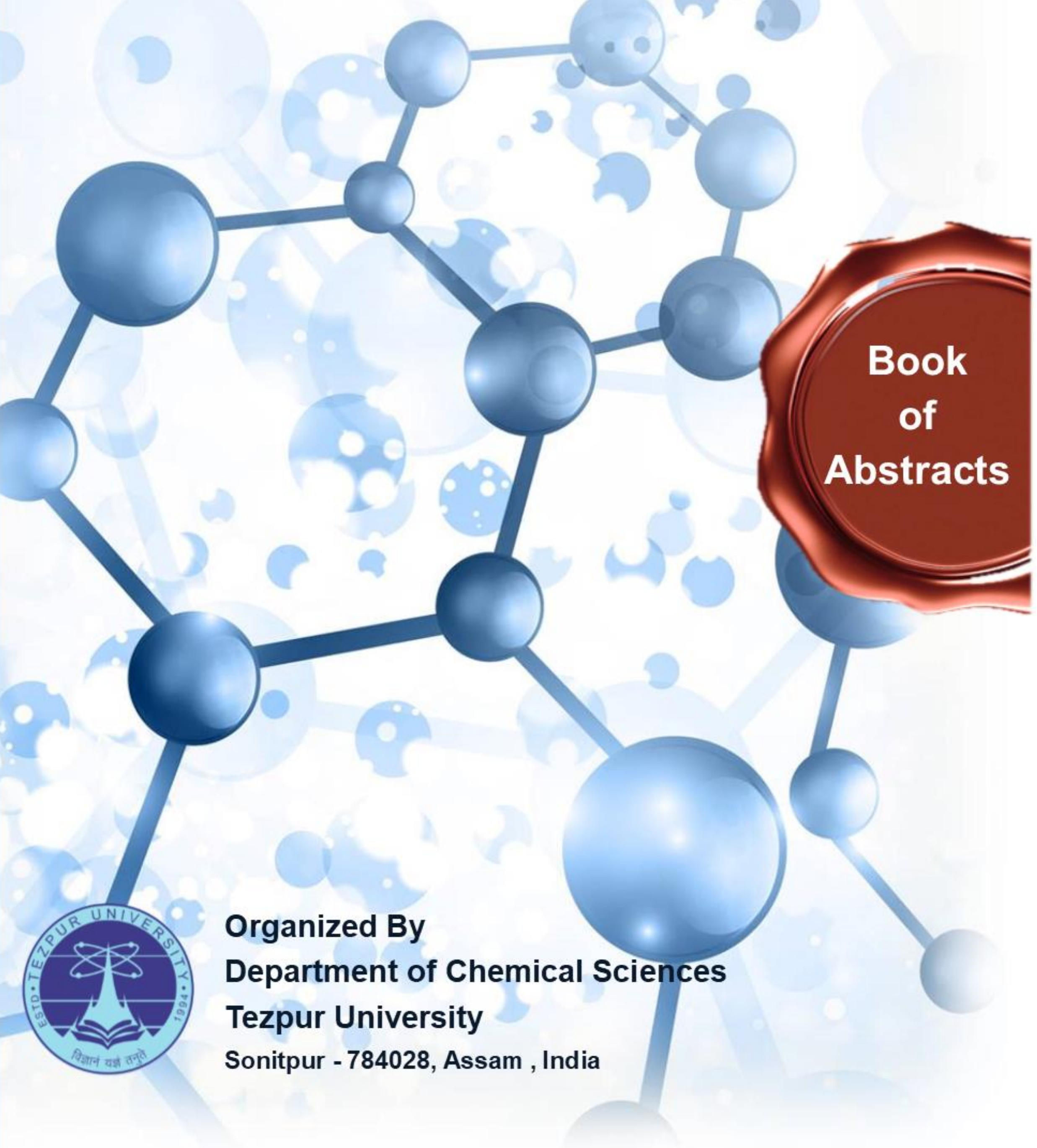
Celebrating 25th Glorious Years of Tezpur University

Organix 2018

An International Conference in Chemistry

20th & 21st December, 2018



Book of Abstracts

Organized By

Department of Chemical Sciences

Tezpur University

Sonitpur - 784028, Assam , India

About Tezpur University: Tezpur University has featured in the top 20 world's best small universities listed by Times Higher Education 2018. TU is NAAC "A" grade university and Visitor's Best University Award 2016 winner. It was established by an Act of Parliament in 1994. The objects of this Central University as envisaged in the statutes are that it shall strive to offer employment oriented and interdisciplinary courses to meet the local and regional aspirations and the development needs of the state of Assam and also offer courses and promote research in areas which are of special and direct relevance to the region and in emerging areas in Science and Technology. (http://www.tezu.ernet.in/)

About the Department of Chemical Sciences: Decorated by well-trained and extremely motivated faculty, technical staff as well as bright students, the Department of Chemical Sciences constantly strives to maintain a culture of excellence in research and uphold the highest standards in chemical education. The Department is supported by DST-FIST and UGC-SAP (DRS-II) level. External funds are received from DST, UGC, CSIR, DBT, DAE, AICTE etc. (http://www.tezu.ernet.in/dcs/)

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About Tezpur University: Tezpur University (TU) was established by an Act of Parliament in 1994, with objectives stating that it shall strive to offer employment oriented and interdisciplinary courses to meet the local and regional aspirations, all the while working towards the development needs of the state of Assam. In addition it offers courses and promotes research in areas which are of special and bear direct relevance to the region and in emerging areas of Science and Technology. It has featured in the top 20 world's best small universities listed by Times Higher Education 2018. TU is NAAC "A" grade university and bagged the Visitor's Best University Award in 2016. (http://www.tezu.ernet.in/)

About the Department of Chemical Sciences: The Department of Chemical Sciences was started in the year 1997, when it offered M. Sc. course in Polymer Science. From July 2006 the Department has been offering M. Sc. program in Applied Chemistry. However, the Department now offers 5-year Integrated M. Sc. in Chemistry, M. Sc. in Chemical Sciences, M. Tech. in Polymer Science and Technology and Ph.D. in the broad areas of Chemistry. Decorated by well-trained and extremely motivated faculty, technical staff as well as bright students, the Department of Chemical Sciences constantly strives to maintain a culture of excellence in research and uphold the highest standards in chemical education. The Department is supported by DST-FIST and UGC-SAP (DRS-II) level. External funds are received from DST, UGC, CSIR, DBT, DAE, AICTE etc. (http://www.tezu.ernet.in/dcs/)

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OrganiX – 2018

An International Conference in Chemistry

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Book of Abstracts

Organized by

Department of Chemical Sciences

Tezpur University, Sonitpur – 784028, Assam
India

Prof. Gautam Radhakrishna Desiraju

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MESSAGE

It gives me great pleasure to participate in OrganiX-2018 which seeks to highlight various aspects of research in organic chemistry, both pure and applied. Organic chemistry is central to chemistry itself and the topics that are being highlighted in this conference only emphasize the very wide scope of this subject. Several experts from India and abroad are attending this meeting which will add to its importance. Tezpur University is an important Central University in the Northeast region and is already gaining accolades and recognition. In general, chemistry in the entire Northeast region needs to be strengthened through new programs, wise faculty hirings and carefully modulated research plans where core and peripheral areas of chemistry are both given importance. Today's peripheral areas become tomorrow's core areas. I am also happy to see adequate representation given to applied chemistry in OrganiX-2018. The Northeast has a unique biodiversity and ecosystem, which need to be properly harnessed in strengthening our research programs. I wish this meeting all success.

GRDesiraju

Prof. Gautam Radhakrishna Desiraju

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MESSAGE

Chemistry is indispensable to Chemical Industry. I am very happy that OrganiX-2018, an International Conference on Organic Chemistry and related subject areas is being organized by Department of Chemical Sciences, Tezpur Central University, Tezpur on December 20-21, 2018 and wish it all success.

M. Lakshmi Kantam

Prof. M. Lakshmi Kantam

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OrganiX-2018

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Web: oganix2018.wixsite.com/tezu

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Dr. Ashim J. Thakur, Prof & Head
Chairperson, OragniX-2018

Dr. Bipul Sarma
Convenor, OragniX-2018

Department of Chemical Sciences
Tezpur University, Assam, India.

Can we think of life without chemistry? Obviously not, because whatever we do that is nothing but chemistry! Specifically, organic chemistry bridges all the branches of chemistry and related interdisciplinary areas.

Hence, it is very important and great necessity to discuss and exchange knowledge in organic chemistry and related areas in details among scientists, users, researchers, students, industries and academia. In order to facilitate that by creating a creative platform, it is our pleasure that the Department of Chemical Sciences, Tezpur University organizes an international seminar OrganiX-2018 purely dedicated to organic chemistry and related areas during Dec 20-21, 2018 at Tezpur University. This is the first one in OrganiX series. This conference will highlight few focused area such as organic synthesis and process development, pharmaceutical research, crystal engineering, surface chemistry and porous materials, catalysis and green chemistry, tea research, polymer and petrochemical research etc. interdisciplinary studies and discussions on future directions of the fields are strongly encouraged. This conference further contemplates to realize a special session to strengthen industry academia relationship.

We were overwhelmed by the immense responses received from the participants.

The support received from Tezpur University in all respects is very commendable, we sincerely acknowledge that.

We are highly thankful to the peers in the area from India and abroad who are going to participate in the seminar. Many companies are also going to showcase their innovative products of interest to the scientific community. The organizers want to express their gratitude to all the sponsors of this event for their generous support.

On behalf of OrganiX-2018 and Tezpur University, we extend our heartiest welcome to the participants of OrganiX-2018. We are looking forward to the success of OrganiX-2018.

Organizing Committee

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OrganiX-2018

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Program Schedule (Tentative)

Day 1 (Date: 20-12-2018)

Time Period	Programme
8:00 AM – 10:00 AM	Desk Registration
Inaugural Session (Council Hall, TU)	
9:00 AM – 9:10 AM (10 min)	Lighting the lamp and release of the book of abstracts
9:10 AM – 9:15 AM (5 min)	Welcome address by convenor, OrganiX-2018
9:15 AM – 9:30 AM (5 min)	Address by the HoD, Chairman, OrganiX-2018
9:30 AM – 9:35 AM (5 min)	Address by Vice Chancellor, Tezpur University
9:35 AM – 9:40 AM (5 min)	Vote of thanks by Joint Convenor
9:40 AM – 10:20 AM (40 min)	**Opening talk** by Prof. Gautam Radhakrishna Desiraju
10:20 AM – 10:55 AM (35 min)	**Keynote Lecture 1** (Prof. Ashwini Nangia)
10:55 AM – 11:05 AM (10 min) Tea Break	
Technical Session-I (Council Hall, TU)	
11:05 AM – 11:40 AM (35 min)	**Keynote Lecture 2** (Prof. Mamoru Koketsu)
11:40 AM – 12:05 AM (25 min)	Invited Talk 1 (Gautam Panda)
12:05 AM – 12:20 PM (15 min)	Short Invited Talk 1 (Navinchandra B. Patel)
12:20 PM – 12:35 PM (15 min)	Short Invited Talk 2 (Ágnes Szegedi)
12:35 PM – 12:50 PM (15 min)	Short Invited Talk 3 (Pranjal K. Baruah)
12:50 PM – 1:00 PM (10 min)	Inauguration of poster session + Photo session
1:00 PM – 2:00 PM (Lunch)	
2:00 PM – 3:00 PM (60 min)	Poster Session (Community Hall, T.U)
Technical Session-II (Council Hall, TU)	
3:00 PM–3:35 PM (35 min)	**Key Note Lecture 3** (Prof. Yusuke Yamada)
3:35 PM – 4:00 PM (25 min)	Invited Talk 2 (Ritu Kataky)
4:00 PM – 4:15 PM (15 min)	Short Invited Talk 4 (Hitesh D. Patel)
4:15 PM – 4:30 PM (15 min)	Short Invited Talk 5 (Bani Kanta Sarma)

4:30 PM– 4:45 PM (15 min) Tea Break		
	Technical Session-III Council Hall, TU	**Technical Session-IV Dept. of Chem Sc. T.U**
4:45 PM – 5:10 PM (25 min)	Invited Talk 3 (Chilla M. Reddy)	Invited Talk 4 (O Mukherjee Singh)
5:10 PM – 5:25 PM (15 min)	Short Invited Talk 6 (Manjit K. Bhattacharyya)	Short Invited Talk 7 (Sanjib Gogoi)
5:25 PM – 5:35 PM (10 min)	OP (Prakash Kanoo)	OP (Sajal K. Das)
5:35 PM – 5:45 PM (10 min)	OP (Anindita Chakraborty)	OP (Anurag Dutta)
5:45 PM – 5:55 PM (10 min)	OP (Pranita Bora)	OP (Blanka Szabó)
5:55 PM – 6:05 PM (10 min)	OP (Kashyap Kumar Sarmah)	OP (Subhasish Roy)
6:05 PM – 6:15 PM (10 min)	OP (Plabita Gogoi)	OP (Rasna Devi)
6:15 PM – 6:25 PM (10 min)	OP (Nazima Sultana)	OP (Subrata Paul)
7:00 PM – 8:30 PM Cultural Evening, Community Hall, T.U		
8:30 PM– 9:30 PM Dinner		

OP= Oral Presentations

Day-2 (Date: 21-12-2018)

Technical Session-IV, (Council Hall, T.U)		
9:00 AM – 9:35 AM (35 min)	**Key Note 4** (Prof. B. M. Reddy)	
9:35 AM – 10:00 AM (25 min)	Invited Talk 5 (Mukut Gohain)	
10:00 AM – 10:15 AM (15 min)	Short Invited Talk 8 (Shardul Sudhakar Kulkarni)	
10:15 AM – 10:30 AM (15 min)	Short Invited Talk 9 (Tejender S. Thakur)	
10:30 AM – 10:40 AM (10 min)	OP (Panchanan Puzari)	
10:40 AM – 10:50 AM (10 min)	OP (Barsha R. Goswami)	
10:50 AM – 11:00 AM (10 min) Tea Break		
	Technical Session-V Council Hall, TU	**Technical Session-VI Dept. of Chem Sc. T.U**
11:00 AM – 11:25 AM (25 min)	Invited Talk 6 (Prodeep Phukan)	Invited Talk 7 (Anil K. Saikia)
11:25 AM – 11:40 AM (15 min)	Short Invited Talk 10 (Pranjal Gogoi)	Short Invited Talk 11 (Pranjal Kalita)
11:40 AM – 11:55 AM (15 min)	Short Invited Talk 12 (Róbert Barthos)	Short invited talk 13 (Anant R. Kapdi)

11:55 AM – 12:05 AM (10 min)	OP (Pranjit Barman)	OP (Kusum K. Bania)
12:05 AM – 12:15 AM (10 min)	OP (Runjun Devi)	OP (Pinaki Bhusan De)
12:15 AM – 12:25 PM (10 min)	OP (Progyashree Goswami)	OP (Manashi Sarmah)
12:25 PM – 12:35 PM (10 min)	OP (Rajarshi Bayan)	OP (Mitu Sharma)
12:35 PM – 12:45 PM (10 min)	OP (Swagata Baruah)	OP (Jahnabi Deka)
12:45 PM – 1:30 PM Lunch Time		
Technical Session-V (Council Hall, TU)		
1:30 PM – 1:55 PM (25 min)	Invited Talk 8 (Jubaraj B. Baruah)	
1:55 PM– 2:10 PM (15 min)	Short invited talk 14 (Naba K. Nath)	
2:10 PM–2:20 PM (10 min)	OP (Rituparna Duarah)	
2:20 PM– 2:30 PM (10 min)	OP (Bably Khatun)	
2:30 PM– 2:40 PM (10 min)	OP (Khairujjaman Laskar)	
2:40 PM– 2:50 PM (10 min)	OP (Pangkita Deka)	
2:50 PM– 3:00 PM (10 min)	OP (Kabirun Ahmed)	
3:00 PM–3:10 PM (10 min)	OP (Aditi Saikia)	
3:10 PM– 3:30 PM (20 min) Tea Break		
Technical Session-VI (Council Hall, TU)		
3:30 PM- 3:55 PM (25 min)	Invited talk 9 (Parthasarathi Das)	
3:55 PM- 4:10 PM (15 min)	Short invited talk 15 (Lakhinath Saikia)	
4:10 PM- 4:30 PM Valedictory Note		
8:00 PM– 9:30 PM Dinner		

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Keynote Lecture

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Opening Talk by:

Prof. Gautam Radhakrishna Desiraju

Indian Institute of Science, Bangalore

Keynote Lectures

Chemical Processes for a Sustainable Industry

Ashwini K. Nangia

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The chemical industry is undergoing a transformation towards processes which are minimal in generating waste, optimize costs and logistics of raw materials sourcing, manage energy, heat and cooling, and carry out the production of chemicals in a safe and economical manner. The shift from batch reactors to flow processes, use of selective catalysis, biomass and crop-waste feedstock, recycling and regeneration of by-products to useful chemicals, energy grid loop, and digitization of chemical processes are integral parameters in this change. In order to mitigate the overuse and dependence on fossil fuels and naphtha, biomass feedstock and biorefinery are the beginning of a new chemistry and chemical industry paradigm. Examples from crystal engineering, catalysis, agrochemicals, biomass, fine chemicals, pharmaceuticals and polymers will be presented as case studies.

Chemistry and Catalytic Applications of Cerium Oxide

Benjaram M. Reddy

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Environmental issues such as air pollution, water pollution, and excessive natural resources consumption represent some of the most formidable challenges facing the global humanity today. Recent developments in nanoscience and nanotechnology are playing a key role in addressing some of the environmental and energy related problems. Selection of a suitable material and an appropriate synthetic methodology ultimately determines the success or failure of a nanostructured material towards application, since the physicochemical properties are heavily dependent upon how they are synthesized. Ceria (CeO_2), an abundant rare-earth metal oxide, has attracted considerable research interest in recent years owing to its extensive utilization in environmental and energy related applications.[1-4] The significance of ceria originates from its remarkable Ce^{4+}/Ce^{3+} redox couple and superior oxygen storage/release capacity (OSC). Ceria serves both as a promoter and as an active catalyst in three-way catalytic converters for abatement of hazardous exhaust emissions.[4-9] As well, the catalytic activity of ceria for soot combustion has also been investigated recently and proven to be a potential material. Therefore, numerous studies were undertaken on the application of ceria-based materials for various reactions. Nevertheless, a significant limitation encountered with pure ceria is its poor thermal stability, resulting in the loss of surface area and OSC, hence poor catalytic performance. An ongoing challenge in this respect is to develop efficient and thermally stable ceria–based catalysts in order to meet more demanding requirements. There are two promising options available for improving the properties of CeO_2, namely, doping of suitable rare-earth or transition metal ion into the ceria lattice and reducing the ceria particle size into nanoscale. Our recent investigations revealed that incorporation of an appropriate dopant into the ceria matrix greatly enhances its redox properties and chemical reactivity. In particular, small ionic size and low valence state dopants show strong influence on the physicochemical properties of the resulting materials. More details of these studies will be elaborated in this presentation.

References

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2. Mukherjee, D. and Reddy, B. M. *Catal. Today* 2018, 309, 227.
3. Mukherjee, D., Swamy, P. V., Devaiah, D. and Reddy, B.M. *Catal. Sci. Technol*. 2017, 7, 3045.

The Era of Organic Selenium Chemistry: Synthesis of Selenophene-based Heteroacene Scaffolds

Mamoru Koketsu

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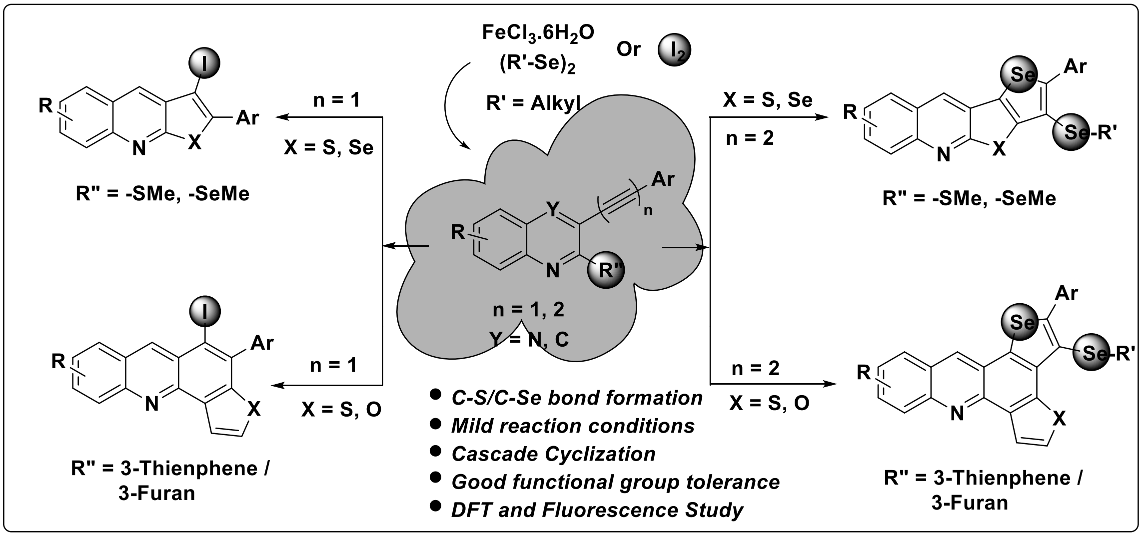
Gifu University, Gifu 501-1193 Japan.

Herein, we are presenting the recent advances in organic selenium chemistry, Biological importance and Novel methodologies. Iodine as well as Fe(III) promoted the regioselective intramolecular cascade cyclization for the construction of quinoline and quinoxaline fused selenophene-based Heteroacene scaffolds. Further their DFT study and fluorescence study was carried out. Diversified internal nucleophiles were used to afforded quinoline and acridine based cores. We believed that this methodology provides a novel pathway for the synthesis of linear alkynes as well as quinoline and quinoxaline fused two and three membered heterocycles.



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Catalysts Utilized for Artificial Photosynthesis with a Molecular Light Harvesting Unit

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Increase of global energy consumption is a critical threat for human beings, because fossil fuels are depletive resources and greenhouse gas is emitted after burning. Production of fuels such as hydrogen and hydrogen peroxide using solar energy by an artificial photosynthesis would be promising to mitigate the threat. Artificial photosynthesis systems for hydrogen evolution usually composed of a photosensitizer, a hydrogen-evolution catalyst and an electron donor. The systems can evolve hydrogen under photoirradiation, however, the electron donor should be replaced by water to realize sustainable society. Thus, highly active water oxidation catalysts should be developed in which water oxidation accompanies with transfer of four electrons and four protons to generate molecular oxygen. I report herein highly active catalysts developed for both hydrogen evolution and oxygen evolution. The catalytic activity of metal nanoparticles active for hydrogen evolution can be tuned by metal particles size, shape and crystal structure.[1] These metal particles can be functionally assembled with a photosensitizer on various solid supports such as porous metal oxides, assembly of metal oxide nanoparticles, and porous protein crystals.[2] Highly active water oxidation catalysts can be obtained using not only mixed metal oxides[3] but also coordination polymers. Artificial photosynthesis employing the coordination polymers as water oxidation catalysts is disclosed to generate hydrogen peroxide from water and molecular oxygen.

References

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Invited Lectures

Stereoselective Synthesis of Heterocyclic Compounds

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Cyclic ethers and their nitrogen and sulphur analogues have undoubtedly attracted the interest of synthetic chemists due to their occurrence in many natural products, and pharmaceuticals.[1] Development of novel highly efficient procedures for the synthesis of these molecules is of current interest. These procedures must be compatible with our environment and should have economical advantages. In such an approach the reduction of number of steps and increase in selectivity is a valuable standard for the quality of a synthesis. A general way to improve synthetic efficiency is the design of a selective transformation either in a regio-, diastereo- or enantio-selective fashion. Recently, we have developed a few methodologies for the regio-, diastero- and enantio-selective synthesis of oxygen, nitrogen and sulphur heterocyclic compounds using Prins, ene and related reactions.[2] Some of these methodologies are used for the synthesis of biologically active molecules. Detailed results will be discussed in the meeting.

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Mechanical Properties of Organic Crystals: Knowing the Limits

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It has been shown recently that certain molecular crystals can be flexed into different shapes by applying suitable external mechanical stress.[1-4] Crystal structure based deformation mechanisms have been proposed for plastic and elastic crystals, while nanoindentation experiments revealed that the elastic modulus (E) of most organic crystals is typically in the range of 0.1-15 GPa and hardness (H), in the range of 0.01 to 1 GPa. The plastic and elastic crystals are known as soft, having these values on the lower side. Our recent nanoindentation and spatially resolved crystal structure analyses of bent crystals revealed that the current understanding of mechanical limits of organic crystals is very poor and there remain many unexplored opportunities for achieving organic crystals that are as hard as soft-metals and ceramics, yet with low weight and mechanical flexibility.

Fig. Elastically bent organic crystal.

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Amino Acids Towards Anticancer Natural Products and Steroidomimetics: Rays of Hope?

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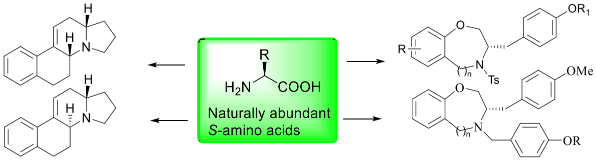
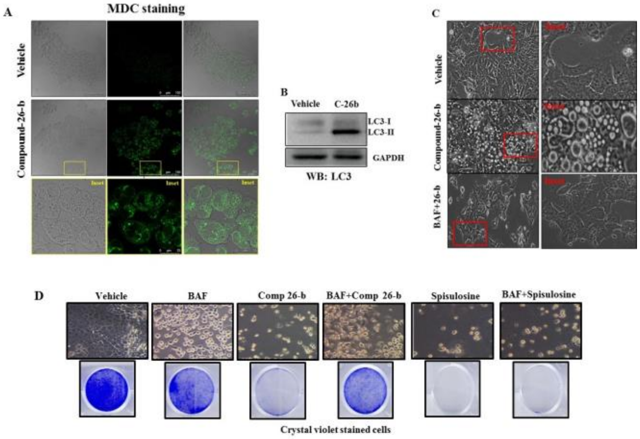
Chirality derived from amino acids based steroidal and non-steroidal architectures provide new and easy to incorporate chiral chemical space which otherwise very difficult to introduce and comprising of several synthetic steps for asymmetric steroids. The different and exciting ligand-receptor interactions arise from the use of each enantiomer of amino acids. The ring A and D of steroidal architectures can be mimicked through phenyl group of amino acid tyrosine. Promising biological activities related to hormonal disorders were observed from these benzofused amino acids derived steroidal and nonsteroidal molecules. Amino acids derived natural products promoted robust autophagic cell death to cancer cells instead of classical apoptosis.





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Dissimilarities in the Fluorescence Emission Properties in Solid-state than in Solution

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The lecture will be on emission properties in solid and solution state of certain critically chosen examples of fluorescent compounds. The role of emission mechanism, conformation, aggregation influencing the fluorescence emission will be discussed. The influence of water molecules and coformers to modulate emission properties will be shown.

Industrial Process Research and Process Development of Active Pharmaceutical Ingredients (APIs)/or Commercial Demand Chemicals

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Process chemistry is the practical application of organic synthesis. The timely supply of high-quality active pharmaceutical ingredients (APIs)/chemicals having commercial demand depends on efficient process chemistry. In process research and development (PR&D), the generation and manipulation of commercially demand chemicals ranges from bench-scale (laboratory) chemistry to pilot plant manufacture to commercial production. For a chemical process to be functional on commercial scales, the developed process should be operationally simple, repeatable, safe, and straightforward. The developed process should be ecofriendly as well. Ideally reactions should use commercially available inexpensive, environmentally benign starting materials, reagents, and solvents and produce the target compound with high yield and high quality as well, with a minimum of impurities that are easily removed, preferably by recrystallization or treatment with suitable solvent/solvent system. If, the process is catalytic, turnover numbers and turnover frequencies must be high and the product must be free of trace contaminants such as heavy metal salts or complexes. However, a few synthetic transformations meet these rigorous criteria. During development, a process chemist needs to understand completely the chemistry involved and conducts reactions aimed at finding the limits of acceptability of critical variables. A broad range of disciplines, including process chemistry (synthesis), analytical chemistry, process engineering (mass and heat transfer, unit operations), process safety (chemical risk assessment), regulatory compliance, IPR, and plant operation, must be effectively applied during process research and development for successful commercial standard process and hence technology for manufacturing of Active Pharmaceutical Ingredients and Commercial Demand Chemicals as well.

Synthesis and Photophysical Properties of New Indole Derivatives

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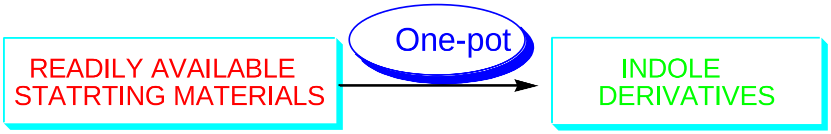
The chemistry of indole is one of the most exciting and challenging area in the field of heterocyclic chemistry.[1] The significant application of indole derivatives in pharmaceuticals, agrochemicals and organic electronics continues to inspire the tireless efforts of synthetic organic chemists since time immemorial. New concepts and methodologies have been developed in recent times to access various indole derivatives.[2]

Thus we have been working on the designing of synthetic methods of indole derivatives staring from easily available synthons[3] and also investigating on the bioactivities of the newly synthesized indoles. Interesting, photophysical properties of certain indole containing Cyan Flourescent Protein chromophore analogs have been reported recently.[4] In this presentation our experience towards the synthesis of new indole compounds will be discussed.



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Expanding the Medicinal Chemistry Toolbox to Access New Chemical Space in Drug Discovery

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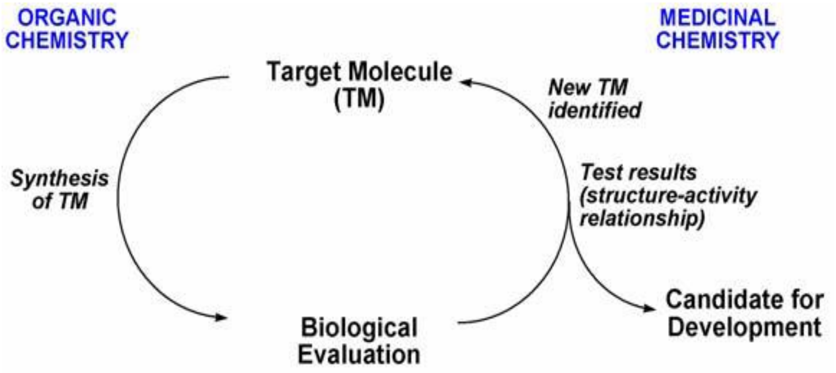
Identification of small molecule leads in drug discovery has been largely dependent on organic synthesis to deliver the designed ligands against target proteins. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered an insurmountable synthetic challenge. In turn, the pharmaceutical industry, where large numbers of molecules are prepared and tested for their therapeutic use became the principal end-users and beneficiaries of this enlarged toolkit. Designing and discussing of various synthetic tools for the synthesis of medicinally important heterocycles and generation of new chemotypes with translational potential will form the basic premise of my presentation.[1]



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Metal-free Amino-functionalization Reactions using $TsNBr_2$

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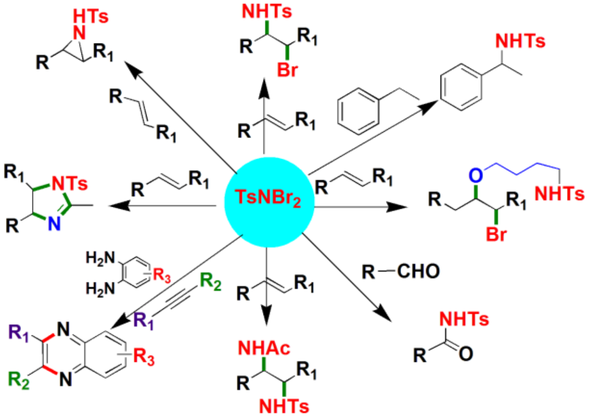
N-Halo-sulfonamides such as NN-dibromo-p-toluene sulfonamide ($TsNBr_2$), are efficient and powerful reagents for various organic transformations. $TsNBr_2$ has been found to be very effective for reactions such as vicinal bromofunctinalization of olefins, oxidation of alcohols, bromination of aromatic compounds, aminofunctionalization of olefins, C-H amination etc.[1] Most importantly, the reactions could be carried out without using any catalyst. This reagent can also be used for generation of sulfonyl nitrene in presence of a base under mild condition. Aziridines could be successfully synthesized via a nitrene insertion process at room temperature within a short time without the aid of any catalyst.[2] This strategy could further be utilized for activation of C-H bond of alkyl aromatics and aldehydes to produce corresponding Ts-amines and amides respectively.[3] Treatment of olefins with the reagent under appropriate condition leads to various amino-functionalized products.[4] Alkynes can be very easily converted to corresponding quinoxalines using this reaction without any catalyst.[5] This presentation highlights the salient findings of our research group in this area.



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Electrochemical Investigations of Interactions at Soft Interfaces

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Interactions at the interface between two immiscible liquids are of interest both for fundamental studies and practical applications. This talk will focus on diverse aspects of interactions at a liquid-liquid interface.

1. Tethered bilayers lipid membranes (tBLMs) are commonly used as model membranes. However in biophysical studies free-standing membranes or 'black' lipid membranes are more realistic models of cellular processes. BLMs modified using two important mitochondrial membrane associated molecules – Ubiquinone-10 (UQ10) and α-tocopherol (VitE) an coupled electron transfer rates with NAD^+/NADH, using electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) will be discussed.
2. The investigation of interactions of drugs with proteins is another area of fundamental importance in drug discovery and toxicity studies. A micro liquid-liquid interface can be used very effectively for quantifying drug-protein interactions. Chiral discrimination of the enantiomers of a basic drug, propranolol, was achieved at a micro liquid-liquid interface, using α1-acid-glycoprotein (AGP) as a chiral acute phase plasma protein.
3. Accumulation of aggregated amyloid-β peptide (Aβ) in the brain is a pathological hallmark of Alzheimer's disease (AD). The Aβ peptide is amphiphilic and accumulates preferentially at a hydrophilic/hydrophobic interface. In this study $A\beta_{42}$ was introduced to an aqueous phase in a two-phase system with 1,2-dichloroethane (1,2-DCE). The interactions of $A\beta_{42}$ with redox active metals ions such as copper were studied at an electrified liquid-liquid interface (interface between two immiscible electrolyte solutions, ITIES). Binding constants were evaluated. Results showed that $A\beta_{42}$ bound two molecules of copper with binding constants of $K = 1.2 \times 10^6$ M^{-1}, $n = 1.6$ and $K = 31.6$ M^{-1}, $n = 1.3$. Further, complexation of Cu-$A\beta_{42}$ with a multifunctional peptidomimetic inhibitor (P6), based on a naturally occurring metal chelating tripeptide (GHK), and an inhibitor of $A\beta_{42}$ aggregation, was monitored at the ITIES. A combination of electrochemical, optical microscopy, circular dichroism and electrochemical methods proved an efficient means to study the aggregation, effects of redox active metal ions and inhibitory drugs.
4. Metallic nanoparticles (NPs) such as gold, silver and copper are used widely in pharmaceuticals, medical and biological applications. The effect of material, size, surface charge and surface charge density have a significant effect on the interaction of NPs with lipid membranes. The work reports the comparison of metal NPs (gold, silver and copper) and their interactions with lipid membranes using electrochemical, impedance and microscopy techniques. Size, charge and incubation time dependent interactions will be presented. The differential behaviour of AuNPs modified with anionic, cationic and zwitterionic ligands will be demonstrated.

Short Invited Lectures

SBA-15 Supported Copper Ferrite Catalysts for Total Oxidation of Toluene

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Catalytic total oxidation is an efficient method for the removal of low concentration of volatile organic compounds (VOCs) including various aliphatic and aromatic compounds from air. Transition metal oxides are alternatives to expensive and poison sensitive noble metals in the supported catalysts of the process. With their high specific surface area and uniform pore structure ordered mesoporous silica materials are excellent supports for transition metal oxide catalysts. Bimetallic oxide catalysts, such as copper ferrite ($CuFe_2O_4$), show favorable catalytic properties as compared to monometallic compositions.

SBA-15 supported mono and bimetallic Cu-Fe catalysts, with 10 wt.% metal content were prepared by incipient wetness impregnation technique with the nitrate salts of the metals. In bimetallic preparations the Cu/Fe atomic ratio corresponded to 1:2, such as in copper ferrites. Catalysts were heat treated for salt decomposition at different temperatures (350-450 °C) and in gas media (air, NO/He).

Textural investigations (XRPD, N_2 physisorption, TEM) revealed that by the applied impregnation method the salts penetrated into the channels of the silica, and hardly any separate oxide phase could be detected. On monometallic catalysts copper oxide with different crystallite sizes, whereas on bimetallic preparation only finely dispersed (< 8 nm) copper ferrite phase was observed. Heat treatment in air resulted in bigger metal oxide particles as well as in stronger interaction with the silica wall, depending on the pore size (6 or 8 nm) and silanol groups density of the support. Salt decomposition in NO/He favored the formation of finely dispersed metal oxide nanoparticles and hindered the formation of metal silicates. Spectroscopic methods (UV-Vis, Mössbauer sp.) supported that ionic metal species and nanosized metal oxide particles are generated in the mesopores of the support.

Catalysts with finely dispersed copper oxide or copper ferrite species showed high catalytic activity in total oxidation of toluene below 350 °C. Copper ferrite catalysts, independently of the pretreatment procedure, exhibited high stability in the reaction due to the peculiar reduction behavior of copper ferrite phase. Reduction of the latter up to 500 °C results in the formation of highly dispersed metallic copper confined and stabilized in a magnetite structure. In contrast, in copper oxide catalysts the agglomeration of oxide particles and fast deactivation cannot be avoided even by confinement of particles in the nanopores of silica support.

Operando FT-IR investigations evidenced the different reaction mechanism of toluene oxidation on the studied catalysts.

Phosphatriazenes: Versatile Ligands for Bio-Active Molecules Modification via Sustainable Palladium Catalysis

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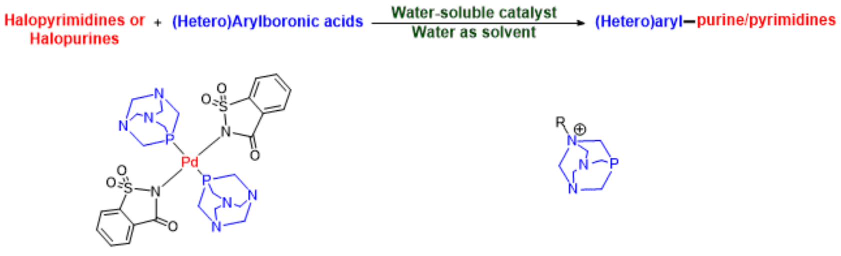
Functionalization of nucleoside heterocycles by transition metal catalysed cross-coupling reactions are important tools to prepare modified nucleoside analogues. Palladium-catalyzed cross-coupling reactions are powerful methods to attach carbon (hetero) atom groups to the heterocyclic base. These nucleoside analogues after modification show high fluorescence and biological activity. The 1st generation palladium complexes allowed the modification of nucleosides in water as the sole reaction solvent for all 4 nucleosides at relatively low catalyst loading. Despite achieving the desired reactivity with the 1st generation catalytic system, column-free isolation of the products or recyclability of the catalyst was not possible. A rational ligand design was therefore needed for the development of 2nd generation Phosphatriazene-based ligands which allowed us to achieve the above objectives. The efficiency of the 2nd generation has also allowed the development of low temperature protocols for accessing useful heteroarenes as well as drugs.



First Generation Water-Soluble Pd-Imidate Complexes

Second Generation Water-Soluble Sultone Ligands

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Carbonyl-Carbonyl Interactions in Small Molecules and Proteins

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The carbonyl group is ubiquitous in both chemistry and biology. Apart from being involved in numerous chemical transformations, it can also participate in various distinct weak noncovalent interactions including hydrogen bonding (C=O⋯H-X)[1], carbonyl-chalcogen interactions[2] (C=O⋯X; X = S, Se, Te) and nucleophile-carbonyl interactions[3] (Nu⋯C=O). In recent years, carbonyl-carbonyl (CO⋯CO) interaction[4] has emerged as an important weak interaction in chemistry and biology. It is known to contribute to the stabilization of many important small- and macromolecules including peptides and proteins.[5] The CO⋯CO interaction is believed to be $n \rightarrow \pi^*$ in origin wherein the lone pair of the oxygen atom of a carbonyl group is delocalized over the π^* orbital of C=O bond of another nearby carbonyl group. Despite its growing importance, many aspects of the this interaction such as dependence of its nature on the relative orientation of the two interacting carbonyl groups, the role of this interaction in the stabilization of polyproline (PPII) helix and the scope of controlling three-dimensional shapes of peptidomimetic oligomers and drug-like small molecules using this interaction are still not clearly understood. Recently, we discovered the “reciprocal” variant of CO⋯CO interaction in small molecules and proteins, especially in PPII helices.[6] Our recent investigations revealed that there are at least six different ways in which two carbonyl groups can engage in CO⋯CO interactions of which only two have been observed in proteins so far.[7] In this talk, I will discuss our current understandings of CO⋯CO interactions with a focus on the “reciprocal” variant. I will also discuss about the various structural motifs of CO⋯CO interactions and put forward a hypothesis that could explain the stabilization of polyproline II helices based on CO⋯CO interactions.

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Liquid Phase Pyrolysis of Wheat Straw and Poplar in Hexadecane Solvent

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There is a need for replacement of fuel, especially transportation fuel, obtained from fossil resources by bio-based alternative. The thermochemical conversion of lignocellulosic material is a feasible method to degrade and partially deoxygenate natural polymeric materials to get bio-oils as fuel precursors. The degradation of lignocellulosic materials in none-hydrogen donor organic solvent referred to as degradative extraction (DE) or liquid phase pyrolysis (LPP). According to LPP method lignocellulosic material is treated at ~350°C under liquid phase organic solvent and inert atmosphere at relatively low pressure (max. 20 bar). The solvent acts as a heat carrier, having high heat transfer rate, and as media for extracting and dissolving degradation products. The method gives three types of solid materials: (i) solvent-insoluble residue (ii) extract insoluble at room temperature (iii) extract soluble at room temperature. Gases, mainly CO_2, and liquid, non-miscible with the applied solvent, mainly H_2O, also form. Our research is focused on the better understanding of the mechanism of lignocellulose degradation in the LPP process. Reactions were executed in Parr-type autoclave. Effect of solid acid and base catalysts, such as BEA zeolite, Nafion®, Amberlyst 15, and Mg,Al-Layered Double Hydroxide on the product yields was examined. The reaction products were analysed by means of CHNO elemental analysis, GC-MS, ^1H and ^{13}C NMR spectroscopy. The carbon and oxygen mass balances were determined in order to optimize the conditions of carbon transfer from lignocellulose to bio-oil. About 40-49 wt% of lignocellulosic carbon was successfully transferred to hexadecane. The best carbon yields were achieved at 350 °C. The main extracted products were alkyl and alkoxy derivatives of phenol and furan derivatives. By comparing seven parallel experiments in presence and absence of the catalysts no or only negligible catalytic effect was observed. The effect of heterogeneous catalysts was manifested only in splitting the primarily extracted macromolecules. The carbon/oxygen mass balances suggest that the extracted compounds have relatively high residual oxygen content.

Acknowledgements

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NCE Development for Therapeutic Use as Anti-Malarial Agent through Computational Chemistry

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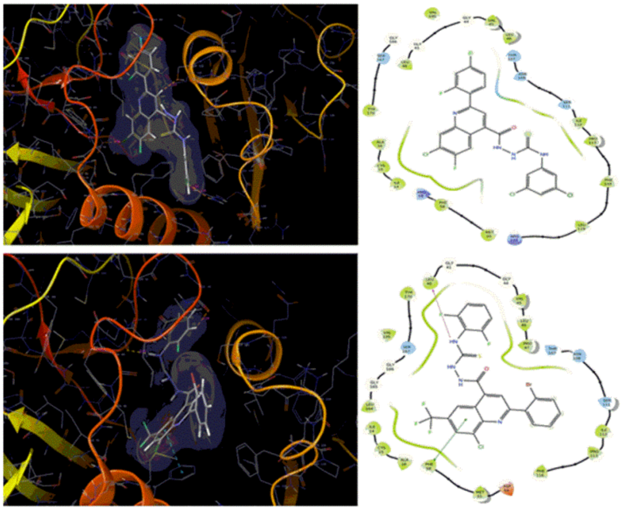
Computational chemistry is playing vital role in the field of the drug discovery, which is known as CADD – Computer Added Drug Design. It reduces the time period of the drug discovery and improves the chances of the success. The easiest way for chemist to design the NCE is, selection of the target structure of the receptor and then design of the ligands (one of the way of CADD). During our research work we have used structures of receptor from RCSB PDB.[1] All designed compounds were synthesised through green chemistry routes, purified and well characterised. The compounds were screen against the *Plasmodium falciparum* by using modified method of microassay protocol.[2] The effectiveness of NCE confirmed by comparison with standard drugs. SAR study of the NCE carried studied by possess of receptor-ligands and the presence of the functional groups.



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$Fe(OTf)_3$: An Efficient Catalyst for Michael Addition Reaction of Homoaromatic C-H Nucleophiles with Nitrostyrenes

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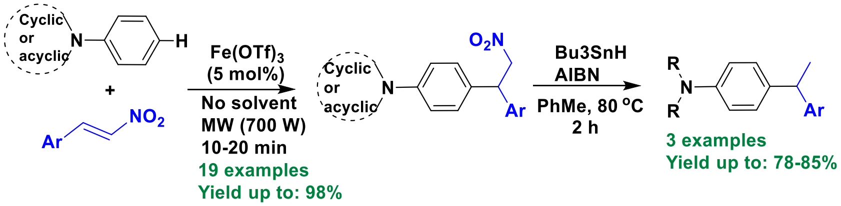
Michael adducts of *N,N*-dialkylanilines/their cyclic analogs with nitrostyrenes constitute an important class of organic compounds as the $-NO_2$ groups present in the molecules can easily be transformed into diverse functionalities. Unlike other subtypes (*aza*-, *phospha*-, *thia*- etc.), Michael addition of homoaromatic C-H nucleophiles with nitrostyrenes are found to be less explored. An $Fe(OTf)_3$ catalyzed methodology for Michael addition of aromatic C-H nucleophiles (*N,N*-dialkylanilines/their cyclic analogs) with nitrostyrenes under microwave irradiation and solvent-free condition has been developed and presented herein. Compared to the few procedures available,[1-4] the current methodology is capable of reducing the time requirement by a huge margin from many hours to a few minutes and is quite general. The regioselectivity of addition of *N,N*-dialkylanilines/their cyclic analogs is observed to be exclusively *para.* The worth of the synthesized Michael adducts is checked by denitrohydrogenating three numbers of our synthesized products to their corresponding alkylated arenes, a set of compounds which can otherwise be synthesized by direct hydroarylation of unactivated olefins.[5-6] However, the two-step approach proposed herein, which consists of Michael addition of nitrostyrenes followed by denitrohydrogenation enjoys a significant advantage over many single-step procedures as it avoids the regioselectivity issue faced in the later. As such, it paves a way for effective regioselective synthesis of *p*-alkylated *N,N*-dilalkylanilines starting from nitrostyrenes & *N,N*-dilalkylanilines in a two-step process.



Scheme 1: Two-step synthetic route for *p*-alkylated arenes

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Cooperative Interplay Involving Weak Supramolecular Contacts in Coordination Solids of Transition Metals

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The construction of supramolecular networks with fascinating structures and interesting properties in crystal engineering is mainly due to the assemblies generated through a variety of cooperative non-covalent interactions.[1,2] The intelligent utilization of cooperative non-covalent interactions to obtain aggregates that function differently from the components of the structures is the paradigm of supramolecular chemistry.[3] Among many non-covalent interactions, those involving halogen, chalcogen and pnicogen atoms have attracted considerable attention in recent years and they are increasingly being recognized by scientists in the field of supramolecular chemistry, crystal engineering and biochemistry.[4] In addition, unconventional sigma- and pi-hole interactions also found important to the stabilities of supramolecular networks and might thus be equally useful for coordination solids.[5]

We have investigated structures of a few coordination solids of transition metals and characterized by single crystal X-ray diffraction, elemental analysis, FT-IR, electronic spectroscopy and TGA. The structures are stabilized by interesting weak non-covalent interactions involving halogen and chalcogen atoms. Cooperative sigma- and π-hole interactions are also energetically significant for a few coordination solids.

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Multi-Stimuli Responsive Smart Molecular Crystal

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Research on stimuli responsive molecular crystals have witnessed tremendous development in last couple of years due to their probable applications as actuators, sensors, dynamic components of micro or nano machineries etc. These mechanically responsive molecular crystals can respond to light and heat by jumping (photosalient and thermosalient effect), bending, coiling, twisting, rolling or even walking.[1,2] In addition to that certain crystals when mechanically impacted undergo elastic or plastic deformation. In recent times, several classes of compounds were discovered, molecular crystals of which display impressive stimuli response. However, these crystals are mostly responsive towards a single stimulus and examples of materials that are capable of responding to multiple external stimuli are scarce. In my presentation, recent discoveries on multi-stimuli responsive molecular crystals by our research group will be focussed. We have discovered several materials, molecular crystals of which display impressive responsiveness when UV light and mechanical force is applied. In addition to that the first example of multi-stimuli responsive smart molecular crystal of a 2:1 cocrystal of probenecid and 4,4′-azopyridine is also demonstrated recently.[3] The acicular crystals of this multi-component material undergo photomechanical bending / unbending, thermomechanical twisting / untwisting and mechanical force induced reversible deformation. An additional property displayed by the crystals is their ability to self-heal upon heating and cooling. All the four properties displayed by the molecular crystals were explored from mechanistic and kinematic point of view.

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In vitro Antimicrobial, Anti-Mycobacterium and Anti-Protozoal Activity of Pyridine and 1,3,4-Oxadiazole Bearing Scaffolds: Their *in-silico* Molecular Docking, Molecular Stimulation and ADME Studies

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Currently, "Neglected Diseases" such as Chagas, malaria, tuberculosis and leishmaniasis disease are still serious public health problems in developing countries and their prevalence continues to increase, because of the constant migratory flow in endemic countries new strategies to speed drug development to treat these diseases are required. Moreover, the increasing rate of bacterial resistance to clinical antimicrobial agents is the major problem that facing world today. For example, fluoroquinolones and third and fourth-generation cephalosporins resistant *Escherichia coli*, Methicillin-resistant *Staphylococcus aureus*, same as in the case of *Mycobacterium tuberculosis*, isoniazid (INH) and rifampicin (RIF) resistant *M. tuberculosis*, was the most commonly observed type. This provides a great opportunity to synthetic chemists for the synthesis of new compounds possessing lower cytotoxicity and with better antimicrobial potency. Compounds containing pyridine and 1,3,4-oxadiazole cores have a broad spectrum of different biological activities. The ability of these heterocyclic compounds to undergo various chemical reactions has made them important for molecule planning, such as, 1,2,4-triazole, Manich base, Schiff base, etc., using various amino benzimidazoles, qunaxolines, benzothiazoles etc. with enormous biological potential. All the newly synthesized scaffolds were subjected to *in vitro* anti-bacterial (*S. aureus*, *S. pyogenes*, *E. coli*, and *P. aeruginosa*), anti-fungal (*C. albicans*, *A. niger*, and *A. Clavatus*), anti-mycobacterial (*M. tuberculosis* $H_{37}Rv$), anti-malerial (*P. falciparum*) anti-tryponosomal (*T. cruzi*) and anti-leishmanial (*L. Mexicana)* activity**.** Moreover, short-term *in vivo* model on *Trypanosoma cruzi* has also been studied with one of the derivative containing 1,3,4-oxadiazole. We have also carried out *in silico* molecular docking study of our targeted compounds with different PDBs as biological target to understand binding interaction of targeted compounds. The molecular dynamics (MD) simulations are performed for up to 20 ns simulation time investigating the stability of a ligand–protein complex. *In silico* ADME properties of all synthesized compounds have also been calculated to determine their drug-likeness properties and compared it with standard drug.

ortho-Functionalizations of Arenes *via* Arynes and Their Applications

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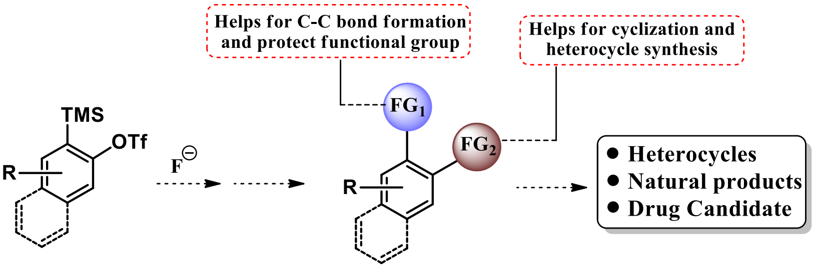
Arynes are one of the most important classes of organic species that have received tremendous attraction to chemist over the past few years and many valuable transformations comprising this intermediate has been developed.[1] Most importantly, this synthetic intermediate have extensively used for the synthesis of several complex natural products. Additionally, they have been used for the direct synthesis of *ortho*-disubstituted arenes through sequential reaction strategy in a single reaction vessel. Such synthetic strategy allows a rapid and straight forward access to benzene derivatives having molecular complexity and structural diversity. Moreover, such transformations help to achieve the synthetic targets in a shorter way by further modifying the newly installed functional groups. Our group has been working on this highly reactive transient intermediates for the one-pot synthesis of 2-formylarylsulfonate, 2-aroyl benzofurans, *ortho*-formyl allyl aryl ethers, 2*H*-chromen-2-ol derivatives, isocoumarin and coumestans derivatives.[2]



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Waste Materials: Heterogeneous Catalyst

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Due to global warming and climate change, more attention is now being paid for renewable feedstocks such as lignocellulosic biomass due to their easy availability for production of platform chemicals such as 5-hydroxymethylfurfural (HMF) and furfural (FF). Such greener routes for producing value-added compounds include liquid bio-fuels in the ranges of C8-C15 through aldol-condensation followed by catalytic hydrogenolysis or hydrogenation or hydrodeoxygenation. In the present work, we have synthesized well-ordered different loading of triflic acid functionalized KIT-5 mesoporous materials. The mesoporosity and structure of synthesized mesoporous materials were characterized by PXRD and HRTEM techniques. Moreover, FTIR and HRSEM-EDS studies confirmed the incorporation of triflic acid into KIT-5 materials. For model reaction, we have taken fructose and xylose as starting material to obatin HMF and FF. The yield of the desired products HMF and FF were found to be 80 and 75% within 6 h, respectively. The yield of the product could be explained on the basis of total acidity of the catalyst.

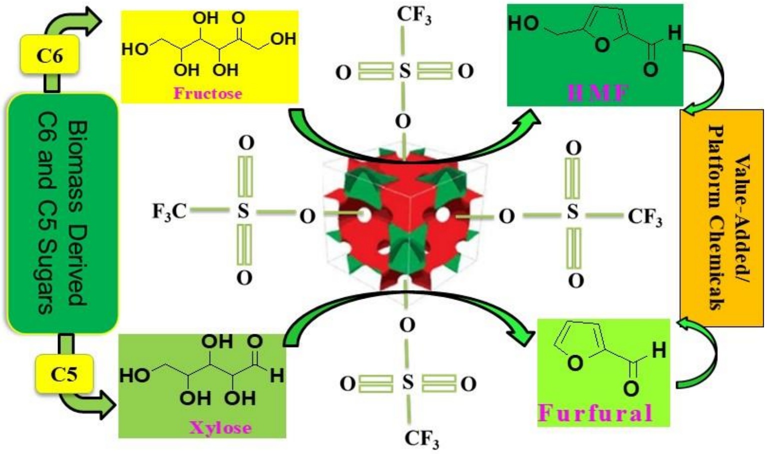

Figure: Conversion of Biomass Derived C6 and C5 Sugars into Value-Added Chemicals

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Novel Methodologies Towards the Synthesis of Heterocyclic Compounds

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Heterocyclic compounds are important because many of them possess wide spectrum of biological activities. 1,3-Oxazine and Indole derivatives exhibit a wide spectrum of biological activities, such as anti-HIV, antibacterial, antitumor, antituberculosis, fungicidal, antihypertensive, antineoplastic, antimitotic agents, hypoglycemic, protein kinase inhibitors, etc. We are interested in developing novel methodologies using the principle of multi-component reaction, C-H functionalization, and cascade reaction for the synthesis of various classes of heterocyclic derivatives.

Metal-Catalyzed Decarbonylative Annulation Reactions for the Synthesis of Important Heterocycles

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In the last few decades, transition-metal-catalyzed C-H bond activation and alkyne annulation reactions have evolved as efficient and atom-economical approaches for the synthesis of several important carbocycles and heterocycles.[1] In particular, the transition-metal-catalyzed decarbonylative C-H/C-C bond activation followed by annulation of alkynes, have been frequently used for the efficient construction of wide range of heterocycles.[2] Very recently, we have developed some unprecedented Ru(II)-catalyzed decarbonylative C-H/C-C activation and annulation reactions for the efficient construction of important heterocycles. For example, we have developed a novel Ru(II)-catalyzed decarbonylative π-insertion reaction of less strained six-membered ring compound which proceeds via C-H/C-C activation, alkyne insertion and decarbonylation reactions to provide good yields of spiro-indenebenzofuranones.[3] Similarly, a Ru(II)-catalyzed C-H activation and annulation reaction, in which the annulation proceeds via cleavage of the triple bond of the alkyne as well as decarbonylation was developed for the construction of substituted quinazolines.[4] These new reactions will be presented in the symposium.

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Microwave Synthesis-An Alternative Synthetic way

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Microwave assisted synthesis has revolutionized chemical synthesis. In Microwave Chemistry, microwave radiations applied in cavity for chemical reactions. Microwave chemistry is major breakthrough in synthetic chemistry. The major advantages of using microwaves are rapid heat transfer, volumetric and selective heating, compactness of equipment, speed of switching on and off and pollution-free environment as there are no products of combustion. Small molecules can be built in a fraction of the time required by conventional methods. In microwave synthesis, microwave radiation is used as a source of heating in chemical synthesis instead of oil bath, heating mental, hot plate as used in conventional technology. The basic mechanisms observed in microwave assisted synthesis are dipolar polarization and conduction. Microwave-assisted synthesis provides clean synthesis with the advantage of enhanced reaction rates, higher yields, greater selectivity, and economic for the synthesis of a large number of organic molecules, have provided the momentum for many chemists to switch from conventional heating method to microwave assisted chemistry.

Microwave-assisted synthesis is rapidly becoming the method of choice in modern chemical synthesis and drug discovery. There are many applications of microwave-assisted synthesis in organic synthesis, inorganic synthesis, polymer synthesis, nanotechnology, peptide synthesis and discuss the basic mechanism involved in microwave heating.

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Polymorph Explorations Guided by the Structural Landscape Studies

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Polymorphs and other crystalline forms of a drug are the endpoints emerging out of a multi-dimensional crystallization reaction coordinate. These crystalline forms together constitute the structural landscape for a given compound. The growth of a particular crystalline form solution is governed by molecular recognition, nucleation and the crystallization kinetics. A thorough understanding of the structural landscape and growth pathway interrelationships can be valuable to the identification and assessment of new polymorphic forms, which hence can be employed in a rational polymorph exploration of the compound. My talk will highlight this issue using the representative examples from our some of the recent studies.

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Oral Presentations

Renewable Resource Based Epoxy/Polyester Blends for Advanced Applications

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Blends are the physical mixtures of two or more polymers with different sets of properties to create a new material with synergistic properties. The most widely used thermoset namely epoxy is used to blend with flexible polymers like polyester. Epoxy resins are most widely used range of polymers for engineering applications. Conversely, the limitations like low toughness and high brittleness characters restrict its use in many advanced areas. On the other hand, polyester resins are also a class of polymers with aliphatic backbone that offer high toughness, elongation and impact resistance. However, both these commercially available polymers are mostly based on petroleum resources derived from fossil fuels that are on the verge of extinction, and causes environmental problems. In the present approach, hyperbranched polymers derived from renewable resources are blended in different proportions through a facile approach and the resultant materials are well characterized. The hyperbranched polymers are globular shape consisting of large number of polar functionalities that offer good crosslinking ability. The results showed the cured thermosets of the blends exhibited excellent set of mechanical properties like toughness, impact resistance and elongation due to the synergism of strength and flexibility. Furthermore, the blends are biodegradable and hence environmental solid waste disposal problem can be addressed. Thus, the studied blends have the potential to be used in different advanced applications.

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MOF/Aminoclay Nanocomposites with Enhanced Functionalities

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Metal-organic frameworks (MOFs) have rapidly developed as a new class of hybrid materials with diverse functionalities.[1] Toenhance the properties and to further introduce new functionalities, a contemporary approach is the fabrication of new high-performance MOF composites. Nanoscale MOFs and their composites have emerged recently and show improved processabilities and functionalities.[2] Here we present a new and facile method to synthesize rigid and flexible MOF nanocomposites in an inorganic nanoclay, namely aminoclay.[3,4]We demonstrate miniaturization of different types of MOFs using aminoclay which acts as a functional matrix to grow and stabilize MOF nanocrystals. Several composites with improved functionalities,such as with enhanced CO_2capture, separation and chemical fixation properties, were synthesized. The strategy is expected to provide new route to prepare composite materials with enhanced properties.

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Benzylidene Barbiturates: A Precursor to Unusual Rearrangement and Substitution Reactions

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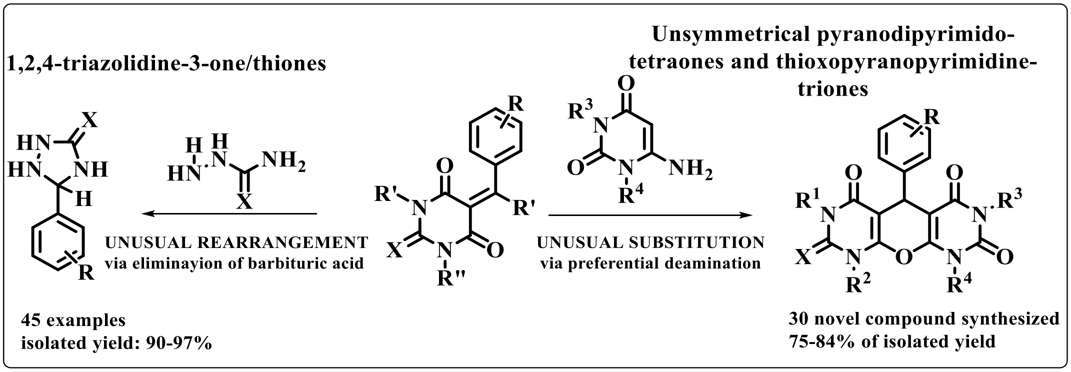
Benzylidene barbiturates, a common Knoevenagel product has been explored for its utility in acid catalysed reactions, directed towards the synthesis of numerous bioactive molecules. In many a cases the products are primarily *bis*-barbiturates or closely following condensed homologues. However, when the reaction conditions are only slightly altered, unusual and obviously unexpected products are formed. Approaching *via*a tandem on-water approach, the work describes the synthesis of **1,2,4-triazolidones/thiones**and **unsymmetrical pyranodipyrimido-tetraones and thioxopyranopyrimidine-triones**. Rapid eco-friendly reactions with high yields, easy work-up procedure as well as chromatography free isolation of product, excellent homogenous media recyclability, high atom economy, and novelty aid to the auxiliary advantages of the protocol.



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Curcumin Modification and its Anticancer Activity

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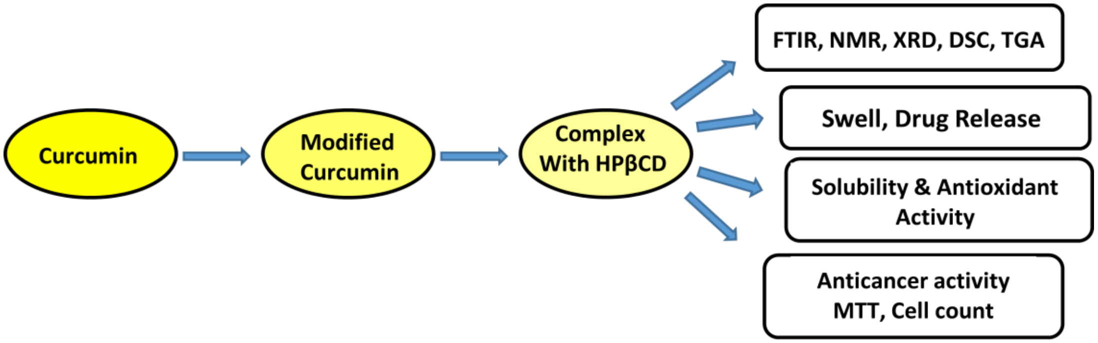
Curcumin, a compound in turmeric, is a well-known anticancer drug. The main difficulty associated with curcumin is the lack of solubility & bioavailability and hence less efficacy. So to increase its effectiveness, curcumin is structurally modified and then complexed with Hydroxypropyl-β-cyclodextrin. Both the structurally modified curcumin and its prepared complex were characterized by Fourier Transform Infrared Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, X-Ray diffractometry, Differential Scanning Calorimetry&Thermogravimetric Analysis. The solubility and antioxidant activity of both the products were checked. Swelling and cumulative release profile of the prepared complex was examined at two different pH (1.2 & 7.4) respectively. The anticancer activity of the products was checked by MTT assay and cell counting using A549 cancer cells. The results indicated that the products had the potential to be used as anticancer agents.



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Role of Biosurfactants in the Stabilization and Color-enhancement of *Mahī*: A Traditional Herbal Ink of Assam

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Assam had a medieval heritage of manuscript writing on *Sāncipāt withMahī*, a unique herbal ink of medieval Assam; which continued till the early 20th century. The durability of *Mahī*without having any binderhas been considered to be its major attributes that attracts the attention of many historians, curators and traditional practitioners. Surface active property of *Mahī*and the role of biosurfactants as green stabilizer on the chromogenic components of *Mahī* have been studied. The color intensification has been studied through interactions of two representative polyphenols present in *Mahī*, viz., gallic acid and quercetin with iron forming iron-polyphenol complexes, and that of the complexes with surfactants of various charge types. The glycosidic surfactants reduce the surface tension of *Mahī*to 46.5mN/m giving a critical micellar concentration (CMC) of 1.4 mg/L. The effect of the surfactants on the iron-polyphenol complexes was found to be highest with the anionic surfactant, similar to glycosidic surfactants present in *Mahī*, than with other types of surfactants. The polyphenolicglycosidic surfactants have been suggested to stabilize *Mahī*through solubilization of the insoluble/sparingly soluble polyphenols.

Conversion of Ethanol to Butadiene over Mesoporous $MgO-SiO_2$ Catalysts

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Ethylene is generally produced by thermal cracking of naphtha in the process involving a complex network of radical reactions resulting in a broad product distribution. 1,3-butadiene is the most important conjugated diene. It is the basis of a wide variety of synthetic rubbers, elastomers and polymer resins. The developments in ethylene production technologies such as oxidative dehydrogenation of ethane lead to lack of butadiene and need for an alternative technologies for butadiene production. Recently the production of 1,3-butadiene from biomass-derived feedstock has a great interest of both academic and industrial research. A possible way to obtain butadiene for the rubber industry goes through the dehydrogenation of ethanol to acetaldehyde then two acetaldehydes link to 3-hydroxybutanal followed by dehydration of 3-hydroxybutanal to yield crotonaldehyde, which is then further hydrogenated and dehydrated to finally yield butadiene. $MgO-SiO_2$ catalysts showed excellent catalytic activities in ethanol to butadiene reaction. Preliminary results showed that the MgO can be more efficiently used as a catalyst by expanding its surface area.It is well known that by using template molecules structured mesoporous materials can be synthesized. Therefore we attempted to synthesize mesoporous magnesia or magnesia-containing materials.We have also prepared two different types of MgO/SBA-15 catalysts. One was conventionally impregnated and in another the Zn was incorporateddirectly into SBA-15 silica framework. The effect of ZnO and In_2O_3 dopants on product selectivities was also investigated. Our presentation will discuss the effect of catalyst structure and basicity on the reaction pathway and product yield in ethanol to butadiene reaction.Structure of catalysts was characterized by means of XRD, TEM and N_2physisorption techniques. The surface basicity of the catalysts was determined by using CO_2 adsorption. The catalytic test reactions were carried out in a fixed-bed, continuous flow glass tube microreactor. Our results showed that $MgO-SiO_2$ catalysts selectively produce butadiene in the one step conversion of ethanol. Addition of In and Zn enhances the butadiene yield (~70% selectivity on ~50% conversion level at 300 °C).

Utilization of Night Blooming Plant Leaves for Removal of Basic Methylene Blue Dye from its Aqueous Solution: Adsorption Study

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The presence of dyes in water poses a significant hazard to human health since many of them are toxic, can cause allergies and irritation to the skin and the intestinal walls, and are mutagenic and carcinogenic. Laboratory investigations, of the potential use of dried plant leaves of *NyctanthesArbortristis,* night blooming flowering plants biomass as an adsorbent for the removal of the basic dye methylene blue from aqueous solution were conducted. This biosorbent was characterized by infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Zeta Potential and Thermal Gravimetric Analysis (TGA). A batch sorption model, based on the assumption of pseudo-first-order and pseudo-second-order mechanisms, was applied to understand the sorption dynamics of MB onto NA and to predict the rate constant of sorption, the equilibrium sorption capacity, and the initial sorption rate when the two process variables were optimized.

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Synthesis of Oxo-PeroxoMolybdenum(VI)-Chitosan Complex and its Catalytic Application in Sulfide Oxidation in Water

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Selective oxidation of organic sulfides tosulfoxides is one of the essential reactions in organic synthesis, whichholds immense interest from both chemical as well as biological perspectives.[1,2] Recently much emphasis has been given to develop environmentally benign and sustainable methodology for such oxidation reactions. In the present work, synthesis and catalytic application of oxo-peroxo molybdenum(VI) immobilized on chitosan biopolymerhas been reported. The complexwas characterized by a set of elemental analysis as well as spectral studies including FTIR, Raman, solid-state ^{13}C NMR,diffuse reflectance UV-Vis, PXRD, Brunauer-Emmett-Teller (BET), SEM, EDX and TGA-DTG analysis. The structure of the chitosan peroxomolybdenum complex (**PMoCh**) was studied by density functional theory (DFT) method. The synthesized catalyst was found to be highly active in the oxidation of a wide range of sulfides to sulfoxides using H_2O_2as oxidant in water, at ambient temperature.In addition to water, the catalyst is also highly compatible with a variety of organic solvents. Further, the present catalytic method offers advantages like elimination of metal leaching, high TOF values (~3670 h^{-1}) in absence of halogenated solvents and reusability with excellent activity and selectivity.

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Structural Landscape and Physicochemical Property Study of Pharmaceutical Solids

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Crystal engineering is the main platform for designing/tuning materials property based on intermolecular interactions.[1] Solid-state chemist widely used crystal engineering as a tool during the last 2-3 decades in order to improve physicochemical properties of a large number of materials including active pharmaceutical ingredients (API).[2] Various solid-state strategies including preparation of cocrystals, salts, solvates, hydrates, eutectics, polymorphs, amorphous formulations etc. are employed in pharmaceutical industries.Most of the drugs are administered as solid oral dosage forms like tablets, capsules, powder etc. Among them more than 50 % are available as salt formulation; however isonizable group is essential for salt preparation. Salification is a simple acid-base reaction where either proton transfer or neutralization must be occurred. Thus it can be assumed that cocrystals and salts can be considered as the two extremities where classification as either a cocrystals or salt is determined by position of hydrogen between the two components. There is another very useful parameter by which we can determine the probability of formation of cocrystals or salts; p*K*a difference, i.e. ΔpKa between the components. $\Delta pKa > 3$, results salt formation; whereas $\Delta pKa < 0$ result formation of cocrystal. ΔpKa value in between 0 to 3 is considered to be gray region where probability of cocrystal vs. salt formation is unclear.[2] In case of salt formation the improvement of solubility as well as dissolution is more compared to cocrystals, solvates, polymorphs etc. due to the presence of the ions.[3]

Here we will discuss about some of the BCS[4] (Biopharmaceutical Classification System) class II drug having lower solubility, for physicochemical property modification as well as structural elucidation.[5]

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Microwave Assisted Synthesis, Characterization and Interaction Studies of 1,3,4-Oxadiazole Derivatives of Fatty Acid with Human Serum Albumin (HSA)

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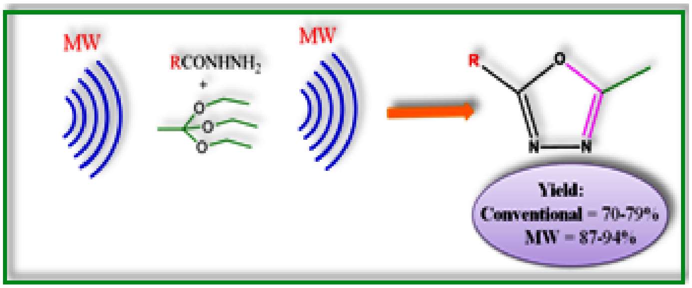
Heterocyclic compounds particularly 5-membered rings have been the subject of significantly adapted because of their versatile pharmacological and biological activities.[1]In particular, 1,3,4-oxadiazoles have been used as 'privileged' scaffolds to produce substances of interest in numerous therapeutic areas. 1,3,4-Oxadiazoles are well known bioisosteres of amides and esters, that can contribute significant pharmacokinetic property due to presence of N=C-O linkage in oxadiazole nucleus which increases the lipophilicity that influence the ability of drug to reach the target by transmembrane diffusion and show remarkable biological activity.[2]In this context, to study the influence of fatty acid chains on the biological activity of organic compounds, we here in reports an efficient synthesis of fatty acid derivatives of 1,3,4-oxadiazole. Further, a comparative study between conventional heating to that of microwave irradiation also described. The synthesis of 2,5-disubstituted 1,3,4-oxadiazoles was carried out utilizing different fatty acid hydrazides and triethylorthoacetate. The newly synthesized compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR and mass spectral analysis.



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Let’s Say No to Poisonous KCN or NaCN for Synthesis of AgCN

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A simple and effective process has been developed for the synthesis of AgCN nanoparticles avoiding the use of toxic sodium cyanide and potassium cyanide. The method that has been suggested here involves the alkyl nitriles especially the acetonitrile as source of cyanide. The thermodynamically stable and kinetically inert C-CN bond of various alkyl nitriles like acetonitile, propionitrile and malonitrile was found to dissociate very easily at 60 °C on treatment with H_2O_2 in presence of silver-sulphur-oxido-vanadium cluster leading to the precipitation of silver cyanide. The silver cyanide nanoparticles were easily separable from the solution by simple centrifugation method at 8000 rpm. The nanoparticles were found to be within the range of 20-50 nm. The residual filtrate left after the formation of silver cyanide particles was well characterized and was found to contain peroxo-vanadate species and unprecipitated silver ions. The filtrate was further treated with 0.1M HCl to abstract the silver ions as silver chloride and the peroxo-vanadate species was used to obtain single phase V_2O_5-nanocrystals.

A Greener NOSE Approach: Comparative Study on Catalytic Activity of Palladium Nanoparticles in C-C Cross Coupling Reactions

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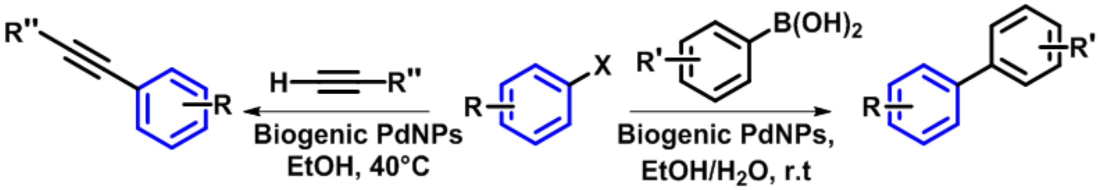
Palladium catalyzed cross-coupling reactions prevails an important methodology for the construction of C-C bonds.[1]Numerous palladium based catalytic systems have been developed for the construction of C-C framework.[2] However, as per green chemistry perspectives various efforts and advances have been made towards simple and cost-effective methodologies. This work describes the effect of substrates on the catalytic activity of palladium nanoparticle (NPs), which are synthesized by using phytochemicals extracted from two common plants species. Comparative studies have been done on the generation of both the *in situ* and *ex situ*Pd NPs and their catalytic activity was investigated in Suzuki-Miyaura and Sonogashira Cross-coupling reaction. Spectroscopic and analytical techniques were performed to confirm the formation of the synthesised compounds and PdNPs.



$R = 4\text{-}NO_2, 4\text{-}OMe, 4\text{-}COMe, 4\text{-}OH, 2\text{-}Me$ etc.
R'= 4-Cl, 4-*t*Bu, 4-Me, 2-Me, 3-Me
R''= 4-Me, 4-OMe, 3-Me, butyl, hexyl, cyclohexyl

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Mixed Ligand Cu(II)-diimine Complexes: Enhanced DNA Binding, DNA Cleavage and Cytotoxicity Effected by Coligands

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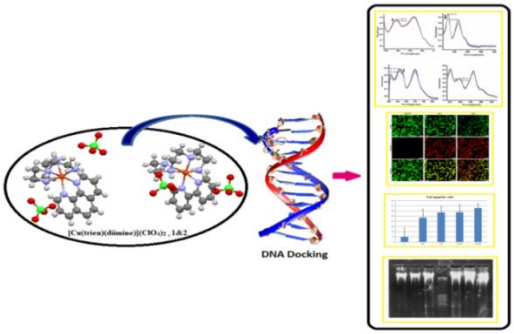
The synthesis of mixed ligand Cu(II) complexes of type $[Cu(trien)(diimine)](ClO_4)_2$**1-4**, where trien is triethylenetetramine and diimine is bipyridine (**1**) or 1,10-phenanthroline (**2**) or 5,6-dimethyl-1,10-phenanthroline (**3**) or 3,4,7,8-tetramethyl-1,10-phenanthroline (3,4,7,8-tmp, **4**) as co-ligand and their DNA binding and cytotoxicity studies are described. The complexes were characterized by elemental analysis, spectral studies and single crystal X-ray diffraction studies. The DNA binding constants obtained by using absorption spectral titration [$K_{b,}$**1**, 3.6×10^3 **< 3**, 2.3×10^4 **~ 2**, 6.6×10^4 **<4**, 2.3×10^5 M^{-1}] and DNA docking studies reveal that the complexes $[Cu(trien)(diimine)](ClO_4)_2$**1-4** bind to CT DNA in the minor groove. Interestingly, the complexes**1** and **2** exhibit higher cytotoxicity against human breast cancer cell line (MCF-7) as well as human lung cancer cell line (A549) than the other two complexes. Also, they display apoptosis in MCF-7 and A549 cancer cells, suggesting that they can be further explored to establish their potential as antitumor drugs.



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Mechanistic Study on Stability Enhancement of Famotidine Drug by Cocrystallization

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Famotidine is one of the highly competitive histamine H_2–receptor antagonists available in the market and is used as a potent inhibitor of gastric acid secretion and pepsin in human body for the treatment of two different kind of peptic ulcer.[1-2]The degradation behaviour of Famotidine drug has been investigated under acidic condition. Hydrolysis of Famotidine results the formation of shiny crystals of decomposed product and confirm by using spectroscopic techniques, Thermal analysis and X-ray diffraction. In contrast, Famotidine is subjected for cocrystal synthesis to prevent their hydrolysis with bronchodilator drug Theophylline and studied degradation under identical conditions. Results suggested the enhanced stability of cocrystal in various experimental conditions and are presented herein. While compared with pure Famotidine, drug cocrystal further improves their bioavailability under same physiological conditions. This new cocrystal with stability enhancement and improved drug pharmacokinetic properties can be projected as viable alternate combination medicine.

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Use of Glutathione-s-transferase in Biomedical Diagnosis and in Pesticide Analysis

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Glutathione S-transferases (GSTs; EC 2.5.1.18) are a multigenicfamily of cytosolic proteins with multifunctional biological roles, widely distributed throughout the body and found in the liver,kidney, brain, pancreas, testis, heart, lung, small intestine, skeletal muscles, prostate and spleen.[1] The important biological functionof GSTs is their catalytic action in detoxification reaction. The *in vivo* detoxification mechanism of GST has been utilized in biomedical diagnosis of drug resistance in cancer patients. The detoxification mechanism can also be studied *in vitro*, which has rendered it possible to apply the same for detection of chemical pesticides or other toxic substances in a solution through electrochemical transduction mechanism. We have developed a method for amperometricbiosensing of a broad spectrum of pesticides using a GST catalyzed reaction *in vitro* as the benchmark. The method was successful in detecting six different classes of pesticides namely - benzamidazole, organochlorine, organothiophosphate, organocarbamate, polyphenol and pyrethroid. The trend of inhibition appears to be competitive for organochlorines, non-competitive for organothiophosphates and mixed type for phenolic and benzimidazole classes.

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Heterogeneous Catalysis on Metal Oxides

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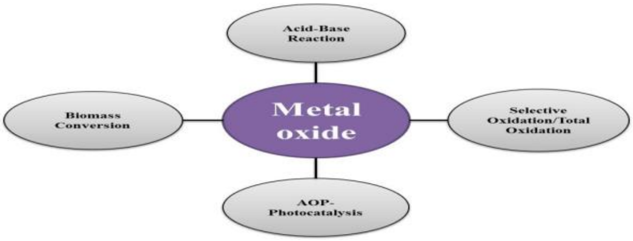
The fundamentals and main domains of heterogeneous catalysis in context of metal oxide catalysts that cover acid-base reactions, selective partial or total oxidation reactions, biomass conversion, and advanced oxidation processes will be discussed.Metal oxides became prominent in the mid-1950s when they were found to effectively catalyze a wide variety of reactions, in particular oxidation and acid-base reactions.Metal oxide catalysts are essential components in many petrochemicals, fine and pharmaceutical chemicals and biomass transformation reactions. These catalysts are also critical to improving environmental quality. The major current industrial applications of bare/supported metal oxide catalysts also will be discussed. We will describe the viewpoints for understanding the catalysts' action and its' applications. The importance of catalyst, description from synthesis to reaction conditions, on main industrial applications in the different domains will be discussed.Following the major types of metal oxide catalysts and the processes that use these catalysts, we consider current and prospective major applications, where recent advances in the science of metal oxide catalysts have major economic and environmental impacts. Although great improvements and new developments were observed in the second part of the 20th century, there remains plenty of room for young researchers from academia and industry to discover and develop new metal oxide catalysts, new preparation procedures, and new or improved processes that highly concern with the world economic and environmental issues.



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Expedient Co-Catalyzed Site-selective C7-Arylation of Indolines with Arylboronic Acids

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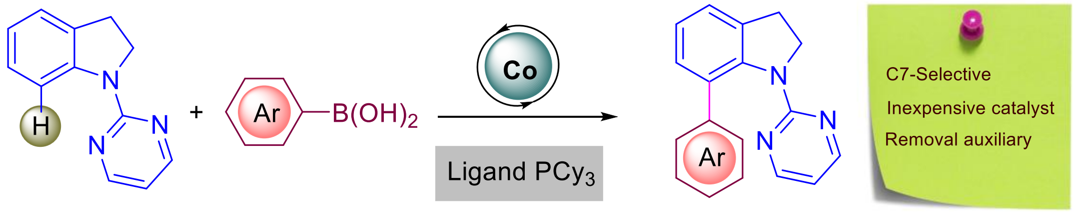
Transition-metal-catalyzed site-selective C-H functionalizations[1] with the aid of chelating group has recently emerged as a potential synthetic tool for the regioselective carbon-carbon bond formation. Among them, the C-H arylation is mostly restricted to Pd and other noble transition metals.[2] Cost-effective and eco-benign Cobalt being a first row transition metal, guided this methodology into new dimension. Expedient cobalt(II)-PCy_3 catalyzed removable pyrimidyl directing group assisted C7 arylation of indolines with arylboronic acids has been developed in the presence of $Mn(OAc)_2{\cdot}4H_2O$ as the oxidant at moderate temperature, which can be readily oxidized with DDQ to furnish C7-arylated indoles in good yields (Scheme 1).[3] This newly discovered reaction provides the advantages of the use of cobalt(II)-PCy_3 complex as the catalyst with broad substrate scope and functional group diversity.



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Silibinin Loaded Xanthan Gum Nanoparticles For Controlled Drug Delivery and Its Application As An Anticancer Agent

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Nanoparticles with suitable bio-compatible coatings using natural polymers are gaining importance recently in biomedicine, particularly in drug delivery applications, magnetic resonance imaging (MRI) and tissue engineering. In this study, silibinin loaded xanthan gum coated nanoparticles were prepared by ionic gelation using calcium chloride ($CaCl_2$). Initially phase separation behavior of xanthan gum was carried out as a function of $CaCl_2$concentration. The prepared nanoparticles were further chemically crosslinked with genipin.Effect of amount of surfactant (Tween80) on different properties of the nanoparticles was investigated. The nanoparticles were characterized by Fourier Transform Infrared spectroscopy (FTIR), X-ray diffractometry (XRD), and Scanning Electron Microscopy (SEM). The average particle size of the nanoparticles was studied by Dynamic Light Scattering (DLS). Swelling of nanoparticles and release rate of silibinin were determined at pH 5 and intestinal pH 7.4 and were found better in intestinal pH.The drug release mechanism was studied for different time periods using a UV-visible spectrophotometer. Cell viability study of the nanoparticles was performed on MCF-7 (breast)andMDA-MB-231 (breast) cancer cell lines at different concentration by MTT assay analysis. The anticancer activities of the nanoparticles were further confirmed by cell-counting on MDA-MB-231 breast cancer cell line. The results implied that silibinin loaded xanthan gum nanoparticles could be exploited as a potential drug carrier for controlled-release applications.

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Pseudo Gated Adsorption with Negligible Volume Changein the Nanospace of PCPs/MOFs

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The design and discoveries of metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) during the past two decades or so have inspired materials scientists to look MOFs/PCPs beyond the scope of traditional porous materials such as zeolites and porous carbon.[1] An intriguing property of the MOFs is flexibility;[2] the later combined with enormous opportunities to tune the nanospaces have made MOFs promising for applications in important areas such as gas technology, catalysis and biomedicines. The nanospaces can be tuned in terms of size, shape and chemical functionality in a desired manner for a targeted function. This report will try to focus on some of the design strategies and mechanistic aspects of some "not so flexible" MOFs/PCPs for efficient and selective capture of gases, in particular CO_2.[3] Improving gas adsorption by utilizing weak interaction in porous compounds is highly attractive for the design of energy efficient storage materials. Inspired with this idea, here we present a rational design for such adsorption process using synergistic functions between dynamic motion in a local module and weak host-guest interaction, viz. halogen bond (XB) in MOFs.

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2D Functionalised Organic Monolayer Surfaces to Control Polymorph Nucleation of Drugs

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Polymorphism, presence of different forms for the same chemical compound, and its control has been regarded as a decisive property in the pharmaceuticalsector.In recent decades, numerous researchers have devoted their interest in selecting and designing heterosurfaces to control crystallizationoutcomes. Thus, the focus of the work is to imply self-assembled monolayer (SAM) templates to control crystallization outcomes of the antimicrobial drug sulfathiazole (SUTH). SUTH having five polymorphic forms generally nucleates concomitantly.SAM surfaces were introduced successfully to nucleate pure polymorphic phases of SUTH. SAM's and resulted crystalline phases on these surfaces were characterized using different analytical techniques.The translation of chemical functionality effect from the surfaces directs the nucleation of specific polymorph is studied and reported.

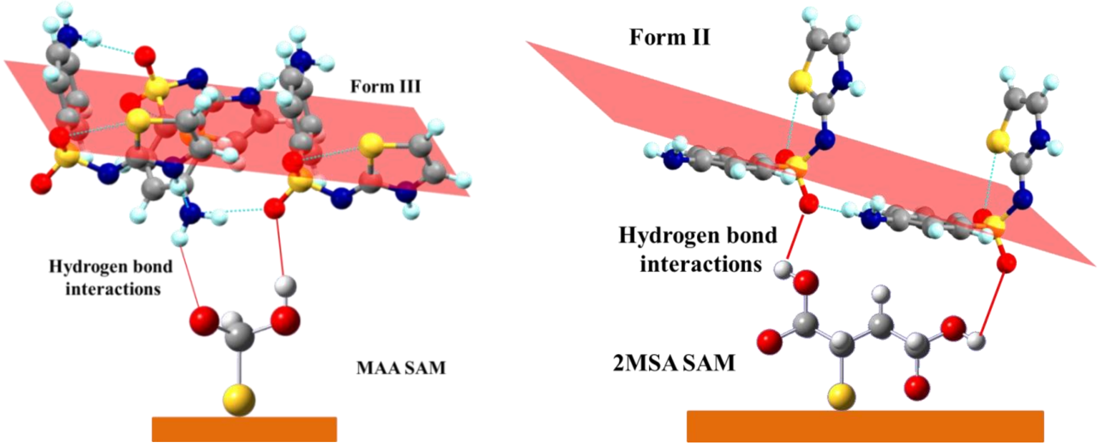

Figure 1 Interaction diagram of MAA SAM (left) to form III and MSA SAM (right) to that with form II of sulfathiazole

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Iodine Catalysed Regioselective Sulfenylation of Unsymmetrical Ketones from Substituted Phenyl Disulfides

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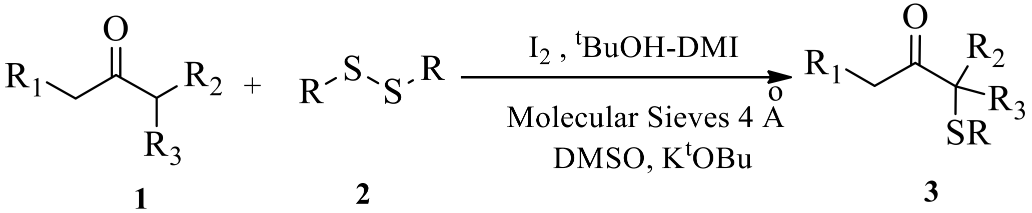
Here, a novel approach for the sulfenylation of unsymmetrical ketone is shown (Scheme 1). A thermodynamically more stable enolate ion is generated from unsymmetrical ketones and reacts predominantly with various substituted disulfides to give α-sulfenylation products, also called as β-ketosulfides. The iodine catalysed method is considered to be of urgent need as it leads to direct access of structurally diverse α-sulfenylation products involving DMSO as an oxidant and potassium tert-butoxide as a base in a solvent mixture of ^{t}BuOH-DMI (7:3). Both linear and cyclic (unmodified) ketones proceed to give β-ketosulfides with ease. The method is low cost, and no hazardous waste products are recovered throughout the process. The method leads to an excellent yield of products, up to 92 % within 2 h.



Scheme 1. Sulfenylation of unsymmetrical ketones.

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Cu(II) Complex with Multidentate N, O, S-Donor Liagands in C-N Coupling Reactions

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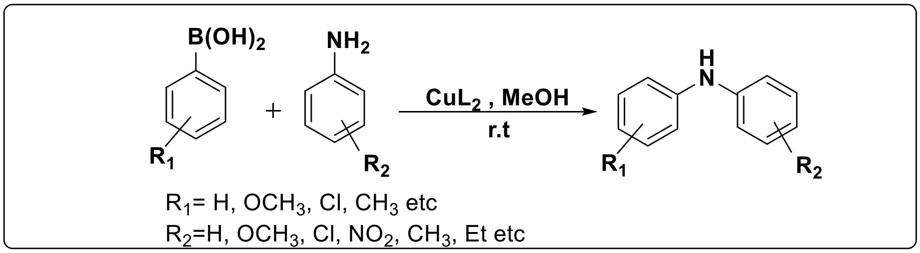
Functional imine synthesis becomes an important and popular topic due to its wide variety of industrial applications in the fields including organic synthesis, analytical, biological, inorganic and coordination chemistry.[1]Mixed-donor Schiff base ligands with hard N and soft S donor atoms provide good coordination property towards wide range of metal ions giving stable and deep coloured compounds.[2]A new ligand 4-nitro-2-(((2-(phenylthio)phenyl)imino)methyl) phenol (L) with O-, N-, S- donors was synthesised and employed for mononuclear Cu(II) complex (CuL_2) formation. The CuL_2 was found to be an excellent catalyst for Chan-Lam C-N coupling reaction in absence of a base (Scheme 1).



Scheme 1. Chan-Lam coupling reaction using CuL_2

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Palladium-Silver-Carbon Dot Nanohybrid and Its Nanocomposite with Hyperbranched Polyurethane: Prospects as Multifunctional Material

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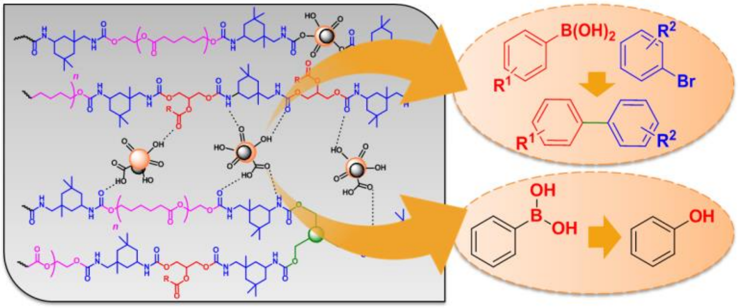
Thepresent work describes the synthesis of bimetallic-cum-carbonaceous Palladium-silver-carbon dot (Pd-Ag@CQD) nanohybrid by a facile UV light-assisted protocol and an *in situ*nanocomposite fabrication with bio-derived hyperbranched polyurethane (HPU). The structural features of Pd-Ag@CQDnanohybrid and its HPU nanocomposite were investigated by analytical techniques like UV-Vis, FT-IR, XRD, EDX, TEM, TGA *etc.* The Pd-Ag@CQDnanohybrid displayed high catalytic efficiency towards Suzuki-Miyaura cross coupling of aryl boronic acids and aryl bromides (80-90% yield, 60-90 min) under ligand-free conditions and ambient conditions. In the same vein, the HPU-reinforcedPd-Ag@CQDnanocomposite exhibited rapid catalytic activity *en route* oxidative *ipso*-hydroxylation of aryl boronic acids (upto 100% conversion, 30-60 min) under ambient conditions. Thus, the design and development of such multifunctional hybrid materials augurs well for a variety of wide-scale applications.



Scheme 1. Multifunctional activity of Pd-Ag@CQDnanohybrid and its HPU nanocomposite

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Synthesis of CoZn-LDH for Photo Enhanced Adsorption of Cationic and Anionic Dyes

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The synthesis of CoZn-LDH was carried out in water in oil microemulsion system using Sodium Dodecyl Sulphate, isooctane and water.[1] The synthesized LDH was characterized by X-ray powder diffraction (PXRD), fourier transform infra red spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetric analysis (DTA) and Bruenuer Emmet Teller (BET) techniques. The characterization techniques showed well defined hydrotalcite layer structure. The LDH was tested for controlled adsorption of a series of cationic and anionic dyes e.g. methylene blue, congo red, malachite green and rhodamine B under dark condition and under irradiation of light. It was observed that light has positive effect over adsorption showing upto 90% adsoption of dyes and adsoption became doubled compared to adsorption under dark condition.

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Starch Modified Hyperbranched Polyurethane Nanocomposites with Diverse Carbon Based Nanomaterials: As Prospective Multifaceted Smart Materials

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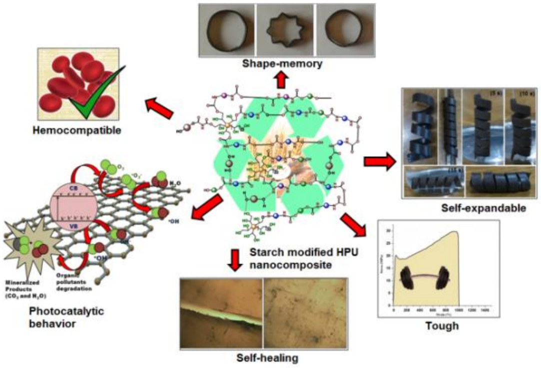
The advancement of a renewable resource-based hyperbranched polyurethane (HPU) nanocomposite with multifaceted attributes of shape memory, high performance and biocompatibility is a challenge in the industrial and scientific domain. In this milieu, smart, biocompatible starch modified HPU nanocomposites were designed, using various carbon based nanomaterials, devoid of any catalyst or plasticizer. FTIR,XRD, EDX, UV-Vis, HRTEM *etc*. were employed to confirm the structural insights of the the nanocomposites. Thefabricated nanocompositesdemonstratedenhanced mechanical and thermal attributes, as well as non-contact triggered self-expandable behaviour. Theydisplayed remarkable photocatalytic degradation of organic pollutants under sunlight, supporting the pseudo kinetics first order model. The nanocomposites also exhibited repeatable solar and microwave induced self-healing abilities. Thus, the developed carbon based HPU nanocomposites possess excellentcapabilitiesfor employement as smart materials for various advanced applications.



Scheme 1. Multifaceted attributes of starch modified HPU nanocomposite

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Synthetic Studies towards 2-Amino-2-(chroman-2-yl)ethanols

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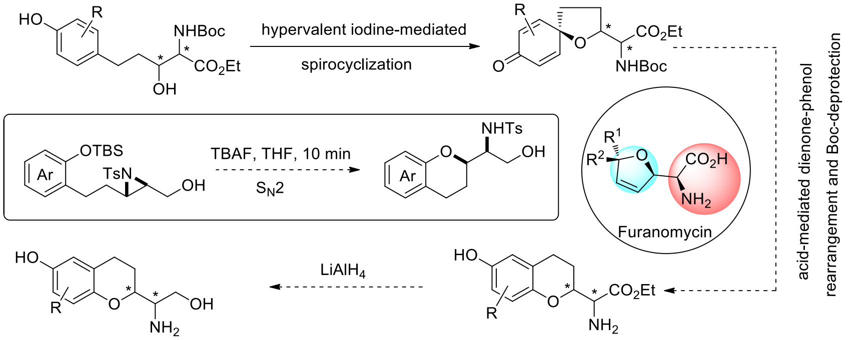
β-Amino alcohol is a privileged motif that serve as an indispensable structural unit in a very large number of bioactive compounds, clinical drugs, agrochemicals, and natural products.[1] Although diverse β-amino alcohols have been synthesized over past several decades, chroman-linked β-amino alcohols have never been reported in the literature. In this line, we have investigated two different synthetic strategies. The first route involving an on-pot dienone-phenol rearrangement and Bocdeprotection as key step was unsuccessful – however, the study provided hitherto unreported spiro-fused cyclohexadienone–tetrahydrofuran-embedded glycine derivatives as a new class of nonproteinogenic α-amino acid derivatives.[2] On the other hand, exploitation of phenolate ion-mediated diastereo- and regioselective intramolecular ring opening of *N*-tosylaziridines furnished the targeted compounds efficiently.[3] Such a study has not only broadened the impact of aziridines as synthetic building blocks, but also unveiled a new entry to the synthesis benzo-fused oxa-heterocycles under transition-metal-free conditions.



Scheme 1. Synthetic Studies towards 2-Amino-2-(chroman-2-yl)ethanols

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Build/Couple/Pair Strategy in the Stereoselective Synthesis of Bridged Tetrahydroquinolines

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Both the tetrahydroquinoline and benzosultam ring systems are found in a large number of biologically active natural products and/or synthetic molecules.[1]Owing to their enormous synthetic and pharmacological utilities, both these scaffolds have become important synthetic targets for organic and medicinal chemists. However, combination of these two privileged scaffolds in one single molecule, which may provide a source of new lead compounds, remains unreported, and is therefore highly desirable. Towards that objective, adiastereo- and enantioselective synthesis of previously unknown tetrahydroquinoline-containing bridged benzothiaoxazepine-1,1-dioxides (Figure 1) has been achieved using build/couple/pair (B/C/P) strategy.[2]In the build phase, a series of both *trans*-3-arylglycidyl tosylates and *N*-aryl-2-fluorobenzenesulfonamides were synthesized.

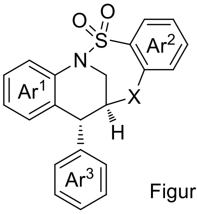

Figure 1

In the couple step, *N*-aryl-2-fluorobenzenesulfonamides were alkylated with *trans*-3-arylglycidyl tosylates in the presence of anhydrous K_2CO_3 in DMF. In the pair phase, two different reactions were employed sequentially to enable two intramolecular ring-forming processes: intramolecular Friedel-Crafts Epoxide-arene cyclization and nucleophilic aromatic substitution (S_NAr). The protocol is experimentally convenient, rapid, and scalable, and requires easily available starting materials, reagents, and catalyst.The detailed synthetic studies towards these molecules will be presented in the Conference.

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Regioselective Etherification of Naphthylamides with Arylboronic Acids Via Picolinamide Directed C(γ)−H Activation

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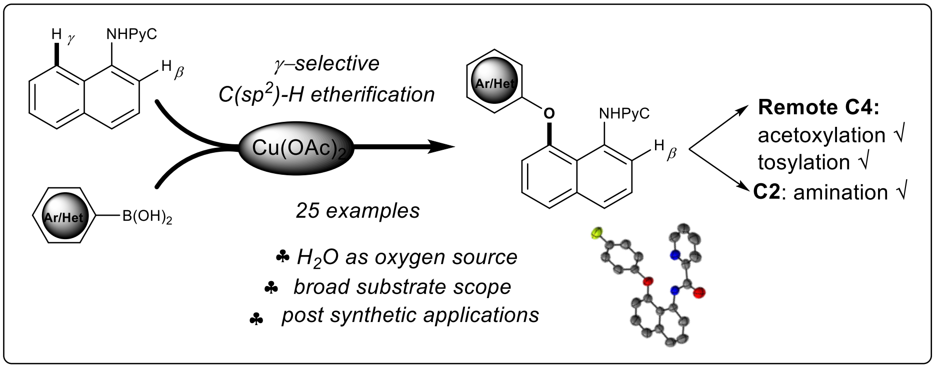
A novel protocol for regioselective etherification of naphthylamides with arylboronic acids has been developed via copper-mediated directed C(γ)−H activation using water as an oxygen source. Structure of one of the desired naphthylether product was confirmed by single crystal XRD analysis. The intermolecular kinetic isotope study suggests that C–H bond activation is the rate-determining step. H_2O^{18} labelling study reveals that incorporation of oxygen is from water. Moreover, the directing group can be removed by base hydrolysis in the presence of NaOH/ EtOH system. The broad substrate scope, functional group diversity and post synthetic utilities are the important practical features.



Scheme 1. Directed C(γ)−H activation of naphthylamides with arylboronic acids

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Atmospheric Degradation Pathways and Kinetics of 2-Difluoroethanol (CHF_2CH_2OH) with Cl Atom: A Theoretical Investigation

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To examine the degradation pathways and kinetics of 2, 2-difluoroethanol (CHF_2CH_2OH) into the atmosphere initiated by Cl atom, three H-abstraction reactions from CHF_2-, -CH_2- and -OH sites are investigated. Geometryoptimization and frequencycalculations are done at BHandHLYP/6-311++G(d,p) level of theory for all stationary points. Energies are further refined by higher level CCSD(T) method along with same basis set. Our analysis suggest that the H-abstraction from -CH_2- site is kinetically and thermodynamically more predominant than the other abstraction sites. The rate coefficients and branching ratios of the reactions and lifetime and global warming potentialof the titled molecule are reported.

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Synthesis of Quaternary Carbon CenteredPyrimidoindolones*via*1,2-Aryl Shift and Ligand-Controlled C-H Activationand Annulation

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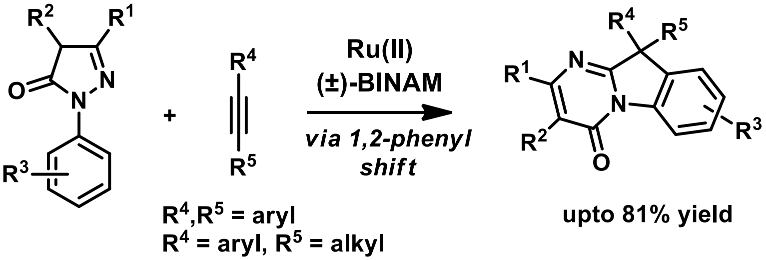
A novel Ru(II)-catalyzed C-H activation and annulation reaction is developed. Unlike the reported metal-catalyzed C-H activation and annulation reactions, in the present bidented amine ligand controlled, C-H activation and annulation reaction of *N*-aryl pyrazol-5-ones and diaryl/arylalkyl substituted alkynes, the annulation occurs *via* 1,2-aryl shift to afford quaternary carbon centeredpyrimidoindolones.



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Poster Presentations

Synthesis and characterization of New Chiral Schiff Base Ligand (1S, 2R)-1-(((E)-3-bromo-5-chloro-2-hydroxybenzylidene)amino)-2, 3-dihydro-1H-inden-2-ol) and It's Cu(II) metal complexes

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A new chiral Schiff base ligand, (1S, 2R)-1-(((E)-3-bromo-5-chloro-2-hydroxybenzylidene)amino)-2, 3-dihydro-1H-inden-2-ol) and its Cu(II) complex were synthesized. The donor site of the ligand are N, O and O which can act as a chelating ligand forming a stable complexes. The chiral ligand was synthesized from (1S, 2R)-amino-2, 3-dihydro-1H-inden- 2-ol and 3-bromo-5-chloro-2-hydroxybenzaldehyde and characterized by UV, FT-IR and NMR. The Cu(II) complex is synthesized both in 1: 1 as well as 2: 1 molar ratio. Now, we are investing the biological applications of the chiral ligand as well as its metal complexes. Melting point of the ligand is ~68°C and that of Complexes is > 300°C. Yield of synthesized ligand is 55-78% and that of metal complexes for Cu (II) is 70-75%.

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Green synthesis of MnSe nanoparticles using Garlic (*Allium sativum*) extracts

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Green synthesis of nanoparticles has gained lots of interest among the scientific community in the last few years. In this study, we report synthesis of manganese selenide nanoparticles using Garlic (*Allium sativum*) extract as green source. Nanoparticles were prepared through hydrothermal process using Manganese chloride-tetra hydrate ($MnCl_2$. $4H_2O$) as Mn precursor. Garlic extract is usedas Se source as garlic is highly rich in selenium. The presence of Mn and Se have been confirmed using energy dispersive X-ray spectroscopy (EDX) and atomic absorption spectroscopy (AAS). Through scanning electron microscopy (SEM) we have visualized the formation of nanoparticles. Structural and optical characterizations of the synthesized samples were done by employing X-ray diffraction (XRD), UV-visible spectroscopy and Photoluminescence spectroscopy.

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Synthesis of Cu-catalysed quinazolinones using a Csp^3-H fuctionalisation/cyclisation strategy

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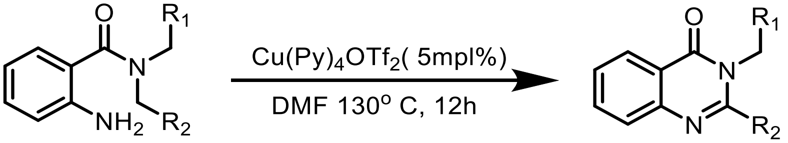
2, 3-disubstituted-4(3H)-quinazolinones were synthesized by copper-catalysed Csp3–H functionalization of 2-amino-N, N-dialkylbenzamides. This strategy allows an easy access to diversely substituted quinazolinones under mild conditions in air. The reaction also exhibits good functional group tolerance and would be of value to heterocyclic researchers as well as pharmaceutical process chemists. The reaction is proposed to proceed through a double SETtype radical mechanism.



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Pt@CD@TiO_2 as an Efficient Catalyst for Methanol Oxidation Reaction

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Noble metal nanoparticles like platinum (Pt) possess excellent catalytic properties, which make them highly desirable for direct methanol fuel cells. [1, 2]However, single component Pt electro-catalyst is acutely prone to CO poisoning. Titanium dioxide (TiO_2), on the other hand, is one of the most studied photo-catalysts3but its application is limited by its light absorption range (UV light). So, there is a huge scope for developing new innovative catalyst designs which can extend the sunlight absorption stretch to the visible region. Incorporating carbon dots (CDs) with TiO_2 can broaden the light response range[4] while a composite of TiO_2 with Pt can significantly enhance the catalytic performance. Herein, we report the structural, optical and electrochemical evaluation of a new photo-electrocatalyst - platinized TiO_2 sensitized with CDs. Reasonably, by combining both photo-catalytic and electro-catalytic mechanisms, the ternary composite catalyst (Pt@CD@TiO_2) under irradiation shows better performance in the methanol oxidation reaction. The performance enhancement can be attributed to the unique up-conversion property of CDs that allows the utilization of the visible solar range, which is otherwise restricted in case only TiO_2 is present.

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Supramolecular Association involving Sigma-hole Chalcogen Bonding Interactions: Experimental and Theoretical Studies

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Studies on the synthesis, structures and properties of coordination complexes including coordination polymers are an important field in chemical research due to their fascinating architectures and potential applications in variety of fields such as luminescent materials, adsorption, catalysis, sensors as well as magnetic materials. [1] The metal-ligand bonds have been widely utilized in organizing diverse supramolecular architectures due to the strength and directionality of coordination bonds associated with metal ions. Hydrogen bonding is a powerful organizing force in designing solids due to its directionality and selectivity. Similarly, chalcogen bond is a non covalent interaction that shares strength with hydrogen bond but exhibits higher directionality. [2]Pyrazoles and bipyridines ligands provide supramolecular interaction sites that assemble through coordination bonds, hydrogen bonds as well as π–π stacking interaction. [3, 4]

Herein, we report Cu(II) and Co(II) coordination complexes involving 3, 5-dimethylpyrazole and 2, 2´-bipyridine. Theoretical studies reveal that the polymeric chain of **1** is stabilized by chalcogen bonding interactions involving the tetrahedral S atom from the sulfate anion as acceptor. To our knowledge, sigma-hole chalcogen bonding interactions involving tetrahedral sulfur atom have not been previously reported in the literature. Various intermolecular hydrogen bonds self assemles **1** and **2** into a 3D and 2D supramolecular architecture respectively. The structure of **3** consists of two crystallographically independent Co(II) complexes. The two independent Co(II) complexes in **3** forms a supramolecular dimer through intermolecular O–H···O hydrogen bonds. The dimers in **3**extend to 2D network structure via π–π stacking and a variety of hydrogen bonds.

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Studies on Removal of Some Metal Ions from Groundwater by Oxidation-Coagulation-Adsorption at Optimized pH

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Removal of some hazardous metals, *viz.,* Cd, Pb, Ni, Cr, Cu, and Co by oxidation-coagulation-adsorptionat optimized pH (OCOP), an efficient and low cost method for simultaneous removal of As, Fe and Mn from groundwater has been studied. $NaHCO_3$, $KMnO_4$ and $FeCl_3$are used in OCOP as pH conditioner, oxidant and coagulant, respectively. The effects of variation of initial concentration and residence time on the removal of these selected metal ions have also been studied. The removal of the chosen metals from initial concentration of 2mg/L by the method has been found to increase in the order Cd (79. 0%) << Co (94. 8%) < Ni (94. 4%) << Cu (98. 0%) <Cr (98. 3%) < Pb (99. 5%). Analyses by AAS, EDX and powder XRD indicate adsorption of the heavy metals on the surface of coagulates/precipitates as oxides and complexes of the metal ions. The highly active absorber coagulates/precipitates formed in FeOOH, $5Fe_2O_3$. $9H_2O$, MnO_2, and Mn_3O_4, also strongly adsorb the metals in addition to removal by precipitations of oxy-complexes in cases of Cd and Pb. The relatively lower removal efficiency observed with Cd has been attributed to its soft acidic nature. On the other hand Cr, being a hard acid is removed very well due to its strong binding FeOOH and MnO2. The present study shows that the OCOP method is capable of removing the heavy metals of Cd, Pb, Ni, Cr, Cu and Co, very well, in addition to efficiently removing As, Fe and Mn from water.

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Diastereoselective Synthesis of *cis*-Fused bis-Chromans/Tetrahydroquinolines/Tetralins via Tandem Semi-pinacol Rearrangement/Double Friedel–Crafts Cyclization

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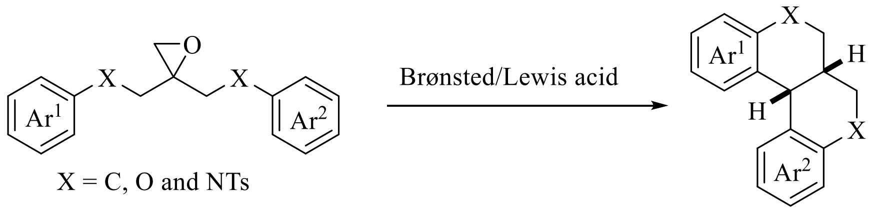
Chroman, tetrahydroquinoline and tetralin scaffolds are a part of the molecular frameworks of a wide range of natural products and synthetic molecules that exhibit a broad spectrum of bioactivities. Owing to their enormous synthetic and pharmacological utilities, these heterocycles have become important synthetic targets for organic and medicinal chemists. However, fusion of any two of these privileged scaffolds in one single molecule, which may provide a source of new lead compounds, remains less studied, and is therefore highly desirable. Along this line, we have developed an efficient route for the diastereoselective synthesis of hexahydrobenzo[c]phenanthrenes and their chroman and tetrahydroquinoline analogs using a domino semi-pinacol – double Friedel-Crafts alkylation as key step (Figure 1).



- domino reactions
- metal-free mild reaction conditions
- high efficiency
- stereoselective
- inexpensive reagents
- broad substarte scope
- high yields

Figure 1

The detailed synthetic studies towards these conceptually new and architecturally interesting molecules will be presented in the Conference.

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Metal-Free C(sp2)-H Functionalization Followed By Suzuki-Cross Coupling Reaction Strategy For The Synthesis Of Highly Substituted 1, 4-Naphthoquinone Derivatives

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Substituted quinones particularly 2, 3-disubstituted-1, 4-naphthoquinones are embedded in several natural products, including menaquinone-6, lapachol, rhinacanthins and in several drugs and therapeutic leads. [1] A synthetic protocol has been developed for the synthesis of 2, 3-disubstituted-1, 4-naphthoquinones which consists of *tert*-butyl hydroperoxide (TBHP)-mediated oxidative benzoylation followed by Pd-catalyzed Suzuki-cross coupling reactions. Benzaldehyde, benzylalcohol and toluene were efficiently used as benzoyl radical source for the benzoylation of 1, 4-naphthoquinones. [2] This synthetic protocol could be effectively used for the synthesis of wide range of 1, 4-naphthoquinones with different substitution patterns with good to excellent yields.

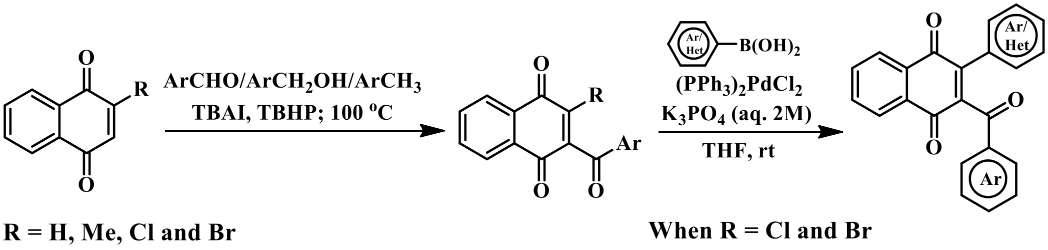

Figure 1: Synthesis of highly substituted 1, 4-naphthoquinone derivatives.

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Molecular electrostatic potential calculation based coformers Selection and development of new crystalline multicomponent forms of Resveratrol

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Multicomponent crystals of an active pharmaceutical ingredient (API) helps in the improvement of itsphysiochemical properties. [1]The experimental screening for multicomponent form development is a time taking and mostly based on trial and error approach. The robust computational screening method can help in solving this issue. [2]In this work we have present, how the molecular electrostatic potential calculationsmethod can be optimized for thecoformer selection for rationalcocrystal screening of a nutraceutical compound resveratrol. Ten new cocrystals with nine different coformers (phenazine, 4, 4′-bipyridine, piperazine, 1, 10-phenanthroline monohydrate, 2-aminopyrimidine, isonicotinic acid, 4-aminosalicylic acid, nicotinic acid, methenamine, 1, 4-diazabicylo[2, 2, 2]octane, succinimide, nicotinamide, 4-cyanopyridine, pyrazinamide, pyrazine, sulfadiazine and N, N-dimethyl-4-aminopyridine) were obtained after computational screening. The newly developed piperazine cocrystal exhibits the highest aqueous solubility among the previously known cocrystals of resveratrol.

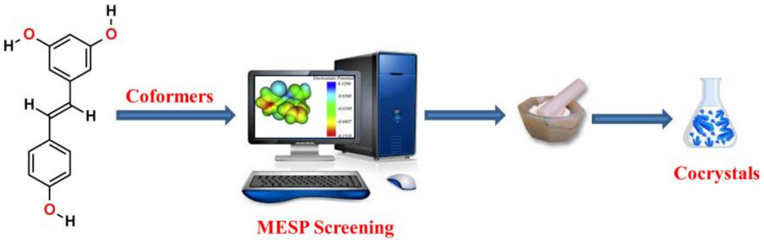

Figure: Procedure for coformer selection to cocrystal formation.

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Drug Mimetic Gelator in Nucleating Pure Drug Polymorphic Phases

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The design and synthesis of low molecular weight organogelators (LMWG) are gaining considerable attention from pharmaceutical research community as they can be used as crystallization media to control drug polymorphs nucleation. [1, 2]This work demonstrates a systematic approach to investigate the role of drug mimetic functionality of organogelsto nucleate specific polymorph of drug molecules. Three new drug mimetic organogels have been designed, synthesizedand characterized by using thermal, microscopic, and spectroscopic techniques. Gelation behaviour has been confirmed by rheological analysis. The gelators are furtherused as crystallization mediafor imide functionalized drugs. Chiralimide functionalised drug thalidomide and barbital have been chosen as model drug compounds for crystallization using the prepared drug mimetic gelators. The crystals obtained from both solution crystallization and gel phase crystallization has been analysed by microscopy, FT-IR, PXRD and/or unit cell determination. The gelators are found to be effective in preventing the concomitant crystallization of drug barbital and thalidomide.

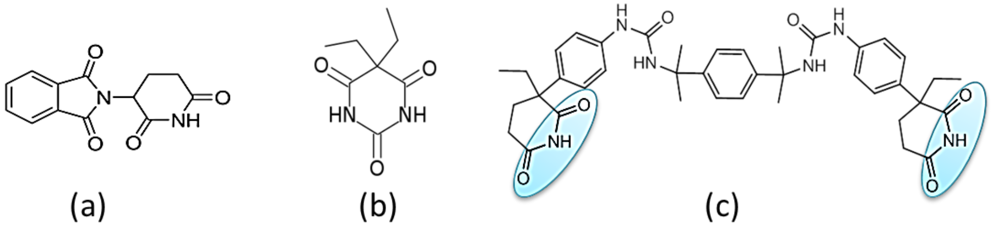

Figure 1. Molecular structures of drug (a) thalidomide; (b) barbital and (c) Imide mimetic functionality on the prepared gelators.

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Enhanced Oxygen Electrocatalysis Over $Mn_3O_4/CeO_2/C$ Nanohybrid Composite

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Superior bifunctional electrocatalysts for advanced oxygen reduction (ORR) and oxygen evolution reaction (OER) are the heart of key renewable energy technologies including water splitting and regenerative fuel cells. The design and synthesis of highly active yet low-cost ORR/OER electrocatalysts with long time durability is extremely desirable. Despite tremendous efforts made by scientific community, it remains challenging. Herein, we report a hybrid material consisting of Mn/Ce oxide nano-composite grown on carbon (Vulcan XC 72-R) as an efficient and high performance bifunctional electrocatalyst for ORR and OER in alkaline media. The prepared nanohybrid is characterized by investigating the crystal structures and electronic properties (XRD, HRTEM, and XPS), morphologies (SEM, TEM), porosities and surface area (BET) and electrochemical properties (Tafel analysis, Koutechy−Levich plots, and constant-current electrolysis). The $Mn_3O_4/CeO_2/C$ nanohybrid exhibits much better ORR activity compared to the benchmark Pt/C and Pd/C in alkaline media. It also tender better OER activity, making it a robust bifunctional electrocatalyst.

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Green synthesized gold nanoparticles for selective detection of arsenic and mercury in aqueous medium

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The presence of heavy metal ions in water is a serious issue for human being. In this work, we present a detection scheme of heavy metal ions in aqueous medium. Gold nanoparticles are synthesized through a green route where chitosan is used as reducing agent. Mangifera indica leaf extract is used to modify the as synthesized gold nanoparticles surface. Upon addition of different heavy metal ions to gold nanoparticles solution, only arsenic and mercury containing vials have shown colour change. This indicates the selective detection capability of these modified gold nanoparticles towards arsenic and mercury among other heavy metal ions. Besides, through UV-vis. spectrometry measurement, the surface plasmon resonance effect of gold nanoparticles upon addition with heavy metal ions are systematically studied and analysed.

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Predictive modeling and parametric optimization of dissolved Arsenic removal by Nanolignin: Calcium alginate hydrogel (LCH) beads using Response Surface Methodology (RSM) and Artifical Neural Network (ANN)

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Three different nanolignin variants were isolated from rice-husk using a chemically amended solvothermal approach and were used for the development of Nanolignin: Calcium alginate hydrogel (LCH) bead variants. The synthesized LCH bead variants were characterized using Photon correlation spectroscopy (PCS) and Fourier transform infrared (FT-IR) spectroscopy and were evaluated for their As removal efficiency using an OVAT (one-variable-at-a-time) based experimental design. A five-level-four-factor Central Composite Design (CCD) matrix was used to further investigate the effect of sorption parameters *viz.* contact time, adsorbate dosage, adsorbent dosage and solution pH concentration on the process of adsorption and derive the optimal set of parametric variables conducive to As adsorption. The trends obtained therefrom were re-assessed using a Multi-layered-perceptron (MLP) based Artificial Neural network (ANN) and the findings from the CCD and ANN process designs were found to be consistent with the experimental observations. The process of adsorption was also simulated using pseudo-first-order and pseudo-second-order rate kinetic equations and modelled using non-linear forms of Langmuir, Freundlich and Sips adsorption isotherms. The studies revealed an optimum As removal efficiency of ~86% for the 3h LCH variant which was found to be largely facilitated via chemisorption across the heterogeneous adsorbent surface. The findings thus demonstrate the significant potential of the synthesized LCH beads as efficient remediates for dissolved As likely to find usage in water purification and remediation applications.

Non-Noble Cu-$CuFe_2O_4$/C Nanohybrid: A Robust Electrocatalysts for Oxygen Reduction Reaction

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Spinel-type ferrites are a class of emerging transition metal oxides that have potential applications in fuel cell oxygen reduction reaction (ORR). However, there is lake of in-depth studies on the influence metal on ferrites (e. g. Cu on $CuFe_2O_4$) for ORR. Herein, we report a facile one-step synthesis methodology of copper ferrites anchored on heteroatom free carbon matrix (Cu-$CuFe_2O_4$/C) as the high-performance ORR catalyst. In the resultant configuration, carbon matrix offers continuous conductive support for electron/ion transfer and chemical interaction between them to enhance synergism of the catalyst. Consequently, the Cu-$CuFe_2O_4$/C electrode exhibits a high limiting current density (4. 35 mA/cm^2) in comparison to the state of the art 20wt% Pt/C (3. 81 mA/cm^2). The Cu-$CuFe_2O_4$/C hybrid, which combines the advantages of metallic copper and chemical interaction of carbon matrix along with the magnetic behavior of the nanohybrid, exhibits enhanced ORR properties.

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Gold Sulphur Oxido-Vanadate Nanoflute as an Efficient Catalyst for Nitro-Arene Reduction

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Gold sulphide embedded in vanadium oxides having nanorod structure is reported herein to be an effective catalyst for catalytic reduction of nitro-arene in isopropanol as solvent. The morphology of the gold-vanadate has hollow nanotube arrangement with the presence of voids giving rise to nanoflute like structure. The material was well characterized by different tools like XPS, TEM, BET, PXRD, Raman etc. analysis. The creation of non-uniform voids having length of ~142 nm and breadth ~70 nm leads to a hollow nanostructured in the material. The nitro-arene was effectively reduced in presence of isopropanol at 100 °C. In the reduction process, isopropanol act as a solvent and reducing agent in presence of KOH. The material was able to oxidize isopropanol liberating sufficient amount of in situ hydrogen for selective reduction of nitro-arene. The ability of the catalyst to oxidize isopropanol was substantiated from electrochemical studies.

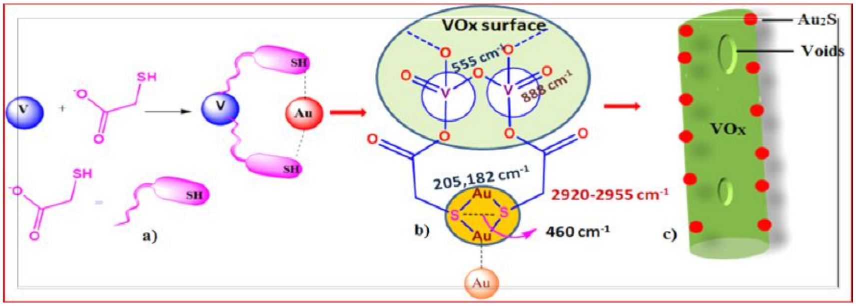

Figure 1. a) Probable interaction of thioglycolic acid with Au and V b) structural representation of AuVNF with some of the important vibrational bands and c) pictorial representation of the nanoflute.

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Sheets Composed of Graphene Oxide and iron as methanol sensing material

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A series of composites based on graphene oxide (GO) cross-linked with ferric hydroxide was developed as methanol sensing materials. GO, which was used as asupporting matrix here, was firstly treated with ferrous sulfate. Then, the ferrous compound cross-linkedwith GO was in situ oxidized to ferric compound by hydrogen peroxide, followed by treating with ammoniumhydroxide. The morphology and composition of the composites were analyzed by X-ray diffraction (XRD), scanning electron microscopy and transmission electron microscopy (SEM). The ferric hydroxide was found tobe homogenously impregnated onto GO sheets in amorphous form. These composites were evaluated as methanol sensing material by means electrical resistivity. The direct current electrical conductivity of the composite was calculated by a four probe technique. It is found that the conductivity dramatically increased to 67. 5 S/m for GO/iron (5 wt. %) composite at ~110 ˚C. The methanol sensing characteristics of the prepared composite was monitored by measuring the change in electrical resistivity on exposure to methanol vapour at different concentrations.

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Moving toward Ylide-Stabilized Carbenes

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The effect of ylide substitution atα positionto the carbene carbon (C_C) atom on the stability and σ-donatingability of a number of cyclic carbenes has been studiedtheoretically. The stabilities of all of the carbenes were investigated from an evaluation of their singlet–triplet energy gaps and stabilization energies. All carbenes were found to have a stable singlet state. The energy of the σ-symmetriclone-pair orbital at the C_C atom increases asa result of the introduction of ylide centers near to the $C_C$atom. This indicates an enhanced σ-donating ability of theylide-containing carbenes. The calculated carbonyl-stretchingfrequencies of the corresponding rhodium complexes, proton affinities and nucleophilicity index values correlatewell with the σ basicity of the carbenes.

RSM based optimization of *in vitro* culture conditions for the mycelial growth of Tea pathogen *E. vexans*

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Tea is one of the most popular beverages consumed worldwide and stands as a major cash crop contributing to the agro based economy of various countries. Among the various factors that affect the production of tea, blister blight is a serious foliar disease caused by the biotrophic pathogen*Exobasidium vexans*. Blister blightaffects the commercial production of tea in terms of both quality and quantity as the fungus *E. vexans* mainly infects young, succulent and harvestable leaves which are the main source for commercial production of tea. Although, exhaustive investigations have been carried out to elucidate the defense mechanism of tea plant against blister blight infections, very little has been known so far about the fungus and its molecular attributes during the state of infection. The major roadblock to such studies owes to the fact that *E. vexans* is an obligate biotrophic pathogen and hence establishment of its *in vitro* cultures is highly challenging. In the present study, statistical optimization of various growth parameters was carried out for the establishment of *E. vexans* culture under *in vitro* conditions. RSM (Response Surface Methodology) based CCD (Central Composite Design) matrix was employed to statistically optimize the variables *viz.* carbon source, tea leaf extract and $CaCO_3$, initial pH and incubation temperature. From the multivariate interaction study czapek dox medium was found to be the most effective medium for the growth of *E. vexans* and the supplemented tea leaf extract played a significant role in the *invitro* establishment of its culture. The optimal pH and incubation temperature required for the growth of *E. vexans* was found to be in the range ~5 – 6 and 25^0C – 27^0C respectively.

Pd_3Cu/C alloy nanoparticle as a highly efficient catalyst for electrochemical formic acid oxidation

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Lack of cost-effective catalysts hinders large-scale commercialization of direct formic acid fuel cells (DFAFCs). Thus, designing novel electrocatalysts for formic acid oxidation (FAO) reaction that occurs at the anode of DFAFCs is noteworthy in the recent years. This work aimed to synthesize carbon-supported bimetallic $Pd_{4-x}Cu_x$ (where x = 1, 2 and 3) nanoparticles (NPs) via solvothermal method to explore its electrocatalytic performance towards FAO reaction. The physicochemical properties of these NPs are confirmed using analytical techniques such as X-ray diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), inductively coupled plasma (ICP), X-ray photoelectron spectroscopy, and transmission electron microscopy (TEM). The electrocatalytic activity of the synthesized NPs was evaluated by cyclic voltammetry (CV) and chronoamperometry (CA) experiments, considering FAO as the model reaction. The current density, mass activity as well as electrochemically active surface area (ESCA)data proves Pd_3Cu/C to be the best electrocatalyst among the as-prepared $Pd_{4-x}Cu_x/C$ NPs towards FAO reaction. Moreover, the prepared Pd_3Cu/C NPs is also found to be superior in electrocatalytic performance as compared to Pd_3M/C (M = Ni and Co) NPs and commercial Pd/C towards the FAO.

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Organocatalyst for Infrequent Wacker-type Oxidation

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The finding of cost effective nitrogen rich porous organic polymer (POP) as an organocatalyst for organic conversion reactions is an alternative to conventional metal catalyst. [1-4]A nitrogen rich microporous polymeric material (MOP-D1) has been synthesised and characterized TGA, BET, SEM-EDX, TEM analytical tools. Characterized MOP-D1is subjected as organic catalyst in performing Wacker type oxidation reaction via radical mechanism. The importance of the reaction conversion arises from puzzling product formation rather than Markovnikov and Anti-markovnikov product.

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Supramolecular Association in the Solid-state Architectures of Cu(II) Coordination Solids: Experimental and Theoretical Studies

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The increasing interest in the field of the crystal design and engineering of multidimensional arrays and supramolecular architecture containing metal ions as nodes have achieved tremendous progress in recent years, which involves both synthetic and theoretical chemists, physicists, crystallographers and materials scientists, is justified by the potential utility of these compounds as zeolite-like materials, catalysts, magnetic materials or antibacterial activities. [1-2]Non-covalent interactions form the backbone of stabilities of supramolecular coordination solids and include hydrogen bond, stacking, electro- static, hydrophobic and charge-transfer interactions as well as metal ion coordination. [3]Analysis of intermolecular interactions using theoretical investigations represent a major advance in enabling supramolecular chemist to gain insight into crystal packing behavior. [4]

Herein, we report crystal structures of two coordination solids of Cu(II). Single crystal XRD studies shows interesting supramolecular layered architectures of the compounds formed by various supramolecular interactions viz. O–H···O, C–H···O, N–H···O and π–π. Theoretical investigations have been carried out on all the supramolecular contacts. The crystal structure, spectral studies and thermal stability of the compounds have been investigated. The antimicrobial activity of the ligand and its complexes has been screened against selected bacteria and fungi.

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Functionalized graphene oxide/ waterborne hyperbranched polyester nanocomposite: An environmentally friendly catalyst

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In recent decades, the design and development of polyester nanocomposite through facile approaches using bio-based and easily available raw materials that reduce the threat to the environment and human have achieved significant attention. Further, their applications in catalysis are significant area in sustainable chemistry as they facilitate environmentally benign catalytic processes. Among various types of catalysts, graphene oxide (GO) gaining greater attention owing to its excellent mechanical and electrical properties, high aspect ratio, high surface area, outstanding thermal conductivity, etc. Thus, GO was incorporated into the waterborne hyperbranched polyester matrix after functionalized with toluene diioscyanate and butane diol through a facile in situ polymerization technique in absence of any compatibilizing agent. The thermoset of the nanocomposite was acquired by curing with hyperbranched epoxy of glycerol and poly(amido amine). [1] This thermosetting nanocomposite was used for Aza-Michael reaction as it is an significant transformation in organic chemistry as these compounds are widely utilized in the synthesis of a different biologically active natural products, antibiotics, chiral auxiliaries, etc. [1]Further, it was also easily recoverable as well as recyclable with the constant catalytic activity. The nanocomposite not only exhibited excellent catalytic activity for this reaction but also showed significant improvement in mechanical (elongation at break, tensile strength, scratch hardness, toughness, Young's modulus and impact resistance) and thermal properties at a low loading of GO. Further, they also showed biodegradation behavior towards *Pseudomonus aeruginosa* bacterial strain. Thus, they can be used as a high performing environmentally benign material in multifaceted applications including heterogeneous catalyst.

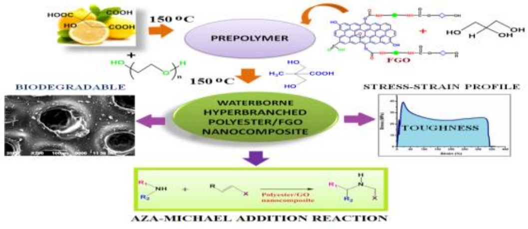

Figure 1. Fabrication of functionalized GO-based tough polyester nanocomposite.

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Structural insight into Conformationally Constrained 2’4’-BNA^{NC} [NH], [NMe] and [NBn] Nucleic Acid Analogue Monomers: A DFT perspective

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Conformationally Constrained 2’4’-BNA^{NC} (2, 4, -bridged nucleic acids) [NH], [NMe] and [NBn] nucleic acid analogues are a remarkable improvement in the area of antisense therapy. Their advantageous properties have even led them to enter human clinical trials. Although the nuclease resistance of these analogues is somewhat better than that of natural DNA, but is significantly lower than that obtained by the PS oligonucleotides, along with inefficient triplex formation and some kind being hepatotoxic. To deal with the observed drawbacks monomers level information of such modifications is very necessary. Thus in this work we have targeted a detailed DFT study of these modifications at the monomer level. All calculations have been performed using the GAUSSIAN09 software package. Full geometry optimization and single point energy calculations were done for isolated bases and at the hybrid M06-2X/6-311G (d, p) level of theory using CPCM solvation model. Calculated geometrical parameters were found to agree well with the available experimental values.

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Prospect and challenges of bio-based biodegradable superabsorbent for multifaceted applications

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Superabsorbent hydrogels are polar, loosely cross linked, hydrophilic network of 3-dimensional polymeric structures, which can absorb and retain several hundred times more water than their dry weights. They have wide spectrum of applications in the fields of personal hygiene materials, soft lenses, controlled drug delivery systems, control release of fertilizers, waste water treatment, enhance oil recovery, environmental remediation, etc. Because of their such remarkable range of applications , the production of these materials in mass sale using facile and greener methodology urge upon great attention to the material scientists. Furthermore, these superabsorbent polymers are commonly prepared by polymerization of acrylic acid and acrylamide based petrochemicals with synthetic cross linking agent. But such superabsorbent hydrogels are non-biodegradable as well as the raw materials are non-renewable and hence cause environmental solid waste disposal problem as well as depletion of pertroleum resources. In this milieu, a biodegradable renewable resource based superabsorbent hydrogels is a demand of the day. But as most of the hydrophilic renewable resource based natural polymers have low capacity of water absorption as well as not easily crosslinked, so obtaining such materials is a real challenge. In this vein, our effort to produce eco friendly, bio based superabsorbent hydrogels by using various polysaccharides such as starch, chitosan, guar gum, etc. demands a special attention as they are expected to be bio degradable and obtain from renewable resources. The results obtained in the regard will be presented in this conference.

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DFT study of Rh(I/III) complexes derived from Salophen ligand

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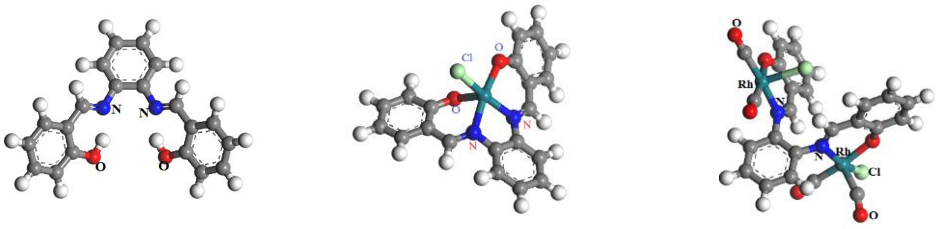
Two new rhodium(I/III) complexes [Rh(η^4-**L**)Cl] (**1**) and *cis*-[$Rh_2(CO)_6Cl_2$(μ^1-N, N-**L**)] (**2**) were synthesized by reacting $RhCl_3$. $3H_2O$ with Salophen ligand [**L** = N, N′-bis(salicylidene)-1, 2-phenylenediamine (**a**)] in 1: 1 molar ratio in dichloromethane solution. The complexes**1** and **2**were characterized by FT-IR and UV-Visspectroscopy. We have also carried out a geometry optimization study for ligand and its complexes using gas-phase density functional theory (DFT) with B3LYP/6-31+G(d) level of theory and using double numerical plus polarization (DNP) basis set as implemented in the program DMol3program package. [1] In order to confirm the stability of the complexes, we performed vibrational frequencies calculations at the optimized structure with the same level of theory. In the vibrational frequency calculations, no imaginary frequency is observed for the compounds which suggests that the optimized compounds signify stable structures *i. e.,* shows local minima in the potential energy surfaces. From the optimized structures (Figure. 1), it is noticed that all the bond lengths of complex **2** are higher than that of complex **1** and the complexes are distorted. HOMO-LUMO gap ($\Delta E= E_{LUMO}-E_{HOMO}$) and hardness ($\Delta E/2$) values suggest that complex **1** is more stable than complex **2** as it has high ΔE and hardness value. The experimental and theoretical IR and UV spectra of complexes corroborates each other. [2]



L **1** **2**

Figure. 1 DFT optimized geometries of ligand and Rh complexes.

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Novel one-pot Synthesis of Cyanamides from DithiocarbamateSalts usingenvironmentally benign reagent Tetrapropylammonium tribromide

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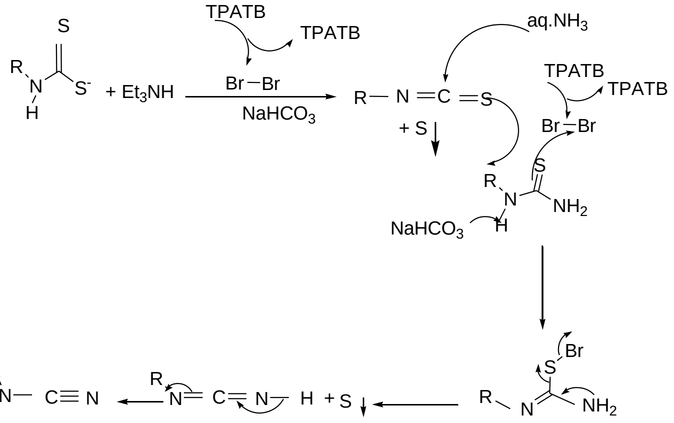
A highly efficient and simple protocol for the synthesis of Cyanamides from their respective amines in the presence of mild, fast, and non-toxic reagent Tetrapropylammonium tribromide is described. High environmental acceptability of the reagents, cost effectiveness and high yields are the important attributes of this methodology.



Scheme: Plausible mechanism for the formation of cyanamide

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Study on Calcineurin Inhibition by Peroxo Vanadium(V) and Niobium(V) Compounds

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The field of modern medicinal chemistry have mostly been dominated by organic drugs. But the serendipitous discovery of cisplatin has changed the paradigm and triggered the development of inorganic medicinal chemistry. Metal compounds have been used in medicine since time immemorial. [1] Based on the singular properties of metal and reactions occurring in the cells, inorganic drugs with therapeutic potential have been designed. Since last decade, Vanadium has been in focus as an attractive choice of metal due to its biological relevance along with its involvement in several cellular signalling pathways. [2] Compared to vanadium, the biological activity of another group V metal, niobium is yet to be explored. The main aspect of niobium is its low toxicity. [3]In the present work, we have investigated the effect of peroxo vanadium and niobium complexes, comprising of monomeric as well as polymer bound macro complexes, on the activity of calcineurin *vis-à-vis* H_2O_2. Calcineurin (protein phosphatase 2B) is a major calmodulin binding serine/threonine phosphatase which plays a critical role in the signaling pathways necessary for T-cell activation, nervous system development and function and cardiac growth. [4]The study showed the competence of both peroxo vanadium and niobium compounds as calcineurin inhibitor. Detailed inhibition kinetic studies reveal that the compounds are uncompetitive inhibitors of calcineurin. [5]

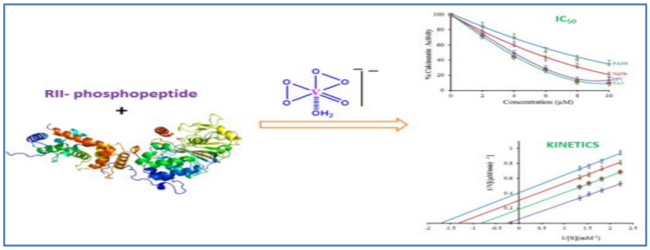

Figure: Graphical representation of Calcineurin inhibition study

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Ru(II)-Catalyzed Annulation of Benzamidines and Alkynes by C-H/N-H Activation: A Facile Synthesis of 1-Aminoisoquinolines

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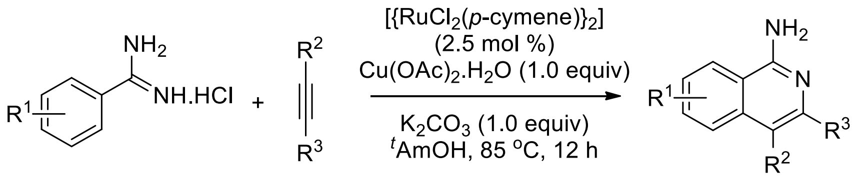
1-Aminoisoquinolines are very important compounds due to the wide range of biological activities exhibited by them. For example, they are the inhibitors of thrombin, factor Xa, rho kinase-I and they display antitumor and antimalarial activities. [1] Because of the high biological profile, there is a continued strong demand for efficient and selective synthesis of 1-aminoisoquinolines for highthroughput drug screening. In the last two decades, the transition-metal-catalyzed organic reactions via C-H activation have evolved as a powerful tool to construct functional molecules. [2]Very recently, we have developed a C−H activation and annulation reaction of readily available benzamidines with disubstituted alkynes catalyzed by inexpensive and readily available ruthenium catalyst [RuCl$_2$(*p*-cymene)]$_2$, for the synthesis of a wide range of 1-aminoisoquinolines (Scheme 1). [3] This work will be presented in the symposium.



Scheme 1. Synthesis of 1-Aminoisoquinolines

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Biodegradable waterborne bio-based polyester: An approach towards environmental remediation

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With growing modernization of today's world, synthetic polymers have started substituting natural materials in almost every area. Among different synthetic polymers, polyesters are one of the significant interests due to their inborn versatile properties along with their wide variety of applications. However, these synthetic polyesters are highly dependent on petroleum-based feedstocks and their preparative protocols involve volatile organic solvents. [1] In this context, synthesis of waterborne polyesters from bio-based resources addresses the shortcomings of the synthetic polyesters as they possess many favourable attributes like no or very low VOC, easy to clean up, non-toxic, non-flammability and low odour. [2] Furthermore, such polyesters with aliphatic structure have attracted significant attention as they are biodegradable and biocompatible. [3]In this milieu, waterborne polyesters were synthesized by using bio-based reactants such as glycerol, citric acid, tartaric acid, sorbitol and dimer acid at different compositions without using any solvent and additional catalyst. The polyester becomes water-soluble on addition of triethanolamine as a neutralising agent, which were then cross-linked with glycerol-based epoxy and fatty-acid based poly(amido amine) to obtain their respective thermosets. The synthesized polyester thermosets showed good performances such as mechanical, thermal and chemical along with hemocompatibility and biodegradability. Therefore, these types environmentally benign polymeric materials can overcome the shortcomings of petroleum based synthetic polyesters as well as they can find applications in different field.

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Waste Chicken Feather Fiber as Reinforcement in Modified Epoxidised Soybean Oil Based Composites

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In recent years, the abundant quantity of chicken feather produced annually by the poultry industry as a waste in worldwide, is a serious threat to the environment as well as society. [1] Health hazards as well as green house pollution arising from the wastes could be minimised by forming composites of these feathers with bio-resins. [2]

In this study, effortswere made to prepare composites with methacrylic anhydride modified epoxidised soybean oil (MAESO), rosin acid derivative i. e., Divinylacrylicpimaric acid (R2) and chicken feather fiber via compression molding technique. Three different percentage of nanoclay were loaded in the composite matrix system and the properties were evaluated. Rosin obtained from pine trees was derivatised and used as a crosslinker. Both MAESO resin and R2 were characterized by ^{1}H-NMR and FT-IR spectroscopy. FTIR, XRD, and TGA studies were employed for the characterization of the prepared composites and the morphological structure was studied by scanning electron microscopy (SEM). Various properties of the nanoclay incorporated composites were found to be improved.

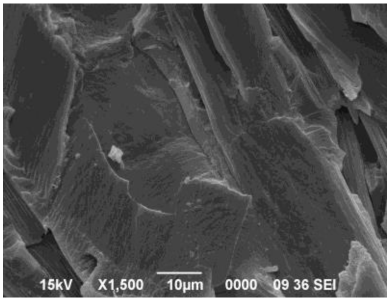

Figure 1. SEM image of chicken feather based composite

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Electrochemically synthesis of graphene quantum dot and its characterization

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In the recent years, the graphene quantum dot has enable to attract the attention of the researchers because of its unique properties like high luminescence, low toxicity, high electrical conductivity etc. and vast range of applications (bio-imaging, sensing, catalytic activities etc). Graphene quantum dot is a zero dimensional carbon system, where all the carbon atoms are bonded in sp^2 hybridized state. In this work, we report the electrochemical synthesis of the graphene quantum dot from commercially available pencil lead graphite. Raman, UV-Visible spectroscopy, DLS, PL/TRPL were employed to characterize the graphene quantum dot.

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A convenient synthesis of oxazolidinone and oxazinanone derivatives via intramolecular ring opening of epoxides

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Biologically active molecules have been obtained through the screening of small-molecule libraries. In this aspect, the library diversity is more crucial consideration. Thus, the diversity-oriented synthesis (DOS) has emerged as a powerful tool for the discovery of biologically active small molecules. [1] Both oxazolidinone and oxazinanone represent important classes of heterocyclic compounds. [2]As a part of our ongoing research interest in developing effective methodologies for the synthesis of biologically relevant heterocyclic compounds using epoxide building blocks, [3] we have synthesized a small libraries of heterocycles **1** and **2** using transition metal-free, intramolecular epoxide-ring opening cyclization as a key step (Figure 1).

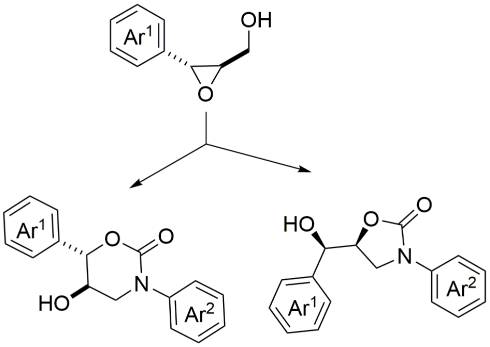

Figure 1

The detailed synthetic studies towards these molecules will be presented in the Conference.

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Cu(II) and Co(II) Coordination Solids involving Phenantroline and Dicarboxylato Ligands: Supramolecular Association and Microbial Studies

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Research in the development of new metal-based compounds with biologically relevant molecules has attracted great interest. [1] Such coordination complexes have much potential for the design of novel remedies with useful properties for practical applications like antibacterial, antifungal, antimicrobial activity where the transition metal ion performs crucial role in terms of structural organization and overall functionality. [2] Coordination compounds with carboxylate ligands are important as building modes for metal organic supramolecular architecture due to thewide variety of coordination modes. Moreover, properties of transition metal carboxylate and the coordination abilities of carboxylate ions can be varied to a large extent using nitrogen donor ligands like 1, 10 phenanthroline (*phen*) with appropriate functionalization [3].

Herein, we report crystal structures of two coordination solids of Cu(II) and Co(II). Single crystal XRD studies shows interesting supramolecular layered architectures of the compounds formed by various weak supramolecular interactions viz. C–H···O, N–H···O and π–π stacking. The crystal structure, spectral studies and thermal stability of the compounds have been investigated. The antimicrobial activity of the ligand and its complexes has been screened against selected bacteria and fungi.

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The efficient role among the inefficient current collector in aqueous aluminium ion batteries

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The current research on rechargeable aluminium-ion batteries has faced many challenges to make it a better alternative than lithium-ion batteries. [1] Many attempts were made to overcome these challenges and one such attempt, is to find a suitable electrode material which can deliver suitable Al^{3+} ion storage capacity in rechargeable aluminium-ion batteries. [2, 3] Here, we showed that one of the essential criteria for correct electrochemical evaluation of aqueous aluminum-ion batteries is theappropriate selection of current collector. Assuming anatase TiO_2as the model electrode material, it is demonstrated that the type of current collector could transform an inefficient electrode material to an efficient one. TiO_2could deliver an initial discharge capacity of 256 $mAhg^{-1}$at a current density of 4 Ag^{-1} with graphite current collector, whereas it is only 82 $mAhg^{-1}$ with titanium current collector at similar current density. Surprisingly, no electrochemical activity could be attained using nickel and stainless steel at any current densities [4].

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Molecular Docking and Molecular Dynamics to identify a potential Human Estrogen receptor inhibitor from polyphenols extracted from *Daucas carrota* seeds

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The seeds of *Daucus carrota* have a long history of use as an anti-fertility agent in United States, European countries and India (1). Scientific in vivo and ex vivo studies suggest that the polyphenolic compounds present in *Daucus carrota* seeds may show anti-fertility effect through impairment of estrogen- progesterone balance (2). Such an impairment can result due to blocking of the receptor binding sites by these compounds thereby affecting the signaling pathway of the sex hormones (3). Although a number of experimental studies have reported the antifertility action of the carrot seed extracts, no attempt has been made so far to reveal the molecular mechanism involved. The present study was undertaken to explore the nature of interaction of these compounds with estrogen receptor using a computational approach. Three major polyphenols viz. catechin, epicatechin, and eridictyol extracted from *Daucus carrota* seeds were chosen to study their interaction with estrogen receptor.

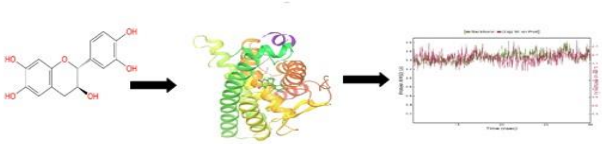

Figure: Catechin undergoing molecular docking and dynamics simulation with ERα.

Molecular docking and dynamics simulation studies were carried out to understand the binding mode and binding strengths of the selected compounds with the receptor. All the three compounds exhibited good binding interaction with the ER, which is ensured by the docking score and the binding affinity values. The present novel study suggested that all three polyphenols extracted from carrot seeds have the potential to compete with the normal substrate binding of ER and interfere with the ER signaling pathway, thus affecting the reproductive function.

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Synthesis of Chroman-Linked Benzothiaoxazine-1, 1-dioxides via Anion Relay Chemistry

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The chroman and benzosultam ring systems are found in a diverse array of compounds, including biologically and therapeutically active agents and natural products. [1]In this regard, molecular frameworks with chroman skeleton linked with benzosultam units should be attractive scaffolds for drug discovery. On the other hand, due to their ready availability in racemic as well as enantiomerically pure forms and capability to undergo inter- and intramolecular ring-opening reactions with diverse carbon and hetero nucleophiles, epoxides have been exploited as versatile building blocks in organic synthesis. Based on the synthetic and biological importance of chroman and benzosultam derivatives, and our fruitful experience in intramolecular epoxide-ring opening chemistry, [2] we became interested in synthesizing chroman-linked benzosultams **1**(Figure 1)employing a protecting group- and transition metal-free strategyvia anion relay chemistry.

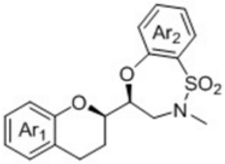

Fig : 1

- Combination of two privileged structure
- Transition metal free C-O bond formation
- Enantio and diastereoselective

The detailed synthetic studies towards these conceptually new and architecturally interesting molecules will be presented in the Conference.

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Simultaneous extraction of hemicellulose and cellulose nanofibers from Kans grass (*Saccharum spontaneum*) using chemical pretreatment method

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Kans grass (*Saccharum spontaneum)* is a locally available grass species that abundantly grows on non-agricultural landmass and has a great potential for the production of high value chemicals due to its high cellulosic content. However, the conversion of the cellulose rich biomass to high value chemicals/precursors is hindered by the highly recalcitrant lignocellulosic microstructure. In order to extract the cellulosic content promote accessibility for diversified usage, these hierarchical structures need to be altered via pretreatment approaches. The current work evaluates the use of *Saccharum spontaneum* as a feedstock for extraction of hemicellulose and cellulose nanofibers simultaneously by integrated chemical pretreatment method. Hemicelluloses were extracted using alkaline extraction (NaOH) and ethanol precipitation. While, cellulose fibers were obtained after subjecting the alkali treated *Saccharum spontaneum* to bleaching treatment. Finally cellulose nanofibers were extracted from these fibers using hydrochloric (HCl) hydrolysis treatment. Yields of hemicellulose and cellulose nanofibers were 58 and 88%, respectively, calculated separately on the basis of their content in *Saccharum spontaneum*. The extracted material after each stage of the treatments was characterized and its chemical composition was determined. The progressive removal of the non-cellulosic constituents was confirmed by Fourier transform infrared (FTIR) spectroscopy. The increased crystallinity with successive treatments was revealed by X-ray diffraction (XRD) analysis. Morphological investigation was performed using scanning electron microscopy (SEM) and the thermal stability was investigated using thermogravimetric analysis (TGA).

Dimensional Stability and Durability Assessment of Phyto Extracts Treated *Bambusa Tulda* Roxb.

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Bamboo is a unique, versatile and widely used lignocellulosic material. It is cheap, possesses adequate mechanical strength, can be utilized readily for a variety of purposes, most important being as construction material. Some drawbacks like its easy susceptibility to biodegradation, dimensional instability etc. limits its utilization. It was reported that bamboos when adequately treated with suitable preservatives, it become resistant to the attack of fungi and insects and give satisfactory service life. However, most of the chemical used as preservatives causes environmental hazards. Phyto extractives are one of the most viable alternatives to chemicals. The effect of phytoextracts viz. *Chromolaenaodorata* (Germany bon), *Clerodendron infortunatum* (Dhopat tita), *Dryopteris adans* (Dhekia bihlongoni), *Polygnum hydropiper* Linn. (Pothar bihlongoni) and the root extract of *Allium sativum* (Naharu) on dimensional stability and termite resistance capacity were studied and the treatment showed positive impact in both the counts. The dimensional stability efficiency of the treated sample in terms of Anti-shrink Efficiency (ASE) and Bulk coefficient(BC) was improved compared to untreated samples. The efficacy of the preservative phytoextracts for the treatment of bamboo samples was evaluated in ground contact against termite and fungus and found to be improved on treatment.

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Uses of Brönsted acidic ionic liquids for multicomponent synthesis of tri and tetra substituted imidazoles under solvent-free condition

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Multicomponents reactions (MCRs) constitute an especially attractive synthetic strategy for rapid and efficient generation of complex library of molecules because the products are formed in a single step and diversity can be achieved simply by varying the reacting components. Furthermore, these reactions are convergent, atom economic, possible structural variations of products, accessible complexity of the molecules and reduction of reaction steps. Designing of the MCRs in presence of Brönsted acidic ionic liquids (BAILs) catalyst also eliminate several drawbacks observed using mineral acid or Lewis acid catalysts. The BAILs can act as dual solvent-catalyst system with negligible vapor pressure, good thermal stability, recyclability in homogeneous phases by dissolving variety of organic and inorganic substrates. The uses of BAIL catalysts are investigated for preparation of tri (I) and tetra (II) substituted imidazoles (Figure**1**) through MCRs in neat condition. Large numbers of imidazoles have been found with several biological and pharmacological activities [2] in addition to uses in material sciences. The structure of imidazole derivatives are established using ^{1}H NMR, ^{13}CNMR, FT-IR analysis and also by melting point.

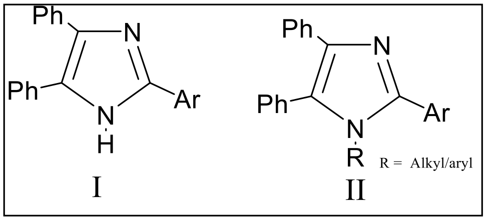

Figure . 1: Structure of tri and tetra substituted imidazole derivatives

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An anionic polymeric chromogenic receptor containing N, S donar sites for selective recognition of HSO_4^- ion

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A new polymeric chemosensor bearing thiourea moieties was synthesised. The chemosensor was found to bind hydrogen sulfate in semi-aqueous solvent systems. Upon continuous addition of 0 to 630 μM of hydrogen sulfate, a shift in the UV-Vis absorption band was observed with a clear isobestic point at 345 nm. The effect of water content on the binding affinity of the chemosensor towards hydrogen sulfate was evaluated, showing that the chemosensor preferentially binds to hydrogen sulfate over the other anions investigated in this study.

Effect of Preparation Method on Properties of Ni/$Ce_{1-X}La_xO_y$ Catalysts

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Carbon dioxide generated by the utilization of carbon-rich fossil fuels (coal, oil, natural gas) is one of the main greenhouse gases. Steam/CO_2 reforming of methane for production of syngas can be considered as an environmentally safe reaction because the main raw materials in this process are greenhouse gases: methane and carbon dioxide. Ni/$Ce_{1-x}La_xO_y$is a good candidate catalyst for this process which is connected with the ability of Ni to break effectively C–C and C–H bonds as well as the contribution of ceria to the activation of the O-H bond. The presence of La promotes Ni dispersion and provides the advanced stability of catalysts [1, 2]. So, in this work, the effects of a preparation method on the physicochemical and functional properties of Ni/$Ce_{1-x}La_xO_y$catalysts were studied. Our strategy was to achieve high catalytic activity and material stability against deactivation by the use of $(CeLa)_{0.8}Ni_{0.2}O_y$ mixed oxides as precursors of Ni/$Ce_{1-x}La_xO_y$catalysts. The Ni/$Ce_{1-x}La_xO_y$samples with different Ce/La molar ratio were prepared by the incipient wetness impregnation (I-series) and polymerizable complex (P-series) methods. To establish the composition-structure-properties correlation, the catalysts were characterized by a group of methods (TG-DTA, BET, XRD, HRTEM-EDX, and H_2-TPR) and tested in the reforming reaction. It was shown that the preparation method and La/Ce molar ratio influence the textural and structural properties of Ni/$Ce_{1-x}La_xO_y$ materials, as well as their reducibility. According to XRD data, the CeO_2 based solid solution with an average crystallite size of 4-6 nm is the main phase of Ni/$Ce_{1-x}La_xO_y$(P)samples, whilethe two-phase system – the CeO_2 based solid solution and NiO was formed in the case of Ni/$Ce_{1-x}La_xO_y$(I)catalysts. The crystallite size, NiO dispersion, and red-ox characteristics are strongly affected by La/Ni molar ratio and conditions of the thermal treatment. The effect of the thermal treatment of Ni/$Ce_{1-x}La_xO_y$catalysts on their coking resistance and functional properties in reforming were studied. The composition-structure-properties correlation was established.

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Effect of Photoluminescent Carbon Dots on the Efficiency of Poly(methyl methacrylate) Based Dye Sensitized Solar Cell

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Dye-sensitized solar cells (DSSCs) are a low-cost alternative to the more expensive traditional silicon based solar cells. However, long term stability and low efficiency are the major problems with DSSCs. In this work, a polymer gel electrolyte (PGE) based on poly(methyl methacrylate) (PMMA) incorporated with carbon dot (CD) is studied. The prepared CDs emits green light which coincides with the absorption range of the dye used in the DSSC. Consequently, the CDs enhance its efficiency by broadening the sunlight absorption range. The PGE is prepared by mixing PMMA with optimum amount of CD in liquid electrolyte. Current density-voltage characteristics plots and impedance spectroscopy are used to characterize the fabricated DSSCs under irradiation of light. The DSSC employing PGE with 0. 14 w/v% CD exhibits an efficiency of 6. 05%, which is noticeably higher than that of the DSSC fabricated with PGE without CDs (2. 83%). Concurrently, significant improvement is also achieved in the current density, the open circuit voltage and long term stability.

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Synergistic catalysis of $Mn_xCo_{3-x}O_4$/C nanostructures for high-performance bifunctional oxygen reduction/evolution reactions

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Transition metal oxides for oxygen reduction (ORR) and oxygen evolution (OER) reactions are most promising catalysts for renewable-energy technologies. Among transition metal oxides, Co and Mn oxides are very active for both ORR and OER and can act as a bi-functional catalyst. But due to their poor electron conductivity, carbon materials are used as supports or mixed with other metal oxides to increase their conductivity that assistances in electrochemical applications. Herein, a series of highly active mesoporous material consisting of $Mn_xCo_{3-x}O_4$(x = 0. 9, 1. 5, 2. 1)nanocrystals grown on carbon (Vulcan XC 72-R) as high performance bi-functional electrocatalysts for both ORR and OER have been synthesized. The synthesized $Mn_xCo_{3-x}O_4$/C catalysts are thoroughly characterized. These nanostructures exhibit much better ORR activity compared to the commercial Pt/C and Pd/C in alkaline media in terms of mass specific activity. The materials are also very active towards OER, making it bi-functional electrocatalysts. The nanostructures follow a 4-electron pathway for ORR. The superior electrocatalytic presentation mainly arises due to the better synergistic coupling effect of Mn_2O_3, Co_3O_4 and carbon.

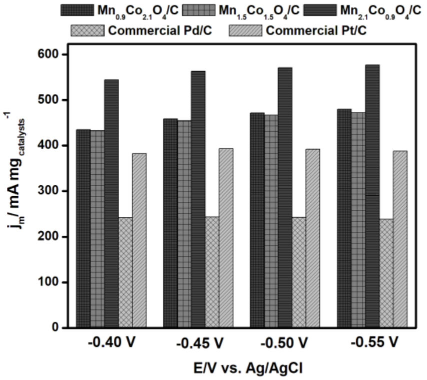

Figure 1: Mass specific activities of $Mn_xCo_{3-x}O_4$/C under different potentials.

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Evaluation of Frostbite Healing Potential of Green Synthesized Silver Nanoparticles

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Frostbite is a cold induced injury which occurs due to exposure of a particular site of body to sub –zero temperature. Past few decades, there had been extensive research in field of wound healing, including burns. However the field of frostbite wound is little explored. Our current work involves development of Aloe based green nanoparticles and evaluation of its frostbite healing potential. We successfully developed the nanoparticles and characterized them using different techniques including DLS, TEM and XRD. We further evaluated their activity on Liquid nitrogen induced frostbite injury. We obtained encouraging results in our investigation as observed by wound healing rate and histopathological analysis.

Switching FromPositive to Negative Axial ThermalExpansion in Two Crystalline Organic Compounds

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Negative Thermal Expansion (NTE) of a material is unusual phenomenon in which the material contractsupon heating and vice versa. Although NTE is relatively common in inorganic compounds, recently few organic compounds have been reported for exceptionally large linear NTE . Switching of thermal expansion is not so common in any material although there are very few reports of some MOFs. Here we present an extraordinary phenomenon of switching from positive to negative axial thermal expansion intwo new diyne-diol-based organic compounds (**1**, **2**). Variable temperature SCXRD experiments from 90K to 270K for compound **1** and 100K to 300K for compound **2** show usual PTE in both the compounds. Surprisingly, the *c* axis decreases with increasing temperature upon further heating from 270K to 350K for compound **1** and from 300K to 400K for compound **2**, whereas *a* and *b* axes expand normally (Fig. **1**). Analysis of crystal structures of both the compounds reveals the mechanism of the unusual phenomena. It has been observed that particular orientation of molecules in the crystal structure and transverse vibration of atoms in the molecules play essential role in the switching of thermal expansion.

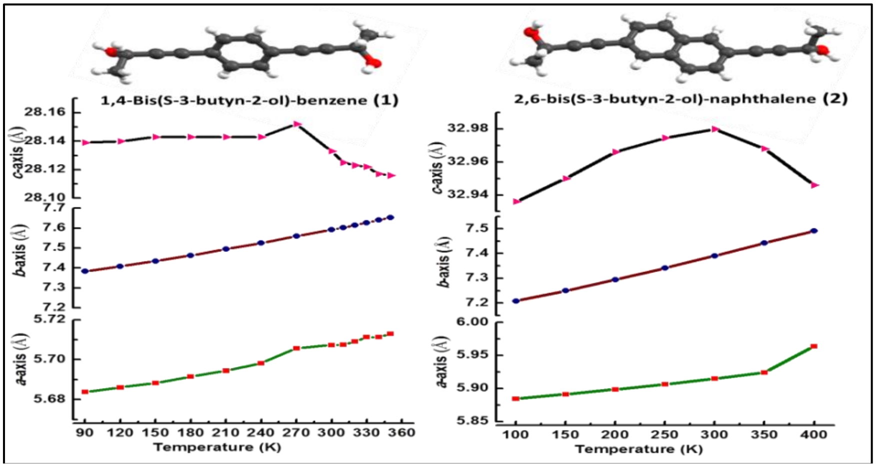

Fig. 1: Change of unit cell with Temperature for two organic compounds. Switching from PTE to NTE is observed for the crystallographic *c* axis.

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Multicomponent eco-friendly synthesis of 3, 4-Dihydropyrimidinone under Microwave condition in the presences of Rhus semialata as a catalyst

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Derivatives of 3, 4- Dihydropyrimidinones were found to possess many biological activities and find an enormous scope in the field of medicinal chemistry. Here in we report the synthesis of 3, 4- dihydropyrimidinone derivatives by the ternary cyclo condensation of various aldehydes, methylacetoacetate and urea in the presences of Rhus *semialata* as an acid catalyst under MW condition.

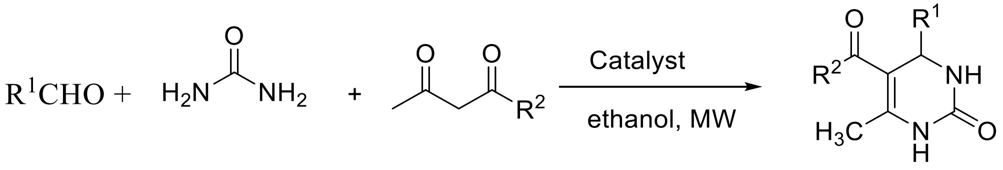

Fig: 1. General Reaction Mechanism

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Remote 'Imidazole' Based Ruthenium(II) Para-Cymene Pre-catalyst for the Oxidation of Alkyl Arenes/Heteroarenes to Aldehydes/Ketones

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The dual role of remote 'imidazole' attached with the pre-catalyst [(*para*-cymene)Ru^{II}(L)Y]$^{+}$ (L = 2-(4-substituted-phenyl)-1H-imidazo[4, 5-f][1, 10] phenanthroline, Y = chloride/solvent) was explored for the selective oxidation of alkyl arenes/heteroarenes to corresponding aldehydes and ketones, in which presence of 'imidazole' was found to be highly effective for the activation of oxidant and release of *para*-cymene from the pre-catalyst, which in turn was not observed without the 'imidazole' moiety. In the present study, we report the synthesis and characterization of phenanthroline derivatives containing imidazole at the remote backbone and their corresponding Ruthenium complexes, in which [Ru(*p*-cymene)Cl]$_2$ was used as the precursor complex. The synthesised complexes were characterized using various analytical techniques like NMR, UV-visible and Emission spectroscopy. The catalytic activity of the complex was studied in the oxidation of alkyl arenes/heteroarenes to aldehydes or ketones. The products were isolated in good to high yields. The kinetics of the reaction with respect to different reaction parameters were investigated through GC-analysis and finally the mechanistic study was done through spectroscopic, kinetic and other controlled experiments.

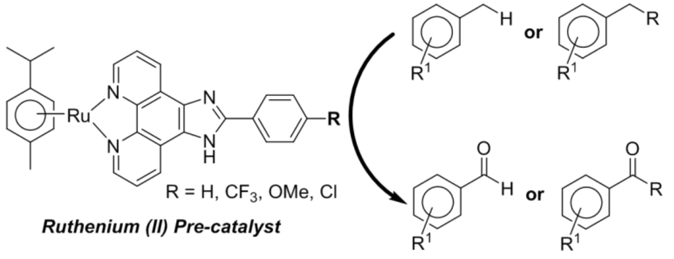

Figure: Ruthenium (II) pre-catalyst mediated oxidation of alkyl/heteryl arenes to aldehydes/ketones

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Pd-Catalyzed Carbonylation of Aryl Halides Using CO Surrogate

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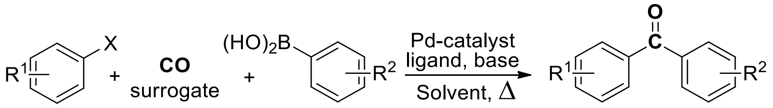
Ketones are key structural building blocks found in pharmaceuticals, agrochemicals, natural products, photo-sensitizers and sunscreen agents. [1] They are ideal starting material for the synthesis of various organic molecules *viz*. oximes, cyanohydrins, carbazones, hydrazones, pinacols, acetals, etc. These potentials of ketones have attracted significant interest in the development of novel and efficient method for their synthesis. [2]In this domain, the palladium-catalyzed carbonylative cross-coupling using carbon monoxide as a C-1 source represents one of the most widely employed methods for the synthesis of ketone derivatives. [3]However, the use of toxic and inflammable carbon monoxide restricts its widespread application. To address these issues, the development of CO-free protocol has gained importance recently. [4]The use of CO surrogates provides a safe and suitable alternative for the synthesis of carbonyl derivatives avoiding the need to use gaseous CO.

Herein, an easily adaptable Pd-catalyzed carbonylation reaction of aryl halides using CO surrogate has been developed under mild reaction conditions. Excellent yields and conversions were obtained under low catalyst loadings.



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A Crystal Engineering Approach to the Synthesis of Six-component Molecular Solids

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The logical design of multi-component molecular solids it has gained in importance in the field of crystal engineering because of their wide applications from materials to pharmaceutical sciences[1]and their synthesis is really a daunting task. Despite this, a number of five and six-component molecular crystals have been synthesized here. A two-step crystal engineering strategy is presented here; the first part is based on the idea that if any molecule is present in two different environments in its lower-order cocrystal, a suitable new molecule can replace the one which is comparatively loosely bound to obtain a higher-order cocrystal. [2]Utilizing this concept, a stoichiometric quaternary cocrystal is obtained from a binary system and the homologation process is ended here. At this stage, the lack of inequivalence does not allow us to move forward and achieve a cocrystal having more than four components. This is only possible when two or more molecules with similar shape and size share a single lattice position and produce a nonstoichiometric cocrystal i. e. solid solution. [3]Followingthis idea, the fifth and the sixth component have been successfully incorporated in the quaternary assembly. [4]

For this crystal engineering exercise, substituted resorcinols such as 2-chloro-, 2-bromo-, and 2-methylresorcinols (having similar shape and size), some ditopic bases, and a few flat polyaromatic hydrocarbons have been used.

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Green synthesis of copper oxide nanoparticles and its antibacterial study

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The present work is attributed to green synthesis of copper oxide nanoparticles (CuONP) using *Banana pseudostem* ash (Kolakhar) extract. The synthesized nanoparticles are characterized by TEM, XRD, SEM, EDX and FTIR analysis. Green synthesized CuONP exhibited strong antibacterial activity against *E. coli* (MTCC-443), *Pseudomonas aeruginosa* (MTCC-741), *Bacillus subtilis* (MTCC-121), *Staphylococcus aureus* (MTCC-3160), *Yersinia enterocolitika* (MTCC -4848) and *Enterobacter aerogens* (MTCC- 111) bacteriaby revealing clear zone of inhibition by Kirby-Bauer agar well diffusion method. These nanoparticles are than applied to fabricate nanocomposites using activated charcoal. The fabricated nanocomposte showed profound antibacterial efficacy against tested bacteria.

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Synthesis of 2-substituted benzimidazole and benzothiazoles using sulfonic acid functionalized activated carbon prepared from matured tea leaf as an efficient green catalyst

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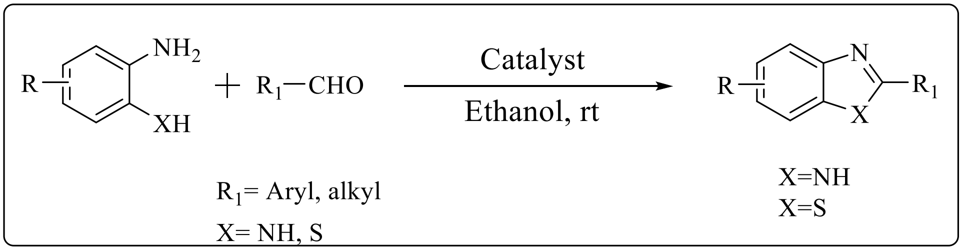
Benzimidazoles and benzothiazoles are the most important heterocyclic compounds since they act as active substructures in many biologicallysignificant compounds. Herein we demonstrate a simple and efficient method for synthesis of both the heterocycles using sulfonic acid functionalized activated carbon as the heterogeneous catalyst. The catalyst was prepared by anchoring SO_3H group on the surface of activated carbon synthesized from matured tea leaf. The reactions were carried out within a short reaction time at room temperature using ethanol as the solvent. After completion of the reaction the catalyst could be recovered easily and reused for seven consecutive catalytic cycles without significant decrease in the catalytic activity. Thecatalytic activity of the catalyst was found to be better than that of a similar catalystprepared from montmorillonite K10.



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Chiral Cobalt Catalyst in Zeolite-Y for Asymmetric Henry Reaction

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Post synthetic method was adopted to introduce hierarchical structure in microporous zeolite-Y to overcome the diffusional restriction of chiral metal Schiff base complexes. [1]The formation of mesopores and cylindrical channels of ~5 nm dimensions were confirmed from the transmission electron microscopy and surface area analysis. Such wider mesoporous channels were suitable for the direct penetration of Schiff base ligand without any structural deformation. Two different chiral cobalt (II) Schiff base complexes with minor variation in the ligand structure were constructed inside the mesoporous zeolite-Y (M-Y) cavity. The synthesized heterogeneous chiral cobalt catalysts were used for asymmetric Henry reaction. At -35 °C, more than 80% ee with S-major nitro-aldol product was achieved within 3h on initial activation with microwave irradiation for 15 min. [1, 2]

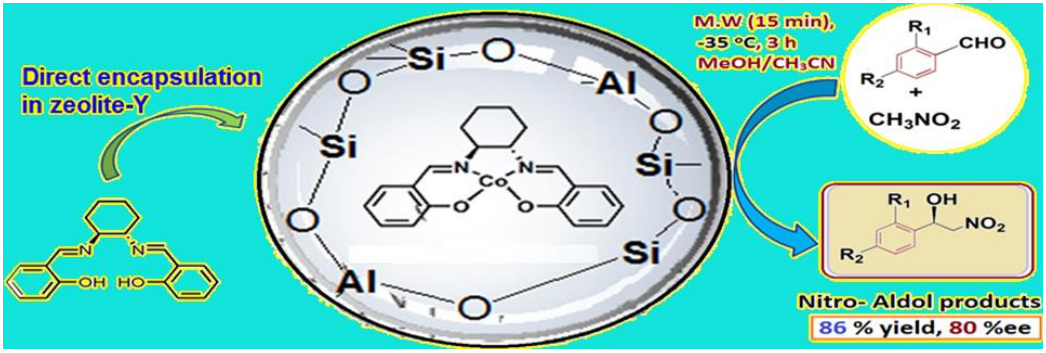

Figure 1. Schematic representation of the asymmetric Henry reaction with zeolite-Y based Cobalt Schiff base catalyst.

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Organocatalytic Asymmetric Michael/Hemiketalization/Acyl Transfer Reaction of 1, 3-Propanediones with (*E*)-2-(2-nitrovinyl)phenols

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The Michael reaction of carbon-centered nucleophiles to nitro olefins represents one of the direct and fascinating routes to nitroalkanes, which are important synthetic intermediates in organic chemistry as diverse transformations of the nitro group into other functional groups could be possible. The organocatalytic asymmetric versions of such processes have been studied extensively in recent years by a large number of synthetic organic chemistry groups. [1] In this regard, (*E*)-2-(2-nitrovinyl)phenols have been broadly utilized as bidentate substrate and a range of asymmetric organocatalytic one-pot double Michael or Michael-cyclization reactions has been developed with the induction of neighboring *ortho* hydroxyl group. [2] Realizing the potential of γ-nitrocarbonyl compounds, an organocatalytic asymmetric cascade Michael/ hemiketalization /acyl transfer reaction between (*E*)-2-(2-nitrovinyl)phenols and 1, 3-propanediones is developed using Cinchona alkaloid derived bifunctional thiourea catalyst. [3]

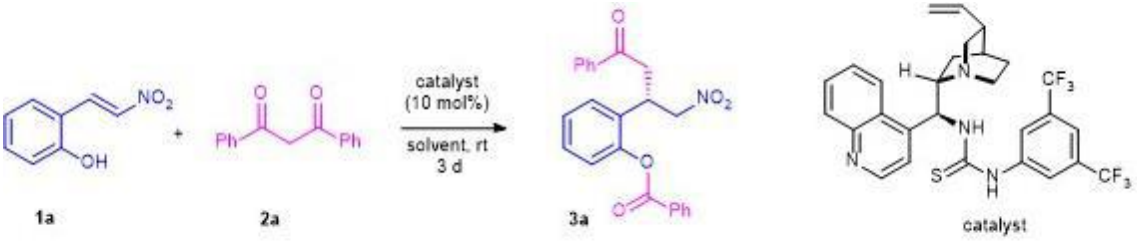

Figure 1. Organocatalytic asymmetric reaction between 1, 3-dicarbonyl compounds and (*E*)nitrovinyl)phenols.

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Study on properties on Nanocomposite Based on Ricehusk and Polyvinyl Chloride

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Polyvinyl Chloride (PVC) and Rice husk were blended with different percentage of Montmorillonite (MMT) 2, 5, 10 wt%. The blended products were compression moldedto prepare the nanocomposite and various properties of the composite were studied. Tharmal, mechanical, flame retardency and morphological features were studied by using through Thermogravimetric analyser (TGA), Zwick tensile tester, limiting oxygen index(LOI) Test and Scanning Electron Microscopy (SEM). Chemical resistance and water uptake properties were checked. The result showed that nanocomposites having 5 phr of MMT exhibited an overall improvement in properties.

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Plastic bendability displayed by molecular crystals of probenecid and its cocrystal with 4, 4´-bipyridine

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Plastic bendability of molecular crystal is an unusual phenomenon as they are traditionally considered to be brittle entities. After the first notable demonstration of plastically bendable molecular crystals by Desiraju et al. in 2005, [1] a handful number of examples are reported till date. Most of these reported examples are obtained serendipitously as predicting plastic bending behaviour of molecular crystals is a formidable task. The most common structural feature found in the crystal structures of plastically bendable molecular crystal is the presence of slip plane, perpendicular to the direction of stress, composed of weak intermolecular interactions. Probenecid, a uricosuric, on crystallization from methanol resulted in elongated plate morphology crystals and these crystals when subjected to stress on the wider faces bend irreversibly. Crystal structure analysis reveals that hydrogen bonded dimmer between carboxylic acid forms stacks of probenecid molecules with slip plane comprising of hydrophobic interactions between *n*-propyl chains thus resulting in plastic bendability. We postulated that by introducing spacer molecule in between the carboxylic acid dimmer of probenecid, the slip plane with hydrophobic interactions between *n*-propyl chains could be retained and therefore, plastic bendability might be extended from single component to multi-component crystals. With this strategy, probenecid was cocrystalized with 4, 4´-bipyridine in 2: 1 molar ratio and crystal structure determination and analysis revealed that as expected the 4, 4´-bipyridine molecules acted as spacer between two probenecid molecules with retention of slip plane compose of hydrophobic interactions. The crystals of the cocrystal of probenecid and 4, 4´-bipyridine were found to be plastically bendable on application of mechanical force as expected. [2]

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Bromo-oxidation of Phenol red to Bromo phenol blue in W-H_2O_2 system: A Comparative study in Aqueous and Micellar medium

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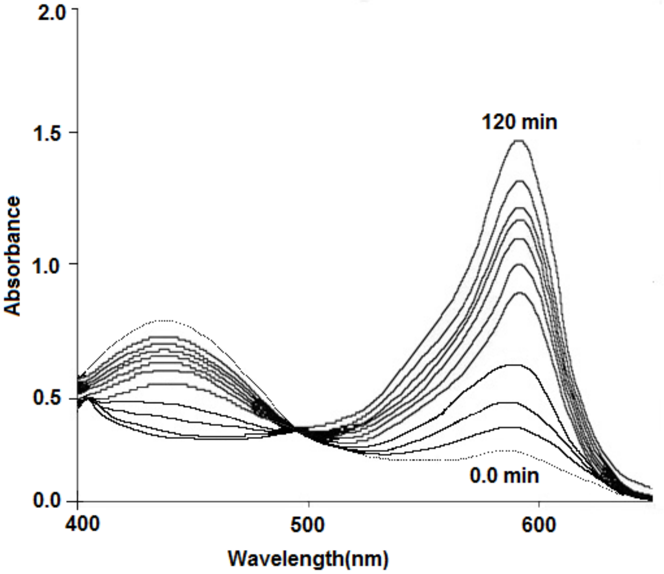
Bromo-oxidation of phenol red in W-H_2O_2 system at physiological pH was investigated spectroscopically in presence and absence of micellar concentration of SDS at different temperature. The conversion of phenol red (λ_{max} 430nm) to bromophenol blue (λ_{max} 590nm) was observed with the gradual increase in the 590nm band and decrease in the 430nm band. It was observed that at constant temperature the reaction time reduces in presence of SDS indicating increase in catalytic efficiency. The rate constant of the reaction increases almost 1. 5 times in presence of SDS above CMC indicating favourable hydrophobic and electrostatic interactions. The reaction was found to be driven by free energy ($\Delta G^o<0$) in aqueous medium and both by entropy ($\Delta S^o>0$) and free energy in micellar medium.



Hydride Pinning Pathway in the Hydrogenation of CO_2into Formic Acid on Small Tin Dioxide Clusters

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Capture of CO_2, and conversion into organic feedstocks, are of increasing need as society moves to a renewable energy economy. Here, a hydride assisted selective reduction pathway is proposed for the conversion of CO_2 to formic acid (FA) over SnO_2 monomer and dimer. Our density functional theory (DFT) calculations infer the strong chemisorption of CO_2 on SnO_2 clusters by forming a carbonate structure, whereas heterolytic cleavage of H_2 provides a new pathway for the selective reduction of CO_2 to formic acid at low overpotential. Among two investigated pathways for reduction of CO_2 to HCOOH, the hydride pinning pathway is found promising with a unique selectivity for HCOOH. The negatively-charged hydride forms on the cluster during the dissociation of H_2 and facilitates the formation of formate intermediate, which determines the selectivity for FA over alternative CO and H_2 evolution reaction. It is confirmed that nanosized SnO_2 clusters exhibit different catalytic behaviour than the bulk and surface equivalents, thus offering promise for future work investigating the reduction of CO_2 to FA via a hydride pinning pathway at low overpotential and CO_2 capturing.

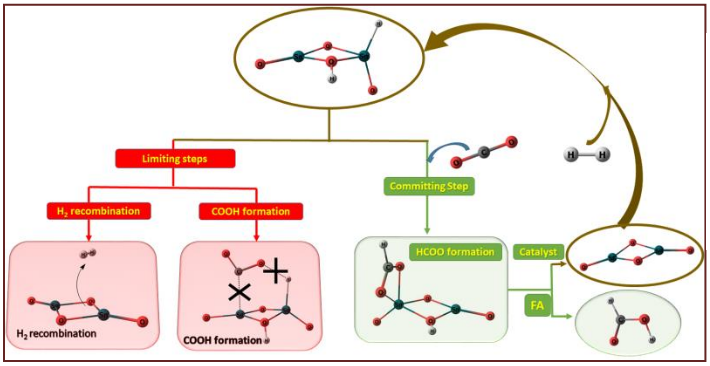

Figure: Representation of different paths involved in the hydrogenation of CO_2 to HCOOH

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A Versatile Multifunctional Smart Molecular Crystal

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In order to assist the normal biological system of life, the requirements of Nature have advanced to a level which can support life in different environments based on their specific biological structure. With this, the interest on stimuli responsive materials has attracted immense attention in materials science due to their exceptional response to external stimuli thus mimicking biological organisms. In recent years, biomimetic crystalline smart materialshas been developed which can bend, jump, walk, crawl, twist and roll under the application of heat, light and mechanical stress. [1, 2] Herein, we focus on the first example of stimuli-responsive smart crystalline material[3] (2: 1 cocrystal of probenecid and 4, 4′-azopyridine) which can respond to three external stimuli UV light, heat and mechanical stress by reversible bending / unbending, twisting / untwisting and elastic deformation respectively. An additional property displayed by the crystals is their ability to self-heal upon heating and cooling. The *trans-cis* isomerization of the azopyridine molecule is the cause of photomechanical bending whereas crystal-to-crystal phase transition results in thermomechanical twisting as well as self-healing. Interlocked molecular packing with fairly isotropic intermolecular interactions thought to be the cause of highly elastic nature of the crystals.

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Towards Knoevenagel condensation using bio-based sustainable heterogenous catalyst

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The Knoevenagel condensation is one of the most important procedures for C-C bond formation in synthetic organic chemistry and allows the production of various important intermediates in the pharmaceutical industry. [1]In recent years, utilization of eco-friendly and reusable heterogeneous catalysts has been emerged as major constituent of green chemistry. [2]Various heterogeneous catalysts have been developed for Knoevenagel condensation including ionexchange resins, mesoporous zirconia etc. [3] but utilization of bio-waste for the preparation of heterogeneous solid-base catalyst leads to newer dimension with opening the scope of chemical fabrication. In this context, herein we developed Calcined burnt peel ash (CBPA) obtained from *Musa balbisiana* Colla peel as an eco-friendly, reusable and cost effective heterogeneous base catalyst. The catalyst then investigated for the first time towards Knoevenagel condensation reaction of benzaldehyde derivatives with malononitrile. The products (benzylidenemalononitrilederivatives) were obtained in excellent yield in shorter period of time and catalyst could be recycled for six runs withloss in the yield can easily be tolerated. It was also observed that, CBPA shows higher catalytic activities of benzaldehyde derivatives with EWG in comparison to those with EDG forproduct formation in catalytic process.

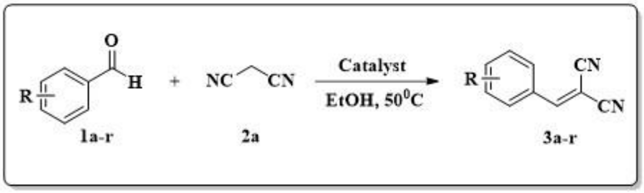

Fig: Synthesis of benzylidenemalononitrile derivatives

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Copper based bimetallic catalyst with low CO selectivity for methanol steam reforming

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Methanol steam reforming is one of the most promising technique for onboard hydrogen production particularly when integrated with Proton Exchange Membrane Fuel Cells (PEMFCs). However, PEMFC requires ultra-pure hydrogen (purity more than 99. 99 %) with CO content less than 10 ppm. Further, PEMFC operates at low temperature hence, a low temperature reforming reaction is more suitable for integration. Steam reforming of methanol can provide hydrogen stream at low temperature with low CO content. Theoretically zero CO content hydrogen stream is also possible from steam reforming of methanol if the selectivity of catalyst is higher towards methanol reforming reaction. However, most of the catalyst reported in the literature yields relatively high CO content (due to methanol decomposition or reverse water gas shift reactions) and operates at relatively higher temperature (~300 to 400 °C). In this work a highly active catalyst which is capable of operating at low temperature (200-300°C) and having low CO selectivity (<10 ppm) has been synthesized, characterized and tested. Copper based bimetallic catalyst was prepared by co-precipitation method and characterized by Energy Dispersive X-Ray (EDX), Brunauer Emmett Teller (BET), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and X-Ray Diffraction (XRD). The prepared catalyst was tested in the temperature range of 150-350 °C, pressure 1-3 bar and with variable steam to methanol (S/M) molar ratio.

Cocrystal polymorphs and unlikepharmacokinetic behaviors at physiological pH environments

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The major bottleneck in pharmaceutical industries is the efficacy and bioavailability of drug molecules in various physiological pH environments. [1, 2] Multicomponent solid forms of drugs has emerged as an alternative formulation for desired properties. We demonstrated here how multi-component crystal technology of an analgesic and antipyretic drug, ethenzamide results three different stoichiometric polymorphs with 2, 4-dihydroxybenzoic acids leading to unlike pharmaceutical properties in terms of solubility and membrane permeation behavior at different physiological pH environments. [3, 4] Prior to property study all product materials were characterized using thermal, spectroscopic and X-ray diffraction techniques and then subjected for aqueous solubility and membrane efflux studies at pH = 1. 2 & 7. 4 environments. Drug···coformer, solute···solvent intermolecular interactions, enhancement in lipophilicity of drug and conformational change upon cocrystal formation of the drug contributed towards enhancement in solubility and membrane permeation and thereby efficacy of the parent drug in their three cocrystal polymorphic phases.

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An expedient, “on water” approach to Chan-Lam coupling at room temperature

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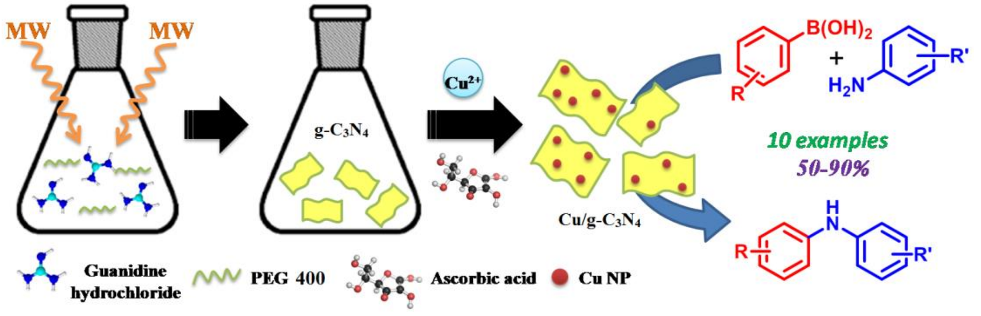
Cu-nano decorated-graphitic carbon nitride (Cu/g-C_3N_4) was developed *via* a facile protocol, using guanidine hydrochloride as the carbon nitride precursor. Connected through tri-*s*-triazine based motifs, g-C_3N_4 is a polymeric assembly of C-N bonds bearing rich surface properties with inherent basic surface sites. This property contributes to its plethoral prospects in the catalytic industry. The most thermally and chemically stable of carbon-nitrides, g-C_3N_4 can tolerate a variety of functional groups, owing to its suitability in sustainable chemistry. The as-synthesized Cu/g-C_3N_4 was characterized by IR, UV, PXRD, TEM, EDX and ICP-AES. The decoration of Cu into the g-C_3N_4 framework opens up a possibility of exploring various catalytic protocols. Its basic surface property was employed in a base-free Chan-Lam coupling between arylboronic acids and anilines at room temperature. A variety of aryl/heteroaryl/polynuclear boronic acids coupled with substituted anilines in water at room temperature. Only 1 wt % of the material sufficiently catalyzed the reaction in moderate to good yields.



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Ru(II)-Catalyzed C-H Activation and Annulation Reaction via Carbon-Carbon Triple Bond Cleavage

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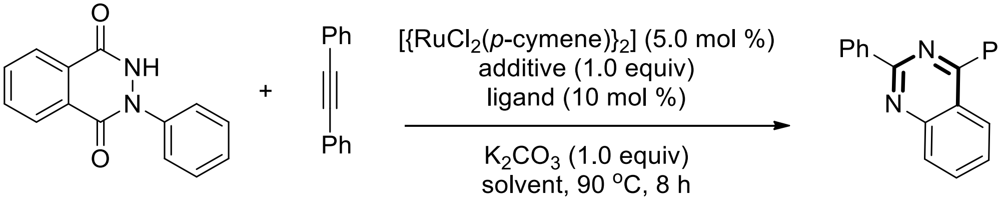
In recent years, transition metal catalyzed annulation reactions which proceed via activation of a C−H bond have revolutionized the construction of cyclic compounds. [1] In particular, the transition-metal-catalyzed C-H bond activation followed by annulation of alkynes, have been frequently used for the efficient construction of wide range of heterocycles. [2] Quinazoline derivatives are known as serine/threonine kinase inhibitors, tyrosine kinase (TK) inhibitors, and vascular endothelial growth factor receptor (VEGFR) inhibitors and they are the essential structural units of many synthetic compounds. [3] Herein, we have developed a novel Ru(II)-catalyzed C-H activation and annulation reaction, in which the annulation proceeds via cleavage of the triple bond of the alkyne. This new reaction of N-aryl pyrazol-5-ones and diaryl/arylalkyl substituted alkynes provided an easy synthetic route for the biologically important substituted quinazolines by accommodating both the fragments of the alkyne in the same product. [4]



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Nano Curcumin: Its synthesis, characterization and application

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In this work, we have synthesized curcumin nano particles from raw curcumin powder by ultrasonication process. The prepared curcumin nanoparticles show good water solubility and high pH stability. The chemical composition of the prepared nano particle was determined by various spectroscopic techniques. Transmission electron microscopy showed the sizes of nanocurcumin exist in 100 nm. Aqueous based nanocurcumin(nanoparticles of curcumin) impregnated guar-gum cellulose fibres(NCGCFs) were developed by a green process. The developed fibres were characterized by Fourier transform infrared spectroscopy. Cumulative releasing studies showed slow and sustained releasing patterns for NCGCFs.

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Revisiting the fluoride binding behaviour of Dipyrrolylquinoxaline in aqueous medium: a Cu(II)-mediated approach

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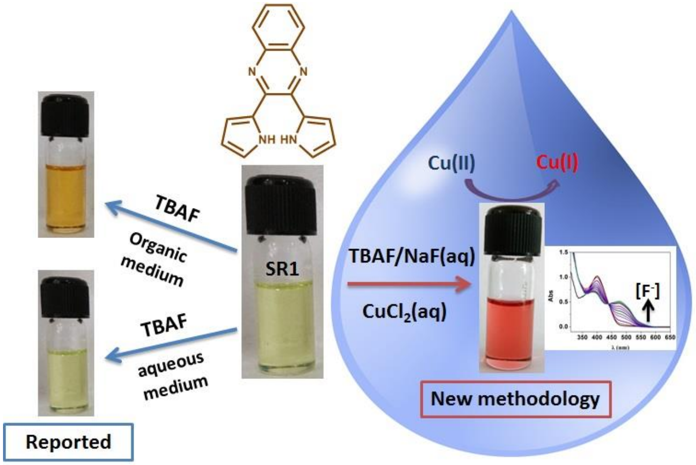
An ion detection methodology employing synergistic interaction between copper(II) ion and fluoride with 2, 3-dipyrrol-2′-yl-quinoxaline (**SR1**) is studied with particular target to detect fluoride in aqueous environment. The theme of the work simultaneously exploits H-bonding and metal-ligand interaction of **SR1** in presence of fluoride and Cu(II) ion in DMSO/water mixture. The cooperative ion detection event in presence of **SR1**and fluoride reveals *in situ* reduction of Cu(II) to Cu(I) species to form a Cu(I) complex [Cu(**SR1)**$_2$OH]$^{2-}$, which instigates a sharp colorimetric change from green to red differentiable to naked eye. The plausible structure of the complex is further supported by DFT calculations. The limit of detection (LOD) is calculated to be 0. 15 ppm. The real time application of the protocol is also tested in ground water samples of the fluoride affected area and toothpaste samples.



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Sensing of anions *via* indole derivatives: scopes and mechanistic aspects

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Anions play vital role in diverse array of biological, medical, and technological processes. [1]Therefore, selective sensing and recognition of anions in a given system is very important in order to keep balancing the required level. Over the past 2-3 decades, one frequently used strategy to produce a colorimetric and fluorometric anion sensor is to functionalize an anion binding group with a chromogenic moiety capable of signaling the binding event through intramolecular charge transfer processes *via* the hydrogen bonding interaction or advanced stage of the proton transfer reactions between binding group and anion. [2] Toward this, development of simple organic molecular frameworks containing N–H as a binding unit are found to be prominent due to their wide applicability, low cost and synthetically easy accessibility. In this regard, herein, we introduce series of indole derivatives viz. bis(indolyl)methanes based on the different electron donating and withdrawing substituent at aryl and indole moiety (**1a-1j**), [2](2, 4-dinitrophenyl)hydrazine (DNP)derivative of4-(di(1H-indol-3-yl)methyl)benzaldehyde (**2a**)[3], 6H-indolo[2, 3-b]quinoline(**3a**) for the selective sensing of anions *via* naked eye as well as spectral change. The mechanism of interaction between chemo sensor and fluoride in all the cases were established from the *in-situ* and ex-situ evidences observed from NMR, UV-vis and theoretical study.

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A dual excitability ‘turn-on’ chemosensor for Al^{3+}responds via two independent emission signals: A case of Al^{3+}-DNA interaction and real time detection of Al^{3+}

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Fluorescence based techniques have emerged as frontrunners in selective and specific recognition of a large variety of target analytes. The possibility of prompt responses, high sensitivities, facile operational procedures and cost effectiveness render fluorometric methods an attractive platform for detection of a large number of analytes. Amongst various target analytes, selective and sensitive detection of Al^{3+} ions deserve special mention owing to its fundamental role in biological as well as environmental domains. Aluminium has, by far, been the most abundant (8. 3% by weight) metallic element and the third most prevalent of all elements (after oxygen and silicon) in the earth’s crust. The detection of Al^{3+} on most occasions has been limited due to its strong hydration enthalpy in aqueous medium and poor coordination ability. [3] Adding to it, the complex level of synthesis and purification processes involved in developing highly selective and sensitive chemosensors for Al^{3+} ions limit its practical applicability. Therefore, designing fluorescent probes, which are amicable to facile synthesis and exhibit high selectivity towards Al^{3+}ions are extremely desirable.

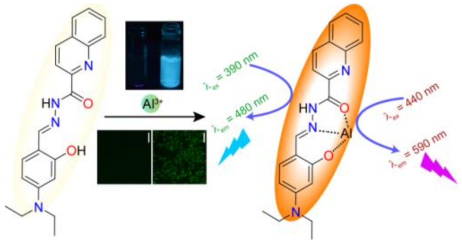

Figure 1. Graphical abstract of dual mode fluorogenic detection of Al^{3+}

Herein, we report a new fluorescent probe for selective and sensitive sensing of Al^{3+} ions. The ligand responds with two different emission signals attributed to two different excitation wavelengths. It is, thus, possible to detect Al^{3+} at two wavelengths separated by over 100 nm using a single probe. The distinctive fluorescence responses were deciphered using the chelation enhanced fluorescence (CHEF) mechanism. The chelation of Al^{3+} ions enhanced the push-pull activity thereby resulting in remarkable fluorescence emission signals. The probable sensing mechanism was reinforced by mass spectrometric and ^{1}H-NMR studies. The rapid sensing of Al^{3+} using the paper strip device enhance the prospect of the ligand in environmental sensing applications. In addition, the probe could render detection of Al^{3+} in cells and specifically track the interaction of Al^{3+} with DNA, which could perhaps be leveraged in future to investigate the toxic implications of the metal in cells.

Experimental and theoretical studies of *cis*/*trans*-bis-(glycinato)palladium(II) complexes for Sonogashira cross-coupling

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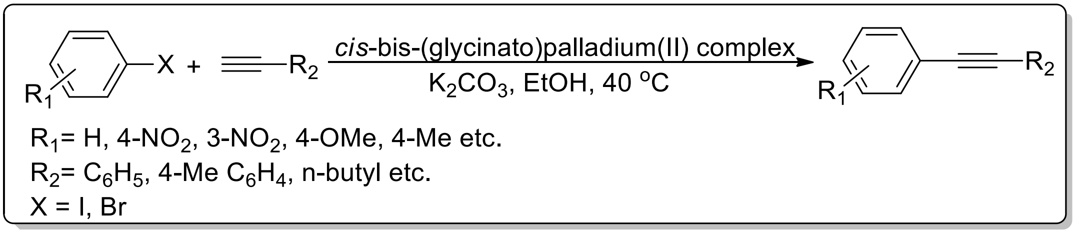
The very important polyfunctionalised alkyne formation *via* the Sonogashira cross-coupling is a well-established reaction which predominantly uses palladium catalyst and copper co-catalyst in presence of excess ammine as base as well as solvent to give the desired product. The key drawback of this traditional method is the use of copper co-catalyst which leads to the formation of Hay/Glaser type homo-coupled by-product of the alkyne thereby reducing the product formation efficiency. Consequently, different methodologies have been reported time to time for this coupling by modifying the traditional methodology. In most of the methodologies, different types of catalyst systems were designed based on palladium and different ligands. The basic goal of these modified methodologies is to avoid the use of copper co-catalyst as well as toxic ammine base and the other harsh reaction conditions. In this report, we have described a simple and facile methodology for the Sonogashira cross-coupling using palladium-glycine complex. The *cis*/*trans*-bis-(glycinato)palladium(II) complexes have been synthesized by using easily available glycine as a ligand with palladium salts and their effectiveness have been examined for the Sonogashira cross-coupling reaction. Both the complexes favours the current reaction, but, with a difference in time in efficiency, to complete the reaction. The *cis*- complex takes a lesser time for the completion of the reaction than the *trans*- complex. This, further, have been confirmed by theoretical investigation which surely evidenced the experimental result. In general, the reaction proceeds at 40 °C with the use of catalytic amount of the complex in presence of K_2CO_3 as a base and ethanol as a green solvent. This developed protocol has been applied to a variety of aryl iodides and aryl alkyne moieties which shows excellent compatibility.



R_1= H, 4-NO_2, 3-NO_2, 4-OMe, 4-Me etc.
R_2= C_6H_5, 4-Me C_6H_4, n-butyl etc.
X = I, Br

DFT based and statistically relevant QSAR models in modeling G-quadruplex binders

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At the telomeres the single-stranded guanine (G) rich sequences can held together by Hoogsteen hydrogen bond and fold in such a way to form the four stranded organization of telomeric G-quadruplexes (G4). [1-3] One of the promising steps in the indirect inhibition of telomerase is through the stabilization of the telomeric G4s. Only a small part of the reported G4 stabilizers comprising planar fused and cyclic or acyclic linked heteroaromatic compounds[4] has entered clinical trial for anticancer therapeutics but failed to reach the market due to bioavailability problems.

Implementation of advanced computational techniques such as pharmacophore modeling, molecular docking, quantitative structure-activity relationship (QSAR) and molecular dynamics (MD) aids to find alternative ways to increase the efficiency and productivity in the discovery of new and potent drug molecules. A large dataset of around 700 G4 stabilizers, with their experimental activity values, was prepared for computational modeling. Geometry optimization of all the collected inhibitors were performed at B3LYP/6-31G(d) and M06-2X/6-31G(d) level of theories. These optimized geometries were used to carry out analogue and structure based modeling. Molecular docking calculations were performed on GOLD docking program using the optimized geometries of all the collected G4 stabilizers. 16 different G4 receptors downloaded from protein data bank (PDB-ID: 4FXM, 5CDB, 1L1H, 1O0K, 5CCW, 5HIX, 4P1D, 4G0F, 3CE5, 3EUM, 3NYP, 3R6R, 3SC8, 3CCO, 3TSE, 4DAQ) were validated. DFT based and statistically relevant QSAR models were generated against 20 different cell lines. The QSAR was performed to find the relationship between the biological activity and physiochemical properties for the collected G4 stabilizers. Optimum number of molecular descriptors were used to understand the representative molecular properties. Effect of docking and conceptual DFT based descriptors on the generated models were analyzed. We plan to predict a few new and promising G4 stabilizers on the basis of our modeling studies.

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Layered Supramolecular Association in Pyridinedicarboxylato Coordination Solids of Ni(II) and Zn(II)

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Recently, the effective combination of coordination bond and weak supramolecular interactions has been applied for engineering metal-organic hybrid materials [1]. The suitable organic ligands make the complexes not only to possess novel structures but also produce unique optical, electrical and magnetic properties [2]. Two coordination solids viz. $[Ni_2(2,\ 6\text{-PDC})(\mu\text{-}2,\ 6\text{-PDC})(H_2O)_5].\ 2H_2O$ (**1**) and$[Zn(2,\ 5\text{-PDC})(H_2O)_4].\ 2H_2O$(**2**) have been synthesized. Hydrogen bonding between coordinated water and the carboxylate oxygen atoms of the PDC^{2-} links the binuclear nickel molecules to form a one-dimensional chain in **1**. Extensive O–H···O interactions involving the lattice water molecules result in a layered supramolecular structure in **2**. The compounds are characterized by elemental, spectral (IR and UV-Vis.), thermal analysis and single crystal X-ray diffraction analysis.

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Catalytic application of biosynthesised gold nanoparticles for synthesis of bis(indolyl)methanes

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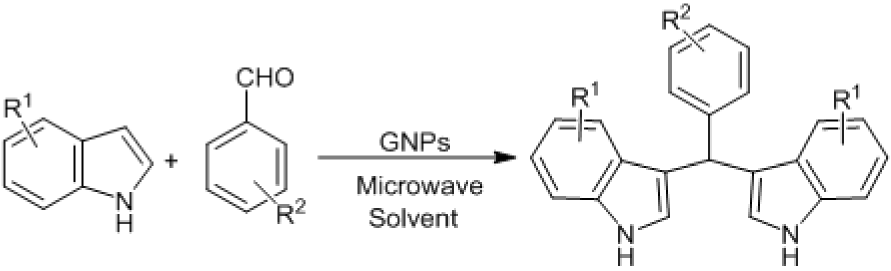
Indole derivatives exhibit their huge significance in drug discovery and medicinal chemistry due to its widespread presence in nature, as fragments in the chemical structureof many bioactive compounds and natural products [1]. Bis(indolyl)methanes (BIMs) are an important type of indole derivatives commonly isolated from marine and terrestrial natural sources such as plants, parasitic bacteria, sponges etc. [2]. Application of gold nanoparticles (GNPs) in mild reaction condition for the synthesis of different substituted BIMs has been studied.



Scheme 1. Synthesis of Bis(indolyl)methanes

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Improving physicochemical properties of the BCS Class II drug Mebendazole by using Crystal Engineering Approach

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Mebendazole (MBZ) is a BCS class II anthelminthic drug which is used in the treatment of parasitic worm infections with a serious problem in its solubility and dissolution properties. By using crystal engineering principle, we have synthesised mebendazole nitrate, mebendazole hydrochloride and a new mebendazole methyl bisulfate (MBZ. CH_4O_4S). [1-2] To increase its bioavailability by improving its permeation through membranes, we opted for different random ethanol-water ratios such as 0: 10, 1: 9, 3: 7, 1: 1, 7: 3, 9: 1 and 10: 0 and demonstrated the physicochemical properties of these salt formulations to get a better formulation than the parent drug molecule. Permeability measurements were done in these ethanol-water ratios along with 1. 2 and 7. 4 buffer solutions. These measurements lead to a result which shows increased solubility as well as permeation behaviour of the salt than the original mebendazole molecule.

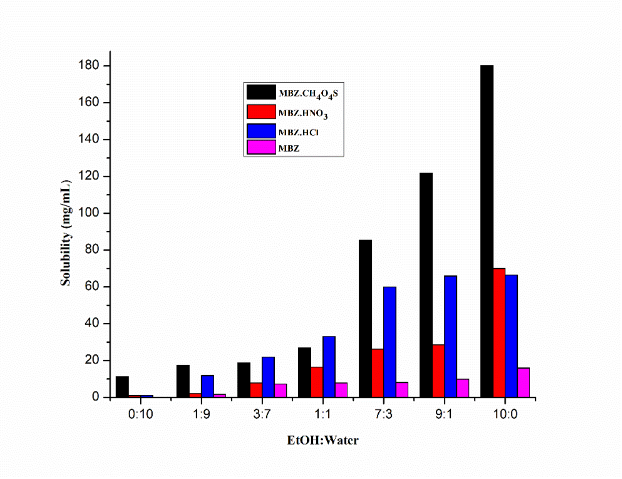

Figure 1. Bar diagram for **(a)** MEB. CH_4O_4S, (b) MEB. HCl, (c) MEB. HNO_3 and(d) MEB in various ethanol-water ratios.

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Theoretical charge density studies of hydrogen bonded cation···cation complexes observed in synephrine salts

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The nature of short intermolecular interactions observed between the same charge species (anion···anion or cation···cation type) are generally considered destabilizing. [1] This has lately become a hot topic of discussion among researchers. [2] The nature and importance of these short interactions appearing in crystals is still unclear. We have observed few hydrogen bonded cation···cation species (**Figure 1**) in the newly characterized crystalline salt forms of (±)-*p*-synephrine by us. We have studied the nature of O–H···Ohydrogen bonds in these cation···cation species foundin the salt crystal with the help of theoretical charge density studies obtained from periodic DFT calculation. The electron density descriptors obtained from charge density studies indicates no significant difference in the topological features of a hydrogen bonded observed for a cation···cation species with a neutral complex.

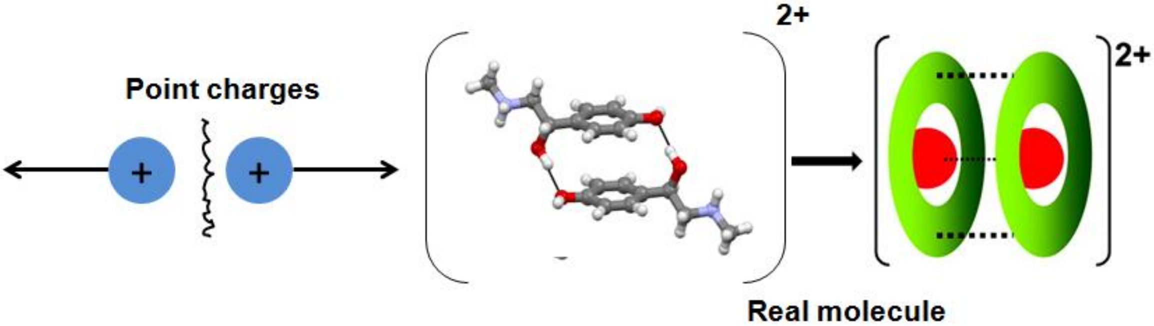

Figure 1: O–H···O hydrogen bonds involving a cation···cation spices

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Development of Non-isocyanate Polyurethane Hybrid/Graphene Oxide Composites and its thermo-mechanical properties

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In this work, we synthesized sunflower oil based non-isocyanatepolyurethane hybrid materials (HNIPU) and its nanocomposites with amine functionalized graphene oxide (AF-GO). Initially, the five-membered cyclocarbonatebased on carbonated sunflower oil (CSFO) was synthesized by the reaction of epoxidized sunflower oil (ESFO) with carbon dioxide (CO_2) at pressure 50 bar and temperature 120 °C. Then, hybrid materials HNIPU were synthesized by using commercial epoxy resin (30 wt% with respect to CSFO) by using isophorone diamine asthe curing agent. Then, the nanocomposites of 30 wt% HNIPU based composition were prepared with different wt% of AF-GO (0. 3, 0. 6 and 1. 0wt%) and were characterized by usingFTIR, ^{1}HNMR, and SEM techniques. These results emphasize the potentiality of this environmentally friendly approach to prepare renewable HNIPU and its nanocomposite materials of highperformances.

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Efficient Ru(II)-Catalyzed Regioselective C-H Amidation of Indolines and Carbazole using Acyl Azides

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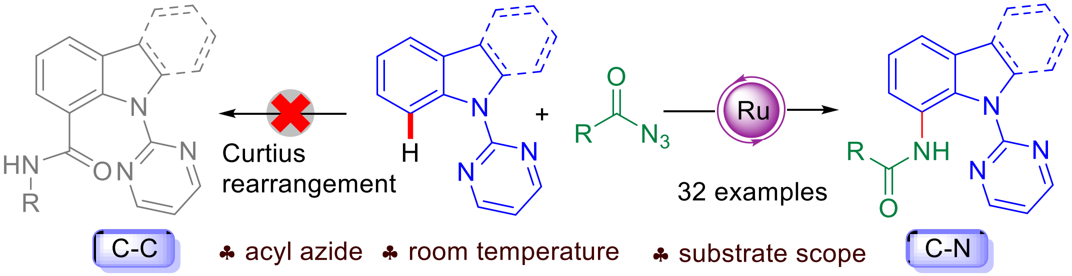
Transition-metal-catalyzed C-H functionalization via chelation supported C-H activation has been turned out to be a prominent approach for carbon-heteroatom bond formation. [1]Herein, we developedan efficient Ru(II)-catalyzed C7-amidation of indolines with the aid of pyrimidyl chelating group using acyl azides[2] as the nitrogen surrogate at room temperature (Scheme 1). [3]The reaction condition was extended to the selective C1-amidation of carbazoles. The broad substrate scope, controlling reactivity, room temperature and oxidant-free are thesignificant practical features.



Scheme 1

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Co(II) Complexes in which Carboxylate Anions do not form Coordination Bonds

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Syntheses and structural characterization of metal-organic compounds involving carboxylic acid anions and substituted pyridine ligands have received considerable attention from both crystal engineering and catalytic points of view. Pyridyl ligands having hydrogen bond acceptors such as $–CO_2^-$ and CN as substituents on the pyridine ring helps in various types of non-covalent links leading to interesting supramolecular architectures. Such non-covalent interactions may also take place by involving other ligands such as RCO_2^- and H_2O that display interesting solid state structure. Herein, we describe the syntheses and crystal structure analyses and physicochemical studies of a few 4-cyanopyridine Co(II) having benzoate or 4-substituted benzoate anions as the other ligands*viz.*, $[Co(4\text{-}CNpy)_2(H_2O)_4]^{2+}[(O_2CR)_2]^{2-}$, where R = C_6H_5 (**1**) and C_6H_4-4-Me (**2**).

Crystal and molecular structures of compounds **1** and **2** have been determined by single crystal X-ray diffraction to find that both the compounds have the cation *trans*-$[Co(4\text{-}CNpy)_2(H_2O)_4]^{2+}$ along with two uncoordinated RCO_2^- counterions. The benzoate anions, RCO_2^- fail to coordinate to the Co^{2+} centre. The presence of the non-covalent intermolecular O–H···O, C–H···O interactions gives rise to a robust supramolecular layered structure in the crystalline state.

Study on the Synthesis, Characterization of ONS donor Schiff Base Complexes of Ruthenium and its Applications

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Chelating ligands of thioether with ONS donor Schiff base and its metal complexes were synthesized. Hydroxyl functionality and sulfur coordination provides more advantageous effect on the formation of chelating ligands with tridentate fashion. Schiff base ligand, HLhaving the chemical formula, $C_{24}H_{19}NOS$ was derived from 1-hydroxy-2-napthaldehyde and 2-(benzylthio) aniline by typical condensation reaction. Electron donating and withdrawing moiety in the aldehydic group impact in formation and also in coordination with metal centers. The imine moiety with E configuration provides structural stability on the chelating Schiff base ligand HL. The Ru (III) complex was prepared with the synthesized ligand HL in 1: 1 and 1: 2 ratios respectively. The synthesized Ru (III) complex was used as a catalyst for the reduction of aldehydes and ketones. All the reactions are completed under mellow conditions and yield of the product are good in sum.

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Tin(IV) Oxide Nanoflake Catalysed Friedel-Crafts Acylation Reaction

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Synthesis of inorganic nanostructures of well defined morphology has attracted considerable attention due to their uniquephysicochemical properties. Owing to such unique properties they are widely used in the various fields of science and technology. In particular, SnO_2nanostructures have potential applications as gas sensor, heterogeneous catalyst, lithium ion electrode material, supercapacitor, etc. Hence, asingle crystalline SnO_2 nanoflake hasbeen successfully synthesized via simple solvothermal method. The synthesized $SnO_2$are characterised by various analytical techniques such asFTIR, XRD, TEM/HR-TEM, BET surface areaetc. XRD profile shows the synthesized oxide adopts rutile type SnO_2 structure (spacegroup No. 136, $P4_2/mnm$). Further, synthesized SnO_2nanoflake is employed for the Friedel-Crafts acylation reaction of aromatic compounds. The product of the reactions is confirmed by NMR and FTIR analysis. The synthesized SnO_2nanoflake exhibit high catalytic activity and reusability for the mentioned reaction with (%) yield maximum about 80%. Finally, the present workon single crystalline SnO_2 nanoflakes catalyzed Friedel-Crafts acylation reaction largely contributes to the fine chemical and pharmaceutical industries.

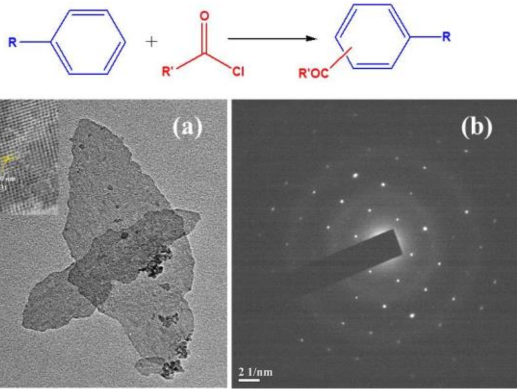

Figure: TEM image (a), SAED pattern (b) of SnO_2 nanoflake; inset (a) HR-TEM image of corresponding SnO_2 nanoflake; top: Reaction scheme for the FC acylation reaction.

Covalently Bonded Hybrid Bilayer of 11-Mercaptoundecanoic Acid and Chitosan on Gold: A Flexible interface for Biosensor Application

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Surface modification with layer-by-layer deposition strategies are gaining much interest in the recent time. Different approaches are followed to obtain surfaces with specific physicochemical properties. Here in this work we have prepared a hybrid bilayer of 11-mercaptoundecanoic acid (MUDA) and chitosan on gold surface using self-assembled monolayer (SAM) formation strategy and functional group activation followed by covalent binding. The self-assembled monolayer of MUDA was prepared on properly cleaned, polish finished gold surface. The carbonyl groups of the monolayer were activated using1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide (*EDC*)and n-hydroxysuccinimide (NHS) in aqueous solution. The primary amine groups of the chitosan molecule form amide bonds with the activated carboxylic groups of the SAM resulting a hybrid bilayer. The prepared bilayer has been characterized using electrochemical quartz crystal microbalance, cyclic voltammetry, impedance spectroscopy, scanning tunnelling spectroscopy, atomic force microscopy, field emission electron microscopy, contact angle measurement and attenuated total reflection infrared spectroscopy. It has been found that the bilayer is highly hydrophilic with an average water contact angle of 20°, which enables it as an excellent support for formation of bilayer lipid membrane. The additional primary amine groups present at the surface of the membrane provide scope for further functionalization.

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Regioselcetive synthesis of substituted 3, 6-dihydropyran from 3-butene-1-ol and aldehydes *via* Prins cyclization mediated by TFA

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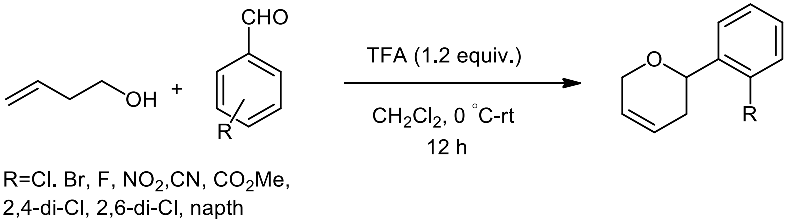

Multicomponent reactions have attracted the considerable attention in synthetic organic chemistry due to their ability to form a series of bonds in a single step. In particular, multicomponent reactions can provide functionalized heterocyclic compounds with high stereoselectivity. Dihydropyran units are valuable compounds of interest for the reason that these units constitute important structural unit in many natural products of biological importance.compounds such asmartirioland salinomycin carry dihydropyran unit in which double bond in cyclic system is responsible for the biological activity. Martiriol for that matter, is a biologically active molecule, isolated from the red algae of the genus *Laurencia*, shows potent activity against various tumour cell lines. Similarly, salinomycin isolated from a culture broth of *Streptomyces albus* is known to possess interesting antibacterial and anticoccidial properties. The presence of double bond in cyclic system is not only responsible for their biological properties but also serve as a functional group for further manipulations in organic synthesis. They can also be used as building blocks in organic synthesis.

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One pot synthesis of indole derivatives via sequential *Claisen Schmidt* Condensation and Michael-like addition using task specific ionic liquid catalysts

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3-Alkylated indole derivatives are produced efficiently in one pot reactions involving acidic ionic liquid (IL) catalyzed Claisen Schmidt condensation of substituted aromatic aldehydes with acetophenone to chalcones followed by Michael-like addition of indoles under solvent-free thermal reactions. The significance of 3-alkylated indole derivatives are recognized from various types of natural products possessing wide range of biological activities like antifungal, antimicrobial, antiviral, anticancer, anti-inflammatory and analgesic activities etc.[1] The acidic properties of –SO3H functionalized ILs are employed to catalyze the two step reactions in one reaction vessel without isolating any intermediate involving throughout the course of reactions to get the desired product selectively. For this purpose, initially we synthesize and characterize few member of 1, 3-disulfo-imidazolium based ILs through different analytical and spectroscopic tools. After that they are examined as reusable catalyst to optimize the sequential reaction conditions without formation of side products. The structures of indoles are confirmed via NMR (^{1}H and ^{13}C), FT-IR and melting point measurements.

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Development of porous TiO_2 photocatalyst for water splitting reaction

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Water splitting reaction is one of the most vital reactions as it is capable of converting solar energy into chemical energy in the form of H_2, a clean and renewable energy source. In present work a porous TiO_2 molecular organic framework (TiO_2-MOF) is synthesised in which water molecules get efficiently absorbed. A coating of reduced graphene oxide (rGO) is applied on TiO_2-MOF to enhance its conductivity. Subsequently, a thin layer of carbon dot (C dots) is applied on it to sensitize the photocatalyst. Using the prepared photoanode as a working electrode and 0. 1 M sulphuric acid solution as electrolyte in a three electrode photochemical cell (PEC) the water splitting reaction is successfully carried out.

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Fluorescent Carbon Nanoparticle and Its Application

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A simple and facile one-step synthesis of fluorescent carbon dots from carbohydrate was performed using the acid and base carbonization method at a mild temperature (60 ^{0}C). The chemical composition and morphological feature of the obtained carbon nanoparticles were characterized using various spectroscopic techniques. The prepared carbons nanoparticles were amorphous in nature, included a large quantity of oxygen functional groups. A composite of carbon nanoparticles with ZnO was used as a photo catalyst for degradation of methylene blue dye under UV irradiation, and the superior photo catalytic activity was demonstrated. Overall, the present preparation method of carbon nanoparticles takes on meaning in the area of eco-friendly synthesis in aqueous solutions, and the product has great potential as a component material in the development of a remarkably efficient catalytic system.

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Evaluation of the efficiency of clathrate hydrates for storing small molecules

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Density functional theory (DFT) based studies are carried out to understand the structure, stability and reactivity of clathrate hydrates with or without hydrogen encapsulation. Allgeometries of clathrate hydrates were fully optimized using B3LYP/6-31G(d), M062X/6-31G(d) and B97D/6-31G(d) level of theories using Gaussian 09 program package. The storage capability of five standard clathrate hydrates cages (5^{12}, $4^3 5^6 6^3$, $5^{12}6^2$, $5^{12}\ 6^4$ and $5^{12}6^8$) is systematically explored to store small molecules like Ar, CH_4, CO_2, H_2, H_2S, Kr, N_2, O_2 and Xe. The capability is depicted in the given Figure. The efficacy of trapping of small molecules inside the cages of clathrate hydrates generally depends upon the cavity sizes and shapes. The interaction energy values indicate the formation of stable gust-host system.

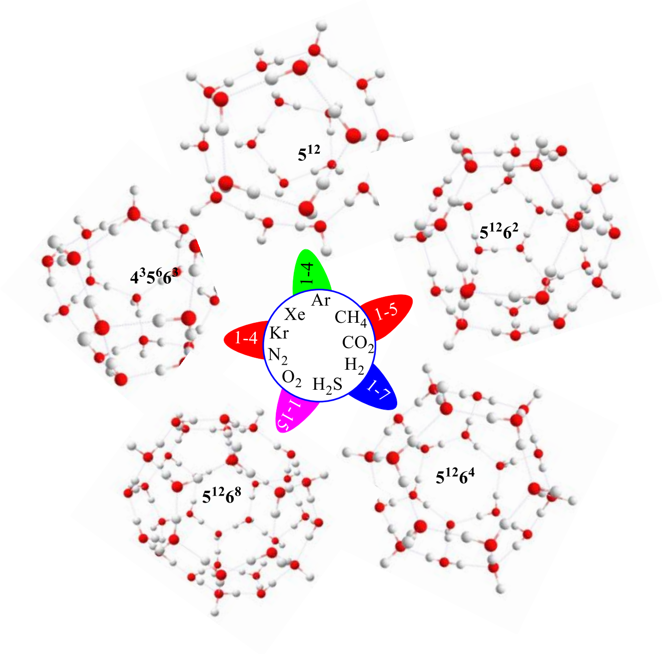

Figure: Capacity of five standard water cavities in the clathrate hydrates with various molecules

Bu_4NI Catalyzed Radical Induced Regiospecific *N* - Alkylation and Arylation of Aryl tetrazole

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Nitrogen center radicals (NCR) are less explored than carbon center radicals due to dearth of operationally simple and clean reaction process for its generation. Most of the nitrogen center radicals are generated under harsh, toxic, expensive and potentially explosive reaction conditions. The search for new proficient protocols for direct catalytic conversion of the N–H bonds of azole into the corresponding NCR under mild reaction conditions has become significant, Yet challenging. Transformation of azoles N▯H bond into NCR and trapping of the generated NCR with appropriate coupling partner will lead to valuable target molecules.

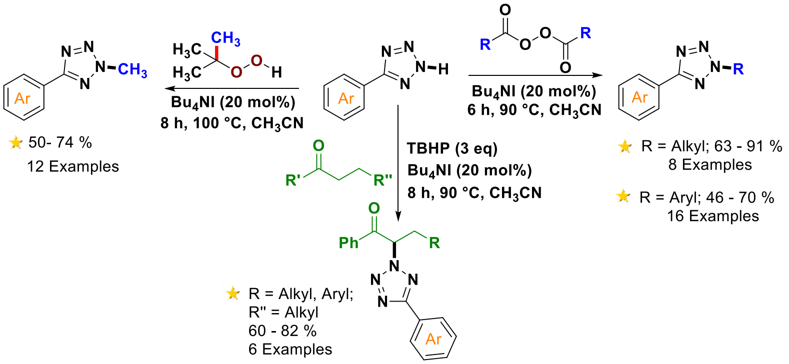

Figure 1. Bu_4NI catalyzed radical induced regioselective *N*-alkylation and arylation of aryl tetrazole.

Herein we have developed a simple and efficient metal-free approach for the synthesis of *N*▯methyl tetrazole from NH-tetrazole *via* radical induced pathway. The process involves effective coupling of nitrogen center radical of aryl tetrazole with CH_3 radical which is generated *in-situ* from *tert*-butyl hydrogenperoxide catalyzed by TBAI. Homologous series of methyl radical and aryl radical were generated from alkyl diacyl peroxide and Aryl diacyl peroxide respectively. Weaker Peroxide bond undergo homolytic cleavage, followed by decarboxylation leads to alkyl/aryl radical this alkyl/aryl radical was trapped by variety of 5-aryl tetrazole makes regioselective 2, 5 disubtituted tetrazole. In addition to that a-amination of ketone was achieved under our methylation condition.

Polyoxometalate based ionic liquid $[MDSIM]_3[PW_{12}O_{40}]$ as heterogeneous catalyst for nitration of aromatics

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The combination of cationic part of ionic liquids and polyanions of polyoxometalates is envisioned to lead to new molecular materials which are of interest as stable heterogeneous catalyst in organic synthesis. This type of “task specific” ionic liquid cation modified polyoxometalate hybrid materials act as effective, recoverable and reusable catalysts for various functional group transformations [1, 2]. As we know most of the nitration methods involve the use of nitrating mixtures require a lot of time, toxic and corrosive acids and are associated with the disposal problems of complex by-products. Traditional method of nitration involves mixture of nitric acid and sulfuric acid (mixed acids) which is unselective and resulting in liquid waste causing a serious environmental problem [3-5]. Therefore, we have synthesized dual –SO_3H functionalized 2-methyl-1, 3-disulfoimidazolium polyoxometalate hybrid salt materials and successfully utilized them in nitration of aromatic compounds. All the synthesized materials were characterized via FTIR, TGA, NMR, UV-visible, DRS spectra, Raman, PXRD and SEM analysis.

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N-substituted Carbazole based *N*-Heterocyclic Carbene ligands-Pd Catalytic System in Synthesis of Stilbene based Boronate Ester via Double-Tandem Protocol

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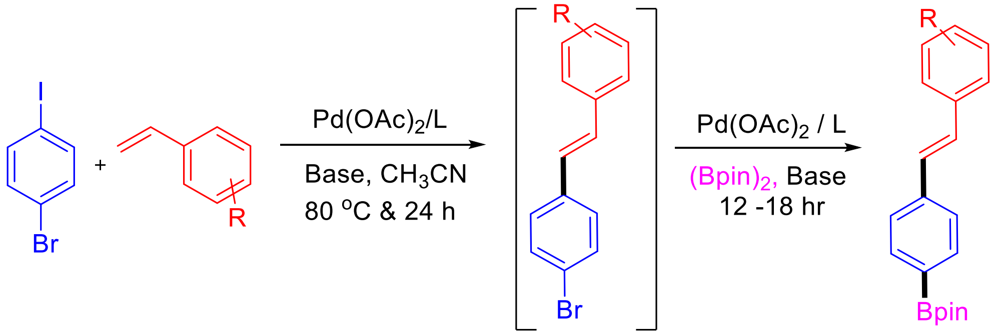
Series of new carbazole based *N*-heterocyclic carbene ligands synthesized via a simple synthetic route and characterized by standard spectroscopic technique. Palladium alongwith carbazole based NHC catalytic system catalyzes double-tandem Heck and Borylation reaction to afford the stilbene based boronate ester at ambient reaction condition. This tandem protocol involves the chemoselctive Heck reaction followed by Borylation to gives desired product with good to excellent yield. The mildness of this protocol successfully explored towards the modification of nucleoside molecule.



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Mechanochemical synthesis of pharmaceutical cocrystals and eutectics of Pyrazinamide

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Crystal engineering is the design and synthesis of molecular solids with desired properties, based on the understanding of intermolecular interactions. [1] It is a matured field with wide application in materials chemistry research. Pharmaceutical cocrystallization is one of the crystal engineering techniques to improve/ alter physicochemical properties of active pharmaceutical ingredients (APIs). [2]The technique involves synthesis of various multi-component solids such as cocrystals, salts, solvates, hydrates etc of an API. In recent times, preparation of eutectics has immerged as an alternative along with the existing multicomponent solid formulations. For preparation of these multicomponent solids, the coformer is selected from the list of benign chemicals for human consumption (generally regarded as safe by the FDA or GRAS).

Pyrazinamide (PZA), a first line anti-tuberculous drug is one of the listed essential medicines declared by World Health Organization (WHO) in a basic health system. It is generally used for the treatment of Tuberculosis (TB) during monotherapy as well as fixed dose combination (FDC) along with other tuberculous drugs. Cocrystallization of anti-tuberculosis drug pyrazinamide (PZA) with severalsubstituted aromatic carboxylic acids as coformers is studied. [3, 4]The combinations are analyzed by powder X-ray diffraction and melting behavior to assess the formation of eutectic versus cocrystal. Benzoic acid, cinnamic acid and N-heterocycle coformers give eutectics whereas majority of their hydroxyl/methoxysubstitutes form cocrystals with PZA. X-ray crystal structures areobtained for somecocrystals and binary phase diagrams are constructed to determine eutectic compositions. Differences in functional group positions andvariations in supramolecular growth are found to dictate the formation of eutectics versus cocrystals. Supramolecular synthon energy calculations on selected combinations validate the formation of eutectic versus cocrystal.

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Silicone containing bio-based hyperbranced polyurethane elastomer with smart attributes

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Designing of stimuli-responsive smart hyperbranched polyurethanes (HBPU) from bio-derived resources have gained tremendous impetus now a day's, owing to their sustainability and environmental safety. [1] Therefore, in the present work author's group wish to report the synthesis of smart silicone containing HBPUs using some bio-based raw materials like monoglyceride of sunflower oil, dimer acid-glycerol modified polyol. [2, 3] Three different compositions of the HBPUs were synthesized by simply varying the silicone-containing moiety. Synthesized HBPUs were characterized using FT-IR, NMR, XRD and SEM analyses. Synthesized HBPUs exhibited very high molecular weight (10^5order). In addition all the HBPUs exhibited outstanding flexibility, adequate tensile strength, good toughness and high impact strength. Furthermore, synthesized HBPUs showed multi stimuli-responsive ultrafast self-healing and shape recover behavior. Most interestingly the HBPUs exhibited self-cleaning behaviour through surface hydrophobicity and showed satisfactory amount of biodegradability under the exposure of *Pseudomonas aeruginosa* bacterial strains. Henceforth the studied HBPUs with the above smart properties have significant potential to be used in many advanced applications.

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Synthesis of shape-tunable ZnO nanoparticles for application as catalyst in the formylation of aromatic amines

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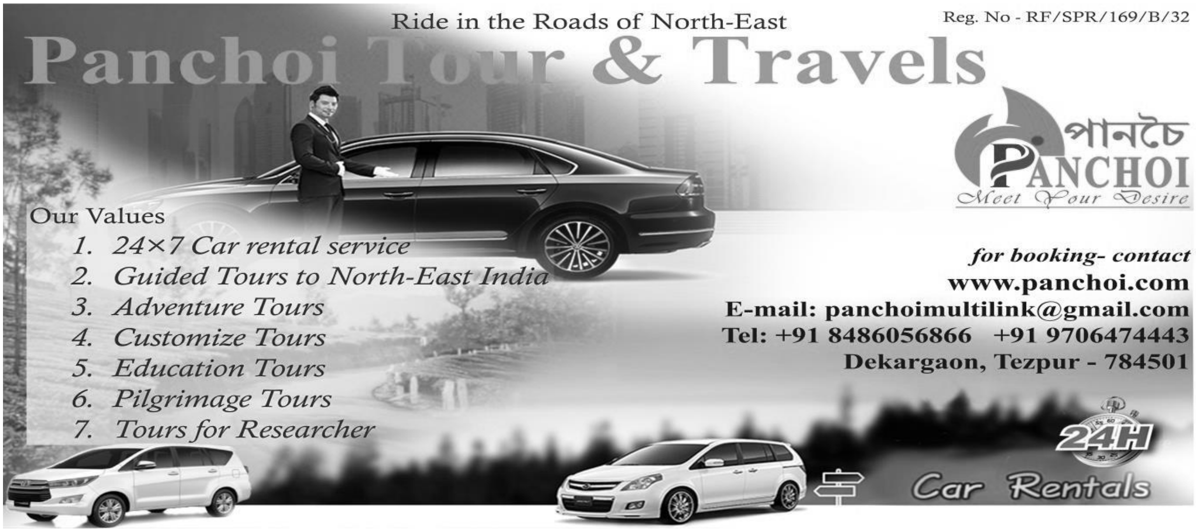
In recent years metal oxide semiconductor materials are gaining importance as a heterogeneous catalyst with profound redox properties in their surfaces. The catalytic activity of these metal oxides can be further enhanced by bringing them in to nano state associated with high surface-to-volume ratio as the surface area of the catalyst plays the key role in heterogeneous catalysis. Herein, we report the synthesis of spherical and rod-shaped ZnO nanoparticles in methanol without using any stabilizer. ZnO nanoparticles were characterized by optical spectroscopy, X-ray diffractometry and electron microscopy techniques. The catalytic activity of these synthesized ZnO nanoparticles were tested in the formylation of aromatic amines. Spherical ZnO nanoparticles were found to be more efficient than the rod-shaped and bulk counterpart. The reaction is very fast giving high yield compared to other reported catalysts. The process is relatively greener and the catalysts are reusable in the formylation of aromatic amines up to few cycles of reaction.



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