



সমানো মন্ত্র: সমিতি: সমানী

# Frontiers in Chemistry 2023 & Prof. C. N. R. Rao Endowment Lecture



**Dept. of Chemistry  
University of North Bengal  
in association with  
CRSI - North Bengal Local Chapter**

**Seminar dates  
13-15<sup>th</sup> March 2023**



## UNIVERSITY OF NORTH BENGAL

Prof. P. Ghosh,  
Professor of Chemistry &  
Director, Research and Development  
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### MESSAGE

It gives me immense pleasure to learn that the Department of Chemistry, University of North Bengal has arranged an International Seminar on "Frontiers in Chemistry-2023 and Prof. C. N. R. Rao Endowment lecture" during 13-15 March, 2023.

The theme of the seminar is really attractive and the speakers will enlighten the recent advancements in frontier areas of Chemical Sciences with deeper insights. This will help growing interests in the young minds to undertake projects towards solving contemporary issues in this arena. Furthermore the visionary ideas from national and international delegates will be enormously beneficial to the young researchers and students.

I believe that the seminar will be a grand success and convey my best wishes to the organisers and participants.

**Prof. Pranab Ghosh**  
Director, Research and Development Cell  
University of North Bengal  
&  
Convenor, CRSI  
North Bengal Local Chapter

# University of North Bengal

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March 10, 2023

## Message

It is matter of great pleasure to me that our department is going to organize an International Seminar on "*Frontiers in Chemistry 2023*" and "*Prof. C. N. R. Rao Endowment Lecture*" on 13-15<sup>th</sup> March 2023 in association with CRSI-North Bengal Local Chapter after the unprecedented halt on academic programs due to COVID-19 pandemic since March 2020. Added to this pleasure is the fact that several renowned speakers from home and abroad will deliver their keynote speech on emerging fields of Chemistry and Material Sciences. Certainly the program will help the learned audiences including students and research scholars to enrich as well as advance their knowledge of Chemical and Material Sciences.

I must thank the university authorities to allow us to convene this seminar in spite of the ongoing financial crunch. I personally thank the conveners and Prof. Pranab Ghosh, Convener, CRSI-North Bengal Local Chapter to take up all the challenges in organizing this seminar. I also thank all my respected colleagues for their cordial support and active participation in organizing this seminar and I do hope that the seminar will have its grand success.

Prof. Biswajit Sinha  
Head & Chairperson of the Organizing Committee  
Department of Chemistry  
University of North Bengal



## International Seminar on Frontiers in Chemistry-2023

&

### Prof. C.N.R. Rao Endowment Lecture

Organized by

Department of Chemistry, University of North Bengal

In association with

CRSI-North Bengal Local Chapter



#### Program Schedule

13/03/2023	2:00 PM - 2:30 PM	Sixtieth years completion of Department of Chemistry: <b>A Celebration</b>
	2:30 PM - 2:40 PM	Oral Presentation
	2:40 PM - 2:50 PM	Oral Presentation
	2:50 PM - 3:00 PM	Oral Presentation
	<b>3:00 PM - 3:15 PM</b>	<b>Tea Break</b>
	3:15 PM - 3:25 PM	Oral Presentation
	3:25 PM - 3:35 PM	Oral Presentation
4:00 PM - 5:00 PM	<b>Invited Lecture-1: Dr. Silvia Diez-Gonzalez</b>	
14/03/2023	10:45 AM - 11:15 AM	<b>Inaugural Session</b>
	11:15 AM - 11:30 AM	Tea Break
	11:30 AM - 12:30 PM	<b>Invited Lecture-2: Dr. S. S. V. Ramasastry</b>
	12:30 PM - 1:00 PM	Oral Presentation
	<b>1:00 PM - 2:00 PM</b>	<b>Invited Lecture-3: Dr. Tatsuya Nishimura</b>
	<b>2:00 PM - 3:30 PM</b>	<b>Lunch and Poster Session</b>
	<b>3:30 PM - 4:15 PM</b>	<b>Invited Lecture-4: Dr. Ranjit De</b>
	4:15 PM - 4:30 PM	Oral Presentation
4:30 PM - 6:00 PM	Cultural Programme	
15/03/2023	10:45 AM - 11:45 AM	<b>Prof. C. N. R. Rao Endowment Lecture: Prof. Souvik Maiti</b>
	11:45 AM - 12:00 PM	Oral Presentation
	12:00 PM - 12:15 PM	Oral Presentation
	12:15 PM - 12:30 PM	Oral Presentation
	12:30 PM - 1:30 PM	Oral Presentation
	1:30 PM - 2:30 PM	<b>Lunch Break</b>
	2:30 PM - 4:00 PM	Oral Presentation
4:00 PM - 4:30 PM	Valedictory	

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<b>Venue:</b>	Department of Chemistry, University of North Bengal
<b>Convenors:</b>	Dr. Kiran Pradhan, Dr. Kinkar Biswas, Dr. Md Selim Arif Sher Shah, Department of Chemistry, NBU
<b>Chairperson:</b>	Prof. Biswajit Sinha, HoD, Department of Chemistry, NBU
<b>Prof. Pranab Ghosh</b>	Convener, CRSI-North Bengal Local Chapter

**INVITED LECTURES**  
**(IL)**

## **IL-01**

### **With or Without You (Copper): Stories in Heterocyclic Chemistry**

Dr. Silvia Diez-Gonzalez

Faculty of Natural Sciences, Department of Chemistry

Imperial College London, United Kingdom

The copper(I)-catalysed selective formation of 1,4-disubstituted-1,2,3-triazoles is broadly considered as the most powerful Click reaction to date. Despite its popularity, this cycloaddition process remains victim of its own success and only little efforts have been focused on developing efficient catalytic systems, preventing numerous applications from meeting the stringent Click criteria.

In this talk, our contribution to the field will be discussed with a comparison of the catalysts developed so far bearing either N-heterocyclic carbene or phosphorous ligands, including the more challenging reaction of azides and iodoalkynes. Furthermore, related azide-alkene cycloaddition reactions have allowed us to access a wider variety of heterocycles under user and environmentally friendly conditions.

## **IL-02**

### **Some of our Contributions to the Metal-Free Chemistry**

Dr. S. S. V. Ramasastry

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Our lab has been actively involved in developing new synthetic strategies to access diverse classes of heterocyclic scaffolds starting from easily accessible starting compounds. In this context, we have developed several metal-catalyzed approaches to synthesize privileged structures.<sup>1</sup> We also have made significant progress in developing metal-free processes to access various classes of carbo- and heterocycles.<sup>2</sup> The major emphasis of my presentation would be on the metal-free strategies developed in our laboratory, viz., (i) enantioselective intramolecular Morita-Baylis-Hillman reaction,<sup>2</sup> (ii) phosphine-catalyzed intramolecular hydroalkylation and hydroacylation of ynones,<sup>3</sup> (iii) organocatalyzed reductive aldol and vinylogous aldol reactions,<sup>4</sup> and related findings.<sup>5</sup>

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### IL-03

## **Development of Organic Spintronics Devices using Precise Synthesis of Helical Poly(phenylacetylene)s**

Dr. Tatsuya Nishimura

Nano Life Science Institute (NanoLSI), Kanazawa University

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The CISS (Chiral-Induce-Spin-Selectivity) effect reported by Naaman et al. has led to much research on spintronics using organic compounds, mainly biopolymers. In the literature, there are few reports on CISS using precisely designed organic compounds. However, it is desirable to diversify the organic molecules for spin polarization measurements and to clarify the CISS effect. On the other hand, we have successfully developed a precise synthetic technique for the chain-end functionalization of poly(phenylacetylene)(PPA)s. This method enables us to design and synthesize different end-functionalized PPAs and to verify the CISS effect from various viewpoints. In this study, we have immobilized the chain ends of PPA derivatives on a device with a unidirectional helical structure and observed the CISS effect in various ways. Then the polarization conversion of the spin polarization by external stimuli has been evaluated.

Helical PPAs (poly-1L and poly-1D) with thiol end groups were synthesized by multicomponent catalytic polymerization using mercaptophenyl boronic acid derivatives as initiator. The device was fabricated by immersing a gold/Ni substrate in THF solution of the polymer for 12 hours. Spin polarization measurements were performed by tunnel magnetoresistance measurement using a self-made probe, magnetic field conductivity AFM measurement (0.5 T), and Hall measurement in aqueous solution. Poly-1L has a very narrow molecular weight distribution ( $M_w/M_n=1.08$ ) with degree of polymerization (DP) about 23 mer, and the length was estimated at around 6 nm from the model. The spin polarizability of the synthesized polymer was measured by AFM conductivity measurement in presence of external magnetic field 0.5 T, and the estimated spin polarizability was around 56%. The same measurement was carried out for the helical poly-1D with right-handed helical alignment of the main chain and upward spin was observed. It is important to mention that polymers with achiral functional groups in the side chains are unable to exhibit spin polarization.

In this presentation, I would like to show other collaborative projects related with the goal of Nano LSI.



## **IL-04**

### **Introduction to Carbon Quantum Dots: Synthesis and Multidirectional Applications**

Dr. Ranjit De

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Carbon quantum dots (CQDs) are graphene family quasi-spherical sub-10 nm sized fluorescent nanomaterials which have gained tremendous attention during the past 15 years. This is mainly due to their expanding applications in various fields, such as, renewable energy harvesting and storage, optoelectronics, biological and medical devices, catalysis, nanomedicine design, *etc.* In this presentation I shall briefly discuss their origin, properties, various synthetic routes, and multipurpose applications. Specifically, their synthesis *via* rapid, one-pot, and cost-effective route will be presented. How doping of CQDs can alter their properties will be explained. Finally, their multidirectional applications, such as, inscription of confidential information, finger imprinting, hosting on cellulose papers, designing of polymeric molds flashing bright fluorescence, cell viability, *in vitro* imaging, detection of reactive oxygen species (ROS) in cellular milieu, will be presented.

**Prof. C. N. R. Rao Endowment Lecture**  
**Correcting and Detecting Genes with Precision: An Indigenous Approach**

Prof. Souvik Maiti

CSIR-Institute of Genomics and Integrative Biology, Delhi

CSIR-National Chemical Laboratory, Pune

CRISPR based genetic correction has moved rapidly into therapeutics with multiple clinical trials currently underway for predominantly monogenic disorders. One of the limitations of first generation CRISPR proteins derived from *Streptococcus pyogenes* (SpCas9) is the rampant off-targeting caused by high propensity to binding genetic loci with some degree of homology to the target. At the biophysical level, this can be explained by the nature of amino acid and nucleobase contacts that the domains of the Cas9 makes with a substrate. In order to make such a Cas protein more specific in targeting the desired gene, several groups have attempted to engineer SpCas9 by reducing possible contacts in the DNA backbone inevitably leading to more specific but less efficient editors that impacts the eventual therapeutic benefit. We have approached this problem from a different route by exploiting the high specificity of an orthogonal Cas protein from *Francisella novicida* (FnCas9). Although this protein has a very high mismatch dissociation ability, its inherent activity on cellular targets was low. To circumvent this, we have engineered residues in the PAM interacting domains of FnCas9 and developed engineered versions of the protein that uniquely combines high specificity and efficiency. We are currently taking this ahead for clinical trials for the genetic correction of hematological and ocular diseases. This talk will feature how such an engineering was done and the eventual outcome on target binding and off-target discrimination.

**References**

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# **ORAL PRESENTATIONS**

## **(OP)**

## OP-1

### **Green Chemistry Protocol for the Synthesis of Some New Scaffolds of Isoxazolidine & Isoxazoline Derivatives via 1,3-Dipolar Cycloaddition Reaction and Potential Biological activities of the Cycloadducts**

Prof. Bhaskar Chakraborty

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One of the excellent examples of spin trapping reagents is nitrones which plays fundamental role in the synthesis of five-membered heterocyclic ring compounds (commonly called isoxazolidine and isoxazoline derivatives) via 1,3-dipolar cycloaddition reactions which are an integral part of many natural products. The medicinal activities of these heterocyclic compounds always finds a tremendous interest to the synthetic organic chemists as they found to exhibit antibacterial, anticonvulsant, antibiotic, antitubercular, antifungal and anticancer activities. Except green chemistry methodologies, majority of the reported procedures for the synthesis of isoxazolidine and isoxazoline derivatives require drastic experimental conditions like high temperature and long reaction times. In addition, these reactions found to suffer from selectivity and also there are possibilities of poor yields as well as development of side products. Majority of these conventional procedures for the synthesis of isoxazolidine and isoxazoline derivatives are replaced successfully nowadays with the inception of green chemistry procedures like solvent free reactions (solid phase reaction), reactions conducted “in water” & “on water”, microwave induced reactions and many more techniques. In the present work, few excellent examples based on stereoselective 1,3-Dipolar cycloaddition reactions using green chemistry protocols have been reported. Good to excellent yields, minimum reaction time, fast & simple isolation of products, environment friendly reaction conditions and stereoselectivities in the reported reactions will certainly attract researchers working in this domain.

**Keywords:** Stereoselective 1,3-Dipolar cycloaddition reaction, New approaches, Green chemistry methodologies, Anticancer activity

## **OP-02**

### **Manipulating electronic structures of Mo<sub>2</sub>C to achieve ultra-high catalytic activity for electrochemical water oxidation**

Md. Selim Arif Sher Shah

*Department of Chemistry, North Bengal University, Siliguri 734 013, West Bengal, India*

Molybdenum carbide is a well-known electrocatalyst for high performance water reduction (i. e., hydrogen evolution reaction, HER) due to its Pt-like electronic structure, high electrical conductivity, stability, and abundance. However, it displays poor catalytic activity for electrochemical water oxidation due to the high overpotential demanded by the sluggish kinetics of the oxygen evolution reaction, OER. Many efforts involving several strategies have been directed to increase the OER catalytic activity of Mo<sub>2</sub>C. Nevertheless, increase in catalytic activity was not up to the mark. In this contribution, electronic structures of Mo<sub>2</sub>C were finely manipulated with the incorporation of two transition metals Co and Fe. It was observed that any single metal could not finely tune the electronic structures of Mo<sub>2</sub>C. The optimized electrocatalyst exhibited excellent OER electrocatalytic activity evidenced by an ultra-low overpotential of 214.8 mV to achieve a current density of 10 mA cm<sup>-2</sup> and a low Tafel slope of 38 mV dec<sup>-1</sup>. Moreover, the electrocatalyst was characterized with long term stability. Density functional theory calculation proved the experimental data. The ultra-high catalytic activity of the electrocatalyst was attributed to the excellent intrinsic catalytic activity evidenced by high electrochemically active surface area, large mass activity and low charge transfer resistance.

### **OP-03**

#### **Bio-modified magnetic nanoparticles as a versatile tool for different applications**

Goutam Biswas

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Purified drinking water has been a main concern for all humans. Nanoparticles have recently emerged as a helpful and inexpensive option for numerous applications in most cases. Biomodified magnetic iron oxide nanoparticles have also emerged as a low-cost and long-term solution for water purification. In our group, we synthesized *Cinnamomum tamala*, *Jatropha curcas*, and *Terminalia arjuna* coated magnetite iron oxide nanoparticles independently and analysed them using TEM, SEM, FTIR, powder XRD, AGM, and other methods. The biomodified nanoparticles that were created were subsequently used to remove different poisonous metal ions, dangerous organic chemicals, and microbiological species.

## OP-04

# Unraveling the Surface Chemistry of Perovskite Nanocrystals for White Light Emitting Applications

Mihir Manna<sup>1</sup>, Tushar Debnath<sup>1</sup> and Satyapriya Bhandari<sup>2</sup>

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Surface modification of perovskite using chemical agents is of paramount interest to tune their optical properties for light-emitting applications especially white light generation.<sup>1-4</sup> Thus, the understanding of the binding nature of chemical agents such as organic ligands and inorganic complexes to the surface of CsPbX<sub>3</sub> (X= Cl, Br, I) perovskite nanocrystals (PNCs) is critically essential for making them a perfect material either for solar cell applications or for white light generation.<sup>1-3</sup> When a small bidentate 8-hydroxyquinoline (HQ) organic molecule functionalizes the surface of a presynthesized CsPbX<sub>3</sub> (X= Cl, Br, I) PNCs, two different binding chemistry are proposed based on the polarizability of the halides and the octahedral cage size.<sup>1</sup> The halogen-hydrogen binding chemistry is observed for HQ-coupled CsPbCl<sub>3</sub> and CsPbBr<sub>3</sub> PNCs, which facilitates the interfacial charge transfer (CT) process between the PNCs and the HQ molecule. While the presence of weak chelation in HQ-coupled CsPbI<sub>3</sub> PNCs inhibits the CT process. Interestingly, a completely different binding chemistry is observed when the calcium complex form of HQ (i.e. CaQ<sub>2</sub> complex) is added to a Mn<sup>2+</sup>-doped CsPbCl<sub>3</sub> PNCs.<sup>2</sup> Notably, the chloride on the surface of CsPbCl<sub>3</sub> PNCs coordinated with the calcium metal centre of the CaQ<sub>2</sub> complex followed by preserving the size, shape and dopant oxidation state of doped PNCs. The combination of orange emission from Mn<sup>2+</sup>-doped PNCs and cyan emission from CaQ<sub>2</sub> complex resulted a bright white light emitting material with a chromaticity of (0.33, 0.32), correlated colour temperature (CCT) of 5483 K, colour rendering index (CRI) of 80, and quantum yield of 54.1%.

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## **OP-05**

### **Autophagy augments chemotherapeutic drug efficacy in human cancer cell lines – an in vitro and in silico study**

Ankita Dutta\*, Anoop Kumar

Advanced Nanoscale Molecular Oncology Laboratory, Department of Biotechnology, University of North Bengal, Siliguri - 734013, West Bengal, India

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Cancer is the most leading cause of death worldwide, and its prevalence is frequently increasing. Higher mortality rate associated mainly with its metastatic potential and resistance to various chemotherapeutic drugs. Although anticancer therapy has improved appreciably, it still has inadequate efficiency for tumour eradication. Most of the chemotherapeutic drugs are nonselective in action and as a consequence it ends up with decreasing normal cell viability also. Continuous exposure of chemotherapeutic drugs like, cisplatin and 5-fluorouracil also develop multidrug resistance (MDR) in cancer cells which eventually leads to chemotherapeutic failure. Considering these factors, a new autophagy based therapeutic approach is developed which enhance the drug mediated cytotoxicity particularly in cancer cells. This study suggests that caloric intake modulation (autophagy) combined with chemotherapeutic drug increased the susceptibility of cancer cells and emerge as a new efficient and low cost strategy to treat cancer. By using a series of in vitro and transcriptome-based in-silico approach we have modified the conventional practice of starvation to get promising result during chemotherapeutic treatment. Under the experimental condition, drugs like- 5-fluorouracil and cisplatin showed significant cytotoxicity towards renal (ACHN) and liver cancer cell (HepG2, HUH-7) growth, with less harm to normal cells (HEK-293, WRL-68). Here, characterization of successful autophagy induction was monitored by fluorescence based assays and quantifying stress response enzymes expression. Further confirmation was achieved by antibody based ELISA technique. Identification of differentially expressed genes (DEGs) and functional interaction between identified novel regulators were analyzed by building protein-protein interaction (PPI) network to unveil the molecular mechanism of autophagy induced cell death. Therefore, our work reinforced the concept of using caloric intake modulation (autophagy) along with chemotherapeutic drug as a potential strategy to specifically target cancer cells.

## **OP-06**

### **Molecular Assembly of Rhodanine with Torus Shaped Cyclodextrins and their Innovative Applications by Physicochemical Contrivance Simultaneously Optimized by Computational Study.**

Antara Sharma<sup>a,b</sup>, and Mahendra Nath Roy<sup>\*,a</sup>

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To increase the bioavailability of Rhodanine (RH), inclusion complexes of RH with both  $\alpha$ -cyclodextrin ( $\alpha$ -CD) and  $\beta$ -cyclodextrin ( $\beta$ -CD) were prepared. The complexes were characterized by different physicochemical as well as spectroscopic techniques thereby indicating encapsulation of RH molecule into the cavities of  $\alpha$ -CD and  $\beta$ -CD cavity. DSC analysis showed that the thermal stability of RH was enhanced after complexation. Computational study suggests the most preferred orientation of RH molecule within both CD cavities. *In vitro* antibacterial activity test illustrates that the IC2 (RH- $\alpha$ -CD) complex displayed better activity than pure RH and IC1 (RH- $\beta$ -CD) complex. IC2 (RH- $\alpha$ -CD) complex (IC 50 = 7.88  $\mu$ M) shows the remarkable *in vitro* cytotoxic activity than pure RH (IC 50 = 44  $\mu$ M) and IC1 (RH- $\beta$ -CD) complex towards human kidney cancer cell line (ACHN). Furthermore, interaction of IC2 (RH- $\alpha$ -CD) complex RH) and IC1 (RH- $\beta$ -CD) complex with CT-DNA was investigated and found that IC2 (RH- $\alpha$ -CD) complex enhances bioavailability of RH to greater extent than that by IC1 (RH- $\beta$ -CD) complex. Additionally, photostability studies reveals that inclusion of RH using  $\alpha$ -CD induces better stabilization of RH as compared to  $\beta$ -CD.

**Keywords:** Rhodanine;  $\beta$ -Cyclodextrin;  $\alpha$ -Cyclodextrin; Molecular docking; *In vitro* biological activity study.

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## OP-07

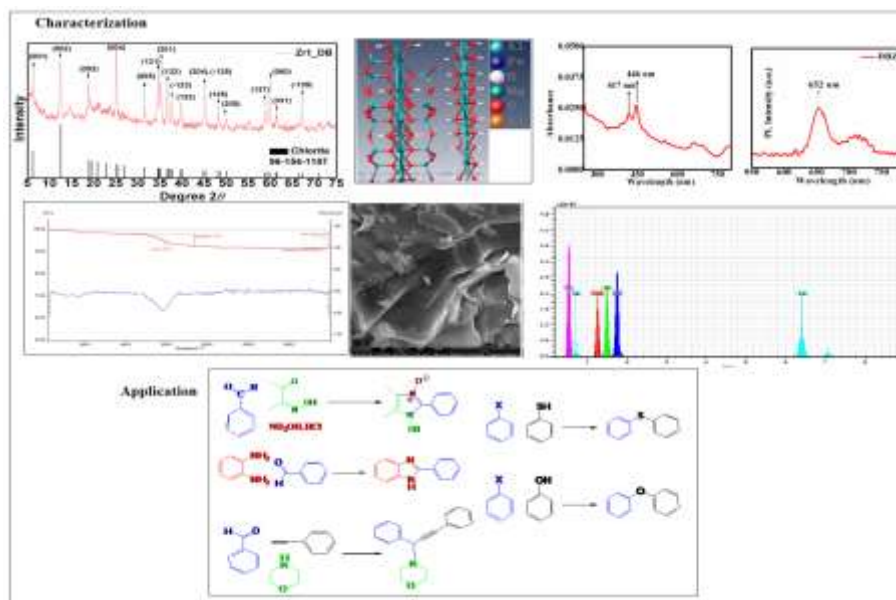
### **Fe-Rich Chlorite mineral as a multifunctional catalyst for C-N, C-O and C-S coupling reactions**

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A locally available chlorite mineral have been identified and characterized using different analytical and spectroscopic tools. After thorough investigation, it was revealed that it belongs to the Fe-rich chlorite among the various naturally occurring chlorite minerals. Its structure has been established by powder x-ray diffraction method and it belongs to the monoclinic crystal system with  $C 1 2/m 1$  space group. The other physico-chemical properties such as surface morphology, BET surface area (pore size), FT-IR, TGA/DTA, ICPOES, Photoluminescence etc of the chlorite minerals have been studied. Furthermore, the catalytic efficacies of the Fe-rich chlorite mineral have been investigated for C-N, C-O and C-S coupling reactions.



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## OP-08

### Solubilization of Aqueous-Insoluble Phenothiazine Drug in TX-100 Micellar Solution and Interactions of Cationic/Anionic Surfactants with Phenothiazine–TX-100 System

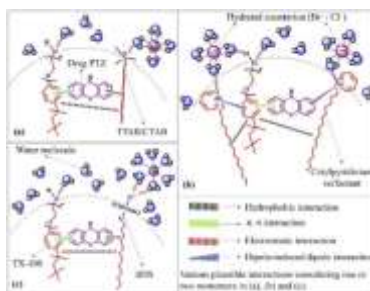
Jackson Gurung<sup>a\*</sup> and Jacqueline Lalhlengliani<sup>b</sup>, and Ajmal Koya Pulikkal<sup>b</sup>

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Poorly aqueous insoluble drug phenothiazine (PTZ) is solubilized in triton X-100 (TX-100) micellar aqueous media at physiological pH and the interaction of surfactants such as hexadecyltrimethylammonium bromide (CTAB), tetradecyltrimethylammonium bromide (TTAB), cetylpyridinium chloride (CPC), cetylpyridinium bromide (CPB) and sodium dodecylsulphate (SDS) in presence of PTZ–TX-100 aqueous media have been investigated through various physicochemical measurements. Conductometric analysis has been used to examine the interactions of surfactants in PTZ-TX-100 media at pH 7.4 (SP buffer) and at three different temperatures. The results reveal the sequence of critical micelle concentration (CMC) values of surfactants as SDS > TTAB > CPC > CPB > CTAB. UV-vis spectroscopy studies were used to study the interactions of surfactants with the drug PTZ in TX-100 aqueous media (at pH 7.4 and 303.15 K) that suggest the interactions are highly feasible (change of Gibbs energy;  $\Delta G_b < 0$ ) and greatly improve beyond the CMC values of corresponding surfactants. Evaluated parameters using the Benesi–Hildebrand equation indicate higher binding constant ( $K_b$ ) for cetylpyridinium surfactants and least for SDS and the drug–surfactant complex formations are found to be in 1:2 stoichiometric ratios. Fluorescence technique has also been employed to study the aggregation number ( $N_{agg}$ ), Stern-Volmer constant ( $K_{SV}$ ) and micro-polarity of TTAB/CTAB/SDS in PTZ–TX-100 systems at 303.15 K. The evaluated thermodynamic parameters such as a change in Gibbs energy ( $\Delta G_m^0$ ), enthalpy ( $\Delta H_m^0$ ) and entropy ( $\Delta S_m^0$ ) of micellization show the process of micellization of all studied surfactants in PTZ–TX-100 aqueous media are spontaneous and exothermic.



## **OP-09**

### **Effect of Globalization on Environment and Biodiversity**

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Globalization means the growing interdependence of the world's economies, cultures and populations. In other words, globalization means the speed-up of movements and exchanges of human beings, technologies or cultural practices all over the planet. For many developing nations, globalization has led to an improvement in standard of living, roads and transportation, improved health care and improved education due to global expansion of corporation. Increased emissions, more fuel is consumed and a greater level of greenhouse gas emission is produced which contribute to pollution, climate change and ocean acidification which broadly impact on biodiversity and environmental degradation. Biodiversity is generally described at three levels i.e. diversity of ecosystems, diversity of species and diversity of genes. During the last 100 years there have been rapid development in science and technology, which caused several distinct pressures on environment and biodiversity. In 1960, started the experiments of selective breeding of crops to fix beneficial traits. It was Dr. Norman Borlaug who able to develop dwarf varieties of high yielding wheat through selective breeding. This was the beginning of Green Revolution during 1970. Today, the selective breeding technology has been widely spread and we find thousands of lucrative varieties of crops, vegetables, fruits and flowers all around. The loss of crop diversity due to mono culture of high yielding varieties and expansion of agricultural fields destroying or fragmenting forests are very dangerous to protect biodiversity. Several organizations have recently become active to conserve wild varieties of crops. Simultaneously, there was tremendous development in the field of molecular biology and biotechnology, which led to the development of genetically modified organisms. So, it is globally agreed by scientific and political concept to protect environment and conservation of biodiversity a global movement should be immediately started. It was found on fossil records that on an average 25% of the species are facing extinction risk due to globalization and its impacts on biodiversity.

**Keywords:** Global expansion, Environmental degradation ,Ecosystem, Green revolution, Extinction.

**References:**

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Anil K De ( 2018 ) : Environmental Chemistry 220-251, 310-325.

## OP-10

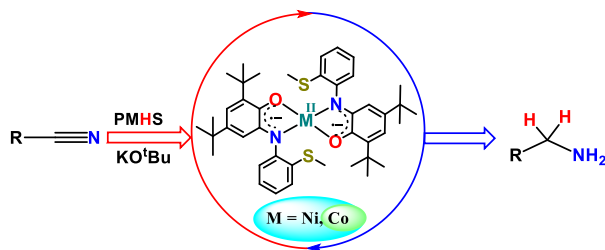
### Non-innocent Quinonoid and Phenalenyl Based Transition Metal Complex Catalysed Organic Transformation and Cross-Coupling Reaction

Krishnendu Paramanik, Hari Sankar Das\*

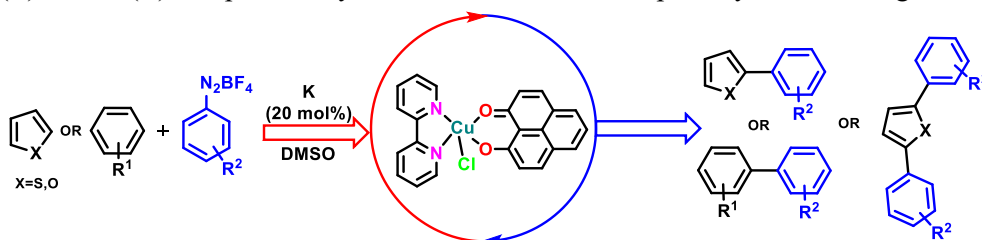
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Quinonoid and phenalenyl are redox active non-innocent ligands (NIL) which function in vital electron transport processes often in conjugation with a transition metal centre. The transition metal complexes with redox active ligands like quinonoid and phenalenyl exhibit delocalized electron distributions, non-integer oxidation states and interesting electronic properties due to the extensive mixing of ligand  $\pi^*$  orbitals with the transition metal  $d\pi$  orbitals. As a result of this, the metal complexes containing redox active ligands play important roles in a variety of fields such as magnetic materials<sup>[1]</sup>, metal-metal coupling, supramolecular chemistry<sup>[2]</sup>, coordination polymers, biological activities<sup>[3]</sup>, bio-mimicking reactions and homogenous catalysis<sup>[4]</sup>. Here in, we have synthesized quinonoid and phenalenyl ligand based Ni(II), Co(II) and Cu(II) complexes. All the compounds were characterized with a suite of spectroscopic methods, cyclic voltammetry and single-crystal X-ray diffraction study. All these transition metal complexes show excellent catalytic activity towards transformation of organonitriles to primary amines using inexpensive PMHS (Scheme 1) and C-C cross-coupling reaction of arenes and heteroarenes with diazonium salt (Scheme 2). The transformation of nitrile to primary amine and C-C cross coupling reaction has great importance in organic and industrial synthesis.



**Scheme 1.** Ni(II) and Co(II) complex catalysed reduction of nitrile to primary amines using PMHS.



**Scheme 2.** Phenalenyl based Cu(II) complex catalysed C-C cross coupling reaction.

## OP-11

### Solvent-Free Synthesis of 4*H*-Benzo[4,5]thiazolo[3,2-*a*]pyrimidine-3-carboxylate, using Humic Acid: A Rarely Explored Green Catalyst

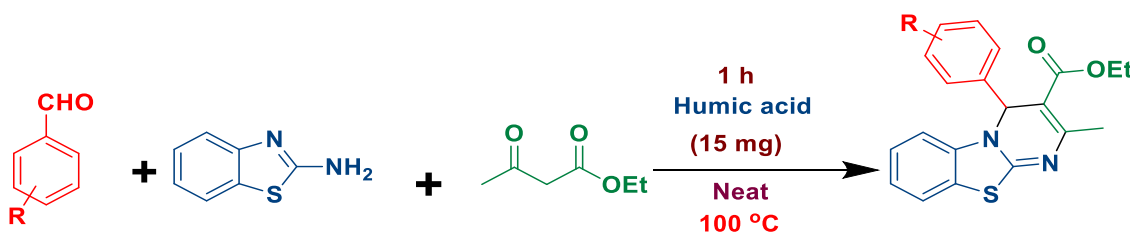
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Humic acid, a rarely used non virulent, easily accessible, inexpensive, environmentally benign, high molecular weight polymer, because of its extraordinary catalytic activity has been explored for the synthesis of functionalized 4*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidine-3-carboxylate and its derivatives. Environmental friendliness, low catalyst loading, outstanding yield, magnificent functional group forbearance and renewability up to fifth run without any noteworthy loss of its activity at the finishing point of reaction, are the cue significances of these methods. It is one of the most feasible techniques for synthesizing a number of such heterocyclic derivatives under the absence of any solvent, taking humic acid as catalyst to activate carbonyl oxygen of respective aldehydes and ester for enhancing the electrophilicity of carbonyl carbon, followed by nucleophilic addition onto that position. The overall mechanism proceeds through Cascade reaction, involving a well-known Knoevenagel and Michael Addition pathway. Since, no metal was used here, so, the overall method was maintained as greener synthetic one. Again, the solvent-free condition, contributes a huge environmental sustainability to the protocol. Humic acid catalyst can be recuperated through easy filtration procedure. So, the basic unique creativity proposition of this methodology, is, the utilization of environmentally benign, easily accessible and low priced humic acid catalyst, instead of any noxious, virulent, exhaustive, hazardous and expensive metal catalyst. This synthetic technique will surely assemble a proper optimistic approach towards the scientists and researchers by creating a magical and significant evolution within the chemical world of medicines, synthetic pathways of natural products and drug industries, on to the upcoming future endeavor.



Humic acid mediated synthesis of functionalized 4*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidin

## OP-12

### **Synthesis, structural characterization, in vitro cytotoxicity activity and ROS assay against ACHN cell-line of a new pyridinium ionic liquid tagged Schiff base and it's Cu (II)/ Zn (II) /Cd (II) - complexes**

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A synergic effect of the metal ion and the ligand system were seen against the ACHN cell-line in their cytotoxicity action and ROS production capacity. Three novel complexes of Cu (II)/ Zn (II)/ Cd (II) ions were synthesized with a novel ligand system of pyridinium ionic liquid tagged Schiff base and characterized by IR, UV-Visible spectroscopy, Magnetic Susceptibility (by Evan's Method), <sup>1</sup>H NMR, <sup>13</sup>C NMR, HRMS, MALDI and PXRD. Diamagnetic Cu (II)- complex (6a) have been assigned to exhibit square planar geometry while diamagnetic Zn (II)- complex (6b) and Cd (II)- complex (6c) are assigned tetrahedral geometry. The Crystallite size of the ligand (5) and it's Cu (II)-complex (6a), Zn (II)-complex (6b) and Cd (II)-complex (6c) are found to be 0.42nm, 0.36nm, 0.34nm and 0.29nm respectively. The degree of Crystallinity of the ligand (5) and it's Cu (II)-complex (6a), Zn (II)-complex (6b) and Cd (II)-complex (6c) are found to be 78.62%, 42.64%, 57.66% and 69.23% respectively. The four synthesized compounds were then, subjected to ACHN cell-line by MTT assay. Among these four compounds Zn (II)-complex (6b) was found to show most cytotoxicity activity with minimum IC<sub>50</sub> value (7.12µg/ml) followed by Cu (II)-complex (6a) with IC<sub>50</sub> (7.96µg/ml) and Cd (II)-complex (6c) with IC<sub>50</sub> (10µg/ml) and the ligand (5) was found to show the least cytotoxicity activity with highest IC<sub>50</sub> (12.82µg/ml). This observation were well supported from their respective ROS production capacity in ROS assay against the same cell-line.

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### OP-13

## **Molecular interaction of selected amino acid in room temperature ionic liquid: A case study of L-proline and L-leucine in aqueous Tetrabutyl Phosphonium *p*-Toluene Sulphonate**

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The study of volumetric and viscometric properties allows investigation into the molecular interaction in solution phase, specifically allows us to understand the nature and strength of the intermolecular forces operating among mixed components. This research work is intimately related to the studies of solute-solute, and solvent-solvent interactions of L-Proline and L-leucine in aqueous Tetrabutyl Phosphonium *p*-Toluene Sulphonate (TBPPTS) solutions at 298.15, 303.15 and 308.15K probed by density, viscosity and refractive index measurements.

Apparent molar volumes ( $\phi_V$ ), viscosity *B*-coefficients and apparent molar isentropic compressibility for L-Leucine and L-Proline in (0.001, 0.003, and 0.005) mol · kg<sup>-1</sup> aqueous tetrabutyl phosphonium *p*-toluene sulphonate solutions have been determined at (298.15, 303.15, and 308.15) K from solution density,  $\rho$ , viscosity,  $\eta$  and at 298.15 K from solution's speed of sound *u* measurements as a function of the concentration of L-Leucine and L-Proline. The limiting apparent molar volume ( $\phi_V^0$ ) and experimental slopes ( $S_V^*$ ) obtained from the Masson equation have been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The viscosity data were analyzed using the Jones-Dole equation, and the derived parameters *A* and *B* have also been interpreted in terms of solute-solute and solute-solvent interactions, respectively, in the mixed solutions. The limiting apparent molar isentropic compressibility ( $\phi_R^0$ ) and experimental slopes, ( $S_R^*$ ) values are also in perfect agreement with the above-mentioned parameters. The refractive index (nD), molar refraction ( $R_M$ ) has also been reported.

The values of the limiting apparent molar volume ( $\phi_V^0$ ), viscosity *B*-coefficients and limiting apparent molar isentropic compressibility indicates the presence of strong solute-solvent interactions which increases with the increase in amount of TBPPTS in solvent mixture and with the increase in the experimental temperature. The refractive index and the molar refraction values suggest that L-Leucine molecules are more tightly packed in the solution leading to higher solute-solvent interaction than L-Glycine.

## OP-14

### Design, Synthesis and In Vitro Cytotoxicity Activity of Copper Complexes of Imine and Amine Ligands

Deboshmita Mukherjee<sup>1</sup>, Rajesh Kumar Das\*<sup>1</sup>

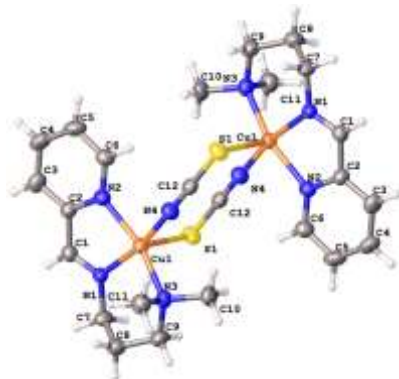
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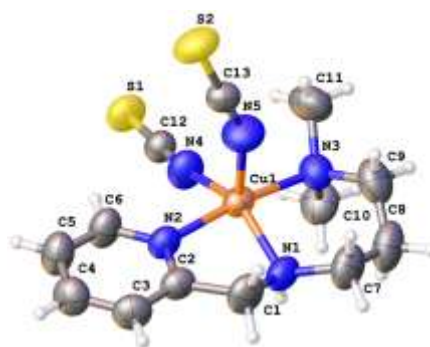
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The development of metal complexes with selected and designed ligands is of great interest in the field of coordination chemistry. Over the years, much effort has been put into exploring complexes of various Schiff base ligands, primarily for pyridine-containing systems. Encouragement for the syntheses of the Schiff bases derived from 2-pyridyl carbonyl compounds and its metal complexes are widely used in a variety of applications, especially as potential antibacterial agents, antifungal agents and antitumor agents. Supporting the idea that copper could be used as a potential tumour-specific target several copper complexes have been now proposed as potential cancer inhibiting agents, as they demonstrate remarkable anticancer activity and show general toxicity lower than platinum compounds. Accordingly, we have synthesized two new Cu(II) complexes of tridentate Schiff base and reduced Schiff base ligands containing two bridging as well as two terminal SCN<sup>-</sup> ligands. Both of the complexes were characterized by various spectroscopic and electrochemical methods along with single crystal XRD techniques. The synthesized binuclear Complex **A** and mononuclear Complex **B** were screened for their *in vitro* anticancer activity against human colon adenocarcinoma cells (HT-29) and human hepatoma cell line (Hep-G2) and HeLa cell line. Activity results proved that has excellent antiproliferative activity against HT-29 whereas Complex **B** is active against Hep-G2 and HeLa cell line.

**Keywords:** Copper (II) Complex; Schiff-base ligands; in vitro; anticancer activity.



Complex A



Complex B

## OP-15

### **Ultra-fast Degradation of Methylene Blue via Fenton-like Process Using Green Synthesized $\text{Mo}_x\text{Fe}_{1-x}\text{O}$ Nanocomposites**

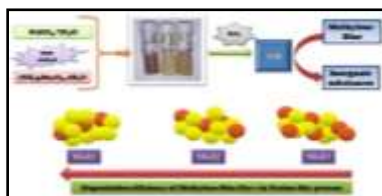
Shatarupa Basak<sup>1</sup>, Salim Ali<sup>1</sup>, Ankita Shome<sup>1</sup>, Mahendra Nath Roy<sup>1,\*</sup>

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In the present work, a series of  $\text{Mo}_x\text{Fe}_{1-x}\text{O}$  ( $x=0.05, 0.10, 0.15$ ) nanocomposite catalysts were prepared via a green method. The synthesized NPs were characterized by scanning electron microscope (SEM), Ultraviolet-Visible spectroscopy (UV-vis), X-ray diffraction (XRD), Energy dispersive X-ray (EDX), Fourier transform Infrared Spectroscopy (FTIR) and Dynamic light scattering (DLS) studies. Catalytic In this study, green synthesis was adopted by using *Punica granatum* peel (PGP) extract for the synthesis of  $\text{Mo}_x\text{Fe}_{1-x}\text{O}$  ( $x=0.05, 0.10, 0.15$ ) nanocomposites with effective degradation of MB. The average crystalline size of  $\text{Mo}_x\text{Fe}_{1-x}\text{O}$  ( $x=0.05, 0.10, 0.15$ ) nanocomposites were in the range 23-47 nm. The  $\text{Mo}_x\text{Fe}_{1-x}\text{O}$  ( $x=0.05, 0.10, 0.15$ ) nanocomposites used for removal of MB dye via Fenton-like reactions as an effective catalysts. Numerous variables, including the amount of catalyst used, changes in the dye's concentration, the pH, the amount of  $\text{H}_2\text{O}_2$ , and the temperature all had a significant impact on the rate of degradation. We studied the degradation rate under a suitable condition of 10 mM to 30 mM of different nanocomposites, 20 mM [ $\text{H}_2\text{O}_2$ ], and temperature 303.15 K. These conditions yield approximately 99% degraded product within 22 minutes of treatment. The activation energy was 7.95 kJ/mol, suggesting the temperature dependence effect of MB degradation is very small. The scavenger quenching experiment demonstrated that  $\cdot\text{OH}$  radicals production regulates the decomposition of MB dye.



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## OP-16

### Spectrophotometric and Conductometric Studies on the Interaction of Surfactant with Polyelectrolyte in the presence of Dye in aqueous medium

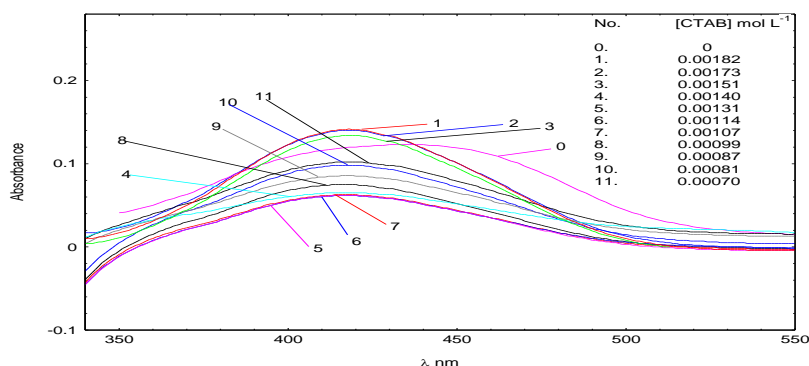
Shiv Narayan Yadav<sup>a,b</sup>, Ajaya Bhattarai<sup>a\*</sup> and Biswajit Sinha<sup>\*b</sup>

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The major goal of this work is to use conductometry and UV-Vis. techniques to investigate the influence of MR on the interactions between cationic surfactant cetyltrimethylammonium bromide (CTAB) and an anionic polyelectrolyte sodium polystyrene sulfonate (NaPSS) in aqueous environments. By observing changes in the dye's spectra and the breaking points of conductometric curves, it is obvious that MR causes the development of surfactant aggregates. Various important thermodynamic parameters were determined by conductivity techniques at  $298.15 \pm 0.2$  K. With increasing CTAB concentrations, the absorption spectra of MR were observed between 430-440 nm for the basic form steadily dropped to 414-421 nm. The CMC of CTAB in water was determined to be  $0.00091 \text{ mol L}^{-1}$  but the CMC\* of CTAB for the CTAB+NaPSS system was determined to be  $0.001438 \text{ mol L}^{-1}$  and CMC\* for the CTAB+NaPSS+MR system was observed to be  $0.001328 \text{ mol L}^{-1}$  by conductivity and  $0.001310 \text{ mol L}^{-1}$  by UV-Vis. spectroscopy at  $298.15 \pm 0.2$  K.

**Keywords:** Conductivity, CTAB, Interaction, Methyl red, NaPSS, UV-Vis. spectroscopy



**Fig.** Absorption spectra of MR in the water [0] and the presence of CTAB/NaPSS at various concentrations of CTAB [from 1-11] for CTAB/NaPSS/MR system at  $298.15 \pm 0.2$  K.

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## **OP-17**

### **Characterization of *Firmiana colorata* (Roxb.) R. Br. leaf extract and its silver nanoparticles reveal their antioxidative, anti-microbial, and anti-inflammatory properties**

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Nanotechnology is the integrative science in the field of physics, chemistry and biology. For the synthesis of silver nanoparticles, a simple approach was applied using *Firmiana colorata* (Roxb.) R. Br. aqueous leaf extract. During the synthesis of this silver nanoparticle, the solution color changes from green to deep brown due to the reduction of silver. The phytochemicals present in the *Firmiana colorata* leaf extract act as a reducing as well as a capping agent. Identifying the presence of bioactive compounds responsible for the reduction of silver was extensively characterized by UV-Visible spectrophotometer, FTIR, SEM, and EDX. Moreover, to know the efficacy of the silver nanoparticles (AgNps) antioxidant and antimicrobial studies were evaluated against the human pathogenic bacteria. Furthermore, in-silico molecular docking was done against the Anti-inflammatory and oxidative protein. Here within this study, a comparative evaluation was done between the *Firmiana colorata* leaf extract and the synthesized silver nanoparticles. Results indicate that ethnomedicinally lesser-known *Firmiana colorata* and AgNps have the potency to act as anti-inflammatory, antioxidative and antimicrobial agents.

**Keywords:** Inflammation, Ethno-medicine, phytochemicals, Nanoparticle, SEM, UV-spectroscopy.

## OP-18

### Organocatalytic synthesis of (Het)biaryl scaffolds via photoinduced intra/intermolecular C(sp<sup>2</sup>)-H arylation by 2-pyridone derivatives

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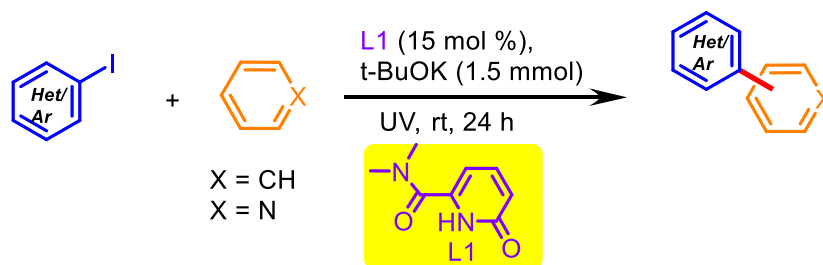
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A unique N,O-bidentate ligand 6-oxo-1,6-dihydro-pyridone-2-carboxylic acid dimethylamide (L1) catalyzed direct C(sp<sup>2</sup>)-H (intra/intermolecular) arylation of unactivated arenes has been developed to expedite access to (Het)biaryl scaffolds under UV-irradiation at room temperature. The protocol tolerated diverse functional groups and substitution patterns, affording the target products in moderate to excellent yields. Mechanistic investigations were also carried out to better understand the reaction pathway. Furthermore, the synthetic applicability of this unified approach has been showcased via the construction of biologically relevant 4-quinolone, tricyclic lactam and sultam derivatives



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## OP-19

### **Target Analyte Interaction with a New Julolidine Coupled Benzoxazole based Dyad: A Combined Photophysical, theoretical and Bio-imaging study**

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A Julolidiene coupled benzoxazole based fluorescence chemosensor is designed and prepared based on chelation induced enhanced fluorescence(CHEF) which can selectively and sequentially recognize  $Zn^{2+}$  ion, an explosive chemical Picric acid(PA)and  $HSO_4^-$  ion when other rival ions of the similar kind are present not only in laboratory limit but also in living cells. Benzoxazole moiety is chosen as our signalling unit to develop our chromogenic & fluorogenic sensor because of its extra ordinary photo physical properties. Solvatochromic properties of the probe are checked both in UV-Visible and fluorimeter. The probe is found to be fluorescence inactive but with the addition of definite volume of  $Zn^{2+}$  ion from zinc perchlorate salt the intensity is almost 16 times increased and LOD is found to be in  $\mu M$  range for  $HSO_4^-$  & PA but in  $\eta m$  range for  $Zn^{2+}$  and under UV at 365nm wavelength the colour changed from colourless to green. The complex formation is supported by Job's plot The (Probe+ $Zn^{2+}$ ) complex can selectively detect  $HSO_4^-$  & PA in other colonial gatherings as fluorescence intensity is quenched on interaction with said anion & mentioned NAC. Depending on this orderly response, the probe can be utilized making two inputs INHIBIT gate & combinational logic gates .Besides ,MTT assay says that the probe can be used as bioanalytical tool also.

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## OP-20

### **A 4-Aminophthalimide Derive Smart Molecule for Sequential Detection of Aluminum Ions and Picric Acid**

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A fluorosensor derived from 4-aminophthalimide, ((E)-5-((2-hydroxybenzylidene) amino) isoindoline 1, 3-dione, AID) working with excited state intramolecular proton transfer (ESIPT) mechanism is synthesized and employed for the selective recognition of aluminum (Al<sup>3+</sup>) ions and picric acid (PA) based on ‘off-on-off’ fluorescence mechanism. The sensor AID shows a turn-on fluorescence response towards Al<sup>3+</sup> ions in 10% (v/v) DMSO/H<sub>2</sub>O with a rapid response time (2 minutes) and exceptional sensitivity (LOD = 0.56 μM). The binding constant (K) of AID with Al<sup>3+</sup> ions is estimated to be  $1.32 \times 10^8 \text{ M}^{-2}$ . The 1:2 stoichiometries of the complex between AID and Al<sup>3+</sup> ions are confirmed through Job’s plot and <sup>1</sup>H NMR spectral analysis. Al<sup>3+</sup>-chelated AID complex is further employed to detect explosive nitroaromatic compounds, especially PA. Furthermore, using these two chemically encoded inputs, viz. Al<sup>3+</sup> and PA and corresponding optical output, we have constructed the INHIBIT molecular logic gate. The AID chemosensor and Al<sup>3+</sup>-chelated AID complex is also applied to map Al<sup>3+</sup> ions and PA in the living cell. The AID chemosensor and Al<sup>3+</sup>-chelated AID complex's performance toward detecting Al<sup>3+</sup> ions and PA demonstrates that they might be used as a signaling tool for the analysis of biological and environmental samples.

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## **OP-21**

### **Determination of Reliable Allosteric Parameter in MWC Model from Hill Coefficient**

Dr. Tridib Mondal

Sukanta Mahavidyalaya, Dhupguri, Jalpaiguri, WB, 735210

Many multi-subunit proteins undergo ligand promoted conformational change either by Monod-wyman-Changuex (MWC) model or Koshland-Némethy-Filmer (KNF) model. Although these two models were proposed a long time ago, some fundamental problems have retarded the use of the MWC and KNF models. One of the difficulties to distinguish between the two models as the ligand binding curves are sigmoidal in nature and insensitive to the different ligation intermediates. Another difficulty to determine the values of the allosteric parameters in a reliable manner as the parameters are very sensitive to the data fitting method and correlated with each other. We have derived a general mathematical equation between the hill coefficient of steady state condition and the parameters of the MWC model. This relationship probably helps to determine true combination of MWC parameters from all possible parameters obtained from data fitting. This approach is applied to fit the allosteric transition of GroEL molecules in the presence of ATP from low-affinity tense state (T) to a high-affinity relax state (R). This method enlightens on the hydrophobic-to-hydrophilic transformation of the GroEL cavity surface on binding of ATP molecules which is vital for its function.

## OP-22

### **Molecular docking studies to validate the efficacy of the indigenous Bioformulation of North East India against the reproductive proteins of the pest, *Tetranychus urticae***

Sandipan Ghosh<sup>1</sup>, Gargi Sen<sup>2</sup>, Indrani Sarkar<sup>2</sup>, Chandra Ghosh<sup>3</sup>, Arnab Sen<sup>1,2,4\*</sup>

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*Tetranychus urticae* (two-spotted spider mite) is a pest infesting multiple crops of agricultural importance. An effective remedy for the prevention and control of this pest is lacking. This study focuses on the identification of the phytochemicals from the indigenously prepared bioformulation by GC-MS analysis. Further, the identified compounds were targeted against the proteins present in the reproductive cycle of the pest by molecular docking. Molecular docking analysis revealed an effective binding score against the vital proteins which will be effective in arresting the multiplication of the two-spotted spider mites. Since the phytochemical affect the reproductive proteins, its further multiplication and spread in the field can be averted. The current *in silico* study depicts the interaction of the mite protein and the phytochemical which also may be effective against other mite pests. This is the first-ever report for the characterization of the bioformulation against pests from this region.

# **POSTER PRESENTATIONS**

## **(PP)**

## **PP-01**

### **Theoretical and computational study of metal capped superatomic clusters**

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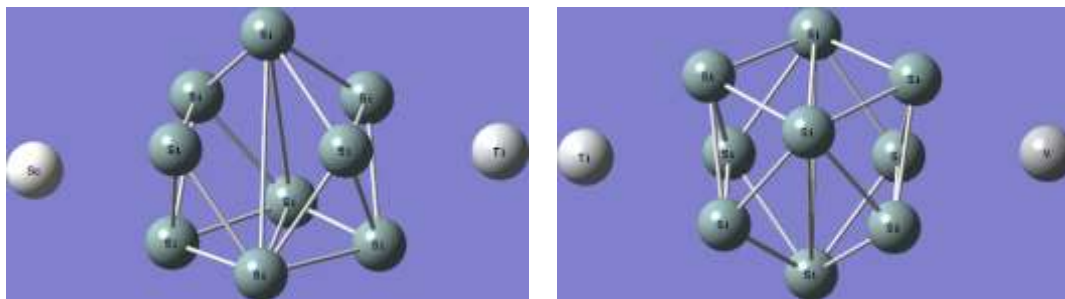
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Superatoms are the tiny clusters which exhibit the properties of elemental single atoms are indeed the most important development in the area of cluster chemistry due to their unique structural and electronic characteristics. It has the potential to be used as building blocks of new materials in the field of optics, sensors, and catalysis etc.

Recent studies reveal that the exploration of atomic structure of the small atomic clusters are difficult compared to the characterisation of the bulk material, where techniques like X-ray diffraction and neutron scattering are routinely used. Density functional theory (DFT) plays an important role in characterising such materials. Obviously, DFT based computations can be an efficient way in predicting the structure and physico-chemical properties of small superatomic clusters.

Silicon based clusters have a great variety of chemical properties and widespread applicability. Bare silicon clusters are not a very good building block for materials and doping of these clusters with metal atoms not only introduce stability but make them important candidates for making building blocks of materials having interesting properties. The present work deals with the exohedral heterometal atom doped neutral  $MSi_9M'$  systems with  $M, M' = Cr, Mn, Fe$  etc. The relative stability of the clusters has been assessed through DFT.

The structures have been optimized in B3LYP/TZV level of theory and are taken for further investigation. The structure and stability have been explored through molecular orbital and bond orbital analyses. The optimized structures show  $C_{2v}$  geometry and represent a stable electronic structure and wavefunction. The analysis of structure and bonding has also been executed with the help of natural bond orbital analysis.



## PP-02

### Synthesis of a tetragonal SnO<sub>2</sub> photocatalyst for Microstructural analysis and visible light driven Fenton-like degradation of Methylene Blue

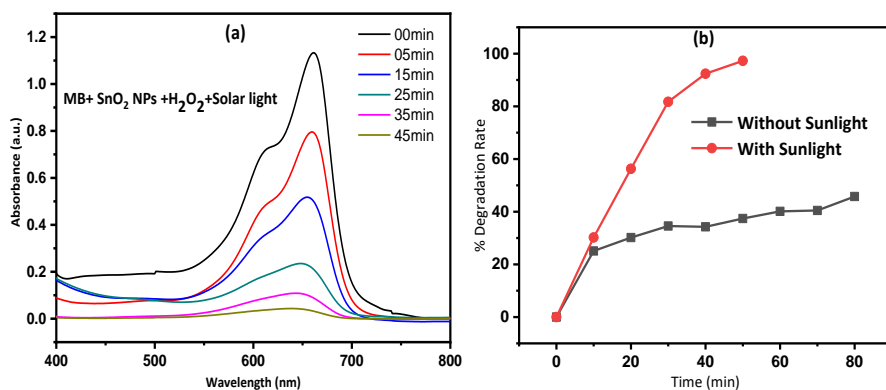
Afroja Banu<sup>1</sup>, Suranjan Sikdar<sup>2</sup> and Biswajit Sinha<sup>1,\*</sup>

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A simple co-precipitation followed by solid state method is employed for the synthesis of tetragonal SnO<sub>2</sub> nanoparticles. The as synthesized nanoparticles were characterized by XRD, FTIR, SEM, HRTEM, EDAX, DLS, UV-vis, and PL techniques to examine the structural properties, functional group, morphological and electronic properties. SnO<sub>2</sub> NPs has been used for Fenton-like degradation of Methylene blue (MB) dye in presence of solar light in aqueous solution. The structural analysis and Rietveld refinement justified the formation of the tetragonal SnO<sub>2</sub> NPs. The mean crystallite size of the synthesized tin oxide nanoparticles was found to be 16.47 nm using the Scherrer formula and strain throughout the crystal was determined by Williamson-Hall method. The degradation of MB dye follows pseudo-first order kinetics with the rate constant  $k_1$  equal to  $7.889 \times 10^{-2} \text{ min}^{-1}$ . The surface area, pore-volume, and pore diameter were measured by Brunauer-Emmet-Teller (BET) surface analysis with nitrogen adsorption-desorption isotherm.



The changes in the concentration of MB Dye in presence of tetragonal SnO<sub>2</sub> nanoparticles and H<sub>2</sub>O<sub>2</sub> at different irradiation time interval in presence of visible light (Figure (a)) and % of degradation in presence of sun light and absence of sun light (Figure (b))

### PP-03

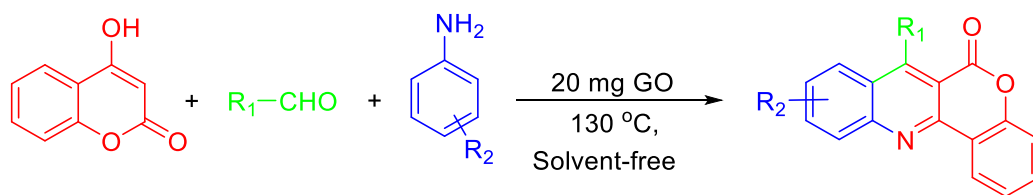
## Novel Greener protocol for one-pot three-component tandem annulation of 4-hydroxycoumarine with aldehyde and aromatic amines using Graphene oxide as an efficient catalyst.

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At this time, rapid synthesis of highly important heterocyclic compounds becomes a great challenge for the synthetic chemists. Multi-component reaction (MCRs) is a great idea for success in this purpose. MCRs has unique advantages such as low cost, high atom-economy, energy saving, smaller reaction time and cheap purification processes. Chromeno[4,3-*b*]quinolin-6-ones are one of the important heterocyclic compound because of the presence of this moiety in various natural product as well as in synthetic product. This heterocyclic compounds are also important in the application of medicine and optoelectronics. Chromenoquinoline derivatives are also widely used in medicinal chemistry as glucocorticoid, selective progesterone receptor modulator, estrogen receptor, anti-inflammatory, bacteriostatic activities and anti-cancer. In our approach we applied Graphene oxide (GO), as a greener carbocatalyst. Graphene oxide is a two dimensional thin layer nanostructure and it has unique chemical properties, high mechanical and thermal resistance. GO contains different kind of oxygen containing functional groups like epoxide, carbonyl, hydroxyl, carboxyl. Due to the presence of these different oxygenated functional groups in GO, it has been reported as moderate acidic and an oxidant catalyst in several reaction. Here we developed a solvent free greener GO catalysed reaction for the synthesis of chromeno[4,3-*b*]quinolin-6-ones using aniline, aldehyde and 4-hydroxycoumarine. The reaction protocol was carried out under mild condition and it taken short reaction time and easily recovered the catalyst from the reaction mixture. The recovered catalyst was reused up to 5<sup>th</sup> cycle without loss of its catalytic activity.



## PP-04

### **ENCAPSULATION OF AN ANTIPLATELET AGENT WITH BETACYCLODEXTRIN FOR BIOCHEMICAL APPLICATION AND DIVERSE AUTHENTICATIONS.**

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Host-Guest inclusion complex of ticlopidine hydrochloride and  $\beta$ -cyclodextrin have profound Antibacterial and cytotoxic activity. In our present study, we aim to develop the inclusion complex of ticlopidine hydrochloride (TCP) with  $\beta$ -cyclodextrin ( $\beta$ -CD) and investigate its invitro bioactivity. The complex was characterized by various physicochemical as well as spectroscopic techniques suggesting the successful inclusion of TCP molecule into the  $\beta$ -CD cavity. TG analysis showed that the thermal stability of TCP was found to improve after complexation. Molecular docking study speculated the most preferred orientation of TCP molecule within the binding pocket of  $\beta$ -CD cavity. In-vitro antibacterial activity test demonstrated that the TCP- $\beta$ -CD complex displayed better activity than pure TCP. TCP- $\beta$ -CD complex ( $IC_{50} = 24 \mu M$ ) also exhibited significant in-vitro cytotoxic activity than pure TCP ( $IC_{50} = 44 \mu M$ ) towards human kidney cancer cell line (ACHN). Furthermore, the complex induces the ROS generation in ACHN cells more pronouncedly than TCP alone, suggesting the increased apoptotic activity of TCP after complexation. These results reveal that inclusion of TCP using  $\beta$ -CD could lead to stabilization of TCP and efficient display of its antibacterial and cytotoxic activities. Thus, TCP- $\beta$ -CD inclusion complex can be a promising approach for designing a novel formulation of TCP in drug delivery, thereby, extending the potential clinical purpose of TCP in pharmaceutical industries and biomedical sciences.

**Keywords:** Ticlopidine hydrochloride;  $\beta$ -cyclodextrin; Thermodynamic analysis; Molecular docking; Cytotoxicity.

**Reference:**

Food Chem Adv1:100015; <https://doi.org/10.1016/j.focha.2022.100015>.

## PP-05

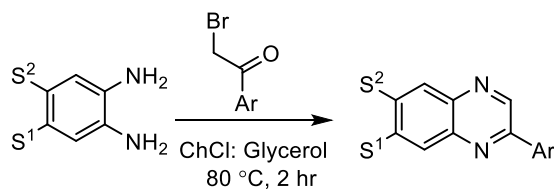
# One-Pot Synthesis of Quinoxaline Derivatives Using Choline Chloride and Glycerol Based Deep Eutectic Solvent (DES)

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**Abstract:** Quinoxaline moieties are frequently encountered in medicinally and biologically active heterocyclic compounds. Quinoxaline moieties exhibit excellent medicinal properties such as anti-cancer <sup>[1]</sup>, anti-viral <sup>[2]</sup>, anti-bacterial <sup>[3]</sup> etc. There are various protocols reported in literature for the synthesis of quinoxaline derivatives. With the rising environmental concern to make more sustainable methodology, we have developed Choline chloride: Glycerol based Deep Eutectic Solvent (DES) catalyzed one pot multicomponent synthesis of quinoxaline derivatives from 1,2-diaminobenzenes and 2-bromoacetophenone. In this synthetic protocol, 1,2-diamino benzene reacts with phenacyl bromide or 3-(bromoacetyl) coumarin at 80 °C for 2 hours in DES medium to give the corresponding quinoxaline derivatives in excellent yield (96-86%) which shown in Scheme 1.



Scheme 1: DES catalyzed synthesis of Quinoxaline derivatives

The role of the DES as a solvent as well as catalyst has been extensively studied. Catalyst free condition, sustainable medium, mild reaction condition, operational simplicity and excellent reaction yield are some of the promising features of present synthetic protocol. The results of this investigation will be presented.

**Keywords:** Deep Eutectic Solvent, Multicomponent Reaction, Quinoxaline

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## **PP-06**

### **A new oxido-rhenium(V) complex with 4-diethylaminobenzaldehyde ligand: Catalytic activity and DFT calculations**

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New oxorhenium(V) complexes containing the 4-diethylaminobenzaldehyde (HL) in chloroform have been synthesized [ReOCl<sub>2</sub>L(PPh<sub>3</sub>)] (1). The product has been characterized by FTIR, NMR and elemental analysis. The molecular structure of the complex was determined to be distorted octahedral by single crystal X-ray analytical method. The Complex crystallizes as triclinic, space group P-1, Z = 2. It contains one bidentate anionic ligand (L<sup>-</sup>), one triphenylphosphine and two chloro ligands at the (ReO)<sup>3+</sup> core, so that a distorted octahedral geometry is adopted by the six-coordinated rhenium(V) center. The halide ligands are in *cis* positions to each other. The gas phase molecular structure has been optimized for the complex with the density functional theory (DFT) method. The theoretically predicted bond lengths and bond angles are in good agreement with the values based upon the X-ray crystal structure data. Computationally determined IR and absorption spectra are correlated with the experimental observed spectra. The complex was applied to the reduction of a variety of aldehydes, producing the corresponding primary alcohols in good yields and good chemoselectivity.

**Key words:** Oxorhenium(V) complex; Catalytic Activity; DFT

## **PP-07**

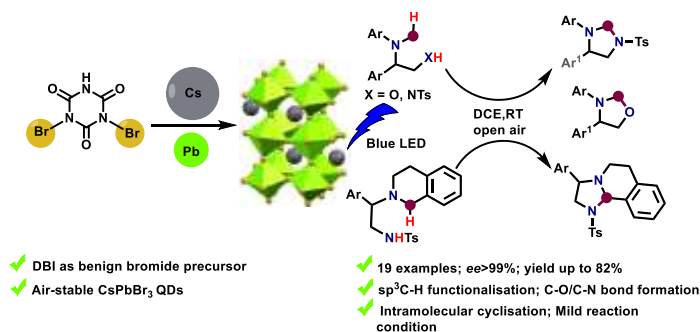
# CsPbBr<sub>3</sub> Perovskite Quantum Dots As An Efficient Visible-Light Photocatalyst For Organic Transformation

Bikram Gurung<sup>1</sup> and Sudarsan Tamang<sup>1</sup>

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In recent years, CsPbBr<sub>3</sub> Colloidal Quantum dots (CQDs) have emerged as an efficient photocatalyst for various organic transformations.[1] Previously, PbBr<sub>2</sub>, molecular bromine, NBS, etc served as a bromide precursor for preparation of CsPbBr<sub>3</sub>. [2] We report a synthetic procedure for preparation of CsPbBr<sub>3</sub> QDs using Dibromoisocyanuric acid (DBI) as benign non-toxic bromide precursor. The as-synthesized QDs possess tunability, ambient air stability and photostability ideal for photocatalysis. A range of bioactive enantiopure bioactive heterocycles such as imidazolidines, fused-imidazolidines and 1,3-oxazolidines were isolated in high yields (isolated yield upto 82%, *ee*>99%) demonstrating QDs as an efficient visible light mediated photocatalyst. The photocatalytic conversion involves the formation of C-N and C-O bonds *via* intramolecular sp<sup>3</sup> C-H bond functionalization as the key step. The use of QDs as photocatalyst under ambient conditions alleviated the challenges of visible light mediated reaction such as use of expensive catalyst, oxidant, stoichiometric amount of base and stringent conditions and was also scalable for industrial purposes. The QDs exhibited high TON (177) and catalytic efficiency (The rate was three times faster compared to conventionally prepared CsPbBr<sub>3</sub> QDs).



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**PP-08**

**Green synthesis of AgNps using saponins extracted from Morus alba plant**

Bishnu Prasad Neupane

*Department of Physics, Tribhuwan University, Damak Multiple Campus, Damak Jhapa*

The green synthesis of AgNps using medicinal plants is of great importance in medicine and agriculture. A new method for synthesizing silver nanoparticles involves the use of saponins. Saponins was extracted using water, ethanol, n-butanol, methanol, and diethyl ether as the solvents by solvent -solvent extraction method. Using Morus alba saponins, the size of AgNps synthesized was found to be 413 nm. The prominent antimicrobial activity of silver nanoparticles is due to their high surface to volume ratio.

## PP-09

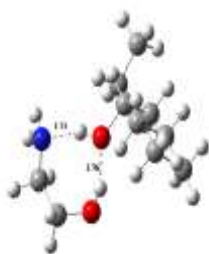
### Binary mixtures of 2-ethyl-1-hexanol and 1, 2-disubstituted ethanes: A Thermophysical, Ultraacoustic and Computational Studies

Dhruba Jyoti Roy<sup>1</sup>, Rajendra Pradhan<sup>2</sup>, Dipu Kumar Mishra<sup>1</sup>, Soumik Das<sup>1</sup> and Biswajit Sinha<sup>2\*</sup>

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Densities ( $\rho$ ), viscosities ( $\eta$ ), ultrasonic speeds ( $u$ ) and refractive indices ( $n_D$ ) of the binary mixtures of 2-ethyl-1-hexanol (2-EH) with ethylenediamine (EDA), 1,2-dichloroethane (DCE) and monoethanolamine (MEA) were measured at  $T = (298.15-318.15)$  K under atmospheric pressure over the entire composition range ( $x_1 = 0 - 1.0$ ). With these experimental data the excess molar volumes ( $V_m^E$ ), viscosity deviations ( $\Delta\eta$ ), excess molar refractions ( $R_m^E$ ), excess isentropic compressibility ( $\kappa_S^E$ ), etc., were determined and discussed in terms of molecular interactions and structural effects well corroborated with IR spectra of the mixtures. Excess molar volumes ( $V_m^E$ ) of the binary mixtures were used to derive partial molar volumes ( $\bar{V}_{m,1}^0$  and  $\bar{V}_{m,2}^0$ ) and excess partial molar volumes ( $\bar{V}_{m,1}^{0,E}$  and  $\bar{V}_{m,2}^{0,E}$ ) at infinite dilution to reveal the volume changes of the binary mixtures. Ultrasonic speeds ( $u$ ) of the binary mixtures predicted using several empirical or semi-empirical theories. Computational studies have also been performed to establish the degree and nature of solvent-solvent interactions theoretically.



**2-EH + MEA (cis)**

**$E_{\text{int}} = -18.00$  kcal/mol**



**2-EH + EDA (cis)**

**$E_{\text{int}} = -12.98$  kcal/mol**



**2-EH + DCE (cis)**

**$E_{\text{int}} = -5.73$  kcal/mol**

References:

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- [2] G.M. Smith, H.C. Van Ness, *Introduction to Chemical Engineering Thermodynamics*, McGraw Hill, New York, 1987.

## **PP-10**

### **Synthesis, characterization and anticancer activity of succinamide compound**

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N<sup>1</sup>, N<sup>4</sup>- Bis(3-(dimethylamino)propyl)succinamide (**DAPS**) has been synthesized and utilized to produce 3,3'-[succinylbis(diazaneyl)]bis(N,N,N-trimethylpropan-1-ammonium) perchlorate (**SAPAP**). Both **DAPS** and **SAPAP** were characterized using different spectroscopic techniques. Structure of the **SAPAP** has been determined using single crystal X-ray diffraction technique. The compound **SAPAP** had excellent anticancer activity against the human colon carcinoma cell line (HT-29), proposing them as a suitable candidate for future anticancer therapies. Docking, Molecular dynamics simulation, pharmacokinetic predictions and ELISA were also employed to evaluate the inhibitory action of the synthesized compound against the said cancer cell line HT-29.

**Keywords:** SAPAP, DAPS, anticancer activity, DFT.

#### **References:**

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## **PP-11**

### **Surfactant-drug interaction in aqueous media at various temperatures**

Dilliram Pokhrel and Abhik Chatterjee

*Department of Chemistry, Raiganj University, Raiganj*

This experimental work on solution properties of surfactant, sodium dodecyl sulfate (SDS) and drug, isoniazid (INH) interaction in aqueous media at various temperatures gives measurement of conductivities, surface tension, viscosity and density at four different temperatures (293K, 298K, 303K and 308K) and 0.05M to 0.001M SDS in 0.001M INH solution. By using these values, cmc,  $X_{cmc}$  and some thermodynamics parameters like enthalpy, free energy and entropy change was also measured.

## **PP-12**

### **Synthesis and Characterization of Inclusion Complex of DL-Aminoglutethimide with $\beta$ -Cyclodextrin and its Application in a Biological System**

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The drug DL-Aminoglutethimide or ( $\pm$ )-3-(4-aminophenyl)-3-ethylpiperidine-2, 6-dione (AGT), is used as an aromatase inhibitor for the treatment of advanced breast cancer and Cushing's syndrome. According to Biopharmaceutics Classification System, it is a class II drug with low water solubility but having good permeability. Cyclodextrins are known to be the good host molecules to accommodate molecules with suitable dimensions to produce inclusion complexes and to increase the solubility. This work tries to explain the feasible inclusion of the drug molecule inside the  $\beta$ -Cyclodextrin molecule with 1:1 stoichiometric ratio. The inclusion complex was characterised by means of various thermodynamic as well as spectroscopic studies. The In Vitro Cell Viability Study was performed and found the inclusion complex to be less toxic at higher concentration compared to the normal drug molecule.

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## PP-13

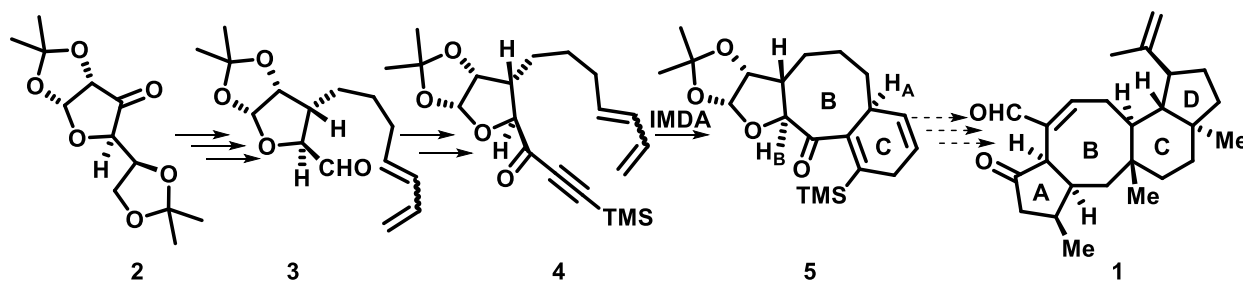
### Construction of Fused Bicyclic 8/6 Ring System of Variecolin Using Intramolecular Diels-Alder Approach

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Variecolin **1** is a sesterterpene isolated from fermentation of *Aspergillus varicolor* MF138.<sup>[1]</sup> It possesses several significant bioactivities such as it is an angiotensin II receptor binding inhibitor, anti-hypertensive agent and suppressor of splenic lymphocytes proliferation induced in mice.<sup>[1,2]</sup> Structurally variecolin is a tetracyclic compound with multiple asymmetric centers and a fused bicyclic 8/6 ring system present at the center. A number of elegant strategies have been developed.<sup>[3]</sup> However, no total synthesis of variecolin has yet been reported.



Scheme 1: Synthesis of Fused Bicyclic 8/6 Ring System

Intramolecular Diels-Alder (IMDA) reaction is one of the most useful tools chemist frequently used for construction of fused bicyclic ring systems.<sup>[4]</sup> Considering this we developed a synthetic approach for the construction of fused bicyclic 8/6 ring system of variecolin employing IMDA reaction. The synthesis is started with the sugar derivative **2** and prepared the IMDA precursor trienone **4** via the diene derivative **3**. Compound **4** was heated in toluene to obtained the fused bicyclic 8/6 ring system. The results of this study will be presented.

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## **PP-14**

### **Title: Design and Synthesis of Cu(II) and Zn(II) Complexes of a Quinoline Based Flexible Amide Receptors as Fluorescent Probe for Dihydrogen Phosphate and Hydrogen Sulphate and Their Antibacterial Activity**

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Quinoline based amide receptor has been designed and synthesized from oxine. The Cu(II) and Zn(II) complexes of the fluorescent receptors have also been synthesized from the amide receptor for the recognition of anions. All the synthesized compounds were fully characterized by spectroscopic technique. Between the Cu(II) and Zn(II) complexes, the later one shows better selectivity towards anions, *viz.* dihydrogen phosphate and hydrogen sulphate as their tetrabutylammonium salts in acetonitrile-water (9:1 *v/v*). Cu(II) complex also binds anions better compared to amide ligand, but with less selectivity. Both the metal complexed receptors show broad spectrum anti-bacterial activity being effective against both gram-positive and gram-negative bacteria. However, Zn(II) complexed receptor is more potent than Cu(II) complexed receptor having lower MIC value against both the bacteria.

**Keywords:** Anion recognition, Cu(II) complex, Zn(II) complex, Fluorescent sensor, Anti-bacterial activity, MIC value.

#### **References:**

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## PP-15

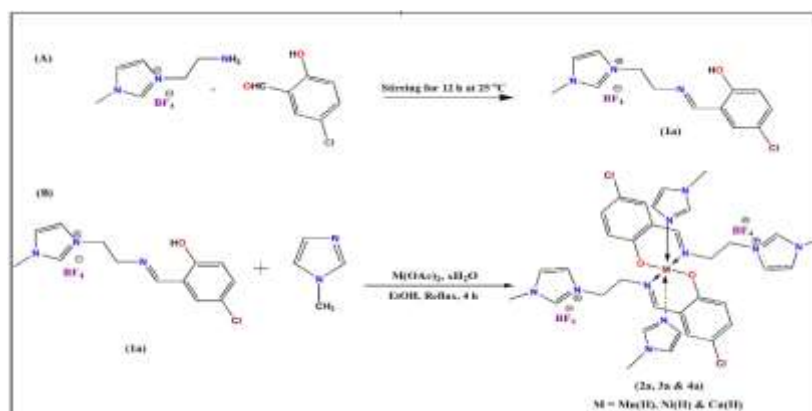
# Mn(II), Ni(II), Cu(II) mixed ligand complexes derived from *environmental affable* Ionic liquid-supported Schiff base and 1-methyl imidazole : Spectroscopic studies and Antimicrobial evaluation

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Mixed ligand Mn(II), Ni(II), Cu(II) complexes with the ionic liquid-supported Schiff base (primary ligand) and 1-methyl imidazole (secondary ligand) and were synthesized and characterized by various spectroscopic and analytical methods. Antimicrobial activity of the mixed ligand complexes with respect to the Schiff base against two gram positive (*Staphylococcus aureus* and *Bacillus cereus*) and two were gram negative (*Escherichia coli* and *Klebsiella pneumoniae*) were conducted to assess their antibacterial activities. The Schiff base along with the mixed ligand complexes exhibited very significant responses. The maximum inhibition zone was produced by Ni(II) complex while the minimum inhibition zone was produced by Cu(II) complex in plates of *Staphylococcus aureus*.



**Keywords:** Mixed ligand complexes, imidazole, ionic liquid supported Schiff base, Antimicrobial Studies.

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## **PP-16**

### **Investigation of Molecular Interactions between Amino Acids and Ionic Liquid in Aqueous Media at Various Temperatures: A Comparative Physicochemical and Theoretical Study**

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Physicochemical studies including density, viscosity and refractive index at four different temperatures of two neutral amino acids namely L-Alanine & L-Isoleucine in an aqueous ionic liquid Benzyltriethylammonium chloride (BTEAC) have been studied to explore the molecular interactions prevailing in the solution media. The strong solute-solvent interaction existed in the solution have been ascertained with the help of some derived parameters such as the limiting apparent molar volume ( $\phi_V^0$ ), viscosity  $B$ -coefficient and limiting molar refraction ( $R_M^0$ ) obtained from Masson equation, Jones-Doles equation and the Lorentz-Lorenz equation respectively. Hepler's method and positive value of  $(dB/dT)$  data suggest that both the solutes (amino acids) are structure-breaking (chaotropic) in nature. The solute-solvent interaction between L-Isoleucine and BTEAC is found stronger than that between L-Alanine and BTEAC according to the investigation. Additionally, Density functional theory (DFT) helps to evaluate the adsorption energies, electrostatic potential maps (ESP) and reduced density gradient plots which also authenticate the experimental findings.

**Keywords:** Benzytriethylammonium chloride; L-Alanine; L-Isoleucine; physicochemical studies; Density functional theory.

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## **PP-17**

### **Performance-based designing of organic polymeric additives for waxy crude oil**

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Crude oil, whether heavy, medium or lighter, is probably the biggest source of energy around the globe. But its extraction, transportation and even storage require lots of struggle due to high density, high viscosity and high pour point.<sup>1</sup> Despite such handling trouble, heavy and even extra heavy crude oil has attracted much attention due to the limited and declining source of medium or light oil. Variety of studies have been performed to tackle these problems from thermal treatment to dilution method and most commonly addition of chemicals as pour point depressants (PPDs), viscosity reducers and extreme–pressure additives.<sup>2</sup> But still it is a challenging aspect of this research area to find out the minimum dosage of the additives with maximum efficiency. Properly designed organic polymers have attracted much attention as efficient chemical additive such as ethylene-co-vinyl acetate, poly (ethylene-butene), polymethacrylates, and modified maleic anhydride copolymers. Homo polymer of decyl methacrylate and its copolymers with styrene and vinyl acetate separately have been successfully evaluated as effective pour point depressant (PPD) for crude oil. Moreover polymer blending is an economic and easy process to develop better polymeric materials with higher thermal and mechanical stability. Polymer blend of two copolymers viz. vinyl acetate-octyl acrylate and dodecyl acrylate-methyl methacrylate showed promising results in terms of viscometric parameters, pour point and shear stability index in crude oil. Ionic liquids (ILs) are the new addition in this area which has got enough potential to be emerged out as an effective, environment friendly multifunctional additive.

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## **PP-18**

### **Investigation on the Minimization of Side Effects of Food Preservatives in Human Body**

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An analysis on the diverse molecular interactions of implausible food preservatives, Sodium benzoate (SBz), Sodium salicylate (Scyt) in the aqueous solutions of Benzyltriethylammonium chloride (BTEACl), Benzyltrimethylammonium chloride (BTMACl) having durable anti-bacterial effect have been explored thoroughly by various physicochemical methodologies such as Density, Refractive index, Viscosity, Electrical conductivity, at five different temperatures ranging from 298.15 K to 318.15 K. Antibacterial as well as the anti-fungal effects of the ternary mixtures, (BTEACl+SBz+H<sub>2</sub>O), (BTEACl+Scyt+H<sub>2</sub>O), (BTMACl+SBz+H<sub>2</sub>O) and (BTMACl+Scyt+H<sub>2</sub>O) were further analysed for better results and found to act synergistically below the MIC of both the food preservative, thus minimises the hazardous threat, caused by unnecessarily excessive consumption of food preservatives. Association constants governed by diverse intermolecular interactions in the solution phase were studied by UV-vis spectroscopy. The genesis of diverse interactions was exposed by measurement of the apparent molar volume ( $\Phi_v$ ), limiting apparent molar volume ( $\Phi_v^\circ$ ), molar refraction ( $RM$ ), limiting molar refraction ( $R^\circ M$ ) viscosity B coefficients and reveals as strong solute-solvent interaction, over the solute solute and solvent-solvent interactions.

#### **References:**

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## **PP-19**

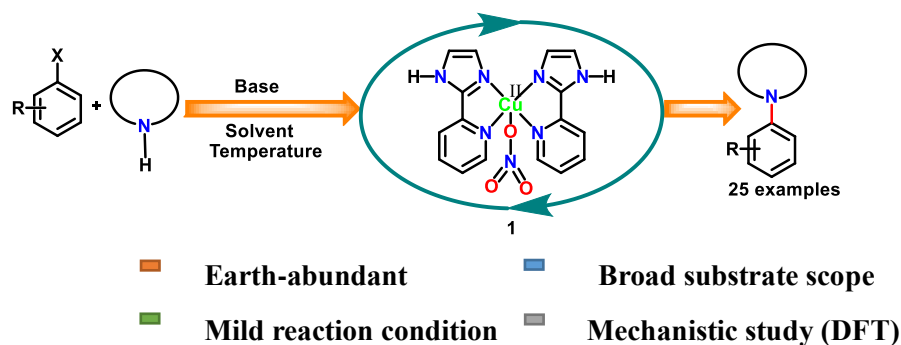
# An Efficient 2-(2-pyridyl)imidazole Based Copper Catalyst for N-Arylations with Aryl-Iodides, Bromides and Chlorides

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Arylated amines have their presence in a wide range of pharmaceuticals, agrochemicals, natural products and organic materials exhibiting exceptionally broad application.<sup>1</sup> The most common classical routes for N-arylation are the copper salt mediated Ullmann–Goldberg reaction.<sup>2</sup> However, this reaction often suffers from harsh reaction condition such as high temperature (>200 °C), use of stoichiometric amount of copper salts, moderate yields and long reaction times.<sup>3</sup> These limitations can be overcome by introducing bidentate chelating ligands.<sup>4</sup> Till date, the most general and efficient Cu-catalyst is 1,10-phenanthroline based complex. To increase the efficiency of these type of catalytic systems, instead of 1,10-phenanthroline ( $L^1$ ) we have used 2-(2-pyridyl)imidazole ( $L^2$ ). The combination of  $Cu(NO_3)_2$  and  $L^2$  leads to the formation of pentacoordinated complex of the type  $[CuL^2_2(NO_3)](NO_3)$ , (**1**) which was characterized by spectroscopically, structurally and electrochemically. The complex **1** is more electronically rich than corresponding  $L^1$  based complex  $[CuL^1_2(NO_3)](NO_3)$ , (**2**) and observed a quasireversible reduction at relatively higher potential ( $E_{1/2} = -0.19$  V with respect to Ag/AgCl) compared to **2**. In N-arylation of nitrogen heterocycles, the complex **1** shows excellent catalytic activity with aryl-iodides, -bromides and even with less reactive -chlorides (scheme 1). A wide spectrum of the common organic functional groups are tolerated in the present catalytic reaction. In addition, a mechanistic cycle of this **1** catalysed N-arylation reaction has been explored on the basis of spectroscopic (UV-Vis,  $^1H$  NMR, EPR) results and DFT calculations.



Scheme 1. Copper catalyzed N-arylation reaction.

## PP-20

### Drug Repurposing against Monkeypox Virus using Computational Approaches

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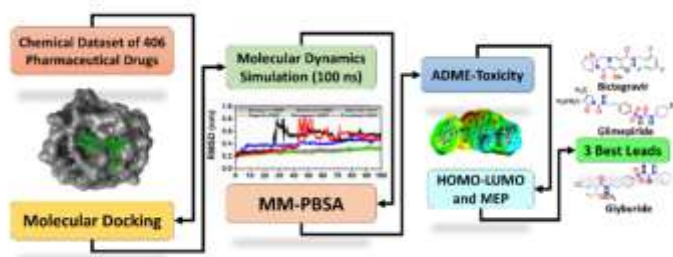
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Monkeypox virus (MPXV) is considered as zoonotic disease with characteristics comparable to smallpox. The disease was confirmed in May 2022 as a global epidemic concern. Tecovirimat, an antiviral drug, was approved by the US Food and Drug Administration (FDA) for MPXV. The aim of this work was to repurpose approved pharmaceutical drugs as potential inhibitors of MPXV. In this study, molecular docking was performed on 406 pharmaceutical drugs, and results were compared with reference tecovirimat. Results showed that seven compounds, bicitegravir, glimepiride, glyburide, lasmiditan, olaparib, rimegepant, and ubrogepant, have satisfied higher negative binding energies compared to the reference. These best hits were further assessed by 100 ns molecular dynamics simulation, and the best results were observed for bicitegravir, glimepiride, glyburide, olaparib, and ubrogepant. The docking analysis was further validated by molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) binding free energy calculations. In addition, pharmacokinetics and density functional theory (DFT) studies were also discussed for these best hits. In conclusion, three compounds, bicitegravir, glimepiride, and glyburide, have satisfied all the criteria for better leads against MPXV.

**Keywords:** Monkeypox virus, drug repurposing; molecular docking; molecular dynamics simulation; DFT, pharmacokinetics.



#### Reference:

1. Sarkar K, Das RK. Repurposing of Existing Pharmaceutical Drugs Against Monkey-pox Virus: An In Silico Study. *Analytical Chemistry Letters*. 2022 Nov 2;12(6):655-70.

## **PP-21**

### **Influence of ortho group in rhodamine B hydrazide based Schiff base for selective recognition of Cu<sup>2+</sup> and Fe<sup>3+</sup> ions: A mechanistic approach by DFT and colorimetric studies**

Kingkar Ghosh, Subrata Basak, Mintu Thakur, Ratan Das and Kinkar Biswas\*

Our work is to find the best way to use the new age computational approach in designing sensor molecules for the selective recognition of Cu<sup>2+</sup> and Fe<sup>3+</sup> ions. Seven rhodamine B hydrazide-based Schiff base derivatives were designed and analyzed their chemosensing properties against Cu<sup>2+</sup> and Fe<sup>3+</sup> ions in ethanol solution theoretically. The theoretical calculations revealed that the selective recognition of Cu<sup>2+</sup> and Fe<sup>3+</sup> ions takes place via spirolactam ring-opening and there is a pivotal role of ortho substituents and N-heteroatoms. The two best chemosensors were synthesized and used for the detection of Cu<sup>2+</sup> and Fe<sup>3+</sup> ions by colorimetric methods. This methodology will definitely help to reduce the chemical consumption in the entire in the entire process and dose follow the basic principles of Green Chemistry. In recent days the new age computational chemistry may be an important tool or play a pivotal role in Green Chemistry research.



## PP-22

### **A coumarin151-derived chemosensors for rapid and sensitive detection of a sarin surrogate, diethylchlorophosphate**

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A coumarin151-derived electron donor-acceptor-based chemosensor has been designed and developed for the selective detection of sarin surrogate diethylchlorophosphate (DCP) in solid, solution, and gas phases, respectively [1]. A ratiometric UV-visible absorption spectral change with a colorimetric change from yellow to colorless is observed in the presence of DCP. A visual cyan color could be seen under 365 nm UV light irradiation, which is also well supported by the color chromaticity diagram. The sensitivity of chemosensor toward the detection of DCP can be possible down to the nanomolar (nM) range from aqueous to the non-aqueous medium. Further, a paper strips-based test kit has been fabricated for the practical utility of the present chemosensor to identify a trace amount of DCP under the stockpiles of related analytes. Also, the dip-stick experiment has been demonstrated for the selective detection of DCP vapor. This turn-on chemosensor has a potential application as a moveable kit for sensing DCP vapour with high sensitivity. The performance of chemosensor toward the DCP proved that it could be exploited as a signal tool for environmental and biological sample analysis.

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**PP-23**

**ULTRASOUND ASSISTED SOLVENT FREE SYNTHESIS OF 1-HYDROXY 1H-IMIDAZOLE 3-OXIDE ON SILICA SUPPORT**

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'Nitrene like' azaheterocycle 1H-imidazole 3-oxides are found to have diverse application in various reactions since it is a valuable synthetic intermediate for the preparation of imidazole based heterocyclic compounds. Many imidazole N-oxides are also found to be potentially biologically active. Thus, we obtained these valuable compounds through ultrasound irradiation which provides higher yield in relatively shorter reaction time- almost 35-fold faster than the conventional method. The reactions were performed at room temperature and under solvent free condition. The simple work up procedure without any tedious purification makes our method a suitable alternative to desirable hydroxy imidazole N-oxide. The reactions are performed on solid silica support, which is inexpensive and reusable and can be easily handled and separated from the reaction mixture, which also contributes to make reactions cleaner, faster and higher yielding.

**Keywords:** Imidazole N-oxides, sonochemistry, silica support, ultrasound, hydroxy imidazole

## **PP-24**

### **A Benzoxazole-based Turn-on Fluorosensor for Rapid and Sensitive Detection of Sarin Surrogate, Diethylchlorophosphate**

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Organophosphorus (OP)-based nerve agents are extremely poisonous. They are too reactive, highly toxic, easy to prepare, and accessible in nature. [1] A benzoxazole-based fluorosensor (**IMP**) has been synthesized and employed for the selective and sensitive detection of sarin surrogate, diethylchlorophosphate (DCP) in solution, and gas phase, respectively. Remarkable turn-on fluorescence is observed due to the introduction of DCP in the solution of **IMP** because of inhibition of the intramolecular charge transfer process and disruption of the excited state intramolecular proton transfer (ESIPT) mechanism. The synthesized **IMP**-based fluorescence sensor exhibits excellent selectivity, high sensitivity, and a wide linear range of 15–60  $\mu\text{M}$  with a detection limit of 44 nM. Low-intense to highly intensified visible violet color could be seen by the naked eye under a portable 365 nm UV lamp due to the addition of DCP in the solution of **IMP**. **IMP**-stained paper strips-based test kit experiment has been demonstrated to detect traces of DCP in stockpiles of related analytes. A dip-stick experiment for the detection of DCP vapor has also been demonstrated. The effectiveness of **IMP** in detecting DCP established that it might be used as a signal tool for real sample analysis. The details experimental result of our findings will be discussed.

#### **Reference**

- [1] R.T. Delfino, T.S. Ribeiro, J.D. Figueroa-Villar, Organophosphorus compounds as chemical warfare agents: A review, *J. Braz. Chem. Soc.* 20 (2009) 407–428. <https://doi.org/10.1590/S0103-50532009000300003>.

## **PP-25**

# Catalytic Fate of Structurally Characterized Manganese(III)-Salen Complexes towards an Efficient Transformation of Primary Amide to Amine

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A convenient and selective hydrosilylative transformation of chemically inert primary amides (26 examples) into the corresponding primary amines with key functional group tolerance has been developed by using simple well-defined O,N,N,O donor salen based earth abundant manganese(III) complexes under mild condition (Scheme1). On a slight modification of the reaction condition by adding the blocking agent secondary amide, the transformation of primary amides to amines stops in the intermediate nitrile state (9 examples). The same catalyst has also the capability to reduce nitriles to amines (15 examples) using inexpensive silane such as polymethylhydrosiloxane (PMHS). Mechanistic studies and DFT calculations are also carried out to understand the reaction mechanism and chemoselectivity. In this catalytic transformation, the manganese catalyst activates the primary amides and the overall reduction proceeds *via* the dehydration of the primary amides into the corresponding nitriles which are then reduced into the corresponding primary amines. The present transformation has great importance in the synthesis of primary amines and nitriles which are used as a key building blocks for the preparation of various important pharmaceutical products, agrochemicals, dyes, pigments, plastics, surfactants, and various fine chemicals.<sup>1-4</sup>



**Scheme 1.** Transition metal-catalyzed hydrosilylative transformation of primary amides to amines.

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## **PP-26**

### **Castor oil based eco-friendly lubricating oil additives**

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The addition of chemical additives in lubricating oil also called lube oil is essential for smooth functioning of modern engine. Lubricants (a combination of additive and lube oil) are generally liquids or semi-liquids which are used to lubricate the automotive engine for their longevity and better performances. The key functions of a lubricant are to keep moving parts apart, reduce friction, protect against wear, transfer heat, prevent rust and corrosion, as antioxidant, as detergents/dispersants etc. The acrylate/vinyl acetate based lubricants exhibit satisfactory performance but they are not environmentally benign. The research on vegetable oils as base stocks or their derivatives as additives for base stocks is increasing significantly due to their biodegradable property and availability in nature. Moreover, they show excellent antiwear properties; enhanced extreme pressure (EP) additives performance; high viscosity index and low volatility. There are lots of research papers where chemically modified vegetable oils have been used as additive for base oil or base stocks in the formulation of bio-lubricant. Castor oil is widely used in different fields such as lubricants, pharmaceuticals, paints, adhesives, rubber, cosmetics, etc. The high flash point and the presence of polar hydroxyl group of castor oil make it efficient in candidate for the synthesis of additives for lubricating oil as well as bio lubricant. However research articles regarding the application of castor oil or its copolymer as lubricant are very scanty. Therefore, in this work we have synthesized homopolymer of castor oil and copolymer of it with styrene in different percentage ratios to get thermally stable, cost effective as well as eco-friendly lubricant additives. Styrene was chosen because the incorporation of it enhances the thermal stability of lubricant. Performance evaluation of the prepared polymeric additives was carried out as viscosity index improver, pour point depressant and antiwear additive according to respective ASTM method.

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## **PP-27**

### **A Combined Experimental and Theoretical Study on *p*-Sulfonatothiacalix[4]arene Encapsulated Sulisobenzene**

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Sunscreen ingredient has the tendency to degrade when exposed to UV-radiation which becomes major problem for their further development and application in cosmetic industry. Host-guest inclusion complexation could be a promising strategy to address this issue. New inclusion system of sunscreen agent Sulisobenzene (SBZ) with macrocyclic host *p*-sulfonatothiacalix[4]arene (TSC4X) was fabricated, and its binding behaviour both in solution and solid states has been investigated by UV-visible spectroscopy, <sup>1</sup>H NMR, DSC, ESI-MS and FT-IR spectroscopy. The 1:1 stoichiometry of the inclusion complex was confirmed by Job plot and mass spectrometry. TSC4X displayed strong affinity for SBZ and the binding process was found to be thermodynamically feasible. FT-IR and <sup>1</sup>H NMR spectroscopic studies demonstrated that the unsubstituted aromatic moiety of SBZ is inserted into the cavity of TSC4X, which is in accordance with the molecular docking study. The aqueous solubility, photostability and thermal stability of SBZ were improved on complexation with TSC4X. The molecular docking study depicted the most feasible conformation of inclusion complex with lowest binding energy. In conclusion, SBZ-TSC4X supramolecular hybrid would enable the investigation of its applications as highly photo-stable sunscreen agent for cosmetic industry.

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## **PP-28**

# Synthesis and Crystal Structure of two copper complexes of 4-substituted benzoic acid and 1, 10 phenanthroline

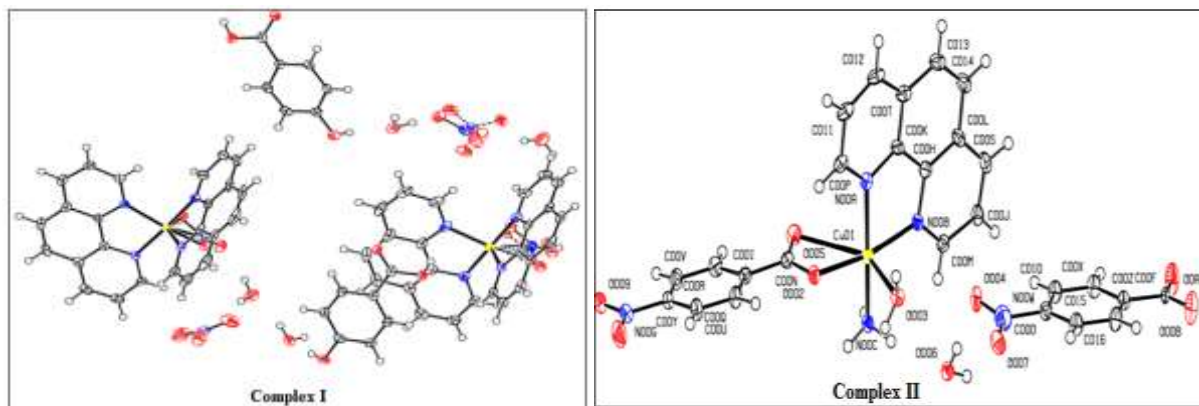
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Two copper (II) complexes of 4-substituted benzoic acid derivatives (namely 4-hydroxybenzoic acid and 4-nitrobenzoic acid) and 1, 10 phenanthroline (I and II) have been synthesized by conventional method. The synthesized complexes have been characterized different analytical and spectroscopic techniques. Suitable crystals for single crystal analysis of the synthesized complexes were collected by the slow evaporation of mother liquor. From the x-ray single crystal analysis (MoK $\alpha$  = 0.71703 Å) it was revealed that the complex (I) crystallizes in monoclinic crystal system with space group P21/c with cell parameters a = 17.4339(1) Å, b = 21.5979 (14) Å, c = 16.5129 (10) Å,  $\alpha^\circ = 90$ ,  $\beta^\circ = 102.828(2)$ ,  $\gamma^\circ = 90$ , V = 60625 (7) Å<sup>3</sup>, and Z = 12. Complex (II) crystallizes in triclinic crystal system with P-1 space group having cell parameters a = 5.5805(4) Å, b = 14.5748 (11) Å, c = 16.2220 (12) Å,  $\alpha^\circ = 95.250$ ,  $\beta^\circ = 92.187(2)$ ,  $\gamma^\circ = 98.646(2)$ , V = 1297.14 (7) Å<sup>3</sup>, and Z = 2. The FT-IR spectra of the complexes (I and II) suggested that the benzoic acid derivatives co-ordinate to the metal centre via bi-dentate fashion utilizing both the oxygen atom of carboxylic group in complex (II) but in complex (I) it has been observed that the carboxylic acid group did not co-ordinate with the metal centre rather they remain as a solvate in the crystal packing.



**Keywords:** p21/c, Copper (II) complex, 4-nitrobenzoic acid, 4-hydroxybenzoic acid, 1, 10 Phenanthroline,

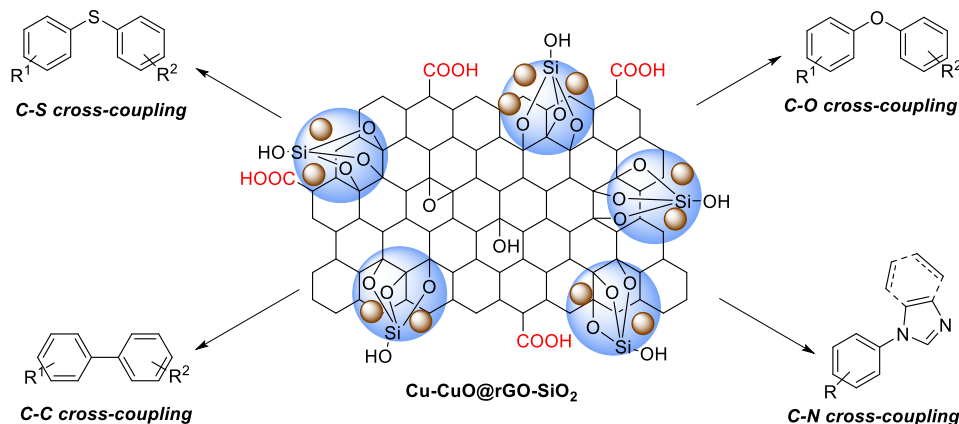
**Cu-CuO@rGO-SiO<sub>2</sub>: A versatile catalyst for multifarious cross-coupling reactions**

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Graphene oxide silica (GO-SiO<sub>2</sub>) has been selected as a heterogeneous solid support for the immobilization of copper and copper oxide species. This ternary nanocomposite (Cu-CuO@rGO-SiO<sub>2</sub>) has been characterized in detail by various spectroscopic and microscopic techniques. The powder X-ray diffraction (PXRD) patterns and X-ray photoelectron spectroscopy (XPS) indicated the presence of Cu and CuO nanoparticles in rGO-SiO<sub>2</sub> matrix. Moreover, the TEM images indicated the homogeneous distribution of Cu and CuO species having average particle size in the range 5-10 nm on the rGO-SiO<sub>2</sub> surface. The nanocomposite has been employed as a versatile catalyst for C-S, C-C, C-O and C-N cross-coupling reactions (Scheme 1). The catalyst exhibited superior catalytic activity and the products were obtained in good to excellent yields. Furthermore, the recyclability of the catalyst has been checked for four consecutive cycles without any significant drop in the yield of the product.



**Scheme 1:** Cu-CuO@rGO-SiO<sub>2</sub> catalyzed C-S, C-O, C-N and C-C cross-coupling reactions.

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## DNA Binding and DNA Cleavage Activities of Newly Synthesized Co<sup>II</sup> and Cu<sup>II</sup> Complexes of a $\beta$ -Cyclodextrin Based Azo-Functionalized Schiff Base

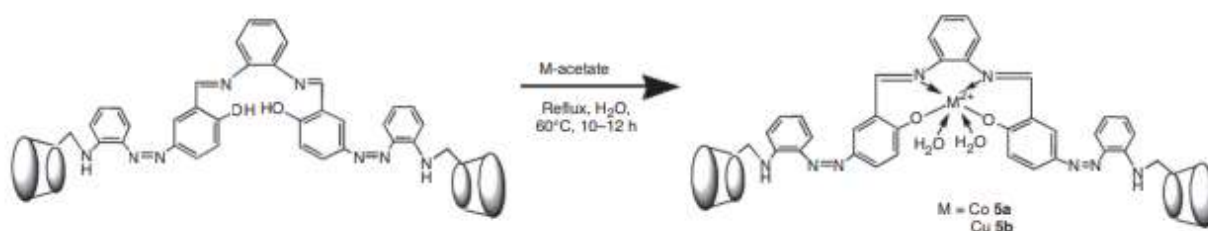
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Of late, there has been an increasing fascination for the development of transition metal complexes of Schiff bases with diverse densities and structures, because such complexes may interact and cleave DNA and thus, they may find potential applications in the field of pharmaceuticals for cancer therapy and in molecular biology, etc. But Schiff base metal complexes are mostly insoluble in aqueous solution and aqueous solubility is a prerequisite for availability in bio-fluids (bio-availability). Therefore, a water-soluble complex with Co<sup>II</sup> and Cu<sup>II</sup> ions were synthesized using a novel  $\beta$ -cyclodextrin based azo functionalized Schiff base as a ligand. The Schiff base and its metal complexes were characterized by different physico chemical and spectroscopic methods. From the analyses of the experimental data, distorted octahedral geometry has been assigned for both the metal complexes. The binding interactions between the metal complexes and DNA were investigated by means of a thermal denaturation study and viscosity measurements as well as by electronic absorption and fluorescence spectroscopy. These studies revealed that both the metal complexes followed an intercalative mode of



binding to calf thymus (CT)-DNA and also effectively cleaved the supercoiled pBR DNA.

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## PP-31

### **Multi-component reactions involving barbituric acid, urea and aldehyde in presence of yttrium nitrate as lewis acid: study molecular docking against protein tyrosine kinase**

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We have reported an efficient Yttrium nitrate catalyzed one pot three component reactions involving barbituric acid, urea and aldehyde to produce simple Biginelli product and in some cases with spirofused heterocycle product. The reaction occur in a green solvent ethanol:water (10:1). Depending upon the reactivity of aldehydes there are possible formation of either normal biginelli product or oxidized form of Biginelli product or *spiro* compound. The reaction was very simple, easy to product isolation and excellent yield of product. All of the synthesized products (1a-1b, 2a-2c, 3c) were characterized by spectroscopic methods. Molecular docking was used to predict the binding energy (-9.1 kcal/mole) and binding interaction between the compound (E)-5-styrylpyrimido[4,5-d]pyrimidine-2,4,7(1H,3H,8H)-trione (2c) and tyrosine protein kinase (PDB Code: 1AD5).

**Keywords:** Biginelli reaction, spirofused-heterocycle, multi component reaction, Yttrium nitrate, Green catalyst, Molecular Docking.

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**A PET and ESIPT-communicated Ratiometric, Turn-on Chromo-fluorogenic Sensor for Rapid and Sensitive Detection of Sarin gas Mimic, Diethylchlorophosphate**

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Fast and precise identification of toxic G-series nerve agents in the solution and vapor phase is urgently needed to save human beings from unwanted wars and terrorist attacks, which is challenging to execute practically. [1] In this article, we have designed and synthesized a sensitive and selective phthalimide-based chromo-fluorogenic sensor, **DHAI**, by a simple condensation process that shows ratiometric and turns on chromo-fluorogenic behavior towards Sarin gas mimic diethylchlorophosphate (DCP) in liquid and vapor phases, respectively. A colorimetric change, from yellow to colorless, is observed in the **DHAI** solution due to the introduction of DCP in daylight. A remarkable cyan color photoluminescence enhancement is noticed in the presence of DCP in the **DHAI** solution, which is observable to the naked under a portable 365 nm UV lamp. The mechanistic aspects of the detection of DCP by employing **DHAI** have been revealed by time-resolved photoluminescence decay analysis and <sup>1</sup>H-NMR titration investigation. Our probe **DHAI** exhibits linear photoluminescence enhancement from 50-400 μM with a detection limit of 69 nM. For practical utility, a **DHAI**-stained test kit employing Whatman-41 filter paper has been fabricated and used as a portable and displayable photonic device for on-site detection of Sarin gas surrogate, DCP. Also, a dip-stick experiment has been demonstrated to identify the vapor of Sarin gas mimics DCP colorimetrically and fluorometrically. The concentrations of DCP in various water samples have been evaluated with the help of a standard fluorescence curve for real sample analysis.

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**Volumetric and viscometric study of caffeine in aqueous D-sorbitol solutions**

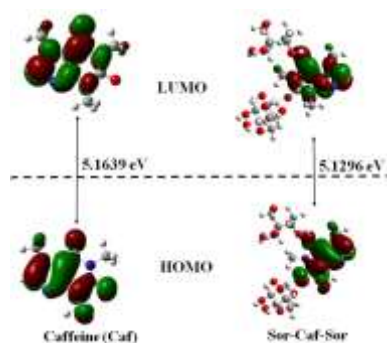
Sachindra Kumar Singh<sup>1</sup>, Debadrita Roy<sup>2</sup>, Somanika Basu<sup>2</sup>, Tanmoy Dutta<sup>3</sup> and Biswajit Sinha<sup>2,\*</sup>

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Densities, viscosities, and refractive indices of caffeine in various molal concentrations of aqueous d-sorbitol solution,  $m = (0.005-0.020)$  mol kg<sup>-1</sup> of d-sorbitol, were measured at  $T = (298.15-318.15)$  K and pressure  $P = 101$  kPa. A number of derived characteristics have been determined from the measured data including apparent molar volume, standard partial molar volume, slope, apparent specific volumes, standard isobaric partial molar expansibility and its temperature dependence, viscosity B-coefficient, solvation number and others. These findings were used to calculate the standard volume of transfer and viscosity B-coefficient of transfer for caffeine from water to aqueous d-sorbitol solutions in order to explain a variety of interactions in the ternary solutions. In terms of solute-solvent and solute-solute interactions, the effects of molality, solute structure, temperature, and taste behaviour were examined. These findings showed that caffeine acts as a structure maker and that solute-solvent interactions dominate the characteristics of the ternary solutions. Further, bond length changes due to interaction between d-sorbitol and caffeine, molecular electrostatic potential maps, Mulliken charge distribution, *etc.*, were also studied theoretically.



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**Synthesis, characterization and *in vitro* anticancer activity of 3-(1,3-dioxoisindolin-2-yl)-N,N-dimethyl propan-1-aminium perchlorate**

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2-(3-(Dimethylamino)propyl)isoindoline-1,3-dione (**DAPID**) has been synthesized and utilized to produce 3-(1,3-dioxoisindolin-2-yl)-N,N-dimethyl propan-1-aminium perchlorate (**DIDAP**). Both **DAPID** and **DIDAP** were characterized using different spectroscopic techniques. Structure of the **DIDAP** has been determined using single crystal X-ray diffraction technique. **DIDAP** found to self assemble in a helical motif in its supramolecular structure with the aid of different hydrogen bonding,  $Cg \cdots Cg$  and short interatomic contacts in the solid state. The compound **DIDAP** exhibited anticancer activity against the human hepatomas cell line (Hep G2) and the activity was further complemented by performing docking study. In addition, the computational studies have also been performed to examine the chemical reactivity of the compound. *Shape index* and *Curvedness* surfaces indicated  $\pi$ -stacking with different features in opposed sides of the molecule. Fingerprint plot showed  $C \cdots C$  contacts with similar contributions to the crystal packing in comparison with those associated to hydrogen bonds. Enrichment ratios for  $H \cdots H$ ,  $O \cdots H$  and  $C \cdots C$  contacts revealed a high propensity to form in the crystal.

**Keywords:** DAPID, DIDAP, anticancer activity, DFT.

**References:**

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## Synthesis, Physico-chemical Characterisation and Theoretical Study of some 2,4,5-triaryl imidazole derivatives

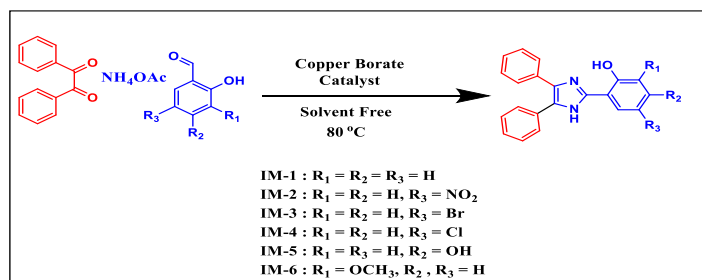
Sailesh Chettri<sup>a</sup>, Biswajit Sinha<sup>b</sup> and Dhiraj Brahman<sup>a\*</sup>

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A series of six 2, 4, 5-triarylimidazole (IM-1 to IM-6) have been prepared by the multi-component condensation reaction of benzil, substituted salicylaldehyde and ammonium acetate under solvent free condition utilizing inexpensive and unconventional CuB<sub>4</sub>O<sub>7</sub> catalyst. The synthesized 2, 4, 5-triarylimidazole derivatives have been characterized by different analytical and spectroscopic techniques. Furthermore, DFT studies such as optimization of gas phase structure, HOMO-LUMO energies, Molecular electrostatic potential, nonlinear optical properties of the synthesized compounds have been investigated. In-silico molecular docking study of the synthesized 2, 4, 5-triarylimidazole derivatives (IM-1 to IM-6) have been carried out to ascertain the inhibitory potential of these molecules against the diabetic protein (PDB ID 1IR3). The molecular docking study showed that the studied compounds have significant inhibitory potential against the protein 1IR3 and the binding energy ( $\Delta G$ ) values of the compounds (IM-1 to IM-6) against the protein 1IR3 found to be -8.7 Kcal/mole, -8.4 Kcal/mole, -8.8 Kcal/mole, -8.0 Kcal/mole, -8.9 Kcal/mole and -7.8 Kcal/mole respectively. In addition, the pharmacokinetic properties (ADMET) of the compounds (IM-1 to IM-6) have also been studied.



**Key words:** 2,4,5-Triaryl imidazole, Benzil, Copper Borate, DFT, FT-IR, In-Situ, 1IR3, Lipinski rule, Pharmacokinetic (ADMET) study.

## PP-36

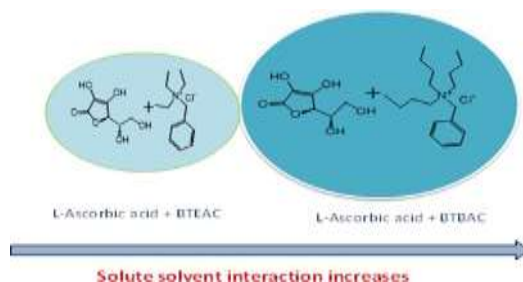
### Exploring Diverse Interactions of Some Ionic Liquids in Aqueous Vitamin-C with the Manifestation of Solvation Consequences

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By identifying the physicochemical parameters; density, viscosity, refractive index, conductivity and surface tension the nature of interaction prevailing in L- Ascorbic acid with two different aqueous ionic liquid solutions named as Benzyltributyl ammonium chloride and Benzyltriethyl ammonium chloride have been studied. The existence of plausible intermolecular interactions in the ternary solution have been evaluated on the basis of apparent molar volume, viscosity A and B co- efficient, molar refraction investigating at four different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K and variation of three different concentration 0.001m, 0.003m and 0.005m. The solute-solvent interaction has enhanced with increasing the concentration of solute and also with increasing temperature and the vitamin shows structure breaking activities in both ionic liquid solutions. All these concepts are well established by the limiting apparent molar volume obtained from Masson equation, viscosity parameters A & B co-efficient from Jones-Doles equation, and molar refraction value from the Lorentz-Lorenz equation. The values of specific conductance( $\kappa$ ) help to assure the ionic nature of the system. According to the result of studied investigations, L-Ascorbic acid and Benzyltributyl ammonium chloride interactions are more predominant over L-Ascorbic acid and Benzyltriethyl ammonium chloride interactions.



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**Self-Assembly of Octyl-2-acetoxybenzoate@ $\beta$ -CD to Reversible Thermoresponsive  
Supramolecular Nanotube**

Sayannita Das, Sahiba Khatun, Susama Chakraborty, Amkana Karmakar, Suraj Mandal, Amitava Mandal\*  
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Self-assembly programmed by molecular structure and guided dynamically by energy dissipation is a ubiquitous phenomenon in biological systems that build functional structures from the nanoscale to macroscopic dimensions [1]. Today nanotechnology has emerged as a new dimension of research towards the synthesis of multistage nanostructured self-assembly [2]. The present work deals with supramolecular host-guest complexation of octyl-2-acetoxybenzoate (OCASP) into  $\beta$ -cyclodextrin ( $\beta$ -CD) which spontaneously self-assembled into a thermoresponsive nanotubular architecture at a molar ratio of 1:1. The formed inclusion complex (IC) was characterized by UV-Vis, FT-IR, WAXRD,  $^{13}\text{C}$  CP/MAS NMR studies. SEM, TEM and AFM revealed the formation of nanotube with a diameter of  $\sim 50$  nm. Reversible switching of assembly and disassembly is triggered by decreasing and increasing of temperature, as is evidenced by the turbidity measurements of a 5% solution of OCASP@ $\beta$ -CD system [3]. This developed stimuli responsive system would permit tailoring of its physical properties and probably it will bring light on the fabrication of novel smart materials.

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## PP-38

### Green protocol for one-pot three-component synthesis of functionalised *N*-amino-3-cyano-2-pyridone

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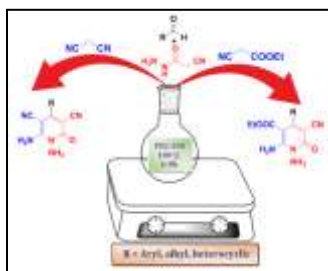
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Nowadays, interest in using green solvent during organic synthesis is multiplying day by day. Besides, one-pot multi-component reaction is a key tool for synthesis of biologically active heterocyclic compounds. MCR removes most of the drawbacks of multi-step procedures owing to its numerous advantages. Functionalised *N*-amino-3-cyano-2-pyridones reveal numerous biological activities such as analgesic, antimalarial, antitumoral, anti-HIV, anticancer, anti-inflammatory, antifungal, antibacterial, antidepressant, adhesives, dye intermediates and so on.

In this research article PEG-200, a green, biodegradable, non-toxic, economical, easily available, robust and recyclable solvent mediated one-pot three-component reaction for synthesis of diverse array of functionalised *N*-amino-3-cyano-2-pyridone having several biological and pharmaceutical activity by the simple reaction of aldehydes, cyanoacetohydrazide and malononitrile or ethyl cyanoacetate has been demonstrated. This protocol is a cascade type reaction that includes the series of Knoevenagel type condensation, Michael addition, intramolecular cyclisation, imine-enamine tautomerization and oxidative aromatization.

We have developed a straightforward and facile eco-friendly synthetic route for the synthesis of an enormous number of 1,6-diamino-4-aryl/alkyl-2-oxo-1,2-dihydropyridine-3,5-dicarbonitrile and ethyl 1,6-diamino-4-aryl-3-cyano-2-oxo-1,2-dihydropyridine-5-carboxylate derivatives using biodegradable solvent PEG-200 which execute the role of catalyst essential for these protocols devoid of using any additional catalyst or metal salt, which intensify the superiority of the protocol. The alternative of toxic, hazardous and pricey metal catalysts by a sustainable, innocuous and economical solvent is the uniqueness of this protocol.



**Structure Dependent Reactivity of Cu(II) Tetra-Pyrrolic Complexes: A Theoretical and Experimental Insight**

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Transition metals are known to exhibit varied redox properties under different ligand environment.<sup>1-2</sup> However, the structural aspects of these redox motifs under the same ligand system are yet to be explored. Likewise, the generalization of catalysts' reactivity to draw a correlation to its structure would help formulate and design an efficient catalytic system. In this context, our work demonstrates the study of different Cu(II) complexes, (**Cu1a-e**), with similar tetrapyrrolic ligand environment having variable steric and electronic attributes. Briefly, **Cu1a-c** resembles a tetrahedrally distorted Cu system about a *bis*-dipyririn ligand (**1a-c**) in comparison to **Cu1d** that holds an ideal square planar geometry with a porphyrin-based ligand (**1d**). The structural refinements of the complexes **Cu1a**, **Cu1b** and **Cu1d** were initially obtained using SCXRD and their relative stability owing to different non-covalent interactions were conducted using Hirshfeld Surface analysis. The cyclic voltammetry (CV) studies reveal irreversible nature of the redox processes with subsequent differences in their electrochemical behavior. The findings have been further supported by single point DFT calculation on these complexes which reveals ligand centric oxidation process and the relative stability of the frontier orbitals being greatly influenced by their structure. Likewise, Natural Bond Orbital (NBO) analysis and spin density calculations suggest the distribution of the metals' residual charge and spin over the ligands in these complexes. Again, the experimental rate for different organic transformations were found to be greatly influenced by the electronic and quantified steric properties of these complexes which further justifies our theoretical correlation.

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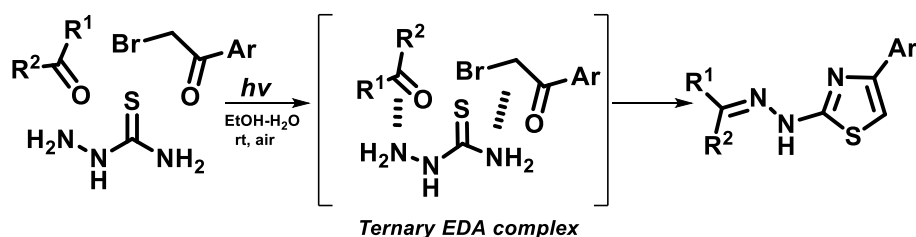
**Metal and Photocatalyst Free Visible-Light-Induced Synthesis of 2-(2- hydrazinyl)thiazole Derivatives via Formation of Ternary Electron Donor-Acceptor (EDA) Complex**

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Hydrazinyl thiazoles are a class of five-membered aromatic heterocycles frequently encountered in many natural products. The hydrazinyl thiazole moiety possesses different bioactivities viz. anti-oxidant, anti-tubercular, anti-inflammatory, anti-HIV, etc. Additionally, it is used as fluorescent chemosensors, semiconducting materials, and OLEDs. In literature, a number of methods are reported for the synthesis of this molecular scaffold<sup>[1-2]</sup> To best of our knowledge there is no report of photochemical synthesis of this molecular scaffold.



**Scheme 1:** Visible light photocatalytic synthesis of Hydrazinyl thiazole

Inspired by the global emphasis on visible light photochemistry for the development of a sustainable protocol, we developed a visible light photocatalytic strategy for the synthesis of 2-(2- hydrazinyl)thiazoles which shown in Scheme 1. The developed protocol proceeds through the formation of photo absorbing ternary EDA complex. A detailed mechanistic investigation was done to have a better understanding of the photocatalytic mechanism. In addition to this some of the synthesized compounds showed potent anti-oxidant and anti-diabetic activity. The results of this investigation will be presented.

**Keywords:** Visible light, EDA complex, Hydrazinyl thiazole

**Reference:**

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## PP-41

### **Supramolecular Chemistry–Synthesis, Characterization and Applications**

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Supramolecular chemistry is a branch of chemistry that deals with various large molecules which encapsulate relatively small molecules. This molecular encapsulation and release are extremely important in pharmacology and drug delivery science in recent years. In this intention various host molecules, such as calixarenes, pillararenes, cucurbiturils, cyclodextrins, etc. have been extensively used as excellent receptors for guest recognition. The host-guest complexes could be applied to construct stimuli-responsive supramolecular materials, where series of external stimuli, such as, enzyme activation, photo sensing, temperature dependence, changes in pH and competitive binding may be employed to operate the release of guest molecules from the inclusion complexes. Macrocyclic host molecules are of immense importance in inclusion complexes as the cyclized and constrained conformation offer the benefit of molecular selectivity. The cyclodextrins are exclusively interesting in this regard, due to their amphiphilic nature. The interest in amphiphiles comes up from their self-assembly in aqueous systems to form well defined structures, such as micelles, nanotubes, nanorods, nanosheets and vesicles, which can be applied in several grounds ranging from nano-devices, drug delivery and cell imaging. In recent times cyclodextrin modified nanoparticles are of great attention as they appreciably improve the characteristics of the assemblies, such as the electronic, conductance, thermal, fluorescence and catalytic properties improving their potential applications as nanosensors and drug delivery vehicles. Various sophisticated probes have been designed for this purpose for their applications in the manufacture of molecular switches, molecular machines, supramolecular polymers, chemosensors, transmembrane channels, molecule-based logic gates and other interesting host–guest systems.

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2. NMR, surface tension and conductivity studies to determine the inclusion mechanism: thermodynamics of host–guest inclusion complexes of natural amino acids in aqueous cyclodextrins, *New Journal of Chemistry*, **2016**, *40*, 651 – 661.

**STUDY OF MOLECULAR INTERACTIONS BETWEEN AN IONIC LIQUID  
BENZYLTRIBUTYLAMMONIUM CHLORIDE AND AMINO ACIDS L-PHENYLALANINE  
AND L-TRYPTOPHAN AT 298.15K, 303.15K, 308.15K**

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The densities, viscosities, refractive index, conductance and surface tension of L-phenylalanine and L-tryptophan in aqueous Benzyltributylammonium chloride (BTBACl) solutions have been measured at 298.15K, 303.15K and 308.15K. Apparent molar volumes and viscosity B-coefficients are obtained from these data supplemented with densities and viscosities, respectively. The limiting apparent molar volumes and experimental slopes derived from the Masson equation have been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The viscosity data have been analyzed using the Jones-Dole equation, and the derived parameters B and A have also been interpreted in terms of solute-solvent and solute-solute interactions, respectively. The structure making/breaking capacities of the solutes in the studied solvent systems have been discussed. Lorentz-Lorenz equation was used to calculate the molar refraction. The specific conductance and surface tension values also explained and supported the interaction properties.

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4. M. N. Roy, etc. Journal of Mol. Liq., 2022, 118800, <https://doi.org/10.1016/j.molliq.2022.118800>

**Application of a Copper (II) Complex Containing an Azo-Functionalized Schiff base in *In-vitro* Fungicidal, Anti-Cancer and Catecholase Activity**

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Nowadays azo-functionalised Schiff bases and their complexes grab special attention for their remarkable importance in the medicinal and pharmaceutical field besides wide use in dye and pigment industries. Focusing on their significant contribution we have designed a new Schiff base ligand and its copper(II) complex [Cu(L)<sub>2</sub>]<sub>2</sub>H<sub>2</sub>O·CH<sub>3</sub>OH] (**1**) (HL = 2-methoxy-6-((Z)-((4-((E)-phenyldiazenyl)phenyl)imino)methyl)phenol) with high catalytic activities and potential therapeutic values, here we explored the catalytic catecholase activity, the fungicidal property against *candida albicans* and the antitumor activity towards the breast cancer MCF-7 cell lines. The copper(II) complex, characterized by different spectroscopic methods along with single crystal XRD, has emerged as a bio-inspired catalyst in the oxidative transformation of 3,5-di-*tert*-butylcatechol (DTBC) to o-benzoquinone in methanol with a high turnover number,  $4.75 \times 10^2 \text{ h}^{-1}$ . Electrochemical analysis of the copper(II) complex in presence of DTBC recommends the generation of catechol/o-benzosemiquinone redox couple in the course of oxidation. The EPR spectral analysis of **1** in presence of DTBC was found silent and suggested the antiferromagnetic interaction between copper centre and benzosemiquinone species. The minimum inhibitory concentration (MIC) value against *candida albicans* was estimated as 230 µg/mL for the copper(II) complex. Under a similar experimental condition, the standard fluconazole shows the MIC value of 6.25 µg/mL. *In vitro* study of cytotoxicity of the copper complex towards the breast cancer, MCF-7 cell lines account for its excellent antiproliferative potency at 15 µg/mL for 24h. The synthesis of azo-functionalized Schiff base-copper(II) complex will certainly enrich the molecular library having copper(II) complex with important catalytic and biological activities.

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## PP-44

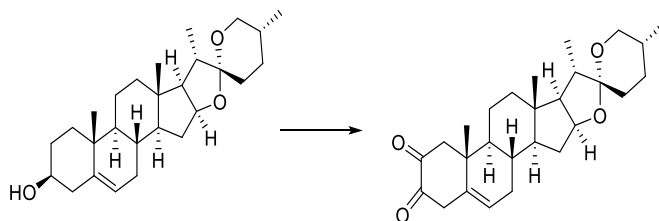
# **Phytochemical Investigation on the Medicinal Plants of Darjeeling Hills: Diosgenin and its Derivatives**

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Diosgenin (DG), a well-known steroidal sapogenin, is present abundantly in medicinal plant such as Dioscorea plant. DG is utilized as a major starting material for the production of steroidal drugs in the pharmaceutical industry. This bioactive phytochemical not only is used as an important starting material for the preparation of several steroidal drugs in the pharmaceutical industry, but has revealed also high potential and interest in the treatment of various types of disorders such as cancer, hypercholesterolemia, inflammation, and several types of infections. Due to its pharmacological and industrial importance, several extraction and analytical procedures have been developed and applied over the years to isolate, detect, and quantify diosgenin, not only in its natural sources and pharmaceutical compositions, but also in animal matrices for pharmacodynamic, pharmacokinetic, and toxicological studies. Numerous studies have reported that DG is useful in the prevention and treatment of neurological diseases. It briefly recapitulates recent advances in structural modification and novel formulations to increase the therapeutic efficacy and brain levels of DG. Thus, the present aims to provide collective information on the most recent pharmacological data on diosgenin and on the most relevant analytical techniques used to isolate, detect, and quantify this compound as well. In our work we try to activate diosgenin and prepare various types of biologically active diosgenin derivatives and to study their potential bioactivity.



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## PP-45

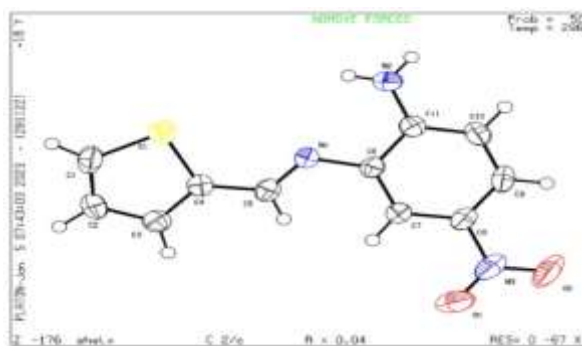
### Exploration of the biological efficacies of (*E*)-4-nitro-*N*<sup>1</sup>-(thiophen-2-ylmethylene)benzene-1,2-diamine Schiff base Zn(II) metal complex

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Schiff bases and their transition metal complexes are one of the important classes of compounds which have many interesting properties and extensive applications in medicinal, agriculture, pharmaceutical fields and material sciences [1]. Therefore a novel Schiff Base Ligand (LH) was synthesized from thiophene-2-carbaldehyde and 4-nitro-*o*-phenylenediamine, and transition metal complex was synthesized using Zn (II) Sulphate Heptahydrate in 1:1 molar ratio. Physico-chemical characterization techniques including Elemental Analysis, Multi-spectral analysis such as Infrared (IR) Spectroscopy, Mass Spectrometry, UV-Vis Spectroscopy, <sup>1</sup>H NMR Spectroscopy, Powder XRD, Molar Conductance investigations etc. were used to characterize the synthesized compounds. The Zn (II) complex was reported to have tetrahedral geometry based on spectroscopic analysis. Furthermore, the biological applications for the synthesized compounds were analyzed through DNA binding study and anti-bacterial activity. Fluorescence Spectroscopy, Viscosity Measurement and Adsorption Measurement were used to investigate the interaction of the Zn (II) complex with CT-DNA. The *in vitro* antibacterial activity against *Escherichia coli*, *Klebsiella pneumoniae*, *Bacillus subtilis* and *Staphylococcus aureus* strains were studied and compared with free ligand and Zn (II) metal complex. In addition, ADMET analysis was used to evaluate the ADMET properties of the ligand and the complex. Based on the Lipinski Rules, the in-silico ADMET properties suggested that the synthesized compounds have substantial drug-likeness character [2, 3].





**Synthesis, Crystal Structure, Hirschfield surface analysis and catalytic activity of New Cobalt (II) complex of 4-Nitrobenzoic acid and 1-Methylimidazole**

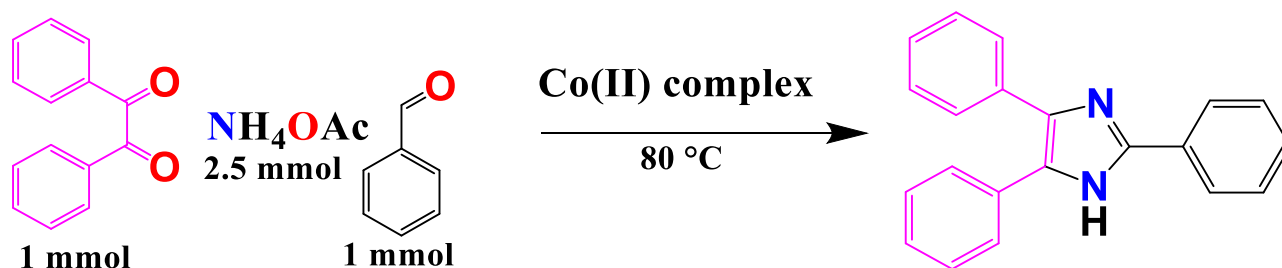
Sumiran Tamang<sup>a</sup>, Kiran Pradhan<sup>b</sup>, Biswajit Sinha<sup>b</sup>, Dhiraj Brahman\*<sup>a</sup>

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A new cobalt (II) complex has been prepared by the reaction of Cobalt (II) Nitrate Hexahydrate, 4-nitrobenzoic acid and 1 methyl imidazole in anhydrous methanol under reflux condition. The complex has been characterized by different analytical techniques and X-ray single crystal structure revealed that the complex crystallizes in monoclinic I2/a space group with following parameters:  $a = 33.046(1) \text{ \AA}$ ,  $b = 19.5363(8) \text{ \AA}$ ,  $c = 15.7773(9) \text{ \AA}$ ,  $\beta = 115.176(2)^\circ$ ,  $V = 9218.3(8) \text{ \AA}^3$ , and  $Z = 4$ . In addition, Hirschfield surface analysis and catalytic activity of the synthesized complex have been studied for the solvent free synthesis of 2,4,5-triarylimidazole derivatives (4a-4o).



**Keywords:** I2/a, Cobalt (II) nitrate hexahydrate, 4-nitrobenzoic acid, 1 methyl imidazole, Hirschfield surface

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## **PP-47**

### **Phthalimide-Based Off-On-Off Fluorosensor for Cascade Detection of Cyanide Ions and Picric Acid**

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Novel methods that can be utilized to identify and detect harmful environmental pollutants still need to be proposed [1]. This article describes the effective design and development of a turn-on photoluminescence probe, T1 [(E)-5-((2-hydroxybenzylidene) amino) isoindoline-1, 3-dione], which is selective and sensitive towards CNions having detection limit nM to  $\mu$ M range. When exposed to CNions, Probe T1 displays a strong fluorescence response under a 365 nm UV light irradiation with a noticeable low to high intense cyan color photoluminescence visible to the naked eye. For the practical utility of the present probe T1, a paper strips-based test kit experiment has been demonstrated as a portable and displayable photonic device for on-site detection of CNions. Furthermore, the T1-CNadduct has been applied for detecting explosive nitroaromatic compounds, especially PA, based on the photoluminescence quenching mechanism. Using CNions, and PA as chemically encoded inputs and corresponding optical output, a molecular logic gate has been constructed. Further, probe T1 has been employed as a bio-analytical tool to map intercellular CNions in live cells. This study invokes a novel approach for designing and developing efficient and selective sensors employing well-known fluorescent probes as signaling units with prior photophysical knowledge. The details experimental results of our findings will be discussed.

#### **Reference**

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**(azanido)-(dihydroxido)- $\mu$ -(3-methylpyridine-2-carboxylato)- $\mu$ -(3-methylpyridine-2-carboxylato)-di-copper and Copper aqua-(5,5'-dimethyl-2,2'-bipyridine)-hydroxido-[1,2,2-trimethylcyclopentane-1,3-dicarboxylato]-cuprate,  
Hydrothermal synthesis, crystal structure and theoretical studies**

Vikas Kr. Dakua<sup>1</sup>, Kanak Roy<sup>1</sup>, Quazi Arif Islam<sup>1</sup>, Mahendra Nath Roy<sup>2</sup>

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Metal-organic hybrid complexes often exhibit large surface area, pore volume, fascinating structures and diversified potential applications. Hence two metal-organic hybrid complex,  $(C_{14}H_{12}Cu_1N_2O_4)_n$  and  $(C_{22}H_{28}CuN_2O_5)_n$  were synthesized hydrothermally. Single crystal X-ray diffraction study of these two crystal suggests that these are three dimensional with space group P 21/c (monoclinic) and P 2<sub>1</sub> 2<sub>1</sub> 2<sub>1</sub> (Orthorhombic), respectively. The  $(C_{22}H_{28}CuN_2O_5)_n$  complex contains a penta-coordinated Cu ion coordinated to one H<sub>2</sub>O molecule, two N-atoms of 5,5'-Dimethyl-2,2'-bipyridine and two O-atom of the carboxylic group of d-Camphoric acid in a distorted square pyramidal geometry and  $(C_{14}H_{12}Cu_1N_2O_4)_n$  complex contain six coordinated Cu ion coordinated to two N-atoms and two oxygen atoms from two different 3-methyl picolinic acid and two oxygen atoms from another two different 3-methyl picolinic acid. These crystal structures achieves its three-dimensional structure and stability through h-bonding and polymeric chains in between moieties. Hirshfeld topology analysis studies revealed it to be a stable complex.

**Keywords:** Hydrothermal synthesis, Single crystal Xray diffraction, metal-organic hybrid complex, Hirschfeld topology

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## PP-49

### Development a controlled release complex for Bisphenol A using cyclic oligosaccharide to lessen its risky effects

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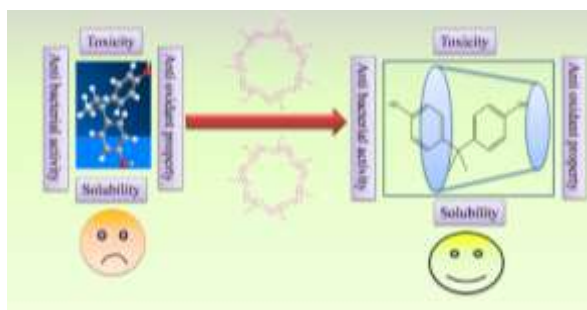
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Herein in order to improve the bioavailability of a non-biodegradable pollutant, inclusion complexation procedures had been used to develop better formulations of this pollutant, Bisphenol A (BPA). In our research, an inclusion complex (IC) of  $\beta$ -Cyclodextrin ( $\beta$ -CD) with BPA was formed to investigate the effect of  $\beta$ -CD on the water solubility, anti-oxidant, anti-bacterial activity, toxicity and thermal stability of BPA. UV-Vis and other spectrometric methods such as NMR, FTIR, and XRD indicated the molecular mechanism of interactions between  $\beta$ -CD and BPA, which was further hypothesised using molecular modelling to confirm preliminary results. Studies of TGA and DSC demonstrated that encapsulation boosted the thermal stability of BPA. This research also makes predictions about BPA's release behaviour when CT-DNA is present. *In vitro* testing of the IC's antibacterial activities showed that it outperformed pure BPA. The *in-silico* study was found to have a considerable decrease in toxicity level for IC compared to pure BPA. Therefore,  $\beta$ -CD-encapsulated BPA can lessen toxicity by raising antioxidant levels. Additionally, as its antibacterial activity increases, it may be employed therapeutically. Thus, this discovery of creating BPA formulations with controlled release and/or protective properties allows for a more logical application of BPA by reducing its hazardous effects through boosting its efficacy

**Keywords:** Anti-bacterial assay, Anti-oxidant study, Bisphenol A, Inclusion Complex, Toxicity



## PP-50

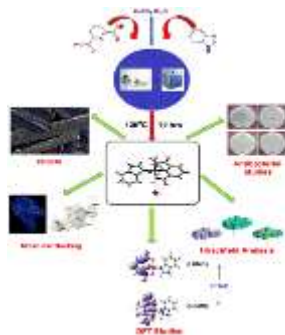
### Penta coordinated Cu(II) based metal-organic hybrid complex: Hydrothermal synthesis, Hirshfeld surface analysis, pharmacokinetic studies, molecular docking, antibacterial studies and DFT studies

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Of late, the synthesis of metal-organic hybrid complexes with intriguing structures and topologies following hydrothermal method has attracted considerable attention globally. In these syntheses, product formation largely depends on the pH, reaction temperature, nature of solvents, counter ions and ligand geometry, *etc.* Metal-organic hybrid complexes quite often have a large surface area, large pore volume, intriguing structures and wide range of potential applications. [1] Hence, aqua(1*H*-benzimidazole- $\kappa$ N<sup>3</sup>)(pyridine-2,6-dicarboxalato- $\kappa^3$ O<sup>2</sup>,N,O<sup>6</sup>)-copper(II) 0.75-hydrate i.e., [Cu(C<sub>7</sub>H<sub>3</sub>NO<sub>4</sub>)(C<sub>7</sub>H<sub>6</sub>N<sub>2</sub>)(H<sub>2</sub>O)]·0.75H<sub>2</sub>O was synthesized hydrothermally. [2] Physico-chemical characterization of the synthesized complex was performed using single crystal X-ray diffraction (SCXRD), FTIR spectroscopy and FESEM. A single crystal X-ray diffraction study indicates that it is three-dimensional structurally, with the space group *P*2<sub>1</sub>/*n* (Monoclinic). The unit cell dimensions are *a* = 8.6388 (17) Å, *b* = 17.692 (4) Å and *c* = 9.783 (2) Å. The 3D structure and stability of the crystal are achieved through extensive intermolecular hydrogen bonding. Hirshfeld surface analysis, pharmacokinetic studies, molecular docking, DFT studies and antibacterial studies of the complex were also performed for this crystal.



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## PP-51

### Synthesis, DNA binding, Molecular docking and ADMET properties of a Novel Zn(II) complex

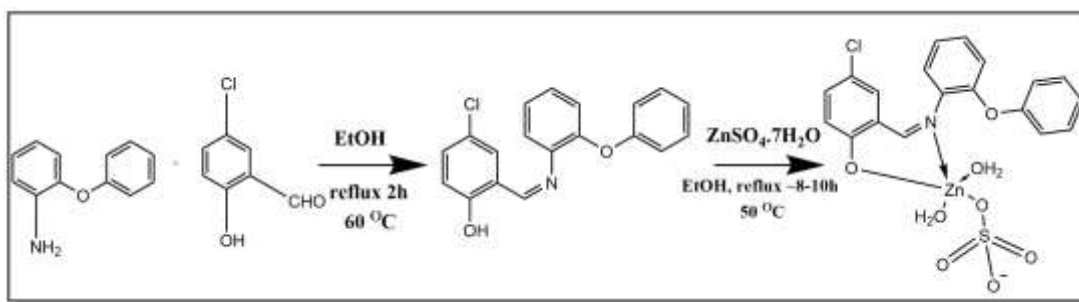
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A new Schiff base ligand (LH) has been synthesized by the condensation reaction of 2-phenoxyaniline and 5-chlorosalicylaldehyde. It has been characterized by elemental analysis, infrared (IR) spectroscopy, <sup>1</sup>H NMR spectroscopy and Mass Spectrometry. Its Zinc complex was synthesized by reacting the ligand (LH) with zinc sulphate heptahydrate in 1:1 molar ratio. The zinc complex was characterized by elemental analysis, molar conductance, electronic spectra, IR spectroscopy and <sup>1</sup>H NMR. The complex's non-electrolytic nature is established by the molar conductance investigation. IR study revealed that the metal ion is coordinated in pentadentate fashion, which was further confirmed by NMR studies. Absorption, fluorescence spectroscopy (EB displacement assay), and viscosity measurements were used to investigate the interaction of the complex with CT (calf thymus) DNA. According to the observations, the synthesized complex binds to DNA in an intercalative way and can reduce the fluorescence intensity of EB bound to DNA. Furthermore, ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity) analysis was used to determine the ADMET features of the ligand and the complex.



**Figure:** Synthesis of Schiff base ligand and its Zn(II) complex.

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## Tuning the Supramolecular Helicity of Aromatic Functional Group Conjugated Short-Peptide-Based Gel Nanofibers

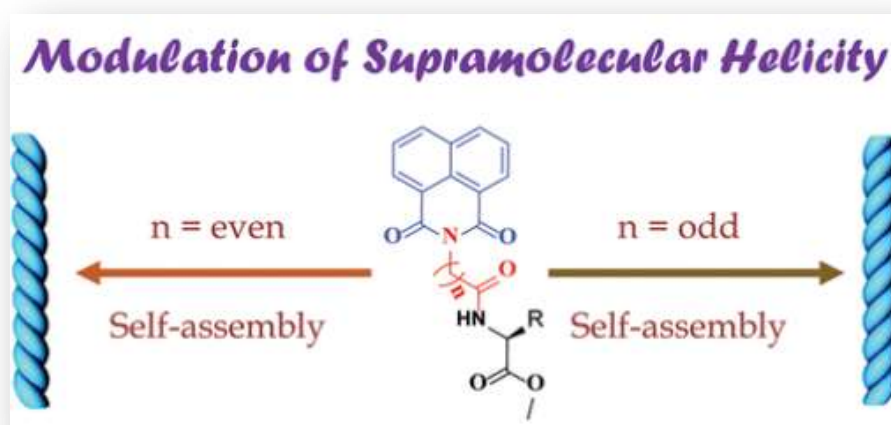
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Helical supramolecular architectures play important structural and functional roles in biological systems. The helicity of synthetic molecules can be tuned mainly by the chiral manipulation of the system. However, tuning of helicity by the achiral unit of the molecules is less studied. In this work, the helicity of naphthalimide-capped peptide-based gel nanofibers is tuned by the alteration of methylene units present in the achiral amino acid. The inversion of supramolecular helicity has been extensively studied by CD spectroscopy and morphological analysis. The density functional theory (DFT) study indicates that methylene spacers influence the orientation of  $\pi$ - $\pi$  stacking interactions of naphthalimide units in the self-assembled structure that regulates the helicity. This work illustrates a new approach to tuning the supramolecular chirality of self-assembled biomaterials.

**Keywords:** Helicity • Inversion • Achiral Chain Length • Naphthalimide



### Reference

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**Journey of Purine-Alkaloids to Ammonia for Plant Growth Promoting Activity: Metabolomic Approach to Validate CTC Tea Waste As Sustainable Organic Fertilizer**

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**Abstract**

Valorization of agro-industrial waste biomass is today's main concern among agrochemists agribiotechnologists. This research was designed to validate tea industrial waste (from CTC tea factory) as a sustainable and renewable resource for waste biomass management. Physicochemical analysis has been carried out to characterize tea waste treated soil. Pot experiment with cowpea [*Vigna unguiculata* (L.) Walp.] was considered to study impact of tea waste on plant growth. Effect of tea factory waste on soil nutrition was found remarkable with increased organic carbon, organic matter, nitrogen, phosphorus, potassium and sulphur content. Pot culture revealed impact of tea waste composted soil on boosted plant growth. GC-MS based metabolite profiling revealed purine alkaloids such as xanthosine and caffeine as major compounds of tea waste. A possible pathway has been proposed to explain the role of xanthosine and caffeine breakdown in fertilization of soil and plant growth. Disposal of tea wastes produced during tea manufacturing can be managed in a sustainable manner if this research is implemented industrially.

**Keywords:** Metabolomics; tea waste; xanthosine; caffeine; waste biomass.



**PP-54**

**Formulation of Herbal Handwash Using Natural Products with Antibacterial Effects**

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**ABSTRACT**

**BACKGROUND:** Currently market is rich with many synthetic handwash which have heavy metals like lead, arsenic, copper, nickel, chromium, and cobalt. During applying these handwash some of those toxic chemicals are absorbed by hands. Herbal based products are very much familiar as well as popular now-a-days. Along with human skin they are beneficial to the environment.

**AIM:** To prepare herbal handwash using natural products which help prevent infectious diseases and compare the quality with marketed herbal handwash available in Indian market.

**METHODS:** Leaves of *Carica papaya* (papaya), *Azadirachta indica* (neem), *Ocimum sanctum* (tulsi), *Aloe vera*, *Sapindus mukorossi* (reetha fruit), and turmeric (product of *Curcuma longa*) and eucalyptus oil (obtained from *Eucalyptus globulus*) were used for the preparation. After formulation, it was evaluated and various parameters such as pH, stability, colour, odour, foam height, foam retention and antibacterial study were determined and reported.

**RESULT:** Results showed that, different evaluation parameter of prepared herbal handwash was resembled with standard values and with marketed formulation.

**CONCLUSION:** Consumers always search for natural-based cosmetics to avoid allergic reactions and any sort of side effects as well as helps to fight various disease-causing agents. Further research is appreciated for formulating the handwash with some other additional advantages of skin benefits.

**KEYWORDS:** Herbal handwash, *Ocimum sanctum*, *Aloe vera*, *Sapindus mukorossi*,  
*Azadirachta indica*, and *Carica papaya*.

**PP-55**

**Preparation and characterization of Polyelectrolyte Complexes of  $\kappa$ -Carrageenan (Neem Seed Oil) and Chitosan**

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An increasing number of articles on Polyelectrolyte complexes reflects the growing industrial interest in pharmaceutical field. These complexes can roughly divided into two types: the first one PECs are complexes of cationic and anionic polyelectrolytes and the second type is PE-serfs complexes of anionic polyelectrolytes with cationic surfactants of vice-versa.

In this study we prepared polyelectrolyte complexes of  $\kappa$ -Carrageenan and Chitosan and done characterization studies. To form polyelectrolyte complexes of  $\kappa$ -Carrageenan extracted from fruits of neem and chitosan were prepared using chemical crosslinking procedure. The PECs were insoluble and at weight ratio of 7:3 the maximum yield was obtained. After extracting the obtained supernatant was clearly representing complete conversion of polysaccharides into PECs. After precipitation of PECs complexation was also evaluated by measuring the viscosity of supernatant. The dried PECs were characterized using FTIR, DSC, zeta potential, water uptake, swelling index and SEM studies. The optimized ratio (7:3) exhibited a zeta potential of -0.535 mV and displayed a porous structure in SEM analysis. Swelling studies show that swelling of PECs occurs more in pH 6.8 as compared to pH 1.2 which may in future be used in pH dependent sustained drug delivery system.

**Key words:**  $\kappa$ -Carrageenan, polyelectrolyte, swelling study.

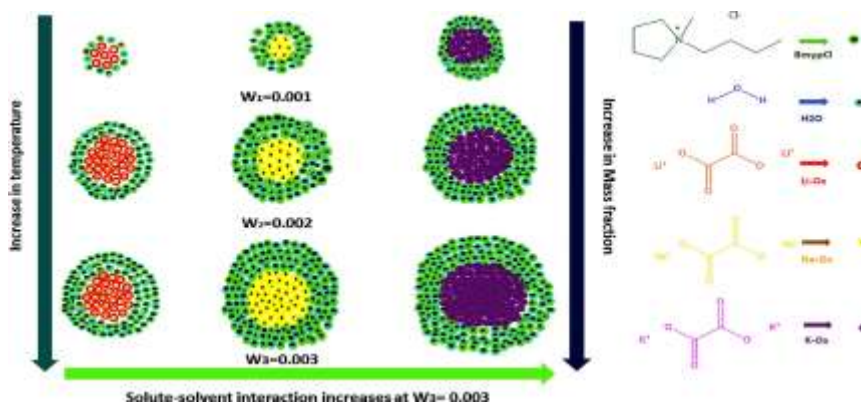
## PP-56

### Physicochemical and computational investigations of some food Chemicals prevalent in aqueous 1-butyl-1-methyl-pyrrolidinium Chloride solutions with the manifestation of solvation consequences

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**Abstract:** Investigating the diverse molecular interactions between implausible food chemicals (potassium Oxalate, sodium oxalate, and lithium Oxalate) and 1-butyl-1-methyl-pyrrolidinium chloride in aqueous Solutions has been presented. The experiments have been discovered thoroughly by different types of Physicochemical methodologies like density, refractive index, viscosity, and electrical conductivity at three different temperatures 298.15 K, 308.15 K, and 318.15 K. The genesis of diverse interactions of the ternary mixtures was exposed by measuring the apparent molar volume, limiting apparent molar volume, Viscosity B coefficient, molar refraction, and limiting molar refraction. The results have revealed the predominant solute–solvent interaction over the solute–solute as well as a solvent–solvent interactions. The ionic liquid strongly interacts with potassium oxalate than sodium oxalate, which in turn is greater than lithium oxalate at a higher range of temperature. Moreover, Density Functional theory calculations were performed to evaluate parameters like adsorption energies, molecular electrostatic potential maps, and mode of binding which corroborate the experimental observations.



Schematic representation of growing interaction taking place between Metallic oxalates and Ionic liquids in ternary systems of their aqueous solution

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## Supramolecular Encapsulation of Nanocrystalline Schiff bases into $\beta$ -Cyclodextrin for Multifold Enrichment of Bio-potency

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### Abstract:

We report the solvent-free green synthesis of two Schiff bases, (E)-2-((2-hydroxy-3-methoxybenzylidene)amino)-4-methylphenol (SL1) and (E)-2-((2-hydroxybenzylidene) amino)-4-methylphenol (SL2), and their inclusion complexes with  $\beta$ -cyclodextrin ( $\beta$ -CD). The encapsulation phenomenon, structural characteristics and hydrolytic stabilities of the SL1, SL2 and their inclusion complexes are determined with a suite of spectroscopic, analytical and crystallographic analyses. Dose and time-dependent cytotoxicity study of SL1- $\beta$ -CD and SL2- $\beta$ -CD against two breast cancer cell lines, Michigan Cancer Foundation-7 (MCF-7) and Metastatic mammary adenocarcinoma1 (MDA-MB-231), exhibit excellent inhibitory activity with significant non-cytotoxic concentrations and ensure a multifold elevation of bio-potency than the parent Schiff base compounds. The annexin-V assay determines the efficacy of these inclusion complexes to trigger apoptosis, suggesting that SL2- $\beta$ -CD possesses better efficacy as an anti-cancer drug. To the best of our knowledge, we, for the first time, report the inclusion of nanocrystalline Schiff bases into  $\beta$ -CD for multifold enrichment of bio-potency.



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**Fomation of carbon quantum dots from tea leaves**

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**Abstract**

Carbon quantum dots (CQDs) are a new class of carbon nanomaterials that have emerged recently and have garnered much interest as potential competitors to conventional semiconductor quantum dots. In addition to their comparable optical properties, CQDs have the desired advantages of low toxicity, environmental friendliness, low cost, and simple synthesis routes. CQDs have found many applications in the fields of chemical sensing, biosensing, bioimaging, nanomedicine, photocatalysis and electrocatalysis. CQDs are prepared from CTC tea using Hydrothermal synthesis. Ground tea powder dissolved in acetic acid and placed in hydrothermal for 4 hours at 180°C. The obtained yellow liquid was filtered twice by a 0.22 µm microfiltration membrane and dried at 80°C. The concentrated solution was lyophilized to get the carbon quantum. A simple, stable, and reproducible nanoparticle-modified glassy carbon electrode would be developed as a sensing probe for the electrochemical determination of tea pesticides. TEM and DLS was performed to study the physical characteristics (particle size, shape, and distribution).

Key words: CQDs, Hydrothermal, Tea, TEM, DLS

**Reference**

Chu, H. W., Unnikrishnan, B., Anand, A., Lin, Y. W., Huang, C. C. (2020). Carbon quantum dots for the detection of antibiotics and pesticides. *Journal of Food and Drug Analysis*, 28(4), 539–557.

## PP-59

### **Nanoencapsulated biopesticides for the sucking pest management in the tea gardens.**

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#### **Abstract**

Biopesticide plays a fundamental role in protecting agricultural crops as well as the environment from indiscriminate application of chemical and hazardous synthetic pesticides. Our study highlighted the potentiality of ginger, neem and black pepper extract as a sucking pest-controlling agent for tea gardens, principally the controlled release of liposome encapsulated bio-pesticides with improved stability and enhanced solubility. Ginger extract has high amounts of zingiberene and gingerol, which act as potent active components for sucking pests control. Azadirachtin present in neem leaves and piperine in black pepper is also an important active ingredient to control sucking pest. Nano-formulations have the capability to upgrade the pest-control ability for a prolonged period of time by prohibiting the early degradation of active ingredients under eco-friendly conditions. To study the efficacy of the liposome encapsulated biopesticides, composed of ginger, neem and black pepper extract were applied on Darjeeling tea clones. Randomized block design (RBD) with three plots per treatment chosen for the field trial. After pre-treatment count, foliar spray applied with a hand operated knapsack sprayer at standard dose. The liposomes were made of a thin film hydration method. The liposome encapsulated biopesticides were prepared by mixing the plant extract with liposomes, Tween 80 (as surfactant), and sucrose (as cryo-protectant). TEM and DLS was performed to study the physical characteristics (particle size, shape, and distribution) of liposomes and liposome-coated bio-pesticides. Post treatment observation for 2 weeks results mean population reduction per treatment.

**Keywords:** Nano-encapsulation, biopesticide formulation, liposome, RBD.

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**Synthesis and Biological Evaluation of  
Some Novel Substituted Quinazoline-4-(3H)-One Analogs**

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Quinazolinones and their substituted derivatives constitutes an important class of heterocyclic compounds and quinazolinone nucleus is found in many natural bioactive natural products as different biological significant pharmaceutical agents like anti-inflammatory , anti-ulcer, anti-depressant, anti-convulsant, immunotropic, anti-proliferative , anti-microbial , antiviral active pharmaceutical ingredient. As this evidents are obtained , an analogous series of substituted Quinazoline -4-3(H)-One are intended to synthesized as anti microbial agent . Primarily , 2-phenyl-1,3,1 benzoxazin-4(3H)-one , skeleton were synthesized by condensation of anthranillic acid and benzyl chloride through a established reaction method , then by refluxing it with thiosemicarbazide in a methanolic mediaum N-[ 2-phenyl-4-3(H)-oxo-quinazolin-3-yl]-thiourea was prepared. Then through a nucleophilic reaction by chloro acetic acid a cyclization reaction was carried out to produce a thiazolidinone ring in place of thiourea and produce 3-[(4-oxo-1,3-thiazolidin-2-ylidino)amino]-2-phenylquinazolin-4-3(H)-one. Then with differen carbonyl compound this substituted phenylquinazolin-4-3(H)-one moiety was substituted with a acceptable range of yeild percantage and characterized by melting point , FTIR, <sup>1</sup>H-NMR, <sup>13</sup>CNMR study . All seven substituted compounds (M-I TO M-VII ) were screened for their antibacterial and anti fungal activities .Compound named M-II , M-III , M-V and M-VI produces a significant antibacterial activity against S.aureus(ATCC-23922) , S.typhi (TY-259 ) , Bacilus subtilis (PZ-6633) and V.cholrae (ATCC -783) and compound M-II . M-V and M-VI shows potent antifungal activity against Candida albicanis (SSKM ) and C.tropicalis (ATCC-750).

**KEY WORDS :** Quinazoline -4-3(H)-One , Condensation , Nucleophilic Cyclization ,FT-IR , NMR , Anti Microbial activity .

**Pre-monsoon air quality index of Darjeeling tea gardens**

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The change in the climate is affecting vegetation especially food crops all around the world with implications for environmental and the well-being of humans. The beverage crop - tea will be correlated with environmental effects on the directionality of crop quality. Our systematic study aims at the relevance to suspended and gaseous particulate matter. Shifts in seasonality, water stress; geography, light factors, altitude, microbes, temperature, and soil factors that are linked to climate change can result in changes in secondary metabolites. Various meteorological factors such as air quality, wind speed, altitude, humidity, temperature, air pressure, soil pH, and air density influence the growth and quality of tea. The climatic and soil conditions affect the metabolite composition of the Darjeeling tea including its flavor, nutrition and overall consumer preference. Thus, in the present study, different meteorological parameters like temperature (T), relative humidity (RH), solar radiation, air pressure, wind speed, and wind direction were monitored with the help of an automated weather monitoring station at the study sites during pre-monsoon season of the analysis period. Assessment of ambient air quality observed by the monitoring of PM<sub>2.5</sub>, PM<sub>10</sub>, and PM<sub>1</sub> along with monitoring of gaseous air pollutants (O<sub>3</sub>, NO<sub>2</sub>, and SO<sub>2</sub>) and monitoring of Air Quality Index (AQI) was monitored during this pre- monsoon season. The mean temperature, relative humidity, solar radiation, and air pressure within 24 hours span were 14.11±0.38°C, 84.78 ± 0.50%, 124.14 ± 7.43 W/m<sup>2</sup>, and 79433.71 ± 23.78 Pa during the studied season. The average concentration of PM<sub>2.5</sub>, PM<sub>10</sub>, and PM<sub>1</sub> was 102.27, 123.43 and 117.60 µg.m<sup>-3</sup>. The air quality index box plots illustrated that the minimum, lower quartile, upper quartile, and maximum values were 81, 134, 313, and 352 µg.m<sup>-3</sup> respectively during the pre-monsoon period.

**Keywords:** Darjeeling tea, pre monsoon, weather monitoring, particulate matter, meteorological parameters, air quality index.



**PP-62**

***Guizotia abyssinica*: a promising local herb as a source of biodiesel in future**

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**Abstract:**

Traditional fossil fuels derived from petroleum have a significant impact on the accelerated exhaustion of energy resources and the rise in energy consumption, and they are also a major contributor to environmental contamination. Myriad research shows that *Guizotia abyssinica* as a promising crop with diverse applications in agriculture, medicine and energy. Its investigation found to have favorable physical and chemical traits, making it a potential source of biodiesel in the globe. Its quality has been assessed, and the results indicate that it is of high quality and suitable for various industrial applications. This study discusses the challenges and opportunities for using its seed as a source of biodiesel in India, including the availability of the crop and the economics of its production.

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## **PP-63**

### **A Ratiometric, Turn-on Chromo-fluorogenic Sensor for Sequential Detection of Aluminium Ions and Picric acid**

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The abundance of aluminium in the earth's crust is highest as metal and third as an element after silicon and oxygen [1,2]. This metal commonly remains in ionic form ( $\text{Al}^{3+}$ ) in the tissues of most animals, plants, and water. For the detection of  $\text{Al}^{3+}$  ions a simple ratiometric, turn-on chromofluorogenic sensor, (E)-2-((2-hydroxybenzylidene) amino)-5-nitrophenol (HBAN), has been developed, synthesized, and characterized by several conventional analytical methods. HBAN is found to be selective for the sequential detection of  $\text{Al}^{3+}$  ions and picric acid (PA), respectively based on fluorescence 'off-on-off' method. UV-visible absorption spectra are found to be red-shifted from 382 nm to 454 nm with a clear isosbestic point located at 414 nm due to the complex formation between the free probe and  $\text{Al}^{3+}$  ions. A visible colorimetric change from colorless to yellowish of the HBAN solution is found in the naked eye due to the chelation of  $\text{Al}^{3+}$  ions with HBAN. A remarkable fluorescence enhancement of HBAN is detected at 540 nm upon binding with  $\text{Al}^{3+}$  ions with a visual yellow color fluorescence under a portable 365 nm UV light irradiation. Among the various tested nitroaromatic compounds, PA selectively quenches the fluorescence of the  $\text{Al}^{3+}$  ions chelated HBAN complex. The formation of the complex between HBAN and  $\text{Al}^{3+}$  ions is found to be in a 1:1 stoichiometric ratio. The mechanistic aspects of detecting  $\text{Al}^{3+}$  ions have been elucidated by different spectroscopic and density functional theoretical analyses. Additionally, a test kit based on paper strips coated with HBAN is demonstrated to selectively detect  $\text{Al}^{3+}$  ions.

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## **PP-64**

### **KA<sup>2</sup> Coupling reaction: Access to synthesis propargylamine: Recent updates and modification with future scope**

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#### **Abstract**

Multicomponent coupling among ketones, amines and alkynes is known as KA<sup>2</sup> (Ketone-Amine-Alkyne) coupling reaction. Tetrasubstituted propargylamine is formed by this reaction which is a unique class of highly useful compounds. When aldehyde is used as the carbonyl partner, it is the A<sup>3</sup> coupling reaction which affords trisubstituted propargylamine. Aldehyde-Amine-Alkyne coupling was largely explored as a convenient reaction methodology to synthesis propargylamines in last decades. Many metal catalysts (Cu, Zn, Ag, Mn, Au) are employed for this KA<sup>2</sup> reaction among them Cu-salt has been used mostly as it is the most suitable way to activate the <sup>SP</sup>C of terminal alkyne. Very recently (2022) KA<sup>2</sup> and A<sup>3</sup> coupling was modified using ynamide as alkyne surrogates and designated the reaction as KYA (modification of KA<sup>2</sup> coupling) and AYA (modification of A<sup>3</sup> coupling) coupling i.e. Aldehyde-Ynamide-Amine and Ketone-Ynamide-Amine coupling. “Green Chemistry” and “sustainable development” are increasingly popular in both academia and industry promising environmental safety. The objective of multicomponent reactions towards “greener approach” typically due to their step economy. But there is still enough scope to establish the KA<sup>2</sup> coupling reaction satisfying most of the principle of green chemistry in a single methodology. In future the reaction may be explored under completely metal-free, solvent-free as well as under ambient condition as unique protocol. After ticking these boxes, a more critical and comprehensive green review over KA<sup>2</sup> coupling reaction will be read with a cup of tea in near future as found in A<sup>3</sup> coupling reaction.

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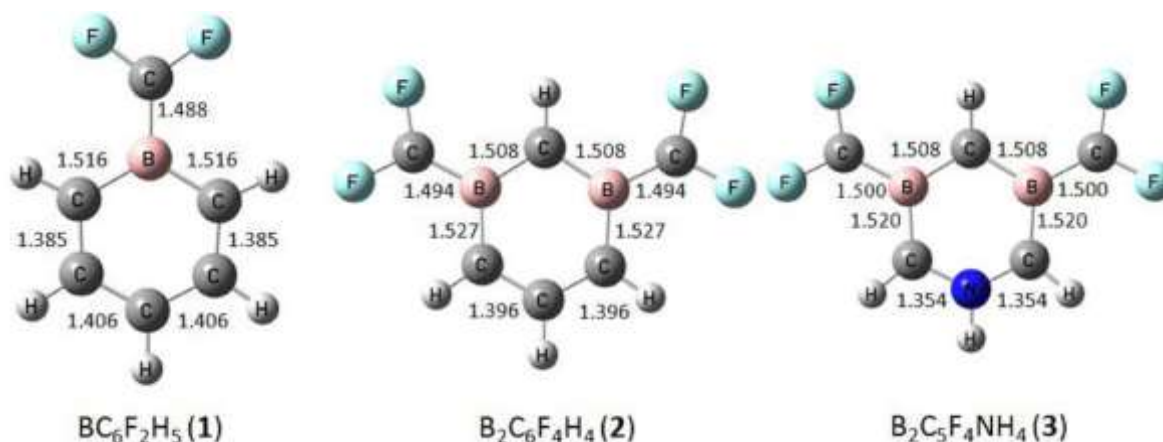
## A New Approach to Design High Spin Organic Systems: Aromatic Stabilization with Exo-cyclic $\pi$ Electrons Plays Crucial Role

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High spin organic molecules have important applications in diverse fields such as organic magnetic molecules,<sup>1</sup> spintronics,<sup>2</sup> magnetic resonance imaging (MRI) contrast agents<sup>3</sup> and so on. We have modelled three systems,  $\text{BC}_6\text{F}_2\text{H}_5$ ,  $\text{B}_2\text{C}_6\text{F}_4\text{H}_4$  and  $\text{B}_2\text{C}_5\text{F}_4\text{NH}_4$ . Each of them contains  $-\text{CF}_2$  unit(s) with one  $p_z$  electron on carbon atom exo-cyclic to the six-membered ring. The first two systems have  $6\pi$  electrons and the last one contains  $7\pi$  electrons in total. An isolated  $-\text{CF}_2$  unit can be considered as a monoradical entity. From computational study we observed that the  $p_z$  electron on the exo-cyclic carbon atom participates in aromatic conjugation, which in turn imparts stability to the designed systems. We found that exo-cyclic conjugation is strong enough to force  $\text{BC}_6\text{F}_2\text{H}_5$  and  $\text{B}_2\text{C}_6\text{F}_4\text{H}_4$  to be closed shell singlets. On the other hand,  $\text{B}_2\text{C}_5\text{F}_4\text{NH}_4$  is in a doublet state where the formation of an aromatic sextet of electrons stabilizes the system, and the extra spin is delocalized over the whole ring, thus forming a stable radical.



**Figure 1.** Optimized structures of  $\text{BC}_6\text{F}_2\text{H}_5$ ,  $\text{B}_2\text{C}_6\text{F}_4\text{H}_4$  and  $\text{B}_2\text{C}_5\text{F}_4\text{NH}_4$ .

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