

References:
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Regioselective three-component synthesis of novel pyrido[2,3-*d*]pyrimidines using 3-cyanoacetylindole

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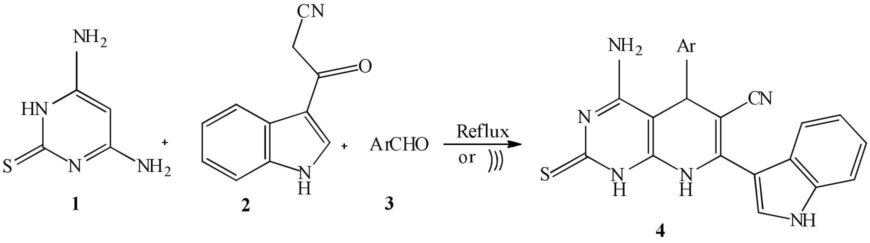
Pyridopyrimidines especially pyrido[2,3-*d*]pyrimidine derivatives are important group of organic materials, which show the diverse range of pharmacological and biological activities such as anti-pyretic, anti-bacterial, anti-histaminic and anti-inflammatory. In recent years, due to biological and pharmaceutical activities of these kind of heterocycles, synthesis of them has attracted many attentions [1,2].

Due to our recent interests in the development of benign methods for the synthesis of medicinally important heterocyclic compounds [3], preparation of novel pyrido[2,3-*d*]pyrimidine derivatives, was investigated via one-pot three-component reaction of 4,6-diaminopyrimidime-2(1*H*)-thione **(1)**, 3-cyanoacetylindole **(2)** and arylaldehyde **(3)** under ultrasonic irradiation and classical conditions (Scheme 1). In this protocol pyrido[2,3-*d*]pyrimidine derivatives **(4)** were synthesized in excellent yields (88-95%) and short reaction times.



Scheme 1

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Using 3-formylchromone as valuable substrate in the synthesis of novel chromeno[2,3-*d*]pyrimidines

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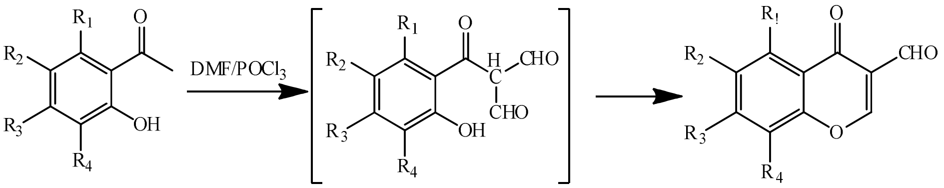
The pyrido[2,3-*d*]prymidines and their oxoderivatives have attracted many interests for their potential biological activities. On the other hand 3-formylchromones are versatile synthons for the synthesis of a variety of novel heterocyclic systems possessing diverse biological activities [1,2]. From a synthetic point of view, 3-formylchromones occupy an important role in the synthesis of various heterocyclic systems, due to the availability of three electron deficient sites. Also, 3-formylchromones are able to serve as a heterodiene as well as a dienophile or a Micheal acceptor.

In continuation of our recent interests in the synthesis of biologically important heterocycles [3], various derivatives of 3-formylchromone were prepared and used in the synthesis of novel chromenopyrido[2,3-*d*]pyrimidines. In this presentation various aspects of this novel methodology are discussed.



Scheme 1

References:

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   (b) R. Hossein Nia, K. Mamaghani, K. Tabatabaeian, F. Shirini, M. Rassa, *Bioorg. Med. Chem. Lett.* 22 (**2012**) 5956.
   (c) M. Mamaghani, A. Loghmanifar, A. Taati, *Ultrason. Sonochem.* 18 (**2011**) 45.

Synthesis of novel pyrimidine derivatives as antimicrobial agent and anti-inflammatory agents

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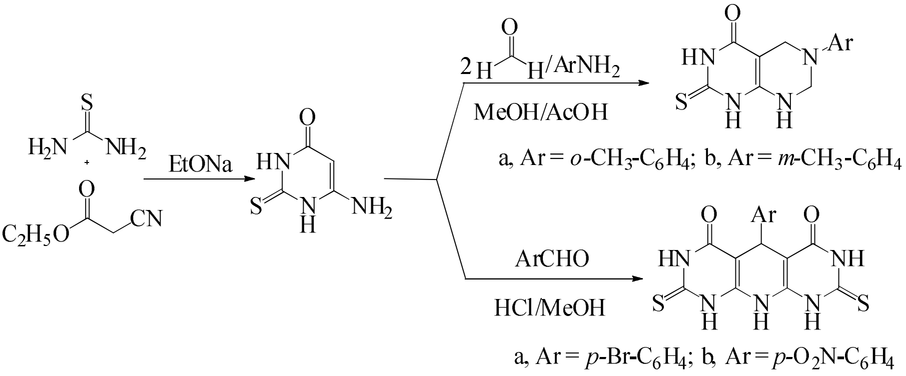
Email:laya5077@gmail.com

The importance of fused pyrimidines, as common sources for new potential therapeutic agent, is well known. Bicyclic and tricyclic compounds containing pyrimidine system are common biologically active structures. Pyrimidine derivatives exhibit a range of pharmacological activities such as antibacterial, anticancer and anti-inflammatory [1,2]. In continuation of our recent studies in the synthesis of biologically important heterocycles [3], a variety of novel fused pyrimidine derivatives were synthesized via the reaction of 6-amino-2-thiouracil with various reagents. The antimicrobial and anti-inflammatory activities of some of the synthesized compounds were also examined.



a, Ar = o-CH_3-C_6H_4; b, Ar = m-CH_3-C_6H_4

a, Ar = p-Br-C_6H_4; b, Ar = p-O_2N-C_6H_4

Scheme1

References:

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Multicomponent click synthesis of *β*-hydroxy-1,2,3-triazoles by heterogeneous copper catalyst

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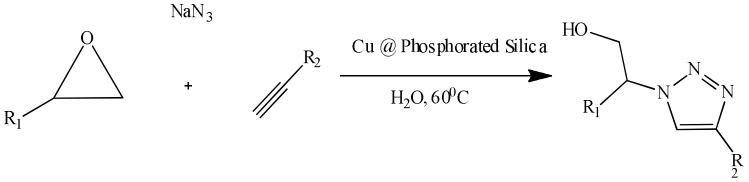
The Huisgen [1], 1,3-dipolar cycloaddition of azides and alkynes has become a synthetic cornerstone since the paramount discovery by the groups of Meldal [2] and Sharpless [3] of its copper (I) catalyzed version (CuAAC). As a result, a plethora of methods have been developed around this reaction with the aim to increase efficiency. In recent years, multicomponent click synthesis of *β*-hydroxy-1,2,3-triazoles have been developed via in situ azidolysis of epoxides in the presence of the alkynes and different heterogeneous catalysis with source metal copper in water [4–7]. The resulting products possess a β-hydroxy-1,2,3-triazoles moiety which is also present in peptide surrogates of HIV-1 protease inhibitors [8].

In this study, we wish report, the modified Cu (I)-silica catalyzed in the cascade reaction. Three component, epoxides, sodium azide and alkynes react via one-pot reaction in water solvent and amount of catalytic from modified Cu (I)-silica. Then the pure *β*-hydroxy-1,2,3-triazoles were obtained as products in excellent yields and short reactions time (Scheme 1).



Scheme 1

References:

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Synthesis of aliphatic polyesters by immobilized lipase

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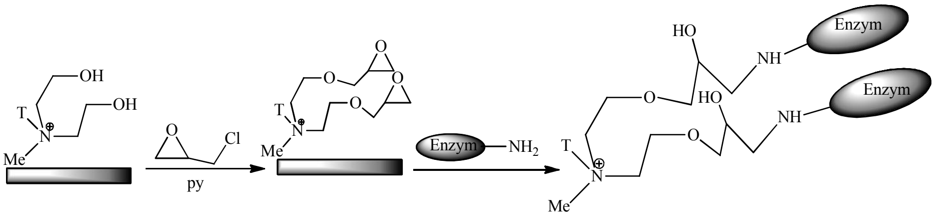
Enzyme-catalyzed polymerization reactions in organic solvents has been important in organic synthesis and has been proven to be a new methodology in polymer synthesis [1]. Characteristic features of enzyme catalysis afforded novel polymerization reactions to produce polymers, which are often difficult to be synthesized by conventional polymerizations. Syntheses of aliphatic polyesters by fermentation and chemical processes have been extensively studied in viewpoint of biodegradable materials science [2]. Lipase is an enzyme which catalyzes the hydrolysis of fatty acids. By utilizing such catalytic properties of lipase, polyester syntheses have been achieved by ring-opening polymerization of lactones [3]. Due to the wide variety of environmental conditions, lipases are often easily inactivated and difficult to be separated from the reaction system for reuse. A lot of effort is still being devoted to the search for new support materials and novel techniques. By an appropriate choice of the immobilization process, operational costs of industrial processes involving lipases can be significantly reduced [4].

In this work immobilized lipase on activated cloisite (Scheme 1) was used for synthesis of aliphatic polyesters. Three different diols, 1,5-pentanediol, 1,4-butanediol and 1,3-propanediol were used to carry out the lipase catalyzed polymerization reaction with glutamic acid and adipic acid . The diacid and the diol was always used in a 1:1 molar ratio, most suitable for AA + BB polycondensation to obtain a high molar mass polyester. Effects of solvent and effect temperature and reusability enzyme were also evaluated in polyesterification reaction.



Scheme 1

References:

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Fe_3O_4-SA-PPCA As novel and effective nanocatalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones

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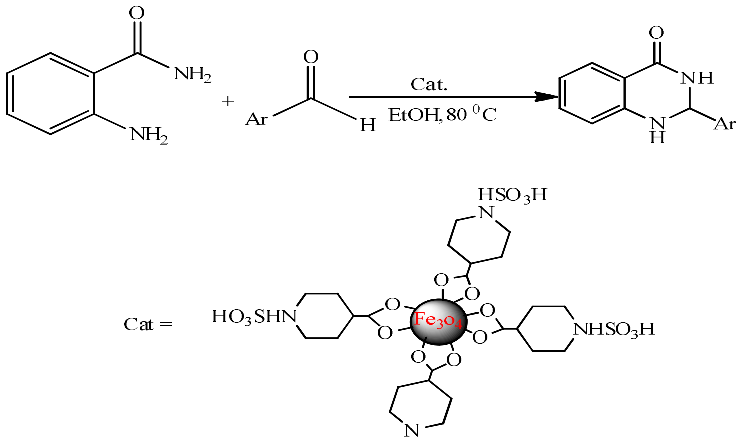
During the past decades, advances in nanoscience and nanotechnology have pushed forward the synthesis of functional magnetic nanoparticles (MNPs), which is one of the most active research areas in advanced materials. MNPs that have unique magnetic properties and other functionalities have enabled a wide spectrum of applications [1]. Iron oxide magnetic nanoparticles (Fe_3O_4-MNPs) are approximately 20–30 nm in size containing a single magnetic domain with a single magnetic moment and exhibit superparamagnetism [2]. Magnetic nanocatalysts can easily be separated and recycled from the products by an external magnet [3].

In this study, we report immobilization of sulfamic acid groups on the magnetic MNPs-PPCA, as a new heterogeneous catalyst for the synthesis of dihydroquinazoline *via* one-pot condensation of 2-aminobenzamide with aldehyde (Scheme 1). This method is an efficient and rapid route for the synthesis of a wide range of dihydroquinazoline.



Scheme1

References:

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Chemical analysis of the essential oil Prangos Ferulacea(L.) Lindl. growing wild in Iran. obtained by using HS-SPME instrument

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The Iranian flora comprises 15 species of prangos, of which 5 are endemic [1]. The plant material was collected from Shahrood, Semnan Province, Iran. Fruits of some Prangos species have been traditionally used in Iran as emollient, carminative and tonic[2]. There are also some reports on antibacterial and antioxidant properties in some Prangos genus [3]. The volatiles compound obtained by head space-solid phase microextraction (HS-SPME) procedures from the crushed dry flowers, leaves and stems of *prangos Ferulacea* (L.)Lindl and analyzed by GC and GC/MS [4].

The major components of the stems oil were α- pinene (36.13٪) and sabinene (14.94٪). The main component of flower oil were α-pinene(42.18٪), β-phelandrene(18.69%), α-phelandrene(12.83%) and sabinene(12.46٪). The predominant components of the leaf oil were α-pinene(49.49%), ß-phlandrene(17.28%), E-β-ocimene(11.4%) and sabinene (7.91%).

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1-(4-Sulfobutyl)-3-methyl imidazolium hydrogensulfate as an efficient catalyst for the synthesis of 4, 10-dinitro-2, 6, 8, 12-tetraoxa-4,10-diazaisowurtzitane (TEX) from intermediate 1,4–diformyl-2, 3, 5, 6-tetrahydroxypiperazine (DFTHP)

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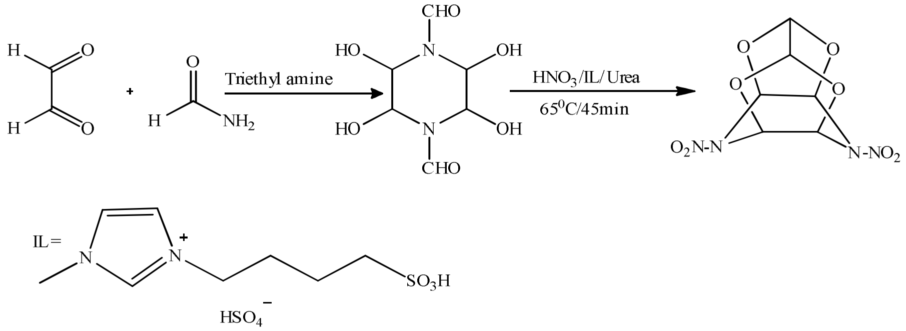
4,10-dinitro-2,6,8, 12-tetraoxa-4, 10-diazaisowurtzitane (TEX) is well known as an efficient insensitive high explosive. It was usually prepared via nitration of 1, 4-diformyl -2, 3, 5, 6-tetrahydroxy piperazine using a mixture of fuming nitric acid and concentrated sulfuric acid [1-4]. However, this traditional liquid acids are toxic, corrosive, hazardous waste and cause product decomposition and low yields despite their high catalytic activity. In this research, the use of an efficient catalyst and mild reaction condition for synthesis of TEX is reported for the first time. Boronosted ionic liquid was employed successfully as catalyst for reaction nitration. (Scheme 1) [5-8]. The influence of the time, temperature, nitric acid and ionic liquid ratio on the yield of TEX was examined and synthesis was optimized.



Scheme 1

References:

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Synthsis of azoic dyes based on 4-hycroxy cumarin

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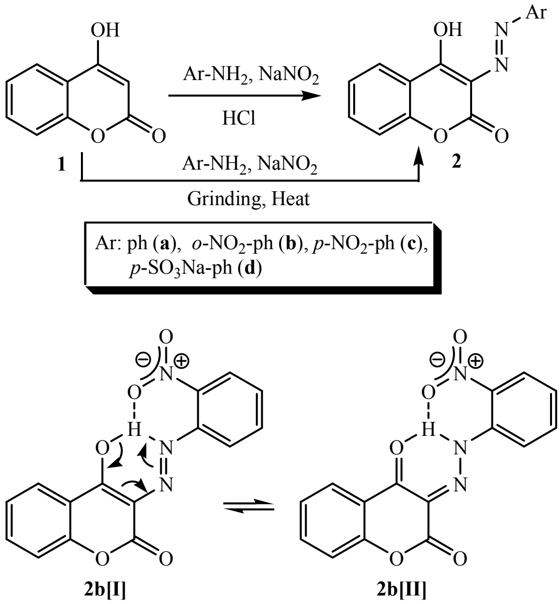
4-Hydroxycoumarin and some its derivatives have been and have evoked a great deal of interest due to their biological properties and characteristic conjugated molecular architecture. Many of them display important pharmacological effects including anti-arthritis, anti-inflammatory,anti-bacterial,anti-cancer properties [1,2].

In this study, the reaction of 4-hydroxycoumarin withdiazinium salts ofanilin and its derivatives such as *ortho*-nitro, *para*-nitro aniline and sulfanilic acid afforded interesting azo dyes. An intramolecular hydrogen bond is formed in these compounds.Azo dye obtained from *ortho*-nitro aniline showed a bifurcated intramolecular hydrogen bond. In this research, tautomeric forms ofenol-azoandketo-hydrozonewere investigated. The synthesis of the mentioned above dyes were also successfully examined under solid phase (Scheme 1).



Scheme 1

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Ultrasound promoted one pot synthesis of 2-amino-4*H*-pyran-3-carbonitriles

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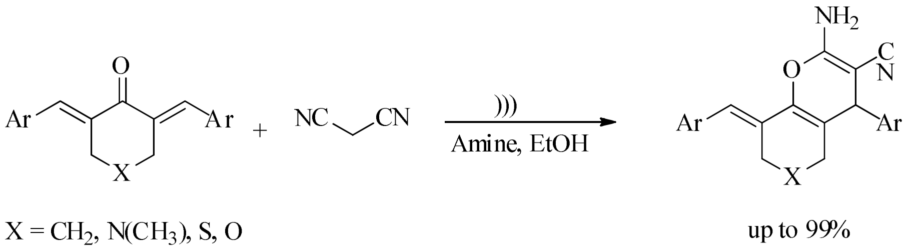
4*H*-pyrans and its derivatives have not only attracted biological, pharmacological properties but also led to pyridine systems as the framework of numerous biologically active alkaloids [1]. 2-amino-4*H*-pyran derivatives have been synthesized by different methods such as under exposure to microwave and using catalyst [2] These methods show varying degrees limitations such as prolonged reaction times, low yields, toxic solvents and cost of catalysts.

Ultrasound irradiation is now used in the synthesis of many organic chemicals under milder and more environmentally friendly condition and shorter reaction times. In continuation of our studies to develop environmentally friendly processes [3] we would like to herein report an efficient protocol for ultrasound promoted one pot synthesis of 2-amino-4*H*-pyran-3-carbonitriles up to 99% yield with using catalytically amount of amine at 5-8 minutes which surpasses those limitations (Scheme 1).



Scheme 1

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Effect of thermodynamical parameters on synthesis of novel polyester for orthopedically applications

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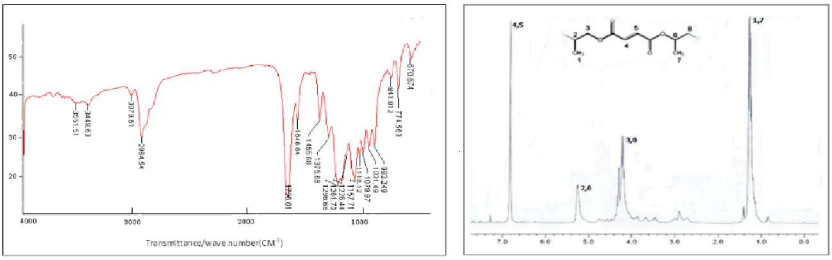
One of the most important biodegradable polymer is poly(propylene fumarate) (PPF), a linear, unsaturated polyester which consists of alternating propylene glycol and fumaric acid units [1]. Main advantage of this polymers is ability to cure the material in vivo, thereby filling skeletal defects of any shape or size with minimal surgical intervention [2]. Many different methods for synthesizing of PPF have been reported [3-5]. However, none of the presented PPF preparations have possessed the optimal physical characteristic.

The purpose of present study is including time and temperature on PPF synthesis. In order to determine effects of synthetic parameters, FTIR analysis has been used. Optimum synthesized PPF characterized by FTIR and NMR analyses. Finally, we introduce the best conditions to PPF synthesis. FTIR and HNMR of the best product have been shown in Fig.1 and Fig.2, respectively. According to our results, suitable products were obtained using 17 hours reaction time and 140°C of temperature.



Scheme 1

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Chemical composition of the essential oil from *Tanacetum Tenuisectum*(Boiss.)Podl., Obtaind by HS-SPME, from Iran

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The Flora of Iran comprises 26 species of *Tanacetum* of which 12 are endemic [3]. *Tanacetum* species are reported to possess anthelmintic, carminative, antispasmodic and anti-migraine properties having a repellent effect against the Colorado potato beetle [1,2].The plant material was collected from south of Shahrood, semnan Province, Iran [3]. The present report deals with the analysis and comparison of composition of the volatiles obtained by head space-solid phase microextraction (HS-SPME) procedures from the crushed dry flowers, leaves and stems of *Tanacetum Tenuicectum* [4]. The composition of the volatile essential oils was investigated by GC-FID and GC-MS [5]. The main component in the flower oils were 1,8-cineole(43.94%) α-pinene(26.02%), and sabinene(19.24%).the major compound in the leaves oil were1,8-cineole(43.87%, α–pinene(33.68%) and sabinene(11.56%). The main component in the stem oils were 1,8-cineole(45.38%), α-pinene(41.00%) and sabinene(3.17%).

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Synthesis of 2-butyl-2-ethyl-1, 3-dinitrat propane as a miscible energetic plasticizer in HTPB

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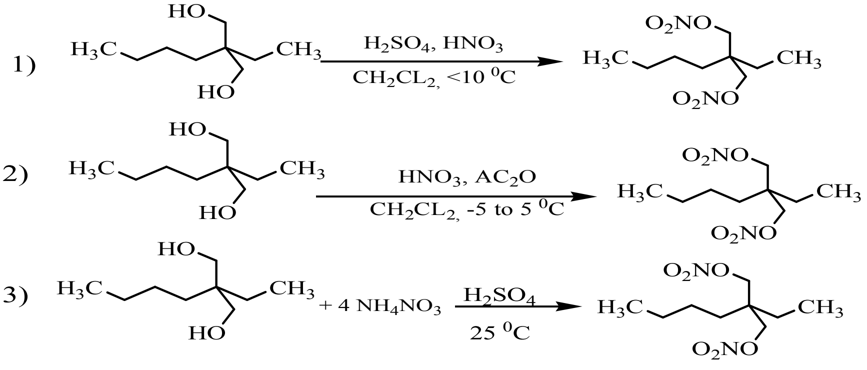
In modern energetic propellant composition, conventional plasticizers is replaced by Energetic ones, but the most important factor that influence the stability of mixture is a miscibility of the plasticizers in a per polymer [1]. Hydroxyl terminated poly butadiene(HTPB) is commonly used as binder in formulations of propellant. HTPB is a neutral polymer and its miscibility with polar plasticizers is low. Here, we have synthesized a new type of nitro plasticizer that its solubility parameter is nearly similar to HTPB and have acceptable miscibility in HTPB [3]. The new type of plasticizer, 2-Butyl -2-Ethyl -1,3-Dinitrat Propane, has synthesized via following three methods:[2-4]. The yield of the reaction in the first and second methods are high. The third method give a mild conditions for processing of the nitration and it is suitable for scaling up of the reaction. Plasticizer has characterized by HNMR, IR spectroscopy. Thermal stability of plasticizer is studied by DSC method and the miscibility of plasticizer is investigated by calculation of solubility parameter via group contribution method. This study shows that The 2-ethyl -2-butyl -1,3-dinitrato propane provide a promising alternative to neutral plasticizer, including DOA and DOS , for increasing the specific impulse of HTPB base propellant.



Scheme 1

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Synthesis and characterization of novel polyimide/α-Fe_2O_3 nanocomposite

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The nanocomposites of polymer metal oxide exhibit a significant increase in thermal stability as well as self-extinguishing characteristics. Advances in magnetic nanoparticles and polymer magnetic nanostructured technology have shown that some of these materials have the potential to play an important role in the diagnosis and treatment of cancer [1]. Other interesting features have been observed when the polyimide (PI) has been loaded with magnetic materials [2] making them as polymer magnetic composites and these materials are supported to have applications as memory devices, magnetic fluids,and magnetic sensors, etc [3]. The work described in this paper deals with the synthesis and characterization of superparamagnetic PI/α-Fe_2O_3 nanocomposite films. The incorporation of different percents of α-Fe_2O_3 nanoparticles into poly(amic acid) (PAA), afforded an opportunity to prepare several novel PI/α-Fe_2O_3 nanocomposites. To this point, firstly PAA derived from 3,3',4,4'-benzophenone tetracarboxylic dianhydride (BTDA) and 3,5-diamino-N-(9H-fluoren-2-yl)benzamide (DFB) in *N,N*-dimethylacetamide (DMAc) as an aprotic solvent. Novel PI containing α-Fe_2O_3 nanoparticles was synthesized through ultrasonic irradiation method. With the aim of a typical silane-coupling agent, 3- aminopropyltriethoxysilane (APTES) was used. The surface of nanoscale α-Fe_2O_3 was modified to decrease aggregation of nanoparticles in polymer matrix. Thermal treatment of the α-Fe_2O_3 doped precursor film converted the PAA into its final PI film with superparamagnetic behavior. Its morphology, microstructure and magnetic properties of samples were characterized by transmission electron microscopy for investigate of the distribution of nanoparticles in the polymer matrix, Fourier transform infrared spectroscopy (FT-IR) and X-ray diffraction for characterize of the nanoparticles and composite films and TGA data demonstrated thermally stable in compare to pure PI. These studies showed the homogenous dispersion of α-Fe_2O_3 in the PI matrix with an increase in the thermal stability of the composite films on α-Fe_2O_3 loadings.

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One-pot synthesis of polyhydroquinoline derivatives in the presence of copper oxide under microwave irradiation

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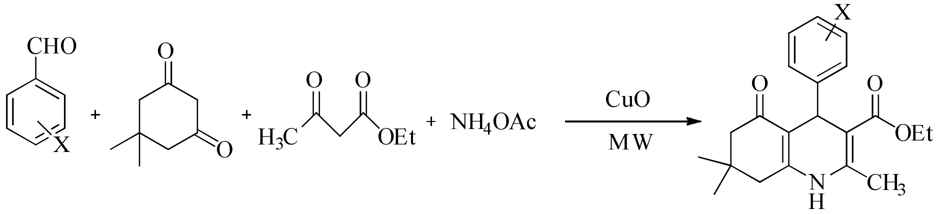
An efficient synthesis of polyhydroquinolines is achieved via a four-component reaction of aldehydes, dimedone, active methylene compounds, and ammonium acetate in one-pot under solvent-free conditions at room temperature on grinding [1,2]. In this method, polyhydroquinoline derivatives have been successfully prepared via four component condensation reactions of an aldehyde, dimedone, ethylacetoacetate and ammonium acetate in the presence of cupper (II) oxide (CuO) and under microwave irradiation. The reactions were performed in water as a green solvent. Simple work up procedure, high yield, short reaction time, easy available chemicals are among the important features of this work, and the procedure could be added to the present methods for the preparation of polyhydroquinoline derivatives (Scheme 1).



Scheme 1

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Application of new solid sulfonic acid nanocatalyst in the Biginelli reaction

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Dihydropyrimidinones have attracted increasing interest due to their divers therapeutic and pharmacological properties [1]. These meterial have been synthesized via biginelli reaction under acidic conditions [2]. Acording in this study the catalytic application of a novel sulfonic acid containing ionic liquid based nanoorgano silica in the biginelli reaction has been developed [2,3]. The catalyst was synthesized via grafting of propylthiol groups on the a prepared nanoorgano silica. fllowed with oxidation with hydrogen peroxide.this catalyst was first characterized with nitrogen sorption analysis and transmission electron microscopy (TEM) then significantly applied in Biginelli reaction of several aldehydes with urea and ethyl acetoacetate and gave good to excellent yields of corresponding coupling products.

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Synthesis of thiourea derivatives by using of benzoyl isothiocyanates

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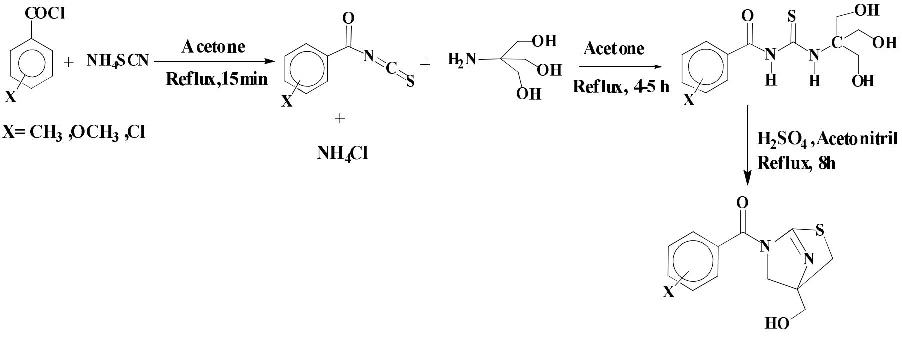
As the thiourea molecule contains one sulphur and two nitrogen atoms, thiourea and its derivatives are potential corrosion inhibitors [1]. The main application of thiourea is in textile processing. Moreover, thiourea reduces peroxides to the corresponding diols [2]. Thiourea is also used in the reductive work-up of ozonolysis to give carbonyl compounds [3]. Some thiourea derivatives display a wide range of biological activity including antibacterial, antifungal, antitubercular, antithroid, antihelmintic, rodenticidal, insecticidal, herbicidal, and plant-growth regulator properties [4].

In this work, reaction of derivatives of benzoyl isothiocyanates with tris(hydroxymethyl)methyl- amine was studied. The products of these reactions are derivatives of 1-tris(hydroxymethyl)-3-(benzoyl)thiourea in high yields and short reaction times. Then, these products under reflux in the presence of acid led to final products (Scheme 1).



Scheme 1

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Synthesis and characterization of novel poly(amide-imide)/α-Fe_2O_3 nanocomposite

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In recent years, polymer/metal oxide nanocomposites have been a center of scientific interest and active multidisciplinary research because of their excellent potential for widespread technological applications such as toners in photocopying, rechargeable batteries, sensors, drug delivery, etc [1]. Poly(amide-imide)s (PAI)s contains both amide and heterocycle imide structures along the main chain of the polymer backbone are a kind of thermoplastic resin, have good high-temperature resistance, outstanding mechanical properties, excellent oxidative stability and hydrogen bonding interaction, being a promising matrix candidate for hybrid materials [2,3]. In this study, a series of PAI was synthesized from the polymerization reaction of pyromellitic dianhydride bis-L-alanine diacid and different aromatic diamines. The obtained polymer/metal oxide nanocomposites composed of PAI/α-Fe_2O_3 were synthesized through ultrasonic irradiation. The formation of PAI was confirmed by ^1H NMR, fourier transform IR spectroscopy (FT-IR). The resulting nanocomposites were characterized by FT-IR, powder X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM) and thermogravimetric analysis (TGA). The TEM and FE-SEM results indicated that the nanoparticles were dispersed homogeneously in PAI matrix on nanoscale. TGA confirmed that the heat stability of the nanocomposite was improved in the presence of α-Fe_2O_3 nanoparticles.

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A study of electronic and magnetic structure of some annulenes based on nuclear magnetic resonance spectroscopy by using density functional theory

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Purpose:35 neutral and ionic structures, mostly annulene, were examined in this study, and stable structure of ground-state was achieved through density functional calculations by Gaussian software after optimizing all the structures, and OPTS, NICS and NMR calculations were made on them.

Methods:The structure of some annulenes was extracted from NIST website and Solomons' book Then, it was plotted by GaussView software to be introduced to Gaussian software (2,4). All preliminary optimizations were accomplished through B3LYP method with 6-31G* basis set and OPT keyword. The preliminary optimized structures were determined through B3LYP method with 6-31++g(d,p) basis set and nmr=giao keyword, and required data were extracted from output and section related to SCF GIAO Magnetic shielding tensor.

Results: The graphs of difference between single and double bond of annulenes shows that benzene, cyclopentadiene anion, etc. possess the conditions of aromaticity. NICSZZ is more exact than isotropic 2, because there is no share of δ bond in it and π electrons spin area is outside molecule plane, thus it is one of the ideal criteria for identifying aromaticity [1,3].

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A simple and efficient pseudo four component synthesis of highly substituted benzenes under solvent free condition

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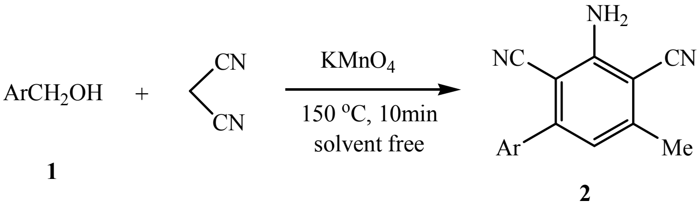
Multi-functionalized benzenes possessing electron-donor substituents such as dicyanoanilines are very important chemicals. They are useful as important substrates for nonlinear optical materials, molecular electronic devices and they are strongly fluorescent [1] and have been reported to exhibit biological activities like antileishmanial activity [2].

This work described an efficient Pseudo four-component synthesis of 3-aryl-2,6-dicyano-5-methylanilines **2**. Thus, a mixture of benzyl alcohol **1** (1 mmol) and malononitrile (4 mmol), in the presence of Potassium permanganate $KMnO_4$ (1 mmol), underwent a solvent free condition at 150 °C to afford the corresponding 3-aryl-2,6-dicyano-5-methylanilines **2** in good to excellent yields. The structures of the isolated products were assigned on the basis of IR, ^1H and ^{13}C NMR, mass spectrometry and elemental analysis (Scheme 1). The mp values, elemental analyses, and spectral data of compounds 2, were also in good agreement with those of authentic samples [3].



Scheme 1

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Synthesis of novel azo dyes derivatives from 3-Hydroxy-naphtalene-2-carboxylic acid and β-naphtole

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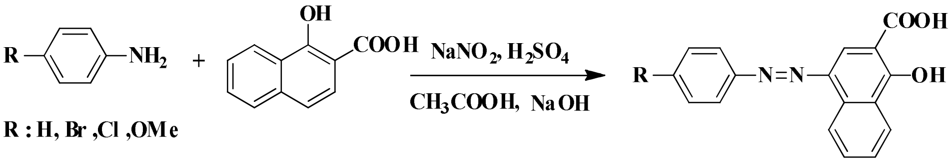
Several novel azo disperse dyes were synthesized by coupling reaction of 3-hydroxy naphthalene-2-carboxylic acid and β-naphthol with diazotized *p*-substituted aniline derivatives as diazo components. The structures of all compounds were characterized by spectral techniques and elemental analysis [1-2].

Ionization constants, pKa, for these dyes were determined using electronic spectroscopic method.



Scheme 1

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New thiazolo Schiff base ligand: Synthesis, characterization and X-ray crystal structure determination

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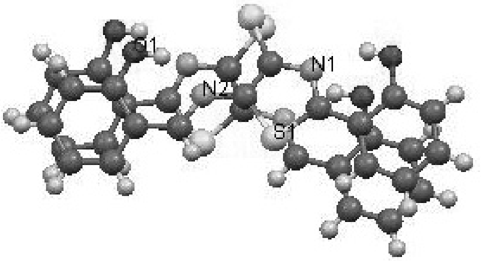
Schiff bases are a group of organic compounds with an activated carbon –nitrogen double bond that are obtained by the condensation reaction between $-NH_2$ and a carbonyl group [1-3]. These compounds, as an important class of organic compounds, have the unique performance against bacteria, fungi and toxins, and show anti-cancer activity [4].

In this work, a new thiazolo Schiff base ligand has been synthesized by using salicylalehyde and dithiooxamide. The structure of synthesized compound has been investigated in $CDCl_3$ solution by ^1H NMR and solid state by X-ray (Scheme 1). The four interamolecular hydrogen bond exist in the crystal structure that lead to 1D supramolecular structure in the direction of the crystal ***b*** axe.



Scheme 1

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DABCO: An efficient catalyst for the synthesis of biscoumarin derivatives

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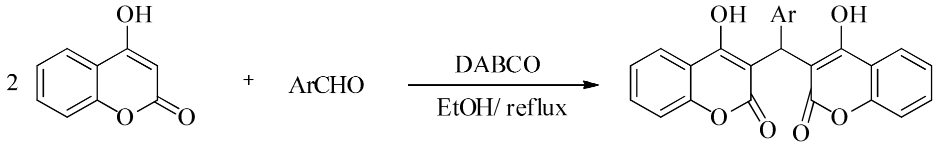
Biscoumarins and dihydropyrano[c]chromenes are of considerable interest due to their widespread biological properties [1–3]. A number of methods have been reported for the synthesis of biscoumarins [4–6]. Most of these methods require use of expensive catalysts and tedious work-up procedure. Herein, DABCO has been successfully applied to perform the reaction of 4-hydroxycoumarin with aldehydes in ethanol at reflux temperature to provide a series of biscoumarin derivatives in excellent yields (Scheme 1).



Scheme 1

References:

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A green and efficient method for diazotization and diazo couplingreaction using nano- BF_3/SiO_2 under mild conditions

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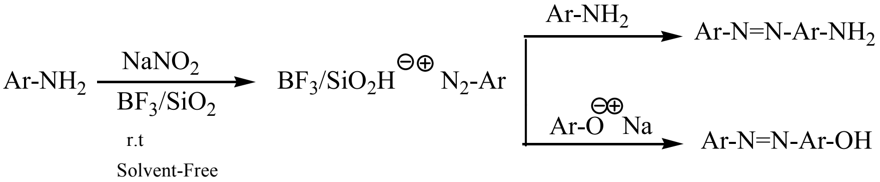
Diazo coupling reactions is one of the most important class of organic reactions which is currently performed with mineral acids as catalysts[1]. Aromatic azo compounds are widely used in various fields. For example, the azo compounds are used as organic dyes, indicators ,radical reaction initiators, and therapeutic and drug delivery agents [2].In recent years, wide attention has been directed toward the application of solid acids in organic synthesis because such reagents not only simplify purification processes but also help to prevent release of reaction residues into the environment. Recently, various solid acids have been used for the preparation of azo dyes [3]. Silica supported boron tri-fluoride ($BF_3.SiO_2$) is a bench-top catalyst which is reusable,cheap, readily available, eco-friendly, versatile and efficient for promotion of many acid catalyzed organic reaction [4].

This work describes simple and efficient method for the diazotization and diazo coupling reaction over BF_3/SiO_2, sodium nitrite and coupling reactants under solvent-free conditions at room temperature (Scheme 1).

The new method uses mild reaction conditions and avoids the use of acids and toxic solvents.



Scheme 1

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Nano-BF_3/SiO_2 solid acid as a mild and efficient catalyst for nitration of aromatic compounds under solvent free conditions

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Email: Bamoniri@kashanu.ac.ir
[b] *Department of Chemistry, College of Science, Yazd University, Yazd, I. R. Iran*

Aromatic nitration reaction is one of the more widely used in organic syntheses and in industrial applications for the formation of aromatic nitro compounds, which are important starting materials for the manufacture of various industrial products such as pharmaceuticals, intermediates, explosives and plastics [1]. Therefore nitration of aromatic compounds is properly one of the most widely studied organic reaction [2]. Moreover, the classical nitration process has some disadvantages, in order to overcome the limitations and drawbacks of the classic methods such as strongly acidic media, tedious work-up, oxidation, poly nitration, safety problems and to develop a high-yielding one-pot synthesis of nitro compounds a novel solid acid was introduced to be a mild and efficient agent [3,4]. The replacement of current chemical processing techniques with more environmentally benign alternatives is an increasingly attractive subject.

In this work, an efficient procedure for the nitration of aromatic compounds using nano-BF_3/SiO_2 was carried out under mild conditions. Nitration reaction was performed in the presence BF_3/SiO_2 as a solid acid catalyst, potassium nitrate and aromatic compound at 70 ^{0}C and solvent-free conditions in excellent yields (Scheme 1).This method has the following advantages: (a) reaction was carried out under mild condition;(b) nitrating agent was mild, highly efficient and chemoselective mono nitrating reagent;(c) the procedure was friendly environment and (d) the work-up was easy.

$$\mathbf{ArH} \xrightarrow[\mathbf{70\ ^0C,\ solvent\text{-}free}]{\mathbf{nano\text{-}BF_3/SiO_2,\ KNO_3}} \mathbf{ArNO_2}$$

Scheme 1

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One-pot synthesis of aromatic α-hydroxyesters under microwave irradiation

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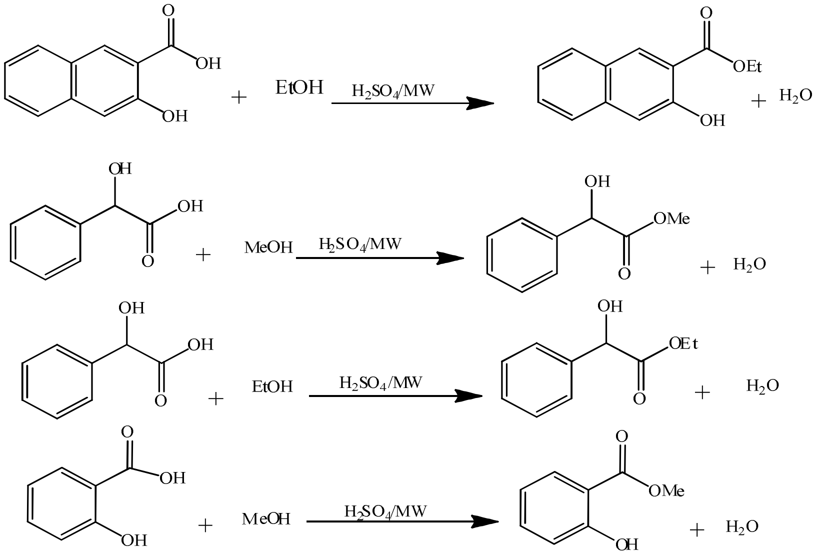
Microwave assisted organic synthesis is a technique which can be used to rapidly explore chemistry space and increase the diversity of compounds produced. Nowadays, it could be considered that all of the previously conventionally heated reactions could be performed using this technique [1]. In this study, has utilized microwave irradiation as an efficient one-pot synthesis to construct a series of aromatic α-hydroxy-esters from aromatic carboxylic acids. Because of the synthetic method properties under microwave irradiation the reaction time has gotten low. This method has a high yields, low cost, easy manipulation, less pollution, short time and simple operation [2]. The analytical methods such as FT-IR, UV and ^{1}H-nmr were utilized to determine the results of the reactions. The features of the products and the reactions will be presented and discussed.



Scheme 1

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NBS as a raeagent for deamnation of aziridine

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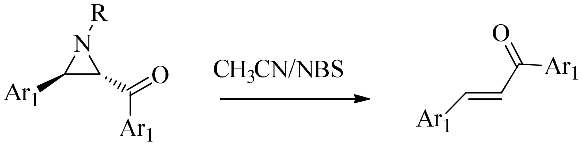
Among the reactions of aziridines, deamination of aziridines has been attractive because of their mechanistic, structural, thermodynamic, and theoretical aspects. Several methods have been described for the deamination of variety of aziridines using some reagents such as N_2O_4, N-nitroso-3-nitrocarbazole, nitrosyl chloride and organosilyllithium reagent have been used [1,2].

In continuation of our recent interest in the use of N-heterocyclic compounds in organic synthesis [3], herein we report the reaction of cis and trans non-activated aziridines using NBS which gave the corresponding trans-alkenes as sole product.



Scheme 1

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MgO Nanoparticles: A highly effective and easily recyclable catalyst for the synthesis of spiro[indoline-3,4-pyrano[2,3-c] pyrazole] derivatives

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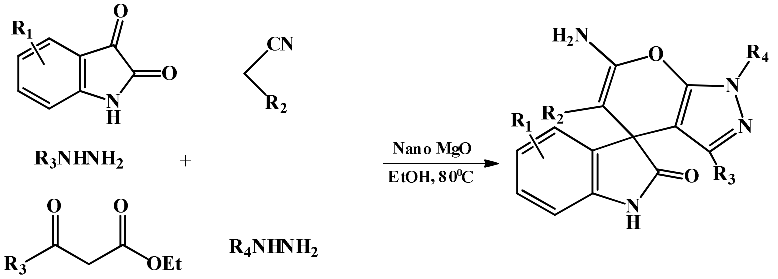
Multicomponent reactions (MCRs) are special types of synthetically useful organic reactions in which three or more different starting materials react to give a final product in a one-pot procedure [1]. Compounds carrying the indole moiety exhibit antibacterial and antifungal activities [2]. The chemical synthesis efficiency can be increased by nano sized catalysts because of their low size and high surface area to volume ratios [3]. The use of environmentally benign nano catalysts represents extremely important green chemical technology procedures from both the economical and synthetic points of view [4]. Among the various nano catalysts MgO found out an extensive application as heterogeneous catalysts in diverse organic reactions. We investigated a four component reaction of hydrazine, ß-keto ester, isatin and malononitrile to afford a series of spiro[indoline-3,4-pyrano[2,3 c]pyrazole] derivatives catalysed by MgO nanoparticles (Scheme 1).



Scheme 1

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Synthesis and characterization of NTA-modified K60-silica for selective recognition of aminoacids

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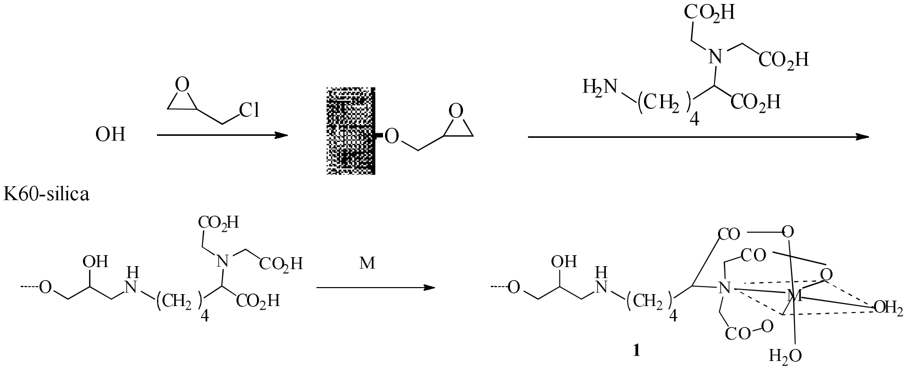
Quadridentate chelating adsorbent play a great rule in Chemistry and Biochemistry [1]. In the present work, we have used a nitrilotriacetic acid (NTA) derivative which occupies four positions in the metal coordination sphere of. e.g., Ni^{2+} and Cu^{2+}. The remaining two ligand positions in the octahedral coordination sphere are disposable for selective complexation of biorelevent molecules such as aminoacids and proteins [2].

We have prepared our chelating adsorbent based on K-60 silica and according to the following scheme.



Scheme 1

After characterization of the adsorbent **1**, our primary results show that the new chelating adsorbent **1** can strongly complex with aminoacids, which have positive residue such as Histidine, Argenine, and Lysine. In the future, we have to investigate the probably selective interaction of our adsorbent with the proteins especially with His-tag proteins.

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Synthesis of multisubstituted imidazoles catalyzed by *L*-pyrrolidine-2-carboxylic acid-4-hydrogen sulfate supported on silica gel

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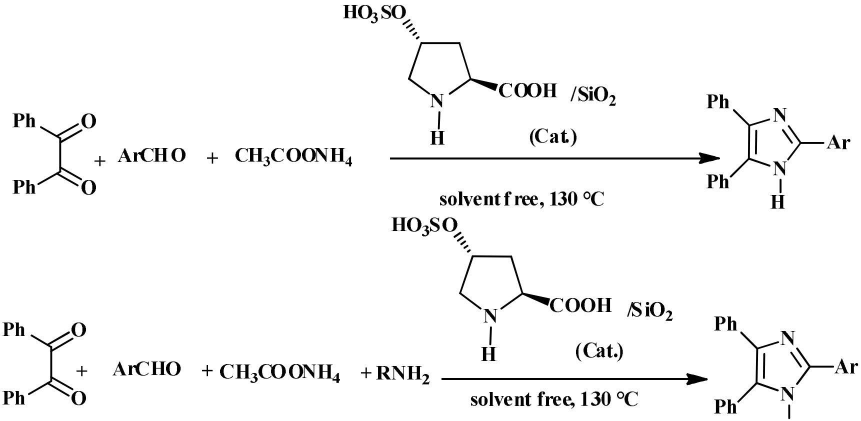
One-pot transformations, particularly multi-component reactions (MCRs) are of current interest to organic chemists. Multisubstituted imidazoles, an important class of pharmaceutical compounds, exhibit a wide spectrum of biological activity [1]. They have emerged as an integral part of many biological systems [2]. Recently a number of methods have been reported for the synthesis of substituted imidazoles in the presence of an appropriate catalyst [3], most of these synthetic methods suffer from one or more serious drawbacks.

In continuing our studies in organic reactions [4-5] we became interested to apply *L*-pyrrolidine-2-carboxylic acid-4-hydrogen sulfate supported on silica gel as an efficient catalyst for the synthesis of 2,4,5-trisubstituted imidazoles and 1,2,4,5-tetrasubstituted imidazoles. In this light benzile, ammonium acetate (or mixture of ammonium acetate and primary amines) and a variety of aldehydes were condensed at 130 °C under solvent-free conditions (Scheme 1).



Scheme 1

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Investigation of the reaction between (thio)barbituric acid and various aldehydes in presence of *N*-methylmorpholin

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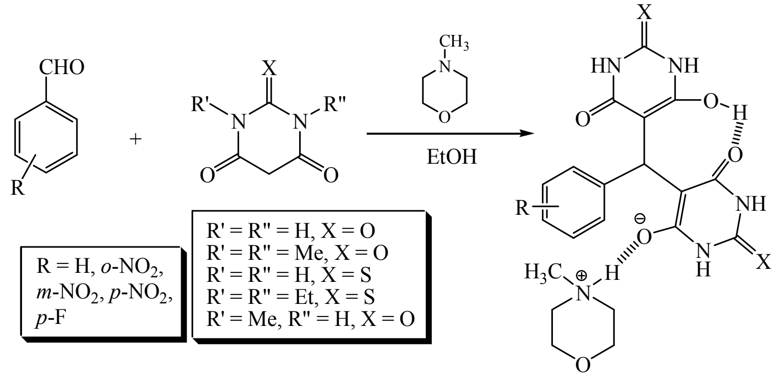
Some quinoline and pyridine bis-barbiturates involving anticancer effect have been reported by Neumann *et al.* and appeared as enolic and zwitterionic form [1]. Based on these concepts, we have developed the synthesis of various bis (thio) barbiturates in the presence of different bases. Many of these compounds exhibit an intramolecular hydrogen bond [2].

In this research, the reaction of (thio) barbituric acids with various aldehydes in the presence of *N*-methyl morpholine produced bis (thio) barbiturates in the ratio of 1:2 at room temperature. These compounds show an eight-membered intramolecular hydrogen bond and also an intermolecular hydrogen bond with *N*-methymorpholin moiety. This project presented the synthesize of new derivatives of bis (thio) barbiturates that we expected having anticancer properties.



Scheme 1

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Synthesis of multi-agent imidazolidine-2,4-diones via an one-pot accumulation method

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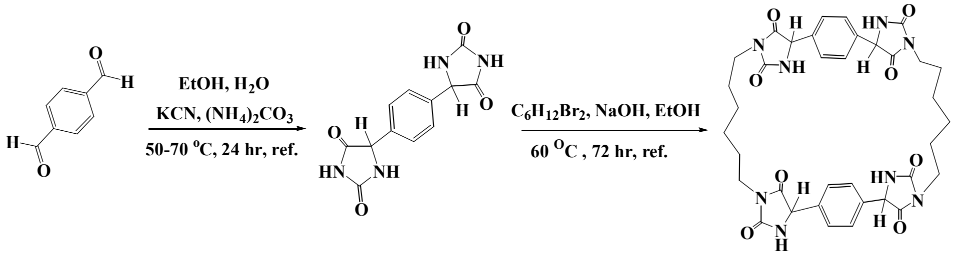
The *bis*-hydantoin compounds are expected to be capable of double therapeutic behavior as *bis*-drugs. Since a wide range of *bis*-heterocyclic compounds have been reported to display superior pharmaceutical and therapeutically activities than their *mono*-heterocyclic counterparts, in this study we decided to prepare some novel multi-agent hydantoins [1-4]. A basic and modified Bucherer Burge's method was applied for synthesis of some 5,5′-substituted mono and bis-imidazolidine-2,4-diones (hydantoins) starting with aldehyde and ketone derivatives [5-7]. In elevated work, the 5,5′-(1,4-Phenylene)bis(imidazolidine-2,4-dione) resulted a new *N*3, *N*′3-substituted tetrakis-hydantoin with alkyl-phenyl linkages throw a versatile one-pot double alkylation route. Synthesis of this compound that has not to our knowledge been previously reported in the literature can be a way toward *multi*-drugs (Scheme 1).



Scheme 1

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An convenient one-pot method for synthesis of symmetrical trithiocarbonates in the presence of KF

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Organic trithiocarbonates are attractive targets due to their high remarkable industrial, synthesis, and medicinal applications [1]. The limited routes for the synthesis of trithiocarbonates which include reactions of thiols with thiophosgene, chlorodithioformates, or with CS_2 and alkyl halides under basic conditions [2]. One of the methods for the synthesis of trithiocarbonates is in situ generated trithiocarbonate anion in the reaction of CS_2 with Cs_2CO_3, KF/Al_2O_3, *n*Bu_4NOH, K_3PO_4, and so forth [3-5].

Here, we report a simple and convenient one-pot synthesis of the title compounds using alkyl halides derivative were treated with CS_2 in the presence of KF at room temperature to generate trithiocarbonate. Good to high yields of thrithiocarbonates are obtained under mild reaction conditions with easy work-up and short time (Scheme 1).

Scheme 1

References:

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Dolomite as an efficient heterogeneous catalyst for the synthesis of 2,3-dihydro-4(1*H*)-quinazolinones

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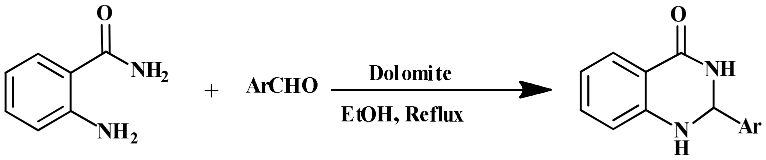
2,3-Dihydro-2-aryl-4(1H)-quinazolinones are a class of fused heterocycles that have drawn much attention due to their potential biological and pharmaceutical activities as anti-tumor, diuretic, and herbicidal agents, as well as plant growth regulators [1]. Many classical methods for the construction of 2,3-dihydro-2-aryl-4(1H)-quinazolinones were reported in the literature [2]. The most common approach for the preparation of 2,3-dihydro-2-aryl-4(1H)-quinazolinones involves condensation of 2-aminobenzamides with aldehydes, acid chlorides, or orthoesters in the presence of various catalysts [3].

Recently, carrying out of the organic reactions with heterogeneous catalysts have been attracted much interest because of their advantages such as cleaner reaction, easy work-up and high selectivity[4]. The advantages of these catalysts encouraged us to the synthesis of 2-aryl-2,3-dihydro-4(1*H*)-quinazolinones via condensation of 2-aminobenzamide with aromatic aldehydes in the presence of a catalytic amounts Dolomite (Scheme 1).



Scheme 1

References:

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Synthesis of diethyl 1,2-dicyano-3-(alkyl-) arylcyclopropane-1,2-dicarboxylate using ethyl cyanoacetate

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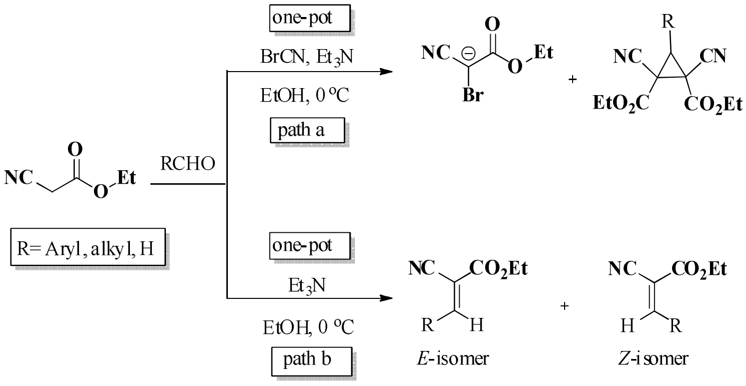
A new, fast and easy method for one-pot reaction of aromatic, Aliphatic aldehydes and dialdehydes with Ethyl cyanoacetate and cyanogen bromide has been developed to afford full substituted 3-arylcyclopropane-1,2-dicarbonitriles-1,2-dicarboxylates in excellent yields in very short time (about 5 seconds) [1-2].

Reaction of Ethylcyanoacetate with cyanogen bromide and various aldehydes in the presence of Et3N afforded 3-arylcyclopropane-1,2-dicarbonitriles-1,2-dicarboxylates at the range of 0 °C to room temperature. All structures was elucidated by ^{1}H, ^{13}C NMR and FT-IR spectroscopy techniques (Scheme 1).



Scheme 1

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Investigation of the reduction reaction of 3-aryl and/or alkyl cyclopropane-1,1,2,2-tetra carbonitrile

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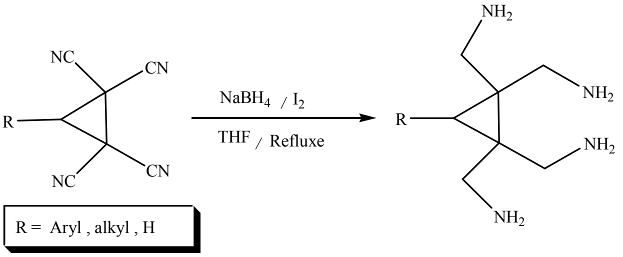
Nitrile hydrogenation is an important method to obtain amines. The most commonly used approaches in nitriles hydrogenation are using strong hydride donors such as lithium aluminum hydride or catalytic hydrogenation. Transforming nitriles to primary amines with high selectivity and yields has become an important field to chemist [1]. Except for a few examples KBH_4 or $NaBH_4$ alone generally could not reduce nitriles to amines. The reducing ability of $NaBH_4$ could be enhanced by introducing I_2 and other special additives for the reaction. Several routes were reported for nitriles [2-4]. Recently, the synthesis of 3-alkyl and/or aryl -1,1,2,2- tetracyano cyclopropanes has been reported in very short reaction time [5].

In this work, a new strategy has been introduced for the preparation of 3-aryl and/or alkyl cyclopropane-1,1,2,2-tetramethaneamines. Reaction with $NaBH_4$, I_2 in THF, reflux under nitrogen gas and then with acid and profits were increasing (Scheme 1).



Scheme 1

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One-pot synthesis of highly substituted imidazoles catalyzed by 2, 4, 6-trichloro-1, 3, 5-triazine

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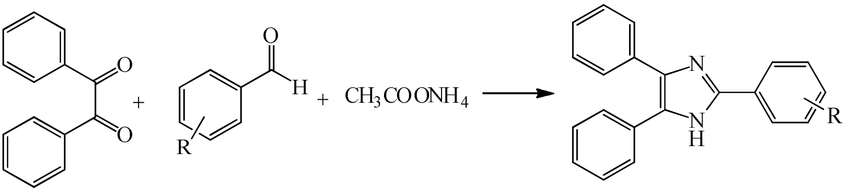
Imidazoles exhibit a wide spectrum of biological activities such as nitric-oxide synthase inhibition, anti-inflammatory, anti-parasitic, antifungal, antidepressant, antitubercular, anticancer and antiviral activities [1].

Therefore, preparation of substituted imidazoles has attracted considerable attention in recent years and numerous methods for their synthesis have been reported [2-3]. Some of these methods are associated with one or more disadvantages such as using expensive reagents, long reaction time, tedious work-up procedures and generation of largeamount of toxicwaste.

Herein, An efficient method for the synthesis of imidazole derivatives by a three-component condensation of benzil, aldehydes and ammonium acetate using 2,4,6-trichloro-1,3,5-triazine under classical heating conditions has been described. The present methodology offers several advantages, such as excellent yields, simple procedures, short reaction times and simple work-up (Scheme 1).



Scheme 1

References:

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Synthesis of hydantoine alkyl acrylate base polymeric bonding agent

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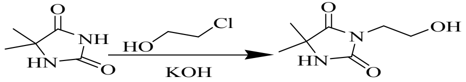
One of the most important methods for increasing the mechanical properties of high solid loading propellant is addition of a bonding agent to propellant formulation. The filler- binder interaction of bonding agent are occurred through adsorbtion of the bonding agent on the surface of filler (oxidizer or energetic filler) and primary covalent bond with matrix binder that is caused to form a coherent and tough polymeric layer around the filler particle. In recent times, studies on the bonding agent have shown that a urea-amide bonding agents have a good interactions with nitramine and perchlorate oxidizer.So, here we introduce a new type of polymeric bonding agents that have a pendant hydantoine group in their polymeric backbone. The new terpolymeric bonding agents are synthesized.

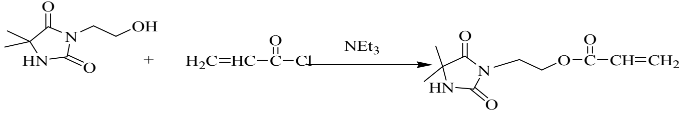
Through radical addition polymerization between 3-(acryloxyethyl)-5, 5-dimethylhydantoin, acrylonitrile and 2-hydroxy ethyl acrylate. Also,The interaction of new bonding agent with ammonium perchlorate and RDX particle have studied by IR spectroscopy [1].

The polymeric bonding agent has synthesized via following methods:

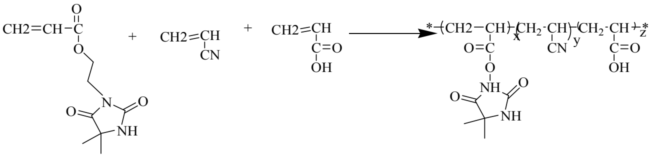
1-Synthesis of 3-hydroxy-5,5-dimethylhydantoine [2].



2-Synthesis of 3-(acryloxyethyl)-5,5-dimethylhydantoine [3].



3-Synthesis of Polymeric bonding agents



Reference:

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One-pot three component synthesis of spiropyrroloqiunoline compound catalyzed by hexamethylenetetramine in water solvent

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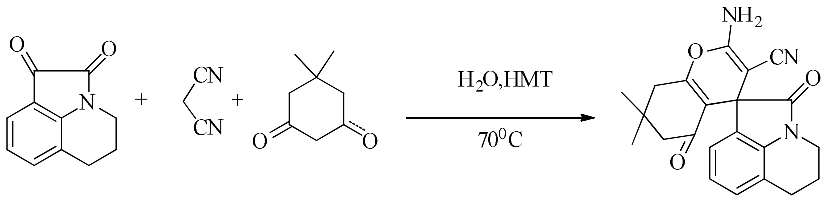
Multicomponent reactions (MCRs) represent a highly valuable synthetic tool for the construction of novel and complex molecular structures because of their environmentally friendly atom economy and high-throughput generation of organic compounds. If such reaction could be run in an innocuous solvent, they would thus comply with most of the green chemistry principles [1]. Spirocyclic systems containing one carbon atom common to two rings are structurally interesting [2]. Over the past few years, Hexamethylenetetramine (HMT) has been shown to be effective, promising and alternative catalyst because of its low price, nontoxicity and stability [3].

Herein, we report HMT-catalyzed three component coupling of 5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinoline-1,2-dione, malononitrile and dimedone for the synthesis of spiropyrroloqiunoline product in water as a green solvent (Scheme 1).



Scheme 1

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A convenient procedure for the direct high-yield glycosylation of ω-functionalized alcohols *via* the use of perpivaloylated sugars

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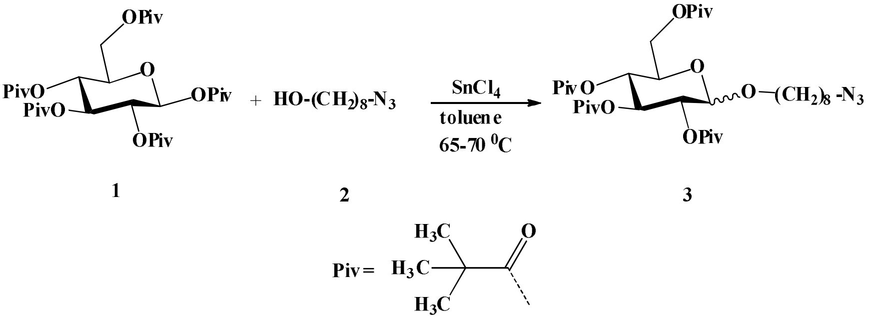
The stereoselective formation of glycosidic bonds is a crucial process in most oligosaccharide and glycoconjugate synthesis [1-2]. A large variety of glycosylation methods has been developed to address the challenges of an efficient (*i.e.* high-yielding, regio- and stereoselective) reaction between a glycosyl donor and glycosyl acceptor [3-4].

In this study, perpivaloylated derivatives of glucose were used. β-Glucose pentapivalate 1, was prepared by triethylamine-catalyzed reaction of glucose with trimethylacetyl chloride in CH_2Cl_2. However, in our hands that procedure primarily lead to the isolation of the thermodynamically more stable α-anomer of glucose pentapivalate. Tin chloride has been shown to be promoter of choice for the glycosylation of ω-azidoalcohol with β-Glucose pentapivalate. Thus, 1 and 2 (1.3 equiv.) were dissolved in dry toluene, and upon addition of $SnCl_4$ the reaction mixture was heated at 65 ^{0}C for overnight. Shorter reaction times lead to an incomplete pivaloylation (Scheme 1).



Scheme 1

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Microwave-assisted efficient synthesis of azlactone derivatives using 2-aminopyridine-functionalized SiO_2 nanoparticles as a catalyst

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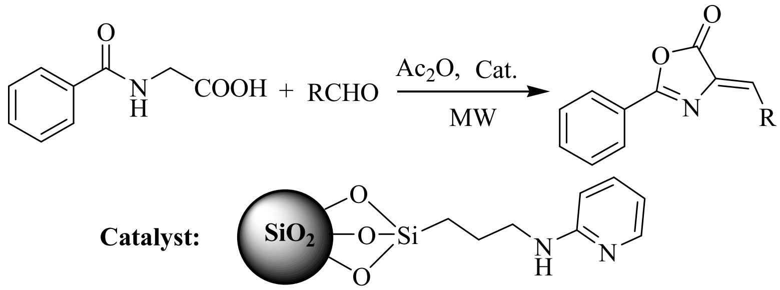
Azalactones, or 2,4-substituted oxazolin-5-ones and their derivatives have been used in a wide variety of reactions as precursors for the synthesis of various bioactive molecules and show a wide range of pharmaceutical properties [1]. They are usually obtained by condensation reactions of different arylaldehydes with hippuric acid in acetic anhydride, in the presence of anhydrous sodium acetate as a basic catalyst, according to the Erlenmeyer method [2]. Although several methods [3-5] for the synthesis of azlactones have been reported, there is still a demand for simple and facile methodologies for the preparation of azlactones using a cheap and readily available catalyst. Nanoparticles-supported catalysts mimic their homogeneous counterparts and can be considered as 'soluble' analogues since they are readily dispersed and exhibit an intrinsically high surface area, attribute that allow excellent accessibility of substrates to the surface bound active catalytic sites.

In the present work, a novel 2-aminopyridine-functionalized SiO_2 nanoparticles was developed as a reusable heterogeneous catalyst for the synthesis of azlactone derivatives from condensation reaction of hippuric acid and aldehydes (Scheme 1). A wide variety of aromatic aldehydes, containing both electron withdrawing and donating substitutes were treated and afforded the corresponding azlactones in good to high yields. Additionally, the catalyst was reused six times without significant degradation in catalytic activity and performance.



Scheme 1

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Rapid, simple and efficient oxidative transformation of thiols to disulfides using $Cu(NO_3)_2.3H_2O$ in $H_2O/AcOEt$

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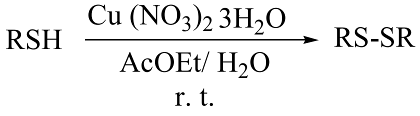
Oxidation of thiols to disulfides without over oxidation is an important process in organic chemistry and biochemistry [1]. Additionally, numerous reagents and catalysts have been applied to oxidize of thiols to disulfides under a range of experimental conditions However, these reagents suffer from disadvantages such as long reaction times, low yields, , toxicity, tedious work-up of products Therefore in this article, a simple and efficient methodology is described for the Therefore in this article, a simple and efficient methodology is described for the preparation of symmetric disulfides from corresponding thiols in the presence of $Cu(NO_3)_2.3H_2O$ and in H_2O/ AcOEt**.** this process is environmentally and economically friendlydue to not using of toxic and expensive reagents.(Scheml).



$$\text{RSH} \xrightarrow[\text{AcOEt/ } H_2O \atop \text{r. t.}]{Cu\ (NO_3)_2\ 3H_2O} \text{RS-SR}$$

Scheme 1

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$FePO_4$ As a green and reusable catalyst for the synthesis of 2-amino-4,6-diphenylpyridine-3-carbonitrile

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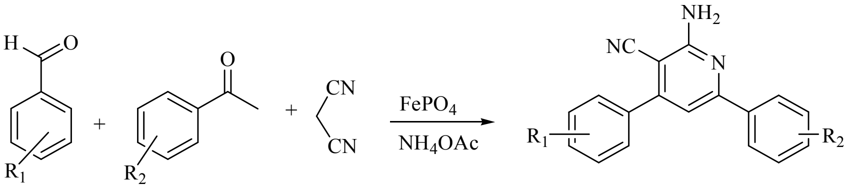
Cyanopyridines have shown an interesting pharmacological and chemotherapeutic activity, such as anticancer, antitubercular, antimicrobial, anticardiovascular, etc. In addition, they have been used as ligands for transitionmetal ions in the formation of complexes, in an IKK-*β*-inhibitor drug [1], and as intermediates for the synthesis of vitamins. Various preparation methods of 2-amino-4,6-diphenylpyridine-3-carbonitrile have been reported such as microwave irradiation [2], ultrasound irradiation, hexadecyldimethyl benzyl ammonium bromide, triethylamine [3], DMF [4], and acetic acid [5]. These reported methods suffered from several drawbacks like prolonged reaction times, low yields and harsh reaction conditions. Therefore, in this work, a new strategy has been introduced for the preparation of 2-amino-4,6-diphenylpyridine-3-carbonitrile via combination of aromatic benzaldehyde, malononitrile and acetophenone in the presence of a catalytic amount $FePO_4$ (Scheme 1).



Scheme 1

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Fe_3O_4@ZrO_2/SO_4^{2-} Nanocatalyst magnetic solid super acid: An efficient and recoverable solid acid catalyst for three component strecker reaction

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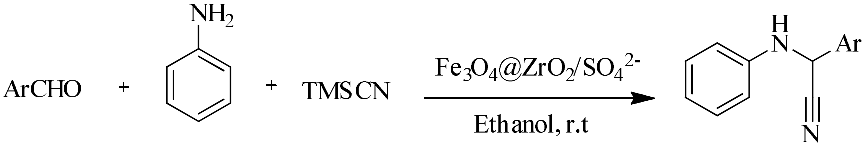
The Strecker reaction, as the first multicomponent reaction [1], provides valuable α-aminonitriles synthons, which are important intermediates for the synthesis of amino acids and nitrogen-containing heterocycles such as thiadiazoles, imidazoles and other biologicallyactive molecules [2].

In this work, a new strategy has been introduced for the preparation of α-amino nitriles.In this regards, Fe_3O_4@ZrO_2/SO_4^{2-} has been synthesized and new applications of this catalyst explored. Therefore a variety of α-amino nitriles have been prepared via combination of aromatic aldehydes, amines and TMSCN in the presence of a catalytic amounts Fe_3O_4@ZrO_2/SO_4^{2-} at room temperature (Scheme 1).



Scheme 1

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Green synthesis of 5,7-dihydroxy-4-methyl coumarine derivatives under solvent-free conditions

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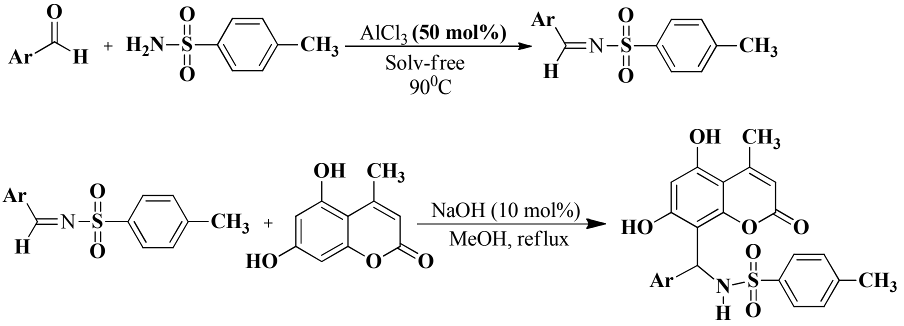
There has been considerable interest in coumarin derivatives, not least because of their value for a variety of industrial, biological, and medicinal chemistry uses. Furthermore, these compounds have shown different pharmacological activities such as anti HIV, antitumor, anticancer, antibacterial, and anti-inflammatory properties [1-3].

According to the more advantages of coumarin derivatives, in this work, a new strategy has been introduced for the preparation of them via the reaction of prepared sulfonimine with 5,7-dihydroxy-4-substituted coumarins in the presence of a catalytic amount of NaOH as a base catalyst at solvent-free conditions.



Scheme 1

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Novel antibacterial silver/ethylene propylene rubber nanocomposites

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Building materials are often defaced and/or adversely affected by bacteria, fungi, molds, algae and other bio-organisms. On another note, nano silver has the potential of being used as a biocide in coated fibrous substrate facers and other construction and/or building substrates. In order to protect against such adversities, we have devised novel formulations of silver nano powder (Ag NP) composites with ethylene propylene rubber (EPR). The Ag NP samples were fabricated through arc discharge with 28nm, 35nm, 55nm, 65nm, 75nm, 85nm, and 100nm average diameters, preliminarily estimated by scanning electron microscopy (SEM). Among them the transmission electron microscopy (TEM) image and X-ray diffraction (XRD) pattern of that with 35nm are shown below which indicate the high purity and good dispersion of the sample. Our DC arc discharge technique involved explosion of movable silver anode and static cathode by a current pulse between 5 to 10A/cm^2. A solution blending method was employed for preparation of Ag NP composites. The Ag NP was first dispersed in toluene using ultrasonic homogenizer and then thoroughly mixed with EPR in the same solvent. Upon fast solvent removal, the dispersed structure of 2 vol% Ag NP in EPR remains. In this article, antibacterial activity against *Staphylococcus aureus* for Ag NP/EPR samples will be compared and contrasted.

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Convenient method for the synthesis of substituted furan-2(5*H*)-one derivatives using ZrP_2O_7 nanoparticles

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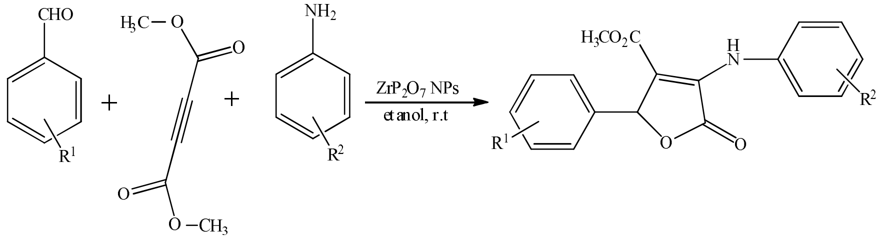
Highly substituted furans play an important role in organic chemistry, not only as key structural units in many natural products, but also as common subunits in pharmaceuticals and biological active compounds [1-3]. Nanoparticles can be utilized as a suitable catalyst in organic reactions due to their high surface-to-volume ratio and coordinated parts which provide a larger number of active sites per unit area in comparison with other catalysts [4].

We wish to report herein a highly efficient procedure for the preparation of 3,4,5-substituted furan-2(5H)-one derivatives from a three-component reaction of aniline derivatives, dialkylacetylenedicarboxylate, and aromatic aldehydes under mild conditions in excellent yields, short reaction times ,easy work-up and environmentally using ZrP_2O_7 nanoparticles (Scheme 1).



Scheme 1

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Synthesis, characterization and crystal structure determination of new bidentate Schiff base ligands derived from 3-ethoxysalicylaldehyde

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The *ortho*-hydroxy Schiff bases derived from the condensation of primary amines with carbonyl compounds are important compounds which show tautomerism via the intramolecular proton transfer from an oxygen atom to the neighboring nitrogen atom. These compounds can exist in three different structures, that is, enol, keto and zwitterionic forms in the solid state. The *ortho*-hydroxy Schiff bases also show thermochromism and photochromism via the intramolecular proton transfer [1, 2].

In this research, we synthesized new bidentate Schiff base ligands by using reaction of 3-ethoxysalicylaldehyde with aniline derivatives in ethanol at room temperature. These ligands were characterized by ^{1}H NMR, IR, UV-Vis and their solid state structures were determined by single crystal X-ray diffraction.

The asymmetric unit of the *Para*-chloro aniline derivative Schiff base ligand, Fig. 1, comprises a potentially bidentate Schiff base ligand. In the crystal structure, intramolecular O–H···N hydrogen bonds make *S*(6) ring motifs. The crystal structure is further stabilized by intermolecular π···π interactions.

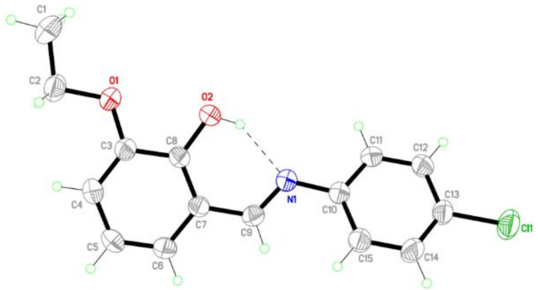

Fig 1

References:

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Efficient and mild synthesis of *N*-substituted pyrroles in the presence of sulfonated multi-walled carbon nanotubes as catalyst in water conditions

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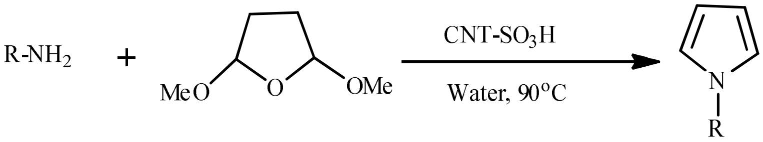
Pyrroles are an important class of compounds with different biological activities [1]. Many methods for the synthesis of diversely substituted pyrroles have been developed [2]. Conjugate addition reactions [3], transition metal-mediated reactions [4] and other multistep operations [5] have been performed for the synthesis of pyrroles. Substitution at nitrogen in the pyrrole has showed the significance of the pyrrole in different biological activities such as antitumor, analgesic, antimycobacterial, antifungal, and anti HIV activities [6].

In this study, we describe a efficient method of synthesis of *N*-substituted pyrroles by treatment of 2,5-dimethoxy tetrahydofuran and various amines in the presence of sulfonated multi-walled carbon nanotubes (0.04 gr) as catalyst in water. In this reaction, pyrroles as products were obtained in excellent yields under green process (Scheme 1).



Scheme 1

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CuI Nanoparticles: A highly active and easily recyclable catalyst for the synthesis of 4,40-(arylmethylene)bis(3-methyl-1H-pyrazol-5-ol) derivatives

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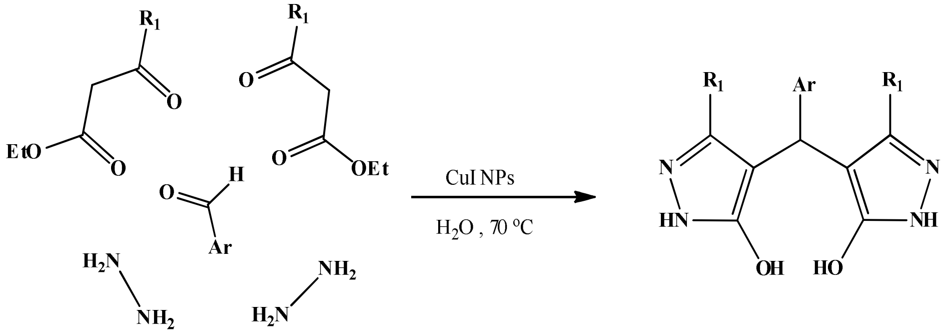
Multicomponent reactions constitute powerful tool to synthesize pyrazole derivatives such as 4,40-(arylmethylene)bis(3-methyl-1H-pyrazol-5-ols) that have a broad spectrum of approved biological activity, being used as anti-inflammatory, antipyretic, gastric secretion stimulatory, antidepressant, antibacterial, and antifilarial agents [1].

Nanoparticles have undergone extensive examination in the past decade. Among various nanoparticles, copper nanoparticles have received considerable attention because of their unique properties and potential application in diverse fields [2].

In this research an efficient synthesis of 4,40-(arylmethylene)bis(3methyl-1H-pyrazol-5-ol)derivatives has been developed via one pot pseudo five component reaction of hydrazine hydrate, ethyl acetoacetate and aldehydes in the presence of CuI nanoparticles in green media.

This present approach offers several advantages such as short reaction time, excellent yields, simple procedure and easy workup.



Scheme 1

References:

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Efficient and selective deoximation catalyzed by a molybdenum glycine Schiff base complex

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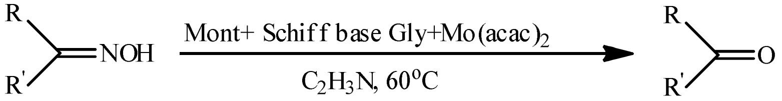
[b] *Faculty of Chemistry, Kharazmi University, Tehran, Iran; E-mail: mahmina_ayoubi@yahoo.com*

Oximes are extensively used for purification and characterization of carbonyl compounds and in the preparation of amides via the Beckmann rearrangement [1]. Their synthesis from noncarbonyl compounds [2] provides an alternative pathway to aldehydes and ketones. Here in, We used a high- yield (70-90%) and selective oxidation procedure for the conversion of oximes with various electron releasing and electron withdrawing substitutions, to corresponding aldehydes and ketones at 60 °C with TBHP and H_2O_2 as oxidant, in the presence of molybdenum complex with Schiff Base Ligand of Glycine Supported on nanolayers of Montmorillonite as catalyst with short reaction times and high yields. The presence of electron releasing and electron withdrawing substituents in ortho or para positions shows that the importance of steric and electronic effects due to high activity of the catalytic systems are lower than expected. The presence of the catalyst seriously affects the deoximation by TBHP and H_2O_2.



R = Aryl
R' = H, Alkyl, Aryl
Scheme 1

References:
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Synthesis of arylidene dihydropyrimidinones using acidic catalysts

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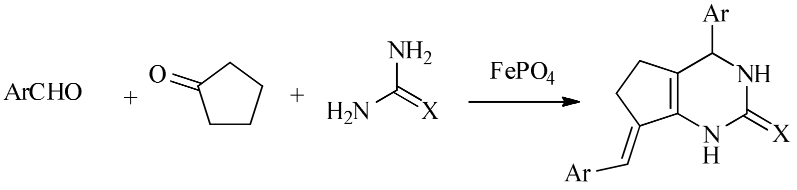
Pyrimidinones are used in various pharmaceutical and biochemical fields [1, 2]. Therefore, an interest for the synthesis of 3, 4-dihydropyrimidin-2(1*H*)-ones (DHPMs) and their derivations is tremendously increasing [3]. One of the most important functionalized pyrimidinones is fused derivatives with an arylidene group. These heterocyclic compounds are significant intermediates for the preparation of many biologically active products. For example, some of them show a broad-spectrum antitumor activity [4]. In most cases, using strong Brönsted acid such as HCl, or base such as sodium alkoxide or potassium hydroxide was necessary for the progression of the reaction [5, 6].

In this communications, we wish to report the synthesis of arylidene dihydropyrimidinones using acidic catalysts in the presence of arylaldehydes, cyclopentanone and urea. Moreover, this approach is known as an important economical and environmentally benign process in synthetic chemistry because it decreases the number of reaction steps, energy consumption and waste (Scheme 1).



Scheme 1

References

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Synthesis of novel quinazolinone derivatives using baclofen as a pharmaceutical γ-amino acid

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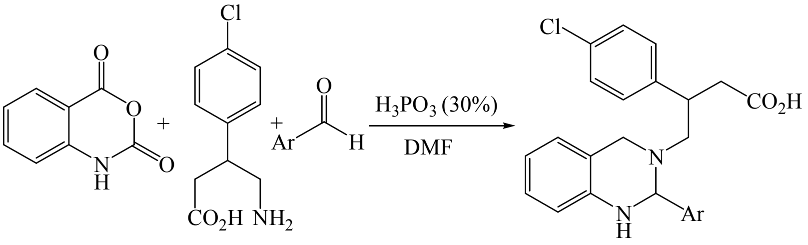
A number of quinazolinones have extended biological activities. The biological activity of these compounds is related to its structure and in some cases insertion of biologically active groups could add its activity. In all reported methods for the synthesis of quinazolinones the three-component reaction of isatoic anhydride, primary amines and aldehydes was used for this synthesis and only the reaction Conditions or the type of Catalyst was changed. In continuation of our research work for the synthesis of biologically active compounds, we wish to report herein three-component reaction of isatoic anhydride, aromatic aldehydes and Baclofene as γ-amino acid in DMF in the presence of Catalytic amount of Phosphorous acid to access the functionalized quinazolinone derivatives. Baclofen is as a drug that primarily used to treat spasticity and it was used at the first time for the synthesis of quinazolinones. The structures of products were determined based on the spectroscopic data. The products have a carboxylic acid which is suitable for further designing of novel sequential reactions based on these products and investigation of their biological activity in progress in our laboratory.



Scheme 1

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Cu/SiO2: A recyclable catalyst for the synthesis of octahydro- quinazolinone

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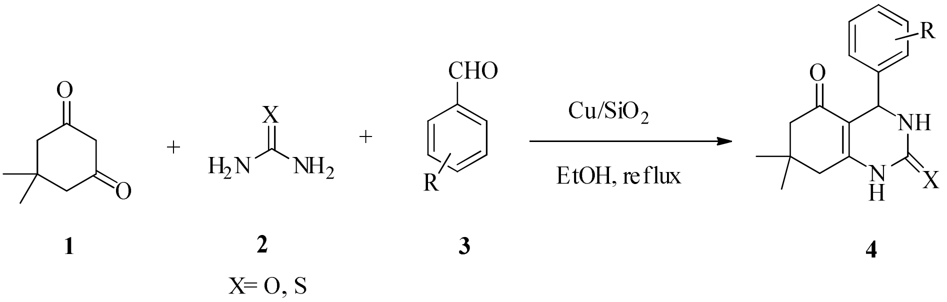
Octahydroquinazolinone derivatives have attracted considerable attention in recent years owing to their potential antibacterial activity against Staphylococcus aureus, Escherichia coli, Pseudomo-nas aeruginosa [1], and also as a calcium antagonist [2]. Synthesis of octahydroquinazolinone derivatives through condensation of dimedone, aldehyde and urea/thiourea using TMSCl has been reported [3].

A simple and one-pot method for the synthesis of octahydroquinazolinone is reported. Cu/SiO_2 in refluxing ethanol catalyzes this three-component condensation reaction to afford the corresponding quinazolinones in good yields. The short reaction time, simple work-up and isolation of the products in high yields with high purities and recyclability catalyst make this approach feasible and attractive for the generation of octahydroquinazolinone libraries (Scheme 1).



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Synthesis of 5*H*-pyrido[2',1':2,3]imidazo[4,5-*b*]indole skeleton *via* copper catalyzed intramolecular C-N coupling

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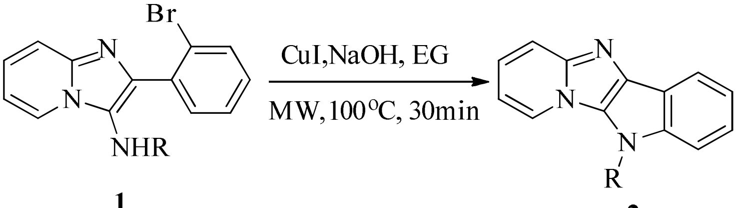
N-heterocycles are widely used as biological and medicinal compounds. They are also used in the plastics industry, for photography, as sensitizers and developers, and in the dye industry. Therefore, the synthesis of *N*-heterocyclic compounds has attracted much attention [1]. In recent years use of copper-catalyzed C-N couplings for formation of different heterocyclic and polycyclic compounds has attracted much attention and combining this with multicomponent reactions (MCRs) has led to many complex new structures.[2]

In this work substrates of type compound **1** are prepared via three component reaction of a suitable N-nucleophile with an aldehyde and an isocyanide (groebke type reaction) and then treated with copper (I) iodide, ethylene glycol and NaOH as a base to give compounds of type **2**.



1 **2**

Scheme 1

Ethylene glycol (EG) has been used as a ligand in several copper-catalyzed cross couplings of different N-nucleophiles with aryl halides [3]. In this reaction it acts both as a ligand for copper and a solvent for the reaction. Low amounts of copper source (5 mol%), use of NaOH as a low cost, efficient, inorganic base, recyclability of the catalyst and short reaction times are benefits of this protocol.

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Alkylation of amidic nitrogen of benzothiazinones on KF/Alumina in Ball Mill

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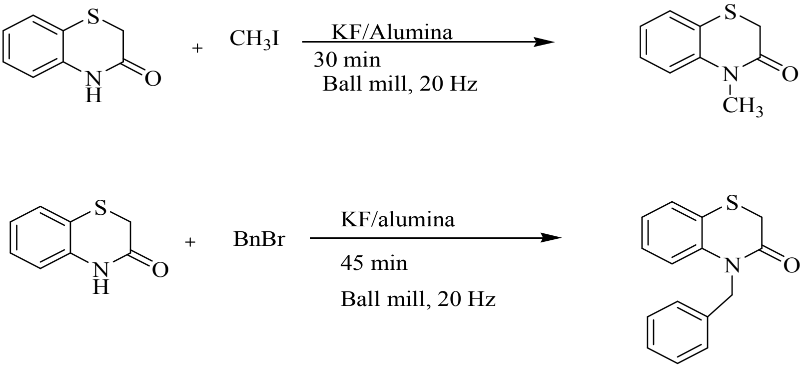
Benzothiazinones are very important group of heterocyclic compounds that have many applications in both pharmaceutical & industrial research [1].

Alkylation of Amidic nitrogen in benzothiazinones is a well-known method in synthesis of different derivatives of this compound. The obtained product can be used in the synthesis of many compounds of biological and pharmaceutical importance [2].

In a typical procedure one can reach the product by heating the reagents for long times using non-green solvents. Using k_2co_3 as a base and acetone as a solvent and heating in 50-60°C for 24h the yield is 70% [3].

In this project, a new strategy has been introduced for the preparation of 1, 4-benzo thiazine-3-one. we have developed an easy and cost-free procedure by omitting the solvent and temperature and lowering the reaction time to 30-45 minutes and all of the rules of green chemistry are preserved.

Using KF/Alumina as a base and ball milling the substrates in room temperature, the amidic nitrogen in 1, 4-benzo thiazine-3-one is alkylated (with methyl iodide or benzyl bromide) in 30 minutes and the yield is 100% **(**Scheme 1**).**



Scheme 1

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Synthesis of pyranochromenes through the addition of 4-hydroxycoumarin to α,β-unsaturated ketones in molten [Et_3NH][HSO_4]

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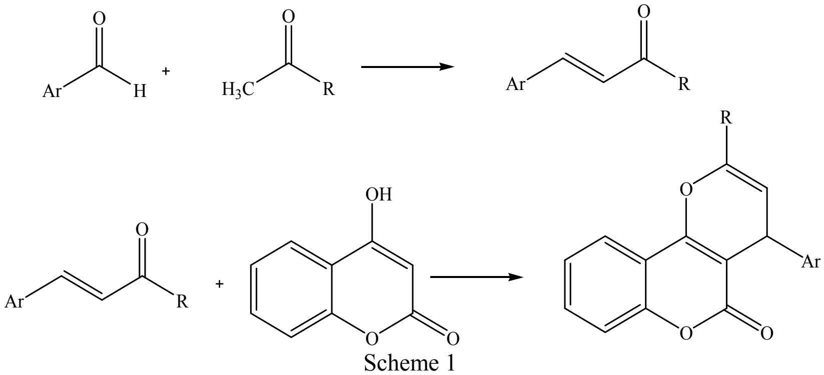
Ionic liquids have attracted considerable interest as environmentally friendly or ‘‘green’’ alternatives to conventional molecular organic solvents because they have very low vapor pressure and are non-explosive and thermally stable in a wide temperature range. Triethylammonium sulfate [Et_3NH][HSO_4] is a simple ammonium ionic liquids, air and water stable, easy to prepare from amine and acid, and relatively cheap[1]. The Michael addition was considered as one of the most powerful and efficient methods for C–C bond formation in organic synthesis. Particularly, the addition of 4-hydroxycoumarin to α,β-unsaturated ketones is a straightforward method to access S-warfarin which is an effective and relatively safe agent for preventing thrombosis and embolism [2].

Due to extending our interest in the development of practical, safe, and environmentally friendly procedures for several important organic transformations [3], herein, we report the conjugate addition of 4-hydroxycoumarin to α,β-unsaturated ketones catalyzed by [Et_3NH][HSO_4] ionic liquid.

Initially, [Et_3NH][HSO_4] ionic liquid has been synthesized. Then α,β-unsaturated ketones have been synthesized through aldol condensation and at the second step 4-hydroxycoumarin has been reacted with them in [Et_3NH][HSO_4] ionic liquid to produce corresponding pyranochromenes (Scheme 1).



Scheme 1

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Using cyclic α-halo ketone for the synthesis of indenopyridines containing densly pyrazole or uracil via three and four component reaction

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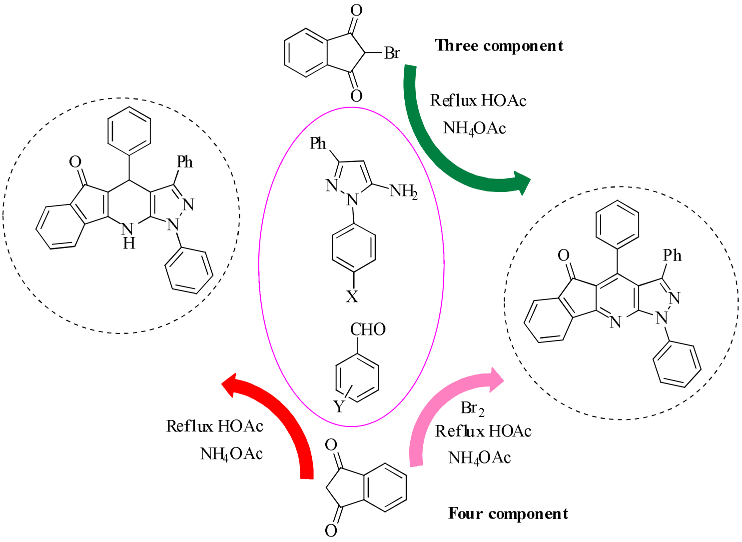
Pyrazole derivatives have gained more attention in recent years for biological [1], medicinal [2] and agricultural [3] reasons. These compounds have been reported to possess a wide spectrum of biologic activities like anti-hyperglycemic, analgesic, anti-inflammatory, antipyretic, antibacterial, hypoglycemic, sedative-hypnotic properties [4]. Pyrazolopyridines are one of important category in pyrazolo fused compound. These compound have been interest due to their wide range of biological and pharmacological properties such as possible antiviral agent, potent p38 kinase inhibitors, HIV reverse transcriptase inhibitors [5].

In this work, a new strategy has been introduced for the preparation of Pyrazolopyridines. we investigated an efficient synthesis of new indenopyridines containing pyrazoles moitly via the three-component reaction of 1,3-diphenyl-1*H*-pyrazol-5-amines, aldehydes and 2-bromo-1*H*-indene-1,3(2*H*)-dione (Scheme 1).



Scheme 1

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Asymmetric synthesis of L-carnitine

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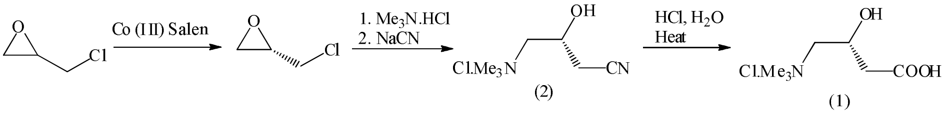
In this research, a practical chemical synthesis of L-carnitine (1) has been accomplished.

Enantiopure isomer of epichlorohydrin was utilized as a chiral starting material to prepare the key intermediate 2. The promising points for the presented methodology are reduction of steps, efficiency, generality, high yields, relatively short reactiontimes, cleaner reaction profile and simplicity.



Scheme 1

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N, N, N-Triphenylselenoisocyanuric acid (NTPSICA): a new electrophilic selenium-containing reagent and its application in direct aldehyde and ketone α-Selenenylation reactions promoted by *L*-prolinamide organocatalysts

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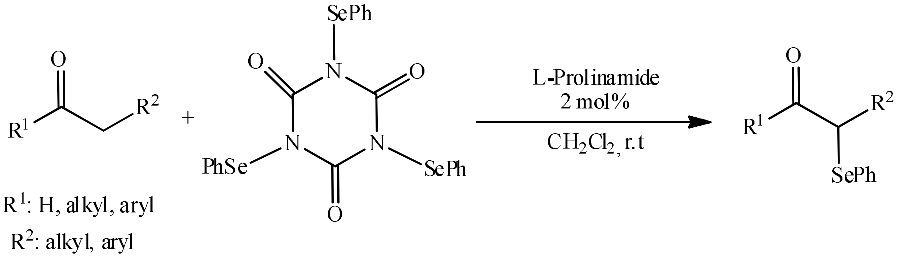
α-Selenylated carbonyl compounds are of great significance in organic synthesis due to the ease in which they are converted to synthetically valuable motifs such as α,β- unsaturated carbonyl compounds, terminal aziridines, α-hydroxy esters, allylic amines, α-amino acids[1]. The most common sources of the PhSe$^+$species are: phenylselenenyl chloride(PhSeCl), phenylselenenylbromide(PhSeBr), diphenyldiselenide(PhSeSePh) and phenylselenocyanate (PhSeCN), (NPSP), (NPSS). These reagents are used directly, as carriers of the electrophilic phenylseleno species (PhSe+), or they are combined with other reagents, to generate in situ electrophilic selenenylatingagents [2].

Here, recently we introduced a novel electrophilic phenylselenenylating reagent, *N,N,N*-triphenylselenoisocyanuric acid (NTPSICA) which is air- and moisture-stable and easily prepared in our laboratory. This reagent was able to react with a series of electron-rich organic molecules such as alkenes, aldehydes and ketones [3 – 4].This reagent was used for α-selenenylation of various aldehydes and ketones mediated by an organocatalyst in high yields.



Scheme 1

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High yield synthesis of mixed 2,6-bis(benzylidene)– cyclohexanone derivatives

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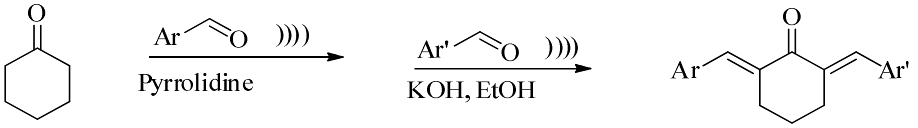
Mixed diarylidenes of cycloalkanones have been reported to have antiinflammatory, analgesic and antipyretie properties [1]. Some of these compounds also possess bactericidal, antifungal and insecticidal activities and some others are reported to be antimutagenic [2].

In this study, a one-pot reaction causes combination of cyclohexsanon and two different aldehydes catalyzed in a solvent-free environment. The first aldehyde is added to the ketone in the presence of by pyrrolidine and then the second one reacts with the *in situ* formed monobenzylidene using potassiom hydroxid to give the final product. Reactions were carried out under ultrasonic irradiation (Scheme 1).



Scheme 1

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Solvent-free synthesis and antibacterial activity of novel sulfonamides derived from p-anisidine

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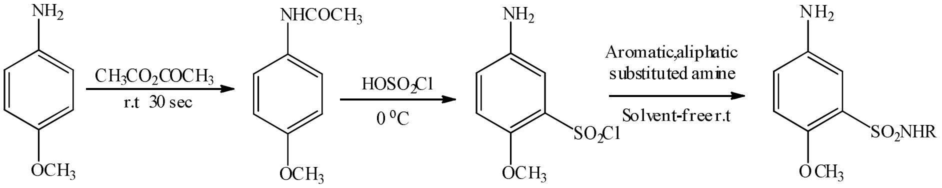
Sulfonamides are a diverse group of pharmaceutically important compounds widely used as, anticancer, anticonvulsant, antiinflammatory and antiviral agents and HIV protease inhibitors [1,2]. The most usual routes to the vast majority of Sulfonamides involve the reaction of an appropriatesulfonyl chloride with primaryor secondary aromatic or aliphatic amine in the solvent-free method [3]. Due to importance of sulfonamides in medical compounds, in this project, new sulfonamides derivatives have been synthesized from *p*-anisidine under solvent-free conditions and their antibacterial properties have been studied (Scheme 1). *N*-(4-Methoxy phenyl) acetamide was prepared by acetic anhydride as an acylation agent with in a simple procedure. It was sulfonated with chlorosulfonic acid as sulfonating agent. Resulting sulfonyl chloride was reacted with various amines in a mild and green and under solvent-free conditions in the presence of sodium hydrogen carbonate to produce sulfonamides. The products were characterized with IR, ^{1}H NMR and ^{13}C NMR methods. All the compounds were screened for their antibacterial activities against Escherichia coli (gram negative) and Staphylococcus (gram positive). N-(4-methyl-3-phenethylsulfamoyl-phenyl)-acetamide, was found to be the most potent compounds against all the tested strains.



Scheme 1

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Efficient synthesis of chiral α-amino alcohols

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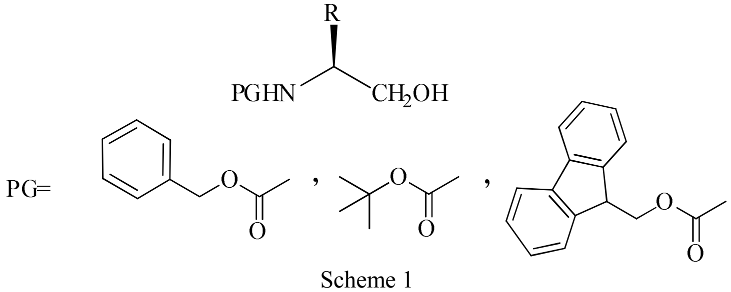
The chiral α-amino alcohols are as an important starting materials in asymmetric organic synthesis.There are different approaches for the synthesis of these compound through conversion of different functional groups such as carboxylic acids, acyl azides, arylbronic anhydrides, cyanurates and *N*-acylbenzotriazoles to alcohols. In all cases the convertion could be done through reducting agent. With this background and in the continuation of our research work for the synthesis of biologically active and functionalized peptides, we wish to report herein efficient synthesis of chiral amino alcohols using protected amino acids to access the novel peptide contaius amino alcohol moiety in their structure.

To achieve this goal, the reaction sequences were done as follows reaction sequences:

a) Protection of *N*- terminal of amino acids using desired protecting groups (Cbz, Boc and Fmoc)
b) Synthesis of methyl ester of protected amino acids
c) Reduction of ester groups to alcohols using suitable reducing agent

Good yields, high diversity, no racemization of chiral center are adventages of the method. More details will explain in the conference.



Scheme 1

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One-pot three-component synthesis of new tri-substituted imidazole derivatives in the presence of ionic liquid catalyst

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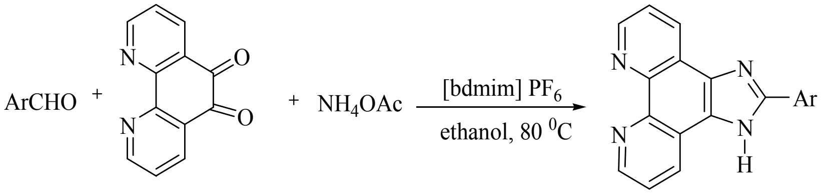
Imidazoles are important class of heterocyclic compounds [1]. Many of the substituted imidazoles were known as inhibitors of p38 MAP kinase, B-Raf kinase, herbicides, fungicides, therapeutic agents, pesticides, plant growth regulators, nitric oxide synthase and cytotoxic activities [2,3].

Imidazoles are found in biological structures, natural products and pharmaceuticals. These compounds are anti-bacterial, anti-tumor, anti-TB, anti-inflamatory, anti-allergic, analgesic and glucagon receptors [1,2,4]. Omoprazole, Pimobendan, Losartan, Olmesartan, Eprosartan and Trifenagrel are some of the leading drugs in the market with diverse functionalization around the imidazole motif [2].

In respect to our continued studies in the synthesis of heterocyclic compounds [5], an efficient procedure for the synthesis of new tri-substituted imidazole derivatives from 1, 10-phenanthroline-5, 6–dione, aldehyde and ammonium acetate in refluxing ethanol and using acidic ionic liquid catalyst was developed (Scheme 1). The desired 2-aryl-1*H*-imidazo [4, 5-f] [1, 10] phenantrolines were synthesized in low reaction times and reasonable yields.



Scheme 1

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Synthesis of nano phosphorus ylide from fullerene

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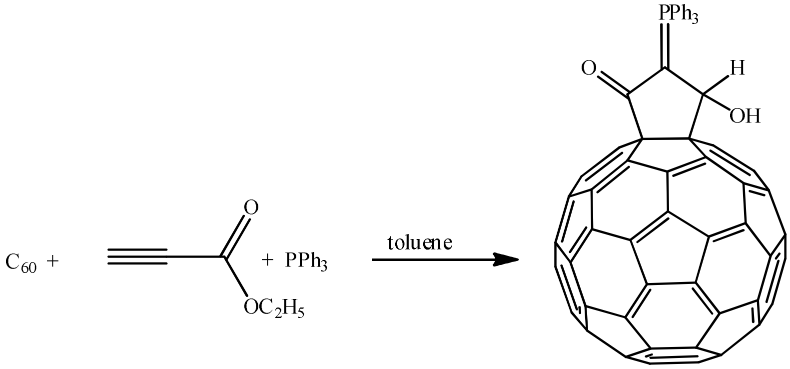
Nanotechnology has penetrated many fields of pharmaceuticals which perhaps the most important result is the compatibility of new drug delivery. Chemical functionalization of fullerenes has attracted much attention for application in material science and biochemistry. In addition, many organic phosphorus compounds are important and well-known biologically active species. Exposure to phosphorus fullerene derivatives are expected to provide interesting activities in biological systems. According to the investigation, the similar synthesized compounds to the resulting product (a) show promising biological activities such as anti-HIV [1], DNA cleavage [2], and cytotoxicity [3]. Here is a method for the synthesis of new derivatives of fullerenes by reaction with C60 and ethyl acetylene in the presence of triphenylphosphine. In this reaction, The main product of this reaction is a phosphorus ylide which attached to the fullerene surface. The effects of various parameters like temperature at optimum conditions were investigated. We used from silica gel column chromatography for separating our main product from other side compounds. The structure of the product has been determined through different spectroscopic methods such as UV, IR, ^{1}HNMR, ^{13}CNMR, ^{31}PNMR.



Scheme 1

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Single-step synthesis of benzimidazoles using magnetic nanoparticle KF/Fe_3O_4 as catalyst

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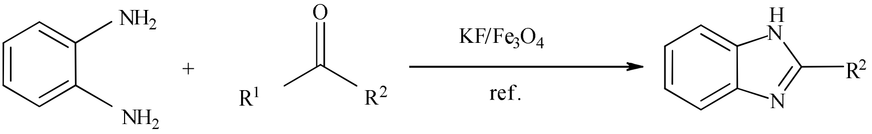
Benzimidazoles are present in various bioactive compounds possessing antiviral, antihypertension and anticancer properties [1,2]. Compounds possessing the benzimidazole moiety express significant activity against several viruses such as HIV [3], Herpes (HSV-1) [4] and influenza [5]. Bisbenzimidazole is DNA-minor grove binding agents possessing anti-tumour activity [6].

In this work, a new strategy has been introduced for the preparation of benzimidazoles. In this regards, magnetic nanoparticle KF/Fe_3O_4 has been synthesized. Therefore a variety of benzimidazoles have been prepared via combination of aldehydes and ketones, 1,2-phenylenediamine in the presence of a catalytic amounts of KF/Fe_3O_4 in reflux (Scheme 1).



R^1, R^2 = alkyl, aryl

Scheme 1

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The triazine-based azo-azomethine dyes; synthesis, biological properties and solvatochromism

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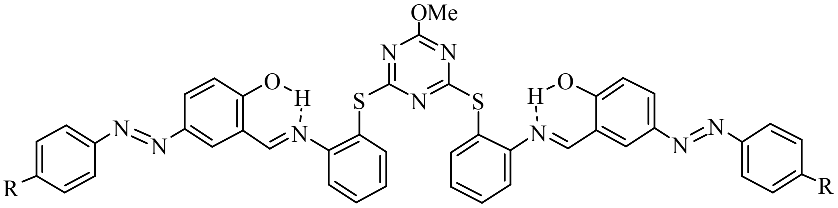
The macrocyclic azo-azomethine dyes 2,2'-((2,2'-(6-methoxy-1,3,5-triazine-2,4-diyl)bis (sulfanediyl)bis(2,1-phenylene))bis(azan-1-yl-1-ylidene)bis(methan-1-yl-1-ylidene)) bis(4-phenyl diazenyl)phenol) and its substituted derivatives were synthesized and characterized by elemental analysis, mass, FT-IR, UV, ^1H and ^{13}C NMR spectroscopy. The solvatochromism of dyes was evaluated in various solvents. The newly synthesized compounds are explained on a basis of positive solvatochromism behavior of compounds due to intramolecular hydrogen bond in enol–ketotautomeric and dipole moment changes. All the compounds were then evaluated for their antibacterial and antioxidant activity. The results show that synthesized compounds did not exhibit any remarkable antibacterial activity. But, they are having electron donating group showed moderate antioxidant activities.



Scheme 1

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Study of reaction between 4-chloro phenol, acetylenic esters and Pph_3, $Asph_3$, $Sbph_3$

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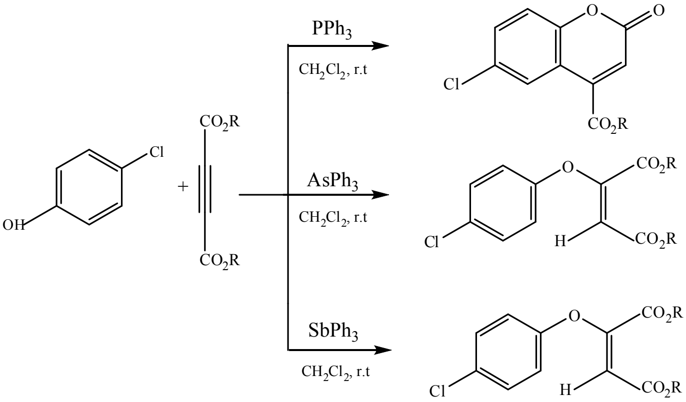
Multi-component reactions (MCRs) are important for generating high levels of diversity, as they allow more than two building blocks to be combined in a practical, time-saving, one-pot operation, giving rise to complex structures by simultaneous formation of two or more bonds [1]. MCRs contribute to the requirements of an environmentally friendly process by reducing the number of synthetic steps, energy consumption, and waste production [2,3]. In this work we reported that the three component reaction between triphenylphosphine, triphenylarsine and triphenylantimonywith acetylenic esters and 4-chloro phenol.



Scheme 1

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Synthesis of imines and Schiff bases using nano BF_3/SiO_2 under mild conditions

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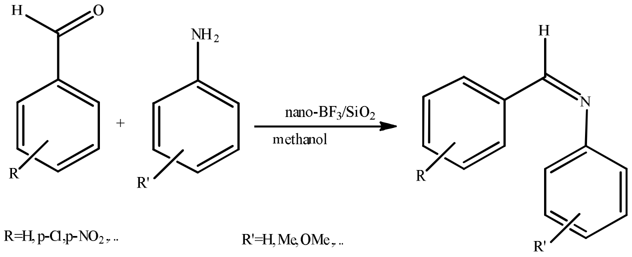
Schiff base ligands, as variety of compounds with imine group, have gained importance because of physiological and pharmacological activities associated with them. They constitute an interesting class of chelating agents capable of coordination metal ions given complex, which serves as models for biological system[1]. Schiff-bases and their metal complexes exhibited important function as catalysts in various biological systems, and they were also considered as active materials used in polymerization, functional dyes ,pigment and medicinal fields[2] . Especially, Schiff-base derivatives were extensively used in research on antimicrobial activity, and so much reported works had been reviewed [3,4]

In this study, BF_3/SiO_2 is found to catalyze Schiff-bases from the reaction of aldehyde compounds with amines efficiently using methanol as solvent. Simple work up, high yield products and short reaction time are some advantages.



Scheme 1

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A simple and convenient approach to the synthesis of 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile derivatives *via* a multi-component reaction with ZrP_2O_7 nanoparticles as catalyst

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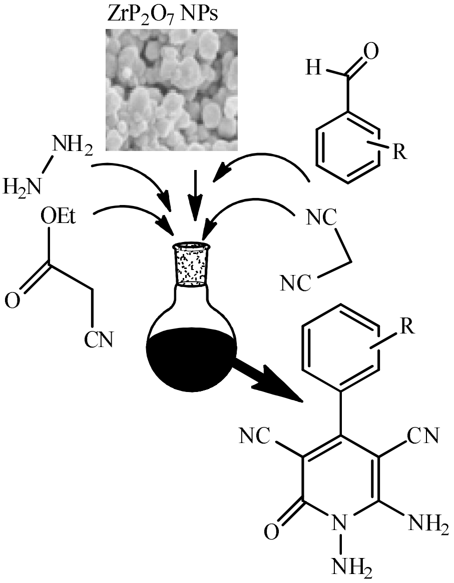
Among a large diversity of heterocyclic compounds, 2-pyridone derivatives are valuable building blocks in natural products synthesis and pharmaceuticals [1-2]. Therefore, the development of simple strategies for the synthesis of 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile derivatives is hot topic of organic chemistry. In recent years, nanoparticles have received considerable attraction in organic reactions [3].

We report herein the synthesis of 1,6-diamino-2-oxo-4-phenyl-1,2-dihydropyridine-3,5-dicarbonitrile derivatives using a four component one pot protocol under mild conditions in the presence of ZrP_2O_7 nanoparticles (Scheme 1).



Scheme 1

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Fe_3O_4@ZrO_2/SO_4^{2-} Nanocatalyst magnetic solid super acid for the synthesis of ß -amino ketones in Mannich reaction

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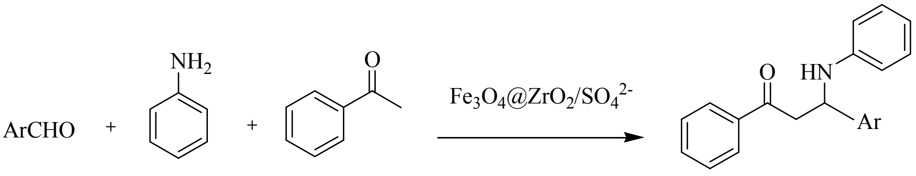
Mannich reaction is a one of the best method in synthesis of ß-amino carbonyl.This reaction is a kind of MCRs that includes three-component reaction of an aldehyde, an amine and a ketone for the preparation of ß-amino carbonyl [1]. ß-amino carbonyl compounds are significant synthesis intermediates for synthesis of natural and pharmacological and biological products [2].

In this work, a new strategy has been introduced for the preparation of ß-amino carbonyl compounds. In this regards, Fe_3O_4@ZrO_2/SO_4^{2-} has been synthesized and new applications of this catalyst explored. Therefore a variety of ß-amino carbonyl have been prepared via combination of aromatic aldehydes, aniline and acetophenone in the presence of a catalytic amounts Fe_3O_4@ZrO_2/SO_4^{2-} at 60 ^{0}C in solvent-free conditions (Scheme 1).



Scheme 1

References:

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A green synthesis of nitrones from diamino glyoxime using pyridine aldehydes

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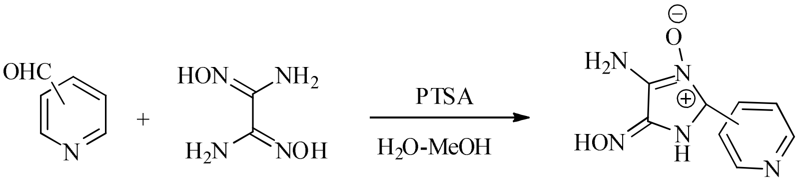
Nitrones as the 1,3-dipolar species are valuable intermediates in organic synthesis[1]. Thermal cycloaddition reactions of nitrones with multiple bond systems is an efficient strategy for providing various heterocyclic five-membered ring systems [2-3].

The reaction of diamino glyoxime with pyridine aldehydes in the presence of *p*-toluene sulphonic acid in H_2O/MeOH mixture at room temperature afforded nitrone derivatives in high yields within 20-100 min (Scheme 1). The nature of solvent and catalyst were evaluated and it was found that the reaction could be performed using strong acids such as H_2SO_4 and HCl in CH_3OH as a protic solvent. The products were characterized by ^{1}H NMR, ^{13}C NMR and IR spectroscopes. The effect of temperature on stability of the products structural isomers has been studied by NMR as well. The results showed that, only one product was observed at high temperatures. The remarkable advantages of this method are the green procedure, short reaction times and high yields.



Scheme 1

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Green synthesis of functionalized 4*H*-chromenes *via* three-component reactions catalyzed by proline

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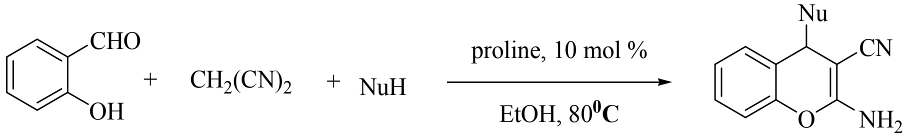
Three-component reactions of salicylaldehyde, malononitrile and a sulfur, carbon, or nitrogen-based nucleophiles were developed, by using proline as a catalyst, which generated various substituted 4*H*-chromene derivatives in good yields. The reactions were performed in ethanol under mild and metal-free conditions. In these reactions, the use of proline as a catalyst was proven to be key for rendering the reactions possible because applying other acid or base catalysts instead of proline resulted in generation of several side products. Many nucleophiles, such as secondary amines, indoles, thiophenols, mercaptans, cyanide and azide were applied at this condition. The current green protocol depends on the nature of the nucleophile used in the reaction (Scheme 1).



Scheme 1

References:

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Polyaniline hybrid nanocomposites with copper oxide nanoparticles: synthesis, characterization and investigation of their physical properties

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Nanocomposites are special class of materials having unique physical properties and wide applications potential in diverse areas. The polymer nanocomposites have attracted great interest owing to their novel properties derived from the successful combination of the characteristics of parent constituents into a single material [1]. Conducting polymers such as polyaniline (PANI) and polypyrrole are becoming increasingly important for their technological importance due to their electrical, optical properties and their high air, chemical and electrical stability at ambient conditions and in field effect transistors [2,3]. Copper oxide (CuO) is a monoclinic n-type semiconductor with narrow band gap energy of 1.5–1.8 eV, and it has very large excitation binding energy (60 meV) at room temperature [4].

In this research work, a serious of PANI/CuO nanocomposites were fabricated by chemical oxidative polymerization method of aniline with various amounts of CuO nanoparticles in the presence of $(NH_4)_2S_2O_8$ as an oxidant at 0°C. Physical properties of nanocomposites were characterized and analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FTIR), and UV-Vis spectroscopy. Structural analysis showed that the crystal structure of CuO was not disturbed in the PANI/CuO hybrid nanocomposites. Surface morphology study showed the uniform distribution of CuO nanoparticles in PANI matrix. FTIR and UV-Visible studies confirmed the presence of polyaniline in emeraldine base form in the nanocomposites and suggested incorporation of CuO in polymer. Four probe point electrical resistivity measurements of nanocomposites revealed that the resistivity of PANI increases with increasing content of CuO nanoparticles.

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Control of pore structure formation in PEBAX membrane by phase inversion method

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Polymer-based membrane for gas separation processes in gas and petrochemical industrial are in developing stages. Polyamide-6-b-ethylene oxide (PEBAX) which consists of a regular linear chain of rigid polyamide segments interspaced with flexible polyether segments has been the best candidate for membrane application. It has been shown that the performance of PEBAX membranes is significantly affected by the pore structure of these membranes. These membranes are commonly formed through a process known as phase inversion method which induces an anisotropic structure. In this work, the effect of different solvents on the pore structure formation in PEBAX membrane was investigated. A series of membranes were produced using butanol, propanol, formic acid, DMAC, and water/ethanol as solvent [1]. Water/ethanol (30:70) was found to be the best solvent to prepare defect free structure PEBAX membrane. Thus, the effect of variables including polymeric solution temperature and concentration (by changing PEBAX weight percentage from 1 to 3 by 0.5 wt% interval) and also the temperature of surrounding environment (temperature range of 25 to 90 °C and 60 °C was selected) on the physical structure formation within the membrane were investigated. The optimum concentration was found to be 2.5 wt. The effect of the above-mentioned parameters on the pore structure formation of the membrane using XRD and SEM techniques was investigated. Good permselectivity ($\alpha CO_2/CH_4$ =25.103) for these membrane obtained.

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Efficient and selective oxidation of alcohols catalyzed by a molybdenum glycine Schiff base complex

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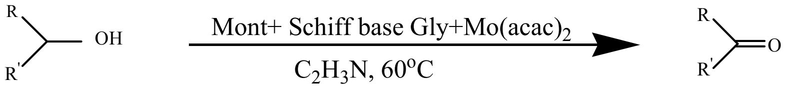
Aldehydes and ketones represent an important class of products and intermediates in the fine chemicals and specialties [1]. The oxidation of alcohols to carbonyl compounds is an important transformation of organic synthesis, and several methods have been explored to accomplish such a conversion [2]. Here in, We used a high- yield (70-90%) and selective oxidation procedure for the conversion of benzylic alcohols with various electron releasing and electron withdrawing substitutions, to corresponding aldehydes and ketones at 60°C with TBHP and H_2O_2 as oxidant, in the presence of Molybdenum complex with Schiff Base Ligand of Glycine Supported on Nanolayers of Montmorillonite as catalyst with short reaction times and high yields. The Presence of electron releasing and electron withdrawing substituents in ortho or para positions shows that the importance of steric and electronic effects due to high activity of the catalytic system are lower than expected. The presence of the catalyst seriously affects the oxidation of alcohols by TBHP and H_2O_2.



R = Aryl
R' = H, Alkyl, Aryl

Scheme 1

References:

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Synthesis of 2,2' arylmethylene bis(3-hydroxy-5,5-dimethyl-2-cyclohexene-1-one) utilizing starch phosphorylase enzyme as an selective and green catalyst

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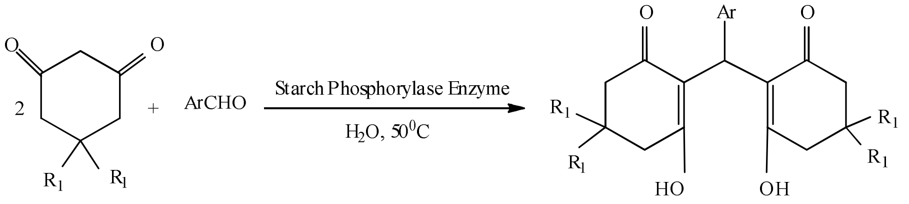
Starch phosphorylase enzyme is an enzyme that can break α(1→4)-glycosidic bond at the end of the starch molecule, producing glucose-1-phosphate and starch chain residue; The reaction can be carried out in reverse order as well, leading a longer starch molecule. Therefore, starch phosphorylase manages a mutual reaction which environmental conditions, particularly the amount of reaction products, affect it. This enzyme is common in plants, while it is more abundant in the cells that produce large amounts of starch, e.g. potato tuber which used in the research. Extraction of starch phosphorylase was done by squashing potato tuber in ice following by heating at 55°C; it was precipitated using ammonium sulfate conducted in a stepwise process. In recent years, polyfunctionalized benzopyrans and their derivatives have attracted strong interest due to their useful biological and pharmacological properties, such as anticoagulant, spasmolytic, diuretic, antianaphylactin, anticancer [1]. In addition, they also constitute a structural unit of a series of natural products and because of the inherent reactivity of the inbuilt pyran ring are versatile synthesis [2].

Interestingly, this structurally complex molecule can be synthesized by a simple one pot tandem reaction between an aldehyde (1 equiv) and dimedone (2 equiv) or cyclohexane-1,3-dione in the presence of a catalyst [3]. However, in the absence of a catalyst and many of unique catalyst the reaction stops just after Knoevenagel type adduct formation, to give an open chain intermediate, 2,2'-aryl/alkyl methylene-bis(3-hydroxy-5,5-dimethyl-2-cyclohexene-1-one (Scheme 1).



Scheme 1

References:

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Polyol-reduction method for the synthesis of ruthenium nanoparticles

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The polyol method is a novel, single-step process for preparing nanostructured materials [1]. It was extended to synthesize ruthenium nanoparticles that exhibit significant activity for ammonia synthesis which is an important process in the petrochemical industry. Ammonia synthesis over Ru-based catalysts is a structure-sensitive reaction depending strongly on ruthenium particle size [2]. In polyol process, the metal precursor(s) are suspended or dissolved in an organic solvent such as ethylene glycol. The resulting mixture is heated under reflux and the metallic moieties precipitated out of solution [3].

In this work, ruthenium nanoparticles were synthesized by $RuCl_3$ reduction by ethylene glycol and deposition on alumina. Well-dispersed and uniform ruthenium nanoparticles with an average diameter of 7 nm were produced as shown by TEM images. It can proceed in two steps: (i) ligand exchange around the Ru^{3+} ions and (ii) reduction of Ru^{3+} to Ru metal (Scheme 1). The concentration of $RuCl_3$ in ethylene glycol and the reduction time were crucial factors that were improved to obtain monodispersed and stable Ru nanoparticles. The catalysts showed good activity in ammonia synthesis (1175 $mmolNH_3/g_{Catalyst}$, h^{-1} at 450 °C, 30 bar and GHSV 2650 h^{-1}).

$$CH_2OH - CH_2OH \rightarrow CH_3CHO + H_2O$$
$$6CH_3CHO + 2Ru^{3+} \rightarrow 2Ru + 6H^+ + 3CH_3COCOCH_3$$

Scheme 1

References:

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Synthesis and characterization of a novel designed cyclophane for the recognition of cyanideion

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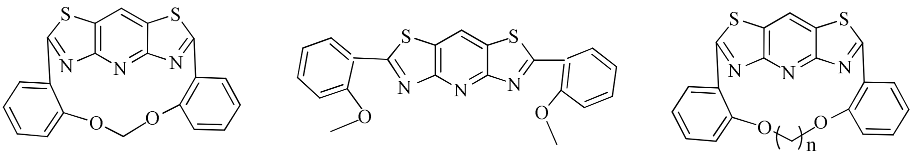
The design and synthesis of cyclophanes possessing rigidly defined cavities and shape-persistent structures attract current interest in view of supramolecular chemistry.[1]

The extreme toxicity of cyanide ion in physiological systems, as well as the continuing environmental concern caused by its widespread industrial use, has led to considerable research into the development of methods for cyanide detection. Optical sensors for cyanide, in which a change in color and/or fluorescence intensity (or emission wavelength) is monitored, have been studied actively over the past ten years due to their simple, inexpensive, and rapid implementation.[2]

Herein we report the design and synthesis of a new cyclophane **1** operating in ‘turn-off-on’modefor selective and sensitive detection of cyanide ions in a water-organic solvent mixture.The sensor **1** is reversible as the emission signal originates from the dynamic equilibration of complex ions.

The sensor **1** can be synthesized under both microwave irradiation and classical heating condition. The reaction is based on the Willgerodt-Kindler reaction to give the corresponding thioamide which further convert to the cyclophane**1**.

There is a big difference between compounds **1** and **2** in recognition of cyanide ion which related to the nonosize cavity of compound **1**. In this regard, we are going to synthesize the other cyclophanes**3** with bigger cavity to study the efficiency of cavity in recognition of cyanide ion.



1

2

3 (n = 2 -5)

Scheme 1

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Removal of sulphure from model gasoline using metal-incorporated mesoporous silica and investigation of process parameters

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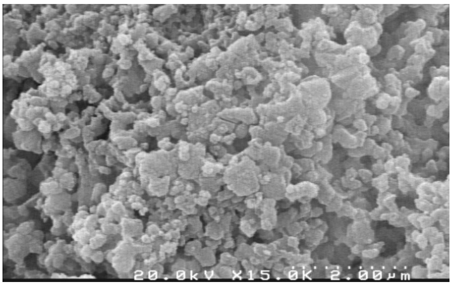
Mobil has patented a family of nanoporous materials (mesoporous molecular sieve) designated as M41S, in which MCM-41 is considered to be the most promising structure. Narrow pore size distribution with size controllable pores over micrometer length scales makes the MCM-41 materials attractive to many applications, e.g., the separation of proteins, selective adsorption of large molecules from effluents [1-3]. More specifically, metals used in catalysis are nanoparticles rather than large single crystals, because of their higher dispersion (fraction of atoms in the surface shell), higher number of defects which provides favorable bonding opportunities for breaking and forming bonds, easier surface reconstruction to adapt to the adsorbates, better interaction with the support, and tunable electronic properties varying particle size.

In this contribution, platinum nanoparticles were incorporated into the MCM-41 structure and the obtained samples was characterized and used as adsorbent for the removal of sulphur (as thiophene) from model gasoline. The effect of three process parameters, i.e. metal content, temperature and liquid hourly space velocity (LHSV) on the removal of sulphur (response) was investigated using response surface methodology (RSM). The obtained results imply that a quadratic model can explain the relation between the before-mentioned parameters and efficiency of sulphur removal. The obtained model was significant according to F-test evaluation and also all the three selected process parameters has significant effect on the response of Model.



SEM image of parent mesoporous silica.

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preparation of magnetic graphene oxide mesoporous silica hybrid nanoparticles with pH-sensitive moiety as nanocarriers for anticancer drug delivery

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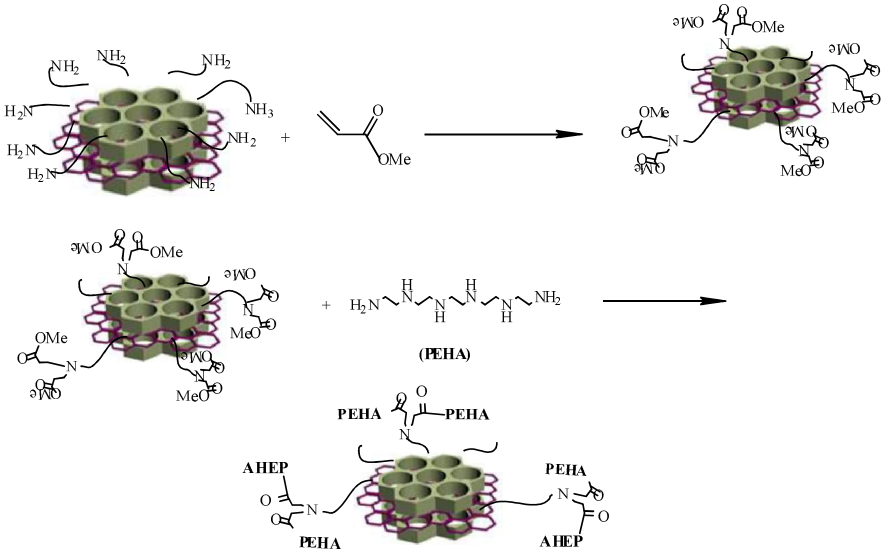
In recent years it has been a growing interest in using nanoparticles as controllable drug carriers. These nanoparticles are suitable for drug delivery systems (DDS) because they could have high drug loading ability, nontoxicity, biocompatibility and availability.

Magnetic graphene oxide nanosheets have some advantages like magnetization for targeting drug delivery, ability of high hydrophile and hydrophobe drug loading, a potential for chemically functionalizing the surface and so on [1-3]. On the other handsince the cancer tissues are inflamed andhave lower pH in comparison with other healthy tissues, using apH-sensitivecarrier for smart release of drug seems reasonable.

In this research we have coupled the advantages of using mesoporous magnetic graphene oxide nanosheets and a pH-sensitivesegment onto the surface of the nanoparticle. The surface of hybrid nanosheets of mesoporous magnetic graphene oxide is altered with methyl-acrylate and pentaethylenehexamine (PEHA), and then drug is loaded inside the nanoparticle (Scheme 1). It is expected that drug will be released in the more acidic medium (pH=5.5).



Scheme 1

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A study on the antioxidant activity of wild pistachio (*Pistacia atlantica)* and wild olive (*Olea europaea)* essences in IRAN and use them for synthesis of nanogold particles

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Ziziphus mauritiana is the group of flowering plants; the fruit is oval and slightly smaller tree or the olive fruit size with sweet and sour tastes. The nutritious fruits rich in vitamin C and good amounts of B vitamins, and contains calcium, phosphorus and iron. In this study the antioxidant effect of the *Ziziphus mauritiana* and also gold nanoparticles synthesis with using the plant extract were analysed.The antioxidant activity of the plant was measured by DPPH scavening method. The results showed that the antioxidant activity of methanolic extract of this plant was desirable and it's increasing when concentrations increase.
45.98mg gallic acid for leaves ±Results: The average of total phenolic was found to be 1061.6 and these result shows that this plant has good antioxidant activity. The results of Transmission electron microscopy, scanning electron microscopy, FT-IR, UV-VIS and X-ray diffraction spectra confirm that the extract leaves of *Zizyphus mauritiana* can synthesis gold nanoparticles.

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Synthesis and characterization of a novel schiff base compound from cinnamaldehyde and 3,4-diaminofurazan

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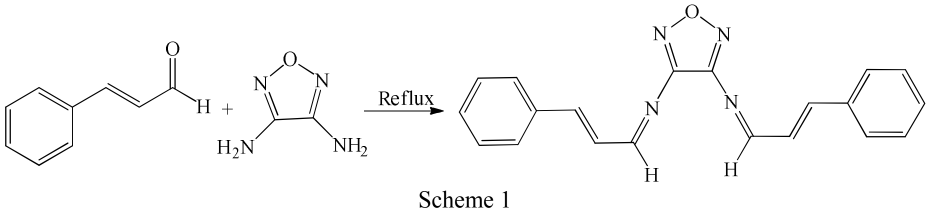
Schiff bases are aldehyde or ketone like compounds in which the carbonyl group is replaced by an imine or azomethine group. They are widely used for industrial purposes and also exhibit a broad range of biological activities [1].

Cinnamaldehyde(**1**) is an aromatic aldehyde and main component of bark extract of cinnamon. The main advantage of Cinnamaldehyde is that this compound has been shown to be active against a range of forborne pathogens bacteria.

3,4-Diaminofurazan (DAF)(**2**) is the precursor to a wide range of energetic substances carrying the furazan ring. Furazans have many desirable properties for an energetic material such as its dense planar structure, stabilizing aromatic nature and energetic oxygen in the ring; many furazan derivatives also have a very high heat of formation [2,3].

In this research, a new Schiff base compound was prepared by condensation reaction between Cinnamaldehyde(**1**) and 3,4-Diaminofurazan(**2**) in aqueous solution. Mixture of compounds **1** and **2** refluxed for 24 hours. After the end of reaction and evaporation excess solvent, needle crystals appeared.

Spectroscopic properties of the synthesized Schiff base were investigated by means of FT-IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis spectroscopy and elemental analysis.



Scheme 1

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Combustion synthesis of nano-crystalline TiO_2

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In this work, Nano-crystalline TiO_2 were synthesized by combustion method using metal nitrate solution and Citric Acid. Microwave irradiation was used as heating source. X-ray diffraction, scanning electron microscopy as well as Fourier transform infrared spectroscopy was performed to characterize the obtained samples. Results from XRD showed that the crystal size was at 15 nm and SEM micrograph showed the bulky-thick flakes morphology. Results demonstrated that solution combustion method is a simple and efficient method to produce pure anatase TiO_2 phase.

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Green synthesis of gold nanoparticles in the present of chitosan/ polyvinylpyrrolidone/TiO_2 under UV irradiation

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Superior gold nanoparticles (Au NPs), in a bionano-composite film, are successfully synthesized by UV irradiation of an aqueous solution containing $AuCl_3$ and chitosan/polyvinylpyrrolidone/TiO_2 [1-3].

This UV irradiation-mediated method is a green and promising route for the synthesis of dispersed and stable Au NPs for several purposes. Important advantages of this method include economic feasibility, easy workups, and nontoxic materials [4]. Characterization of the bionano-composite film is carried out via SEM, TEM, FT-IR, XRD, and TGA.

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A new preparation of pyrano[2,3-*d*]pyrimidinone derivatives via one pot tree component reaction

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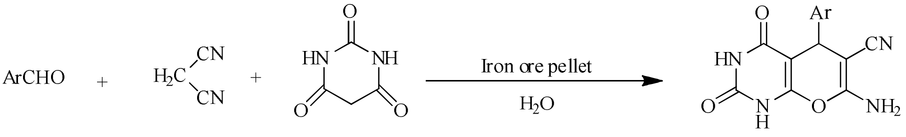
Pyran derivatives are ordinary structural subunits in a variety of important natural products, including carbohydrates, alkaloids, polyether antibiotics, pheromones, and iridoids [1]. Uracil and its fused derivatives, such as pyrano[2,3-d]pyrimidines, pyrido[2,3-*d*]pyrimidines or pyrimido[4,5-*d*]pyrimidines are well recognized by synthesis as well as biological chemists. Compounds with these ring systems have diverse pharmacological properties such as antiallergic, antihypertensive, cardiotonic, bronchiodilator, antibronchitic, or antitumour activity [2-4].

Iron ore pellet is used as natural catalyst for a simple and efficient one-pot synthesis of aryl substititued pyrano[2,3-*d*]pyrimidinone via initial Knoevenagel, subsequent Micheal and final heterocyclization reactions of aryl aldehyde, malononitrile and barbituric acid in water with excellent yields. This method has the advantages of high yields, simple methodology, short reaction times and easy work-up (Scheme 1). The structures of some products were deduced from their spectroscopic data (FT-IR, ^{1}H-NMR).



Scheme 1

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Synthesis and characterization poly(amid-imide)/ SiO_2 nanocomposite

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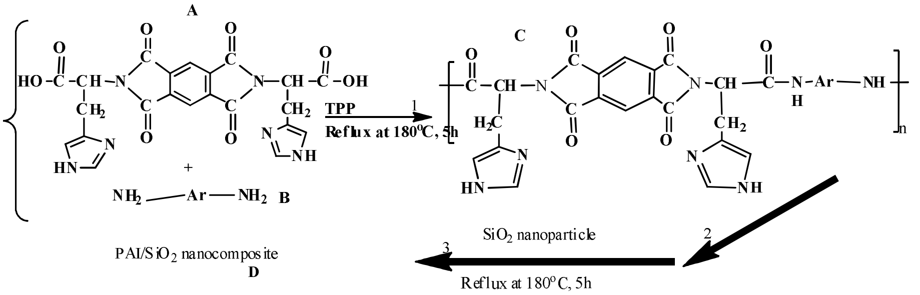
In the past two decades, organic/inorganic nanocomposite materials prepared by sol-gel process have drawn a great deal of attention in material science because of their unique properties[1].Nanocomposite based on organic polymers and inorganic nanoclay minerals consisting of silicate layers are among the most promising composite systems[2-5].

In this study, Poly(amide-imide)/silica (PAI/SiO_2) nanocomposites were prepared by in-situ polymerization process. In a first step, a monomer containing two chemically pre-formed imide rings has been synthesized. The monomer was then used to synthesized poly(amide-imide) (PAI) and were finally reacted with varying a mounts of silica nanoparticles in a in-situ polymerization reaction in order generator the poly(amide-imide)/SiO_2 Nano composite. The prepared monomer, PAIs and poly(amide-imide)/silica Nano composites were characterized by ^1H nuclear magnetic resonance (NMR) spectroscopy, Fourier transform infrared(FT-IR), thermo gravimetric analysis(TGA), X-ray diffraction(XRD), scanning electron microscopy(SEM). The SiO_2 phase was dispersed in the polymer matrix. DSC and TGA results showed that these PAIs and PAI/silica Nano composites had excellent thermal stability. (Scheme 1).



Scheme 1

References:

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Silanization of silver nanoparticles and its application in ethylene propylene robber nanocomposites

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In order to probe usability and dispersion of metal nanoparticles in nonpolar polymers, surface modification is done [1]. Silanization is one such method where the silanol group on silane coupling agents (SCAs) reacts with surface species and can be used to create an ultrathin single molecular layer on the surfaces of nanoparticles [2-3].

In this article, the surface of silver nanoparticles (AgNPs) is modified through trapping Ag+ ions by triethoxyoctylsilane in ethanol, followed by reducing with sodium borohydride. Fourier transform infrared spectroscopy (FT-IR) spectrum shows silane groups on AgNPs. A solution blending method is employed for preparation of AgNPs composites. The AgNPs is first dispersed in toluene using ultrasonic homogenizer and then thoroughly mixed with EPR in the same solvent. Upon fast solvent removal, the dispersed structures of 2%, 4%, 6%, and 8 vol% AgNPs in EPR remain. The products are characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD).

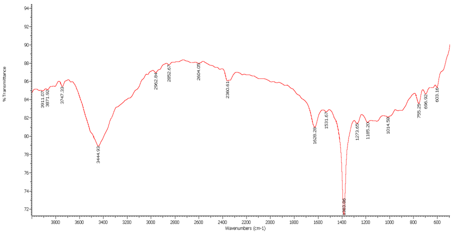

Fig.1- FT-IR spectrum of AgNPs with silane

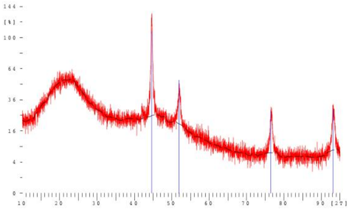

Fig.2- XRD pattern of AgNPs/EPR

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Functionalization of carbon nanotubes with anthraquninone pigments

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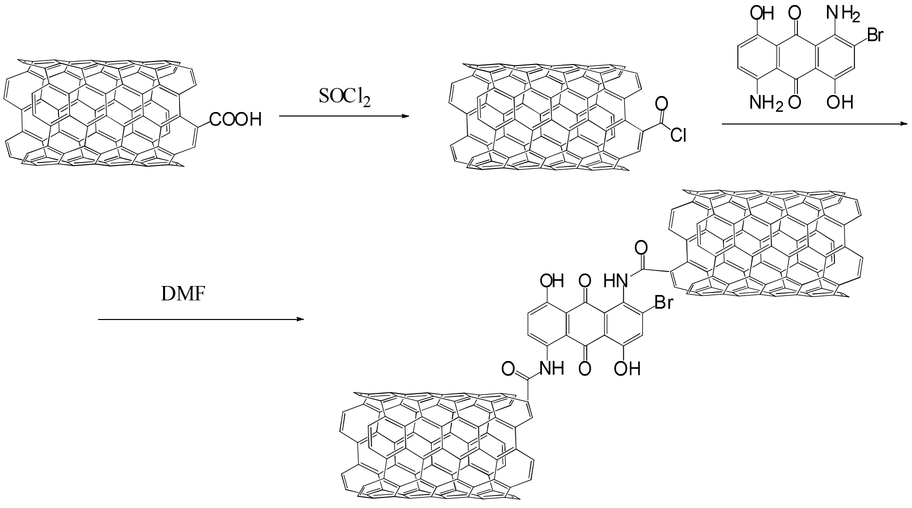
Carbon nanotubes (CNTs), a new member of the carbon family, were first discovered by Iijima in 1991[1]. Functionalization of multi-walled carbon nanotubes are one of the best ways to improve the properties of them. Treatment of them in the presence of acidic environment can produce oxygenated species on the end wall nanotubes[2].
Anthraquinone is the base structure of Disperse dyes which have good stability they can have the covalent binding with nanotubes.

Carbon nanotubes due to structural characteristics, mechanical, electrical and thermal is very attractive for many researchers. The anthraquinone dye effects and perspective by placing the electron donor groups such as amino, hydroxyl and .... At positions 1,4,5 and 8 will change and they can be made light blue until shade red[3]. At first multi-walled carbon nanotubes functionalized (MWCNTsCOOH) has been changed to the acyl halide and by a subsequent reaction amid to connect Disperse Blue 56(scheme1). The structure of the product has been analysed and determined through different spectroscopic methods such as UV, IR, ^{1}HNMR, Raman, SEM.



Scheme1

Reference

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Rhodium catalyzed enantioselective synthesis of cyclopropanated pyrroles and furanes via in-situ preparation of diazo compounds from triazoles

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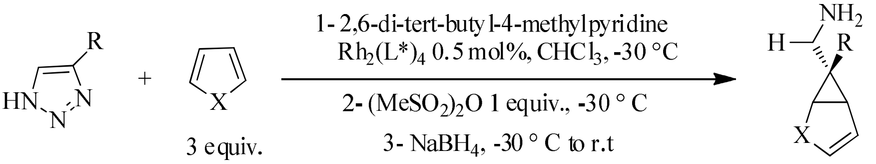
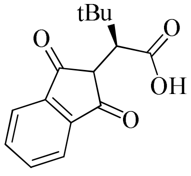
We previously reported the copper-catalyzed stereoselectivecyclopropanation of pyrrole and furane using diazo esters and subsequent ozonolysis of the cyclopropanatedpyrroline as a simple preparation of chiral α,β-amino acids [1]. The same method can be applied on furane to produce cyclopropanatedcarbaldehydes.

Diazo compounds are highly carcinogenic and explosive therefore these processes are potentially hazardous and cannot be easily scaled up. In-situ preparation of diazo compounds is a much safer method rather than synthesis and isolation of hazardous diazo compounds. Folkin and colleagues have reported the in-situ generation of diazo compounds via rearrangement of triazoles as a safe and efficient method for cyclopropanation of alkenes [2,3]. We have extended the same protocol for the Rhodium catalyzed stereoselectivecyclopropanation of pyrrole and furane derivatives. The reaction produces imino-cyclopropanatedpyrrole and furanes which is reduced to the corresponding amino cyclopropanated product in the presence of sodiumborohydride.





L*

	X	R	yield%	e.e
1	NBoc	Ph	41	90
2	NBoc	3-thiophene	32	81
3	O	Ph	44	85
4	O	3-thiophene	37	80

Scheme1

References:
1. O. Reiser, et. al. *J. Org. Chem.* (**2000**) 8960.
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Efficient and selective deoximation catalyzed by a molybdenum thiosemicarbazid schiff base complex

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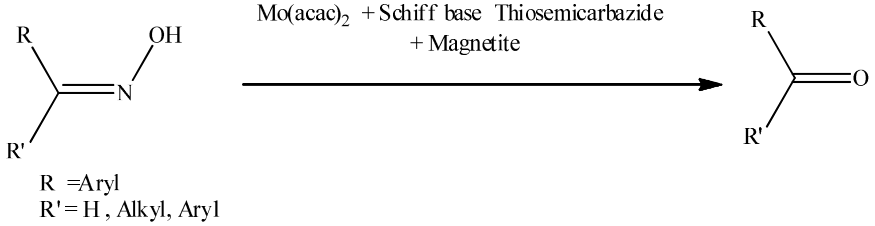
In recent years considerable effort has been directed towards the transition metal complex catalyzed oxidation of organic compounds. Among these, Deoximationto aldehydes and ketones has specially been attended a lot, since carbonyl compounds are important intermediates in organic synthesis. Here in, We used a high- yield (65-95%) and selective Deoximation procedure for the conversion of Oximes with various electron releasing and electron withdrawing substitutions, to corresponding aldehydes and ketones at 60°Cwith H_2O_2 as oxidant, in the presence of Molybdenum complex with Schiff Base Ligand of ThiosemicarbazidSupported on Magnetite as catalyst with short reaction times and high yields. The Presence of electron releasing and electron withdrawing substituents in ortho or para positions shows that the importance of steric and electronic effects due to high activity of the catalytic system are lower than expected. The presence of the catalyst seriously affects Deoximationby H_2O_2.



Scheme 1

References:

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Synthesis, characterization and crystal structure of a new Schiff base

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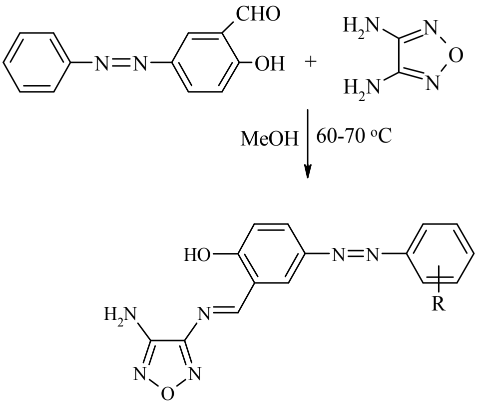
Schiff bases are important class of ligands in coordination chemistry and have extensive applications in different fields [1]. Schiff bases are versatile ligands which are synthesized from the condensation reaction of amines and aldehyde or ketone compounds. [2]

In this work we synthesis new Schiff base 2-[(4-amino-1,2,5-oxadiazol-3-ylimino)methyl)-4-(phenyl diazenyl] phenol. The UV-Vis absorption spectra indicated positive solvatochromism in these compounds which is dependent on the substitution, nature of solvent, PH, and environment temperature.



Scheme 1

The structure of new Schiff base was confirmed by X-ray structural analysis.

References:

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Oxidation of sulfides to sulfoxides using new modified nanomagnetic Fe_3O_4 catalyst

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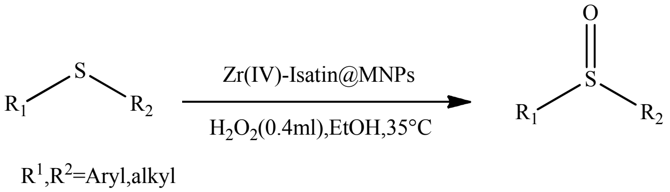
Recently, magnetic nanoparticles have been extensively employed as alternative catalyst supports, in view of their high surface area. In this light nano catalyst Fe_3O_4 could easily be separated and recover from the reaction mixture with an external magnet and reused several times [1].

Sulfoxides are valuable synthetic intermediates for the synthesis of chemically and biologically important and significant molecules. The main synthetic route for the preparation of these valuable materials is oxidation of the corresponding sulfides [2,3].

In this work, oxidation of sulfides to sulfoxids using Zr(IV) modified Fe_3O_4 has been reported in 35 °C temperature.



Scheme 1

References:

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An efficient synthesis of 2,3-dihydroquinazoline-4(1H)-ones using heteropolyacid as green and eco-friendlyacidic catalyst under solvent-free conditions

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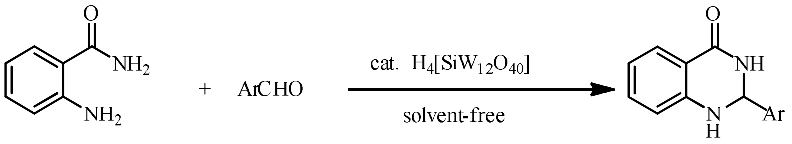
Recently much attention has been devoted towards 4(3H)-quinazolinones derivatives due to their significant therapeutic and medicinal properties such as anti-inflammatory [1], antimalarial [2] and antiparkinsons activities [3].

Heteropolyacids are widely used in variety of acid-catalyzed reactions such as esterification, alkylation and dehydration [4].

In continuation of our research program to develop the green, efficient and recyclable catalyst in organic synthesis [5,6], it is therefore of interest to examine the behavior of heteropolyacids catalyst in solvent-free conditions for synthesis of 4(3H)-quinazolinones. Herein we wish to report a simple and an efficient synthetic method for 4(3H)-quinazolinone derivatives using a recyclable green catalyst, heteropolyacid under mild reaction conditions (Scheme 1).



Scheme 1

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Grafting of copper complex in MCM-41 matrix: a highly efficient catalyst for the coupling thiols by UHP

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Many metals are immobilized/grafted into MCM-41. Among these metal, copper modifications are of considerable importance, because copper is a known metal which shows redox properties. Copper ions have been introduced to mesoporous silica by means of impregnation, and grafting. Recently scientist had widely been studied in this field, for example Evans et al. observed the aziridination of *trans*-stilbene when transition-metal–aquo complexes such as Cu^{+2}aquo were used [1]. Ghadiri et al. reported the post-synthetic grafting of copper complexes [2]. Karandikar et al. reported the immobilization of copper–Schiff base complex onto the $-NH_2$ modified MCM-41 [3]. Schiff bases have been widely used in the development of coordination chemistry. They easily form stable complexes with most transition metal ions with different oxidation states. We have successfully grafted 3,4-dihydroxybenzaldehyde ligand onto the inner walls of amino functionalized MCM-41, made the strong host for copper (II) . Grafting of 3,4-dihydroxybenzaldehyde as ligand and then copper(II) salt on nanosilica increasing the dispersion of the acidic sites and so increase the catalytic activity. This supported catalyst can use efficiently in a wide variety of organic reactions like, coupling of thiols to disulfides.

In this research Cu-MCM-41 has been synthesized as an active catalyst and then it has been research in the coupling of thiols to disulfides in the presence UHP as oxidant at room temperature (Scheme1). A simple filtration followed by removal of the solvent from the filtrate gave the product in acceptable purity. The Cu-MCM-41 catalyst has been recovered from reaction mixture and has been reused successively several times under the same reaction conditions.

$$\mathrm{RSH} \xrightarrow[\text{Ethanol, r.t}]{\text{Cu-MCM-41/UHP}} \mathrm{RSSR}$$

Scheme1

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Electron transfer, free activated energies and kinetics process study of [Zn[Pc-β(OBz-$(CF_3)_2)_4$]].[Cn] nano-structure complexes

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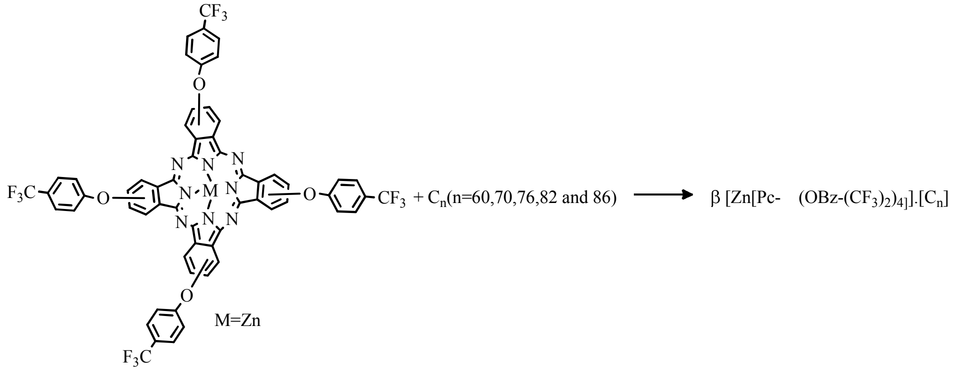
Phthalocyanine is an intensely colored macro cyclic compound that is widely used in dyeing. Phthalocyanines form coordination complexes with the most elements of the periodic table.Fullerenes Cn , are a Class of spherical Carbon allotorope group with unique properties. Various empty Carbon fullerenes (Cn) whith different Carbon atoms have been obtained and investigated.Electron transfer between fullerenes and other molecules is thought to involve the transfer of electrons between molecules surrounding the fullerene cage[1-2]. In this study ,to establish agood relationship between the structures of (Zn[Pc-β(OBz-$(CF_3)_2)_4$]) with fullerenes Cn(n=60,70,76,82 and 86),with create [Zn[Pc-β(OBz-$(CF_3)_2)_4$]].[Cn] was utilized the number of Carbon atoms within the fullerenes as an index[3].the relationship between the number of Carbon atoms and the free energies of electron transfer ($\Delta G_{et(1)}$- $\Delta G_{et(4)}$) are assessed using the Rehm-Weller equation for [Zn[Pc-β(OBz-$(CF_3)_2)_4$]].[Cn]supramolecular complexes have investigated (Scheme1).the calculations have presented on the basis of the four reduction potentials ($^{Red}E_1$ to $^{Red}E_4$) of fullerens Cn. the results used to calculate the four free-energies of electron transfer ($\Delta G_{et(1)}$- $\Delta G_{et(4)}$) of [Zn[Pc-β(OBz-$(CF_3)_2)_4$]].[Cn] supramolecular complexes as well as the first to fourth free activation energies of electron transfer and kinetic rate constants of the electron transfers $\Delta G^{\#}_{et(n)}$ and k $_{et(n)}$ (n=1-4),in accordance with the Marcus theorem for fullerens C_{60} to C_{100}.



Scheme 1

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Magnetic nanoparticle-supported as a recyclable and recoverable ligand for the $Cu(NO_3)_2$ catalyzed for synthesis of 2,3-dihydroquinazolin-4(1H)-ones

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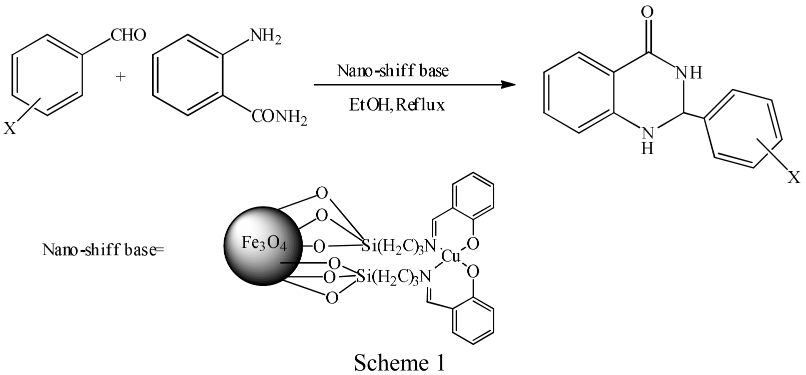
Nanoscale materials have been a subject of particular inter-est due to properties, which differ from their bulk counterparts. They have been used extensively in chemistry, physics, biology, and catalysis. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. In contrast to the difficulty observed in recov-ering and reusing most solid catalysts, core–shell nanostructure magnetic catalysts can be easily retrieved under the influence of a magnetic field and used in subsequent reactions [1,3].

In this work, a new strategy has been introduced for the preparation of 2,3-dihydroquinazolin-4(1H)-ones. In this regards, Schiff base complex of metal ions functionalized Fe_3O_4 nanoparticle has been synthesized and new applications of this catalyst explored. Therefore a variety of 2,3-dihydroquinazolin-4(1H)-ones have been prepared via combination ofaromatic aldehydesand 2-aminobenzamide.



Scheme 1

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Room temperature synthesis, characterization and gas sensitivity study of polythiophene hybrid nanocomposites with SnO_2 nanoparticles

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Recently people have witnessed the development of the society. The prosperity of the society relies on the combustion of fuels, which can produce some toxic gases, such as NO*x* (mostly NO, little NO_2 and N_2O_4). The presence of NO*x* in the atmosphere tends to produce acid rain and photochemical smog, which are harmful to environment. The Office of Air Quality Planning and Standards has set National Ambient Air Quality Standards for NO_2 at 0.053 ppm [1]. To protect the environment, the monitoring and control of polluted gases has become increasingly important. SnO_2 has been studied extensively and has emerged as economical sensor for monitoring toxic gases [2,3].

In this research work, a serious of polythiophene (PTP) nanocomposites with nanodimensional SnO_2 was fabricated by *in situ* oxidative polymerization method, using $FeCl_3$ as oxidant. These nanocomposites were characterized by FT-IR, UV-vis, XRD, TGA, SEM, and TEM techniques. The obtained results showed that SnO_2 nanoparticles have been encapsulated by PTP matrix. The composites were used for gas sensing to NO*x* at different working temperature. It was found that PTP/SnO_2 materials with different PTP mass percent (1%, 5%, 10%, 20% and 30%) could detect NO*x* with very higher selectivity and sensitivity at much lower working temperature than the reported SnO_2. The PTP/SnO_2 nanocomposites responded to NO*x* at concentration as low as 10 ppm. PTP/SnO_2 composite containing 5 mass% PTP showed the highest sensitivity at room temperature. The sensing mechanism of PTP/SnO_2 nanocomposites to NO*x* was presumed to be the effects of p-n hetero- junction between PTP and SnO_2.

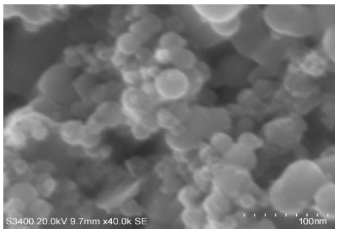

Fig. 1. SEM photograph of PTP(30%)/SnO2 nanocomposite

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Indirect chemically attachment of $–SO_3H$ groups on multiwalled carbon nanotubes surfaces

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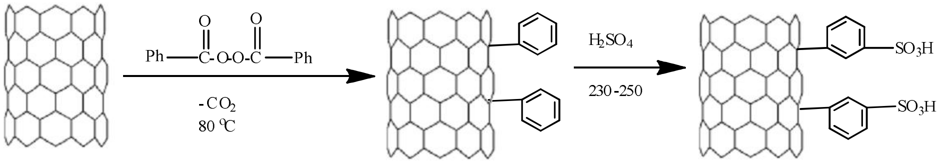
Carbon nanotubes (CNTs) represent a relatively new class of carbon-based nanomaterials, currently under deep scrutiny for applications in materials and biomedical fields [1]. Chemical functionalization is based on the covalent linkage of functional entities onto carbon scaffold of CNTs. It can be performed at the termini of the tubes or at their sidewalls [2]. Because of unique properties of carbon nanotubes such as high surface area, and stability in hard reaction conditions, they can be used as catalyst supports [3, 4]. functionalization of carbon nanotubes by acidic groups such as $-SO_3H$, convert them to a solid acid for chemical reactions and other scientific fields [5].

In the present study, we have attached sulfonic acid groups on the surfaces of multi-walled carbon nanotubes by chemical bonding. Firstly, we used of benzoyl peroxide for attachment of phenyl groups on the carbon nanotubes surfaces. Then, indirect sulfonation of carbon nanotubes occure at high temperature in the presence of 98% sulfuric acid (Scheme 1).

Functionalized CNTs were identified by X-ray diffraction (XRD), infrared spectroscopy (FTIR), scanning electron microscope (SEM) and Raman spectroscopy.



Scheme 1

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Preparation of photochromic functionalized polymeric nanoparticles based on spiropyran and acrylic copolymer by emulsion polymerization

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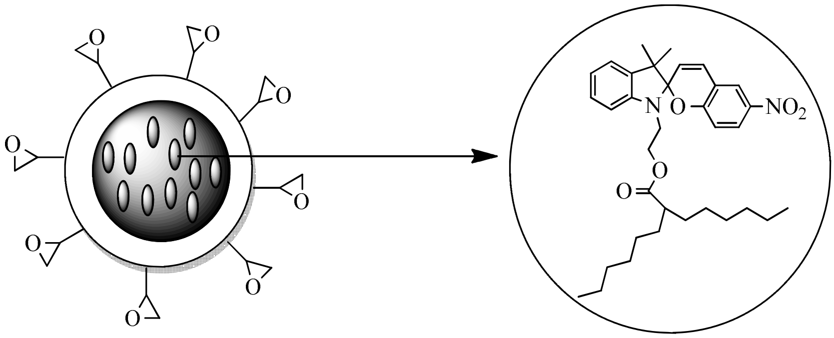
Photochromic nanoparticles have found wide applications in the fields of electronics, biological and cells tracking systems, because of the their ability to protect the photochromic dye against environmental degradation and maintaining their properties [1]. Spiropyrans dyes in the hydrophobic nanoparticles have reversible color changes, which is induced by UV-Vis light [2].

In this study, a spiropyran dye containing hydroxyl functional group was synthetized and characterized [3], and then modified with acrylic groups [4]. In order to prepare hydrophobic core, the prepared modified spiropyran was copolymerized with methyl methacrylate through emulsion polymerization technique. In the next step a shell containing epoxy groups on the hydrophobic core was formed by adding methyl methacrylate/glycidyl methacrylate monomers. The sizes of these nanoparticles were 50-100 nm to maintain its optical properties. Due to the surface functionalization of nanoparticles with epoxy groups, they could be used as a nanodetectorfor attaching to the substrate surfaces efficiently.



Scheme 1

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Selective removal of carbon dioxide from methane via facilitated transport membranes containing carboxymethyl derivative of chitosan as carrier

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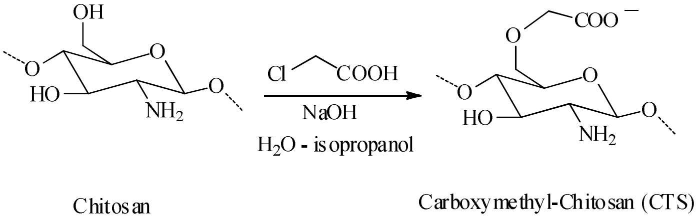
Thin film composite (TFC) membranes are preferential structure for membranes because of low thickness of separating layer and subsequently high flux [1-2]. Fixed facilitated transport mechanisms are a solution for conventional membranes which enhances gas permeability as well as gas pair selectivity [3-5].

In this work a carboxymethyl derivative of chitosan containing amino and carboxylate functional groups (Scheme 1) as a new membrane material was prepared for facilitated transport of CO_2 across PVA/PS TFC membrane. The membranes were prepared at different content of carboxymethyl derivative and performance was evaluated using binary CO_2/CH_4 gas mixture. Gas permeability and CO_2/CH_4 selectivity of membranes was measured at different operating conditions.



Scheme 1

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Synthesis and characterization of molecularly imprinted polymer-based nanoparticles (MIP-NPs) for target and controlled release of isosorbide dinitrate

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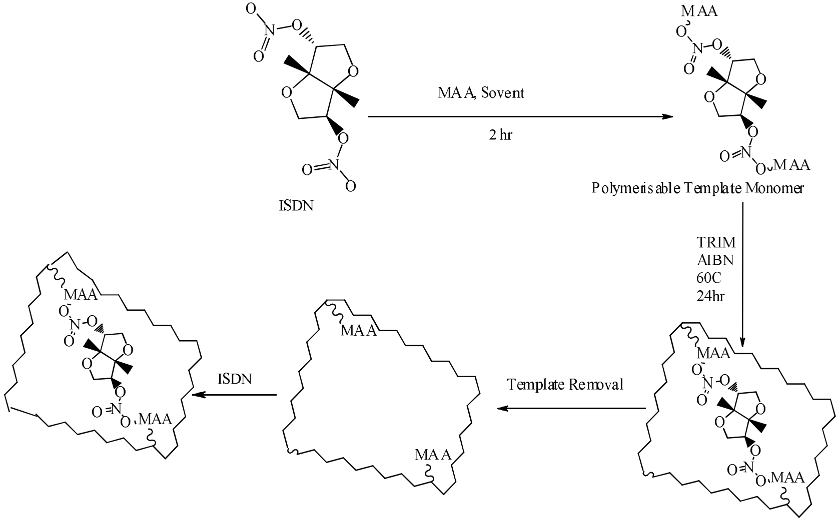
Isosorbide dinitrate is a promising pharmaceutical agent that has vasodilative effects as a NO donor. To study the complex and wide-ranging roles of NO and to facilitate its therapeutic use, a great number of synthetic compounds (e.g., nitrosothiols, nitrosohydroxyamines, N-diazeniumdiolates, and nitrosyl metal complexes) have been developed to chemically stabilize and release NO in a controlled manner. Although NO is currently being exploited in many biomedical applications, its use is limited by several factors, including a short half-life, instability during storage, and potential toxicity. Additionally, efficient methods of both localized and systemic *in vivo* delivery and dose control are needed. One strategy for addressing these limitations and thus increasing the utility of NO donors is based on nanotechnology.

In this work, we describe how to prepare a highly selective imprinted polymer by a precipitation polymerization technique and non-covalent bonding. We used IsoSorbide DiNitrate (ISDN) as the template, TRIM as the cross linker, MAA as the monomer.



Scheme 1

Results show that this imprinted sorbent exhibits good recognition and high affinity for ISDN. Controlled release of ISDN from MIPs was investigated through in vitro dissolution tests and by measuring by (HPLC).

References:

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Structural and configurational properties of tetramethyltetraaza[8] pericycline, tertaphospha[8]pericyclineand tetraarsena[8]pericycline. A hybrid-density functional theory study and natural bond orbital (NBO) interpretation

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Pericyclines are macrocyclic structures, in which saturated corner atoms are connected by ethynyl linkages [1]. In this work, we have investigated the structural parameters, aromatic characters and hybridized orbitals of the various forms of tetramethyltetraaza[8]pericycline (1), tetramethyltetraphospha[8]pericycline (2) and tetramethyltetraarsena[8]pericycline (3) by means of hybrid-density functional theory based method (B3LYP/6-31G*) [2] and natural bond orbital (NBO) interpretation [3].

The anti-aromatic characters of compounds 1-3 are attributed to their great NICS (0.0) values. The decrease of the C-M-C bond angle from compound **1** to compound 3 can be justified by increase of the p orbital percentage of the hybridized orbitals of the M atom of M-C cyclic bond and the decrease of the contribution of the corresponding s orbital from compound **1** to compound **3**.

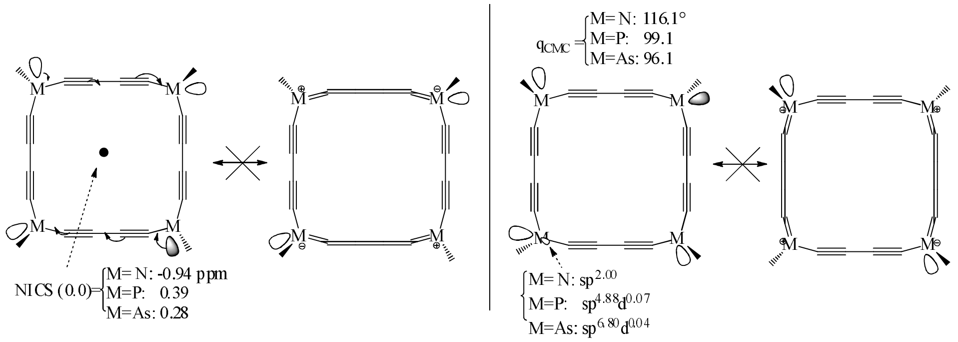

Figure1: M = N (1), P (2), As (3)

References:

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Ultrasound effect for an efficient three-component synthesis of 1*H* spiro[furo[3,4-*b*]pyridine-4,3'-indoline]-3-carbonitriles

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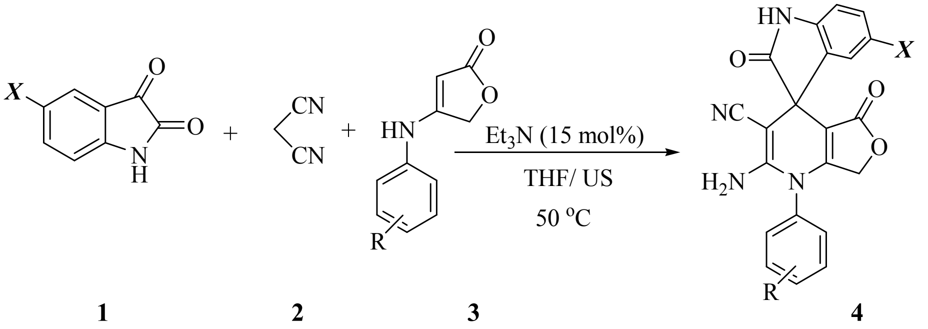
[b]*Reproductive Immunology Research Center, Avicenna Research Institute, ACECR, Tehran,Iran*
[c]*Nanobiotechnology Research Center, Avicenna Research Institute, ACECR, Tehran, Iran; Email: R.ghahremanzadeh@yahoo.com*

Multicomponent reactions (MCRs), in which multiple starting materials react together *via* a one-pot procedure to form a final product without isolating the intermediates, are special types of synthetically important organic reactions in combinatorial and medicinal chemistry [1-2]. Recently, the application of ultrasound as a powerful technique in synthetic organic chemistry became extremely efficient and attractive. The prominent features of the ultrasound approach are enhanced organic reaction rates, formation of purer products in high yields, mild reaction conditions, and considered a processing aid in terms of energy conservation and waste minimization compared with traditional methods [3]. Spirooxindole unit is a privileged heterocyclic motif that forms the core of a large family of alkaloid and natural products, with interesting structural properties and wide range of useful pharmacological properties and biological activities, such as antimicrobial, antitumoral, antibiotic agents, inhibitors of human NK-1 receptor, and inhibitors of microtubule assembly [4-5].

In this research, we report a highly efficient one-pot, three component condensation reaction for the synthesis of 1*H*-spiro[furo[3,4-*b*]pyridine-4,3'-indoline 3-carbonitrile derivatives **4** through a three-component condensation reaction of isatins **1**, malononitrile **2,** and anilinolactones **3** in the presence of catalytic amount of Et_3N as an inexpensive and available catalyst in THF under ultrasound irradiation in high yields.



Scheme1

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Synthesis and characterization of some new ligands from bis ((o-allyl)cresyl)sulfoxid and praper diamine with nano biological property as [ONS] donor

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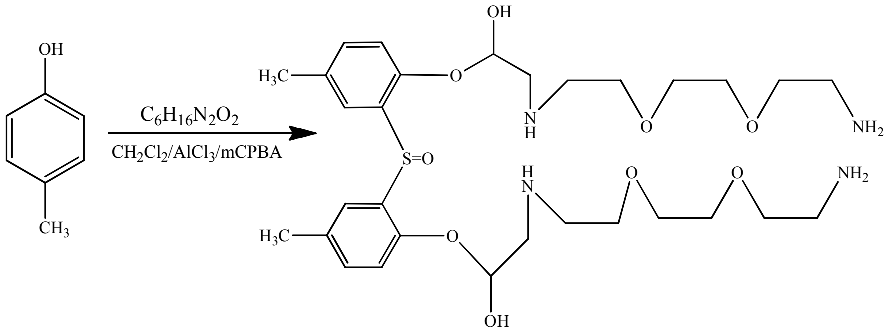
Podands with anti-cancer properties show their properties with making possible to interact DNA with N-free ring in their skeletons. Podands are open-chain analogs of crown ethers; in the recent years, they have attracted increased attention due to their accessibility, fairly high efficiency, and the possibility for controlling their properties of complexion over a wide range via structural modifications[1-2]. Our purpose in this research work was synthesis a new podand as a ligand with nano biological property as [ONS] donor. At First, p-cresol in presence of $ALCL_3$ and thionyl chloride in dichloromethane as solvent result to sulfoxide (1) and then compound (1) reacted with allyl bromide and potassium carbonate to prepare bis allyl (2) which underwent an oxidation reaction by means of mCPBA to be changed into epoxide (3) reacting with diamine ($C_6H_{16}N_2O_2$) to produce our podand (4). The structures of all prepared compounds have been recognized by IR, ^1H NMR and ^{13}C NMR.



Scheme 1

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The synthesis of 5-(3,3,6,7-tetramethyl-3H-indol-2-yl)pyrimidin-2(1H)-one

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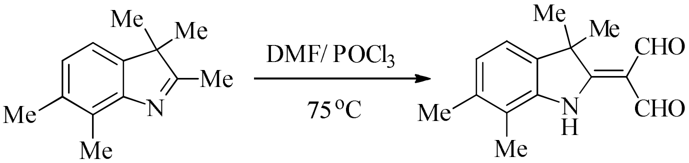
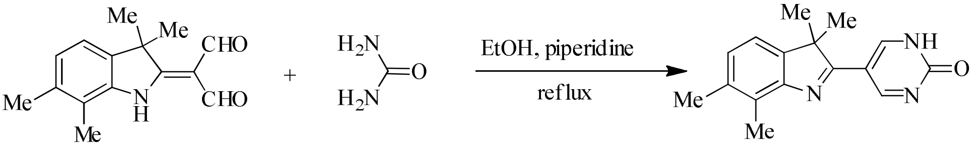
In 1959, Fritz [1] reported the N-formylation of the 3,3-disubstituted 3H-indole (indolenine) with using the Vilsmeier reagent DMF and $POCl_3$. No further studies of the formylation of these types of compound have been reported since.

In this research, we synthesized the novel diformyl compounds from 2,3,3,6,7-pentamethyl -3H-indole by the action with Vilsmeier reagent at 75 °C in excellent yield [2].



Scheme 1

Condensation of corresponding diformyl with urea produced 5-(3,3,6,7-tetramethyl-3H-indol-2-yl) pyrimidin-2(1H)-one in excellent yield [3].



Scheme 2

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A simple and expedient method for the one-pot synthesis of 2-(thiophen-2-yl)-4*H*-benzo[*d*][1,3]oxazin-4-ones

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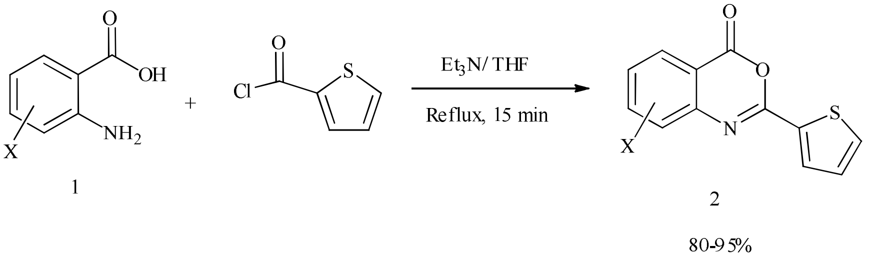
2-Substituted 4*H*-3,1-benzoxazin-4-one and its derivatives are used directly or indirectly in many clinical applications [1]. One of the most important features in 4*H*-3,1-benzoxazinones chemistry is their use as key starting materials for further transformations in design and synthesis of biologically active compound [2-6]. The reactivity and chemical behavior of 4*H*-3,1-benzoxazin-4-ones are due to the susceptibility of the C-4 carbonyl to nucleophilic attack.

Herein, an expedient method for the one-pot synthesis of the title compounds is described. The reaction of anthranilic acid derivative **1** with thiophen-2-carboxylic acid chloride in THF leads to the desired compounds 4*H*-3,1-Benzoxazin-4-ones **2** (Scheme 1). Good to high yields of **2** are obtained under mild reaction conditions with easy work-up.



Scheme 1

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Magnetic nanoparticles Fe_3O_4 coated silica sulfuric acid as an efficient and recyclable nanocatalyst for the acetylation of alcohols with acetic anhydride

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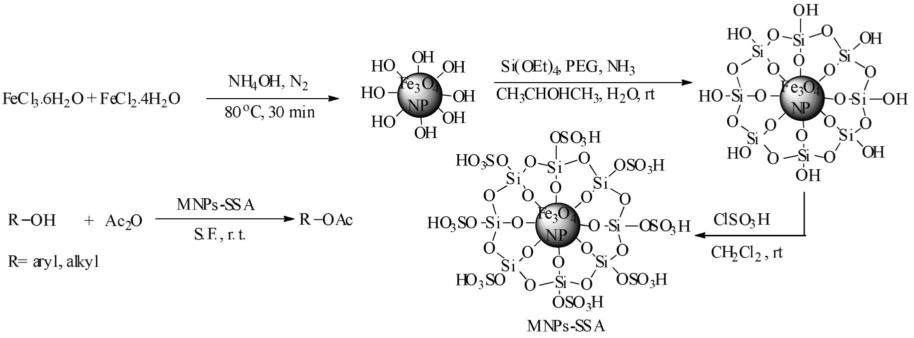
Magnetic nanoparticles (MNPs) are considered as ideal supports for the heterogenization of homogeneous catalysts, since they can be recovered by using an external magnet and reused for several time without significant loss of their catalytic efficiency [1].

The acylation of alcohols is one of the most frequently used transformations in organic synthesis, as it provides an efficient and inexpensive means for protecting hydroxy groups in a multistep synthetic process [2].

In continuation of our systematic studies about application of magnetic nanocatalysts in organic synthesis [3], herein, we prepared magnetic nanoparticles supported silica sulfuric acid (MNPs-SSA) according to Scheme 1. The MNPs-SSA was characterized with TGA, SEM, XRD and FT-IR techniques and was used as a novel, efficient and reusable nanocatalyst for the acetylation of alcohols and phenols with acetic anhydride at room temperature under solvent-free conditions (Scheme 1).



Scheme 1

In summary, the notable advantages of this method are mild and green reaction conditions, simple work-up procedure, short reaction time, good to high yields of products and using non-toxic, high activity, recoverable and reusable catalyst.

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A new method for synthesis of PEG lated chitosan and its application as a carrier for weakly water soluble drugs

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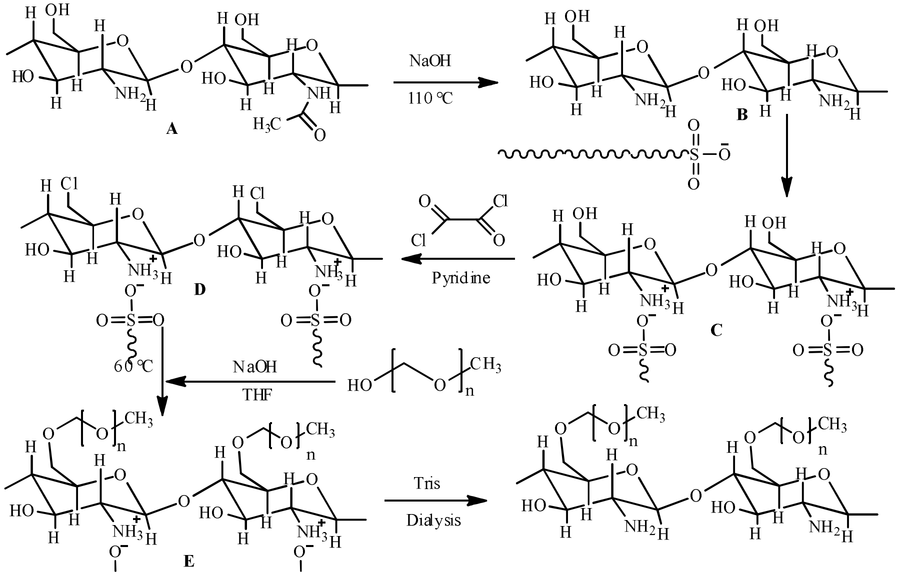
Chitosan is a cationic polysaccharide which has wide application in biotechnology, pharmaceutical, textile, food, cosmetics, and agriculture due to its abundant availability, inherent pharmacological properties polycationic, nontoxic, biodegradable and biocompatibility properties[1-3]. Unfortunately, chitosan is soluble only in aqueous at pH higher than its pKa (~pH 5.5-6.5). Present study introduced a facile new method for conjugating methoxy polyethylene glycol (mPEG) to C6 position of chitosan under mild condition to improve the biocompatibility and water solubility of chitosan is introduced (Scheme 1). Current methods for preparation of PEGylated chitosan have limitations such as harsh de protecting step and several purification cycles. For this purpose chitosan is modified using a new method in which the C6 position of chitosan grafted to mPEG. The chemical structure of prepared polymer was chrectrerized by FTIR and ^{1}HNMR spectroscopy. The TEM, SEM, AFM and DLS techniques were used to characterize prepared particles size. In vitro investigation of ibuprofen release from nanoparticles was carried out to evaluate nanopraticles potential as nano carrier for oral delivery of Ibuprofen as model drug of poorly water soluble drugs.



Scheme 1

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Efficient and selective deoximation catalyzed by a molybdenum alanine Schiff base complex

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Oximes are often used in organic synthesis as protected forms of carbonyl compounds [1] or as carbonyl derivatives for purification and characterization purposes [2]. Oximes were oxidized to the corresponding carbonyl compounds in good to high yields with t-butyl hydroperoxide (TBHP) and (H_2O_2) as oxidant in acetonitrile in the presence of molybdenum alanine Schiff base complex supported on the montmorillonite. This work is performed with the aim to find a way to control the oxidation of various organic compounds and their conversion to the corresponding aldehydes and ketones. To achieve this goal, first a heterogeneous molybdenum catalyst was prepared and then its catalytic activity was investigated in deoximation with (TBHP) in acetonitrile as solvent. The reaction shows good results in the case of oximes. It is noticeable that the reaction was preceded selectively for all the oximes to the corresponding aldehydes and ketones. All of the products were characterized with gas chromatography. Advantages of this method are the high performance, process as well as the relatively short time and good yield of the reaction. Finally, this work resulted in the introduction of a new method for controlled oxidation of organic compounds.

R = Aryl
R' = H, Alkyl, Aryl

Scheme 1

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Synthesis of Ag/AgCl/polyaniline nanocomposites in Polyvinylalcohol matrix

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Polyaniline (PANI) is one of the most important conducting polymers due to its high stability, ease of preparation, low monomer cost, high conductivity, different redox states and a large variety of applications especially in light-emitting diodes and electronic devices and chemical sensors [1]. Inorganic nanoparticles, silver nanoparticles (NPs) and silver chloride (AgCl) related materials such as AgCl nanoparticles and silver (Ag) nanograin decorated AgCl nanoparticles have received a great deal of attention because of their unique electrical and optical properties as well as extensive applications in preparation of photographic paper, photocatalyst, bone cements, and fabrics owing to its antibacterial property [2]. Although many groups have synthesized Polyaniline/silver nanocomposites by utilizing various methods, still it is a challenge to explore the various interesting properties of nanocomposites. To application of polyaniline composites in the living system for continuous monitoring of the level of main metabolites such as sugar, cholesterol etc., it is essential that composite to be biocompatible. Poly (vinyl alcohol) (PVA), a water soluble hydrophilic polymer, is widely used in industries owing to its excellent chemical and physical properties, non-toxicity, excellent chemical resistance, good film formation capacity, biocompatibility and high crystal modulus [3]. In this work, we synthesized Ag/AgCl/PANI nanocomposites in PVA matrix. The procedure involves oxidative polymerization of aniline in the presence of Ag NPs and PVA. The resulted nanocomposites were characterized by scanning electron microscopy (SEM), ultraviolet visible spectra (UV-vis) (Fig.2), x-ray diffraction (XRD) (Fig. 2), energy-dispersive X-ray spectroscopy (EDX), and fourier transform infrared spectroscopy (FT-IR).

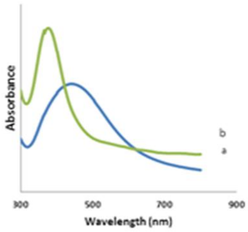

Fig. 1

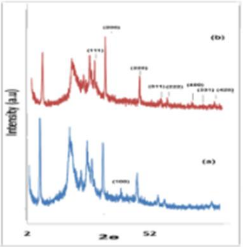

Fig.2

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The oxadiazole-based azo-azomethine dyes; synthesis, solvatochromism, computational and biological properties of some 2,2'-((1E,1'E)-((1,2,5-oxadiazole-3,4-diyl)bis (azanylylidene))bis(methanylylidene))bis(4-(phenyldiazenyl)phenol)

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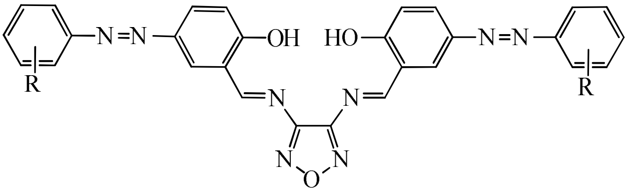
The azo-azomethine dyes based on oxadiazole rings were synthesized by condensation reaction of 5-((4-R-phenyl)diazenyl)-2-hydroxybenzaldehyde with 3,4-diamino-1,2,5-oxadiazole. Substitution, solvent environment and acidity dependence of the electronic absorptions of the synthesized compounds have been studied. The absorption maxima of these dyes show bathochromic shift (positive solvatochromism) in DMF and DMSO than THF solvent. Theoretical calculations results for hydrogen bonding in agreement with experimental data. Due to presence of -CH=N-, –N=N- and OH functional groups in the structure of synthesized dyes these compounds are potentially multidentate ligand and could be used in preparation of coordination polymers.



a) R=H **b**) R=4-Me **c**) R=4-Et **d**) R=3,5 di-Me

e) R=4-iPr **f**) R=4--OMe **g**) R=4-NO_2 **h**) R=4-SO_2-OH

Scheme 1

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Regioselective direct ortho C-acylation of phenols catalyzed by $ZnCl_2$ supported on multi-walled carbon nanotubes as catalyst under solvent-free and microwave conditions

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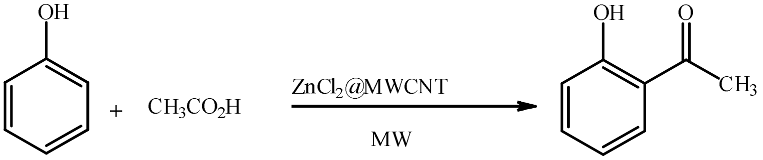
Acylated phenols and naphthols are an important structural motif found in a diversity of bioactive molecules, especially in the synthesis of natural compounds (some examples in Figure 1). Also they serve as protecting groups [1], polyfunctional molecules such as nucleosides, carbohydrates, peptides [2] or modified peptideand bond such as; isoesters [3] steroids [4]. *ortho*-Hydroxyacetophenone is a key intermediate for producing 4-hydroxycoumarin and warfarin, which are both used as anticoagulant drugs [5], and it has been also employed for obtaining flavones [6].

The goal of the present work is to study and compare various processes of the *ortho*-acylation of hydroxyaryl compounds with organic acids, catalyzed by $ZnCl_2$ supported on MWCNTs as new catalyst, and to evaluate the influence of these treatments on the catalytic performances of $ZnCl_2$@MWCNTs catalysts for selective acylation. The direct *ortho* *C*-acylation of phenol formed the phenylacetate intermediate, which is consecutively transformed via intermolecular phenol/phenylacetate *C*-acylation. Reactions were accomplished in the absence of solvent, to afford the corresponding *ortho*-acylated hydroxyaryl compounds, in high yields (scheme 1).



Scheme 1

References:

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Modification of magnetic polymers particles with poly(2-acrylamido-2-methyl-1-propansulfonic acid)

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Ion exchange containing polymers have been studied extensively in many research fields such as drug delivery system, separation and absorption materials [1, 2]. In this work modification of magnetic particles by a polymer matrix containing ion exchange resins was carried out. Firstly, iron oxide was encapsulated with poly (styrene-divinyl benzene- HEMA), which called magnetic polymer particles (MPP) or core particle. In the second stage, MPP was encapsulated with poly(2-Acrylamido-2-Methyl-1-Propansulfonic Acid) (poly AMPS) using inverse emulsion polymerization technique to create -SO3H groups on the MPP surfaces (MPP-AMPS). FTIR spectra and powder XRD pattern were shown in Figures 1 and 2, respectively. FTIR spectra and XRD spectrum of synthesized particles shows characteristic peaks of maghemite and AMPS. So it is confirmed the embedment of magnetic particles in the polymer matrix.

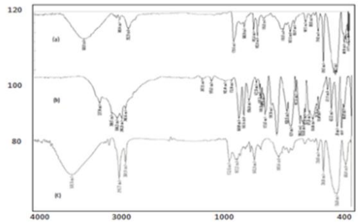

Fig. 1: IR spectra of (a) MPP
(b) AMPS (d) poly(MPP -co-AMPS)

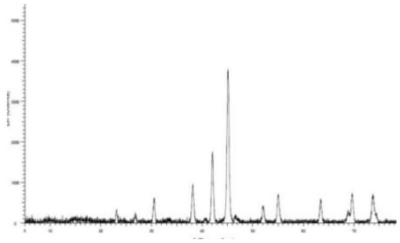

Fig.2: XRD of poly(MPP- co-AMPS)

References:

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The synthesis of benzoxazole derivatives using $Fe(ClO_4)_3/SiO_2$

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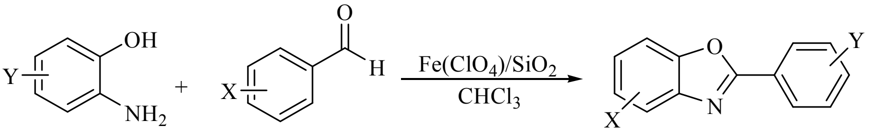
Benzoxazole ring moieties are often found in compounds that exhibit biological activities, including antitumor, antimicrobial, and antiviral properties [1]. There are two general methods for synthesizing 2-substituted benzoxazoles. One is the coupling of 2-aminophenols with carboxylic acid derivatives, which is either catalyzed by strong acids [2] or requires microwave conditions [3]. The other is the oxidative cyclization of phenolic Schiff bases derived from the condensation of 2-aminophenols and aldehydes. In the latter reactions, various oxidants such as DDQ [4], $Mn(OAc)_3$ [5], HPAs [6] and $PhI(OAc)_2$ [7] have been used. However, all of these oxidants are required in stoichiometric or excess amounts relative to their respective substrates. Therefore, a more effective process is needed.

Therefore, we wish to report the synthesis of benzoxazoles using $Fe(ClO_4)_3/SiO_2$ in the presence of arylaldehydes and 2-amino phenols in $CHCl_3$ at ambient temperature. (Scheme 1).



Scheme 1

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Synthesis and characterization of nanocatalyst Husk rice / CuS / Ni (II) and investigation its photocatalytic behavior in degradation of azo dyes

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Dyes wastewater treatment by photodegradation was successfully done over composite of husk rice activated carbon supported CuS nanoparticles which was doped with Ni^{2+} . The prepared catalyst was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) scanning electron microscopy (SEM) analyses and BET. The catalytic activity of this nanocomposite was investigated for degradation of methyl orange. The effect of different pH, contact time and catalyst dosage were investigated. Under the optimized conditions, the best degradation of dye was 6×10^{-5} M dye concentration, pH of 12 and 0.15 mg/L catalyst dose. It was observed that the nanocomposite exhibits the better photocatalytic activity compared with CuS nanoparticles

Co-precipitation method was used followed by direct encapsulation with husk rice coating. The nanocomposite was synthesized in aqueous phase at 100 °C temperature using husk rice as the coupling agent. Different solutions of 0.02 M copper acetate, 0.02 M Na_2S and husk rice were prepared. 0.1 g of husk rice was added to 100 mL of 0.02 M copper acetate solution at room temperature with constant stirring for 30 min. 0.02 M Na_2S (100 mL) was added drop wise to the above solution. Finally, the mixture was stirred at 100 ◦C for 12 h and then cooled to room temperature After reaction, the black precipitates were separated and washed with distilled water. The precipitates were dried in hot air oven for 24 h [1-3].

Ni-doped CuS/C nanocomposite was prepared as a photocatalyst in degradation of methyl orange. Rice husk after pyrolized was used as a support for CuS NPs. The new synthesized catalyst was cylindrical in shape and hexagonal crystalline network as the results of SEM images and XRD patterns were obtained respectively. The TEM images of this nanocomposite showed that the majority of the particles are cylindrical with the size of 20-40 nm. Also the broad peak was resulted from XRD pattern, confirmed the nanostructure of CuS in new composite. In order to investigate the photocatalyst activity of the new nanocomposite, degradation of methyl orange was studied under UV and visible irradiations.

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Photocatalytic degradation of methyl orange dye by CdS/Cu^{2+} nanoparticles supported on activated pine cone

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Large amounts of colored dye wastewaters released into environment mainly by dyestuff and textile industry lead to severe surface water and groundwater contamination [1,2]. Conventional methods such as physical methods, chemical methods or their combinations are used for decolorization of these dyes [3]. Nevertheless, these methods are usually non-destructive, inefficient, costly and result in secondary pollution. Thus, it is necessary to develop treatment methods that are more effective in eliminating dyes from wastewaters. Cadmium sulfide (CdS) is a kind of semiconductor with narrow band gap of 2.5 eV, and its valence electron can be easily evoked to conduction band under visible light irradiation. Therefore, CdS semiconductor nanoparticles (NPs) have attracted intense interest due to their unique photochemical and photophysical properties. However, CdS NPs are easy to aggregate in aqueous solution and this metal sulfide is prone to photocorrosion. Biological synthesis of CdS NPs by yeasts and bacteria has been reported earlier in 1989, and its photocatalytic activity has been verified.

The detailed information of pine core activated carbon/CdS preparation is described as follows: 0.2mg pine core activated carbon were dispersed in 100 mL 0.01 mol/L Na_2S solution, and then a stoichiometric amount of $Cd(NO_3)_2$ solution was injected dropwise into the above mixture with continuous stirring, at room temperature. After that, the obtained suspension was heated and refluxed for about 11 h under stirring. The final products were filtered and washed repeatedly with distilled water and then vacuum dried at 60 °C.

Cu-doped CdS/C nanocomposite was prepared as a photocatalyst in degradation of methyl orange. pine cone after pyrolized was used as a support for CdS NPs. In order to investigate the photocatalyst activity of the new nanocomposite, degradation of methyl orange was studied under UV and visible irradiations.

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Tungstophosphoric acid supported on diamine-functionalized cobalt nanoparticles, as novel magnetically-recoverable nanocatalysts in acylation of alcohols, phenols, amines and thiols

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Heteropoly acids (HPAs), especially the Keggin-type, as multi-electron oxidants or strong acids have attracted much attention in the recent three decades. Their acid strength is usually higher than many mineral or conventional solid acids [1]. Supported HPA catalysts are important, since they can be easily recovered from reaction mixtures and reused [2]. Nanoparticles have also come into view as high surface area heterogeneous catalysts and catalyst supports; however, they are frequently difficult to remove from the product mixture. Recent studies show that magnetic nanoparticles are excellent supports for various catalysts and can easily be separated and recycled from the products by an external magnet [3,4].

We report the synthesis and characterization of polyoxometalate-diamine functionalized cobalt nanoparticles as novel nanomagnetically-recoverable catalysts and evaluate their catalytic activity in acylation of alcohols, phenols, amines and thiols under solvent-free conditions at 80 °C.

$$\mathrm{RXH} + \mathrm{Ac_2O} \xrightarrow[80\ ^{o}\mathrm{C,\ solvent\text{-}free}]{\mathrm{Cat.\ (0.030\ g)}} \mathrm{RXAc}$$

$$X = O, NH, S$$

Scheme 1

SEM and TEM analyses indicated that nanoparticles were the relatively uniform spherical nanoparticles and average size of catalyst was approximately 65 nm.

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Synthesis of indole derivatives via Fischer indole synthesis catalyzed by boric acid

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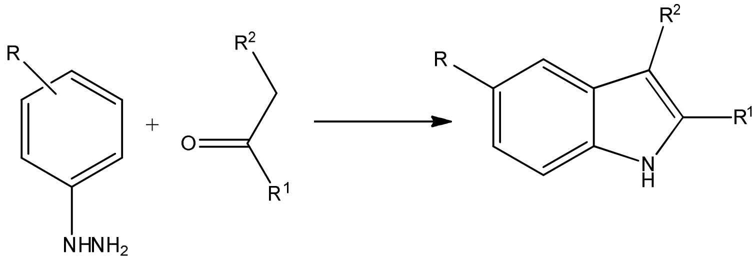
A wide variety of important biological activities havebeen featured by heterocycles containing indolenucleus. Indole frameworks have attracted a plethora ofresearch areas due to the vast applications in materialsciencesand pharmaceuticals. Particularly, anti-inflammatory and anti-tumour activities of some indolederivatives have been proved [1].

In spite of reporting various methods for the synthesis of indoles, Fischer indole synthesis is probably themost widely investigated synthesis of indolederivatives and a large number of newsyntheses or modifications and applications of knownmethods continue to be reported [2-3].

Herein, we wish to reporta facile protocol for the preparation of indolederivatives in high yields from the reaction ofphenylhydrazine derivatives and different carbonylcompounds in the presence of a catalytic amount of boric acid.



Scheme 1

References:

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Synthetic applications of N-Isocyaniminotriphenylphosphorane (Ph3NNC)

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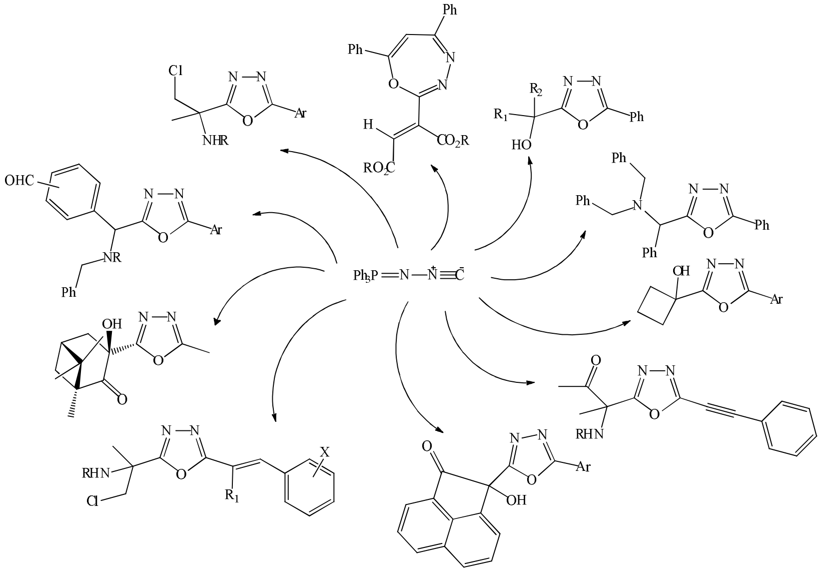
Iminophosphoranes are important reagents in synthetic organic chemistry, especially in the synthesis of naturally occurring products, compounds with biological and pharmacological activity. In recent years, several methods have been reported for the preparation of N-isocyaniminotriphenylphosphorane (Ph3NNC). There are several reports on the use of Ph3NNC in the synthesis of metal complexes. However, the application of Ph3NNC in the synthesis of organic compounds is fairly rare. Ph3NNC has valuable synthetic potential because it provides a reaction system in which the iminophosphorane group can react with a reagent having a carbonyl functionality [1].

As part of our ongoing program to develop efficient and robust methods for the synthesis of heterocyclic compounds, we introduce here some of the synthetic applications of N-isocyanoiminotriphenylphosphorane in the synthesis of heterocycles.



Scheme 1

References:
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2. M. Rouhani, A. Ramazani, S. W. Joo, *Ultrason. Sonochem*. 21 (**2014**) 262.