

## **Welcome to International Conference**

*Advances in Chemistry for Diverse Applications: Bridging Basic, Translational Research and Health Sciences for a Sustainable Future*

*ICACDA-2026*

**The Department of Chemistry is organizing International Conference on Advances in Chemistry for Diverse Applications: Bridging Basic, Translational Research and Health Sciences for a Sustainable Future during Feb 24-26, 2026.**

**The International Conference *ICACDA-2026* is organized with the vision of highlighting the transformative role of chemistry as a bridge between fundamental research and real-world applications. Chemistry today serves as a powerful driving force in advancing healthcare, sustainable technologies, industrial innovation, and environmental protection.**

**This conference brings together eminent scientists, academicians, researchers, industry experts, and young scholars from diverse disciplines to exchange knowledge, foster interdisciplinary collaboration, and inspire innovative thinking. By integrating fundamental discoveries with applied research, the event aims to strengthen the link between science and society.**

**Through keynote lectures, invited talks, oral and poster presentations, the conference provides a dynamic platform to discuss emerging trends and recent advancements across various domains of chemical sciences.**

**We sincerely thank all contributors, speakers, participants, organizing committee members, and sponsors for their valuable support in making this event a success.**

***We are especially grateful to RUSA 2.0 for their generous financial support for this conference.***

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# INVITED LECTURES

## **Prof. Alberto Bianco**

Dr. Alberto Bianco received his PhD in 1996 from the University of Padova (Italy). As a visiting scientist, he worked at the University of Lausanne (Switzerland), the University of Tübingen (Germany) (as an Alexander von Humboldt fellow), the University of Padova and Kyoto University (Japan). He is currently Distinguished Director at the French National Center for Scientific Research (CNRS) in Strasbourg. His research interests focus on the design of multifunctional carbon



and 2D nanomaterials for therapy, diagnostics and imaging. He is also interested on their health impact, particularly on the immune system. He has published more than 350 articles (h-index: 102, >60000 citations). In 2017 he has been elected Fellow of the European Academy of Science and in 2020 of the Academia Europaea, and in 2019 he has obtained the CNRS Silver Medal. Since 2011 he is Editor of the journal CARBON. He has given more than 200 lectures in different conferences.

# Carbon Nanomaterials for Biomedical Innovation

**Alberto Bianco**

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Over the past quarter century, new allotropic forms of carbon—namely carbon nanotubes and graphene—have attracted significant attention for their exceptional properties and promising biomedical applications, as well as for concerns regarding their potential toxic effects on living systems, including mammals, and on the environment.<sup>1</sup> While the use of carbon nanotubes remains the subject of intense debate, with some questioning whether they should be definitively banned, graphene has raised similar concerns due to its shared graphitic nature. However, graphitic carbon materials are not uniform in their interactions with biological systems, nor in their impact on human health and the environment.<sup>2</sup>

In this lecture, I will present our research focused on the design and development of carbon nanotubes and graphene tailored for safe biomedical use, including applications in diagnostics, drug delivery, and regenerative medicine.<sup>3</sup> The health risks associated with the structural similarity between carbon nanotubes and asbestos fibers can be mitigated through appropriate chemical modifications, which not only reduce toxicity but also promote biodegradability and controlled biological interactions.<sup>4</sup> Assessing the potential impact of graphene-based materials on health and the environment is likewise a critical step in translating these materials into clinical and technological applications. In this context, I will discuss the potential risks of graphene-based materials and outline strategies to overcome them, with the ultimate goal of enabling their registration as new and “safe” chemicals for biomedical and related applications.<sup>5</sup>

Keywords: Carbon materials, functionalization, cancer therapy, safety

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## **Prof. Nobuo Kimizuka**

Nobuo Kimizuka is a Professor at the Graduate School of Engineering, Kyushu University, Japan, specializing in molecular self-assemblies, photochemistry, and nanomaterials. He received his B.S. (1982), M.S. (1984), and Ph.D. (1990) in Synthetic Chemistry from Kyushu University under Prof. Toyoki Kunitake. He worked as a postdoctoral fellow at Mainz University (Prof. Helmut Ringsdorf's group) in 1990. He was promoted to Full Professor in 2000. Since 2000, he has led research



on synthesis, structure, properties and functions of molecular self-assemblies and nanomaterials. The recent focus involves the development of photo functional molecular systems showing the interplay between excited singlet and triplets, singlet & triplet energy migration in organized chromophore systems, and the development of self-assembly-based photon up conversion systems.

Citations = 14,216, h-index = 65, Publications = 373

# Maximizing the Power of Self-Assembly for Advanced Triplet–Triplet Annihilation Upconversion

**Nobuo Kimizuka**\*<sup>a</sup>

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Solar energy reaching the earth's surface is scarce (ca. 1 kW/m<sup>2</sup>), and the development of new technologies to effectively harvest, store, and utilize solar energy is one of the most critical issues for the sustainable prosperity of humankind. Based on this perspective, we have been involved in molecular systems science research to link molecular self-assembly to useful work over the past several years. We developed molecular systems that show photon-up conversion based on self-assembly. Triplet-triplet annihilation-based photon upconversion (TTA-UC) is a promising methodology that can be applied to many sunlight-based energy conversion systems. Fundamental studies of TTA-UC have focused on the diffusion of excited triplet molecules in organic media, which limits their applications. Inspired by biological photosynthetic systems, we integrated the concepts of self-assembly and energy migration to develop efficient photon-upconverting molecular systems.<sup>1,2</sup> Interestingly, some of the molecular self-assemblies dispersed in solution or organogels revealed oxygen barrier properties, which allowed TTA-UC even under aerated conditions.<sup>3,4</sup> In this talk, we will discuss our recent development on the TTA-UC molecular systems with controlled energy landscapes, the design of visible-to-UV upconversion materials.<sup>5,6</sup> Also, recent challenge towards living Frenkel/Charge-Transfer hybrid exciton materials<sup>7</sup> and singlet fission directed by chiral molecular self-assembly<sup>8</sup> will be introduced.

Keywords: Self-Assembly, Triplet, Photon Upconversion

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### **Prof. Amitava Das**

Amitava Das obtained his Ph.D. from Jadavpur University, Kolkata, in 1989, followed by postdoctoral research at the Universities of Birmingham and Bristol, UK, with Prof. Jon A. McCleverty and Prof. M. D. Ward. He began his independent research career at CSIR–CSMCRI in 1993 and retired in 2019 as its Director and Distinguished Professor of AcSIR. He also served as Chief Scientist at CSIR–NCL, Pune, from 2013 to 2016. From 2020 to July 2025, he was Senior Professor of Chemical Sciences at IISER Kolkata and currently continues there as a Visiting Professor. He is an elected Fellow of all three major Science Academies of India and a recipient of several prestigious honours, including the ANRF–J. C. Bose National Fellowship (since 2017) and the CRSI Bronze (2009) and Silver (2017) Medals. His research interests span supramolecular chemistry, biomolecular recognition, and therapeutic nanostructures. He has been serving as an Associate Editor of *iScience* since 2022.



# Supramolecular Integration of N-capped Short Peptides for Multivalent Molecular Recognition and Therapeutic Applications

**Amitava Das**

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Recent research in therapeutic design is converging on a central goal of delivering active agents or reactive species precisely at disease sites, maximising efficacy while minimising systemic toxicity. The key challenge lies in balancing therapeutic potency with site-specificity. One promising solution is the creation of *stimuli-responsive therapeutics*—molecules and assemblies engineered to activate selectively in response to disease-specific cues.<sup>1</sup> Advances in molecular recognition-based synthons have accelerated the development of tailored drug delivery systems, enabling improved therapeutic indices and reduced off-target effects. Building on these advances, our work focuses on the rational design of short, purpose-built peptides as versatile scaffolds for therapeutic innovation.<sup>2</sup> In this lecture, I will present proof-of-concept studies where we have developed prodrugs and molecular composites that respond to defined biological triggers, offering new strategies for the treatment of challenging diseases.<sup>3</sup> These efforts highlight how rationally engineered peptides and their assemblies perhaps transform precision therapeutics, bridging the gap between molecular design and clinical relevance.

Keywords: N-capped Short Peptides, Multivalent interactions, Therapeutics.

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## **Prof. Anil Kumar**

Dr. Anil Kumar, Professor of Chemistry, has been selected for the prestigious CRSI Bronze Medal in recognition of his contribution to research in Chemistry by the Chemical Research Society of India (CRSI), Bangalore. The medal will be presented to him either at the 26th CRSI-National Symposium in Chemistry (NSC-26) to be held at VIT University, Vellore, during February 6-9, 2020, or at the 27th CRSI-National Symposium in Chemistry (NSC-27) to be held at IISER, Kolkata, during July 16-19, 2020. The CRSI was established in 1999 as part of the 50th anniversary celebrations of the country's independence by Bharat Ratna Prof. C. N. R. Rao and is the largest chemical society in our country.



Prof. Kumar is also the recipient of Prof. S. Vankateswaran Faculty Excellence Award from BITSAA for (2017), Dr. Arvind Kumar Memorial Award (2014) from Indian Council of Chemists, ISCB Young Scientist award in Chemical Sciences (2013) from Indian Society of Chemists and Biologists, and Harrison McCain Foundation award (2012) from Acadia University, Canada. Prof. Kumar works in the areas of synthetic organic and medicinal chemistry while focusing on development of new synthetic methods for heterocyclic compounds through C-H activation/ functionalization. He has guided 10 PhD students and currently supervising five PhD students. Prof. Kumar has published 155 research articles in journals of international repute with over 3400 citations and h-index of 28. Additionally, to his credit he also has one US patent. He has handled several major projects funded by DST, UGC, CSIR and Ranbaxy Labs. He has also delivered several invited talks in various national and international conferences.

# Dehydrogenative C–H/X–H Annulation under Transition-Metal Catalysis: Efficient Access to Polyheterocyclic Frameworks

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Transition-metal-catalyzed dehydrogenative C–H/X–H annulation has become a robust and atom-efficient approach for the construction of polycyclic architectures in recent years.<sup>1</sup> The direct coupling of unactivated C–H bonds with X–H functionalities (X = N, O, S) eliminates the need for pre-functionalized substrates, offering improved atom- and step-economy and sustainability. Among polycyclic architectures, polyheterocyclic compounds are vital structural motifs which are core structures in natural products, pharmaceuticals, and functional materials. Conventional synthetic routes for these compounds often rely on pre-functionalized substrates, compromising atom economy and step efficiency. Our research explores catalyst design and reaction development for transition-metal-catalyzed dehydrogenative annulation of heteroarene with different coupling partners, offering access to structurally complex and functionally rich frameworks (Figure 1).<sup>2</sup> This lecture will present recent developments in catalyst systems, mechanistic insights, and reaction design, with emphasis on selectivity control and redox-economical processes. Mechanistic insights derived from these studies contribute to the broader understanding of C–H functionalization chemistry and demonstrate the potential of dehydrogenative annulation as a robust method for constructing polyheterocyclic architectures. Representative applications in the synthesis of structurally complex heterocycles of relevance to medicinal and materials chemistry will be highlighted.



Figure

1: Transition-metal-catalyzed dehydrogenative annulation reactions.

Keywords: Transition metal, dehydrogenative annulation, heterocycle, C-H bond functionalization.

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### **Prof. Anindya Datta**

Prof. Anindya Datta, is Director of the Institute of Nano Science and Technology (INST), Mohali since December 4, 2025, and former Professor at IIT Bombay. He received his B.Sc. (1992), M.Sc. (1994) from University of Calcutta and Ph.D. (1998) from Indian Association for the Cultivation of Science, Kolkata. He worked as a Postdoctoral Researcher from 1998-2000 at Iowa State University, USA. He was promoted to Full Professor in 2012. He is an Elected fellow of the Indian Academy of Sciences, Bangalore (Jan 2026); Bronze Medallist, Chemical Research Society of India (2018); Fellow of National Academy of Sciences, India (2017). His research focuses on the photophysics of fluorescent molecules and nanomaterials, with expertise in ultrafast dynamics.



Publications : 181

# Rational design of molecules and experiments to unravel the intertwined interactions in fluorogens

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## Abstract

Fluorogenic molecules have diverse potential applications, e.g. in fluorescence sensing and as solid state emitters. The key to control their light emitting properties is in the design of conditions that suppress nonradiative deactivation pathways of their excited states. Dimethyl-2,5-bis(4- (methoxyphenyl) amino) terephthalate (DBMPT) is a fluorogen which exhibits Aggregation Induced Enhancement in Emission (AIEE). Pairing it with appropriate blue emitters result in white light emission. Curiously, such white light emission with thioflavin T-containing amyloid fibrils involves a disruption of the fibrils by the nanorods [1]. More recently, the role of polarity and aggregation on the fluorescence of a lipophilic derivative of DBMPT has been explored. It has been shown to have promise in tracking lipid droplets in live cells. Hence, fluorescence lifetime imaging microscopy (FLIM) has been used to monitor ferroptosis in mammalian cells [2]. The photophysics of a library of derivatives of DBMPT have also been explored in order to understand their suitability for applications in studies of biomolecular interactions [3, 4]. Another class of compounds that will be discussed are Schiff bases, which become strongly fluorescent upon rigidification and also exhibit room temperature phosphorescence under favorable conditions [5].

Keywords: Fluorogens, time resolved spectroscopy, live cell imaging

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## **Prof. Arvind Kumar**

Dr. Arvind Kumar is a distinguished Chief Scientist and Professor at the CSIR-Central Salt & Marine Chemicals Research Institute (CSMCRI) in Bhavnagar, India, specializing in ionic liquids, solution thermodynamics, and sustainable chemical technology. He completed his Ph.D. in chemistry from Kurukshetra University, India. He heads the Salt and Marine Chemicals Division, focusing on high-purity salt production, biomass processing, and green, sustainable, industrial applications. He is a recipient of the DAAD Fellowship (Germany, 2004-05), CSIR-Raman Research Fellowship (USA, 2011-12), and the CSIR Rural Technology Award (2008). Dr. Kumar has published over 100 research papers, contributed book chapters, and held several patents related to his work in chemical science and technology. His research aims to solve environmental and industrial challenges, such as saline effluent management and sustainable resource recovery.



## **Salt and Marine Chemicals Technologies: Current status, Bottlenecks and improved processes**

**Arvind Kumar**\*<sup>a</sup>

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### **Abstract**

Globally India is positioned third after China and USA in solar salt production with an annual production of higher than 40 MMT. More than 60% of the salt produced worldwide goes for industrial use (mainly chloralkali industry) and rest for edible and other usage. Almost all of the common salt in the country is produced from seawater/sub-soil brine or small quantities from Lake brines. The basic operation of a solar salt field incorporates the progressive evaporation and concentration of brine in specially designed solar pans. During the process of evaporation of brines a series of salts crystallizes out in the concentration ponds, the process being governed by the solubility products of the individual salts dissolved in it. The principal impurities in the salt are divalent ions, mainly, calcium and magnesium cations and sulphate anion. Over the last several years a series of inventions have taken place which have enabled to vastly improve the quality of solar salt – be it produced for industrial, edible or specialty applications. Bittern (left out liquor after salt production) is rich source of marine chemicals viz. potassium, magnesium, bromine and other trace minerals. Processes for utilization of sea bittern as resource for recovery of marine chemicals, major challenges and improved technologies will be covered in the presentation.

**Keywords:** Ionic interactions, solubility, solar salt; chloralkali industry; industrial grade salt, edible salt; low sodium salt marine chemicals.

## Prof. Ayyappanpillai Ajayaghosh

Prof. Ayyappanpillai Ajayaghosh, currently S. S. Bhatnagar Chair Professor, SRM Institute of Science and Technology, Kattankulathur, Chennai, is the former Director of CSIR-NIIST and a J. C. Bose National Fellow at CSIR-NIIST, Thiruvananthapuram, India. He obtained masters and Ph. D. in chemistry from Calicut University. His research interests are in the areas of organic materials such as fluorescent materials, photoresponsive materials, organogels, molecular probes, covalent organic frameworks etc. He introduced a new class of soft materials namely  $\pi$ -gels and studied the fundamental science behind the creation of such materials, which was widely accepted by the scientific community. His research contributions are recognized with several prestigious awards including the Shanti Swarup Bhatnagar Prize for Chemical Sciences (2007), the Infosys Science Prize (2012), Khwarizmi International Award 2012, the Silver Medal of the Chemical Research Society of India (2013), the TWAS Prize for Chemistry 2013 and the Goyal Prize (2019). He was a Swarnajayanti Fellow and Ramanna Fellow of the DST, Govt. India and a DAE Outstanding Researcher. He is a recipient of The Thomson Reuters India Research Front citation award and the Clarivate Analytics (Web of Science) citation award. He is a Fellow of the three major Science Academies of India, an honorary fellow of the Kerala Academy of Sciences and a fellow of the World Academy of Sciences. Currently, he is a J. C. Bose National fellow of the DST-SERB, Govt. India. Prof. Ajayaghosh is in the editorial board of several international and national journals. His research findings and publications are well cited with around 20000 citations with an h-index of 70. He has published 201 peer reviewed research papers, contributed to six book chapters and granted/filed 28 patents. Some of his patents have been sold to industries. He has mentored 37 Ph.D. researchers. He has published the highest number of research papers in the journal *Angewandte Chemie* by an Indian scientist and his author profile have been featured in the same journal.



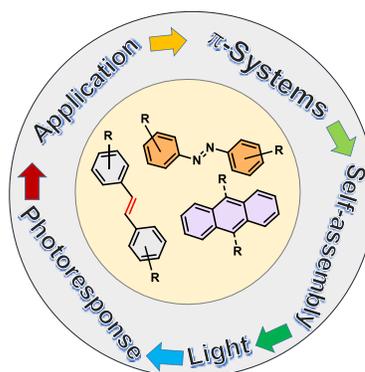
# Photoresponsive Supramolecular Systems for Thermo-responsive Smart Windows

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Integration of photoresponsive units into  $\pi$ -systems are meant to address key challenges in developing responsive and adaptive soft functional materials that dynamically respond to light. Photoresponsive dynamic supramolecular systems are one of the preferred choices in the emerging domain of smart materials, particularly in the field of photonics and nanoarchitectonics. Our expertise in supramolecular chemistry and photochemistry helped us in the construction of small molecules based supramolecular assemblies<sup>1,2</sup> for energy transfer,<sup>3,4</sup> chiral inversion,<sup>5</sup> morphology modulation<sup>6</sup> and device application.<sup>7</sup> Recently we have shown that photocycloaddition and photoisomerization reactions can be applied to modulate the Lower Critical Solution Temperature (LCST) of molecular assemblies<sup>8</sup> for the construction of smart windows that can regulate the heat generating near-IR and IR radiations.<sup>9-11</sup> LCST phenomenon is a thermo-responsive property exhibited by amphiphilic polymers and small molecular  $\pi$ -systems which can be modulated by incorporating photoresponsive moieties. This talk is mainly focused on the use of photoisomerization and photocyclization reactions to modulate LCST property of  $\pi$ -systems for their application in the construction of energy saving smart windows.



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## Dr. Debabrata Patra

Dr. Debabrata Patra is an Associate Professor of Chemistry at IISER Mohali. He earned his M.Sc. (2005) from IIT-Bombay and then Ph.D. (2010) from University of Massachusetts Amherst, USA. He worked as a postdoctoral fellow at Pennsylvania State University (2011 – 2013); Texas A&M University (2013 – 2014) and University of Zurich (2015 – 2016) Zurich, Switzerland.



Currently his group is focusing on (i) Self-powered supramolecular assembly (ii) Self-powered enzyme biosensors for lab-on-a-chip based detection (iii) Self-assembly at liquid-liquid interface (iv) Macroscopic self-assembly. He has published ~50 papers in reputed journals.

# Active Fluidics: Translating Molecular Activity into Macroscopic Motion

Debabrata Patra\*

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**Abstract:** Active fluids are intrinsically non-equilibrium systems in which continuous internal energy transduction drives autonomous flow, transport, and function. This work demonstrates how these principles can be harnessed to engineer self-powered fluidic systems that translate molecular-scale events into macroscopic motion and directly readable outputs. Biocatalytic micropumps that generate sustained fluid flow via enzymatic reactions are introduced, enabling label-free sensing of inhibitors and analytes through simple monitoring of macroscopic flow responses. To expand substrate scope and functionality, supramolecular micropumps are developed that enable programmable cargo transport while amplifying molecular recognition events across length scales, from “host-guest” interactions to macroscopic fluid motion, thereby achieving highly sensitive detection. Building on these concepts, light-powered micropumps are designed to operate without chemical fuel consumption or waste generation, offering a sustainable platform for integration into microfluidic and point-of-care diagnostic technologies.

Keywords: active fluidics, self-powered micropumps, powerless microfluidics.

## Dr. Durga Prasad Hari

Dr. Durga Prasad Hari is an Assistant Professor at Indian Institute of Science Bangalore. Durga Prasad Hari received his MSc degree from IIT Madras in 2010. He then moved to the University of Regensburg, Germany, where he pursued his Ph.D. with Prof. Burkhard König. In 2014, following his graduate education, he was a postdoctoral fellow in the laboratory of Prof. Jerome Waser at EPFL, Switzerland. In 2018, he joined the Aggarwal group at the University of Bristol as a Marie-Curie research fellow.



Since March 2021, he is holding an assistant professor position at the Indian Institute of Science Bangalore. His research group aims to discover and develop novel reaction strategies, which will enable access to versatile reactive intermediates for the mild and sustainable synthesis of useful molecular scaffolds.

Publications = 41, Citations = 5,926, h-index = 23

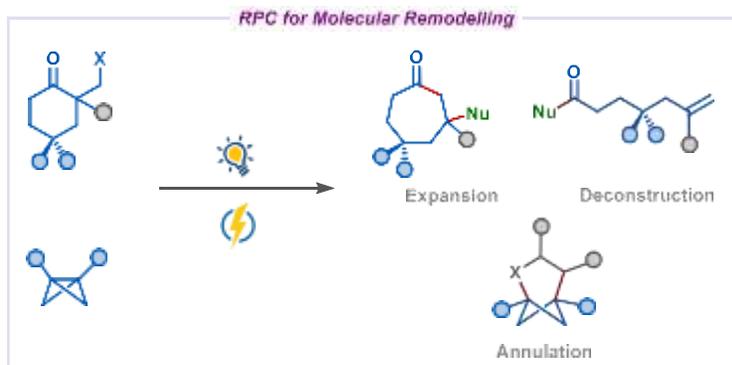
# Radical-Polar Crossover for Molecular Remodelling

**Durga Prasad Hari**

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Radical-Polar Crossover (RPC) is an effective method in organic synthesis that integrates both radical and ionic species. Since the reactivities of radical and ionic intermediates are orthogonal, using these two mechanisms in sequence offers significant advantages in molecular remodelling. In this lecture, I will first discuss a photoredox-catalyzed Dowd-Beckwith ring-expansion/RPC strategy for synthesizing functionalized medium-sized carbocyclic compounds.<sup>1</sup> Recently, deconstructive strategies have garnered attention as efficient methods for molecular remodelling. However, the selective cleavage and functionalization of inert C–C bonds, particularly within unstrained cycles, remains a considerable challenge. In the second part of the lecture, I will present an RPC Interrupted Dowd–Beckwith reaction, which provides a robust approach for C–C bond cleavage and functionalization.<sup>2</sup> This deconstructive strategy is applicable to medium-sized (hetero)carbocycles and macrocycles, thereby expanding its utility for challenging synthetic transformations. Finally, I will discuss a strain-enabled RPC strategy for the unified synthesis of spiro-, fused-, and enantioenriched aza/oxa-bicyclo[3.1.1]heptanes.<sup>3</sup>



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## Prof. D. B. Ramachary

Prof. Ramachary graduated with a M.Sc. degree in Chemistry from the University of Hyderabad and obtained a PhD in synthetic organic chemistry from the Indian Institute of Science, Bangalore in 2001. He subsequently held a postdoctoral position at the Scripps Research Institute for Catalysis, prior to joining the University of Hyderabad in January 2005, where presently he is a full professor of organic chemistry. He has been the recipient of many awards including Fellow of the National



Academy of Sciences (Allahabad, 2021), Fellow of the Royal Society of Chemistry (London, 2020) and Fellow of Indian Academy of Sciences (Bangalore, 2018). He has guided 20 PhD students, 13 PDFs and out of them, 5 got Eli Lilly & Company Asia Outstanding Thesis Awards. He is an Editorial Advisory Board Member for Organic & Biomolecular Chemistry (2013-present), European Journal of Organic Chemistry (2017-present) and Tetrahedron Chem (2021-present). Prof. Ramachary has published more than 113 research papers, 2 books on emerging organocatalysis areas, delivered over 130 lectures in national/international conferences and has a few chemical reactions named after him. His research findings and publications are well cited with around 6717 citations with an h-index of 44.

## Constructing Chiral Molecules *via* Low-loading Organocatalysis

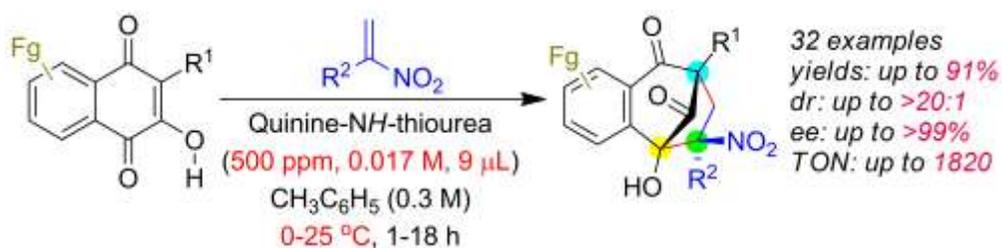
**Sr. Prof. Dhevalapally B. Ramachary\***

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Recently emerging approaches for novel chemistry developing based on the bio-based/renewable feedstock, sustainable catalysis for a circular and sustainable chemical sector.

In this regard, recently, we have discovered an organocatalytic, ppm-level, asymmetric enol–olefin [3+2]-annulation reaction of a variety of enolizable 3-alkyl lawsones with nitroethylenes under the ambient conditions.<sup>[4]</sup> The ppm-level, catalytic asymmetric [3+2]-annulation reaction accommodates amazing features, such as low catalyst loading, high rate and selectivity, mild reaction conditions, easily available substrates with simple operation, and excellent yields, *ee*, *dr* with a broad spectrum of substrates.<sup>[4]</sup> It accolades the previously known annulation reactions.<sup>[1-3]</sup> More details on this new catalytic asymmetric annulation reaction will be discussed how this reaction is under the category of sustainable catalysis for a circular and



sustainable chemical sector.

**Scheme:** Catalytic asymmetric annulations under the low-loading of organocatalysts

**Keywords:** asymmetric catalysis; organocatalysis; ppm-loading; lawsone; nitroethylenes

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## **Prof. Dilip K. Satapathy**

Dilip k. Satapathy is a Professor in the Department of Physics, IIT Madras. He completed his B. Sc. (1997) from Nayagarh College, Utkal University, Bhubaneswar, India; M. Sc. (2000) from Department of Physics, Utkal University, Bhubaneswar, India; M. Tech (2002) from Department of Physics, Indian Institute of Technology (IIT), Delhi, India; Ph.D. in Physics (2005) from Paul-Drude-Institut and Dept. of Physics, Humboldt University, Berlin, Germany. He subsequently held a postdoctoral position with Prof. Dr. Christian Bernhard (2009 – 2012) at Department of Physics, University of Fribourg, Switzerland; with Prof. Dr. J. F. van der Veen (2006 – 2009) at Swiss Light Source (SLS), Paul Scherrer Institute, Villigen PSI, Switzerland.



His research interests include Polymer physics, X-ray and neutron scattering, Responsive soft matter, Self-assembly of colloids, Soft thermoelectrics for energy harvesting. He is a recipient of Early Career Institute Research and Development Award (IRDA), IIT Madras (2018), Young Scientist Awards (YSA), Academy of Sciences, Chennai (2017), Young Faculty Recognition Award (YFRA), IIT Madras (2017) and DAE Young Scientist Research Award (DAE-YSRA) for the project entitled “Glass Transition in Confined Polymers” (2014).

## **Bioinspired Soft Actuators and Flexible Thermoelectrics for Wearable and Adaptive Technologies**

**Dillip K. Satapathy**

*Soft Materials Laboratory, Department of Physics, IIT Madras, Chennai-600 036, India*

This talk will highlight recent advances from our group on the design and fabrication of soft thermoelectric materials for wearable and flexible electronics. By strategically selecting and optimizing composite materials, we have successfully harnessed temperature differences between the human body and the environment to *generate significant voltages*, under realistic operating conditions. In addition, I will discuss our work on moisture-driven, fully reversible protein-based soft actuators that exhibit rapid, sub-second responses. This performance is achieved through precise control of the intrinsic microstructure and mechanical properties of the protein films, without the need for complex external stimuli. The talk will further highlight the role of advanced fabrication strategies, including 4D printing, in enabling programmable and responsive material systems.

## Dr. Ekambaram Balaraman

Ekambaram Balaraman, is an assistant professor at Indian Institute of Science Education and Research, Tirupati. He completed his Ph.D. in 2008 from the University of Hyderabad. He is recipient of Swarnajayanti Fellowship, DST (2020), CRSI Bronze Medal (2019), Dr. A. V. Rama Rao (AVRA) Young Scientist Award (2018), Elected Fellow of the Indian National Young Academy of Sciences (INYAS), New Delhi (2018), Fellow of the Royal Society of Chemistry (FRSC). Dr. Ekambaram



Balaraman's research interest mainly includes mechanistic approach to design and development of novel catalysts/catalytic materials for fundamentally important organic transformations which are of industrial importance. In particular dehydrogenation of feedstock chemicals (hydrogen generation), C-1 chemistry (includes CO<sub>2</sub> to value added chemicals and polymer), and development of novel donors in Ziegler-Natta polymerization catalysis. He has published ~140 papers in reputed journals.

Citations = 9375, H index = 51

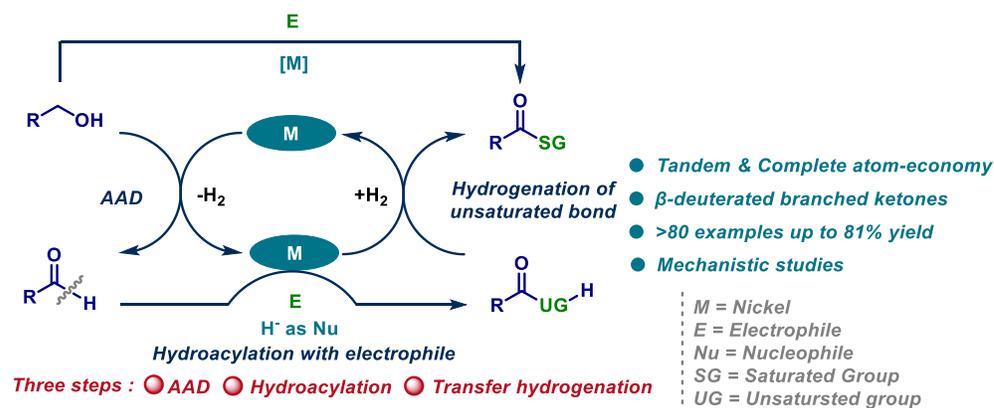
# Advancing Sustainable Chemical Production via Dehydrogenation Catalysis

Ekambaram Balaraman\*<sup>1,2</sup>

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In the realm of synthetic organic chemistry, the pursuit of novel methods for complex chemical synthesis presents both intriguing opportunities and formidable challenges. Traditionally, alcohols serve as alkylating agents in forming C-C and C-N bonds through a dehydrogenative borrowing hydrogen approach in transition-metal catalysis. However, their use as acylating agents in C-C bond formation is notably difficult and infrequently documented. This study introduces the dehydrogenative coupling of benzylic alcohols with internal alkynes under nickel(II) catalysis, employing alcohols as acylating agents. The process yields an array of  $\alpha$ -branched aryl ketone derivatives, achieving zero waste via an umpolung borrowing hydrogen technique. Additionally, the study showcases the versatile applications of the resulting  $\alpha$ -di-substituted ketones as precursors for other valuable compounds, including the large-scale production of  $\beta$ -deuterated branched ketones. To shed light on the underlying reaction mechanism, a series of spectroscopic analyses, the identification of intermediates, and density functional theory calculations were conducted.



**Figure 1.** Nickel-catalyzed dehydrogenative coupling of alcohols with internal alkynes.

## Dr. Gokulnath Sabapathi

Dr. Gokulnath Sabapathi is an Associate Professor of Chemistry at IISER Thiruvananthapuram. He earned his B.Sc. (2000), M.Sc. (2002) and then Ph.D. (2009) from IIT Kanpur focuses on near-IR applications and solar cell materials. He further pursued a postdoctoral stint in the laboratory of Prof. Hiroyuki Furuta at Kyushu University, Japan in March, 2009, in exploring the unique properties of N-Confused Porphyrinoid systems. In 2012, he moved to National University of Singapore to join the research group of Prof. Chi Chunyan to work in the area of  $\pi$ -conjugated systems targeting n-type semiconductor materials based on acenes and heteroacenes. In 2013, he joined Inorganic and Physical Chemistry at Indian Institute of Chemical Technology (CSIR-ICT, Hyderabad, India as a DST-Inspire Faculty and worked until August, 2015. His research area covers synthesis of planar p-conjugated macrocycles for near-IR applications, molecular probes for toxic elements, exploring new DSSCs and heteroditopic receptors. He has published ~50 papers in reputed journals.



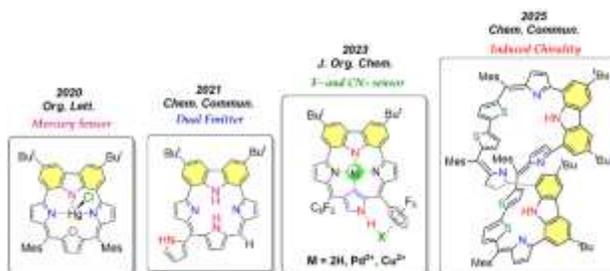
# Carbazole Embedded Macrocyclic Systems with Multifaceted Properties

**Gokulnath Sabapathi**\*<sup>a</sup>

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The synthesis of a new class of carbazole based porphyrin-like macrocycles via [3+1] acid condensation along with its metal complexes will be presented. All the macrocycles showed partial aromatic character and red-shifted emission starting from 600 nm which makes them unique in comparison to other carbazole based modified porphyrins reported.<sup>[1,2]</sup> The presence of porphyrin-like cavity allowed us to conduct the metal binding studies and observed the colorimetric changes that these macrocycles could be used as selective Hg<sup>2+</sup> ion sensors.<sup>[3a]</sup> Further, an inverted pyrrole incorporated macrocycle showed anion binding property in a reversible manner in a nanomolar scale.<sup>[3b]</sup> During our continuous efforts in constructing new macrocycles incorporated with carbazole as a subunit, an unprecedented formation of *meso*-pyrrole embedded carbazole-based porphyrin was obtained which was structurally characterized. Such introduction lowers the structural symmetry and exhibits dual emission, which strongly depends on the excitation wavelength and temperature. The origin of dual emission induced by NH-tautomerism is confirmed by photophysical and DFT calculations.<sup>[3c]</sup> Lastly, I will discuss about an unprecedented formation of carbazole-embedded decaphyrin through acid-catalyzed condensation. Single crystal X-ray diffraction analysis revealed that the macrocycle adopted a ‘figure-of-eight’ structure, wherein two pyrrole and thiophene rings were inverted. The absorption spectrum of the macrocycle exhibited ill-defined band and shows specific affinity towards soft metal ions such as Ag<sup>+</sup> and Hg<sup>2+</sup>.<sup>[3d]</sup>



**Keywords:** Ion-sensors, dual emitters, helically chiral macrocycles

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## **Prof. Jayamurugan Govindasamy**

Govindasamy Jayamurugan is a Professor at Institute of Nano Science and Technology, Mohali, India. He received his B.Sc. in 2001, M.Sc. in 2003 and Ph.D. in 2009 from Indian Institute of Science (IISc), Bangalore, India. He worked as a postdoctoral fellow at ETH-Zurich, Switzerland (Prof. François Diederich) from 2010-2012 and at University of Cambridge, United Kingdom, (Prof. Jonathan R. Nitschke). He is recipient of Ramanujan Fellowship, Early Career Research (ECR) Awards. His research interests include New synthetic methods, Functional organic materials, Supramolecular chemistry and Polymer chemistry. He has published over 50 papers in reputed journals.



# Functional Organic Materials: From Molecular Design to Broad Applications

**Govindasamy Jayamurugan\***<sup>a</sup>

<sup>a</sup> Institute of Nano Science and Technology, Sector-81, Mohali-140306, Punjab, India

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Functional organic materials engineered through molecular design and nanotechnology offer versatile solutions across energy, environment, health, and sensing. In this presentation, I highlight key advances from our Functional Organic (Nano) Materials Lab, where supramolecular chemistry, polymer science, and nanoscale engineering converge to create highly functional organic systems. Our research bridges fundamental molecular design with practical applications, emphasizing controllable structure–property relationships that enable performance across diverse platforms.

We have developed push–pull urea chromophores for selective ion and fluoride sensing and engineered organic fluorescent materials for live-cell imaging.<sup>1</sup> These molecular systems extend into hybrid nanomaterials, including sustainable Cu-nanostars derived from sporopollenin and biocidal carbon dots with antibacterial and imaging capabilities.<sup>2</sup> Additionally, our work on polymer-based magnetic nanoformulations and cellulose-grafted nanoparticles demonstrates translation into targeted drug delivery and therapeutic functions.<sup>3</sup> Across these projects, molecular tuning and supramolecular interactions have been central to achieving desired functionality. The presentation connects innovative design strategies with application outcomes, underscoring how tailored organic architectures can address pressing technological and societal challenges. This talk will provide a cohesive perspective on the design, development, and broad utility of functional organic materials.



**Keywords:** Functional Organic Materials, Self-Assembly, Hybrid Nanostructures, Nanotechnology

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## **Prof. Nilmoni Sarkar**

Nilmoni Sarkar is a Professor at Indian Institute of Technology (IIT) - Kharagpur, India. He received his B.Sc. in 1986, M.Sc. in 1988 from University of Burdwan and Ph.D. in 1994 from Indian Association for the Cultivation of Science- 1994, Under the supervision of Prof. Kankan Bhattacharyya. He worked as a JSPS short-term postdoctoral fellow- March 1996, with Professor K. Yoshihara at the Institute for Molecular Science (IMS), Japan Postdoctoral fellow- June 1996 - February 1998, with



Professor H. Hayashi at RIKEN, Japan. JSPS postdoctoral fellow- March 1998 - June 1998, with Professor T. Tahara at IMS, Japan. He is an elected Fellow of the National Academy of Sciences, India (NASI), 2018.

# Understanding The Self-Assembly of Biological Building Block Molecules and Their Potential Applications

**Nilmoni Sarkar\***

*Department of Chemistry*

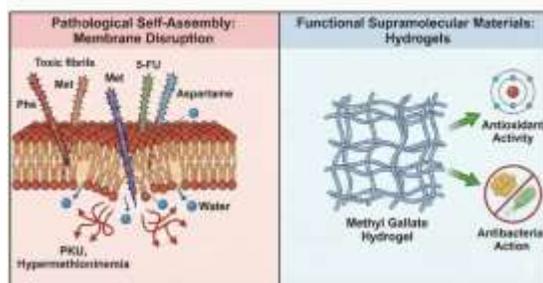
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## Abstract

The pathological deposition of amyloid-like fibrillar assemblies is recognized as a critical factor in the etiology of various neurological and metabolic disorders. To unveil the molecular mechanisms underlying these pathologies, the self-assembly of amino acids—specifically Phenylalanine, Tryptophan, and Methionine—and their derivatives, such as the artificial sweetener Aspartame and the drug 5-Fluorouracil, was characterized. The interaction of these assemblies with artificially synthesized lipid membranes (DMPC, LAPC, and Oleic acid) was investigated using a combination of time-resolved spectroscopy and high-resolution microscopy. It is indicated by the cumulative results that the integral rigidity is strongly hampered and the hydration dynamics of the model membrane are altered by these fibrillar assemblies. A molecular rationale is thus provided for amyloid-induced disorders, such as Phenylketonuria (PKU) and Hypermethioninemia. Crucially, the role of morphological polymorphism is highlighted, wherein membrane toxicity is shown to be governed by metastable fibrillar forms rather than thermodynamically stable crystals, and the enhanced virulence of cross-assemblies is revealed. Complementing this pathological investigation, similar supramolecular principles were harnessed to engineer functional biomaterials. The ultrasound-assisted hydrogelation of polyphenolic molecules, specifically Methyl Gallate, is presented. Unlike the toxic amino acid fibrils, excellent cytocompatibility, potent antioxidant activity, and dual antibacterial efficacy against both *S. aureus* and *E. coli* are demonstrated by these engineered supramolecular hydrogels. Furthermore, "crosstalk-assisted" assemblies of Gallic Acid and Methyl Gallate, which exhibit enhanced cytotoxicity against cancer cells, are discussed. The gap between deciphering the membrane-active toxicity of metabolite assemblies and utilizing controlled self-assembly to design novel therapeutic hydrogels will thus be bridged by this presentation.



## **Prof. Nitin T. Patil**

Dr. Nitin T. Patil, is a Professor at Indian Institute of Science Education and Research Bhopal. He received his B.Sc. (1995), M.Sc. (1997) from North Maharashtra University, Jalgaon and Ph.D. (2002) from University of Pune, Pune. He worked as a Postdoctoral Researcher at University of Gottingen, Germany and JSPS Post-Doctoral Fellow, Tohoku University, Japan. He is an elected fellow of Indian Academy of Sciences (FASc) – 2026; Indian National Science Academy (FNA) – 2022, The National Academy of Sciences (FNASc) – 2021. He is recipient



of CNR Rao National Prize for Chemical Sciences – 2024; J. C. Bose National Fellowship – 2023; Chemical Research Society of India (CRSI) Bronze Medal – 2018. The key research area are Organic Synthesis, Metal Catalysis, Organocatalysis, Photoredox Catalysis, Electro-organic Synthesis, Asymmetric Catalysis, Total Synthesis.

Total Publications: 178; Total Citations: 10300; h-index: 57; i10-index: 135

## Enantioselective Gold Redox Catalysis

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Traditionally, gold complexes have been recognized as Lewis acid catalysts for the activation of C-C multiple bonds (Scheme, LHS). Over the years, there has been a considerable shift, and Au(I)/Au(III) redox catalysis is now recognized as an established technique for achieving cross-coupling reactivities (Scheme, RHS). The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple ( $E_0 = +1.41$  V) and to facilitate two-electron redox cycle in gold catalysis. Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes. Recently, ethynylbenziodoxolones (EBXs) have also been used for accessing redox gold catalysis serving dual role as oxidant and alkyne surrogate.

All the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remained forbidden. In recent years, ligand-enabled gold redox catalysis have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will present some of our recent work on enantioselective gold redox catalysis.

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## **Prof. Pannuru Venkatesu**

Dr. Pannuru Venkatesu was awarded PhD in 1995 at Sri Venkateswara University, Department of Chemistry, Tirupati, Andhra Pradesh, India. In 1995, Research Associateship awarded by CSIR, New Delhi and in 2006, he was also awarded Fast Track Young Scientist by DST, New Delhi. He has post-doctoral research experience from Warsaw University of Technology (Poland), The University of Texas Medical Branch (UTMB) USA, Academia Sinica (Taipei, Taiwan),



National Taiwan University of Science and Technology (Taipei, Taiwan). Dr. Venkatesu is a recipient of Bronze Medal– 2017 from Chemical research Society of India (CRSI), Bangalore and Professor S. S. Katiyar Endowment Lecture award (2016-2017) from the Indian Science Congress Association, India. His general research focused on thermodynamic and physicochemical properties of novel class of ionic liquids and liquid mixtures, protein folding / unfolding in presence of co-solvents (osmolytes, denaturants and ionic liquids), Effect of polymer chain or IL in coexisting liquid phases. Dr. Venkatesu has published 162 research papers in internationally reputed journals.

## **Sustainable Solvents for Pharmaceuticals: Role of Ionic Liquids/ Deep Eutectic solvents in Pharmaceutical Formulations**

**Pannuru Venkatesu\***

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The design of biologic and synthetic drugs in the pharmaceutical industry is facing three key challenges, namely, ensuring bioavailability, solubility, and stability. Ionic liquids (ILs) and deep eutectic solvents (DESs), classified as designer solvents, have emerged as excellent solvents for improving the permeability and stability of biotherapeutic drugs. Moreover, they have shown remarkable solubilizing effects for synthetic drugs, particularly in solubilizing active pharmaceutical ingredients (API) and are known as eco-friendly solvents. Thus, we have reported the development of designer formulations in pharmaceutical industries and examined the underlying strategies for designing the most efficient formulations for both biotherapeutics and synthetic drugs. All over, for the first time, with different experimental approaches, the impact of each biomaterial individually and in combination is explored to study their effect on the stability of antibodies. Thus, better efficient formulations can be designed for the storage/packaging of IgG-based drugs which ultimately will have more applicability in pharmaceuticals.

**Keywords:** Sustainable Solvents, Eco-friendly solvents, Antibodies

### **References:**

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## **Prof. Rajneesh Misra**

Rajneesh Misra is currently a Senior Professor in the Department of Chemistry, Indian Institute of Technology (IIT) Indore. He received his master's degree from the University of Gorakhpur, after that, he moved to the Indian Institute of Technology (IIT) Kanpur for his PhD in chemical sciences (2007). After two successive postdoctoral stays at the Georgia Institute of Technology, Atlanta, USA, and Kyoto University, Japan, he joined IIT Indore, India, as an Assistant Professor in 2009.



In 2017 he was promoted as full Professor. His research interests lie in the areas of organic photonics, organic electronics, Supramolecular Chemistry, and Organometallic Chemistry.

## Mechanochromism, Peizochromism and Room Temperature Phosphorescence in Isomeric Phenothiazines

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The solid-state emission of fluorophores can be enhanced by minimizing the  $\pi$ - $\pi$  Stacking.<sup>1</sup> Phenothiazine is having a butterfly shape and its derivatives undergoes rapid conformational change, under external stimuli. In this presentation, I will be talking about the strategies for tuning the emission and room temperature phosphorescence of phenothiazine derivatives.<sup>2,3</sup>

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## Prof. Sanjay Singh

Sanjay Singh is a Professor in the Department of Chemical Sciences at the Indian Institute of Science Education and Research (IISER) Mohali. He earned his B.Sc. (2000) from Banaras Hindu University M.Sc. (2002) from Indian Institute of Technology Kanpur and then Ph.D. (2006) from University of Goettingen, Germany. He further pursued postdoctoral stints at University of Cambridge, UK, (Advisor: Prof. Dominic S. Wright) and University of Goettingen, Germany, (Advisor: Prof.



Dr. Herbert W. Roesky) between 2006-2007. He joined IISER Mohali as an assistant professor in 2008. He is Elected as Young Associate of the Indian Academy of Sciences, Bangalore for 2009-2013. He specializes in inorganic chemistry, specifically in the synthesis of novel organometallic compounds, and molecular catalysts. His research often involves X-ray crystallography and catalytic applications of main group elements.

# Phosphazane Based Macrocycles: From Molecular Design to Tunable Properties

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Abstract: The area of organic macrocycles such as crown ethers, calixarenes, and cryptands is well. In contrast to this, the area of inorganic macrocycles is still in its infancy. The different valence and oxidation state of the constituent *p*-block inorganic atoms in the backbones of macrocycles have a profound effect on the size of the macrocycle, donor-acceptor properties, and overall bonding arrangement.<sup>1</sup> However, the targeted synthesis of inorganic macrocycles is not an easy task due to the lack of general synthetic routes and the difficulty in purification of the cyclic.<sup>1</sup>

This work will swirl around a variety of novel macrocycles involving the popular dichlorocyclodiphosph(III)azane, [ClP(N-tBu)]<sub>2</sub> as the building block (for example **A**, Figure 1).<sup>2</sup> Using a systematic strategy the reaction of the dimer [(Cl)(E=)P(μ-NtBu)]<sub>2</sub> with sodium metal gave the macrocyclic, E-bridged hexamer [(E=)P(μ-NtBu)<sub>2</sub>P(μ-E)]<sub>6</sub>, via head-to-tail cyclisation of the intermediate anion (E = S, Se) (**B**, Figure 1).<sup>3</sup> Inspired by the three-dimensional cavities and strong encapsulation properties of [2.2.2] cryptands, the first cyclodiphosphazane (P<sub>2</sub>N<sub>2</sub>)-based bicyclic macrocycles adopting a cryptand-like topology [TEA<sub>2</sub>-{P<sub>2</sub>(μ-N<sup>t</sup>Bu)<sub>2</sub>}<sub>3</sub>] and [TREN<sub>2</sub>-{P<sub>2</sub>(μ-N<sup>t</sup>Bu)<sub>2</sub>}<sub>3</sub>] (TEA = triethanolamine, TREN = tris(2-aminoethyl)amine) have also been synthesized (**C**, Figure 1) overcoming long-standing synthetic barriers that have hindered access to bicyclic phosphazane systems.

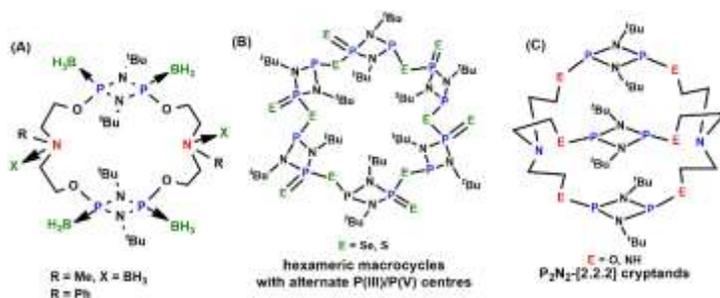


Figure. Selected examples of P<sub>2</sub>N<sub>2</sub> framework containing macrocycles.

Keywords: Macrocycles, Phosphazanes, Cryptands, Chalcogens, Host-guest Complexes

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## **Prof. Saptarshi Mukherjee**

Saptarshi Mukherjee is a Professor at Indian Institute of Science Education and Research, Bhopal, India. He received his B.Sc. (1999), M.Sc. (2001) from Jadavpur University, Kolkata, India and Ph.D. (2006) from Indian Association for Cultivation of Science, Kolkata, India. He worked as a postdoctoral fellow at Center for Photochemical Sciences, Bowling Green State University Ohio, USA (2006-2008). He is a recipient of INSA Medal for Young Scientists, 2012 from Indian National Science Academy.



Publications = 131, Citations = 3,640, h-index = 34

# Intracellular Subdegree Temperature Sensing and Dynamics by Thermo-responsive Silver Nanoclusters as Molecular Probes

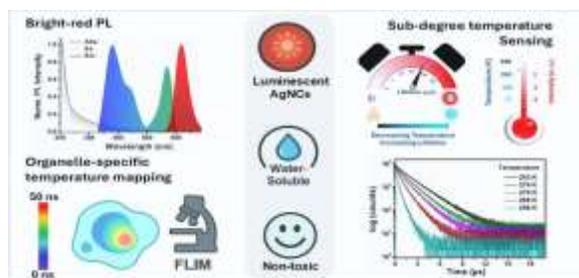
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Noble metal nanoclusters (MNCs) have emerged as promising alternatives to organic dyes and quantum dots due to their robust stability, superior biocompatibility, and tunable physicochemical properties.<sup>1,2</sup> However, their full potential in theranostics, sensing, and biological imaging has yet to be realized. Here, we report long-lived, red-luminescent silver nanoclusters (AgNCs) stabilized by the small-molecule ligand thiolactic acid, which exhibit exceptional stability (shelf-life exceeding three years, photostability ~100%), water-solubility, and high biocompatibility, making them suitable for diverse applications such as sensing and live-cell imaging.<sup>3</sup> AgNCs display extremely sensitive ( $>2\% \text{ K}^{-1}$ ) and reversible luminescence responses to temperature, enabling subdegree ( $<0.5 \text{ K}$ ) precision in local thermal mapping through simultaneous monitoring of emission intensity and excited-state lifetime. Cellular assays, including MTT viability tests, confocal fluorescence imaging, and fluorescence lifetime imaging microscopy (FLIM), suggest that the non-cytotoxic AgNCs specifically stain lysosomes in live mammalian cells, functioning as an organelle-specific biomarker and providing critical insights into lysosomal dynamics and intracellular temperature fluctuations.<sup>3</sup> The unique properties of these AgNCs, corroborated by detailed mechanistic studies, open new avenues for studying nanoscale subcellular physiology and developing temperature-sensitive diagnostics and preservation strategies.



The schematic representation of the work, reflecting the salient features of the present investigation.

## **Dr. Soumit Sankar Mandal**

Dr. Soumit Sankar Mandal, is an Assistant Professor at Indian Institute of Science Education and Research, Tirupati. He completed his Ph.D. in 2013 from Indian Institute of Science, Bangalore. He worked as a postdoctoral fellow at Technical University of Munich, Germany. He is an Alexander von Humboldt Fellow, Germany. The main focus of their research group is to investigate the correlation between the structure and function of multidomain proteins using Spectroscopic and Single Molecule Optical tweezers technique.



# Surface-Engineered MXenes as Advanced Electrodes for Enhanced Charge Storage and Transport

**Soumit Sankar Mandal**<sup>\*a</sup>

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MXenes are a unique class of two-dimensional transition metal carbides and nitrides. They have attracted significant attention as alternative electrode materials due to their high electrical conductivity, tunable surface chemistry, hydrophilicity, and large electrochemically active surface area.

In this presentation we will describe how MXene has been utilized as an alternative electrode material to overcome limitations associated with slow charge transport and limited surface functionality. Pristine MXene was synthesized using a fluorine-based etching. Following this, solvothermal functionalization with lysine and glutamic acid were performed to introduce chemically distinct surface charges and modulate the interfacial properties of this MXene.

Structural, thermal, and surface characterization of pristine and functionalized MXenes was carried out using XRD, TGA, SEM, Raman and XPS spectroscopy, confirming successful etching, functionalization, and structural stability. Electrochemical characteristics were evaluated using cyclic voltammetry and electrochemical impedance spectroscopy. The functionalized MXene electrodes exhibited improved electrochemical performance compared to pristine MXene as evidenced by lower charge transfer resistance ( $R_{ct}$ ) and favorable diffusion coefficients ( $D$ ).

The reduced  $R_{ct}$  and enhanced  $D$  indicate efficient charge transport and improved charge storage capability at the electrode–electrolyte interface, highlighting the beneficial role of amino acid functionalization. These findings demonstrate that surface-engineered MXenes represent a promising material for next-generation electrodes in energy storage and sensing applications.

Keywords: MXene, Surface functionalisation, Charge transport, Storage

## **Prof. Tharamani C. Nagaiah**

Tharamani C. Nagaiah is Professor and Head of the Department of Chemistry at IIT Ropar, specializing in electrochemistry, fuel cells, and nanostructured materials for energy storage. She is a highly decorated researcher, holding an AvH Postdoctoral Fellowship and the Ramanujan Fellowship, with significant contributions to sustainable energy research. She completed her PhD (2005) from Bangalore University, with postdoctoral experience at the University



of Saskatchewan, Canada, and Ruhr University Bochum, Germany (AvH Fellow). She is a recipient of the Chemical Research Society of India (CRSI) Bronze Medal 2023, ECSI METROHM National Award 2023, and A.V. Rama Rao Prize for women 2024. She is Editor of ACS Chemistry of Materials (Jan 2024) and editorial board member of Sustainable Energy and Fuels. She is Fellow of the Royal Society of Chemistry (RSC) and Elected Fellow of the Indian Chemical Society.

## Designing greener energy conversion system for a sustainable future

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Global energy requirements are touching new meridians with the gradual advancement in the living standards and the day-by-day growing world population. This necessitates the exploration to seek for greener and sustainable energy reservoir systems which ought to be environmentally agreeable for such an intriguing purpose. Electrochemical energy conversion and storage devices offer some most alluring aptitudes for providing clean energy. To name a few of these include fuel cells, rechargeable metal-air/peroxide batteries and HCl/ H<sub>2</sub>S electrolysis and likewise.<sup>1,2</sup> Oxygen being central to the processes in these devices, a lot of attention has been focused upon the study of oxygen chemistry in terms of oxygen reduction reaction (ORR) and also Hydrogen evolution reaction (HER) and thence to the melioration of the associated electrocatalysts. In the past decade research has depicted tremendous improvement towards the betterment of fuel cells/Zn based batteries/hydrogen production in its legions of shortcomings or corrigible features.<sup>3,4</sup> But still an infinite pursuit towards the exploration of effective, sturdy and energy efficient catalysts continues. The talk addresses,

- several strategies pursued to replace noble-metal free electrocatalysts for ORR/HER.
- Zn based batteries
- visualization of local electrocatalytic activity by SECM.

Keywords: ORR, HER, electrocatalyst, Zn based batteries, SECM

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# Oral Presentations

## OP-1 Photocatalytic Pathways for the Remediation of Persistent Organic Pollutants

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### **Abstract**

The escalating concentration of Persistent Organic Pollutants (POPs), such as pesticides, industrial chemicals, and novel pharmaceutical residues, are a severe threat to the world ecologies, since they are highly toxic, bioaccumulative and not readily degraded by conventional wastewater treatment methods. Photocatalysis has become an ideal candidate solution to the cleanup of these invisible menaces, where light energy is used to catalyse the total mineralization of the complex organic structure to harmless byproducts such as H<sub>2</sub>O and CO<sub>2</sub>. Fundamental photocatalytic pathways of degrading POPs are examined in this presentation including the activation of semiconductor catalysts (e.g., TiO<sub>2</sub>, g-C<sub>3</sub>N<sub>4</sub>, and ZnO). When light is received, pairs of electrons and holes are created (e<sup>-</sup>/h<sup>+</sup>) triggers a redox cascade and generates highly reactive oxygen species (ROS) including hydroxyl radicals (\*OH) and anions of superoxide (\*O<sub>2</sub><sup>-</sup>). These species indiscriminately react with the strong chemical bonds of POPs and cleaves robust aromatic rings and halogenated chains which are not counteracted by biological processes. New developments in band-gap engineering and the creation of heterojunctions are pointed out as having the ability to extend the catalytic activity to a visible light spectrum and this will fully utilize the available solar energy. Moreover, photocatalysis is addressed in the context of a circular economy and discussed in terms of its opportunity to purify water cheaply and in a decentralized manner. Photocatalytic reaction bypassing the energy-demanding physical separation and utilizing light to catalyse chemical destruction provides a solid and sustainable move towards restoring polluted aquatic and terrestrial environments.

**OP-2 Decoding Thermoluminescence through First-Principles Modelling: Defect Chemistry and Emission Mechanisms in CaSO<sub>4</sub>: Dy , LiF-Based Phosphors and Optically Stimulated Luminescence (OSL) dosimeters.**

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Thermoluminescent dosimeters (TLDs) are indispensable tools in radiation protection, personnel monitoring, and environmental radiation surveillance. Despite decades of experimental investigations, the atomic-scale mechanisms governing trap formation, charge carrier dynamics, and luminescence emission remain incompletely understood at the microscopic level. This comprehensive review synthesizes recent advances in applying Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) to elucidate defect-induced trapping and recombination phenomena in benchmark TLD phosphors: CaSO<sub>4</sub>:Dy, LiF:Mg,Ti, and Al<sub>2</sub>O<sub>3</sub>:C (OSL). We examine defect formation energies, charge transition levels, dopant-host interactions, and electronic band structure engineering, with emphasis on correlating first-principles predictions with experimental glow-curve temperatures. This review addresses critical research gaps by synthesizing defect physics principles, computational methodologies, & mechanistic insights essential for rational design of next-generation radiation dosimeters with enhanced sensitivity, thermal stability, and dosimetric linearity. We conclude by highlighting the transformative potential of DFT-guided defect engineering in advancing radiation protection technologies for nuclear facilities, medical diagnostics, and environmental monitoring.

**Keywords:** Density Functional Theory, Thermoluminescence, Optically Stimulated Luminescence, Dosimetric Phosphors, CaSO<sub>4</sub>:Dy, LiF:Mg,Ti, Al<sub>2</sub>O<sub>3</sub>:C, Glow Curves, Radiation Dosimetry

## OP-3 Photoactivatable Ruthenium–Nitrosyl Nanocarriers for Controlled Nitric Oxide Delivery in Cancer Therapy

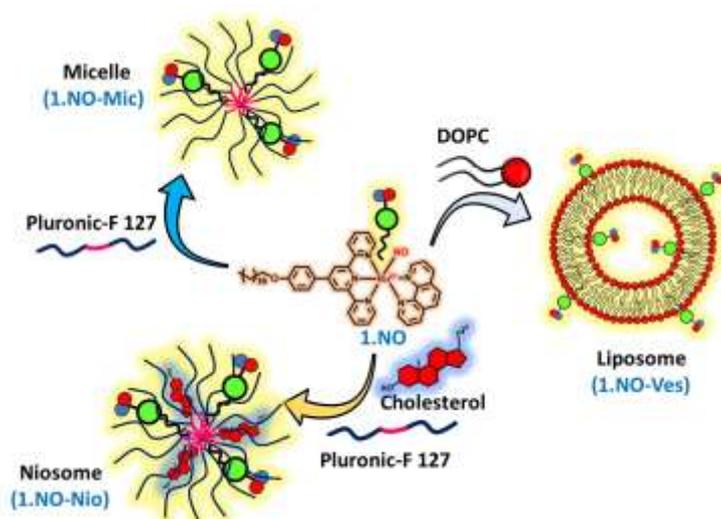
**D. Amilan Jose\***

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Nitric oxide (NO) has emerged as a critical signalling and therapeutic molecule, yet its biomedical application is hindered by rapid degradation, limited biocompatibility of conventional donors, and poor control over release. In this work, we present a newly synthesized amphiphilic ruthenium nitrosyl complex (**1.NO**) as a photoactivatable NO donor, along with its integration into three nanocarrier architectures: vesicles (**1.NO-Ves**), micelles (**1.NO-Mic**), and, for the first time, niosomes (**1.NO-Nio**). The NO-release profiles of free and encapsulated **1.NO** were systematically examined using UV–Vis spectroscopy, Griess assay, and DAF-FM DA fluorescence under 420 nm blue-light irradiation. Free **1.NO** generated up to 11  $\mu\text{M}$  NO, whereas nanoencapsulation enabled significantly prolonged and controlled release across all carrier types.

In vitro studies against the 4T1 breast cancer cell line revealed strong photo-induced cytotoxicity for the nanocarrier formulations, with **1.NO-Ves** demonstrating the highest therapeutic efficacy. These findings highlight the critical influence of nanocarrier design on the release kinetics and bioactivity of Ru–NO photodonors. Overall, this study establishes **1.NO**-based nanoplatforms as promising candidates for spatiotemporally controlled NO delivery in cancer therapy



**Keywords:** Nitric oxide delivery; Photoactivatable NO donor; Ruthenium nitrosyl complex; Nanocarriers; Phototherapy; Cancer therapy.

## OP-4 Photon-Primed Organic Electrosynthesis Enabled by Oxidation of Photon-Induced Intermediates

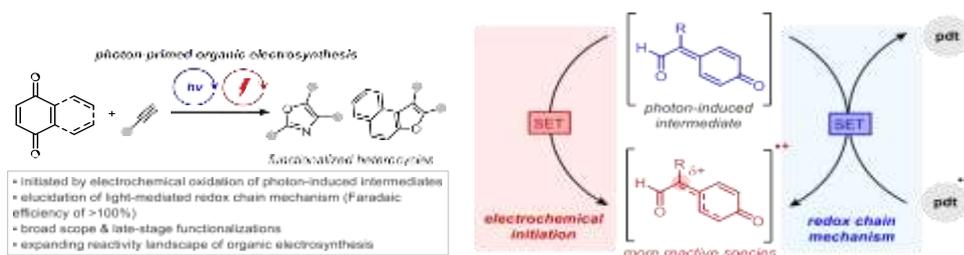
Ahhyeon Choi<sup>1</sup>, Doyeon Kim<sup>1</sup>, Daniel Yim<sup>2</sup>, Jungjin Park<sup>3</sup>, Arun Sharma<sup>4\*</sup>, Woojae Kim<sup>3\*</sup>, Hyungjun Kim<sup>2\*</sup>, Hyunwoo Kim<sup>1\*</sup>

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We present a catalyst-free photoelectrochemical protocol that integrates light-driven excitation and anodic oxidation to activate unreactive substrates. Photoexcited intermediates oxidize to electrophiles, reacting with weak nitrile and arene nucleophiles to form diverse heterocycles like dihydrofurans and pyrroles under mild conditions. Mechanistic studies reveal a redox chain mechanism enabling Faradaic efficiencies >100% through photon-amplified propagation. The method excels across >50 substrates (65-98% yields), including bioactive scaffolds, tolerating sensitive groups. This synergy expands photoelectrochemical landscape for sustainable heterocycle production in pharma and materials chemistry.



**Keywords:** Electrocatalysis, Photoelectrocatalysis.

Reference:

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## OP-5 Synthesis, Characterization and Biological Evaluation of Biguanide based Cobalt(III) Complexes Containing Substituted Benzoates

**Bhupesh Kumar<sup>a</sup>, Ritu Bala<sup>\*a</sup>, Vinit Prakash<sup>b</sup> and Amalija Golobič<sup>c</sup>**

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<sup>b</sup>Department of Applied Sciences, Global Group of institutes, Amritsar-143501, Punjab, India

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### Abstract

An anion-templated supramolecular strategy based on anion coordination-driven assemblies (ACDA) has been developed using biguanide–cobalt(III) complexes as functional building units. In this approach, benzoate anions (**ABA**: *p*-aminobenzoate, **NBA**: *p*-nitrobenzoate, **MBA**: *p*-methylbenzoate and **MEBA**: *p*-methoxybenzoate) act as directing agents, promoting self-assembly with complex cation, [Co(Hbig)<sub>3</sub>]<sup>3+</sup> (Hbig: biguanide) via hydrogen bonding and  $\pi$ – $\pi$  stacking between adjacent substituted benzoates. SCXRD studies also elucidated that *para*-substituted benzoates exhibit varying numbers of hydrogen bonding interactions with the complex cation as well as with lattice water molecules. These interactions collectively facilitate the construction of ACDA and contribute to the overall stability of the supramolecular architecture. These resulting architectures were systematically characterized by using spectroscopic studies (UV-Visible, FTIR & NMR), confirming successful ACDA formation. Anion binding studies were performed to quantify the binding affinities of the biguanide–cobalt(III) cation toward *para*-substituted benzoates, signifying strong and selective anion coordination. Additionally, the ACDA were evaluated for biological activities, revealing promising anticancer and antimicrobial properties. In both biological evaluations, the newly constructed ACDA demonstrated superior potential compared to standard drugs. Morphological evidence for apoptosis induction in MCF-7 cancerous cells was examined using fluorescence microscopy techniques, including DAPI staining, rhodamine-123 staining and dual acridine orange/ethidium bromide staining. These findings highlight the effectiveness of anion-directed coordination strategies for constructing functional metal-based supramolecular systems with combined structural and biological relevance.

**Key Words:** Anion Coordination Chemistry, Anticancer, Antimicrobial, Benzoates, Biguanide-cobalt(III) Complexes and Supramolecular Assemblies.

## OP-6 Sustainable development in Surfactant Chemistry

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### **Abstract**

Recent upsurge in the field of surfactant Chemistry is associated with its sustainable development which encompassing environment safety and circular economy goals. Sustainable development is acting as an influential driver for the finding of new smart surfactants and its mixtures with high surface activity and enhanced performance properties along with its green chemistry principles. For the determination of future viability of surfactant markets, Academic and industrial research is targeted on innovation and product development of surfactants which includes a wide range of environmental, social and economic factors also. In lieu of this, synthetic surfactants are getting replaced by ecofriendly, biodegradable surfactants which are being widely used in cleansing formulations, in synthesis of nanostructure materials and pharmaceuticals. Raw materials derived from natural or synthetic feedstock (petrochemical), or a combination of the two can be a good alternative to meet the challenging demand of surfactant market and end of life impact. Smart tailoring of surfactants and its solutions by employing renewable feedstocks, energy efficient synthesis routes can lead to overall sustainability of a value chain by promoting process efficiency and the use of fewer overall resources, whether energy, water or other materials, and often reducing levels of more hazardous components required. To match the efficiency, of conventional synthetic surfactants with respect to its economic and performance parity, surfactant research meeting sustainability criteria is still a challenging field of research which demand for collaborative efforts of scientific community and surfactant industry.

Keywords: Sustainability, Smart Surfactants, Surfactant mixtures, Green Chemistry.

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## OP-7 Acetylcholine Structure-Inspired Synthetic Fluorescent Substrate for Rapid and Selective Detection of AChE and BChE

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### **Abstract**

Early detection of Alzheimer's disease (AD) is crucial for timely therapeutic intervention and improved disease management. Dysregulation of cholinesterases particularly acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) is closely associated with AD pathogenesis and progression. Here, we report the rational design and development of structure-inspired synthetic fluorescent substrates based on a 1,8-naphthalimide scaffold for the selective and sensitive detection of AChE and BuChE.

Using an “acetylcholine-mimic” strategy, we first engineered a series of naphthalimide-based fluorogenic probes for specific AChE detection while minimizing interference from BuChE. The optimized probe, Naph-3, exhibited 20-fold fluorescence enhancement upon activation by AChE, including both *Electrophorus electricus* AChE and native human brain AChE heterologously expressed in *Escherichia coli* and purified in active form. To complement selective AChE sensing, we developed a parallel series of activatable probes for BuChE detection through systematic cycloalkyl ester engineering (cyclopropyl, cyclobutyl, cyclopentyl, and cyclohexyl) combined with self-immolative linkers to spatially decouple the fluorophore from the enzymatic trigger. Among them, the cyclopropyl ester derivative JCB-3 exhibited superior performance, showing high selectivity for BuChE over AChE, a low detection limit of 0.84 U/L, and rapid fluorescence activation within 20 minutes. Molecular docking studies supported favorable binding of JCB-3 within the BuChE catalytic pocket. In live-cell imaging, JCB-3 displayed excellent cell permeability, low cytotoxicity, and robust activation by endogenous BuChE.

Collectively, this work establishes a structure-guided fluorogenic platform enabling differential and selective monitoring of AChE and BuChE in biological systems. These probes provide powerful chemical tools for cholinesterase profiling, inhibitor screening, and potentially for early diagnosis and mechanistic investigation

**OP-8 Shape-Controlled Preparation of Ternary Ag@AgCl<sub>x</sub>Br<sub>1-x</sub> Nanocomposites in Mixed Micelle Aqueous System with Enhanced Photocatalytic Efficiency For Water Remediation**

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Novel strategies and new materials are always desired by the scientific community, which contribute towards different catalytic applications in more efficient ways. Silver halide nanoparticles and their nanocomposites with plasmonic metals for photocatalytic applications have been surveyed for a long time, but there is always something left unexplored in material science. Ternary silver halides (TSH) possess photosensitive qualities of silver halides but in an enhanced manner, owing to the mixed nature and the presence of two halide ions in the structure (AgCl<sub>x</sub>Br<sub>1-x</sub>). We report one-pot synthesis of nanocomposites of TSH with Ag NPs, stabilized by a mixed micelle system of two cationic surfactants, which also act as donors for the halide ions. We have utilized cetyltrimethylammonium chloride (CTAC) as Cl<sup>-</sup> precursor and a nicotinium-based surface active ionic liquid (SAIL) previously reported by our group (Nic-Br), which is a Br<sup>-</sup> precursor as well as a reducing agent for *in-situ* photoreduction of Ag<sup>+</sup> ions on the surface of TSH to yield Janus- shaped Ag@AgCl<sub>x</sub>Br<sub>1-x</sub> NPs. These particles are characterized by their structural and electrical properties. These NPs, with shape and size controlled precisely by a mixed micellar structure, are probed for their photocatalytic properties against the degradation of harmful dyes, and are found to show remarkably high activities in comparison to the conventional Ag@AgX NPs previously reported. This study opens doors to exploring more strategies for the preparation of such anisotropic TSH-based nanomaterials with new characteristic properties and possessing great catalytic abilities.

## OP-9 Stereochemical Control of Molecular Packing in IT-Based Organic Semiconductors

**Meenal Kataria**,\* Masaki Nobuoka, Yusuke Tsutsui, Takayuki Tanaka, Rajendra Prasad Paitandi, Yuta Takemasa, Wookjin Choi,\* Shu Seki\*  
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Stereochemistry plays a vital role in controlling molecular packing and charge transport in organic semiconductors. In this work, we examine the influence of stereoisomerism on ladder-type indacenodithieno[3,2-b]thiophene (IT)-based small molecules functionalized with  $\beta$ -methylphenethylamine. Enantiopure (RR/SS), meso (RS), racemic, and achiral derivatives were synthesized and comparatively studied to evaluate the effect of chirality on solid-state organization and optoelectronic behavior. While all stereoisomers display similar optical properties in solution, notable differences are observed in their crystalline forms. Single-crystal analysis reveals tighter  $\pi$ - $\pi$  stacking and denser molecular packing in the enantiopure systems. Consequently, time-resolved microwave conductivity measurements show nearly two-fold enhanced photoconductivity for the enantiopure derivatives compared to racemic and achiral analogues. These findings demonstrate that stereoisomerism significantly influences supramolecular packing and charge transport without modifying the conjugated backbone. This study highlights stereochemical control as an effective strategy for designing high-performance chiral organic semiconductors for advanced electronic and spintronic applications.

*Keywords: Stereoisomerism, Molecular Packing, Organic Semiconductors, Charge Transport, Chiral-Induced Spin Selectivity (CISS)*

*References: M. Kataria,\* M. Nobuoka, Y. Tsutsui, T. Tanaka, R. P. Paitandi, Y. Takemasa, W. Choi,\* S. Seki\*Aggregate, 2025; 6:e70230*

**OP-10 Implementation of the Extended McAllister Interaction Model for Predicting the Density and Ultrasonic velocity of advanced solvents at Different Temperatures**

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**Abstract**

Density and Ultrasonic velocity are the important fundamental properties of liquid mixtures, providing information about molecular packing, intermolecular interactions, and structural organization in the system. In the present study, the density and ultrasonic velocity of advanced solvents containing ionic liquids (ILs) and deep eutectic solvents (DES) is computed over a range of compositions and temperatures using extended McAllister interaction model (MAIM). The McAllister Interaction Model (MAIM) is a semi-empirical model initially used to predict the thermodynamic properties of binary liquid mixtures, particularly viscosity and density. Our research group extended the McAllister interaction model (MAIM) from third order to ninth order successfully and employed on some chosen advanced solvents to predict density and ultrasonic velocity. The significant decrease in the absolute average percentage deviation (AAPD) was observed for the higher order MAIM. The obtained results signify the validity of MAIM to compute density and ultrasonic velocity for the chosen solvents.

**Keywords:** Density modelling, Ultrasonic velocity, McAllister interaction model (MAIM), ionic liquids (ILs), deep eutectic solvent (DES)

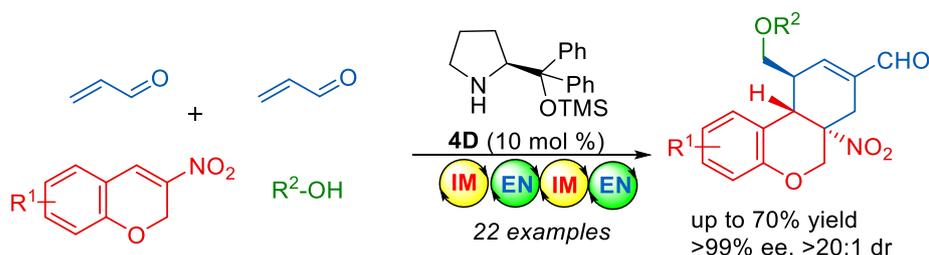
## OP-11 Asymmetric Synthesis of Tricyclic Chromanes via Organocatalyzed Quadruple Domino Sequence

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Functionalized tricyclic chromanes bearing multiple stereogenic centers have attracted much attention of synthetic as well medicinal chemists because of their significant biological activities and structural complexity<sup>1-2</sup>. Due to its interesting biological and medicinal properties, we have developed an elegant organocatalyzed quadruple domino sequence for the construction of highly functionalized tricyclic chromanes bearing three contiguous stereogenic centers including a tetrasubstituted stereocenter. The quadruple domino sequence involves -oxa-Michael/Michael/Michael/aldol condensation between nitrochromenes, alcohol and 2 equivalents of acrolein by employing secondary amine catalyst and acetic acid as additive. There are some key features of this reaction include excellent stereoselectivities (99% *ee*, 9:1 to >20:1 *dr*) along with moderate to good yields (20-66%) of tricyclic chromanes, wide range of substrate scope, successful gram-scale reaction and further functionalization of the chromane product without compromising stereoselectivity.



**Keywords:** Tricyclic Chromanes, Quadruple domino reaction, Asymmetric

### References:

- (1) Sung S. H.; Kim, Y. C. *J. Nat. Prod.* **2000**, *63*, 1019.
- (2) Shirota, O.; Takizawa, K.; Sekita, S.; Satake, M.; Hirayama, Y.; Hakamata, Y.; Hayashi, T.; Yanasawa, T. *J. Nat. Prod.* **1997**, *60*, 997.

## OP-12 Thermodynamic Stability of Ionic Liquids for Green Chemistry Applications

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Ionic liquids (ILs) have emerged as promising alternatives to conventional organic solvents due to their negligible vapor pressure, high thermal stability, and tunable physicochemical properties, making them attractive for green chemistry applications. The present study focuses on the thermodynamic stability of selected ionic liquids to evaluate their suitability as environmentally benign solvents. Key thermodynamic parameters such as Gibbs free energy, enthalpy, entropy, heat capacity, and phase behavior have been analyzed using experimental data and theoretical models. The influence of cation–anion interactions, alkyl chain length, and functional group substitution on the thermal and chemical stability of ionic liquids has been critically examined. Results indicate that strong electrostatic interactions and hydrogen bonding significantly enhance the thermal stability and resistance to decomposition at elevated temperatures. Additionally, the low volatility and high heat capacity of ionic liquids contribute to improved process safety and energy efficiency in chemical reactions. Thermodynamic analysis further reveals that many ionic liquids exhibit favorable solvation characteristics and stability over a wide temperature range, supporting their use in catalysis, separation processes, electrochemistry, and biomass processing. However, the study also highlights the importance of selecting ionic liquids with optimized structures to balance stability, biodegradability, and toxicity. Overall, this thermodynamic assessment underscores the potential of ionic liquids as sustainable solvents and reaction media, reinforcing their role in advancing green chemistry and environmentally responsible industrial processes.

**Keywords:** Ionic liquids; Thermodynamic stability; Green chemistry; Gibbs free energy; Sustainable solvents; Thermal properties

### References

1. Welton, T. *Ionic liquids in green chemistry*. **Green Chemistry**, 1999, 1, 1–7.
2. Plechkova, N. V.; Seddon, K. R. *Applications of ionic liquids in the chemical industry*. **Chemical Society Reviews**, 2008, 37, 123–150.
3. Rogers, R. D.; Seddon, K. R. *Ionic liquids—Solvents of the future?* **Science**, 2003, 302, 792–793.

## **OP-13 In silico studies for designing new ZSTK-474 derivatives**

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Till now there is not a single marketed drug available for PI3K  $\alpha$  anti cancer activity. There are more than a dozen molecules which are in clinical trial for anti-cancer PI3K activity from them ZSTK-474 has been selected to address its toxicity issue. ZSTK-474 has a core moiety of triazene ring with two morpholine group. In order to design better ZSTK-474 inhibitors molecular modeling studies were taken into consideration. Through molecular docking studies the binding interaction and binding pocket analysis of the molecule was done with respect to the PI3K $\alpha$  protein. Through this analysis certain derivatives were proposed, synthesized and further biologically validated for their anti-cancer activity of PI3K.

## Op-14 Systems Chemistry of Molecular Self-Assembly: From Equilibrium Order to Nonequilibrium Dynamics

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Molecular self-assembly has traditionally focused on forming ordered architectures under thermodynamic equilibrium. Bioinspired systems such as peptides and amino acids can organise into  $\beta$ -sheet-rich nanofibers, nanospheres, and hydrogels with promising applications in biotechnology and drug delivery. In our earlier work, we investigated the molecular mechanisms underlying amyloid-like assembly, beginning from dimer nucleation stabilised by non-covalent interactions and progressing to higher-order structures.

Recognising that nature regulates function through dynamic assembly-disassembly processes, we extended this paradigm to non-equilibrium systems. Using compartmentalised reaction–diffusion setups, we engineered controlled interactions between metal ions and organic linkers to generate tubular “MOF garden” architectures with diameters up to 50  $\mu\text{m}$ , structures inaccessible via conventional solvothermal routes.

Building on this systems perspective, we developed a minimalist enzyme-mimetic platform based on a single-step synthesis of a copper-tyrosine (CuY) supramolecular assembly. Structural characterisation confirms the formation of an ordered nanotubular architecture. The CuY network exhibits pronounced peroxidase-like activity toward *o*-phenylenediamine, as quantified by Michaelis–Menten analysis. Importantly, catalytic performance is not solely determined by copper coordination but is strongly modulated by the network's dynamic self-assembled state. Coordination-driven remodelling of the tyrosine assembly induces nonlinear regulation of catalytic activity, revealing a direct coupling between supramolecular organisation and enzyme-like function.

This work highlights molecular self-assembly as a central regulatory element in minimalist catalytic systems and provides new design principles for life-like, metal–amino acid functional materials.

# OP-15 Interface-Controlled Charge Dynamics in Biogenic Ag@g-C<sub>3</sub>N<sub>4</sub> for Rapid Reduction of Nitroaromatics and X-Ray Shielding

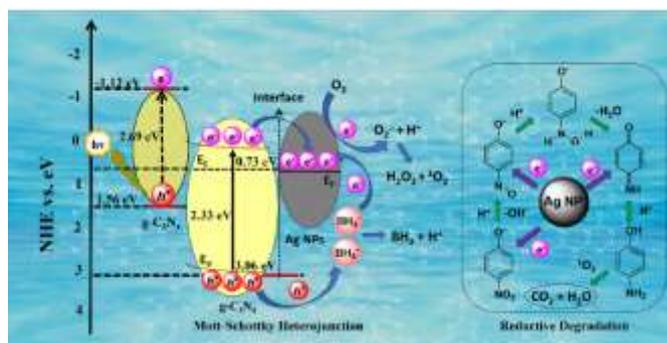
**Sandeep Kumar, Jyoti Rani**

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## Abstract

Silver nanoparticle-decorated graphitic carbon nitride (Ag@g-C<sub>3</sub>N<sub>4</sub>) nanocomposites were developed via chemical and biogenic routes and systematically investigated for multifunctional applications in environmental remediation and radiation shielding. Structural and spectroscopic analyses confirmed the successful immobilization of Ag nanoparticles on g-C<sub>3</sub>N<sub>4</sub> with pronounced band-gap narrowing from 2.69 to 2.33 eV, enabling enhanced visible-light absorption. Under visible light irradiation and in the presence of NaBH<sub>4</sub>, biogenic Ag@g-C<sub>3</sub>N<sub>4</sub> exhibited outstanding catalytic performance, achieving more than 95% reductive degradation of toxic nitroaromatic pollutants (p-nitrophenol, dinitrophenol, picric acid, and dinitrophenylhydrazine) within 5 min at neutral pH, following pseudo-first-order kinetics. Mechanistic investigations revealed that interfacial charge separation and Ag-mediated electron transfer dominate the hydride-assisted reduction pathway, while reactive oxygen species play a negligible role. In addition to catalytic activity, Ag@g-C<sub>3</sub>N<sub>4</sub> demonstrated significantly improved low-energy X-ray attenuation properties, with higher mass attenuation coefficients and effective atomic numbers, and reduced tenth value layers compared to pristine g-C<sub>3</sub>N<sub>4</sub> in the 30–150 keV range. The combined results highlight biogenic Ag@g-C<sub>3</sub>N<sub>4</sub> as a sustainable, efficient, and lightweight multifunctional material for rapid detoxification of hazardous pollutants and advanced radiation shielding applications.



**Figure.** Photocatalytic degradation mechanism of nitroaromatic using *b*-Ag@g-C<sub>3</sub>N<sub>4</sub>

**Keywords:** Biogenic; Silver nanoparticles, Graphitic Carbon nitride; Nitroaromatics, Photodegradation.

**OP-16 Elucidating Antibacterial activity of 3-(Pyridine-3-yl)-2-Oxazolidinone derivatives through QSAR and Molecular Docking Approaches**

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**Abstract**

The high occurrence of multidrug-resistant bacterial stains necessitates the development of innovative antibacterial agents with increased potency. Linezolid has a strong antibacterial action and a satisfactory therapeutic effect. However, due to its widespread use, the advent of bacterial resistance, and the risk of myelotoxicity, its use has been limited. More research is needed on new oxazolidinone molecules with higher efficacy and reduced toxicity. In this study, a variety of 3-(Pyridine-3-yl)-2-oxazolidinone derivatives were studied to determine their antibacterial properties utilizing Quantitative Structure-Activity Relationship (QSAR) modeling and molecular docking techniques. The QSAR models were generated against four gram-positive strains: *S. aureus* (ATCC25923), *S. pneumoniae* (ATCC49619), *E. faecalis* (ATCC29212), and *S. xylosus* (ATCC35924). All of the models showed high predictive performance and acceptable validation parameters ( $R^2$ ,  $Q^2$ , RMSE, and external validation metrics). Molecular docking studies were carried out on the 50S ribosomal subunit of *Haloarcula marismortui* (PDB code: 3CPW). The docking studies also revealed that all of the medicines had significant binding affinity and interacted with the PTC region of the 50S ribosomal subunit. The models can be used to develop novel Oxazolidinone molecules with higher activity and reduced toxicity.

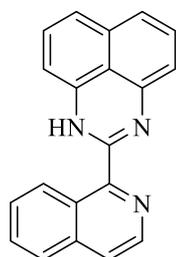
## Op-17 Smartphone-assisted sensing and quantification of Fe<sup>3+</sup> by perimidine derivative

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Department of Chemistry, Multani Mal Modi college, Patiala 147001, Punjab, India

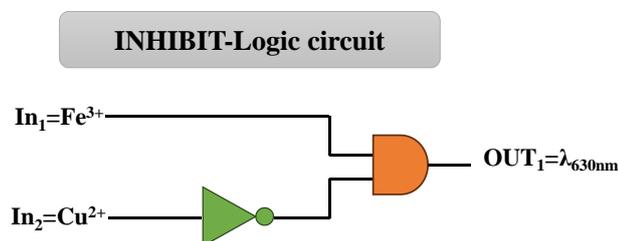
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A one-step reaction between 1,8-diaminonaphthalene and 2-quinolinecarboxaldehyde resulted in the formation of 2-(isoquinolin-1-yl)-1*H*-perimidine **1**. The perimidine derivative **1** was found out to be stable under a pH range of 2-12. The study of the chromo-fluorescent properties of the developed perimidine derivative **1**, unveiled its capability of selectively sensing Fe<sup>3+</sup> via colorimetric change from colorless to yellow as well as fluorescence turn-on response (from non-fluorescent to bright red fluorescence, under UV lamp). The fluorescence titration profile was deployed for calculating binding constant and LOD as 1.3 × 10<sup>4</sup> M<sup>-1</sup> and 7.4 nM, respectively. The fluorescence studies of **1**.Fe<sup>3+</sup> ensemble were also conducted which showed its potential for sensing Cu<sup>2+</sup> ions, which was accompanied by fluorescence turn-off response. Considering the fluorescence turn-on response of **1** towards Fe<sup>3+</sup> ions, we used our portable smartphone device for sensing and quantification of Fe<sup>3+</sup>. This could be beneficial in resource-limited areas and could also be used as an alternative for complex instrumentation. Alongwith smartphone-assisted sensing of Fe<sup>3+</sup> ions, we developed an INHIBIT logic circuit for the fluorescence response of **1** towards Fe<sup>3+</sup> and Cu<sup>2+</sup> ions



2-(isoquinolin-1-yl)-1*H*-perimidine

**1**



# Op-18 From Complexity to Chirality: Solvent-Driven Chirality Modulation and Morphological Transitions in Hierarchical Co-Assemblies

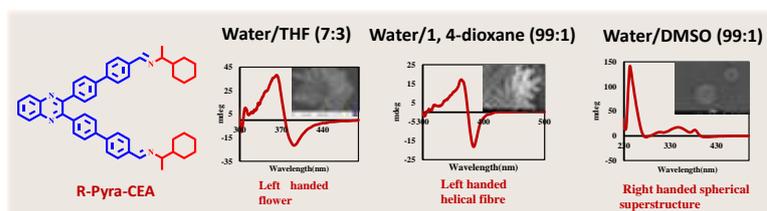
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Programming the solvent-mediated hierarchical organization and chirality transition in organic–inorganic co-assembled hybrid materials is attractive but still a challenge.<sup>1-2</sup> The present work demonstrates the development of solvent-responsive **R/S-Pyra-CEA** building blocks which exhibit distinct absorption and chiroptical behavior in the presence of Lewis base co-solvents (THF/1,4-dioxane/DMSO) in self-assembled/co-assembled state in mixed aqueous media. The study reveals a simple strategy to exploit subtle solvent characteristics as external controls to direct the co-assembly of a well-designed organic building block, inorganic component [Au (III) ions], and chiral inducer (cysteine) through multiple hierarchical growth pathways, leading to diverse chiral superstructures in aqueous media. Strikingly, **R/S-Pyra-CEA** assemblies promoted the in situ reduction of Au (III) ions to Au (0) nanoparticles, while in the presence of cysteine the process was regulated to stabilize Au (I) species, leading to the formation of enantioselective chiral assemblies.<sup>3</sup> The outcome of this investigation provides fresh insights for designing solvent-sensitive building blocks to prepare nature-inspired, hierarchically organized chiral hybrid materials with potential applications in nanomaterials research.



**Keywords:** Hierarchical co-assembly, Chiral Superstructures, Solvent sensitivity, Supramolecular assemblies

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2. Bioinspired chiral inorganic nanomaterials, N. H. Cho, A. Guerrero-Martínez, J. Ma, S. Bals, N. A. Kotov, L. M. Liz-Marzán and K. T. Tam, *Nat. Rev. Bioeng.*, 2023, DOI; 10.1038/s44222-022-00014-4, (I.F = 37.6) [Nature Portfolio, Published online 27/01/2023].

## **OP-19 BioMOF: A Biomolecule-Derived Metal-Organic Framework**

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### **Abstract-**

Metal-organic frameworks (MOFs) are ultra-porous, crystalline materials composed of metal nodes linked by organic ligands. Known for tunable pore sizes and high structural variability, they are used for gas storage/separation, catalysis, drug delivery and sensing. Because of the progressive development of MOFs synthetic processes and considerable potential applications in last decade, integrating biomolecules into MOFs has recently gain considerable attention. The incorporation of biomolecules—including enzymes, proteins, nucleic acids, and other therapeutic agents—into MOFs has emerged as a promising approach for developing multifunctional hybrid materials. Biomolecule–MOF composites can be fabricated through in situ encapsulation, surface immobilization, or post-synthetic modification methods, ensuring preservation of biological activity while enhancing structural stability. Biomolecule–MOF hybrid structures have wide range of applications such as drug delivery, biocatalysis, bio-imaging and biosensing. They have enhanced stability, high loading capacity, enhanced sensitivity and selectivity, biocompatibility and low toxicity etc. Additionally, the development of biocompatible and biodegradable MOFs further supports their potential in pharmaceutical and clinical applications. Although challenges such as long-term physiological stability, scalability, and precise control over biomolecule loading remain, ongoing research continues to address these limitations. By integrating biomolecule with MOFs, it has overcome many existing challenges and generate more practical applications. **Keywords-**Metal-Organic Framework, Bio-MOF, Hybrid materials, Porous materials, Biomolecule functionalisation, Crystalline Framework.

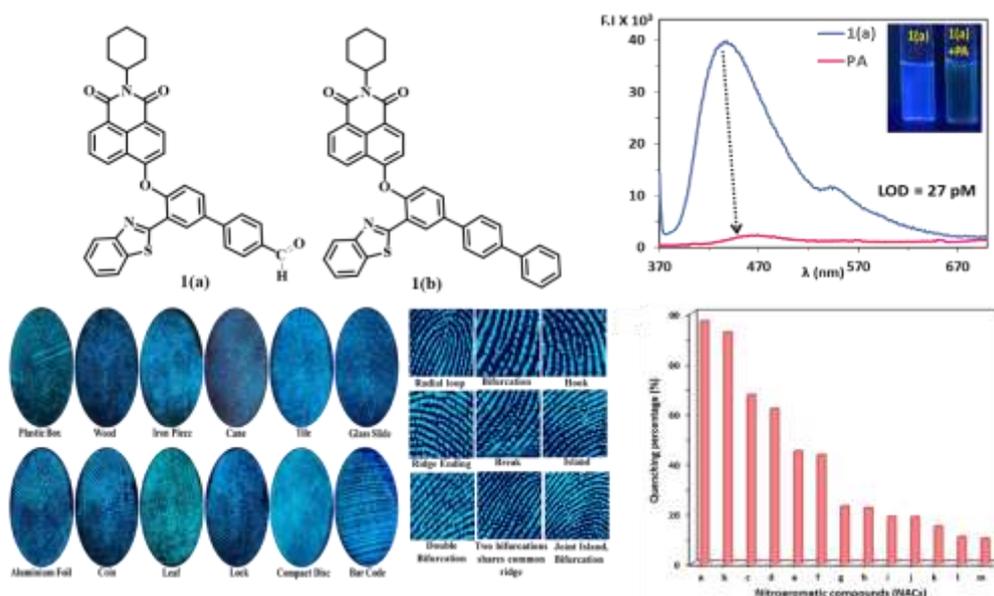
# OP-20 Modified Benzothiazole-Naphthalimide Based Fluorescent Hybrids for Picomolar Detection of Picric Acid in water and visualization of latent fingerprinting

**Vishakha Thakur<sup>a</sup>, Navdeep Kaur<sup>a</sup> and Prabhpreet Singh<sup>\*a</sup>**

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A series of modified benzothiazole-naphthalimide hybrids (1a-1b) were synthesized and evaluated as fluorescent probes for the picomolar detection of picric acid in water. The characterization and photophysical properties including theoretical and solid state properties of compounds (1a-1b) and their complexation with PA and NB have been evaluated by spectroscopic techniques (NMR, IR); optical techniques (Fluorescence, UV-Vis); Thermal Gravimetry (TG); Powder-X-ray diffraction (WXR) AND atomic force microscopy (AFM). These fluorescent derivatives were further explored for visualization of the LFPs on different substrates up to level 3 and for differentiating the subjects based on ridge patterns of fingerprints. The studied compounds showed detection limits of 27 pM and 49 pM (compound 1a); 30 pM and 122 pM (compound 1b); for picric acid and nitrobenzoic acid, respectively. The high value for stern- Volmer quenching constant ( $K_{SV} = 10^6 M^{-1}$ ) revealed strong interactions of compound 1a-1b with PA and NB.



**Keywords:** benzothiazole, naphthalimide, fluorescent, complexation, picric acid, nitrobenzoic acid, stern- Volmer, latent fingerprinting.

## References:

1. P. Singh, V. Thakur, *J. Mol. Struct.*, 2026, 1359, 145377.
2. V. Thakur, N. Kaur, P. Singh, manuscript under progress.

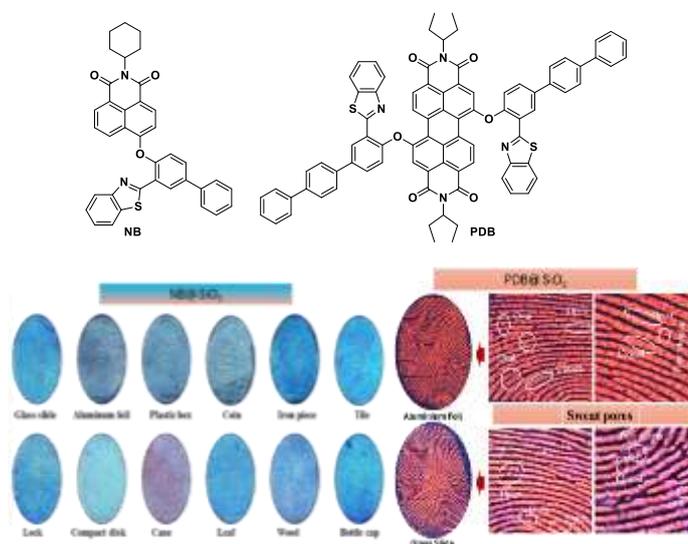
# Poster Presentations

# PP-1 Luminescent Naphthalimide– and Perylene–Benzothiazole Conjugates for High-Resolution Latent Fingerprint Visualization

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based electron deficient and  $\pi$ -conjugated aromatic imides possess heat and light stability and explored for various applications in optoelectronic devices and chromo-fluorescent materials for visualization of latent fingerprints (LFPs). We have designed and synthesized 1,8-Naphthalimide (**NB**) and perylene diimide (**PDB**) based aromatic imide derivatives and characterized by NMR techniques. The solid powders of NB and PDB derivatives exhibited blue and red coloured fluorescence under 365 nm UV illumination. Owing to strong solid-state fluorescence, **NB** and **PDB** fluorophores were adsorbed onto silica nanoparticles to produce **NB@SiO<sub>2</sub>** and **PDB@SiO<sub>2</sub>** fluorescent powders and were employed for visualization of LFPs. The strong fluorescence responses provided high-contrast images of Level 1 (ridge patterns like loops, whorls etc.), Level 2 (bifurcations, overlap etc) and Level 3 (sweat pores) fingerprint features with excellent resolution. Fingerprint imaging was further evaluated under simulated environmental conditions, including thermal exposure, aging, and UV light irradiation. Case study experiments revealed effective visualization of LFPs from male and female subjects using **NB@SiO<sub>2</sub>** and **PDB@SiO<sub>2</sub>** fluorescent powders.



**Keywords:** Naphthalimide, Perylene diimide, Case study, latent fingerprint

## References:

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2. N. Kaur, P. Singh, *New J. Chem.*, 2023,47, 16322-16326.

## PP-2 Beyond Solvation: Hydrolysis-Driven Structure Formation in Coordination Polymers from N, N-Dimethylformamide

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### **Abstract**

N, N-Dimethylformamide (DMF) is a widely employed polar aprotic solvent in solvothermal crystal growth of coordination polymers, valued for its high boiling point and remarkable ability to dissolve both metal salts and organic ligands. Despite its utility, DMF is recognized as a potent hepatotoxin, readily absorbed through skin, inhalation, or ingestion, highlighting the importance of understanding its chemical behavior under solvothermal conditions. Beyond functioning as a reaction medium, DMF undergoes hydrolysis at elevated temperatures to yield dimethylamine (DMA) and formic acid—products that can decisively influence crystal growth and framework topology. This study demonstrates the structure-directing role of DMF hydrolysis products across multiple coordination polymer systems. Earlier reports on thorium-based frameworks demonstrated that solvothermal reactions of thorium salts with trimesic acid (H<sub>3</sub>btc) in DMF produced structures in which DMF either directly coordinated to the metal center, fragmented to yield DMA incorporated as neutral species, or protonated to form dimethylammonium (HDMA<sup>+</sup>) cations. In all cases, these DMF-derived species enhanced hydrogen bonding interactions within the framework. In-situ-generated HDMA<sup>+</sup> cations acted as charge-balancing agents, whereas DMA molecules engaged in hydrogen bonding with the carboxylate groups of trimesic acid, thereby stabilizing the lattice. Similarly, formate species derived from DMF hydrolysis coordinated to metal centers, contributing to charge balance and extending the dimensionality of the framework. Single-crystal X-ray diffraction, supported by complementary techniques, confirmed the incorporation of formate, underscoring the critical role of DMF-derived hydrolysis products in directing framework assembly.

## PP-3 Polymer-Supported Recyclable Catalyst for Reduction of Nitroaromatic Compounds

**Akash T,<sup>1</sup> Sindhu I Sanakal,<sup>1</sup> Anubhab Das<sup>1</sup> and Samarendra Maji<sup>1\*</sup>**

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### Abstract

Heterogeneous catalysis has great potential in various fields due to its wide range of applications.<sup>1</sup> Metal nanoparticles (MNPs) as heterogeneous catalysts have drawn the attention of both commercial and academic research due to their unique characteristics, which include high reactivity, stability, ease of separation and purification, and strong recyclability.<sup>2</sup> Heterogeneous catalysts often have lower catalytic efficiency and after recovery suffer from metal leaching, loss of surface area, and deterioration after multiple cycles. To achieve these features, MNPs require certain supports, such as silica, metal oxides, clay, and polymer.<sup>3</sup> Polymer-supported heterogeneous catalysts are attracting substantial attention due to their inertness, non-toxicity, non-volatility, stability, flexibility, and ability to be reused.<sup>4</sup> Nitroaromatic compounds (NACs) are extremely mutagenic and many of them are recognized as carcinogenic.<sup>5</sup> p-Nitrophenol (p-NP) is a major organic and environmental pollutant in industrial and agricultural wastewater. According to the US Environmental Protection Agency (EPA), p-NP is a non-biodegradable contaminant. It is critical to detoxify p-NP via reduction in the presence of a catalyst. Extensive research has been conducted on the catalytic reduction of p-NP using NaBH<sub>4</sub> as the hydride source, resulting in the effective production of para-aminophenol (p-AP). In our present work, we plan to develop a polymer-based recyclable catalyst for the reduction of nitroaromatic compounds. The catalyst will be synthesized and characterized using various characterization techniques, including X-ray photoelectron spectroscopy (XPS), energy dispersive X-ray (EDX) spectroscopy, transmission electron microscopy (TEM), and scanning electron microscopy (SEM). As a proof of concept, we will investigate the catalyst for the conversion of p-NP to p-AP and compare the results with the reported catalyst. Finally, the recyclability and catalytic activity of the catalyst will be investigated.

**Keywords:** Heterogeneous catalyst; Catalytic efficiency; Reusability; Nitroaromatics; reduction.

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## PP-4 Structural and Electrochemical Properties of Zn doped Tin Ferrite Nanoparticles

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### **Abstract**

Zn-doped tin ferrite (SnFe<sub>2</sub>O<sub>4</sub>) nanoparticles were synthesized via sol-gel process for prospective energy storage applications. The structural properties of the synthesized samples were studied using X-ray diffraction (XRD), which indicated the synthesis of spinel ferrite structure. FESEM showed approximately spherical nanoparticles with minor agglomeration, while EDS confirmed the existence and uniform distribution of Zn, Sn, Fe, and O elements with no impurity phases. The electrochemical behavior of Zn-doped tin ferrite electrodes was tested utilizing a three-electrode setup in Na<sub>2</sub>SO<sub>4</sub> aqueous electrolyte. Cyclic voltammetry (CV) experiments showed excellent redox activity and capacitive performance. Electrochemical impedance spectroscopy (EIS) revealed low charge transfer resistance, indicating increased conductivity due to Zn inclusion. Galvanostatic charge-discharge (GCD) study revealed good specific capacitance and cycling stability.

### **Keywords:**

Tin ferrite, sol-gel synthesis, electrochemical studies, supercapacitor.

## PP-5 Self Assembly of Anionic Surfactant in Deep Eutectic Solvents

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### **Abstract**

Deep eutectic solvents (DESs) are increasingly recognized as green and tunable solvent systems due to their strong hydrogen-bonding networks and unique transport properties. In this work, the conductivity and surface tension behavior of sodium lauryl sulphate (SLS), an anionic surfactant, were investigated in a deep eutectic solvent composed of ethylene glycol and lactic acid in a 1:2 molar ratio, at different DES–water compositions. The measurements were carried out in aqueous solutions containing 10%, 30%, and 50% (v/v) DES, along with pure water for comparison. The primary objective was to study the effect of DES concentration on the micellization and interfacial properties of SLS. Electrical conductivity and surface tension techniques were employed to determine the critical micelle concentration (CMC) in each solvent system. A continuous decrease in surface tension with increasing surfactant concentration was observed, followed by a plateau indicating the onset of micelle formation. Notably, the CMC of SLS was found to decrease with increasing DES content in the solvent mixture. This behavior is attributed to reduced ionic mobility and increased viscosity of the medium at higher DES concentrations, which favor earlier aggregation of surfactant molecules. The conductivity results further revealed a systematic decrease in charge transport with increasing DES fraction, confirming the restricted mobility of ions in the hydrogen-bond-rich DES environment. Compared to pure water, DES–water mixtures significantly modify the solvation and interfacial behavior of SLS, highlighting the strong influence of solvent structure on surfactant self-assembly. The combined analysis provides valuable insights into the role of solvent composition in controlling micellization phenomena and demonstrates the potential of DES-based mixed solvents for applications in green chemistry, colloidal formulations, and sustainable industrial processes.

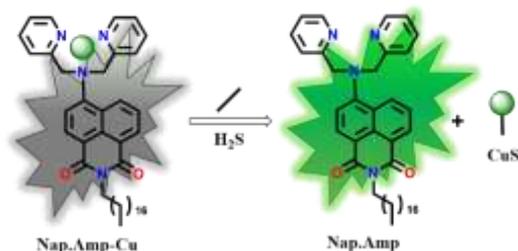
## PP-6 An Amphiphilic Tridentate Nanosensor for Sequential Detection of $\text{Cu}^{2+}$ and $\text{H}_2\text{S}$ and Potential Application in Hydrogel Beads

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### Abstract

$\text{H}_2\text{S}$  is an important gaseous signaling molecule and slight change in the concentration of  $\text{H}_2\text{S}$  within the mammals can cause various diseases. Therefore, the development of a new sensing system that is fast responsive, water soluble and non-toxic to the biological environment is highly significant. So, herein we report the synthesis of a new naphthalimide-based amphiphilic compound, termed **Nap.Amp**. Nanoscale fluorescent liposomes (**Nap.Lipo**) were successfully formed by incorporating **Nap.Amp** within the phospholipid DOPC. **Nap.Lipo** exhibited a fluorescence quenching (turn-Off) response in the presence of copper ions. Interestingly, the resulting in-situ copper complex (**Nap.Lipo-Cu**) displayed a selective fluorescence enhancement (turn-On) response specifically in the presence of  $\text{H}_2\text{S}$ , with a limit of detection (LOD) of 1.62  $\mu\text{M}$ . Owing to its excellent selectivity, **Nap.Amp** was further employed for  $\text{H}_2\text{S}$  detection in a double-compartment gas assay. Additionally, paper-based strips were developed to enable simple, visible detection of  $\text{H}_2\text{S}$ .



**Keywords:** Optical sensor; Liposome;  $\text{H}_2\text{S}$  sensor; Fluorescence

## PP-7 1,2-Diketones as Precursors for Knoevenagel-Type Deconstructive Carbonyl Olefination

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### Abstract

In organic synthesis, carbonyl olefination is a cornerstone approach to construct C=C bond. Since the landmark Wittig carbonyl olefination in 1953,<sup>1</sup> various research groups have developed different carbonyl olefination methods such as Knoevenagel, Horn-Wadsworth-Emmons, Peterson, and Julia.<sup>2</sup> Knoevenagel olefination often lead to side reaction such as Canizzaro, generating copious amount of side products. Other methods generally used non-native molecules as coupling partners such as ylides (Wittig),<sup>3</sup> phosphonates (Horner-Wadsworth-Emmons),<sup>4,5</sup> silyl carbanions (Peterson),<sup>6</sup> and sulfones (Julia)<sup>7</sup>, thus generating stoichiometric amount of by-products along with the desired olefin. Therefore, many groups have developed methods that utilized alcohols as the carbonyl surrogates to avoid side reactions. However, these methods are generally transition-metal assisted. Keeping these aspects in view, we have uncovered a transition-metal-free Knoevenagel-type deconstructive carbonyl olefination of 1,2-diketones to access olefins.

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## PP-8 Synthesis of copper oxide nanoparticles by green method using *Hibiscus rosa-sinensis* leaves extract, characterisation and antibacterial potential

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### Abstract

The copper oxide nanoparticles (CuO NPs) were phytofabricated using *Hibiscus rosa-sinensis* commonly called China rose leaves ethanolic (70%) extract as a reducing and capping agent and tested for antibacterial potential against food pathogenic bacteria. The leaves extract was prepared via Soxhlet extraction method. As per GC-MS analysis, china rose leaves extract consisted of 32 compounds with 5-hydroxymethylfurfural (49.95%) and 3,5-dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one (31.51%) as major compounds. CuO NPs were fabricated with sol-gel formulation procedure by optimizing various physiochemical parameters like precursor salt CuSO<sub>4</sub>·5H<sub>2</sub>O concentration (0.1 M), amount of bio-reductant extract (10 mL), pH (12), temperature (80°C) and heating time (3 hours). UV-visible spectrum showed absorption band at 274 nm characteristic of CuO NPs. Fourier transform infrared spectrum of CuO NPs confirmed functionalisation of NPs with the extract. X-ray diffraction diffractogram of NPs revealed the average crystallite size of 15.01 nm and monoclinic crystal lattice. Energy Dispersive X-ray Spectroscopic analysis showed peaks of Cu, O and C elements. Morphological analysis from Scanning Electron Microscopy and Transmission Electron Microscopy micrographs showed aggregated spherical NPs which had diameter in the range of 15-36.94 nm. CuO NPs exhibited higher antibacterial activity than china rose leaf extract as the MIC values of CuO NPs (10-100 mg/ml) were less than that of extract (50-200 mg/ml) against bacteria *Escherichia coli*, *Proteus mirabilis*, *Staphylococcus aureus* and *Bacillus subtilis*. Hence, CuO NPs fabricated by using China rose leaves extract may be used as a natural antibacterial agent as a substitute for its synthetic analogue as an approach towards sustainable development.

**Keywords:** *Hibiscus rosa-sinensis*, nanoparticles, extract, antibacterial, GC-MS

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# PP-9 Thiosemicarbazone-Based Chemosensors for Highly Sensitive Electrochemical Detection of $\text{Cu}^{2+}$ and $\text{Hg}^{2+}$ .

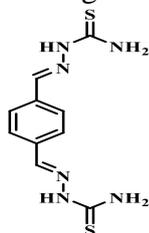
**Anshita Pangotra, Rohit Luna, Inderpreet Kaur\***

*Department of Chemistry, Centre for Advanced Studies, Guru Nanak Dev University Amritsar, 143005, Punjab, India.*

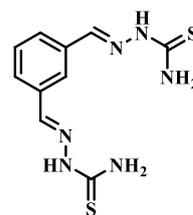
E-mail address\* : nderpreet11@yahoo.co.in

## Abstract

Thiosemicarbazone-based chelators TPB and IPB, incorporating different donor heteroatoms (N and S), were designed, synthesized, and characterized, and subsequently investigated for their metal-ion sensing behaviour through pseudo-cavity-assisted complexation [1]. Preliminary UV-Visible and fluorescence studies revealed that both chelators exhibited high sensitivity towards  $\text{Cu}^{2+}$ , while IPB additionally showed sensitivity towards  $\text{Hg}^{2+}$ . Electrochemical investigations further demonstrated that both TPB and IPB displayed pronounced voltammetric responses towards  $\text{Cu}^{2+}$ , with low detection limits of 4.7 nM and 11.4 nM, respectively. Notably, chelator IPB also exhibited a sensitive electrochemical response towards  $\text{Hg}^{2+}$  with a detection limit of 7.19 nM. The formation of stable metal–chelator complexes  $\text{TPB}+\text{Cu}^{2+}$  and  $\text{IPB}+\text{Cu}^{2+}/\text{Hg}^{2+}$  was supported by large binding constants and associated negative Gibbs free energy changes, indicating spontaneous complexation. The binding mechanism of chelators TPB and IPB with respective metal ions was further confirmed by  $^1\text{H}$  NMR studies. To enable practical application, carbon paste electrodes (CPEs) modified with chelators TPB and IPB were fabricated and found to exhibit near-Nernstian responses, excellent selectivity, and were successfully applied for the determination of  $\text{Cu}^{2+}$  and  $\text{Hg}^{2+}$  in groundwater.



**TPB**



**IPB**

**Keywords:** Thiosemicarbazide, Pseudo cavity, Dual sensor, Voltammetric sensor, Carbon paste electrode.

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## **PP-10 Development of Self-emulsifying Drug Delivery Systems of Mirtazapine for Solubility Enhancement and In vitro Evaluation**

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### **Abstract**

Mirtazapine (MTZ) is a BCS class II drug having poor aqueous solubility, low oral bioavailability, and high first-pass metabolism. It is predominately a noradrenergic and specific serotonergic antidepressant (NaSSA) that blocks 5-HT<sub>2</sub> and 5-HT<sub>3</sub> receptors and antagonizes adrenergic receptors. The aim of the present research was to develop mirtazapine loaded self-emulsifying drug delivery system (MTZ-SEDDS) to enhance its solubility and hence overall bioavailability. Prior to the development of MTZ-SEDDS, the solubility of MTZ was evaluated in various oils, surfactants and co-surfactants and the selected excipients were used for the construction of pseudoternary plots to analyze the performance of the developed formulations. The optimized formulations were investigated for in vitro release and kinetics of drug release to help predict how the formulation may behave in vivo. Since, in vivo studies are important to understand the pharmacokinetic parameters of drug in a biological system, a High-Performance Liquid Chromatography (HPLC) chromatogram was prepared in plasma as a base for future investigations.

**Keywords:** Mirtazapine, Depression, HPLC, Pseudoternary diagrams, Solubility

## PP-11 Insights into Multifunctional PVA Hydrogel Electrolytes for Flexible Supercapacitors

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### Abstract

The development of flexible, safe, and high-performance gel electrolytes is critical for next-generation wearable and portable energy-storage devices. In this work, three complementary hydrogel-based electrolyte systems—Illite/PVA composite hydrogels, PVA-cellulose–LiCl hydrogel, and PVA–H<sub>2</sub>SO<sub>4</sub> hydrogel—are reviewed and conceptually integrated to highlight their collective advances. Illite-reinforced PVA hydrogel exhibits enhanced mechanical robustness, high tensile strength, and improved ionic conductivity owing to strong interfacial interactions within the polymer–clay framework.<sup>1</sup> The PVA/cellulose/LiCl system demonstrated excellent compressive resilience, stable electrochemical performance, and high ionic transport capability enabled by synergistic hydrogen-bonding networks and LiCl-induced plasticization.<sup>2</sup> Meanwhile, the PVA–H<sub>2</sub>SO<sub>4</sub> hydrogel delivers fast autonomous healing, stable proton conduction, and reliable device-level performance through reversible dynamic bonding and acid-mediated ion mobility.<sup>3</sup> Together, these studies illustrate how polymer-filler coordination, multifunctional cross-linking, and ionic modulation can be strategically combined to yield hydrogel electrolytes with high mechanical durability, strong self-healing capacity, and excellent electrochemical properties. This integrated perspective provides a promising framework for the fabrication of next-generation flexible supercapacitors and other soft energy-storage technologies.

**Keywords:** Polyvinyl alcohol, Improved ionic conductivity, Synergistic effect, Self-healing.

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## PP-12 Ultrasonic energy promoted synthesis of bisthioglycolic acid derivatives in deep eutectic solvents-A greener approach

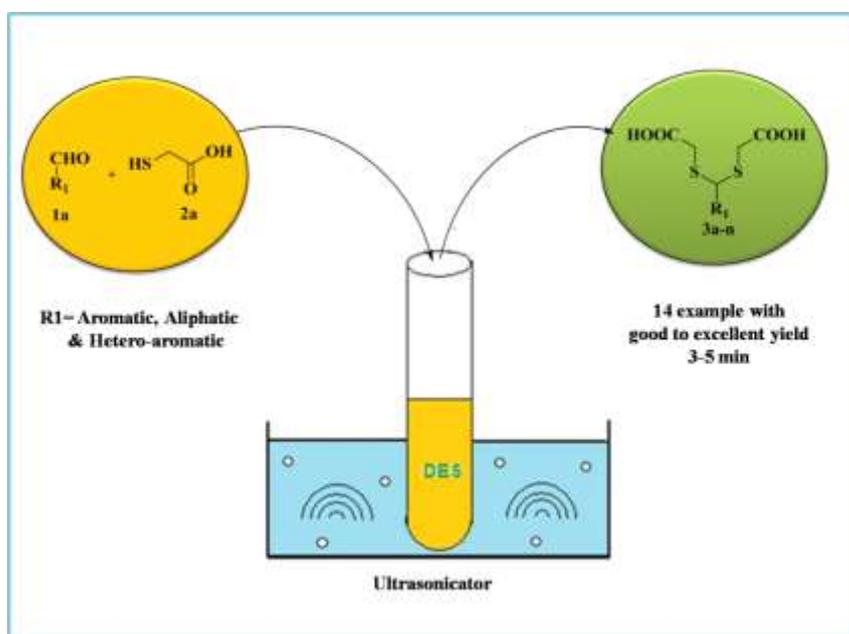
**Archna,<sup>a</sup> Gobind Kumar,<sup>a</sup> Rupesh Kumar,<sup>a</sup> Gaurav Bhargava\*<sup>a</sup>**

<sup>a</sup>Department of chemistry, I. K. Gujral Punjab Technical University  
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### Abstract

Carbon-Sulfur bond formation strategies are significant due to the importance of linkages in the sulfur-containing scaffolds which are found in biologically active compounds.<sup>1</sup> Sulfones, and sulfonamides are common sulfur-containing scaffolds that are found in medicinal drug. For instance, 1,3-oxathiolan-5-one has shown antiviral activity, and PLA2 inhibitory activity.<sup>2</sup> Moreover, bisthioglycolic acid and its derivatives have been reported to play a significant role as a precursor in the formation of many sulfur-containing heterocyclic compounds.

The present methodology explored the effectiveness and versatility of deep eutectic solvent with ultrasonic energy as an eco-friendly protocol for the synthesis of bisthioglycolic acid derivatives. Bisthioglycolic moiety holds its role as a potent scaffold in sulfur-containing drugs. The presented strategy offers significant advantages such as green catalyst as well as solvent, excellent yield, short reaction time, and simple reaction workup. This methodology shows a wide range of substrate scope that contain both electron-donating as well as electron-withdrawing groups.



**Keywords:** ultrasonic energy, green chemistry, bisthioglycolic acid, deep eutectic solvent, Carbon-Sulfur bond formation.

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## PP-13 Eco-Friendly Fabrication and Electrochemical Characterization of Lignin@ZnO Nanocomposites

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### **Abstract**

In this study, lignin-doped zinc oxide (LG@ZnO) nanocomposites were synthesized through an environmentally friendly approach to explore their structural and electrochemical characteristics. Lignin was extracted from rice husk using Soxhlet extraction with ethanol as the solvent, serving as a renewable biopolymer matrix. Zinc oxide nanoparticles were synthesized via the sol-gel method and subsequently combined with lignin to form LG@ZnO nanocomposites. The composites were prepared by keeping the lignin amount constant while varying the ZnO concentration. Comprehensive characterization was carried out using Fourier Transform Infrared Spectroscopy, Scanning Electron Microscopy, Energy Dispersive X-ray Spectroscopy, and X-ray Diffraction to analyze the structural, morphological, and elemental features of the nanocomposites. FTIR confirmed the interaction between lignin functional groups and ZnO, while XRD patterns indicated the crystalline structure of ZnO within the composite. SEM and EDS analyses further verified the homogeneous dispersion and elemental composition, confirming successful lignin incorporation. Cyclic voltammetry (CV) was employed to investigate electrochemical properties and redox behavior. Based on the CV data, the current density was calculated by dividing the peak current values by the geometric surface area of the working electrode, providing a deeper understanding of the electrochemical activity of the prepared nanocomposites.

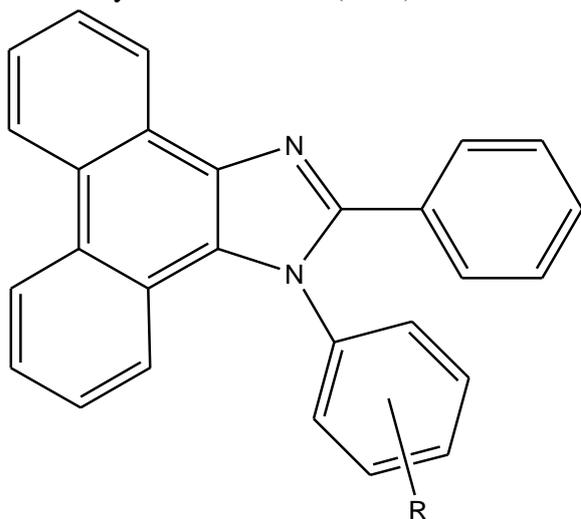
# PP-14 Design and Synthesis of Phenanthro[9,10-d] Imidazole Derivatives for Evaluation of Their Antibacterial Activity

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## Abstract

A series of phenanthrol [9,10-d] imidazole derivatives were designed and synthesized through an efficient, one-pot multicomponent reaction to address the global challenge of multidrug-resistant bacterial strains. The synthesis was achieved by the condensation of phenanthrene-9,10-dione with various substituted benzaldehydes and aniline in the presence of ammonium acetate and acetic acid. Under optimized reflux conditions, the target compounds were obtained in high yields ranging from 78% to 85%. All synthesized derivatives were characterized using modern spectroscopic techniques, including <sup>1</sup>H and <sup>13</sup>C NMR, to confirm their structural integrity. These compounds serve as promising heterocyclic scaffolds for further evaluation against a range of Gram-positive and Gram-negative bacteria to determine their minimum inhibitory concentrations (MIC).



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## PP-15 Fabrication and characterization of Berberine-loaded nanoemulsion reinforcing electrospun scaffolds for the management of wounds

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### Abstract

Electrospun polymeric nanofibers have emerged as an advanced class of wound dressings due to their structural resemblance to the native extracellular matrix (ECM), which facilitates cellular adhesion and proliferation, thereby promoting efficient wound repair. Berberine, an isoquinoline alkaloid pigment, possesses notable anti-inflammatory, antimicrobial, antioxidant, and wound-healing properties. However, its poor aqueous solubility and photosensitivity limit its clinical applicability, necessitating the development of a suitable delivery system to enhance its stability and therapeutic performance. The present study aimed to develop berberine-loaded nanoemulsion (BBR-NE) incorporated electrospun polymeric scaffolds, wherein the nanoemulsion was employed as a nanofiller within the fibrous matrix to achieve reinforced and sustained drug delivery. The prepared scaffolds were systematically characterized for physicochemical properties, morphology, drug encapsulation efficiency, and stability. The results confirmed successful incorporation and stable encapsulation of berberine within the nanofibrous system. *In vivo* evaluation using an incision wound model in Wistar rats demonstrated that the BBR-NE loaded nanofiber mats significantly enhanced wound healing. The micro-nanostructured architecture of the scaffold promoted accelerated wound closure, improved collagen deposition, and enhanced re-epithelialization. Overall, the findings suggest that bioengineered asymmetric wettable nanofibrous scaffolds incorporating berberine nanoemulsion represent a promising and effective therapeutic strategy for the management of wounds.

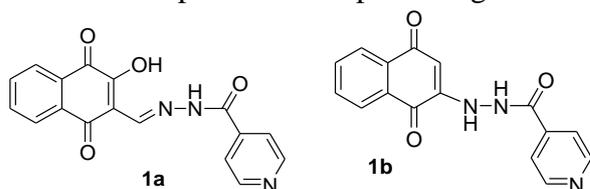
## PP-16 Synthesis, Molecular Docking and Antitubercular activity of Lawsonone derivatives

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### Abstract

The development of novel drug candidates through strategic structural modification of existing drugs has emerged as an effective approach to combat the growing problem of drug resistance. In this context, a new series of Lawsonone derivatives were synthesized by varying the substituents, affording the desired compounds in good yields. These conjugates were evaluated for their antitubercular activity against the M. Tb 7H9OADC. Among the twelve synthesized compounds, two demonstrated excellent minimum inhibitory concentration (MIC) values. Compound 1a showed an MIC of 5 µg/ml, while compound 1b exhibited a remarkable MIC of <0.156 µg/ml, which is comparable to that of isoniazid. Cytotoxicity evaluations further indicated that these compounds are less toxic. In silico docking studies of compounds **1a** and **1b** at the active sites of InhA demonstrated favourable interactions, with docking scores superior to isoniazid. Additionally, ADMET analysis confirmed that these molecules possess promising drug-like properties. Overall, these investigations provide a strong rationale for further development of this promising series of antitubercular agents.



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## PP-17 Skutterudite thermoelectrics for mid-temperature application

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### Abstract

The escalating global demand for fossil fuels and the associated environmental challenges have accelerated the development of clean and sustainable energy technologies. Among these, thermoelectric (TE) technology has emerged as a promising approach due to its capability to directly convert waste heat into electricity without greenhouse gas emissions. Thermoelectric materials are attractive for diverse applications because of their solid-state operation, scalability, and environmental compatibility. The energy conversion efficiency of TE materials is governed by the dimensionless figure of merit,  $ZT$ , which depends on the Seebeck coefficient, electrical conductivity, thermal conductivity, and absolute temperature. However, the large-scale implementation of TE devices remains constrained by relatively low  $ZT$  values and high material costs.

CoSb<sub>3</sub>-based skutterudite thermoelectric materials have attracted significant interest due to their cost-effectiveness, structural versatility, and relatively straightforward synthesis. Strategies such as chemical substitution and filler atom incorporation effectively enhance phonon scattering and optimize carrier concentration, thereby improving thermoelectric performance and stability in the intermediate temperature range (473–773 K). Consequently, these materials are promising candidates for automotive waste heat recovery applications. Although a high figure of merit ( $ZT \approx 2$ ) has been achieved in n-type single-filled CoSb<sub>3</sub>-based antimonides, the performance of p-type skutterudites remains comparatively limited. In this study, filled p-type skutterudites with composition  $M_y\text{Co}_{1-x}\text{Fe}_x\text{Sb}_3$  (where M represents the filler element) were synthesized in bulk form using a powder metallurgy route within a short processing time. The prepared samples exhibit single-phase characteristics and intrinsic p-type thermoelectric behavior, with a power factor of approximately  $0.5 \text{ mW m}^{-1} \text{ K}^{-2}$  at 473 K. The processed  $M_y\text{Co}_{1-x}\text{Fe}_x\text{Sb}_3$  samples display soft magnetic behavior and positive magnetoresistance. Temperature-dependent measurements of the Seebeck coefficient ( $S$ ), electrical conductivity ( $\sigma$ ), and power factor ( $S^2\sigma$ ) reveal that filler incorporation significantly enhances the thermoelectric performance in the mid-temperature range. Detailed investigations of the electronic, magnetic, and optical transport properties of  $M_y\text{Co}_{1-x}\text{Fe}_x\text{Sb}_3$  will be presented.

**PP-18 Role of novel drug delivery system in enhancing iron bioavailability and reducing gastrointestinal side effects in iron deficiency anemia**

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**Abstract**

**Objective**

The primary objective of this review is to comprehensively analyze advancements in novel drug delivery systems, including carrier-based approaches, M cell targeting, and controlled and sustained release formulations, which have been developed to improve iron bioavailability and minimize gastrointestinal side effects commonly associated with conventional iron therapies.

**Significance**

Iron deficiency anemia is a widespread health issue, disproportionately affecting women, children, and vulnerable groups, with serious maternal and population health impacts. This review includes current research, clinical trials, and patented inventions to illustrate the advantages, limitations, and potential future directions of these technologies used in managing IDA. Understanding these advanced systems is crucial for developing safer and more effective iron formulations.

**Key findings**

Advanced drug delivery system including carriers such as liposomes, hydrogels, microspheres, nanoparticles, solid lipid nanoparticles, and sucrosomial iron. They significantly increase intestinal absorption and systemic availability of iron compared to conventional therapies. M cell targeting enhances iron absorption by facilitating efficient transcytosis across the intestinal epithelium, leading to improved bioavailability. Additional benefits from controlled release and gastroretentive dosage forms, which maintain release at absorption sites while reducing adverse effects.

**Conclusion**

Novel drug delivery systems represent a transformative approach in iron supplementation therapy, overcoming the dual challenges of poor bioavailability and gastrointestinal intolerance. By optimizing delivery, absorption, and release kinetics, these systems enhance therapeutic efficacy and patient acceptability. Ongoing research and clinical trials of such technologies hold great promise for developing next-generation iron formulations with enhanced bioavailability, superior safety, and effectiveness profiles.

**PP-19 Triclosan-Isatin Hybrids as Potent Anti-proliferative Agents  
Inducing S-Phase Arrest *via* DNA Gyrase Inhibition in Triple-Negative  
Breast Cancer**

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Triple-negative breast cancer (TNBC) is a particularly aggressive subtype of breast cancer, defined by the absence of estrogen receptors (ER), progesterone receptors (PR), and human epidermal growth factor receptor-2 (HER2). It accounts for approximately 15-20% of all breast cancer cases.<sup>1</sup> Although, FDA-approved selective estrogen receptor modulators (SERMs) such as doxorubicin (DOX), tamoxifen, and raloxifene are commonly used in breast cancer treatment, their clinical utility is frequently hampered by adverse effects-including myelosuppression, insomnia, dizziness, hot flashes, and an elevated risk of endometrial cancer<sup>2</sup>. Despite extensive research, there remains a dearth of therapeutic agents capable of effectively targeting both TNBC and non-TNBC subtypes<sup>3-5</sup>. This underscores a critical need for the development of innovative therapeutic strategies and novel anti-cancer agents capable of addressing the unique challenges posed by this complex disease.

The present work highlights a series of new isatin-triclosan-based hybrids strategically designed and synthesized *via* a copper-promoted click reaction, as illustrated. The resulting compounds were systematically evaluated for their anti-proliferative activity against triplenegative breast cancer (TNBC) cell lines MDA-MB-231 and MDA-MB-468, while their cytotoxicity was assessed using non-cancerous HaCaT keratinocyte cells. Mechanistic investigations revealed that the promising compounds induced caspase-mediated apoptotic cell death in MDA-MB-468 cells, suggesting activation of programmed cell death pathways. Additionally, DNA gyrase inhibition studies showed significant enzymatic suppression, with *in silico* studies supporting a strong binding affinity of the active compounds to the gyrase B active site.

## PP-20 Ni-Doped CuO Nanostructures: Structural Evolution and Enhanced Antimicrobial Activity

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Nickel-substituted CuO nanostructures containing 0, 1, and 3 mol% Ni were fabricated through a high-energy ball milling process followed by thermal treatment at 500 °C. X-ray diffraction analysis verified the formation of a single-phase monoclinic CuO structure without detectable secondary phases, confirming successful Ni incorporation into the CuO lattice. A progressive shift of diffraction peaks toward higher  $2\theta$  angles, supported by Rietveld refinement, indicated a slight contraction of lattice parameters and unit cell volume with increasing dopant concentration. Williamson–Hall analysis revealed reduced crystallite size and enhanced microstrain, suggesting increased defect density upon Ni substitution. Transmission electron microscopy demonstrated irregularly shaped nanoparticles with no significant morphological alteration after doping; however, the average particle size decreased from approximately 39 nm for pristine CuO to about 31 nm for Ni-doped samples, consistent with XRD results. High-resolution TEM confirmed lattice fringes corresponding to the (111) plane, while selected area electron diffraction patterns established the polycrystalline nature of the materials. The antibacterial efficacy against *Escherichia coli* and *Staphylococcus aureus*, assessed using the agar well diffusion method, showed improved bactericidal performance with higher Ni content. The enhanced activity is attributed to particle size reduction, increased structural defects, greater generation of reactive oxygen species (ROS), and suppressed electron–hole recombination. Overall, Ni doping effectively modulates the structural characteristics of CuO nanostructures, leading to superior antimicrobial properties.

### Keywords:

CuO nanostructures, Transition Metal Doping, Antimicrobial activity

## PP-21 Development and Mechanistic Approach Of Doped Semiconductor Photocatalysts for Ciprofloxacin Degradation

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### **Abstract**

The extensive use of ciprofloxacin, a widely prescribed fluoroquinolone antibiotic, has led to its persistent occurrence in aquatic environments due to poor removal by conventional wastewater treatment processes. Its environmental accumulation poses significant ecological risks and contributes to the growing challenge of antimicrobial resistance. Advanced photocatalytic technologies have emerged as effective strategies for the degradation of such recalcitrant pharmaceutical contaminants. This study provides an overview of recent progress in ciprofloxacin degradation using semiconductor-based photocatalytic systems, including TiO<sub>2</sub>, ZnO, graphene-based composites, doped photocatalysts, and biologically assisted approaches. The role of catalyst modification in enhancing visible-light absorption, charge separation, and reactive oxygen species generation is critically discussed. Key degradation pathways involving hydroxyl and superoxide radicals and their interactions with ciprofloxacin's molecular structure are highlighted. Comparative evaluation of different photocatalytic systems reveals improvements in degradation efficiency, stability, and reusability through material engineering and hybrid process integration. Furthermore, emerging photocatalysis-biological coupling strategies are briefly examined for their potential to improve mineralization and reduce toxic by-products. Overall, this work emphasizes the importance of advanced photocatalytic systems as sustainable and promising solutions for mitigating antibiotic contamination in water treatment applications.

## PP-22 Design of a 2-Hydroxy-naphthalene Thiophene Hydrazone Based Dual-Mode Chemosensor for Cu<sup>2+</sup> and Al<sup>3+</sup> Detection

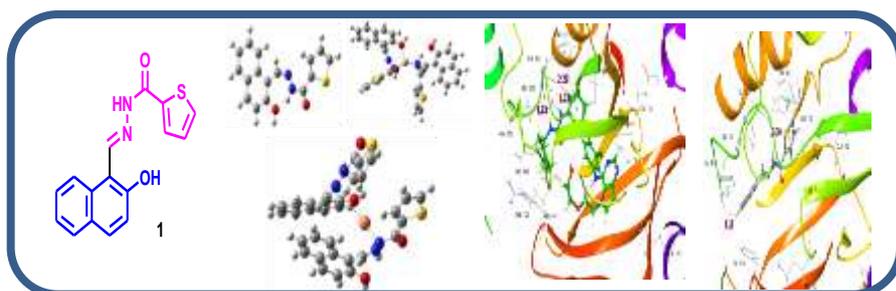
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### Abstract

A novel chemosensor (Probe 1) was synthesized by condensing 2-hydroxynaphthaldehyde with thiophene-2-hydrazide for selective sensing of Al<sup>3+</sup> and Cu<sup>2+</sup> ions in aqueous media. Probe 1 exhibited a fluorescence “turn-on” response with a visible yellow-to-colourless change for Al<sup>3+</sup>, while Cu<sup>2+</sup> induced a yellow-to-green colour change without fluorescence enhancement. The binding constants were  $7.5 \times 10^8 \text{ M}^{-1}$  for Al<sup>3+</sup> and  $1.43 \times 10^{11} \text{ M}^{-2}$  for Cu<sup>2+</sup>, with detection limits of 97 nM and 141.4 nM, respectively. A 2:1 binding stoichiometry for both ions was confirmed by Job’s plot, ESI-MS, and DFT studies. DFT analysis revealed that Al<sup>3+</sup> coordination enhances intramolecular charge transfer and fluorescence by reducing the HOMO–LUMO gap, whereas Cu<sup>2+</sup> forms a more stable complex leading to fluorescence quenching. Probe 1 showed low cytotoxicity (IC<sub>50</sub> = 1 mM), effective intracellular Al<sup>3+</sup> imaging, and weak protein interactions in molecular docking studies, indicating good biocompatibility and potential biological applicability.



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## PP-23 Electrochemical Impedance Investigation of Sustainable Carbon Dots in Mixed Acid-Salt Electrolytes

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### Abstract

Incorporation of nanotechnology allowed for the transformation of biowaste into useful materials with least side effects, that too with lower cost, reduced toxicity and improved stability. The so formed nanomaterials not only contributed to the waste management, but also had applications in fields like energy storage. This study investigates the electrochemical behaviour and energy storage performance of six different acid-salt mixtures (i)  $\text{H}_2\text{SO}_4 + \text{NaCl}$ , (ii)  $\text{H}_3\text{PO}_4 + \text{NaCl}$ , (iii)  $\text{H}_2\text{SO}_4 + \text{H}_3\text{PO}_4 + \text{NaCl}$ , (iv)  $\text{H}_2\text{SO}_4 + \text{Na}_2\text{SO}_4$ , (v)  $\text{H}_3\text{PO}_4 + \text{Na}_2\text{SO}_4$ , and (vi)  $\text{H}_2\text{SO}_4 + \text{H}_3\text{PO}_4 + \text{Na}_2\text{SO}_4$ , when combined with carbon dots (CDs). The CDs were synthesized from banana peel waste using a simple carbonization process. By utilizing Electrochemical Impedance Spectroscopy (EIS), the charge transfer resistance, equivalent series resistance, and Warburg impedance characteristics of each system were thoroughly evaluated. The acid-salt mixture which is best suitable for the real world applications and had balanced characteristics were found through this study. Thus found CD-electrolyte exhibited the lowest ESR, indicating minimal internal losses and enhanced charge transfer capability, making it to be more superior over the other mixtures. These findings provide valuable insight for the selection of electrolytes in supercapacitor and energy storage applications, by following a simple and inexpensive method while at the same time ensuring environmental safety.

**Keywords:** Biowaste, Carbon Dots, Electrochemical Impedance, Acid-Salt Electrolytes, Supercapacitors

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## **PP-24 Biginelli-based organic nanoparticles as probe for detection of alkali metal ions**

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### **ABSTRACT**

Nanoparticles of organic compounds offer remarkable sensing systems for environmentally and biologically significant analytes on account of their facile synthesis, prompt response, superior photostability and biodegradability. Further, the use of fluorescent sensors provide more accurate and swift sensing. The detection of alkali metal ions in environmental and biological samples is a crucial task for regulating the concentration of these metal ions. Any departure from the allowed concentration of these metal ions may lead to deleterious impacts on health or environment.

The current report discusses the synthesis of Biginelli based compounds and their transformation into stable water-based organic nanoparticles (ONP) using reprecipitation method. The characterization of these organic nanoparticles was done using TEM and DLS. These Biginelli-based organic nanoparticles, ONP were explored as fluorescent nanoprobe for selective and sensitive estimation of alkali metal ions. The proposed nanosensors displayed low detection limit and could efficiently work in the wide pH range of 3 to 12, which is excellent for the analysis of environmental and biological samples. The selectivity for alkali metal ions was further established by performing interference studies which further confirmed the absence of any interference from other analytes. Moreover, real sample analysis was done which confirmed the practical applicability of the offered nanoprobe in biological and environmental samples. The discussed nanosensor provides a facile, non-intrusive, selective, sensitive and economic system for the detection of alkali metal ions.

## PP-25 Green and Sustainable Synthesis of Dihydroquinazolin-4(1H)-ones Using a Deep Eutectic Solvent

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A safer, greener, and more effective reaction methodology for the synthesis of dihydroquinazolinones (DHQs) has been developed. The deep eutectic solvent (DES) ZnCl<sub>2</sub>/urea employed in this study efficiently accelerated the cyclization of 2-aminobenzamide with different aldehydes (aromatic and heteroaromatic) to afford the target scaffolds without the generation of any oxidized product. This method has exhibited remarkable advantages such as quick reaction time, mild reaction conditions, high yield (82%–98%), operational simplicity, and selectivity. The approach was observed to be tolerant to electron-donating and electron-withdrawing functional groups. Green metric parameters (AEf, OE, AE, RME, CE, etc.) determined further aided this greener chemical approach.

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## PP-26 Atomistic Tuning of Optoelectronic and Chiroptical Properties in $\pi$ -Conjugated Systems

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### Abstract

Tuning of optoelectronic and chiroptical properties in heteroaromatic  $\pi$ -conjugated systems by an atomistic approach is an important area of research from the viewpoint of designing materials for the advancements in organic electronics. Enhancement of triplet yields in organic materials is intriguingly challenging, though it could have manifold utility in several applications like singlet fission (SF), thermally activated delayed fluorescence (TADF), room-temperature phosphorescence (RTP), etc. Recently, it was known that improvement in those applications could be attained by using materials that are aromatic in their first excited triplet state. But synthetic developments of such stable systems are non-trivial, which can be comprehended from their scarce examples in literature. Diheterolodiheteroles are such  $4n\pi$  antiaromatic systems which are stable in ambient conditions. However, any development towards modulating the triplet yield or the rate of intersystem crossing require further research. Therefore, we have designed, synthesised, and structurally characterized a series of fluorene-based diheterolodiheteroles to understand the problem. Additionally, we could alter the heteroatoms of the  $\pi$  conjugated systems to understand the result through the photophysical characterizations (Abs, Em,  $\tau$ ,  $\phi_{PL}$ ) in combination with computational analysis through density functional theory (DFT), etc. In addition, chiroptical activity have also been amplified by changing the hetero atoms in chalcogenophenyl substituents in multi-substituted acenes, leading to the development of circularly polarised luminescence (CPL) emitters. In short, we have synthesized and explored photophysical properties and the chiroptical activity of these tetraaryl tetracenes in an atomistic manner by varying the heteroatoms in the chalcogenophenyl substituents, which could be a potential candidate for CPL emitters.

**Keywords:** Singlet fission; diheterolodiheteroles; chiroptical activity; tetraaryl tetracenes; fluorene

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## PP-27 Computational Design of Bio-Inspired Molecular Catalysts for Sustainable Hydrogen Production

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### **Abstract**

The global transition toward clean and sustainable energy has intensified research on hydrogen as a carbon-neutral fuel. The present study focuses on the computational design of bio-inspired transition metal complexes as efficient catalysts for the hydrogen evolution reaction (HER). Density Functional Theory (DFT) calculations were employed to investigate electronic structure, adsorption energetics, charge transfer characteristics, and proton-coupled electron transfer mechanisms associated with hydrogen generation. Particular emphasis was placed on ligand environment tuning and the use of earth-abundant metal centers such as Fe, Co, and Ni to replace noble metals. Reaction free energy profiles and key intermediate stabilization energies were analyzed to establish structure–activity relationships governing catalytic efficiency. The findings provide mechanistic insights into rational catalyst design and contribute to the development of cost-effective and sustainable systems for green hydrogen production.

### **Keywords**

Green hydrogen; Hydrogen evolution reaction; Density Functional Theory; Bio-inspired catalysts; Sustainable energy

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## PP-28 In-silico based designing of novel Isatin–Thiazole derivatives as Antihyperuricemic Agents

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### **Abstract**

Xanthine oxidase (XO) is a key enzyme involved in purine metabolism and uric acid production, and its overactivity is associated with hyperuricemia and gout. The development of novel xanthine oxidase inhibitors remains an important therapeutic strategy. In the present study, Isatin–Thiazole derivatives (**1–15**) were designed and evaluated for their inhibitory potential against xanthine oxidase using a molecular docking approach. The crystal structure of xanthine oxidase was retrieved from the Protein Data Bank and prepared for docking studies. All designed ligands were optimized and docked into the active site of the enzyme. Among the screened compounds, **Compound 13** exhibited the best docking performance with a docking score of **–32 kJ/mol** and a ligand efficiency of **0.33**, indicating strong and efficient binding. The compound showed significant hydrogen bonding and hydrophobic interactions with key active site residues and demonstrated binding affinity comparable to the standard drug febuxostat. Furthermore, Compound 13 was found to comply with Lipinski's rule of five, suggesting favorable drug-likeness. These results highlight Isatin–Thiazole derivatives as promising lead molecules for further experimental evaluation.

## PP-29 A Polyaniline-Functionalized Mg/Fe-LDH for High-Capacity Sequestration of Fluoroquinolones

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### **Abstract**

The persistence of fluoroquinolone antibiotics (e.g., ciprofloxacin, norfloxacin) in aquatic systems necessitates advanced remediation strategies. This study presents the development of a novel composite adsorbent by modifying magnesium-iron layered double hydroxide (Mg/Fe-LDH) with polyaniline (PANI) to enhance antibiotic removal. Comprehensive characterization (FTIR, XRD, FESEM) confirmed the successful integration of PANI, which improved the composite's crystallinity, surface morphology, and functional group density.

The PANI-Mg/Fe-LDH composite demonstrated superior and rapid adsorption of ciprofloxacin and norfloxacin from aqueous solutions compared to pristine LDH. This enhanced performance is attributed to synergistic mechanisms, including  $\pi$ - $\pi$  interactions, hydrogen bonding, and electrostatic attraction facilitated by the conjugated PANI chains and LDH layers. The composite also exhibited excellent regenerative capability and stability over multiple cycles.

Our findings highlight PANI-modified Mg/Fe-LDH as a promising, cost-effective, and sustainable adsorbent material for the efficient removal of pharmaceutical contaminants, contributing to the advancement of eco-friendly wastewater treatment technologies.

**P-30 Entropically Favoured ‘Through Space Charge Transfer’ Assemblies: A Lighted Photosensitizer for Regulated Oxidation of Alcohols and Aldehydes**

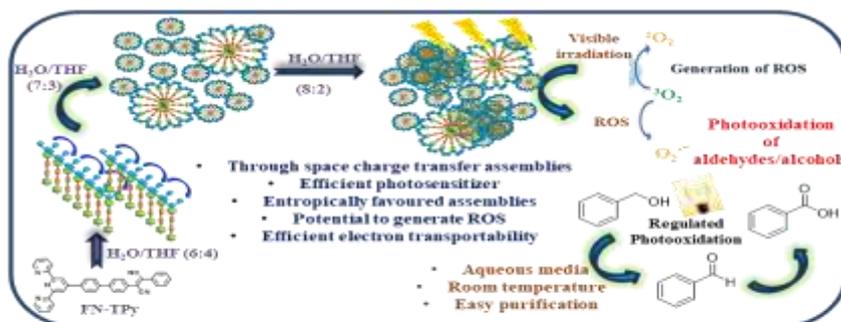
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**Abstract**

Visible light driven sensitized oxidation of organic compounds is a sustainable approach for preparation of synthetically important building blocks.<sup>1-2</sup> Photosensitization enables activation of oxygen to generate reactive oxygen species (ROS) which eventually act as the potent ‘oxidants’ in the oxidative organic transformations. Thus, we developed strong acceptor- weak acceptor FN-TPy which undergoes solvent dependent self-assembly in mixed aqueous media to generate through space intermolecular charge transfer assemblies. The as prepared entropically favoured assemblies of FN-TPy exhibit excellent photostability and photosensitizing properties in the assembled state to activate aerial oxygen for efficient generation of reactive oxygen species (ROS) through Type-I and Type-II pathways. The FN-TPy exhibits excellent potential for regulated oxidation of alcohols and aldehydes under mild reaction conditions (visible light irradiation, aqueous media, room temperature) using aerial oxygen as the ‘oxidant’.<sup>3</sup> The present study demonstrates the potential of FN-TPy assemblies to catalyse controlled oxidation of benzyl alcohol to benzoic acid.



**Keywords:** Photosensitizer, Through Space Charge Transfer, Reactive Oxygen Species

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**PP-31 Source Apportionment of Uranium Prevalence in  
Groundwater of a Hotspot in Southwest Punjab**  
**Guneet Kaur Bhatia<sup>1</sup>, Satvir Singh<sup>2</sup>, P.K. Sahoo<sup>3</sup>, B.S. Bajwa<sup>4,\*</sup>,  
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**Abstract**

High prevalence of uranium in southwest region of Punjab poses significant health risks like cancer, kidney damage, lung disease and other chronic health issue [1]. Groundwater samples were analyzed for major ions and trace metals to understand the hydrogeochemical processes and contaminant sources in southwest Punjab. The study area was systematically investigated using two grid-based sampling approaches of  $12 \times 12 \text{ km}^2$  and  $6 \times 6 \text{ km}^2$  to identify groundwater contamination hotspots in Bathinda and Mansa districts. Based on the spatial assessment, Jalal village was identified as a major hotspot in Bathinda, where 20 groundwater samples were collected from a newly drilled borewell and a detailed borehole investigation revealed two distinct subsurface layers: a semi-impermeable oxidized clay layer between 120 and 140 ft and a fully impermeable compact clay layer at approximately 235 ft depth, indicating depth-wise variations in groundwater quality. The groundwater was found to be alkaline with TDS ranging from 604 to 3100  $\text{mg L}^{-1}$ . The concentration of uranium and fluoride fell within the range of 72.64-463.78  $\mu\text{g L}^{-1}$  and 1.80-4.97  $\text{mg L}^{-1}$ . The study found that 100% of samples exceeded the uranium and fluoride concentration limit of 30  $\mu\text{g/L}$  and 1.5  $\text{mg L}^{-1}$  as recommended by the WHO (2022) [2]. Uranium enrichment at shallow depth (>125ft) was 2-3 times more than the deeper groundwater (<235 ft.), suggesting that anthropogenic activities may enhance uranium mobilization in the groundwater at the hotspot location.

**Keywords:** Groundwater contamination, Hydrogeochemistry, Depth distribution, Subsurface layers.

**References:**

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**PP-32 Elucidating Hydrophobic Interactions in Phenanthrene–Imidazole Derived Chiral Scaffolds for Supramolecular Assembly.**

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**Abstract:** Researchers are exploring ways to control chiral fluorescent self-assembly through dynamic supramolecular interactions, a promising route for designing smart luminescent materials<sup>1</sup>. In this work, a new phenanthrene–imidazole derivative has been synthesized, using menthol and cholesterol as chiral building blocks and a carbamate bond as the connecting link. This molecular scaffold is able to organize itself into ordered structures when placed in a mixed water–dioxane environment. Interestingly, the assembly doesn't stay fixed over time or with changes in temperature, it shifts from a kinetically trapped form into a more stable thermodynamic arrangement.

**Keywords:** *supramolecular self-assembly, luminescent chiral materials, supramolecular interactions*

**References:**

1. Cheng, Y.; Liang, B.; Cao, W.; Wei, X.; Wang, P.; Xia D. Modulating fluorescent and chiral properties of luminescent self-assemblies by supramolecular interactions, <https://doi.org/10.1021/acsami.5c23186>.

## PP-33 Multicomponent Synthesis and Characterization of a DHPM Scaffold

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### **Abstract**

Dihydropyrimidinones (DHPMs) are valuable heterocyclic scaffolds with broad pharmacological potential. They are commonly synthesized through the Biginelli reaction, a classical multicomponent reaction first reported by Pietro Biginelli in 1893. This acid catalyzed condensation of ethyl acetoacetate, benzaldehyde, and urea or thiourea provides 3,4-dihydropyrimidin-2(1H)-one or thione derivatives and is widely appreciated for its simplicity and structural diversity in drug discovery. In this study, ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM) was synthesized under reflux in ethanol using acid catalysis. The reaction was monitored by TLC and afforded the product in good yield. Structural confirmation was achieved by melting point determination,  $^1\text{H}$  and  $^{13}\text{C}$  NMR, UV-Visible, and IR spectroscopy. The versatility of the Biginelli reaction continues to support its relevance in medicinal chemistry and related fields, including the development of biologically active molecules and functional materials.

**PP-34 Achieving white light emission from a hydrazone through three different channels: AIE, solvatochromism and excitation wavelength**

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**Abstract**

Reported herein is a hetero-bis-hydrazone that comprising two different diones which emit independently in the blue and orange regions, resulting in white light emission in solution. Two ESIPT moieties simultaneously emitting in the blue and orange regions led to white light. The presence of four tautomers, two from each, was crucial to achieve this. Interestingly, the white light emission was achieved using three channels: AIE, solvatochromism, and tuning of the excitation wavelengths in a partially aggregated solution (fw = 30%). These results will pave the way for designing new molecular frameworks that can emit white light under multiple experimental conditions.



**Keywords:** white-light emission, ESIPT

**References:**

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## PP-35 Investing the ion sensing capability of catechualdehyde conjugated 1,2,3 triazole towards cerium ions

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<sup>b</sup> *Department of Chemistry, Shanti Devi Arya Mahila College, Dinanagar 143531, Punjab, India*

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### **Abstract**

A novel protocatechualdehyde-tethered 1,2,3-triazole-based fluorescent probe (PCT) was synthesized through Cu(I)-catalyzed click chemistry for the selective detection of Ce<sup>3+</sup> ions in an acetonitrile:water (4:1) medium. The probe was thoroughly characterized using FTIR, NMR (<sup>1</sup>H and <sup>13</sup>C), and GCMS spectroscopic techniques. PCT exhibited selective UV-vis chemosensing behavior along with a fluorescence turn-off response toward Ce<sup>3+</sup> ions, attributed to a photoinduced electron transfer (PET) mechanism. Fluorescence studies indicated a low limit of detection (LOD) of  $1.38 \times 10^{-7}$  M for Ce<sup>3+</sup> ions, while the Benesi-Hildebrand plot showed a favorable association constant ( $K_a$ ) of  $4.03 \times 10^6$  M<sup>-1</sup> for the [PCT-Ce<sup>3+</sup>] complex.

The binding mode and 1:1 stoichiometric ratio between PCT and Ce<sup>3+</sup> were confirmed through FTIR analysis, LCMS spectra, and Job's plot experiments. The probe effectively quantified cerium ions in real water samples and was further applied in the design of a reversible INHIBIT molecular logic circuit. The optimized geometries of PCT and the [PCT-Ce<sup>3+</sup>] complex were obtained using the B3LYP method with the 6-311G++(d,p)/SDD basis set implemented in Gaussian 09. DFT calculations revealed a reduction in the frontier molecular orbital (FMO) energy gap upon Ce<sup>3+</sup> binding, supporting the formation of a stable [PCT-Ce<sup>3+</sup>] complex.

# PP-36 Design, Synthesis, and Antibacterial Evaluation of Sesamol-Based Indole Hybrids

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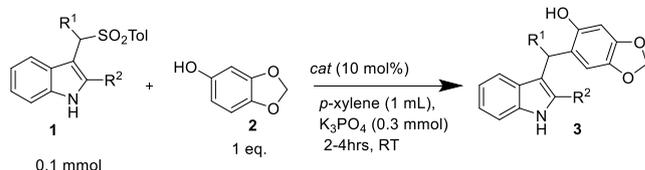
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## Abstract

The indole nucleus represents one of the most privileged heterocyclic scaffolds, widely present in biologically active natural products and pharmaceutical agents [1]. Among indole derivatives, 3-substituted indoles have attracted significant attention due to their diverse biological activities, leading to the development of various synthetic methodologies. Sesamol, an electron-rich natural phenol, is another important structural motif known for its antioxidant and antimicrobial properties and serves as an excellent nucleophile in Friedel–Crafts alkylation reactions [2]. In the present study, a series of novel sesamol-based indole derivatives were synthesized through Friedel–Crafts reactions involving in situ generated vinylogous imine intermediates.

The antibacterial potential of the synthesized compounds was evaluated against selected Gram-positive and Gram-negative bacterial strains, including *Staphylococcus aureus*, *Bacillus subtilis*, *Escherichia coli*, and *Klebsiella pneumoniae* [3]. The antibacterial activity was assessed using the agar well diffusion method. Preliminary results indicate that several compounds exhibit promising antibacterial activity, highlighting the potential of sesamol-derived indole frameworks as antibacterial agents.

This study demonstrates an efficient synthetic approach combined with biological evaluation, offering valuable insights into the development of new antibacterial molecules based on indole-sesamol hybrids.



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**PP-37 ESIPT-active benzothiazole based fluorescent spray for  
Advanced fingerprint applications**

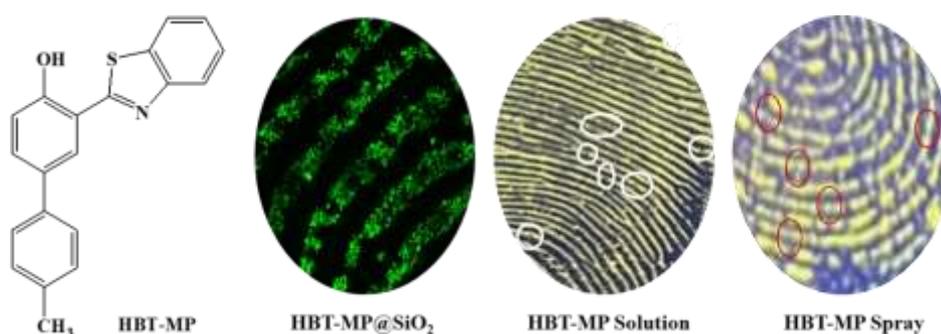
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**Abstract**

HBT derivatives exhibit dual iconic features of aggregation-induced emission (AIE) and excited-state intramolecular proton transfer (ESIPT) process to contribute exceptional luminescent properties. Herein, we designed and synthesized a novel methyl phenyl substituted 2-(2-hydroxyphenyl) benzothiazole (**HBT-MP**) derivative and characterized by  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and Powder X-Ray Diffractograph. **HBT-MP** exhibited AIE assisted ESIPT phenomenon at >70%  $\text{H}_2\text{O}$ -ACN mixture and ESIPT in non-polar solvents with bright yellow fluorescence due to more stabilized keto form. These prominent features were explored for fingerprint visualization at all 1-3 levels using solution and spray-based methods. Further, silica-incorporated **HBT-MP** (**HBT-MP@SiO<sub>2</sub>**) solid powder also depicted advanced latent fingerprint visualisation through powder dusting method. In all cases, the developed fingerprints revealed intense yellow fluorescent features of levels 1-3 with high-contrast and resolution under UV illumination. The enhanced ridge to furrow contrast occurs due to strong  $\pi$ - $\pi$  stacking and H-bonding interactions of **HBT-MP** with lipidic and amino acid components of fingerprint residues that were further evidenced by separately dusting the solutions of sweat components with **HBT-MP@SiO<sub>2</sub>** powder. We also explored the versatility of **HBT-MP** to assess the tape lifting and anticounterfeiting applications. Even, the visualized fingerprints retained ridge resolution before and after heat exposure at wide range of temperatures. The highly crystalline **HBT-MP** revealed the formation of spheres as confirmed by AFM studies.



**Fig.1.** Chemical Structure of **HBT-MP**, photograph for sweat pores from LFPs developed on glass slide using **HBT-MP@SiO<sub>2</sub>** and on aluminum foil using **HBT-MP** ( $10^{-4}$  M) solution and spray in 95% aq. solution captured by CLSM and mobile camera under UV light respectively.

**Reference:** J. Singh, P. Singh, ESIPT-active benzothiazole based fluorescent spray for Advanced fingerprint applications (Under Preparation).

**PP-38 Design, Synthesis, and Biological Evaluation of Triazole-Linked Lignan–Monoterpenoid-Based Hybrid Molecules as Xanthine Oxidase Inhibitors with Potent In Vivo Efficacy**  
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A novel series of triazole-tethered monoterpenoid–lignan hybrid molecules has been designed to target xanthine oxidase (XO), the enzyme responsible for hyperuricemia when it is up-regulated, resulting in gout and other metabolic disorders. Designed molecules were synthesized and initially evaluated for their XO inhibitory potential, and MT7 was most active (XO: IC<sub>50</sub> = 0.263 ± 0.06 μM) with radical scavenging efficacy. MT7 showed higher cytotoxic potential against XO harboring cancer cells (MBDA-MB-231 breast cancer cells) than non-XO-harboring cells (A547 skin cancer cells), confirming intracellular XO inhibition. MT7 was nontoxic to mouse fibroblast cells (L929) and had favorable pharmacokinetic profiles. In vivo investigations in rodent-based animal models revealed the LD<sub>50</sub> (300 mg/kg) value of MT7 and a dose-dependent reduction in serum uric acid. Overall, this suggests MT7 as an effective lead molecule for further investigations as a potential clinical candidate for the management of hyperuricemia via XO inhibition.

**Keywords:** Xanthine oxidase, hyperuricemia, triazole, eugenol, sesamol.

## PP-39 Studies in the Development of Chiral Materials and Evaluation of their Self-Assembly behaviour

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**Abstract:** Self-assembly is a process where monomers of the building block come together to organize into highly ordered structures via non covalent forces such as H-bonding,  $\pi$ - $\pi$  interactions, dipole-dipole, van der Waals interactions etc. During organisation the molecules arrange into different shapes such as spheres, nano-fibers, sheets etc.<sup>1, 2</sup> To mimic nature inspired chirality transition and advanced biological functions, we aimed at regulating self-assembly behavior of synthetic building blocks in water. Our study is focused on regulation of self-assembly using solvent as stimuli, thus previously we had achieved development of superhelix in mixed aqueous media in **Pyra-Chol** having carbamate unit for H-bonding. Building block shows Aggregation Induced Quenching<sup>3</sup> and was found to be Circularly Polarised Luminescence inactive. CPL active materials are important due to their applications in advance optical functionality like OLEDs, optical fibers etc. Following same we further designed and synthesized **Pyra-O-Chol**, having ester linker unit between pyrazine-based core and cholesterol chiral handle. **Pyra-O-Chol** shows helical type morphological structure development upon self-aggregation in mixed aqueous media and showed Aggregation Induced Absorption Enhancement as well as was found to be Aggregation Induced Emission Emissive in nature. We have also regulated excited state chirality in different solvent mixtures. Since **Pyra-O-Chol** was found to be CPL active so it could have potential in photo optics.<sup>4</sup>

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4. *Nanoscale Adv.*, **2026**, DOI: 10.1039/D5NA01038A

**PP-40 Sustainable Synthesis and Structural Characterization of  
Nb<sub>2</sub>AlC MAX Phase and Nb<sub>2</sub>C MXene for Energy Storage Applications**

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**Abstract :**

Nb<sub>2</sub>AlC MAX phases and their two-dimensional MXene derivatives have attracted significant attention due to their layered structure, chemical stability, and multifunctional materials properties. In the present work, a sustainable and reproducible route is reported for the synthesis of Nb<sub>2</sub>AlC MAX phase and its subsequent conversion into Nb<sub>2</sub>C MXene. Nb<sub>2</sub>AlC was prepared via a solid-state reaction. Selective etching of the aluminum layer used a mild fluoride-salt/acid system to reduce hazardous exposure, enabling the production of multilayer Nb<sub>2</sub>C MXene. The transformation from MAX to MXene was verified through changes in diffraction behavior, morphology, and surface chemistry. X-ray diffraction showed a characteristic shift and broadening of peaks after etching, indicating layer separation and structural modification. Spectroscopic analysis definitively confirmed the removal of aluminum and the introduction of surface groups. The combined results demonstrate an effective MAX-to-MXene conversion with clear structural correlation between precursor and derived material. This study provides a practical and environmentally considerate framework for preparing Nb-based MXenes and supports their further exploration in advanced materials and electrochemical device applications.

**Keywords:** MAX phase, Nb<sub>2</sub>C MXene, Selective etching, Advanced materials, Energy storage, Structural characterization



## PP-42 Coordination Polymers: A Versatile Platform for Next-Generation Energy Technologies

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### **Abstract**

Coordination polymers (CPs), constructed from metal ions interconnected by organic ligands have emerged as versatile materials for advanced energy storage and conversion technologies. Their tunable architectures, high porosity, strong adsorption capacity, and abundance of redox-active sites render them particularly attractive for applications in electrocatalysis and supercapacitors. In present work, two transition metal-based CPs;  $[\text{Cu}(\text{ANBA})(4,4'\text{-bipy})(\text{NO}_3)]_n$  (Cu-CP) and  $[\text{Zn}(\text{ANBA})_2(4,4'\text{-bipy})]_n$  (Zn-CP) were synthesized via a facile hydrothermal approach using 2-amino-5-nitrobenzoic acid (ANBA) and 4,4'-bipyridine (4,4'-bipy) as organic ligands. Comprehensive structural, spectroscopic characterizations, such as single-crystal XRD, infrared spectroscopy (IR), UV-visible spectroscopy, and thermogravimetric analysis (TGA) confirmed the successful formation of the target CPs. The functional properties of these materials were subsequently evaluated in hydrogen evolution reaction (HER) electrocatalysis and supercapacitor energy storage. Cu-CP exhibited notable HER catalytic activity highlighting its potential as a cost-effective alternative to conventional noble-metal catalysts, while Zn-CP demonstrated electrochemical performance, including favorable specific capacitance and stable cycling performance. The enhanced performance of both CPs can be attributed to the synergistic interactions between the metal centers and organic linkers, which facilitate efficient electron transfer and provide abundant active sites. Furthermore, the interconnected porous frameworks promote electrolyte penetration and ion transport, thereby improving overall electrochemical efficiency. These findings highlight the potential of coordination polymers as cost-effective and multifunctional materials for advancing sustainable energy technologies, particularly in hydrogen production and high-performance energy storage systems.

**Keywords:** Coordination polymers, Hydrogen evolution reaction, Supercapacitor, Electrochemical studies.

**PP-43 Synthesis and Photophysical Studies of Cu<sup>2+</sup> Selective  
Fluorescent Schiff bases**

**Smile Sharma<sup>a</sup>, Navdeep Kaur<sup>a</sup>, Punita Tiwari<sup>a</sup> and Kuljit Kaur<sup>a\*</sup>**

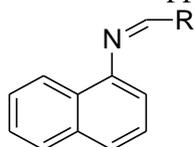
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**Abstract**

Schiff bases are versatile compounds widely explored for their coordination ability and sensing applications due to the presence of azomethine (–C=N–) functional groups. In the present study, a series of Schiff bases were synthesized via condensation reactions between substituted aldehydes and primary amines under mild conditions. The synthesized compounds were characterized using FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and mass spectrometry to confirm the formation of the imine linkage. The sensing behaviour of the synthesized Schiff bases toward Cu<sup>2+</sup> ions was systematically investigated using UV–Visible absorption and fluorescence spectroscopy. Upon addition of Cu<sup>2+</sup> ions, significant spectral changes were observed, including bathochromic shifts in UV–Vis spectra and pronounced fluorescence quenching, indicating strong coordination between the azomethine nitrogen and Cu<sup>2+</sup> ions. The binding interaction was further supported by titration studies, which demonstrated good selectivity and sensitivity toward Cu<sup>2+</sup> in the presence of other competing metal ions. Theoretical studies of these Schiff bases for studying the binding energy with Cu<sup>2+</sup> ions have also been done to support the mechanisms of interaction.

The sensors exhibited a rapid response, high selectivity, and a low detection limit, highlighting its potential application for environmental monitoring and biological analysis of copper ions. These findings suggest that the synthesized Schiff bases serve as efficient and cost-effective chemosensors for Cu<sup>2+</sup> detection. Theoretical studies of these Schiff bases for studying the binding energy with Cu<sup>+</sup> ions have also been done to support the mechanisms of interaction between them.



R= -Aryl, -Naphthyl

# PP-44 Dual-Action Isoxazole Derivatives: Integrating Synthesis and Computational Insights for Sustainable Antibacterial Therapy

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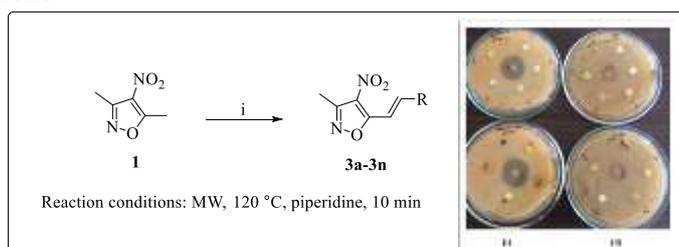
## Abstract

The rapid emergence of multidrug-resistant (MDR) bacterial strains represents a critical global health challenge, demanding innovative therapeutic strategies [1,2]. In this study, a series of structurally diverse isoxazole derivatives were rationally designed and synthesized as potential dual antibacterial and antioxidant agents. Structural elucidation was carried out using standard spectroscopic techniques.

The in vitro antibacterial activity was evaluated against selected Gram-positive and Gram-negative strains, including MDR isolates, using the agar well diffusion method. Several derivatives exhibited significant antibacterial potency, with selected compounds demonstrating zones of inhibition comparable to or exceeding ciprofloxacin. Halogen-substituted derivatives showed enhanced activity, emphasizing the role of electronic and steric modulation in antibacterial efficacy [2].

To elucidate the molecular basis of activity, docking studies were performed against *Escherichia coli* Peptide Deformylase and DNA gyrase, revealing favorable binding interactions through hydrogen bonding and hydrophobic contacts. In silico ADME predictions suggested acceptable pharmacokinetic properties and favorable oral bioavailability [3].

**Novelty:** This work integrates synthetic chemistry, biological screening, and computational modeling to develop dual-functional isoxazole derivatives targeting antimicrobial resistance and oxidative stress, presenting a translational framework for sustainable therapeutic development.



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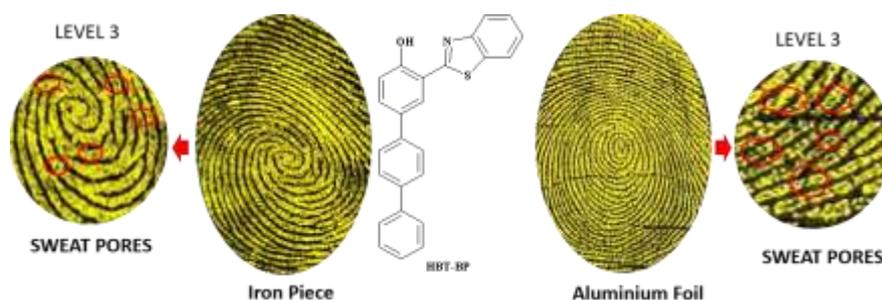
## PP-45 Silica-Supported HBT-BP for durable latent fingerprint applications

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Herein, We designed and synthesized a novel biphenyl appended 2-(2-hydroxyphenyl) benzothiazole (**HBT-BP**) and characterized through  $^1\text{H}$ ,  $^{13}\text{C}$  NMR and powder-XRD techniques. Strong bright yellow fluorescence for **HBT-BP** under UV light intertwined its excellent use for LFP applications. Silica incorporated **HBT-BP** (**HBT-BP@SiO<sub>2</sub>**) was explored to visualize bright yellow fluorescent ridge details on various porous and non-porous substrates. The developed fluorescent latent fingerprints revealed distinct features of level 1 ridge pattern, level 2 minutiae points and level 3 sweat pore details. **HBT-BP@SiO<sub>2</sub>** was further successfully employed for tape lifting applications using adhesive tape. Moreover, highly resolved and good contrast fluorescent LFP images fulfil forensic demands. Moreover, the fingerprints with well resolved ridge details, developed before and after thermal exposure to broad temperature range demonstrated high thermal robustness for forensic purposes.



**Fig.** The photograph for sweat pores of developed latent fingerprint using **HBT-BP@SiO<sub>2</sub>** solid powder and captured through mobile camera under UV light.

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**PP-46 Light-driven Uncaging of Gem-dithiol based Fluorogenic Donors: Influence of Aggregation on Hydrogen Sulfide (H<sub>2</sub>S) Release Kinetics**

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**Abstract**

Hydrogen sulfide (H<sub>2</sub>S) is recognized as a vital gasotransmitter involved in numerous physiological and pathological processes, including neurodegenerative disorders and cancer. However, the development of biomimetic systems capable of controlled and spatiotemporal H<sub>2</sub>S delivery remains a significant challenge. Photoactivated donors offer precise temporal control, yet their efficiency can be strongly influenced by molecular aggregation, which is often overlooked.

Herein, we report a light-driven, fluorogenic H<sub>2</sub>S donor based on gem-dithiol-protected carbonyl scaffolds that exhibit aggregation-caused quenching (ACQ) behavior. The donor molecules were synthesized via thiol protection of fluorophore-containing aldehydes and ketones to generate photo-labile gem-dithiol precursors. Upon irradiation at 365 nm, photo-uncaging leads to the formation of gem-dithiol intermediates, which are inherently unstable, particularly in aqueous environments, and spontaneously decompose to release H<sub>2</sub>S.

Importantly, systematic spectroscopic investigations reveal that molecular aggregation significantly suppresses fluorescence and reduces the rate of photoproduct formation compared to non-aggregated systems. This aggregation-dependent behavior directly influences the uncaging efficiency and subsequent H<sub>2</sub>S release kinetics, demonstrating a clear correlation between supramolecular state and photochemical reactivity. Unlike conventional detection methods that rely on external assays such as the methylene blue method, the present system enables intrinsic, self-reporting monitoring of H<sub>2</sub>S release through fluorogenic response.

These findings establish gem-dithiol-based fluorogenic donors as mechanistically tunable, aggregation-modulated photo-responsive platforms for controlled and self-indicating H<sub>2</sub>S release.

**Keywords:** Hydrogen sulfide, light induced, fluorescence, donors

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## PP-47 Sequential Precipitation-Assisted Selective Recovery of Gold and Copper from E-Waste

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### Abstract

The recovery of noble metals from e-waste is critical for sustainable industrial operations. This study presents a sequential, precipitation-assisted extraction method for the selective recovery of gold and copper from aqua regia leachate of waste CPU pins. Gold was selectively precipitated as tetraphenylphosphonium tetrachloroaurate (TPPAuCl<sub>4</sub>) via precipitate reaction (or) double displacement reaction, achieving 99% recovery at trace levels (0.5 ppm) and a high precipitation capacity of 466 mg/g. Copper was subsequently recovered as Cu(DDTC)<sub>2</sub> with 98% efficiency through pH-controlled coordination precipitation. The recovered complexes were characterized by XPS, HR-MS, and UV-Vis spectroscopy, and reduction of TPPAuCl<sub>4</sub> produced metallic gold of 99.8% purity (23.94 karats). Unlike conventional liquid-liquid extraction, the method avoids volatile organic solvents, minimizing secondary pollution. The use of a commercially available and recyclable reagent (TPPBr) enhances operational simplicity and industrial scalability. This approach combines high efficiency, selectivity, and environmental compatibility, offering a practical and sustainable strategy for multi-metal recovery from e-waste in industrial applications.

**Keywords:** E-waste, sequential precipitation, gold and copper recovery, tetraphenylphosphonium bromide, sodium diethyldithiocarbamate, sequential precipitation.

## PP-48 Bimetallic Coordination Network for Supercapacitor Energy Storage Applications

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### **Abstract**

Supercapacitors are emerging as key players in energy storage because of their rapid charge-discharge capability, long cycle life, and enhanced safety compared to traditional batteries [1]. Meeting the growing demands of modern energy systems requires advanced electrode materials that combine high electrical conductivity, large surface area, and robust electrochemical stability [2]. One exciting direction involves bimetallic coordination polymers (COPs), which combine two synergistic effects of two different metals to achieve stronger frameworks and improved electrochemical performance. In this study, we report the synthesis of novel bimetallic COP, CsZn-COP  $[\text{Cs}_2\text{Zn}_1(\text{BTC})\cdot\text{H}_2\text{O}]_n\cdot 3\text{H}_2\text{O}$ , constructed from zinc ( $\text{Zn}^{2+}$ ), cesium ( $\text{Cs}^+$ ), and benzene-1,2,4,5-tetracarboxylate (BTC) ligands. The crystal structure features  $\text{Zn}^{2+}$  in a tetrahedral coordination environment, linked to  $\text{Cs}^+$  ions via oxygen atoms, with  $\text{Cs}^+$  further stabilizing the extended network. This design improves both conductivity and mechanical strength. Electrochemical performance was comprehensively analyzed using cyclic voltammetry (CV), galvanostatic charge–discharge (GCD), and electrochemical impedance spectroscopy (EIS). The CsZn-COP electrode showed a high capacitance of 1227.2 F/g at 1 A/g. In an asymmetric supercapacitor configuration, it delivered 107.1 F/g, with an energy density of 29.2 Wh/kg and a peak power density of 6999.9 W/kg. These results highlight the material's ability to combine high energy storage with rapid power delivery, making it a promising candidate for future supercapacitor technologies.

**Keywords:** Bimetallic coordination polymer, supercapacitor, energy density, electrochemical performance, reversibility, robust network

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# PP-49 Deep Eutectic Solvent in Thermoacoustic Studies: A Comprehensive Review of Application, Properties, and Recent Advances

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## **Abstract**

Deep eutectic solvents (DES) are a new type of green solvents that have exceptional physicochemical characteristics that render them appealing alternatives to conventional organic solvents and ionic liquids. The paper is a review on the use of thermoacoustic in thermoacoustic studies, its volumetric, acoustic, and thermodynamic characteristics. Recent development in natural deep eutectic solvents (NADES), choline-based DES systems, and applications are discussed in the review in the pharmaceutical, food and material science industries. The studies of Thermoacoustic indicate important understanding of molecular interactions, solvation behavior, and structure of systems composed of DES. The characterization techniques are given special consideration, and this is associated with ultrasonic velocity measurements, density determination, and derived thermodynamic parameters. The review presents the existing information on the use of DES in the fields of drug solubility, biomolecule preservation and analytical chemistry and determines the further directions of research into this rapidly changing area.

**Keywords:** Deep eutectic solvents, Natural deep eutectic solvents, Thermoacoustic, Choline chloride, Volumetric analysis, Molecular interactions, Green solvents, Ultrasonic methods.

## PP-50 Photocatalytic and energy storage application of Ni<sup>2+</sup> doped Mg-spinels and its composites.

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### **Abstract**

Herein, Ni-doped Mg spinel ferrites (Mg<sub>1-x</sub>Ni<sub>x</sub>Fe<sub>2</sub>O<sub>4</sub>) were synthesized using the sol-gel auto-combustion method and calcined at 800 °C for 4 h. The Rietveld refined of X-ray diffraction (XRD) data confirmed single-phase cubic spinel structure for all compositions, except for x = 0.0, which showed the presence of a minor impurity peak. The lattice parameter (a) and unit cell volume (V<sub>cell</sub>) exhibited a decreasing trend with increasing Ni<sup>2+</sup> concentration, attributed to the smaller ionic radius of Ni<sup>2+</sup> compared to Mg<sup>2+</sup>. FTIR spectra revealed the characteristic absorption bands corresponding to Fe-O stretching vibrations at tetrahedral (A-site) and octahedral (B-site) positions, confirming the spinel structure. The highest dielectric constant value (~5500) was observed for x=1.0. Furthermore, the Ag/AgBr/Ni<sub>0.4</sub>Mg<sub>0.6</sub>Fe<sub>2</sub>O<sub>4</sub> nanocomposite was synthesized via a modified deposition-precipitation followed by photoreduction method. The nanocomposite exhibited good photocatalytic activity by degrading methyl orange dye within 50 minutes under 400-W UV irradiation.

# PP-51 V<sub>2</sub>O<sub>5</sub>/COF Composite as an Efficient Electrochemical Platform for Sensitive Ascorbic Acid Sensing.

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## **Abstract**

Sensitive and selective detection of ascorbic acid (AA) is crucial due to its significant role in biological, pharmaceutical, and food systems. In this work, a novel electrochemical sensor based on a vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) and covalent organic framework (COF) composite was developed for efficient ascorbic acid detection. The V<sub>2</sub>O<sub>5</sub>@COF composite was synthesized to combine the high redox activity and electron transfer capability of V<sub>2</sub>O<sub>5</sub> with the large surface area, porous structure, and abundant active sites of COF, resulting in enhanced electrochemical performance. The electrochemical behavior of the fabricated electrode was investigated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). DPV was employed for the quantitative detection of ascorbic acid due to its higher sensitivity and better resolution. The V<sub>2</sub>O<sub>5</sub>@COF modified electrode exhibited a strong and well-defined oxidation peak for ascorbic acid, indicating excellent electrocatalytic activity. The fabricated sensor displayed a good sensitivity, and excellent reproducibility and stability. The enhanced sensing performance is attributed to the synergistic interaction between V<sub>2</sub>O<sub>5</sub> and COF, which promotes rapid electron transport and effective adsorption of ascorbic acid molecules. Moreover, the sensor showed good selectivity in the presence of common interfering species. This study highlights the potential of V<sub>2</sub>O<sub>5</sub>@COF composite as a promising electrochemical sensing platform for sensitive and reliable detection of ascorbic acid, with possible applications in biomedical analysis, pharmaceutical monitoring, and food quality control.

**Keywords:** V<sub>2</sub>O<sub>5</sub>, Covalent Organic Framework (COF), Electrochemical sensor, Ascorbic acid detection.

# PP-52 Formation of stable radical anions from modified benzothiazole functionalized Perylene diimide derivatives

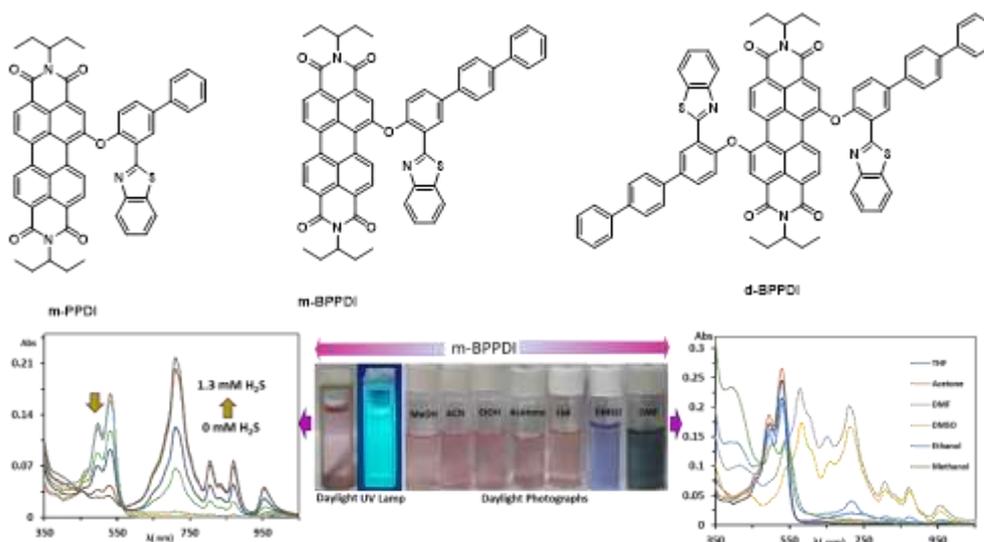
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## Abstract

Perylene diimides (PDIs) possessing electron-deficient  $\pi$ -conjugated system have tunable features through ortho, peri and bay-functionalization. The formation of PDI based radical anions has gained more recognition due to outstanding role in organic electronics, catalysis, and light-driven energy conversion processes. Therefore, Phenyl and biphenyl substituted benzothiazole moieties were introduced onto mono- and di-bromo perylene diimides as **m-PPDI**, **m-BPPDI** and **d-BPPDI** derivatives. We investigated the radical formation properties of **m-BPPDI** and **d-BPPDI** derivatives in different solvents. Favourably, **m-BPPDI** and **d-BPPDI** radical anions exhibited pronounced stability in aqueous medium.



**Keywords:** phenyl, biphenyl, benzothiazole, radical, perylene diimide, aqueous

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## **PP-53 Self-Assembly Behavior of Bio-Based Surfactants and their Role in the Concentration-dependent Enhancement of Enzymatic Activity**

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### **Abstract**

3-Quinuclidinol bio-based surfactants with alkyl chain length of 8, 12, 16 carbons and one amide functionalized have been prepared. 3-Quinuclidinol is a derivative of Quinuclidines which have anti-microbial, antioxidant and medicinal properties. The self-assembly behavior of these surfactants has been studied by different techniques namely conductometry titrations, Fluorescence measurements, Surface tension, Dynamic light scattering (DLS), Nuclear magnetic resonance ( $^1\text{H-NMR}$ ). The activity of the Cytochrome-c was analyzed in the prepared aqueous solution of surfactants. The enzyme-surfactant interactions were studied at below and above *cmc* for all the surfactants. The activity of Cytochrome-c was found to be 35% higher as compared to that observed in buffer. The surface properties of these surfactants have been found to be better compared to conventional cationic surfactants. The ease of synthesis combined with biocompatible functional design and excellent surface properties makes them useful for several industrial and biological applications.

# PP-54 Isatin-Nitroimidazole 1*H*-1,2,3-Triazole Tethered hybrids-: Synthesis, Docking, and Anti-Proliferative Evaluation against Breast Cancer

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Cancer is responsible for approximately 8.2 million deaths and remains as the most difficult disease to treat worldwide.<sup>1</sup> Rapidly dividing cells such as breast, skin, and uterine cells are at higher risk of mutations compared with cells which do not divide and thus are more prone to develop cancer. Breast cancer (BC) is one of the most frequently occurring cancers leading to significant morbidity and mortality among women.<sup>2</sup> One of the significant approaches for the treatment of BC comprises the selectively inhibiting the binding of estrogen with estrogen receptors (ER $\alpha$  and ER $\beta$ ) and resulted in the identification of selective estrogen modulators, SERMs. Estrogen has been reported to play a vital role in the growth and development of mammary glands. Interaction of estrogen with estrogen receptors (ER $\alpha$  and ER $\beta$ ) stimulates the proliferation of mammary cells. MCF-7 cells, being ER $\alpha$  dependent, are found to be sensitive to SERMs while MDAMB-231 cells which are ER- $\beta$  dependent are characterized by the absence of immune-histochemical expression of estrogen, progesterone, and HER2 receptors.<sup>3</sup>

1*H*-1,2,3-Triazole tethered imidazole-isatin conjugates were synthesized and evaluated against MCF-7 and MDA-MB-231 cell lines. Antiproliferative activities of the synthesized conjugates revealed an optimum combination of longer alkyl chain length as spacer and a halogen-substituent on the isatin ring as a prerequisite for good activity. The compound 6g with an optimum combination of chloro-substituent at C-5 position of isatin ring and a butyl chain length proved to be most active and noncytotoxic with IC50s of 54.25 and 26.12  $\mu$ M against MCF-7 and MDA-MB-231 cell lines, respectively.

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**PP-55 Regulating the Morphology Dependent Chiroptical Properties and Photoconductivity in Supramolecularly Orchestrated Phenazine based Assemblies in Aqueous Media**

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**Abstract**

Morphology dependent tuning of chiroptical properties in supramolecular helical assemblies is an area of interest.<sup>1-2</sup> Here, phenazine based derivatives has been synthesized by incorporating menthol group as chiral handle(s) and carbamate unit(s) as linkers. These synthesized scaffolds undergo self-assembly in mixed aqueous media (THF/water), forming distinct supramolecular architectures due to different molecular packing, leading to significant changes in morphological behaviour. This structural modulation further influences the chiroptical response and photoconductivity behaviour of the resulting assemblies. The study highlights the role of rational molecular design in controlling morphology and associated chiroptical properties in chiral supramolecular systems.

**Keywords:** Chiral assemblies, Double Helix, Superhelix, Photoconductivity, Circularly Polarized Luminescence.

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# PP-56 Molecular-Level Insights into Quinone-Capped Silver Nanoparticles: A Combined Experimental and DFT Study

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## **Abstract**

In the present study, a quinone molecule was employed as a stabilizing and capping agent for the synthesis of silver nanoparticles through a chemical reduction method. The formation of quinone-capped silver nanoparticles was investigated to understand the interaction mechanism at the molecular level. Density Functional Theory (DFT) calculations were performed to provide theoretical insight into the stabilization process. Geometry optimization, frontier molecular orbital (HOMO–LUMO) analysis, and adsorption energy calculations were carried out to evaluate the binding affinity between the quinone molecule and the silver surface. The theoretical results indicated strong coordination through the carbonyl oxygen atoms and significant charge transfer from silver to the quinone molecule, leading to enhanced stability of the nanoparticle system. The reduced HOMO–LUMO energy gap upon interaction further supports electronic stabilization of the nanocomposite. The combined experimental and computational approach provides comprehensive insight into the design of stable organic–metal hybrid nanomaterials for potential applications in catalysis, sensing, and optoelectronic devices.

## **Keywords:**

Silver nanoparticles; Quinone; Density Functional Theory; HOMO–LUMO analysis; Nanocomposites

## **References:**

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## PP-57 Ether-Based Electrolyte Systems: A Review of Molecular Interactions and Thermo-Acoustic Studies of Energy Storage Applications

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### **Abstract**

This review examines molecular interactions between ethers and carboxylates using ultrasonic and thermoacoustic approaches. Acoustic, volumetric, and thermodynamic parameters are analysed to understand intermolecular forces and structural behaviour in different solvent systems. The study highlights the influence of molecular composition and solvent effects on physicochemical properties, stability, and functional performance. Experimental challenges and interpretation of thermoacoustic data are discussed. The review also identifies research gaps and future opportunities for improving understanding of ether-carboxylate systems. These findings contribute to the development of advanced functional materials with applications in pharmaceuticals, materials science, biomedical research, and industrial formulations involving ultrasonic technologies.

**Keywords:** *Ultrasonic velocity, Thermoacoustic parameters, Ether solvents, Carboxylate solutes, Intermolecular forces, Volumetric properties, Solketal, Dimethyl isosorbide, Transcutol P, Zinc acetate, Magnesium acetate, Citrates, Gluconate, Molecular interactions.*

# PP-58 Sustainable Synthesis of Rice Husk-Derived Lignin Doped ZnO Nanocomposites for Enhanced Photovoltaic Applications

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## **Abstract**

Sustainable bio–inorganic nanocomposites are gaining significant attention for photovoltaic applications. In this study, lignin was extracted from rice husk using an ethanol-based Soxhlet extraction method and utilized as a natural dopant for zinc oxide (ZnO). ZnO nanoparticles were synthesized via the sol–gel method using zinc acetate in an ethanolic medium, followed by incorporation of extracted lignin to form LG@ZnO nanocomposites. The prepared samples were characterized using X-ray diffraction (XRD) for phase identification, Fourier-transform infrared spectroscopy (FTIR) for functional group analysis, UV–Visible spectroscopy for optical properties and band gap estimation, scanning electron microscopy (SEM) for surface morphology, and thermogravimetric analysis (TGA) for thermal stability. Structural results confirmed the hexagonal wurtzite structure of ZnO and successful interaction between lignin and ZnO. Optical studies showed enhanced light absorption after lignin incorporation. Photovoltaic performance evaluation revealed improved photocurrent response of LG@ZnO compared to pristine ZnO, attributed to enhanced charge separation and reduced recombination, demonstrating its potential for sustainable solar energy applications.

**PP-59 Isoniazid-Derived Vanillin and Salicylaldehyde Hydrazones:  
Promising Antimycobacterials with KatG-Dependent Activation**

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**Abstract**

Tuberculosis (TB) is a highly contagious airborne disease and a leading global cause of mortality, caused by *Mycobacterium tuberculosis* (*Mtb*). A series of hydrazone derivatives based on vanillin and salicylaldehyde scaffolds and incorporating isoniazid (INH) and related analogues were designed and synthesized. The compounds were evaluated for activity against *Mtb*. INH-containing hydrazones showed strong antimycobacterial activity with minimum inhibitory concentration (MIC) values of 0.078–0.625 µg/mL. Salicylaldehyde derivatives displayed the highest potency and some analogues reached MIC values as low as 0.078 µg/mL. Vanillin-based compounds showed slightly lower activity which may reflect structural or linker effects. Analogues prepared from nicotinic hydrazide or pyrazine-2-carbohydrazide were inactive which highlights the importance of the INH pharmacophore. Cytotoxicity studies using THP-1 macrophages showed that active compounds were non-toxic at concentrations below 10 µg/mL and therefore indicate a favourable safety window. UV–visible spectroscopic analysis demonstrated that the representative salicylaldehyde hydrazone 5d remained stable under mildly acidic conditions. These results suggest that pH-triggered hydrolysis and release of free INH are unlikely in intracellular environments. The loss of activity against INH-resistant KatG mutant strains supports a KatG-dependent activation mechanism similar to that of INH. These findings show that Schiff base hydrazones represent a promising scaffold for the development of safe and potent antimycobacterial agents. Further mechanistic studies and structural optimization are required to clarify scaffold contributions and to support future therapeutic development.

**Keywords:** Isoniazid, *Mycobacterium tuberculosis*, InhA, Hydrazones, KatG.

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**PP-60 In dept evaluation of Covalent organic framework as a biocompatible material**

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**Abstract**

A covalent organic framework (COF) was synthesized by a solvothermal route using two triazine- cored precursors by imine linkage. Various physicochemical techniques such as FTIR, XRD, FESEM, TEM and XPS were performed to characterize COF which revealed successful synthesis of COF material with spherical morphology. Further, the as synthesized COF material is being conjugated with the hemoglobin protein to obtain their composite that will be used for the assessment of biocompatibility of present COF with the conjugated protein through various techniques including UV-visible, Fluorescence, CD, FTIR, Raman, SEM and TEM. Outcomes from this study will help in understanding that can these COF materials be utilized as biomaterials for various biomedical and bio-based applications.

**Keywords:** Covalent organic framework, hemoglobin, triazine, biomaterial

**References:**

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# PP-61 Direct recovery of Cu from E-waste using agriculture waste derived biochar and its conversion to Cu<sub>2</sub>O for electrochemical application

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## Abstract

The growing volume of electronic waste has intensified the need for sustainable and selective metal recovery technologies. This work presents a green and integrated approach for copper recovery from waste printed circuit boards (WPCBs) using oxidatively modified torrefied biochar derived from banana peels, followed by the synthesis of Cu<sub>2</sub>O@biochar nanocomposites. The modified biochar, enriched with oxygen-containing functional groups, acts as an efficient sorbent for Cu(II) ions released during oxidative leaching, enabling a simultaneous leaching–sorption process in a mild aqueous system. Captured copper species are strongly bound within the porous carbon matrix through complexation and ion-exchange interactions. The Cu-loaded biochar is subsequently converted into Cu<sub>2</sub>O-decorated biochar via chemical reduction, producing a stable nanocomposite. Structural and morphological analyses using XRD, SEM, and EDS confirm the formation and uniform dispersion of crystalline Cu<sub>2</sub>O nanoparticles on the biochar surface. The developed strategy demonstrates a closed-loop and environmentally benign route that combines biomass valorization with urban mining, offering a scalable platform for copper recovery and the generation of value-added functional nanomaterials for catalytic and electrochemical applications.

**Keywords:** Waste printed circuit boards (WPCBs); Biochar; Cu<sub>2</sub>O@biochar

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**PP-62 Combining entomopathogenic bacteria with new chemistry insecticides to control *Spodoptera litura* (Fabricius)**

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**Abstract**

*Spodoptera litura* (Fabricius), commonly known as tobacco caterpillar, is a highly polyphagous lepidopteran pest that threatens over 389 plant species, including major crops like cotton, soybean, groundnut, maize, and vegetables. *S. litura* can inflict devastating losses, reaching up to 100% in economically important crops. Conventional pest control primarily relies on synthetic insecticides (e.g., carbamates, organophosphates, pyrethroids), which although effective, have led to negative environmental, health, and resistance concerns. Thus, there is a pressing need for sustainable alternatives. The integration of selected entomopathogenic bacteria with new-chemistry insecticides offers a promising, eco-friendly pest management strategy against *S. litura*. This study investigated the combined effects of entomopathogenic bacteria *Comamonas* sp. C2, *Rhodococcus* sp. MG1, *Planococcus* sp. KIC5 with new chemistry insecticides (broflanilide and cyantraniliprole) against *S. litura* larvae, aiming to enhance pest control while reducing chemical load. The study also demonstrated the potential genotoxic effects of combination treatments. These integrated treatments can achieve high efficacy at reduced insecticide load, lower environmental and health risks, conserve beneficial insect populations, and potentially delay resistance development.

## PP-63 Synthesis, Molecular Docking and Antitubercular activity of Lawsonone derivatives

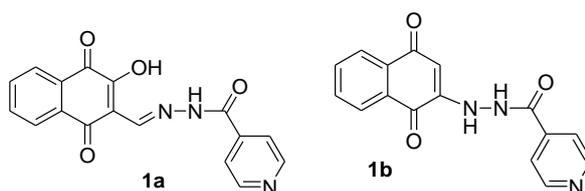
**Prabhdeep Kaur, Avkash Singh, Hardeep Kaur\***

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### Abstract

The development of novel drug candidates through strategic structural modification of existing drugs has emerged as an effective approach to combat the growing problem of drug resistance. In this context, a new series of Lawsonone derivatives were synthesized by varying the substituents, affording the desired compounds in good yields. These conjugates were evaluated for their antitubercular activity against the M. Tb 7H9OADC. Among the twelve synthesized compounds, two demonstrated excellent minimum inhibitory concentration (MIC) values. Compound 1a showed an MIC of 5 µg/ml, while compound 1b exhibited a remarkable MIC of <0.156 µg/ml, which is comparable to that of isoniazid. Cytotoxicity evaluations further indicated that these compounds are less toxic. In silico docking studies of compounds **1a** and **1b** at the active sites of InhA demonstrated favourable interactions, with docking scores superior to isoniazid. Additionally, ADMET analysis confirmed that these molecules possess promising drug-like properties. Overall, these investigations provide a strong rationale for further development of this promising series of antitubercular agents.



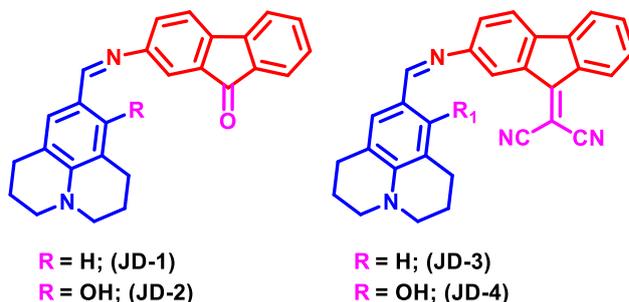
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**PP-64 Synthesis, Non-linear Optical Properties, and Sensing applications of Fluorenone-based Donor Acceptor molecules**  
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**Abstract**

A Julolidine Schiff's base ligands, specifically (Z)-2-(((2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-9-yl)methylene)amino)-9H-fluoren-9-one (JD-1), 2-(((8-hydroxy-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-9-yl)methylene)amino)-9H-fluoren-9-one (JD-2) has been synthesized *via* condensation of 2-amino-9H-fluoren-9-one with 2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline-9-carbaldehyde. The  $\pi$ -extension with some electron-withdrawing moieties like malononitrile is in continuation to prepare (JD-3) and (JD-4). The metal ion sensing capabilities of these ligands were investigated using UV-Vis. spectroscopy. The interactions of JD-1 and JD-2 with various metal ions, including ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Li}^+$ ,  $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Cr}^{+2}$ ,  $\text{Co}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Cr}^{3+}$ ) were evaluated in DMSO media. The JD-2 showed selectivity for  $\text{Fe}^{2+}$  over other metal ions suggesting a high sensitivity and potential application as a  $\text{Fe}^{2+}$  specific chemosensor. Additionally, their photophysical properties, including the first hyperpolarizability, will be analyzed to assess their potential as non-linear optically active materials.



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# PP-65 Systems Chemistry of Molecular Self-Assembly: From Equilibrium Order to Nonequilibrium Dynamics

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## Abstract

Molecular self-assembly has traditionally focused on forming ordered architectures under thermodynamic equilibrium. Bioinspired systems such as peptides and amino acids can organise into  $\beta$ -sheet-rich nanofibers, nanospheres, and hydrogels with promising applications in biotechnology and drug delivery. In our earlier work, we investigated the molecular mechanisms underlying amyloid-like assembly, beginning from dimer nucleation stabilised by non-covalent interactions and progressing to higher-order structures.

Recognising that nature regulates function through dynamic assembly-disassembly processes, we extended this paradigm to non-equilibrium systems. Using compartmentalised reaction–diffusion setups, we engineered controlled interactions between metal ions and organic linkers to generate tubular “MOF garden” architectures with diameters up to 50  $\mu\text{m}$ , structures inaccessible via conventional solvothermal routes.

Building on this systems perspective, we developed a minimalist enzyme-mimetic platform based on a single-step synthesis of a copper-tyrosine (CuY) supramolecular assembly. Structural characterisation confirms the formation of an ordered nanotubular architecture. The CuY network exhibits pronounced peroxidase-like activity toward *o*-phenylenediamine, as quantified by Michaelis–Menten analysis. Importantly, catalytic performance is not solely determined by copper coordination but is strongly modulated by the network's dynamic self-assembled state. Coordination-driven remodelling of the tyrosine assembly induces nonlinear regulation of catalytic activity, revealing a direct coupling between supramolecular organisation and enzyme-like function.

This work highlights molecular self-assembly as a central regulatory element in minimalist catalytic systems and provides new design principles for life-like, metal–amino acid functional materials.

## PP-66 Multi-colour and red emissions from a small donor-acceptor molecule by breaching Kasha's rule

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### Abstract

We present a compact organic fluorophore (MW 260 Da) that defies Kasha's rule by exhibiting dual excited-state emissions. Built on an acenaphthylene scaffold with donor-acceptor substitution, the molecule shows simultaneous S1 and S3 emissions, enabling excitation-dependent colour variation from blue to red. This behaviour is accompanied by huge Stokes shifts ( $>5000\text{ cm}^{-1}$ ) and minimal spectral overlap, ensuring distinct multicolour outputs. In solution, the emission is strongly charge-transfer in nature and highly sensitive to solvent polarity, while in the solid state, the molecule retains efficient red emission. Time-dependent density functional theory (TDDFT) calculations support the experimental findings, revealing two bright states separated by a dark intermediate that suppresses internal conversion and stabilizes dual emission pathways. This study highlights how a small molecular design can achieve versatile photophysical behaviour typically reserved for larger systems. The results open avenues for practical applications in multicolour OLEDs, ratiometric bioimaging, anti-counterfeiting technologies, and photodynamic therapy. By combining simplicity of structure with complex excited-state dynamics, this work establishes a new benchmark in molecular photophysics.

**Keywords:** Anti-kasha, multicolour emission, charge transfer

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**PP-67 Transfer of Mechanical Energy from Crystals to Polymer Composites: A new way to achieve Photo/Thermo actuation**

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**Abstract**

Transfer of strong mechanical effect from dynamic crystals to hybrid polymer composite is an evolving field of research and holds high potential for actuation and energy harvesting. Organic counter anion stabilized nitropentaamminecobalt(III) complexes showing fast photo/thermomechanical motions under UV light (365 nm) and heat were synthesized. Detailed experimental and theoretical studies attribute the photomechanical motion to the formation of metastable nitrito-coordinated species after irradiation where as dehydration induced structural transformation was responsible for thermomechanical motion. Different crystal-polymer composite films were fabricated using the dynamic crystals with polyvinylalcohol (PVA), polyvinylidifluoride(PVDF) and agarose polymers by solution casting method. The composite films show quick and excellent photo/thermo-actuation, though the extent of actuation varies with the types of polymers used. The actuation of the composite films starts immediately (<2-3 s) and can be deflected up to 90° within a few seconds of the onset of UV light/heat. Dynamical transfer of photomechanical energy from crystal to composite films leads to successful assembly of a prototype photo-switch. The presented work provides a new dimension towards the development of smart functional composite materials as photo/thermo actuators.

**Keywords:** Polymer Composite, Actuator, Dynamic Crystal, Photo/thermomechanical

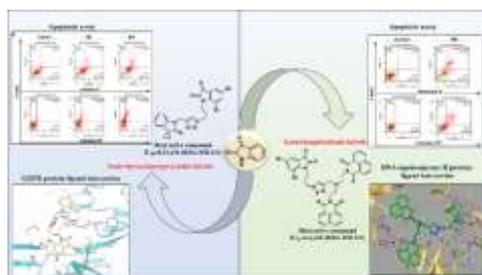
# PP-68 Triazole-Tethered Isatin Hybrids as promising candidates for Triple Negative Breast cancer

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## Abstract

Triple-negative breast cancer (TNBC) is one of the most aggressive and clinically heterogeneous subtypes of breast cancer, defined by the lack of estrogen receptor, progesterone receptor, and HER2 expression. In the present study, a series of isatin-spirocyclopropyl oxindole and isatin-bisnaphthalimide hybrids incorporating a 1*H*-1,2,3-triazole linker were synthesized *via* a copper-promoted click reaction and evaluated for their antiproliferative activity against TNBC cell lines. Structure–activity relationship analysis demonstrated that both halogen substitution and linker length significantly influenced anticancer potency. Hybrids bearing dibromo substitution along with a propyl spacer exhibited the highest activity against MDA-MB-231 cells, with IC<sub>50</sub> values of 8.23 ± 1.87 μM (isatin-spirocyclopropyl oxindole) and 4.4 ± 0.3 μM (isatin-bisnaphthalimide), surpassing the activity of 5-fluorouracil. Importantly, these compounds showed favorable selectivity indices of ~2 when compared to normal keratinocytes (HaCaT). Mechanistic studies indicated that the lead compounds induce caspase-mediated apoptosis. Molecular docking analysis revealed strong binding interactions of the isatin-bisnaphthalimide hybrid with DNA topoisomerase II, comparable to doxorubicin, whereas the isatin-spirocyclopropyl oxindole hybrid demonstrated promising binding affinity toward epidermal growth factor receptor (EGFR). Collectively, these findings highlight the therapeutic potential of these hybrids as promising candidates for TNBC treatment.



**Keywords:** Apoptosis, Click reaction, Domino Corey-Chaykovsky reaction, Triazole ring, Triple negative breast cancer.

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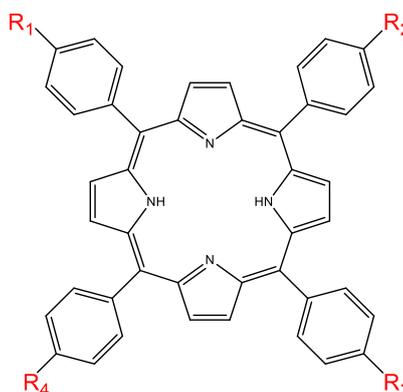
## PP-69 Synthesis and Characterization of mono and Tetra-(Aminophenyl) Porphrin.

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### Abstract

Mono- and tetra-aminophenyl substituted porphyrins were synthesized through an efficient synthetic route starting from nitro-substituted tetraphenylporphyrin precursors. The nitro derivatives were prepared via condensation of pyrrole with substituted benzaldehydes under controlled conditions . These intermediates were subsequently reduced to convert the nitro groups into corresponding amino functionalities at the meso positions of the porphyrin macrocycle. The optimized reaction conditions provided mono-and tetra-substituted aminophenyl porphyrins in satisfactory yields, offering a simple and reliable approach for preparing functionalized porphrin derivatives .



Mono: R1, R2, R3,= H, R4=NH<sub>2</sub>

Tetra: R1, R2, R3, R4=NH<sub>2</sub>

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## PP-70 Design, Synthesis and In-vitro Antibacterial Activity of Naphthalimide-Triazine-Benzimidazole Hybrids

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### **Abstract**

The escalating threat of antimicrobial resistance (AMR) and the diminishing efficacy of current antibiotic therapies necessitate the urgent development of novel antibacterial agents. In this study, we addressed this challenge by designing and synthesizing a new series of hybrid pharmacophores integrating naphthalimide, benzimidazole, and triazine skeletons. These scaffolds were selected for their proven biological relevance and were further derivatized via secondary amine substitutions to optimize bioactivity. The target compounds were synthesized in good yields and fully characterized using <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and HRMS spectrometry. The series was subsequently screened for antibacterial activity against a panel of Gram-positive and Gram-negative bacterial strains. Among the synthesized derivatives, compound **8c** emerged as the lead molecule, exhibiting broad-spectrum potency with Minimum Inhibitory Concentrations (MICs) ranging from 1.56 to 3.125 µg/mL. These results suggest that molecular hybridization of naphthalimide, triazine, and benzimidazole motifs offers a promising strategy for developing next-generation antibiotics capable of overcoming bacterial resistance.

## PP-71 Surfactant free Microemulsion as an Efficient Catalytic Medium for Cytochrome-c.

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### **Abstract**

Deep eutectic solvents (DES) and ionic liquids (ILs) are great alternative to conventional organic solvents for the preparation of microemulsions, where one can even construct surfactant free microemulsion (SFME). In the present study, a SFME was prepared using a DES based on natural components, L-arginine and lactic acid as the polar phase, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonylimide), a hydrophobic ionic liquid (HIL), as the non-polar phase and ethanol as an amphiphilic solvent. The system was extensively characterized to establish its structural organization and molecular interactions revealing ethanol does not form an effective barrier layer, instead it forms H-bonded solvent domains interacting with HIL and DES, thereby stabilizing the nano-interface. The prepared SFME has been employed as nano-reactors for exploring the catalytic activity of Cytochrome-c (Cyt-c). The variation in phase composition markedly affected the enzyme activity, with the DES/HIL phase of SFME providing an optimal nano-environment that stabilized Cyt-c and enhanced its catalytic efficiency upto 6.5 folds as compared to the buffer system. The favorable cation- $\pi$  and hydrogen bonding interactions of arginine and lactic acid at the DES-ethanol interface stabilize the structure of Cyt-c. This study provides new insights into the structural and functional aspects of SFMEs, encouraging the development of new SFME systems for a broad spectrum of several biocatalytic applications.

# PP-72 A Mechanistic Insight into the Emission Behavior of Boron Difluorohydrazone (BODIHYs): Suppression of Kasha's Rule

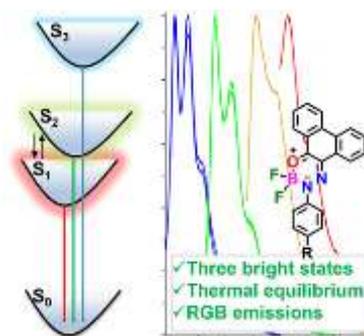
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## Abstract

Single-component luminophores showing excitation-wavelength-dependent emissions are highly attractive for both fundamental studies and advanced optoelectronic applications. Such systems often deviate from Kasha's rule, enabling emission from higher excited states. Herein, we report boron difluorohydrazone (BODIHY) derivatives that exhibit clear excitation-dependent multicolor fluorescence, covering the full red-green-blue (RGB) range. Combined experimental and theoretical investigations reveal that this unusual color tunability originates from three emissive ("bright") excited states, namely  $S_1$ ,  $S_2$ , and  $S_3$ . Time-dependent density functional theory (TDDFT) calculations show that the energy gap between  $S_2$  and  $S_3$  exceeds  $3000\text{ cm}^{-1}$  (0.37 eV), which favors radiative decay from  $S_3 \rightarrow S_0$  over competing internal conversion. For BODIHY 1, the smaller gap between  $S_1$  and  $S_2$  ( $< 2000\text{ cm}^{-1}$ , 0.25 eV) suggests partial thermal equilibrium between these two states. In contrast, BODIHY 2 exhibits three well-separated emissive excited states, allowing independent fluorescence from each state. Distinct excitation spectra, fluorescence lifetimes, and photoluminescence quantum yields (PLQYs) for the emission bands further support the presence of three independently emissive excited states, leading to unprecedented excitation-controlled RGB luminescence in small organic molecules.



**Keywords:** BODIHY, Excitation-wavelength dependent emission, anti-Kasha.

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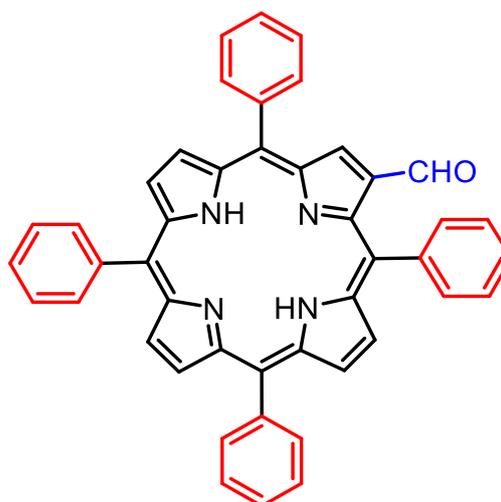
## PP-73 Synthesis, Characterization and Applications of $\beta$ -Substituted Porphyrins

**Rakshita<sup>a</sup>, Aastha<sup>a</sup>, Prabhjot Kaur, Nivedita Chaudhri\***

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### Abstract

A highly efficient synthesis of 2-formyl-5,10,15,20-tetraarylporphyrins was carried out. The procedure involves copper(II) chelation to facilitate highly selective electrophilic substitution. After Vilsmeier–Haack formylation of the copper(II) porphyrins, the resulting iminium salt intermediate is demetalated before undergoing base-mediated hydrolysis to produce the corresponding free-base 2-formylporphyrin. Importantly, this approach minimizes the formation of undesired by-products that commonly arise when the formyl group is exposed to acidic conditions. The presence of the formyl (–CHO) group enables further modification through various reactions [1]. Extension of  $\pi$ -conjugation in the porphyrin was achieved through alkene substitution using Knoevenagel condensation and Schiff base reactions at  $\beta$  position. This structural modification resulted in enhanced optical absorption and improved electronic properties [2].



2-formyl-5,10,15,20-tetraphenylporphyrin

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## PP-74 Soft Eutectogel Formation via Micellization of Surface-Active Ionic Liquids in Deep Eutectic Solvent

**Ravi Dutt, Omish Sethi, Manvir Kaur, Tejwant Singh Kang\***

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### Abstract

The efforts to make chemical processes more sustainable have led to an increasing interest in green chemistry, particularly in the fine chemicals, biocatalysis and pharmaceutical industries. Eutectogels comprising a deep eutectic solvent (DES) of choline chloride and urea (1:2) gelled by self-assembled structure of surface active ionic liquids (SAILs) viz. [C<sub>16</sub>Emim] [Cl], [C<sub>12</sub>Emim] [Cl], [C<sub>12</sub>Amim] [Cl], [C<sub>16</sub>mim] [Cl] have been prepared and characterized. The prepared gels have been examined using freeze-fracture transmission electron microscopy (FF-TEM) and polarized optical microscopy (POM). Further, the phase behaviour of the formed gels has been studied with respect to concentration of SAILs and temperature. The eutectogels have also been checked for their thermal stability over a wide temperature range using the thermogravimetric analysis (TGA). The rheological characteristics of these gels, including their storage ( $G'$ ) and loss modulus ( $G''$ ), have been analyzed with respect to strain ( $\gamma$ ), frequency ( $\omega$ ), and temperature (T). The eutectogels have  $G' > G''$ , indicative of the strong electrostatic as well as *H*-bonding interactions between SAILs and DES components. Also, the  $\gamma$  value at  $G' = G''$  lies in the range of 1-10% provides the acceptable mechanical behaviour of these gels. Owing to their greener and more facile preparation along with their multifunctional properties these gels could be utilized for different applications.

# PP-75 Synthesis, Characterisation and catalytic application of 2-benzoylpyridinethiosemicarbazone based Pd(II) complexes in Suzuki–Miyaura Cross-Coupling reaction

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## Abstract

Palladium(II) complexes based on 2-benzoylpyridinethiosemicarbazone ligands (bzpytsc-N<sup>4</sup>HR) of the type [Pd(N<sup>1</sup>,N<sup>2</sup>,S-bzpytsc-N<sup>4</sup>HR)Br] (where R = H, Me) have been synthesized and characterized using UV-visible, FT-IR, and NMR spectroscopy. The structures of these complexes have been elucidated with the help of single crystal X-ray diffraction. The ligand is coordinated to the central metal atom in the tridentate manner (via pyridyl N<sup>1</sup>, imine N<sup>2</sup> and thiolate S atom) and fourth position is occupied by bromide ion forming distorted square planar structure. Both the complexes act as highly efficient catalysts for Suzuki–Miyaura cross couplings of various aryl halides (Ph-X, *p*-NC-C<sub>6</sub>H<sub>4</sub>-X, *p*-MeO-C<sub>6</sub>H<sub>4</sub>-X and *p*-Me-C<sub>6</sub>H<sub>4</sub>-X (X = Br, I)) with phenylboronic. These reactions are carried out without any additional ligand under mild conditions (50 °C, soft base) in an aerobic atmosphere using the green solvent system of water and ethanol. It is noteworthy that catalysts are used under one-pot conditions without any separation and system could be easily reused with good turnover number.

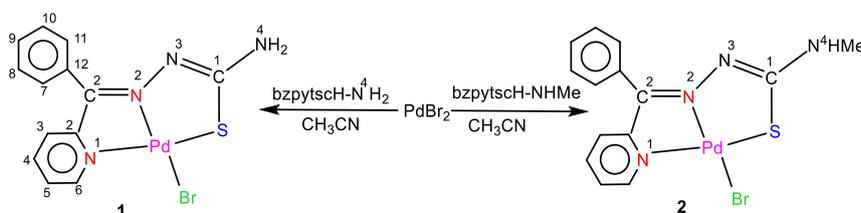


Fig 1. Synthetic route of preparation of complexes (Labeled Cat 1 and Cat 2)

**Keywords:** 2-benzoylpyridinethiosemicarbazone; NMR spectroscopy, Suzuki-Miyaura cross-coupling; Palladium dibromide, X-ray crystallography.

## PP-76 Bridging Gaps in Fungal Keratitis Management: Novel Diagnostics, Drug Delivery Systems, and Gene Therapies

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### Abstract

Globally, fungal keratitis has become a major health concern, particularly in tropical and humid regions. The disease burden is exacerbated because of the underlying complexity of fungal pathogens, delayed or insufficient diagnosis, and limitations in existing therapeutic strategies, often leading to progressive corneal damage and impaired vision. Additional challenges include insufficient therapy optimization and variable efficacy of topical and systemic antifungal treatments, which may be influenced by factors such as rapid ocular drug clearance, ineffective ocular penetration, and the increasing prevalence of antifungal resistance. Conventional diagnostic techniques, such as microscopy and culture, continue to serve as reference standards but have limitations due to comparatively modest sensitivity and the prolonged turnaround times. In comparison, recent advances in diagnostic techniques, including CRISPR-based assays, PCR, MALDI-ToF MS, and *in vivo* confocal microscopy, as well as the novel drug-delivery nanocarriers, have been reported to show noticeable improvements in diagnostic accuracy and therapeutic outcomes. Furthermore, emerging DNA-based gene therapies and RNA-based therapeutics, along with advanced ocular drug carriers, have shown promising outcomes in preclinical research and early-phase clinical trials, suggesting potential advantages in enhanced tissue targeting and reduced therapeutic resistance. However, before widespread clinical acceptability, extensive clinical validation, long-term safety evaluations, and cost assessments are required, as existing findings are mainly limited to short-term and experimental research. This review focuses on the pathophysiology of fungal keratitis while underscoring the unmet diagnostic and therapeutic needs. It further explores the potential for developing translatable technologies aimed at predictive diagnosis and the effective management of this sight-threatening condition.

**Keywords:** Fungal keratitis, Fungal endophthalmitis, Diagnosis, Nanocarrier-based drug delivery, Gene therapy, CRISPR/Cas

**PP-77 A Benzimidazole–Malononitrile-Based Fluorescent “Turn-ON”  
Probe for Selective and Quantitative Detection of Human Serum  
Albumin in Urine**

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**Abstract**

This study provide detailed insight into the differential response of a benzimidazole–malononitrile-based fluorescent “turn-ON” probe toward two structurally similar serum albumin proteins, human serum albumin (HSA) and bovine serum albumin (BSA). Compound **6** exhibits pronounced sensitivity toward both serum albumins, whereas this responsiveness is completely abolished in compound **7**, obtained via structural modification of compound **6**, highlighting the critical role of substitution in modulating protein interaction. In aqueous medium, compound **6** forms aggregates exhibiting an absorption maximum at 385 nm and a weak emission band centered at 565 nm. Upon gradual addition of BSA (200 μM), a new emission band emerges at 475 nm accompanied by a slight enhancement in the original 565 nm emission. In contrast, addition of HSA (50 μM) also induces formation of the 475 nm band; however, approximately 50% quenching of the 565 nm emission is observed. Notably, the fluorescence enhancement at 475 nm in the presence of BSA is nearly four-fold higher than that observed with HSA, clearly demonstrating a differential fluorescence response toward the two structurally analogous proteins. The mechanism of interaction between compound **6** and serum albumins was systematically investigated using fluorescence lifetime measurements, site-selective drug displacement assays, dynamic light scattering (DLS), FE-SEM, FT-IR spectroscopy, drug displacement assay and molecular docking studies. Furthermore, the practical applicability of compound **6** was demonstrated through quantitative detection of HSA in human urine samples. The high binding affinity, excellent sensitivity, selectivity, and clear differential fluorescence response toward HSA and BSA underscore the potential of probe **6** for biomedical and diagnostic applications.

# PP-78 Dual-Functional ZIF-67 Metal-Organic Framework for Fluoroquinolone Antibiotic Removal from Water and CO<sub>2</sub> Capture from Gaseous Media

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## Abstract

This study evaluates the potential of the zeolitic imidazolate framework ZIF-67 as a high-performance adsorbent for the removal of antibiotic contaminants from wastewater. The adsorption behavior of two widely used fluoroquinolone antibiotics, ciprofloxacin (CFX) and norfloxacin (NFX), was investigated. ZIF-67, synthesized using Co<sup>2+</sup> ions and imidazole ligands, was thoroughly characterized by FT-IR, XRD, SEM, TEM, and BET analyses, confirming its high crystallinity, porous structure, and exceptionally large surface area of 1288.99 m<sup>2</sup> g<sup>-1</sup>. Batch adsorption experiments optimized through Response Surface Methodology demonstrated rapid and efficient adsorption under optimal conditions, with equilibrium achieved within 20 minutes. Adsorption isotherm studies revealed that the Langmuir model best described the process, indicating monolayer adsorption on a homogeneous surface. Remarkably high maximum adsorption capacities of 3716.07 mg g<sup>-1</sup> for CFX and 3423.5 mg g<sup>-1</sup> for NFX were obtained, surpassing many previously reported adsorbents. Kinetic studies showed that adsorption followed a pseudo-second-order model, suggesting a chemisorption-controlled mechanism. Thermodynamic analysis confirmed that the adsorption process is endothermic and entropy-driven, with improved performance at higher temperatures. Additionally, ZIF-67 exhibited effective CO<sub>2</sub> adsorption capacity, highlighting its dual functionality for removing both aqueous and gaseous pollutants.

## PP-79 Exploring Detection of Environmentally Toxic Anion (Nitrite) Using Organic Fluorescent Molecule

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### **Abstract**

Nitrite ions ( $\text{NO}_2^-$ ) in soil are an intermediate product in the nitrogen cycle, formed during nitrification (conversion of ammonium to nitrite) and further converted to nitrate ( $\text{NO}_3^-$ ). While they are a temporary source of nitrogen for plants, their accumulation can be harmful. High concentrations of nitrite ions are toxic to plants, disrupt soil microbial balance, and can leach into groundwater, causing environmental and health concerns. These nitrite ions ( $\text{NO}_2^-$ ) can be detected using fluorescence probes, a sensitive and selective method widely employed in environmental monitoring, biological research, and analytical chemistry. Amines are widely employed for the detection of nitrite ions. The latter reacts with amines in the presence of acid, resulting in the deaminated product/alcohol depending on the reaction conditions. Due to this chemical transformation, a dramatic change in the fluorescence properties of the probe can be observed, allowing the detection and quantification of the same. Therefore, we aim to synthesise amino derivatives as a fluorescence probe to detect  $\text{NO}_2^-$  present in the soil.

**Keywords:** *environmental pollution, health hazards, nitrite sensing; fluorescent probes*

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## PP-80 Structural Modulation of Donor–Acceptor Building Blocks for Enhanced ROS Generation and Photocatalytic Activity

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### Abstract

Metal-free organic photosensitizers capable of harvesting visible light have emerged as efficient and sustainable systems for green oxidative transformations.<sup>1</sup> Upon light irradiation, these sensitizers activate aerial oxygen to generate reactive oxygen species (ROS) through type I (electron transfer) and/or type II (energy transfer) pathways, thereby facilitating oxidation reactions under mild and environmentally benign conditions.<sup>2</sup> Our research focuses on the rational design and synthesis of donor–acceptor (D–A) building blocks and the investigation of their self-assembly behavior in mixed aqueous media. Building on our previously reported systems,<sup>3-4</sup> which exhibited efficient red-light-driven photosensitization via regulation of excited-state dynamics and halogen-assisted intersystem crossing, we have designed a new derivative by introducing subtle structural modifications within the same donor–acceptor framework. We expected that these structural modifications can further modulate charge-transfer characteristics and enhance ROS generation efficiency for improved photocatalytic activity.

**Keywords:** Reactive Oxygen Species, Photosensitizer, Photocatalytic activity

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## **PP-81 Enhanced Metronidazole Release via Ni-UiO-66@Nb<sub>2</sub>CTx Composite for Controlled Drug Delivery**

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### **Abstract**

Drug delivery is crucial in modern medicine and essential for improving the efficacy of drug administration to the intended target. In this context, MXene is a promising material for Metronidazole (MTZ) drug release. Here, an MXene (NbCTx)-based composite was fabricated using Ni-UiO-66. The fabrication of the composite was confirmed through several spectroscopic and microscopic techniques (FTIR, PXRD, FESEM, HR-TEM, and XPS), which reveal that MXene was successfully delaminated. DFT theory was used to check the formation of the nanocomposite as well as the interaction with metronidazole at the molecular level. The composite was evaluated for drug delivery applications. The drug delivery response was calculated to be 90% for the composite of MXene.

**Keywords:** MXene, Metal organic framework, Drug delivery.

# PP-82 Green Alternatives to Classical Organic Reactions: A Sustainable Approach to Modern Chemistry

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## Abstract

It is natural that classical organic synthesis has paid so much attention to the efficiency and high yield at the expense of the environment and human health. Most of the classical organic reagents like acetone, DMSO, DMF, and other aromatic compounds has great contribution to environmental pollution but still used at wide range. In the classical organic processes, we do extensive use of heavy metal catalyst, toxic solvents and high energy conditions which raise a serious issue towards human health and ecological conditions. So, we need to shift towards one of the most effective concepts of chemistry to sustain ecology and health i.e. **Green Chemistry**. It is the manufacturer of the chemical processes that reduce the generation of hazardous and toxic substances via bio-catalysis, alternative solvents and alternative repeatable raw material. It aims to decrease the use of such hazardous substances and replace them with less toxic ones. Its main approach is to perform the reaction in solvent-free and highly concentrated conditions but if for any process solvent is really necessary, then it can be replaced with alternative reaction solvents (water, ionic liquid, supercritical fluids). The concept of sustainable or green chemistry comprises full utilization of raw material, reducing or eliminating the use of toxic substances. *Paul Anastas* and *John Warner*, in 1998, introduced twelve principles of green chemistry to form the framework design of new chemical processes for human health and ecological sustainability.



**Keywords:** Green Chemistry, Sustainable Chemistry, Environmental Pollution, Hazardous Substances, Toxic Solvents, Bio-catalysis, Alternative Solvents, Solvent-free Reactions, Supercritical Fluids, Ionic Liquids.

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# PP-83 Immobilized Mononuclear and Binuclear Copper(II) Complexes on Chitosan–PVA Based Composite Films as Dip Catalyst for Dual Enzyme Mimicry

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## Abstract

Structural and biomimetic studies of two copper(II) complexes, [Cu(2,4-DCBz)<sub>2</sub>(pic)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>] **1** and [Cu<sub>2</sub>(2,4-DCBz)<sub>4</sub>(pic)<sub>4</sub>] **2**, immobilized on chitosan–polyvinyl alcohol (CPVA) matrix, yielding composite films for heterogenous dip catalysis are presented for the first time. As a part of research interest of our group in polymer and copper(II) chemistry,<sup>1–4</sup> purposely, complexes **1** and **2** were isolated under ambient reaction conditions and characterized by spectroscopic and X-ray diffraction methods besides theoretical evaluation (DFT), disclosing the distinct coordination nature of monomeric and dimeric copper(II) complexes, respectively. Both complexes **1** and **2** were strategically incorporated into CPVA-based matrix via *in-situ* solution casting methods, owing to biological relevance of these complexes (*in-vitro* antibacterial and *in-silico* molecular docking analysis). The biopolymer CPVA infused copper(II) complexes-based composite films, namely CPVA0 (blank), CPVA1 (complex **1**), and CPVA2 (complex **2**), were substantiated by advanced characterization techniques, including SEM, CV, UV-Vis, FT-IR, *etc.* The significant potentials of composite films as antibacterial and dip catalyst were assessed by *in-vitro* antibacterial and oxidase enzyme mimetic activities. CPVA1 and CPVA2 showed high catalytic efficiency with large  $K_{cat}$  for oxidative transformation of o-aminophenol to aminophenoxazinone (2794.8 and 3022.2 h<sup>-1</sup>) and 3,5-di-tert-butylcatechol to 3,5-di-tert-butylquinone (2137.8 and 2690.4 h<sup>-1</sup>). Both polymeric films demonstrated remarkably high reusability of more than ten consecutive cycles, offering an effective, cost-efficient, and sustainable solution with enhanced catalytic performance and reusability. The details shall be presented.

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## PP-84 Toxicological Profile of 2,4-Dinitrophenol and Synthetic Strategies for its Coordination Complexes

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### Abstract

2,4-Dinitrophenol (DNP) is a synthetic compound historically employed in industrial applications and, controversially, as a weight-loss agent due to its ability to uncouple oxidative phosphorylation. Although effective in increasing metabolic rate, DNP poses severe toxicological risks that have led to its prohibition for human consumption.<sup>1</sup> Mechanistically, DNP disrupts the proton gradient across the inner mitochondrial membrane, resulting in uncontrolled energy expenditure and hyperthermia. This uncoupling accelerates mitochondrial respiration, increases oxygen consumption, and produces excessive heat owing to inefficient energy conversion. DNP acts as a proton ionophore, shuttling hydrogen ions (H<sup>+</sup>) across the inner mitochondrial membrane in an uncontrolled manner. This increases proton leakage, bypasses ATP synthase, and collapses the proton gradient essential for ATP production. Several derivatives of DNP with alkali metals such as Li, Na, K, and Cs have been reported in the literature, though most research has focused on the crystal structures of NaDNP and KDNP, but not on their biological applications. DNP was complexed with alkali metals such as sodium (Na) and potassium (K), forming coordination complexes that are less harmful than free 2,4 DNP. Alkali metals decrease the acute toxicity of DNP by limiting its ability to act freely as a protonophore. In this study, coordination complexes of DNP, namely sodium dinitrophenolate (NaDNP) and potassium dinitrophenolate (KDNP), were synthesized via a hydrothermal method. Single-crystal X-ray diffraction (PXRD), infrared (IR) spectroscopy, thermogravimetric analysis (TGA), and optical measurements provide comprehensive insights into their structural and physicochemical properties.

**Keywords:** 2,4-dinitrophenol, uncoupler, hyperthermia, oxidative phosphorylation

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**PP-85 Evaluation of serum adiponectin in metabolic syndrome among patients of T2DM in a tertiary care center of Kumaon region of Uttarakhand**

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**Abstract**

The prevalence of metabolic syndrome (MS) and type 2 diabetes mellitus (T2DM) has reached epidemic levels. Thus there is a need to study novel biomarkers involved in their etiopathogenesis and associated cardiovascular complications. Adiponectin, an adipokine has been implicated in insulin resistance, inflammation, obesity, and atherosclerosis associated with metabolic syndrome. In the Kumaon region of Uttarakhand, studies regarding adiponectin and its relationship in T2DM and MS patients are lacking. With this the present study was planned. Eighty seven newly diagnosed T2DM patients, enrolled in this study were divided into 2 groups. Group I comprised 48 cases of MS and rest 39 patients without MS were included in group II. All of the study subjects were assessed for anthropometric, clinical, and biochemical parameters. Lower levels of adiponectin were found in group I than in group II ( $p < 0.001$ ). A significant and inverse correlation of adiponectin was observed with BMI, WC, HOMA-IR, hs-CRP, and triglyceride levels while a significantly positive correlation was seen with HDL-C in both the study groups. However, a stronger and better correlation was observed in the MS group than without the group. Adiponectin was found to be decreased and significantly correlated with raised BMI, insulin resistance, hs-CRP, and dyslipidemias in the study subjects.

**PP-86 Chemical composition and antifungal potential of *Nyctanthes arbor-tristis* leaves extract/fractions against rice pathogenic fungi**

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**Abstract**

The ethanol extract (70%) of *Nyctanthes arbor-tristis* (Harsingar) leaves was prepared using the Soxhlet extraction technique. Gas chromatography-Mass spectrometry (GC-MS) analysis of leaf extract revealed the presence of 2,6-dimethoxy-4-vinylphenol (6.32%) and 7-Tetradecenal (21.43%) as major compounds. The crude extract was subsequently fractionated using column chromatography into petroleum ether, ethyl acetate and n-butanol fractions based on polarity. The *in-vitro* antifungal potential of ethanol extract and its fractions was assessed against *Drechslera oryzae* and *Fusarium fujikuroi*, responsible for brown leaf spot and bakanae disease in rice respectively using poison food technique. The ethyl acetate fraction showed the highest percent inhibition in both the tested fungi with minimum ED<sub>50</sub> values of 450 and 520 µg/ml against *Drechslera oryzae* and *Fusarium fujikuroi* respectively followed by butanol fraction, crude ethanol extract and petroleum ether fraction. These findings highlight the potential of *Nyctanthes arbor-tristis* as a safe, natural and eco-friendly alternative to synthetic fungicide as an approach towards sustainable agriculture.

**Keywords:** *Nyctanthes arbor-tristis*, extract, antifungal, GC-MS, synthetic fungicide

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# PP-87 Propellant Free Pressurized Spray System of Etodolac to Manage Acute Pain Conditions: In Vitro and In Vivo Evaluation

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## Abstract

This study aimed to develop a propellant-free topical spray formulation of Etodolac (BCS-II), a potent NSAID, which could be beneficial in the medical field for the effective treatment of pain and inflammation conditions. The developed novel propellant-free spray formulation is user-friendly, cost-effective, propellant-free, eco-friendly, enhances the penetration of Etodolac through the skin, and has a quick onset of action. Various formulations were developed by adjusting the concentrations of different components, including lecithin, buffering agents, film-forming agents, plasticizers, and permeation enhancers. The prepared propellant-free spray formulations were then extensively characterized and evaluated through various *in vitro*, *ex vivo*, and *in vivo* parameters. The optimized formulation exhibits an average shot weight of  $0.24 \pm 0.30$  ml and an average drug content or content uniformity of  $87.3 \pm 1.01\%$  per spray. Additionally, the optimized formulation exhibits an evaporation time of  $3 \pm 0.24$  min. The skin permeation study demonstrated that the permeability coefficients of the optimized spray formulation were 21.42 cm/h for rat skin, 13.64 cm/h for mice skin, and 18.97 cm/h for the Strat-M membrane. When assessing its potential for drug deposition using rat skin, mice skin, and the Strat-M membrane, the enhancement ratios for the optimized formulation were 1.88, 2.46, and 1.92, respectively against pure drug solution. The findings from our study suggest that the propellant-free Etodolac spray is a reliable and safe topical formulation. It demonstrates enhanced skin deposition, and improved effectiveness, and is free from any skin irritation concerns.

## PP-88 Rationally designed aromatase inhibitors and development of their polymeric micelle based delivery system

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### **Abstract**

Aromatase, an enzyme that facilitates the last stage in oestrogen synthesis, has been recognised as a potential target for therapeutic advancement. This study focuses on designing, synthesis and evaluating potential of aromatase inhibitors containing triphenylethylene and indole moieties. Among the synthesized molecules, compound **7d** demonstrated superior inhibitory activity against aromatase, with an IC<sub>50</sub> value of 54.0 nM, and significant tumor growth inhibitory activities of these compounds were also observed against breast cancer cell lines. Further, the physico-chemical experiments including plasma protein binding, HSA binding, kinetic studies, solubility, ADME properties and molecular modelling studies supported the drug like features of the compounds.<sup>1</sup> To enhance its bioavailability and therapeutic efficacy, compound **7d** was further formulated into a drug delivery system using mixed micelles composed of amphiphilic copolymers. The micellar formulation significantly enhanced its solubility, stability, % growth inhibition and cellular uptake. Apoptosis studies supported the micellar system's efficacy over free drug. These findings provide direction for the integration of structure-guided synthesis with nanocarrier delivery systems and give viable approach in overcoming the limitations of existing aromatase inhibitors (AIs) and offer a novel therapeutic avenue for breast cancer treatment.<sup>2</sup>

**Keywords:** Aromatase inhibitors, Bioavailability, Cellular uptake, Drug delivery system, Molecular modelling, Triphenylethylene.

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# PP-89 Heteroleptic Zinc Catalyzed Regioselective 1,2- hydroboration of N-Heteroarenes Under Solvent-Free Conditions

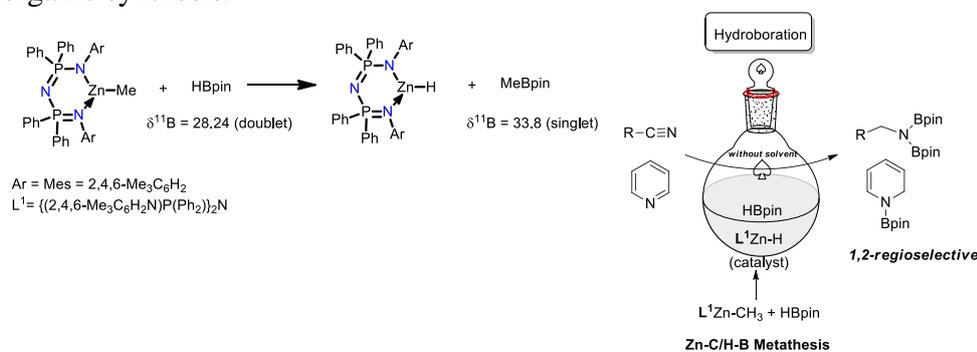
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## Abstract

Zinc, an environmentally benign and earth-abundant base metal, has garnered significant attention in catalysis due to its affordability, biocompatibility, and mild nucleophilic properties. In recent years, Zinc complexes have emerged as a versatile catalysts, facilitating key transformations such as hydrosilylation, hydroboration, and hydroamination of unsaturated substrates.<sup>1-2</sup> Ligand design is a critical determinant of catalyst reactivity and selectivity. In this work, we report a series of low-coordinate, neutral zinc complexes supported by bis(phosphinimino)amide ligands, strategically engineered to provide both thermodynamic and kinetic stabilization. These zinc complexes exhibit high catalytic efficiency in the 1,2-regioselective hydroboration of N-heteroarenes and enable the dihydroboration of nitriles, as well as the hydroboration of imines, carbonyl compounds, esters, and pyridines. Mechanistic investigations, supported by control experiments, reveal key reaction intermediates, which were characterized using NMR spectroscopy, high-resolution mass spectrometry, single-crystal X-ray diffraction, and computational studies. Collectively, these findings demonstrate the potential of zinc-based complexes as sustainable and effective catalysts for selective transformations in advanced organic synthesis.



**Keywords:** Zinc alkyl, Hydroboration, N-heteroarenes, Reaction mechanism.

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**PP-90 Generation of 2-(4-Oxo-but-3-enyl)-isoindole-1,3-dione and their [4+2] cycloadditions with 1,3-diazabuta-1,3-dienes: Synthesis of Functionalized pyrimidinones as Dipeptidyl peptidase IV inhibitors**

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**Abstract**

The manuscript describes a facile methodology for the synthesis of 5-(ethylisoindole-1,3-dione) pyrimidinones *via* [4+2] cycloaddition reactions of functionalized 1,3-diazabuta-1,3-dienes as  $4\pi$ -components with 2-(4-oxo-but-3-enyl)-isoindole-1,3-dione, as  $2\pi$ -components generated *in situ* from Phthaloylbutyric and tosyl chloride using triethylamine as a mild base. The functionalized 5-(ethylisoindole-1,3-dione) pyrimidinones were then investigated for amine deprotection, yielding various 5-ethylamino pyrimidinones. The functionalized 5-(ethylisoindole-1,3-dione) pyrimidinones have also been found as dipeptidyl peptidase IV inhibitors. The 5-(2-Amino-ethyl)-2,3-diphenyl-6-pyrrolidin-1-yl-3H-pyrimidin-4-one was found to be the most potent dipeptidyl peptidase IV inhibitor during the biological screening process.

**Keywords:** Pyrimidinones, [4+2] cycloadditions, Ketene, 2-(4-oxo-but-3-enyl)-isoindole-1,3-dione, Dipeptidyl peptidase IV inhibitors, anti-diabetic agent.

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## PP-91 Strategic Development of Peptide-Based DPP-4 Inhibitors for Antidiabetic Applications

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### Abstract

We designed and synthesized small peptide-based DPP-4 inhibitors for management of type 2 diabetes. A total of eighteen peptides were synthesized, and their inhibitory activity was assessed. Compound **8** emerged as most potent DPP-4 inhibitor (IC<sub>50</sub> 0.12 nM) and exhibited favourable drug-like features, including solubility, plasma stability, and ADME properties. Compound **8** binding constant ( $K_a = 3.56 \times 10^6 \text{ M}^{-1}$ ) with enzyme was determined by ITC and kinetic studies reveals its competitive mode of inhibition. The *in vivo* anti-diabetic efficacy was evaluated by employing a diabetic model of STZ/NA-induced Wistar rats. Compound **8** normalized glucose levels and enhanced serum lipid parameters, liver enzymes, and renal parameters at medium (20 mg/kg) and high doses (40 mg/kg). Histopathological analysis of kidney and pancreas tissue demonstrates its curative effect. Compound **8** demonstrates selectivity for DPP-4, determined by binding energy calculated through post-dynamic analysis. The MM-GBSA value for the compound **8** complex in DPP-4 is nearly double that of DPP-8 and DPP-9.

**Keywords:** Type 2 diabetes mellitus, Dipeptidyl peptidase-4, Peptides, Molecular modelling, Glucose, Drug-likeness, Histopathology

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# PP-92 Exploring Bifunctional Organocatalysts for Isatin Schiff Bases and Biologically Important 3-Aminooxindoles: Molecular Docking and Antimicrobial Studies

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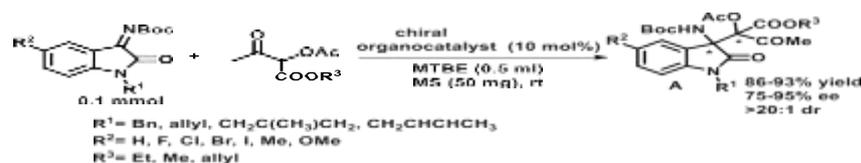
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## Abstract

Nature harbors a diverse array of bioactive compounds, among which 3-Aminooxindole stands out as a core structure present in numerous natural products and bioactive molecules like AG-041R, SSR-1494153, and NITD609.<sup>1</sup> Given its medicinal significance, organic chemists have endeavored to develop methods for its asymmetric synthesis.<sup>2</sup> Reported methods include amination of 3-monosubstituted oxindoles, sequential reactions of 3-isothiocyanato-2-oxindole with various electrophiles, and nucleophilic addition to isatin imine, with the latter being the more straightforward and convenient approach for synthesis.

Our research group actively employs chiral organocatalysts to achieve the enantioselective synthesis of 3-substituted-3-aminooxindole derivatives.<sup>3</sup> In this pursuit, we have devised an organocatalytic asymmetric pathway for synthesizing 3-aminooxindoles through the reaction of isatin imine with  $\alpha$ -acetoxy- $\beta$ -ketoesters. Utilizing the bifunctional Cinchona-derived thiourea as a catalyst, the reaction of  $\alpha$ -acetoxy- $\beta$ -ketoester derivatives with isatin imine yielded compound A in yields of up to 93%, with 95% enantiomeric excess and a diastereomeric ratio exceeding 20:1. Furthermore, the synthesized isatin-based Schiff bases and their corresponding 3-aminooxindole derivatives were systematically evaluated through molecular docking studies and in vitro antimicrobial assays to assess their biological potential.<sup>3c</sup>



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## PP-93 Sustainable Approaches Toward the Design and Green Synthesis of Anticancer Pyrazole Scaffolds

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### **Abstract**

Pyrazole derivatives have a large class of nitrogen-containing heterocycles with a broad range of pharmacological profiles, including strong anticancer activity, which is one of pyrazole derivatives greatest attributes. In prior work, pyrazole derivatives have been synthesized employing toxic solvents, long operational reaction times, and high energy costs which present safety and ecological challenges. Recently, a more sustainable alternative using the principles of green chemistry has been developed for the efficient synthesis of pyrazole derivatives. Between the years 2020 and 2025, a number of publications have been released concerning this topic. The present paper focuses on both the classical and green methods, including synthesis techniques, and gives particular attention to the synthesis of pyrazole derivatives by mechanochemistry, ultrasonically, and microwave-assisted synthesis techniques. In ultrasonic synthesis, reaction times and product purity are improved. In microwave-assisted synthesis, rapid and uniform heating is achieved. Between and among methods, mechanochemical methods are free of solvents and energy-saving. Analyzing the cancer cell line, IC<sub>50</sub> values, and reference medicines, along with the pyrazole derivatives, a comparative table summarizes the green methods for next-generation anticancer agents. Researchers working on anticancer medications, particularly those containing pyrazoles, will find this review helpful.

**Keywords:** Pyrazole derivatives, Anticancer property, Green Synthesis, Microwave Assisted Synthesis, Ultrasonic Assisted Synthesis, Mechanochemical Synthesis, Sustainability

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# PP-94 Aggregation-Modulated Solvatochromic Azo-Fluorophore as a Dual-Mode Colorimetric and Fluorogenic Sensor for Hydrogen Sulfide (H<sub>2</sub>S)

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## Abstract

Hydrogen sulfide (H<sub>2</sub>S) is an essential biological gasotransmitter involved in numerous physiological and pathological processes, necessitating the development of sensitive and reliable detection systems. Herein, we report a donor–acceptor (D–π–A) azo-based fluorogenic probe that exhibits pronounced solvatochromism, aggregation-caused quenching (ACQ), and selective response toward H<sub>2</sub>S. The probe was rationally designed by integrating an electron-donating dimethylamino moiety with an electron-withdrawing sulfonate-linked fluorophore, enabling strong intramolecular charge transfer (ICT) and environment-sensitive optical behavior.

Spectroscopic investigations revealed significant solvatochromic shifts in different solvent systems, confirming the ICT-driven excited-state characteristics of the probe. Furthermore, the molecule displays aggregation-dependent photophysical behavior, where aggregated states lead to fluorescence quenching and reduced photoreactivity compared to non-aggregated conditions. Upon interaction with H<sub>2</sub>S (Na<sub>2</sub>S as a source), the probe exhibits distinct colorimetric and fluorogenic changes, indicating a specific chemical interaction that modulates the electronic structure of the chromophore.

The aggregation state was found to influence the sensing efficiency, with dispersed systems showing faster and more pronounced optical response than aggregated media. This highlights the crucial role of supramolecular organization in regulating probe performance. The dual colorimetric and fluorescence response enables rapid, visual, and spectroscopic detection of H<sub>2</sub>S without the need for additional indicators.

Overall, this study presents a solvatochromic, aggregation-sensitive fluorogenic probe as a mechanistically tunable platform for selective and dual-mode detection of H<sub>2</sub>S in complex chemical and biological environments.

**Keywords:** Hydrogen sulfide, sensors, aggregation, solvatochromism, fluorescence, colorimetric.

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**PP-95 A Water-dispersible Eu-MOF was synthesized by hydrothermal technique to enable the specific and precise detection of TNP in water samples.**

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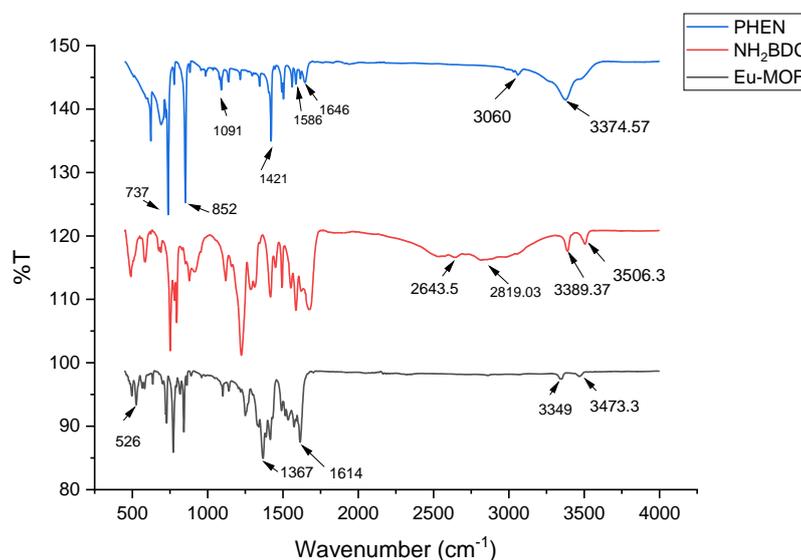
**Abstract**

A dual ligand Eu-based metal organic framework (ENP) with irregular morphology was produced by hydrothermal method using 2-aminoterephthalic acid and 1,10-phenanthroline ligands. Crystalline nature of synthesized ENP was confirmed by PXRD technique and the presence of oxygen, nitrogen, carbon and europium is confirmed in the synthesized ENP by the elemental analysis. MOF was employed as selective and sensitive sensor for ultra-trace detection of 2,4,6-trinitrophenol (TNP) in aqueous matrix, even in coexistence with other competitive nitroaromatic analytes. DFT calculations and electrostatic interactions (i.e. ionic interaction, H-bonding and  $\pi$ - $\pi$  interaction) indicated that electron and energy transfer processes play a key role in turn-off quenching response of ENP. Thus, the present work provides the quick and precise identification of TNP using



a new fluorescent MOF.

**Fig.1** FE-SEM Image of synthesized MOF



**Fig.2** FT-IR Spectra

## PP-96 Chitosan-Based Drug Delivery Systems: Mechanisms, Applications and Recent Advances

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### **Abstract**

Chitosan, a cationic chitin biopolymer, has gained significant importance in the development of improved drug delivery due to its biodegradability, biocompatibility, mucoadhesion, and chemical modification. Various types of chitosan architectures have been created, such as nanoparticles, nanocapsules, hydrogels, films, and microparticles, to deliver small-molecule drugs as well as biomacromolecules, including proteins, peptides, and nucleic acids. These systems increase drug stability, water solubility of poorly water-soluble compounds, and controlled, localised release. The major benefit here is the pH-responsive properties of chitosan: it can stabilise therapeutics at acidic gastric pH and release therapeutics at intestinal pH, which enhances oral absorption and overall bioavailability. Tissue targeting and enhanced mucoadhesion, as well as incorporation into co-delivery systems to combine therapies, by chemical tailoring, are also supported.

Recent studies also put emphasis on theranostic design and stimuli-responsive vectors that fit the customised therapy plan. The inherent antibacterial properties of chitosan, coupled with enhanced targeting and decreased systemic toxicity in antimicrobial therapy, show potential in the treatment of drug-resistant infections. The versatility of the platform is evidenced by the growing body of in vivo applications in gene delivery and regenerative medicine. Nevertheless, there are still issues regarding the high level of consistency of release profiles, reduction of possible immunogenicity, upscaling, and clinical translation.

All in all, chitosan-based delivery systems are a sustainable and versatile way to overcome the drawbacks of traditional formulations. Their application in targeted, efficient and patient-friendly therapeutics is likely to be enhanced even further by continued innovations in nanotechnology, modulation of materials and structure, and development of forms.

## PP-97 Synthesis and Characterization of CQD from Biowaste using Microwave Technique

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### Abstract

In recent years, the synthesis of Carbon Quantum Dots (CQDs) with the aid of green and sustainable approaches has attracted much attention for the environmental application and biomedical use. This study reports on the synthesis of fluorescent CQDs leading to rapid one-pot microwave-assisted synthesis from biowaste precursors such as hibiscus leaves as well as papaya seeds and coffee grounds. Compared to the traditional hydrothermal methods, when microwave irradiation is used in the carbonization process, the carbonization time can be condensed from several hours to seconds and minutes; compared to traditional carbonization processes, the energy consumption is greatly reduced; moreover, the carbonization particles can be precisely controlled in terms of size. Characterization based on TEM, DLS and XRD shows monodispersed quasi-spherical nanoparticles (2-12 nm) with polycrystalline, graphitic structure. Optical analysis using UV-Vis and fluorescence spectroscopy is used to verify the existence of strong excitation-dependent photoluminescence with quantum yields up to 31.6% by nitrogen or sulfur co-doping. Furthermore, the focus by FTIR and XPS detect oxygen-rich surface groups (-OH, -COOH, -NH<sub>2</sub>), providing for good aqueous stability, for efficacy of "turn-off" sensing for heavy metals such as Fe<sup>3+</sup>/Pb<sup>2+</sup>. Given their low toxicity and high biocompatibility, these CQDs prepared from biowaste are excellent fluorescent bioimaging agents. This "waste-to-wealth" approach is a scalable and environmentally safe approach for creating high performing nanomaterials important for advanced environmental monitoring and clinical diagnostics.

## PP-98 Synthesis of a 1,2,3-Triazole-Based Chemosensor for Selective Co<sup>2+</sup> Detection

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### **Abstract :**

This study presents the synthesis of a novel quinoline-based 1,2,3-triazole (QBT), synthesized by Click Chemistry. The molecule was made via a Copper(I)-catalyzed alkyne-azide cycloaddition (CuAAC) process, which is a very selective and effective way to make five-membered triazole rings. Different spectroscopic methods, such as IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and mass spectrometry, were used to confirm the synthesis of QBT. The chemosensing behavior of QBT was analyzed by performing UV-Visible titrations in a CH<sub>3</sub>CN: H<sub>2</sub>O (4:1, v/v) solution. The ligand was evaluated with a number of metal ions, such as Mn(II), Hg(II), Cd(II), Pb(II), Cu(II), Fe(II), Zn(II), Ba(II), Cr(III), Co(II), K(I), and Na(I). The results demonstrated that QBT only reacts to Co(II) ions. The probe was very selective for Co(II), even when other metal ions were present. The limits of detection (LOD), with a value of  $10.55 \times 10^{-6}$  M for Co(II), and the analysis of the job's plot indicated the formation of a metal-ligand complex in a 1:1 ratio.

**Keywords:** Click chemistry, CuAAC, 1,2,3 triazole, Ion sensor.

## PP-99 Tuning the Physicochemical and Electrochemical Properties of Natural Deep Eutectic Solvents via Water Addition and HBD Selection

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Today, Deep eutectic solvents (DESs) have emerged as a promising class of sustainable solvents and a green alternative to organic solvents and conventional ionic liquids. Among them, natural deep eutectic solvents (NADESs), formed through the complexation of hydrogen bond acceptors (HBAs) and donors (HBDs) derived from natural compounds such as amino acids, sugars, and organic acids, are particularly gaining attention due to their low cost, simple preparation, wide availability, and low toxicity. Recently, binary mixtures of NADES with water have gained significant attention for diverse industrial applications because they exhibit physicochemical properties distinct from those of their individual components.<sup>1,2</sup> A comprehensive investigation of the thermophysical properties of NADESs and their aqueous mixtures is therefore essential to elucidate the underlying intermolecular interactions and to expand their potential application scope.

In this study, a series of NADES based on choline chloride as HBA and various HBDs, including ascorbic acid, glucose, citric acid, and oxalic acid, have been prepared and characterized using FTIR and TGA analysis. The physicochemical parameters have been thoroughly investigated in relation to temperature, the nature of HBDs, and the alkyl chain of the constituents. Several thermodynamic parameters have been assessed to determine the level of intermolecular interactions in NADESs systems at different temperatures. Furthermore, the relationship between molar conductivity and dynamic viscosity has been studied using Walden plots to determine the ionicity of the NADESs. The electrochemical performance of these NADESs has also been investigated to ascertain their potential for electrochemical applications.

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## PP-100 Synthetic applications of chiral aldehydes from amino acids

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### **Abstract:**

The Poster demonstrates the use of chiral aldehydes derived from commercially available  $\alpha$ -amino acids for the synthesis of various natural products and bioactive compounds containing an amino group and one or more hydroxyl groups. While the amino groups in the target molecules come from the starting materials, the hydroxyl groups are installed by diastereoselective hydroxylation reactions.

The synthesis of *D-threo*-sphinganine, *L-erythro*-sphinganine, (–)-spisulosine, and various clavaminols from *L*-aspartic acid and *L*-alanine using proline-catalyzed asymmetric  $\alpha$ -hydroxylation of aldehydes and Wittig reaction as key steps. It also deals with the synthesis of (–)-bulgecinine and its *5-epi* diastereomer from *L*-glutamic acid using *D*-proline-catalyzed asymmetric  $\alpha$ -hydroxylation and BF<sub>3</sub>·OEt<sub>2</sub> mediated intramolecular epoxide ring opening with an amine as the key steps. Additionally, Iminocyclitols derived from polyhydroxy pyrrolidines or polyhydroxy piperidines having a 2-aryl substituent are a class of compounds that have gained attention due to their potential for being glycosidase inhibitors. The synthesis of such compounds from an aldehyde derived from (*R*)-*p*-hydroxy phenylglycine. Simple transformations including Wittig reaction, dihydroxylation of olefins and cyclization through S<sub>N</sub>2 reactions has allowed the diastereoselective synthesis of various 2-aryl iminocyclitols.

**Keywords:** Asymmetric synthesis, diastereoselective, amino acids, Iminocyclitols

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# Studies in the development of $\pi$ -conjugated fluorescent materials in sensing, pesticide mimic and targeted antibacterial PDT.

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**Abstract:** The development of  $\pi$ -conjugated fluorescent probes with high luminescence in aqueous medium and solid state as well have gained attention for *in vitro* and *in vivo* sensing of analytes having biological importance. We have designed and synthesized perylene bisimide (PBI) based supramolecular assemblies which could selectively detect organochlorine 2,6-dichloro-4-nitroaniline (DCN) and organophosphate chlorpyrifos (CPF) pesticides in mixed aqueous medium. The assemblies of PBI probe showed ‘on-on’ response towards DCN owing to inhibition of ESIPT and aggregation induced emission enhancement (AIEE) phenomenon and ‘turn-on’ response towards CPF. The biological applications of the probe to detect DCN and CPF in MG-63 cell lines show their ability to restrict the DCN and CPF-induced cell death. These assemblies also show affinity for acetylcholinesterase (AChE) which endow the PBI molecules with mixed inhibitory potential to restrict the AChE catalysed hydrolysis of acetylthiocholine (ATCh) in MG-63 cell lines (*in vitro*) and in mice (*in vivo*). The insecticidal potential of PBI probe has been examined against *Spodoptera litura* (*S. litura*) with excellent insecticidal activity. Further, we synthesized water soluble carbazole based probe which forms *H*-aggregates in water and show excellent type I photosensitizing potential under day light and upon photoirradiation in aqueous media. The *in vitro* cell imaging studies using dihydroethidium (DHE) dye in HeLa cell line and *in vivo* image guided investigation in *C. punctata* fish indicates the high potential of assemblies of compound as safe PDT agent. The *in vitro* antibacterial activity of photosensitizer also shows the high potential for safe antibacterial photodynamic therapy.

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