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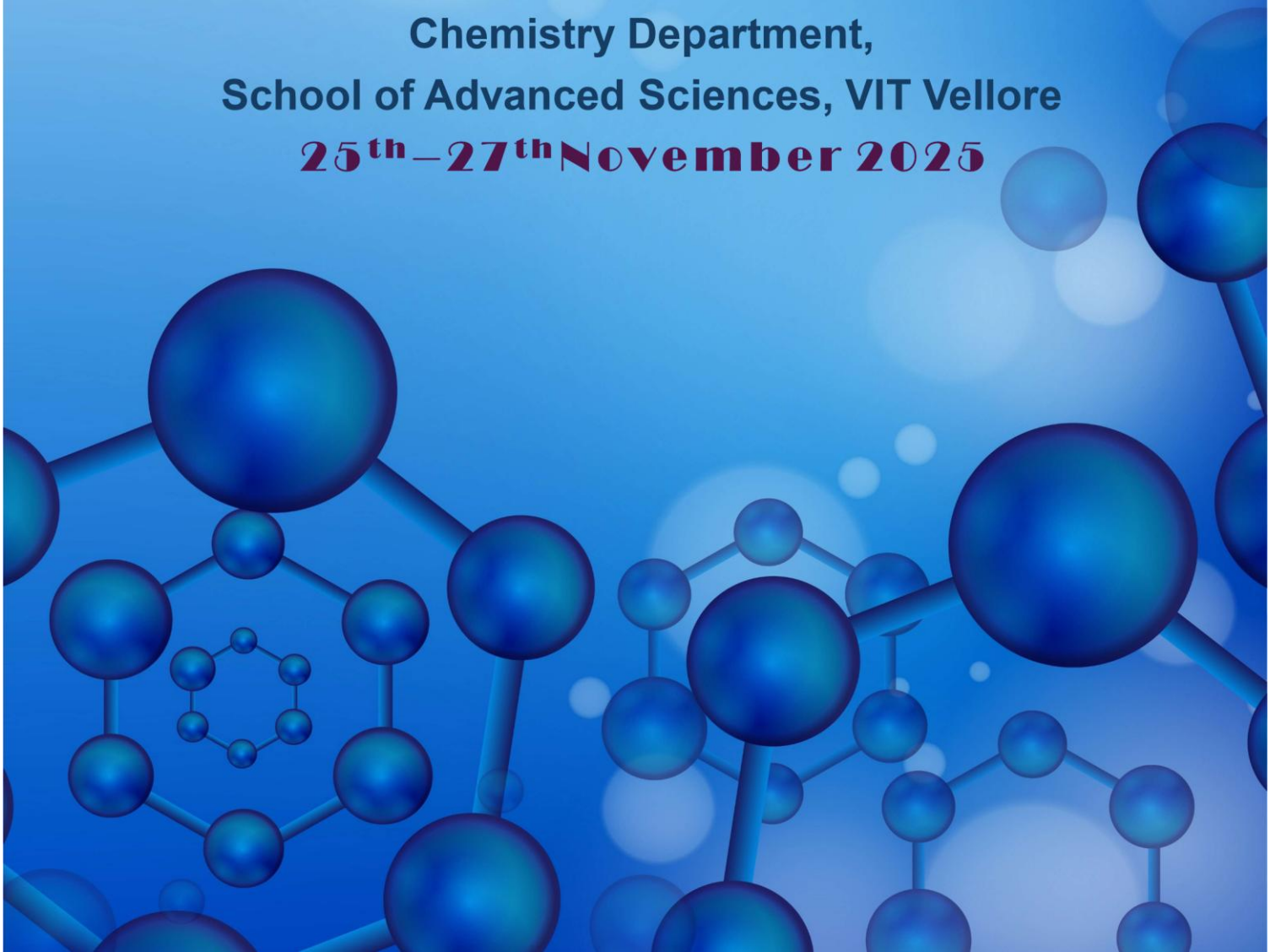
ABSTRACT BOOK

Organised by

Chemistry Department,

School of Advanced Sciences, VIT Vellore

25th–27th November 2025



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ABOUT VIT

Vellore Institute of Technology (VIT) was founded in 1984 as Vellore Engineering College by the Honorable Chancellor Dr. G. Viswanathan. The institution has grown steadily since its humble beginning. VIT attracts students from all over India and abroad because of its excellence. VIT has emerged as one of India's best institutes and aspires to become a global leader in education. In Engineering and Technology, VIT is ranked 142nd in the World and 9th in India (QS World University Rankings by Subject 2025). In Data Science and AI subject areas, VIT is within the top 100 in the world, whereas five subjects (CS, Information Systems, Electrical, Electronics and Material Science) have been ranked among the top 200 in the world (QS World University Rankings by Subject 2025). It is within the top 2 in India and top 600 in the world (Shanghai ARWU ranking 2025). VIT achieved NAAC Accreditation with A++ grade in the 4th cycle. VIT is within the top 20 in University, Research and Engineering categories in India (NIRF Ranking, Govt. of India 2025). It secures rank 396th in the world and 8th in India (QS World University Rankings: Sustainability 2025).

ABOUT THE CONCLAVE

The conclave will feature scientific talks by distinguished international speakers from top 100 QS-ranked universities, as well as national lectures delivered by eminent faculties from IISc, IITs, IISERs, and NITs. Emphasizing interdisciplinary approaches, the event will bring together experts to address global challenges at the interface of health and environment. Expert lectures complemented by interaction sessions with scholars and students will foster future growth and collaborations. Editorial insights will be shared by leading journal editors, while participants will showcase their work through oral and poster presentations evaluated by external experts. Exciting prizes from RSC, Wiley, and ACS will be awarded. Participants will also benefit from career prospect session by these organizations, along with opportunities for publication and membership. The program further includes IR office and laboratory visits, culminating in a brainstorming discussion and faculty interaction aimed at formulating joint Indo-Foreign proposal submissions.

ABOUT CHEMISTRY DEPARTMENT

Chemistry department comes under the School of Advanced Sciences (SAS), which was established in the year 1984. Department of Chemistry's vision is to provide quality teaching and research which would make an impact at a global level. The department consists of a total of 71 experienced and energetic faculty. Most of them are experts in their research fields, evident from their publications and research funding. The Department is recognized by DST-FIST to establish sophisticated instrumental facilities. It is also equipped with necessary instruments for research and also offers services to other institutions as well. After graduation, students are placed in reputed companies in India and abroad, and they have been securing admissions in India and abroad for their higher education. We offer 2 years MSc and 5 years integrated MSc program in Chemistry. Our MSc program (2 years) offers specialization in Analytical/Inorganic/Organic/General/Pharmaceutical Chemistry. Our MSc Chemistry program is Accredited by RSC. The subject Chemistry in VIT is ranked within the top 13 in India and top 401-450 in the world as per QS World University Rankings by Subject 2021 and 14th place at National level with 4 STAR rating in QS World Ranking. In India, VIT has been ranked 15th among the top universities in Chemistry in Best Global Universities ranking by U.S. News & World Report.

TOPICS OF THE CONCLAVE

- Theoretical Chemistry & Spectroscopy
- Organic & Medicinal Chemistry
- Bio-inorganic and Organometallics
- Innovative Materials
- Drug Delivery
- Polymers
- Catalysis

SCOPE OF THE CONCLAVE

IC-HEIAC aims to promote interdisciplinary innovation in chemistry that addresses critical challenges in health and the environment. The conclave focuses on integrating chemical sciences with biology, medicine, materials science, and environmental technology to foster sustainable innovations that support public health and mitigate environmental challenges.

CALL FOR PAPERS

The participants are requested to submit the extended abstracts including manuscript title, author(s), affiliation(s) and contact details, with a clear indication of research work, methodology, major results and conclusion. The committee will evaluate the abstracts and will decide whether the paper will be presented as oral or poster, also considering the preference of the authors.

PUBLICATIONS

The registered and successfully presented papers in the conclave will be considered for publication in the Scopus Indexed International journals after the peer review process.

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Plenary Lecture- PL

PL-1

Design of Pt(iv) Anticancer Complexes, Screening In 3d Spheroids and Delivery to Animal Cancer Models

Giorgia Pastorin*

Department of Pharmacy & Pharmaceutical Sciences, Faculty of Science, National University of Singapore, Singapore 117544, Singapore

The discovery of cisplatin as a Platinum (Pt)-based anti-cancer drug in 1965 was an important milestone. Nowadays, cisplatin and its analogues, all acting at the nuclear DNA as their main biological target, are still used in more than 40% of all chemotherapy treatments. However, these drugs have toxic side effects (e.g. kidney dysfunction and peripheral neuropathy) [1].

Hence, we have conceived novel dual-targeting platforms to ensure strategic delivery of dual-action Pt(IV) prodrugs: the first targeting was established by nanoencapsulation of Pt complexes to attain high accumulation at the tumor site. To achieve that, we developed a nanoscale drug delivery system with high drug loading and decreased off-target accumulation [2]. After the release of the Pt prodrug inside cancer cells, a second stage of targeting directed the Pt prodrugs to the mitochondria [3]. Our data demonstrated minimal peripheral neuropathy *in vivo*, which is often the dose-limiting step in platinumbased drugs [4].

A spatial analysis was also performed to rationalize drug behavior and efficacy in a 3D tumor model: after 24 and 72h, spheroids were evaluated for changes in viability, expression of proliferation marker ki67, mitochondrial membrane potential and platinum accumulation. Images of fluorescently labelled spheroids enabled the discovery that one Pt(IV) complex uniquely induced permanent mitochondrial damage in spheroids after 24h. This extensive mitochondrial damage was corroborated through *realtime* observation of a rapid and increased intracellular platinum accumulation [5].

The Pt complexes showed excellent activity, characterized by low micromolar cytotoxicity and tumor remission *in vivo*, accompanied by reduced kidney toxicity and lack of peripheral neuropathy [4]. One of them has shown the ability to be used as the first-in-kind oral Pt drug [6]. Taken together, these research findings provide insights into the potential of nanomedicine [7] to reach the diseased area, protect the incorporated bioactive molecules from premature deactivation and enhance delivery of Pt(IV) drugs at the mitochondria while decreasing their side effects.

References

[1] J. X. Kee, J. N. N. Yau, R. P. K. Muthuramalingam, X. Wang, W. H. Chng, A. Lopez-Sanchez, K. K. W. Tay, L.-W. Deng, D. Gibson, H. C. Bertrand, G. Adriani, W. H. Ang,* and G. Pastorin*. **Colorectal Cancer at the Crossroads – the Good, the Bad and the Future of Platinum-based Drugs.** *Chemical Reviews*, 2025, In Press.

[2] T. Babu, R.P.K. Muthuramalingam, W.H. Chng, N. Yau, S. E. Acharya, N. Feldman-Goriachnik, S. Lev, G. Pastorin, A. Binshtok, M. Hanani, D. Gibson. **Multi-targeting prodrugs that combine cisplatin and paclitaxel display in vivo anticancer efficacy without neuropathic pain.** *J. Med. Chem*, 2025, 68, 1608−1618.

[3] M. V. Babak, Y. Zhi, B. Czarny, T. B. Toh, L. Hooi, E. K.-H. Chow, W. H. Ang, D. Gibson, G. Pastorin. *Angew. Chemie Int. Ed*., 2019, 58, 1-7.

Biography:

Giorgia Pastorin received her Ph.D. in Medicinal Chemistry in 2004 from the University of Trieste (Italy). She spent two years of her postDoc at the CNRS in Strasbourg (France), where she specialized in drug delivery.
She joined the National University of Singapore (NUS) in June 2006, as Assistant Professor in the Department of Pharmacy-Faculty of Science. She was promoted to Associate Professor in 2011, Assistant Head in 2014, Deputy Head in 2016 and Full Professor in 2024; she is currently Head of the Department of Pharmacy & Pharmaceutical Sciences at NUS.
Her research interest is focused on drug delivery, with the purpose of enhancing the pharmacological effects of bioactive agents (such as Pt-based anticancer complexes) while minimizing undesirable side effects. Recently, her BioNanoTechnology (BNT) group developed cell-derived nanovesicles (CDNs) and biohybrids as novel biocompatible Extracellular Vesicle mimetics for targeted drug delivery. Her approach of using unconventional yet efficacious cell-derived nanocarriers has become her signature program, resulting in new invention disclosures, industry engagements and even an international BioDrone award in 2021. She is the sole and co-Editor, respectively, of two books related to drug delivery and author in more than 170 articles in internationally peer-reviewed journals. She also holds several international patents. For the work performed by her BNT group in NUS, she received the Young Scientist Award (2015) in NUS and she has been invited at prestigious international conferences as plenary or keynote speaker.

PL-2

Designing Smarter Metal Complexes: Overcoming Cellular Sequestration and Hypoxia Limitations in Cancer Therapeutics

Arindam Mukherjee*

Department of Chemical Sciences and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research Kolkata, Mohanpur campus, 741246, India

Cancer is a disease fueled by dysregulated signaling and sustained genetic mutations—forces of evolution that drive inflammation, malignancy, and cellular plasticity while enabling immune evasion. Metal-based therapeutics, particularly platinum(II) complexes, have long been the cornerstone of chemotherapy, with other metals gradually expanding this landscape in recent years. However, a major challenge persists: Designing complexes that retain biological activity even after metal dissociation through ligands endowed with intrinsic targeting or therapeutic functions. This objective is the flagship focus of our group (SMTL@IISER-K). Early in our investigations, we identified cellular thiol sequestration as a key factor underlying the deactivation of metal-based drugs. Our work provided mechanistic insights into overcoming this limitation while directing metal complex reactivity toward biologically relevant targets. Specifically, we have explored imidazole- and benzimidazole-based ligands, demonstrating that their –NH groups critically modulate metal reactivity and therapeutic performance under physiological stimuli. Through systematic development, we have advanced Ir(III)–indazole complexes that exhibit photoactivity even in hypoxic tumor environments. These systems leverage excited-state proton-coupled electron transfer (ES-PCET) processes rather than reactive oxygen species, thereby overcoming hypoxia-induced resistance. This strategy not only broadens the scope of metal-based anticancer agents but also paves the way for dual-targeting, stimuli-responsive therapeutics with enhanced precision and efficacy.

Keywords: cancer therapeutics, metal complex, kinase inhibitor, NF-kB inhibitor, cancer Stem cell killing agent

References

[1] Banshi Roy, Shilpendu Ghosh, Soumee SenGupta, Shamik Chanda, Shantanu Saha Roy, Sangita Sen, Rahul Das, Moulinath Acharya, and Arindam Mukherjee*. **Indispensable Role of Indazole −NH in Cyclometalated Ir(III) Complexes to Drive ES-PCET with High Phototherapeutic Index**. J. Am. Chem. Soc. 10.1021/jacs.5c15369.

[2] Mukherjee, Sujato; Ghosh, Shilpendu; M, Renuga Devi; Roy, Souryadip; Roy, Shantanu Saha; Acharya, Moulinath; Kumar, Bokara Kiran*; Mukherjee, Arindam*. **Peroxiredoxin Depletion and Oxidative Stress by Cyclometalated Ir(III)-Isatin Complexes Renders Ferroptosis and Autophagic Cell Death in Triple-Negative Breast Cancer**, J. Med. Chem. 2025, (68): 21201–21223.

[3] Ghosh, Shilpendu; Paul, Soumya; Ghosh, Sayar; Mukherjee, Sujato, De, Priyadarsi, Das, Rahul*; Mukherjee, Arindam*. **Limantrafin-BODIPY Conjugates Reduce Stemness and Metastatic Potential via Superoxide Driven Phototherapy in Triple Negative Breast Cancer**, Small, 2025, 21, 33, 2505316.

Biography:

Arindam Mukherjee is currently a Professor of Chemistry at IISER Kolkata where he joined during 2009. He completed his PhD from IISc Bangalore in 2005 followed by postdoctoral research as a Marie Curie Research Fellow at University of Edinburgh and University of Warwick (2005-2009). His group's research centers on the design of small-molecule therapeutics against cancer, specifically to prevent their sequestration and deactivation by thiol-rich proteins and other molecules in cells. He started his independent career as a biomimetic chemist. Since 2015, the team showed how the differences in electronic parameters control reactivity towards cellular thiol rich molecules. The group also modulates their targeting strategies by use of metabolite and clinical drug modifications in ligands, use of imidazole/benzimidazole/indazole/pyrazole motifs in ligands to promote kinase inhibition, impede angiogenesis and evaluate the impact on cancer stem cell (CSC) gene expression, emphasizing the importance of understanding CSC dynamics in anticancer efficacy. Their research perspective holds the thiol resistivity in the design aspect while evolving to target proteins and transcription factors through incorporation of suitable ligands. They hypothesize and investigate various ways to increase ES-PCET feasibility in metal complexes and organic molecules to develop the next generation PDT agents that would be active in hypoxic solid tumors.

PL-3

Chemical Tools for Mucopolysaccharidosis Therapeutic Development

Vito FERRO*

School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, QLD 4072, Australia

Mucopolysaccharidosis disorders are lysosomal storage diseases caused by mutations in the genes encoding enzymes that sequentially degrade glycosaminoglycans (GAG), including heparan sulfate (HS). This results in accumulation of GAG in the lysosome which leads to significant cell, tissue and organ damage and, in severe cases, neurological decline and shortened lifespan. There are no cures for MPS disorders, although enzyme replacement therapies are available for some subtypes. However, these are limited by their inability to cross the blood-brain barrier or to penetrate into joints. Various gene and stem cell therapies are also under clinical evaluation or in various stages of development. Advancement to clinical trials is a significant step forward, however, issues remain including exclusion of patients from gene therapy trials due to pre-existing antibodies to the vectors, the necessity of invasive, high-risk procedures, and anticipated loss of gene expression with time. Small molecule approaches for the treatment of MPS disorders, such as pharmacological chaperone therapy or substrate reduction therapy, are therefore desirable. In this presentation I will describe some of our efforts to develop such small molecules with therapeutic potential for MPS disorders.[1] I will also discuss the development of a quantitative LC-MS/MS assay for HS in biological samples,[2,3] and the efficient synthesis of various fluorogenic substrates[4] for assaying lysosomal enzymes involved in MPS disorders. These assays underpin our drug discovery efforts and are useful for monitoring the efficacy of potential new therapies.

Keywords: mucopolysaccharidosis (MPS), lysosomal storage diseases, heparan sulfate

References

[1] Tan S. L. et al., **Substrate reduction using a glucosamine analogue in *Drosophila melanogaster* and mouse models of Sanfilippo syndrome.** *Mol. Genet. Metab*., **2025**, *145*, 109112.

[2] Pan Y. et al., **Synthesis of a deuterated disaccharide internal standard for LC-MS/MS quantitation of heparan sulfate in biological samples**. *Carbohydr. Res*., **2024**, *545*, 109270.

[3] He Q. et al., **Synthetic disaccharide standards enable quantitative analysis of heparan sulfate in MPS IIIA murine brain regions.** *ACS Chem. Neurosci*., **2019**, *10*, 3847-3858.

[4] Pan Y. et al., **Efficient synthesis of fluorogenic substrates for Mucopolysaccharidosis (MPS) IIIA and IIIB via aromatic α-glycosylation with thioglycosyl donors**. *Org. Biomol. Chem*., **2025**, 23, 6446-6455.

Biography:

Vito Ferro completed his PhD at the University of Western Australia under the guidance of Bob Stick in 1992. Following postdoctoral studies at the Carlsberg Laboratory (with Klaus Bock and Morten Meldal) and the University of British Columbia (with Steve Withers) he returned to Australia in 1996 to join Progen Pharmaceuticals where he spent 12 years in various positions, including Director of Drug Discovery. Following a brief period at QUT in the CRC for Polymers he moved to the University of Queensland in 2010 where he is a Professor and the Biomolecular and Medicinal Chemistry Theme Leader in the School of Chemistry and Molecular Biosciences. His research interests are in carbohydrate and medicinal chemistry, with a focus on the synthesis of compounds to probe and/or inhibit carbohydrate-protein interactions involved in disease processes. Of particular interest is heparan sulfate (HS) and the development of HS mimetics as potential drugs for cancer, infectious diseases and lysosomal storage disorders.

Keynote Lecture- KL

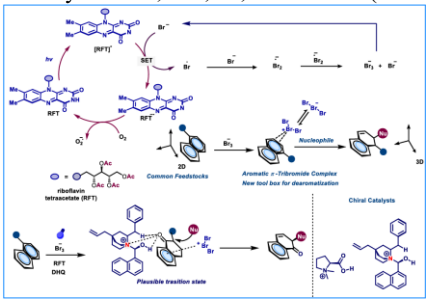
KL-1
Rise of Tribromide Tools – Precision Dearomatisation for 3D Molecular Frameworks

Dr. Debayan Sarkar*
Professor, Department of Chemistry, IIT Indore

Dearomatization reactions have nowadays become interesting chemical transformations in organic synthesis that facilitate the generation of three-dimensional structures from two-dimensional precursors. The transformation relies on conversion of readily available aromatic motifs to three dimensional polycyclic structures. Aromaticity imparts extraordinary stability to the structures due to delocalization of pi electrons. Mostly the aromatic rings are susceptible to undergo substitution reactions which generally do not disrupt the aromaticity of the ring. In this regard many synthetic protocols of dearomatization are available. However still a general platform for the oxidative aromatization of common feedstocks is fewer. In this context our group has reported the first recognition of Phenyl Trimethyl Ammonium Tribromide as an effective reagent for spiro-cyclizations proceeding via oxidative dearomatization. The experiment exhibits economic, metal and ligand free one-pot accomplishment of these significant transformations. In this project we aim to develop a catalytic, visible-light-driven strategy for transforming abundant and inexpensive planar Arenols and other aromatic cores—crucial building blocks in pharmaceuticals, agrochemicals, and materials—into valuable, complex three-dimensional chiral scaffolds via dearomatization. Its significance lies in overcoming the inherent stability of aromatic rings using a novel in situ generated electrophilic tribromide catalyst (Br_3^-), formed synergistically via photo redox processes. The tribromide is sufficiently electrophilic to break inherent aromatic stabilization of 2D cores to provide access to 3D core skeletons in one pot transformation.

Reference

Acs Catalysis 2025 (Accepted); Org. Lett. 2025 doi/10.1021/acs.orglett.5c00744;Chem. Commun., 2024,60, 9206; Advanced Synthesis and Catalysis 2024, https://doi.org/10.1002/adsc.202400117; Org. Lett 2023, 25, 7733; ChemSusChem 2024 (Just Accepted), J. Org. Chem 2023, 88, 13, 7977-7987; J. Org. Chem 2023, 88, 13, 7977-7987; Chem Photo Chem 2023 87, (Accepted Article) doi/abs/10.1002/cptc.202200335; J. Org. Chem 2022. 87, 21, 13529–13541; J. Org. Chem 2022 87, 15, 9729–9754; J. Org. Chem 2021, 86, 23, 16369-16395; J. Org. Chem 2022, 87, 15, 9729-9754; J. Org. Chem 2022, 87, 21, 13529-13541; Asian Journal of Organic Chemistry 2021, 10, 1786-1794; Organic and Biomolecular Chemistry 2020, 18, 4619-4627; European Journal of Organic Chemistry 2020, 11, 1727-1731; Tetrahedron Letters ,2020 (cover page Article), 61, 151646; European Journal of Organic Chemistry 2020, 397-401; European Journal of Organic Chemistry 2020, 7, 891 896 ; Organic Letters 2019 21, 11, 4132-4136; Advanced Synthesis and Catalysis 2019, 361, 24, 5648-5653. (Most Downloaded Paper 2020)



Biography:

Dr. Debayan Sarkar is presently an Professor of Chemistry and Head of Centre of Rural Development and Technology (CRDT) at the Indian Institute of Technology Indore (IIT Indore). Before this he worked as an Associate Professor in the Department of Chemistry at National Institute of Technology, Rourkela, Odisha, India. He has completed his M.Sc with Organic Chemistry specialisation from University of North Bengal (NBU) in the year 2005 followed by a Ph.D in Organic Synthesis from Indian Association For The Cultivation of Science (IACS) in the year 2011, Jadavpur Kolkata under the supervision of Prof. R. V.Venkateswaran. After that he travelled to carry out his post-doctoral studies at Stanford University (USA) under the mentorship of Prof. Barry M Trost (20122013). He was deputed as a Visiting Senior Assistant Professor at Graduate School of Pharmaceutical Sciences, Tohoku University (Japan) under the mentorship of Prof. M. Yamaguchi (Dec 2015- March 2016). He was at the University of Leipzig Germany as a DAAD Research Professor with Prof. Christoph Schneider (2018-2019). He worked with Prof. Burkhard Koenig at University of Regensburg Germany as an ICMR International Fellow from JanDec 2020.

Recently he has been Awarded with the NATIONAL TEACHER AWARD 2025 by Honourable President of India. He has been recipient of prestigious awards like IIT Indore Best Research award 2024, Chemcomm Pioneering Investigators 2023, SERB TETRA Award, RC Tripathy Research Excellence Award by Orissa Chemical Society, DST Inspire faculty award (2013),BRNS-DAE Young Scientist Award (2014), Indo-US Research Award(2012), DAAD Visiting Professor (2018). Research interest includes Visible Light Catalysis, Asymmetric Dearomatisation reactions, Atom Economic couplings, Complex total synthesis of natural products. He has 60 research publications in International Journals of Repute, 2 Patents and guided 10 Ph.D students and 14 Ph.d students are presently undergoing their doctoral studies under his supervision.

KL-2

Cyclometalated Iridium Complexes and Their Biological Aspects

Srikanta Patra*

School of Basic Sciences, IIT Bhubaneswar, Argul, Jatni-752050, Orissa, India
Email: srikanta@iitbbs.ac.in

Cyclometalated iridium complexes have been the point of attraction for the past few decades for their exciting photophysical properties and applications in diverse fields of science and technology. Construction of rationally designed molecular architecture with desired ligand frameworks is crucial to manipulate the energy of the frontier orbitals, tune properties like solubility, biocompatibility, selectivity, stability, etc. In this conclave, we will discuss design and development of various C^N and N^N chelating ligands and their corresponding iridium/ruthenium-based molecular architecture as well as their photophysical properties and biological activities.

Keywords: Iridium, Ruthenium, Benzimidazole, polypyridyl. Anticancer activity,

References

[1] Tripathy S. K., De U., Dehury N., Pal S., Kim, H. S.* and Patra S.* Dalton Trans., 2014, 43: 16597.

[2] Tripathy S. K., De U., Dehury N., Laha P., Panda M. K., Kim, H. S.* and Patra S.* Dalton Trans., 2016, 45: 15122.

[3] Laha P, De U., Chandra F., Dehury N., Khullar S., Kim, H. S.* and Patra S.* Dalton Trans., 2018, 47: 15873.

[4] Mishra S., Tripathy S. K., Paul D., Laha P., Santra M. K.* and Patra S.* Inorg. Chem., 2023, 62: 7003.

[5] Mishra S. and Patra S.* Dalton Trans., 2024, 53: 8214.

Biography:

Dr. Patra is a native from Hooghly District, West Bengal. After graduating from Belur Ramkrishna Mission Vidyamandira, he pursued his masters from MSU Baroda. He then moved to IIT Bombay for his doctoral studies where he did his PhD in Coordination Chemistry under the mentorship of professor Goutam Kumar Lahiri. After completing his PhD, he went to University of Iowa, USA and Pusan National University, South Korea for postdoctoral studies. He joined IIT Bhubaneswar in 2009 and continuing. His primary research interest aims in developing iridium/ruthenium based homo and heterodimetallic systems and exploring their photo(catalytic) and biological aspects.

KL-3
Target-Based Screening, Identification and Optimization of Entry Inhibitors Targeting SARS-CoV-2 Spike–ACE2 Interaction

Dr. Arindam Talukdar*

Organic and Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology (IICB), 4, Raja S. C. Mallick Road, Jadavpur, Kolkata-700032, INDIA

The urgent need for effective antivirals during the COVID-19 pandemic accelerated drug repurposing and screening efforts to identify inhibitors of SARS-CoV-2 entry. In this study, we employed a target-based screening approach focusing on the spike protein's receptor-binding domain (RBD) interaction with the human ACE2 receptor. Screening a curated library of FDA-approved drugs led to the identification of Bazedoxifene, a selective estrogen receptor modulator, and Umifenovir (Arbidol), a known fusion inhibitor, as potent entry blockers with IC_{50} values of 2.0 μM and 9.0 μM, respectively, in SARS-CoV-2-infected cell assays. Both compounds share an indole-based core but differ in key substitution positions, offering a platform for deep structure–activity relationship (SAR) analysis.

Using rational medicinal chemistry, systematic SAR exploration was performed to identify pharmacophores essential for viral entry inhibition. Mechanistic validation through lentiviral pseudovirus assays confirmed their role in entry blockade, while RT-qPCR and immunofluorescence imaging demonstrated suppression of viral replication and spike protein expression. Further lead optimization incorporated ADME screening, in vivo pharmacokinetic profiling, and toxicological assessments, culminating in efficacy studies in a SARS-CoV-2-infected hamster model. The findings provide compelling evidence for Bazedoxifene-derivatives and Umifenovir-based analogs as promising entry-targeted therapeutics with potential to counter current and future coronavirus threats through variant-resilient antiviral strategies.

Keywords: SARS-CoV-2; Entry Inhibitor; Targeted Screening; Rational Design; Optimization

References

[1] Hoque I., Singh N., Dastidar U.G., Martin A.K., Joshi A., Sardana Y., Chawla R., Das N., Patra B., Devi R., Das S., Das D., Ringe R.P., Kumar B.K., Thakur K.G.,* Talukdar A.* **Strategic Design and Optimization of Umifenovir Analogues: Balancing Antiviral Efficacy and hERG Toxicity against SARS-CoV-2**. J. Med. Chem., 2025, (68): 9371-9406. https://doi.org/10.1021/acs.jmedchem.4c03093

Biography:

Dr. Arindam Talukdar is a trained Medicinal Chemist with more than 20 years of research experience. He obtained his Master's degree in Pharmaceutical Chemistry from Panjab University, Chandigarh and PhD degree in Chemistry from the National Chemical Laboratory (NCL), Pune. He spent six years in USA as a postdoctoral fellow and obtained training in glycobiology and various aspects of drug discovery. Thereafter, in 2010, Dr. Talukdar started working in the Industry as a Senior Research Scientist at Albany Molecular Research Inc, Singapore, where he was instrumental as an inventor in the development and validation of first-in-class epigenetic target small molecules from high-throughput screening into the pre-clinical stage. Dr. Talukdar joined CSIR-Indian Institute of Chemical Biology (IICB) in January 2013 and currently, his position is Senior Principal Scientist. His research lab aims to answer fundamental questions at the interface of chemistry and biology to perform rational design, synthesis and validation of novel chemical entities to unravel the molecular mechanism and develop a potential treatment for human diseases. He has a network of collaborations within IICB and other research laboratories in India and internationally.

KL-4
Contrasting Structures in the Art of Electrocatalyst Design

Sayan Bhattacharyya*

Department of Chemical Sciences, and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur - 741246, India

The recent literature is abundant with earth-abundant electrocatalysts that have shown the ability to surpass the noble metal benchmark for driving the redox reactions such as water splitting for green hydrogen generation, carbon dioxide reduction to value added fuels and nitrogen/nitrate reduction to ammonia. A successful architecture of these multi-metallic electrocatalysts relies on the overall electronic structure, optimization of the active centers, elemental ratio, heterogeneous localization of the elements, coordination environment, shape and size of the nanostructures, and the atomic scale defects. However, alloying the metals with dissimilar crystal structures and unmatched crystallographic facets is a non-trivial task. Therefore, an effective multi-metallic catalyst design needs a substantial all-round knowledge of chemistry, especially the branches of basic inorganic chemistry and solid state chemistry, besides electrochemistry. This lecture will highlight a part of our efforts in making the multi-metallic heterogeneous alloys having immiscible lattices of the metal components for water electrolysis,[1-6] CO_2 reduction and nitrate reduction to ammonia. Our electrocatalysts are typically composed of two metals that mutually tune the electronic structure to have a profound impact on the overall catalytic activity.[7-9] The implementation of these systems at the industrial scale will be also mentioned.

Reference

[1] S. Parvin, M. Maji, R. Majee, S. Bhattacharyya, *ACS Catal*. **2025**, *15*, 11818-11851.
[2] S. Mondal, S. Dutta, V. Hazra, S. K. Pati, S. Bhattacharyya, *Nano Lett.* **2025**, *25*, 1296-1304.
[3] M. Maji, S. Dutta, R. Jena, A. Dey, T. K. Maji, S. K. Pati, S. Bhattacharyya, *Angew. Chem. Int. Ed.* **2024**, *63*, e202403697.
[4] S. Mondal, S. Dutta, S. Mal, S. K. Pati, S. Bhattacharyya, *Angew. Chem. Int. Ed.* **2023**, *62*, e202301269.
[5] S. Parvin, N. Bothra, S. Dutta, M. Maji, M. Mura, A. Kumar, D. K. Chaudhary, P. Rajput, M. Kumar, S. K. Pati, S. Bhattacharyya, *Chem. Sci.* **2023**, *14*, 3056-3069.
[6] S. Mondal, R. Saroha, M. Maji, S. Mal, A. K. Mishra, S. Banerjee, S. Bhattacharyya, *ACS Mater. Lett*. **2025**, 10.1021/acsmaterialslett.5c01164.
[7] R. Majee, A. Kumar, T. Das, S. Chakraborty, S. Bhattacharyya, *Angew. Chem. Int. Ed*. **2020**, *59*, 2881-2889.
[8] S. Parvin, A. Kumar, A. Ghosh, S. Bhattacharyya, *Chem. Sci*. **2020**, *11*, 3893-3902.
[9] A. Sahasrabudhe, H. Dixit, R. Majee, S. Bhattacharyya, **2018**, *Nat. Commun*. *9*, 2014.

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Research Interest:

The Advanced Functional Materials Laboratory (AFML) led by Prof. Sayan Bhattacharyya focuses on an interdisciplinary research on functional nanomaterials. The current research interests are: (A) Photovoltaics: Nanocrystal-assisted Metal-halide Perovskite Solar Cells; (B) Electrocatalytic and Photocatalytic Hydrogen Generation, N2 & CO2 Reduction; (C) Zinc-air Battery and Photorechargeable battery.

Academic Background:

- Ph. D. (Solid State Chemistry), Indian Institute of Technology Kanpur (IIT Kanpur), 2006
- M. Sc. (Physical Chemistry), Department of Chemistry (University of Kalyani), 1998
- B. Sc. (Honours) (Chemistry (H), Physics (P), Mathematics (P)), Maulana Azad College (University of Calcutta), 1996

Positions:

- Professor, IISER Kolkata (current)
- Associate Professor, IISER Kolkata (2015 - 2019)
- Assistant Professor, IISER Kolkata (2010 - 2015)
- Postdoctoral Researcher, Drexel Nanotechnology Institute, Drexel University, Philadelphia, PA, USA (2008 - 2010)
- Postdoctoral Fellow, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel (2006 - 2008)

Selected Publications:

- Hazra, Vishwadeepa; Mandal, Arnab and **Bhattacharyya, Sayan**. 2024."Optoelectronic Insights of Lead-free Layered Halide Perovskites." *Chem. Sci.*, 15, 1
- Maji, Mamoni; Dutta, Supriti; Jena, Rohan; Dey, Anupam; Maji, Tapas Kumar; Pati, Swapan K. and **Bhattacharyya, Sayan**. 2024."Hydrogen Evolution in Neutral Media by Differenttial Intermediate Binding at Charge-Modulated Sites of a Bimetallic Alloy Electrocatalyst." *Angew. Chem. Int. Ed.*, 63, e202403697

KL-5

Bio-inspired Wettability to Derive Functional Interface

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The nature-inspired wettabilities that either extremely repelled or allowed effortless sliding of different liquids (oil/water) in air or underwater are with immense potential for various prospective applications. In common practice, essential chemistry and appropriate topography
that conferred the special liquid wettabilities were mostly and generally achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issues. In the literature, very few designs are capable of providing durable bio-inspired wettability—but fabrication processes remain generally complex. Moreover, the integration of various other
relevant physical properties with such durable liquid wettability is highly challenging to achieve. Hence, design of robust bio-inspired liquid wettability following a simple fabrication process that would allow to integrate different and relevant physical properties is utmost important for various fundamental and applied contexts. Related to this, recently, our research group has extended 1,4-conjugate addition reactions between amine and acrylates at ambient conditions to develop tolerant and functional liquid wettability.[1-10] The controlled tailoring of different bio-inspired liquid wettability from the chemically reactive interfaces (either porous or smooth)—following strategic post modulation of the chemically reactive interfaces will be discussed in this invited lecture. A strategic association of adequate crosslinkers can provide a highly tolerant and hard superhydrophobic coating on geometrically complex and soft materials. Such a simple chemical approach also allowed to reveal important fundamental aspects related to different bio-inspired wettability. In this presentation, design of a rewritable and liquid-selective wettability pattern will be discussed in details.[3]

Keywords: Bio-inspired wettability, chemically reactive coating, pattern interface, 1,4-conjugate addition reaction, slippery property

References

1. Mishra, C.; Sarkar, D.; Barman, N.; Kumar, S.; Tenjimbayashi, M. and Manna, U.* *Adv. Mater.*, 2025, In Press.
2. Sarkar,D.; Kara, U. I.; Singh, R.; Phukan, A.; Mondal, P.; Paily,R. P. Wang, X. and **Manna U.*** *Adv. Func. Mater.*, 2**024,** 2419049.
3. Dhar, M.; Sarkar, D.; Das, A.; Rahaman, S. K. A.; Ghosh, D. and **Manna, U.*,** *Nature Communications,* **2024***, 5838.*

Biography:

Prof. Uttam Manna, Fellow of Royal Society of Chemistry (FRSC), is currently a professor at Department of Chemistry—and also affiliated with Centre for Nanotechnology in Indian Institute of Technology, Guwahati (IITG). He completed his Integrated PhD from IISc Bangalore in 2011. He pursued his post-doctoral research from University of Wisconsin-Madison, USA. He is recognized as an emerging investigator by Journal of Materials Chemistry A (2018), Chemical Communications (2020), Nanoscale (2021) and Chemical Society Reviews (2022). In 2023, Chemical Communications journal also recognized him as a pioneering investigator. He received the CRSI Bronze Medal for the year 2023. He is also a recipient of the Humboldt Research Fellowship for Experienced Researchers in 2021. He became International Excellent Fellow of KIT,
Germany in 2024.

https://uttammannaiitg.wixsite.com/polymericlab

summary of your research interests

His research team is interested in designing functional and durable coatings embedded with bio-inspired wettability through the strategic association of robust and facile chemical approaches for energy, environment and health related different applications— including efficient oil/water separation, improving performance of water splitting, self- cleaning, chemical sensing, programmed release of small molecule, anticounterfeiting, no-loss liquid transport, strain sensing, joule heating etc.

KL-6

Metal–Drug Conjugates: Rediscovering the Dual Roles of Metal Ions as Therapeutics and Delivery Vehicles in Cancer Therapy

Rakesh Kumar Pathak*

Department of Chemical Sciences, Indian Institute of Science Education and Research Berhampur, Odisha India.

Metal ions are indispensable regulators of biological function, with catalytic and homeostatic roles governed by reversible coordination to proteins and small biomolecules. Inspired by this natural use of metal-binding "cargos", we exploit metal ions as modular scaffolds to construct metal–drug conjugates (MDCs). Because metal ions support variable coordination numbers and geometries, they can host multiple drug ligands, and judicious control over metal–ligand bond lability enables site-specific, bioorthogonal release of one or more active payloads. In this lecture, I will conceptually distinguish two often conflated classes of metal-derived therapeutics: (i) metal-based drugs, in which kinetically inert complexes act as the primary pharmacophore, and (ii) MDCs, in which more labile metal–drug bonds are deliberately designed to cleave under defined biological or stimulus conditions. I will discuss how systematic stability studies inform whether a given complex should be developed as a stand-alone metal drug or as a drug-delivery platform. I will further highlight the dual roles of metal ions within MDCs: as active therapeutic centres or as nominally "innocent" carriers. In both cases, auxiliary drugs/bioactive molecules/prodrugs can be coordinatively attached, enabling activatable, combination therapy from a single, well-defined scaffold. This strategy directly addresses the pharmacokinetic and bio-distribution mismatches that hinder conventional co-administration of free drug cocktails. Using Zn^{2+}, Co^{3+} and Pt^{2+}/Pt^{4+} platforms conjugated to bioactive molecules such as gossypol, probenecid and chrysin, etc., I will showcase how rational MDC design modulates potency versus toxicity in vitro and in vivo. Finally, I will present recent data demonstrating that selected MDCs and their nanoformulations can also engage innate immune pathways, opening avenues for integrated chemo-immunotherapeutic interventions in cancer.

Keywords: Metal–drug conjugates, Coordination chemistry, Combination therapy, Chemo-immunotherapy, Drug Delivery.

References

1. Arora, K.; Sheehy, T.; Schulman, J.; Loken, J.; Lehmann, Z.; Kimmel, B.; McAtee, C.; Bharti, V.; Stone, P.; Weaver, A.; Tyska, M.; **Pathak, R. K.**; Wilson, J. T.* *"Macromolecular Diamidobenzimidazole Conjugates Can Activate Stimulator of Interferon Genes*." **J. Am. Chem. Soc. 2025**, 147, 38, 35149–35163.
2. Shukla, P.#; Choudhury, K. K.#; Kajol, Behera, S.; Panigrahy, J.; **Pathak, R. K.*** "*Development of a Tumor Microenvironment-Responsive Co(III)-Chrysin Prodrug: Synthesis, Activation Profiling, and In Vitro Antineoplastic Evaluation*" **ChemMedChem 2025**, 20, e202500232.https://doi.org/10.1002/cmdc.202500232.
3. Bose, S.; Saha, P.; Alam, M. T.; Chatterjee, B. Sarkar, M.; Dixit, A.; Kumar, D.; **Pathak, R. K.**; Tripathi, P.' Srivastava, A.* "*Inhibition of DNA polymerase eta mediated translesion DNA synthesis with small molecule sensitizes ovarian cancer stem-like cells to chemotherapy*" **British. J. Pharmacol. 2025**, 1–18. https://doi.org/10.1111/bph.70037.
4. Biswas, M.; Chaudhary, K.; Padhi, S. S.; Banerjee, A.; Bharathavikru, R. S. Bandaru, S.; Panda, S. J.; Purohit, C. S.; Das, N. R.; and **Pathak, R. K.***.; "*TTFA-Platin Conjugate: Deciphering the Therapeutic Roles of Combo-Prodrug through Evaluating Stability–Activity Relationship*" **J. Med. Chem., 2024**, 67, 23, 20986–21008. DOI: 10.1021/acs.jmedchem.4c01545.

Biography:

Name Rakesh Kumar Pathak, Ph.D.
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Career Profile

Dr. Pathak earned his Ph.D. from the Indian Institute of Technology Bombay (2006 to 2011), focusing on the synthesis and bio-interaction of calix[4]arene, a protein/enzyme mimic supramolecular system, in a pathological context under the guidance of Prof. C.P. Rao. Afterward, he joined the Nanotherapeutic Lab at the University of Georgia as a postdoctoral fellow, contributing to design, synthesis, and therapeutic applications of prodrugs, polymeric NPs, and mitochondria-targeted formulations for treating various cancers. In 2015, Dr. Pathak joined the Ohio State University and received the prestigious Pelotonia Postdoctoral Fellowship. This fellowship facilitated his transition from a postdoc fellow to an independent researcher. In 2017, he became an Assistant Professor in the Department of Chemical Sciences and is currently working as Associate Professor at IISER Berhampur, where he is currently establishing a Laboratory of Biological Inorganic Chemistry and Nanomedicine. Dr. Pathak's research focuses on the convergence of synthetic chemistry, biology, and nanotechnology within the broader realm of traditional bioinorganic chemistry.

Significant awards/achievements

- (2016) Pelotonia Postdoctoral Fellowship awarded by The James Comprehensive Cancer Centre The Ohio State University USA.
- (2018) Ramanujan Fellowship Awarded by the DST-SERB-2018-2023.
- (2019) Early Career Research Award by DST-SERB India (ECRA-2019)
- (2024) ICMR-DHR international Fellowship (ICMR-DHR-2024)

KL-7
Sustainable Chemical Production via Catalytic Dehydrogenation

Ekambaram Balaraman*

[1] Department of Chemistry, Indian Institute of Science Education and Research (IISER) Tirupati, Tirupati-517619, Andhra Pradesh, India.

[2] DST-Nodal Center for APIs and KSM production under the Therapeutic Chemicals Program, IISER-Tirupati, Tirupati-517619, Andhra Pradesh, India.

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 α-branched aryl ketone derivatives, achieving zero waste via an umpolung borrowing hydrogen technique. Additionally, the study showcases the versatile applications of the resulting α-di-substituted ketones as precursors for other valuable compounds, including the large-scale production of β-deuterated branched ketones.

Keywords: Nickel, Dehydrogenative coupling, Branched ketones, Deuteration, Mechanistic insights

References

[1] Subaramanian, M., Gouda, C., Roy, T. K., Sivakumar, G., Banerjee, S., Vanka, K., Balaraman, E. ACS Catal., 2024, (11), 8294.

[2] A Process for the Preparation of Selective β-Deuterated Branched Ketones. Subaramanian, M., Gouda, C., Balaraman, E. PCT/IN2025/050720 (06 May 2025).

Biography:

Dr. E. Balaraman received his Ph.D. from the University of Hyderabad and subsequently served as an FGS-Postdoctoral Fellow at the Weizmann Institute of Science. In July 2013, he began his independent career as a Senior Scientist at CSIR-NCL, Pune. In Dec'2018, he joined IISER Tirupati as a faculty member in the Department of Chemistry. Balaraman's research focuses on the design and development of catalytic materials for hydrogen generation from feedstocks, sustainable chemical synthesis, and the conversion of CO_2 into value-added productss.

KL-8
Biomimetic Studies on Metal Detoxification

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Methylmercury (Me–Hg^{+}) is a potent neurotoxin that bioaccumulates in seafood, posing serious health risks. Another organomercurials of concern is ethylmercury (Et–Hg^{+}), commonly used in the form of Thimerosal in vaccines. Certain microbes have evolved detoxification strategies against these toxic species. Bacterial lyase MerB catalyzes the cleavage of the Hg–C bond of R–Hg^{+}, releasing CH_4 and Hg^{2+}, which is then reduced to volatile elemental Hg^0 by MerA, completing the detoxification process. On the contrary, arsenic–a widespread environmental toxin and human carcinogen–is detoxified via enzymatic methylation rather than demethylation. The enzyme **ArsM** (in microbes) or **AS3MT** (in animals) catalyzes the stepwise methylation of arsenite (iAs^{III}) using **SAM** as a cofactor, producing less toxic species such as $DMAs^{V}$ and $TMAs^{V}$. Although significant progress has been made in understanding **ArsM-mediated arsenic methylation**, key mechanistic questions remain. Notably, ArsM enzymes from diverse organisms, differing in size and sequence, show variable methylation efficiencies, pointing to structural and functional diversity.

These natural detox pathways have inspired **biomimetic strategies** for remediating environmental pollutants by mimicking natural enzymes. In this talk, we will discuss the development of synthetic organo-chalcogens for the detoxification of organomercurials and inorganic arsenic.

Keywords: Methylmercury, Organomercurial Lyase (MerB), Arsenic, As^{III} SAM Methyltransferase

References:

[1] Rai, R. K.; Islam, A.; Pati, R, S.; Roy, G* *Chem. Eur. J*., **2025**, 31, e202403483.
[2] Das, R.; Karri, R.; Chalana, A.; Roy, G* *Inorganic Chemistry*, **2024**, 63, 10455.
[3] Karri, R.; Das, R.; Rai, R. K.; Gopalakrishnan, A.; Roy, G* *Chem. Comm.* **2020**, 56, 9280.
4. Banerjee, M.; Karri, R.; Rawat, K. S.; Muthuvel, K.; Pathak, B.; Roy, G.**Angew. Chem. Int. Ed.,* **2015**, 54.

Biography:

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Education & Professional Experience

Jan2020-	**Professor**, Department of Chemistry, IIT Tirupati, Tirupati, A.P.
Jan2020–Dec 2023	**Associate Professor**, Dept. of Chemistry, IIT Tirupati, Tirupati, A.P.
July 2018–Jan 2020	**Associate Professor**, Shiv Nadar University, U.P.
Nov2012 – June 2018	**Assistant Professor**, Shiv Nadar University, UP.
Nov2011–Sept2012	Research Associate, The Scripps Research Institute, San Diego.
Jan2008–Nov2011	Postdoctoral Fellow, Dept. of Physiology and Pharmacology, Oregon Health and Science University, Oregon, USA.
Aug2002–Oct2007	Ph.D, IPC, IISc, Bangalore, India.

Research

Research in our laboratory mainly focuses on two major areas, chemistry, and biology, at the interface of chemistry and biology. Our laboratory is involved in the chemical detoxification of various toxic heavy metals such as mercury, arsenic, and copper. Organomercurials are highly neurotoxic environmental pollutants that preferentially accumulate in the glia of the central nervous system. Thus, the detoxification of organomercurials is of critical importance. On the other hand, copper ion is essential in our lives and used as a cofactor in several vital processes. However, high concentrations of copper can be harmful as they promote Fenton-like reactions, thereby increasing the cellular ROS levels and leading to the oxidative damage of cellular constituents like proteins, lipids, and nucleic acids. Thus, it is essential to control copper concentration strictly in the body. We aim to understand how methylmercury, an extremely neurotoxic organomercurial, exerts its neurotoxicity and try to understand the detoxification pathways in the biological system. Our research group focuses on understanding the homeostasis of essential metals and the detoxification pathways of toxic heavy metals in the cellular system.

Representative Publications:

Inorg. Chem., **2025**, xx, xxxx; *Inorg. Chem.*, **2025**, 64, 18206; *Chem. Eur. J.*, **2025**, 31, e202403483; *Inorg. Chem.*, **2024**, 63, 10455; *J. Agric. Food Comm.* **2022**, 70, 9730; *Chem. Comm.* **2020**, 56, 9280; *Chem. Eur. J.*, **2019**, 25, 12810; *Inorg. Chem.*, **2019**, 58, 6628; *ACS Appl. Mater. Interfaces*, **2019**, *11*,

KL-9

Biography:

Dr. Chithirai Pon Selvan

Director – Research
Head of Faculty
Head of School – Science and Engineering

Professor Chithirai Pon Selvan has extensive experience in teaching engineering students and has worked in academia for over twenty-three years. He has published/presented more than 150 research articles in journals and conferences. He has been invited and honoured as keynote speaker, session chair, resource person, and technical committee member of various conferences held in UAE, India, Thailand, Malaysia, Germany, Italy, Australia, and the UK. His research interests are in the areas of machine design, optimization techniques, manufacturing practices, renewable energy, and engineering sustainable development. He is the approved supervisor of many universities including Curtin University, Australia to guide PhD scholars and has produced many PhDs. He is a member of many professional societies including SAE, ASHRAE, IMechE, ASME, EI, ASQ, and ISTE. He is also a Senior Fellow of the Higher Education Academy (SFHEA), UK.

Prof Pon has received several prestigious awards in the UAE including the following.

- "Teaching Excellence Award (2013-2014)" from Manipal University, Dubai.
- "Dubai Award for Sustainable Transport (2017)" from Road Transport Authority (RTA), Govt. of Dubai.
- "Dr Kalam's International Excellence Award for Education (2017)" from Dr APJ Abdul Kalam Lovers Foundation, UAE.
- "Distinguished Conservation Project Award (2018)" from Dubai Electricity and Water Authority (DEWA), Govt. of Dubai.
- "Alleem Sustainability Researcher Award (2018)" from Alleem Research and Development Centre, Sharjah.
- "Sustainability Ambassador Award (2019)" from Road Transport Authority (RTA), Govt. of Dubai.
- "Research Excellence Award (2020)" from Curtin University, Dubai.
- "TAG Founders Award – Academic of the Year (2021)" from Transnational Academic Group (TAG), Dubai.
- "Curtin Global Award (2022)" from Curtin Global, Curtin University.

Prior to joining Curtin University Dubai in July 2018, he served for 10 years in the UAE with Manipal University Dubai and Amity University Dubai.

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Invited Lecture- IL

IL-1

Nitrate/Nitrite Reduction to Nitric Oxide: A Biomimetic Modelling and Mechanistic Investigation

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Nitric oxide (NO) plays a crucial role in various physiological processes, including neurotransmission, vascular regulation, platelet aggregation, and immune response to multiple infections.[1] Therefore, to maintain an optimal concentration of NO, nitrate reductase (NR), nitrite reductase (NiR)[2], and NO synthase (NOS)[3] enzymes are available for NO biosynthesis. If overproduced, NO Dioxygenase (NOD) enzymes convert NO to biologically benign NO_3^-. The reductive process of NO biosynthesis begins with NR, which catalytically transforms NO_3^- to NO_2^- via the O-atom transfer (OAT) reaction using Mo/W-based enzymes. Meanwhile, NiR enzymes catalyze the conversion of NO_2^- to NO in the presence of acid (H^+).[2] Here, we will explain the reduction of NO_2^- to NO via acid-induced reaction on Co/Fe/Cu centers.[4] A new pathway for NiR enzyme activity was observed with one equivalent proton (H^+) generating M-NOs (or NO generation) with H_2O_2 (which further decomposes to H_2O). Also, VCl_3-induced NO_3^-/NO_2^- reduction was confirmed on the Co-center.[5] In addition, we will also be presenting the NO oxidation reaction of {CoNO}^{8} to understand the mechanistic aspects of base-induced NO mono-oxidation to NO_2^- with H_2 evolution.[6]

Keywords: Nitrite Reductase; Nitrate Reductase; NO Oxidation; O-atom Transfer

References

1) (a) R. F. Furchgott, *Angew. Chem., Int. Ed.*, 1999, **38**, 1870-1880. (b) L. J. Ignarro, *Angew. Chem., Int. Ed.*, 1999, **38**, 1882-1892.
2) E. I. Tocheva, F. I. Rosell, A. G. Mauk, M. E. Murphy, *Science*, 2004, **304**, 867-870.
3) R. G. Knowles, S. Moncada, *Biochem. J.*, 1994, **298**, 249-258.
4) (a) P. Y. M. Ajmal, S. Ghosh, Y. Narayan, Y. Yadav, C. S. Sahoo, P. Kumar, *Dalton Trans.*, **2019**, 48, 13916. (b) Kulbir; Das, S.; Devi, T.; Ghosh, S.; Sahoo, S.; Kumar, P.* *Chem. Sci.*, 2023, 14, 2935-2942 (c) Bhardwaj. P.; Kulbir; Devi, T.*; Kumar, P.* *Inorg. Chem. Front.,* **2023**, *10*, 7285-7295
5) K. Kulbir, S. Das, T. Devi, M. Goswami, M. Yenuganti, P. Bhardwaj, S. Ghosh, S. C. Sahoo, P. Kumar, *Chem. Sci.,* **2021***, 12*, 10605.
6) S. Das, K. Kulbir, S. Ghosh, C. S. Sahoo, P. Kumar, *Chem. Sci.,* **2020***, 11,* 5037.

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Dr. Pankaj Kumar Koli completed his Ph.D. in 2013 from the Indian Institute of Technology, Guwahati. He was a WCU Postdoctoral fellow at the Center for Biomimetic Systems, Department of Chemistry and Bioinspired Science, Ewha Womans University from 2013-2016. In 2017, he joined M. M. University, India, to work as an assistant professor in the Department of Chemistry from 2016-2017. In the same year, he started his independent career at IISER Tirupati. Presently, he has been an associate professor at the institute since 2023. Dr. Koli works on intermediates biologically important small molecule activation, i.e., O_2, NO, CO, CO_2, and H_2S, etc., with transition metal ions to mimic in-vivo enzymatic systems responsible for various biological reactions and working to develop the probes for their detection. Also, he is working on biomimetic modeling and intermediates mimic and stabilize, i.e., Metal-Oxo /-Peroxo /-Superoxo, Metal-Nitrosyl, and Metal-Carbonyl. His research experience helped him to secure several research grants from SERB (3), GAIL, AvH (Humboldt Experienced Research Awards, 2021-2024), DAAD (Experienced Research Award, 2021), and also mentoring a project for WISE-DST Scientist (2024-2027).

Selected Publications:

J. Am. Chem. Soc., **2025**, *147,* 36442
J. Am. Chem. Soc., **2024**, *146*, 21729
Chem. Sci., **2023**, *14*, 2935
Inorg. Chem. Front., **2023**, *10*, 7285-7295
Chem. Sci., **2022**, *13*, 1706
Chem. Sci., **2021**, *12*, 10605
Chem. Sci., **2020**, *11*, 5037
Inorg. Chem. Front., **2020**, 7, 4872-4882.
Dalton. Trans., **2019**, 48, 13916.
Angew. Chem. Int. Ed. **2016**, *55*, 12403
J. Am. Chem. Soc., **2016**, *138*, 7753
J. Am. Chem. Soc., **2015**, *137*, 4284
J. Am. Chem. Soc., **2010**, *132*, 7846
Dalton. Trans., **2019**, 48, 13916.

IL-2

Development of Sustainable Methods; from Plastic to Fine Chemicals

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Abstract: Plastic waste poses a significant challenge to achieving a sustainable future, highlighting the urgent need for innovative approaches to convert it into value-added products. Current recycling methods are limited. The mechanical recycling often results in downgraded materials, and chemical processes typically require high energy input and expensive, precious-metal catalysts.[1] Our research group is dedicated to developing sustainable catalytic strategies for the upcycling of plastic waste, particularly polyolefins. While iridium-based systems for the dehydrogenative degradation of polyethylene are well established, their reliance on precious metals presents economic and environmental drawbacks.[2] To address, we have developed a ruthenium-catalyzed dehydrogenation approach based on hydrogen atom transfer (HAT), enabling efficient functionalization of polyolefins. The dehydrogenated polymers were further transformed into long-chain alkenes via controlled metathesis, yielding valuable chemical feedstocks. Building on this foundation, we further explored the use of earth-abundant 3d transition metals and successfully developed a copper-catalyzed dehydrogenation strategy. This method effectively overcomes the drawbacks associated with precious metal catalysts and enables scalable, one-pot, and cascade transformations. Importantly, our protocol has been validated on real-world plastic waste, demonstrating its potential for practical application in the sustainable production of high-value chemical feedstocks.

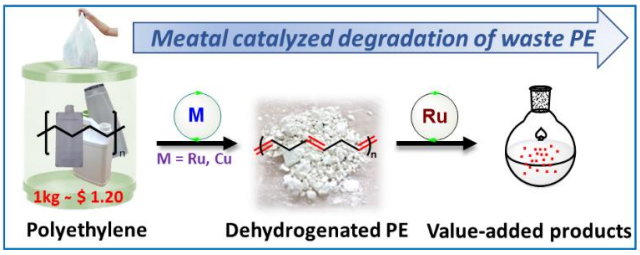

Figure 1. Transition metal catalyzed degradation of polyethylene to value added products.

Keywords: Metal catalysis, degradation, postconsumer polyethylene, upcycling, waste polyethylene, linear aliphatic di-aldehydes and alkenes

References:

[1] Khopade, K. V.; Chikkali, S. H.; Barsu, N. *Cell Reports Physical Science* **2023**, 4, 101341.
[2] Sun, J.; Dong, J.; Gao, L.; Zhao, Y.-Q.; Moon, H.; Scott, S. L. *Chem. Rev.* **2024**, 124, 9457–9579.
[3] Padhi, G.; Khopade, K. V; Moyilla, N.; Rangappa, R.; Chikkali, S. H.; Barsu, N. *Angew. Chemie Int. Ed.* **2025**, 64, e202422609.
[4] Padhi, G.; Moyilla, N.; Purohit, P.; Barsu, N. Submitted **2025** (*under review*).

Biography:

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Dr. Nagaraju Barsu obtained his M.Sc. in Chemistry from Banaras Hindu University in 2012. He then pursued his Ph.D. at the Indian Institute of Technology Kanpur (IIT Kanpur) under the guidance of Prof. Dr. Basker Sundararaju, completing it in 2019 with a specialization in organometallic chemistry and catalysis. In the same year, he joined the Max-Planck-Institut für Kohlenforschung in Germany as a postdoctoral researcher with Prof. Dr. Alois Fürstner, where he continued his research until 2021. He is currently serving as a Senior Scientist at CSIR–National Chemical Laboratory in Pune, Maharashtra.

Awards/Fellowships

1. Awarded the ECRG grant from ANRF
2. Selected for the prestigious Ramanujan Fellowship
3. Max Planck Group Fellowship for postdoctoral research
4. Selected as young scientist to participate in prestigious 67th *Lindau Nobel Laureate Meeting.*

IL-3

Bio-inspired Transition Metal Complexes for Solar Fuel Generation

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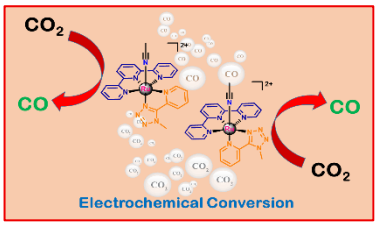
Rapid globalization of the 21st century has urged the scientific community to transcend current exhaustible fossil fuel sources and consider clean and sustainable alternatives. One of the central issues involved in scalable solar energy conversion to meet future energy demands is the direct conversion of solar radiation into chemical substances that can be easily stored, transported, and converted to energy on demand. Artificial photosynthesis is often proposed as a promising substitute for solar energy harvesting by mimicking the essential aspects of natural processes. Therefore, the target reactions are the sunlight-driven splitting of water into molecular oxygen and hydrogen; and light-driven CO_2 to CO reduction or other reduced forms of carbon. The principles of designing transition metal-based redox catalysts for solar fuel production, the development of new, effective, and rapid molecular catalysts for the reduction of CO_2 and the advancement of electrochemical and photoelectrochemical cells in practical devices will be covered in this talk. The detailed mechanistic investigation of the catalytic cycle by properly characterizing potential intermediates for understanding the model systems is to be discussed. Simultaneously, scrutiny of the interplay between steric and electronic effects caused by strategic ligand modifications determining the complexes' reactivities will also be addressed.

Keywords: Sustainable Energy, Bioinspired Catalysis, Carbon Dioxide Reduction, Reaction Mechanisms



References

1. D. Z. Zee, T. Chantarojsiri, J. R. Long, C. J. Chang, Acc. Chem. Res. 2015, 48, 2027-2036.
2. H. Takeda, C. Cometto, O. Ishitani, M.Robert, ACS Catal. 2017, 7, 70– 88.
3. B. A. Johnson, H. Agarwala, T. A. White, E. Mijangos, S. Maji and S. Ott, Chem. Eur. J., 2016, 22, 14870–14880.
4. B. Giri, A. Mahata, T. Kella, D. Shee, F. De Angelis, S. Maji, J. Catal. 2022, 405, 15-23.

Biography :

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Dr Somnath Maji is currently Associate Professor in the Department of Chemistry, IIT Hyderabad. He obtained his B.Sc. and M.Sc. degrees from the University of Burdwan and earned his Ph.D. from IIT Bombay under the supervision of Prof. G.K. Lahiri. Before joining IIT Hyderabad, he was a postdoctoral fellow at ICIQ, Spain working with Prof. Antoni Llobet and Uppsala University, Sweden working with Prof. Sascha Ott. His research focuses on Synthetic Coordination/ Bio-Inorganic/ Organometallic Chemistry. Small molecule activation/ DNA Binding/ Cleavage/ Anti-Cancer Activities / Designed Photoactive Transition Metal Nitrosyl for site-specific NO delivery /Metal catalyzed Water Splitting/ Carbon Dioxide Reduction/ Hydrogen Generation for solar fuel production.

IL-4
Twist, Transfer, and Triplets: Tailoring Molecular Luminescence through Quantum-Chemical Approaches

Pandiselvi Durairaj, Sunandan Sarkar*
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This lecture presents a computational perspective on how molecular conformation and strategic functionalization govern excited-state properties in organic molecules using time-dependent density functional theory (TD-DFT). We explored the PTZ-DBPHZ-PTZ (D–A–D) triad, where conformational twisting of donor units induces a transition from locally excited to charge-transfer character in the S_1 state, enabling multicolor luminescence and thermally activated delayed fluorescence (TADF). Rate constant analysis revealed that axial–axial conformers favored prompt fluorescence, while equatorial–equatorial conformers exhibited efficient triplet harvesting via multi-resonant reverse intersystem crossing (*r*ISC).

Moreover, we investigated halogenated perylenes to elucidate how heavy atom substitution and π-system distortion influence ISC. Bromine at the *bay* position induced π-twisting, enhanced spin-orbit coupling (SOC), and accelerated ISC, leading to fluorescence quenching. In contrast, *ortho* and *peri* substitutions preserved planarity, suppressed SOC, and maintained strong emission. Multi-brominated systems with *bay* distortion exhibited ISC rates up to 10^{11} s^{-1}, highlighting that heavy atom effects are maximized by π-distortion. These findings provided mechanistic insights and computational design principles for metal-free organic optoelectronic materials.

Keywords: Fluorescence, Intersystem Crossing, Spin-Orbit Coupling, TADF, TD-DFT

References

[1] Pandiselvi Durairaj, Kiruthika Samuthirapandi, and Sunandan Sarkar. A First-Principles Investigation of Structure-Luminescence Activity of Donor−Acceptor−Donor Organic Triad, J. Phys. Chem. A, 2023, (127): 3330−3338.

[2] Pandiselvi Durairaj, Durga Mukkonathil, and Sunandan Sarkar. Heavy Atom at Bay of Perylene Significantly Improves Intersystem Crossing, J. Phys. Chem. A, 2024, (128): 10193−10201.

Biography :

Dr. Sunandan Sarkar is an Assistant Professor in the Department of Chemistry at the National Institute of Technology, Tiruchirappalli (2018 onwards). He leads the PCESMLab, focusing on physical, theoretical, and computational chemistry with a strong emphasis on electronic structure theory. Their research deals with electronic, optical, and transport properties of semiconductor nanostructures, carbon nanostructures, and related nanoscale systems for light-harvesting and light-emitting applications. Dr. Sarkar earned his Ph.D. from Visva-Bharati in 2014 and has held postdoctoral fellowships at RCPTM, Palacký University during 2014-15 (Czech Republic) and Kent State University during 2016-18 (USA). He has authored 48 publications and maintains active collaborations across interdisciplinary domains.

IL-5
Mechanochemistry: An Opportunity to do disorder Engineering in Metal Organic Frameworks

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Mechanochemical synthesis exhibits enormous potential for the clean, economic, environmental-friendly and efficient route for the structural transformation of molecules and materials. Our recent work based on an attempt to design and synthesis of new phase pure Metal Organic Framework (MOF) materials by solid state hand grinding or ball mill method. Additionally, our research group also focused to do the ball mill induced mechanical engineering on the various MOFs to acquire new type of structures with unique properties. These types of approach are very rare and not attempted earlier in this area of research.

We have developed a unique series of pure phase MOFs (ZnTIA-1mc, CuTIA-1mc and CoTIA-1mc) synthesized exclusively by mechanochemical (mc) grinding method (Figure 1). The same synthesis was also attempted in each case by using solvothermal procedure, which result the phase impure mixture of two different MOFs crystals. Kinetics study with the function of grinding time during the mechanosynthesis process revealed that the formation of variety of new metastable phases. Less crystallinity and short of mechanical defects in the structure of synthesized mechanochemical MOFs showed enhanced electrocatalytic activity towards oxygen evolution reaction (OER).

In our next work, a novel zeolitic tertrazolate framework (ZTF-8) has been synthesized by green and facile mechanochemical ball mill method with exceptional acid/base stability. The structure of ZTF-8 adopts the zeolitic sodalite (SOD) topology with uncoordinated N-heteroatom sites and resembles with the structure of the well-known zeolitic imidazole framework ZIF-8. Directly used ZTF-8 is the unique report among all the MOFs for the selective electrochemical sensing of dopamine (DA) in the presence of highly concentrated common interferents. Additionally, ZTF-8 electrochemical sensor is the best among all the MOFs in terms of its ability to detect DA in a very wide linear range (5-550 μM) of concentration with excellent sensitivity. DFT study, strongly support our experimental result, revealed that the ZTF-8 framework has a higher binding energy and stronger interaction with dopamine than its isostructural ZIF-8 structure.

Keywords: Metal Organic Frameworks, Solid Solutions of MOFs, Electrocatalysis, Photocatalysis, Sensing and Separation.

References

1. A. Warrier, P. Jhariat, M.Varghese, Tamas Panda, Small, 2025, 36, e06837
2. P. Jhariat , A. Warrier, M.Varghese, Tamas Panda,J. Mater. Chem. A, 2025,13, 23893-23901

Biography:

Dr. Tamas Kumar Panda is an Assistant Professor of Chemistry at VIT Vellore, India. He obtained his Ph.D. in Chemistry from CSIR–NCL Pune in 2014 under Prof. Rahul Banerjee, followed by prestigious postdoctoral fellowships at Kyoto University, Japan (JSPS, 2014–2016) under Nobel Laureate Prof. Susumu Kitagawa, and New York University Abu Dhabi (2016–2018) under Prof. Pance Naumov. During his doctoral studies, he was trained in X-ray crystallography and carried out advanced investigations on Metal–Organic Frameworks (MOFs) for selective carbon dioxide and hydrogen storage. His postdoctoral work further advanced the field by introducing a mechanochemical approach for creating solid solutions of MOFs, pioneering an eco-friendly and industrially scalable method for incorporating bifunctionality.

At VIT, Dr. Panda leads a research group dedicated to the design and synthesis of porous frameworks such as Metal–Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), and Covalent Triazine Frameworks (CTFs) for applications in energy conversion, electrocatalysis, and environmental remediation. His group has demonstrated enhanced triboelectric nanogenerator (TENG) performance using novel nitrogen-rich ZTF-8, developed core–shell MOF nanoarchitectures for humidity sensing, and reported novel viologen-based ionic COFs as a bifunctional electrocatalysts for oxygen reduction, oxygen evolution, and hydroxide conduction.

Dr. Panda has authored 40 publications (h-index 20, >1700 citations), filed two patents, secured national research funding (SERB, CSIR), and received multiple awards for research excellence. He has delivered invited talks internationally, nationally and actively contributes to academic workshops and conferences.

IL-6
Selective Antibacterial activity of Functionalized Nano-antibiotics

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Developing material-based antibiotics can be the most potent alternative due to the increasing resistance against conventional antibiotics. However, one of the important parameters in the development of antibacterial agents is Gram/strain selectivity, which is seldom explored in the case of nano-antibiotics. The multimodal action of surface-functionalized nanomaterials can exhibit strain-selective and enhanced antibacterial activity. Two-dimensional MoS_2 nanosheets (2D-MoS_2) have been widely used in many biological applications due to their distinctive physicochemical properties. In the past, it was theorized that chemically exfoliated MoS_2 can be modified using thiol chemistry. In this regard, we provided the first experimental evidence for this process using a facile solution-based method. By chemically engineering the ligands, we then showed the ability to modulate the surface of the MoS2 sheets. In doing so, we have developed several strategies to demonstrated the ability to tune the surface of the conjugates for selective enzyme targeting, inhibition, and antibacterial activity. Those strategies are based on different proportions of positively and negatively charged functionalized ligands, tethered amino acids/peptides, conjugation of Ni-nanocluster, photo-controlled gating of selective bacterial membrane interaction, etc. Taken together, we have prepared simple and efficient Gram-selective 2D-MoS_2-based antibacterial agents, which can also be extended to other systems with antimicrobial properties.

Keywords: Functionalized nanomaterials, Nano-antibiotics, TMDs, Gram-selectivity

References

1. Pandit, S.; Karunakaran, S.; Boda, S. K.; Basu, B.; De, M. ACS Appl. Mater. Interfaces **2016**, *8*, 31567-31573.
2. Karunakaran, S.; Pandit, S.; Basu, B.; De, M. *J. Am. Chem. Soc.* **2018**, *140*, 12634-12644.
3. Bhattacharyya, S.; Ali, S. R.; Venkateswarulu, M.; Howlader, P.; Zangrando, E.; De, M.; Mukherjee, P. S., *J. Am. Chem. Soc.* **2020**, *142*, 18981-18989.
4. Sahoo, J.; Sahoo, S.; Subramaniam, Y.; Bhatt, P.; Rana, S.; De, M., *Angew. Chem. Int. Ed.* **2024**, *63*, e202314804.
5. Kaur, N.: De, M. *ACS Infect. Dis.* **2024**, *11*, 249-261.
6. Solra, M.; Jaiswal, K.; Srivastava, A.; Mishra, S.; Kamra, A.; De, N.; Rana S. *Adv. Healthc. Mater.* 2025, 2500835.

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Mrinmoy De is an associate professor at the Department of Organic Chemistry at the Indian Institute of Science, Bangalore, India. He completed his BSc degree from Vidyasagar University with Gold medal. He received his M.Sc. from the Indian Institute of Technology, Bombay, and Ph.D. from the University of Massachusetts at Amherst under the supervision of Prof. Vincent M. Rotello. He was a CCNE (Center of Cancer Nanotechnology Excellence) and NSEC (Nanoscale Science and Engineering Center) postdoctoral fellow at Northwestern University. Since 2014, he has been at the Indian Institute of Science, Bangalore, where he is an associate professor in the Department of Organic Chemistry. His research focuses on the preparation of various nanomaterials and their application toward the development of biomaterials, nanoantibiotics, nanozymes, sensors, photocatalysis etc. Mrinmoy De is the associate member of American Material Research Society (MRS), American Chemical Society (ACS), Material Research Society of India (MRSI), Chemical Research Society of India (CRSI) and Society of Biological Chemists, India (SBCI). He is recipient of Young Scientist Award by Science and Engineering Research Board (SERB), Outstanding Researcher Award by NSF Nanoscale Science & Engineering Center, CRS Silver Medal and CRSI Bronze Medal.

IL-7

Stimuli-responsive Turn-on Fluorogenic Prodrugs of Anticancer Drugs

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Specific bioanalyte-responsive drug delivery from suitable prodrugs of the commercially available anticancer drugs has attracted wide research attention in the recent past owing to the enormous side effects of many chemotherapeutic drugs during their direct administration.[1] Moreover, the direct drug administration as well as the non-fluorogenic prodrugs lack the proper and consistent monitoring of drug delivery in the real-time. Interestingly, the development of specific stimuli-activatable turn-on fluorogenic prodrugs is advantageous for the convenient and real-time monitoring of the drug delivery processes with high level of sensitivity and reduced off-target side effects. The present talk will mainly be focused on our recent strategies towards the development of specific bio-analyte-responsive prodrugs for the delivery of anticancer drugs with turn-on fluorescence.[2]

Keywords: Drug delivery, Reactive Oxygen Species, Anticancer Drugs, Self-immolation, Turn-on Fluorescence.

References

1. Malet-Martino, M.; Jolimaitre, P.; Martino, R., The Prodrugs of 5-Fluorouracil. *Curr. Med. Chem. Anticancer Agents* **2002,** *2* (2), 267-310.

2. (a) Kesarwani, R.; Pal, N.; Bhabak, K. P., Stimuli-responsive biotin-anchored prodrug for the targeted delivery of anti-cancer agent NBDHEX with turn-on NIR fluorescence. *Chem. Commun.* **2024,** *60* (25), 3397-3400; (b) Badirujjaman, M.; Thummer, R. P.; Bhabak, K. P., Esterase-Responsive Self-Immolative Prodrugs for the Sustained Delivery of the Anticancer Drug 5-Fluorouracil with Turn-On Fluorescence. *Chem. Asian J.* **2025,** *20* (2), e202400846; (c) Misra, R.; Barman, P.; Bhabak, K. P., Esterase-Responsive Fluorogenic Prodrugs of Aldose Reductase Inhibitor Epalrestat: An Innovative Strategy toward Enhanced Anticancer Activity. *ACS Appl. Bio Mater.* **2024,** *7* (10), 6542-6553.

Biography:

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Professional Experience

Jun, 2021 - Present	Associate Professor, Department of Chemistry, IIT Guwahati, Assam, India
Apr, 2015 - Jun, 2021	Assistant Professor, Department of Chemistry, IIT Guwahati, Assam, India
Feb, 2013 - Apr, 2015	Assistant Professor, Department of Chemistry, Presidency University, Kolkata, India.
Nov, 2012 - Feb, 2013	Post-doctoral Researcher, University of Oxford, United Kingdom
Jul, 2010 - Oct, 2012	Post-doctoral Researcher (Alexander von Humboldt Fellow), Humboldt University, Berlin, Germany

Education

Aug, 2006 - Jul, 2009	Ph.D., Department of Inorganic & Physical Chemistry, IISc Bangalore, India (Supervisor: Prof. G. Mugesh)
Aug, 2003 - Apr, 2006	M.S. in Chemical Science, IISc, Bangalore, India
Aug, 2000 - Jul, 2003	B.Sc. (Chemistry Hons.), Ramakrishna Mission Residential College, Narendrapur, University of Calcutta, India

Awards/Fellowships

Jan, 2013	INSPIRE Faculty Award by Department of Science and Technology (DST), India
Dec, 2010	Best Thesis Award by Eli Lilly and Company Outstanding Thesis Award 2010 in Asia
Mar, 2010	Alexander von Humboldt Fellowship for Post-doctoral Researcher by Alexander von Humboldt Foundation, Germany

Research summary

The major research interests of the group are in the field of (i) developing fluorogenic and non-fluorogenic donors of hydrogen sulfide (H_2S) and studying their biological implications; (ii) targeted delivery of anti-cancer/anti-inflammatory agents/drugs using fluorogenic drug delivery systems; (iii) design and synthesis of potential bio-active organochalcogen compounds towards their anticancer activities.

IL-8
Sustainable Transformation of Waste to Wealth for Energy Application

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Developing highly efficient materials is crucial for advanced energy applications, particularly in response to the increasing demand for sustainable, cost-effective, and scalable energy solutions.[1] Here, we have synthesized nitrogen-doped graphitic carbon using biowaste leaves, imposing a cost-effective chemical activation strategy, followed by pyrolysis at different temperatures in tubular furnace under an inert atmosphere. Synthesized material shows an excellent electrocatalytic activity towards oxygen reduction reaction (ORR), and as an anode material in Li ion battery. During the ORR studies, synthesized material shows a comparable onset potential and limiting current density to that of standard electrocatalyst (10 wt% Pt/C). It has also been tested for anode material in a half-cell configuration, which shows a specific capacity of 509 mAh/g at a 0.05 C, with 100% columbic efficiency. Tubular furnace consumes conventional power i.e., electricity. In order to resolve this, we have developed a simple, low-cost, and energy-efficient reaction setup for the first time to synthesize highly graphitized carbon materials from waste precursors using sunlight as the sole energy source, ensuring zero external power consumption. This work highlights the strategic use of biowaste leaves as a sustainable precursor, demonstrating how natural waste can be converted into a highly efficient material through zero power consumption for energy applications.

Keywords: Waste to wealth, Cost-effective, Graphitic Carbon, ORR, Li-ion battery

References

[1] Sharma, A.; Majee, P.; Pooja; Pawar, R.; Banothu, Y. N.; Pradhan, M., **Conversion of Waste Tecoma Leaves into Heteroatom Doped Graphitic Carbon via a One-Step Chemical Activation Method for the Catalytic Oxygen Reduction Reaction and Supercapacitor Application**. *ACS Sustainable Resource Management* 2024**,** *1* (12), 2564-2574.

Biography

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Research Areas

- Catalyst (composites) for generation of hydrogen from water
- Energy storage (super-capacitor & battery) application
- Novel composite nanomaterials synthesis
- Oxygen reduction reaction

Awards and Accolades

- CSIR-UGC NET, 2007
- DST INSPIRE Faculty Award, 2016
- GATE, 2007
- IBS Research Fellowship, 2013
- NTU Research Fellowship, 2016

Publications

1. Sharma, A., Banothu, Y. N., Majee, P., Kumar, S., Prajapati, M., Kumar, K., & Pradhan, M. (2025). Redox-mediated synthesis of Cu2O/CuO/Mn3O4/C quaternary nanocomposites as an efficient electrode material for oxygen reduction reaction and supercapacitor application. *Journal of Physics and Chemistry of Solids*, *196*, 112402.
2. Chakraborty, R., Sharma, A., Maji, P. K., Rudra, S., Nayak, A. K., Chatterjee, P. N., ... & Pradhan, M. (2024). Nitrogen and oxygen self-doped hierarchical porous carbon nanosheets derived from turmeric leaves for high-performance supercapacitor. *Inorganica Chimica Acta*, *567*, 122056.
3. Sharma, A., Majee, P., Pooja, Pawar, R., Banothu, Y. N., & Pradhan, M. (2024). Conversion of Waste Tecoma Leaves into Heteroatom Doped Graphitic Carbon via a One-Step Chemical Activation Method for the Catalytic Oxygen Reduction Reaction and Supercapacitor Application. *ACS Sustainable Resource Management*, *1*(12), 25642574.
4. Rudra, S., Das, S., Maji, P. K., Nayak, A. K., Negishi, Y., Pradhan, M., & Nandi, U. (2023). Redox-guided synthesis of Au–V2O5–MnO2 nanoflower composites with enhanced electrical conductance for supercapacitor applications. *ACS Applied Nano Materials*, *6*(3), 1648-1659.

IL-9
Bismuth-based Semiconductor Photocatalysts for Wastewater Remediation

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Photocatalysis as an advanced oxidation process offers a tremendous possibility for the environmental remediation of organic pollutants present in aqueous media. Particularly, TiO_2 and ZnO have shown promising results in the degradation applications. But their poor absorption in the visible region and high electron-hole recombination limit their practical application. Hence, suitable visible light active materials are required for practical applications. In this context, many visible light active materials have been explored by researchers all over the world. Particularly, bismuth-based semiconductors are a unique and promising group of recently developed advanced photocatalytic materials. They have been widely applied in several areas, including the hydrogen production by splitting water, decomposition of organic and inorganic pollutants in both wastewater and polluted air, and organic synthesis through harvesting the energy of light. The electronic structure of bismuth-based semiconductors confers them with a suitable band gap for visible-light response and a well-dispersed valence band composed of hybrid orbitals of Bi6s and O2p, making them a promising candidate when compared to other metal oxide semiconductors. In addition, they are simple to operate and prepare with controlled morphologies, making them attractive as potential photocatalysts.

Keywords: wastewater remediation, photocatalysis, organic pollutants, bismuth-based photocatalysts

References

[1] Priya, A., Prabhakaran Arunachalam, A. Selvi, J. Madhavan, Abdullah M. Al-Mayouf, and Mohamed A. Ghanem. **A low-cost visible light active $BiFeWO_6/TiO_2$ nanocomposite with an efficient photocatalytic and photoelectrochemical performance,** *Optical Materials* 2018 (81): 84-92. (Journal)

[2] Mageswari, Kumar, Peethambaram Prabukanthan, and Jagannathan Madhavan. **Microwave-assisted synthesis of ZnO nanoparticles using different capping agents and their photocatalytic application**, *Environmental Science and Pollution Research* 30, 2023, (14): 40174-40188. (Journal)

[3] Bavani,T, Mani Preeyanghaa, Neppolian, B, Madhavan, Balaji, D, **A Hybrid S-Scheme WS_2/BiOI heterojunction photocatalyst for wastewater treatment,** *ChemPhotoChem* 2023, 7.8: e202300024. (Journal)

[4] Malathi, A., and J. Madhavan. **A review on $BiVO_4$ photocatalyst: activity enhancement methods for solar photocatalytic applications**, *Applied Catalysis A: General* 2018, (555): 47-74. (Journal)

[5] Malathi, A., Prabhakarn Arunachalam, Andrews Nirmala Grace, J. Madhavan, and Abdullah M. Al-Mayouf. **A robust visible-light driven $BiFeWO_6$/BiOI nanohybrid with efficient photocatalytic and photoelectrochemical performance**, *Applied Surface Science* 2017, (412): 85-95. (Journal)

Biography:

Dr J. Madhavan is a Physical Chemist who specializes in Materials Chemistry, teaches postgraduate Chemistry and is a Professor and Head in the Department of Chemistry, Thiruvalluvar University, Vellore, India. He received his Ph.D. in the Department of Energy, University of Madras in 2007 and worked as a post-doctoral fellow at the School of Chemistry, University of Melbourne, Australia (2008–2010). Madhavan and his group have developed a number of novel photo- and electrocatalysts as major contributions in the field of energy and environmental remediation. His recent research also involves dye-sensitized solar cells, the hydrogen evolution reaction, electrocatalysis, photocatalysis, and nanomaterials for energy and environmental applications. Dr Madhavan received the DST Young Scientist Award in 2012. He has received four major research projects from Indian government funding agencies such as DST-SERB, DAE-BRNS, DBT-MST, CMRG for a worth of Rs. 1.4 Crores to support his research work. He has published 162 refereed papers in internationally reputed SCI journals, 12 book chapters and 3 patents; and delivered many invited lectures at international conferences and academic institutions. As of now, his research has achieved over 11,967 citations, an h-index of 60, and an i10-index of 145, according to Google Scholar. So far, he has produced 9 Ph.D. and 14 M.Phil. graduates. He placed his footprints on the Stanford's 2% Top Scientist list for a consecutive of 5 years. He has served as a member of many administrative and advisory committees of Thiruvalluvar University and other scientific organizations. He has visited various countries like Australia, South Korea, China, Malaysia, and Sri Lanka.

IL-10

Role of minuscule force in immune cell-pathogen interactions

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Constantly patrolling immune cells recognize and destroy any pathogenic foreign material in our body. Macrophages are a type of innate immune cell; they interact with pathogenic materials and extracellular matrix with tiny submicron size protrusion structures called podosomes [1]. Macrophages use podosomes as sensors during pathogenic recognition. The molecular level understanding of how podosomes mechanically interact with the external substance was unclear because of their fast dynamics, very small force, and tiny size. Using fluorogenic DNA probe, capable of sensing and reporting diminutive force as low as a few piconewton (pN), we have studied the integrin molecular force in podosome and its effect on the structural maturation of podosome. We found that the presence of membrane-bound DNase X, that can destroy dsDNA, the canonical DNA-based tension probe cannot be used in this case [2, 3]. In place of dsDNA, we used DNA/PNA hybrid that is not only stable against DNase-activity but also holds all the mechano-sensing features like dsDNA sensor [4]. We revealed that the formation and structural maturation of podosome unlike focal adhesion, is dispensable of external integrin tension.

Later we employed the DNase-resistant tension sensor to answer the following question: how do macrophages perform phagocytosis when pathogens are strongly adhered to the surface? We found that the cumulative integrin tension is being used by the macrophages in phagocytic cup to overcome the physical barrier and engulf the pathogenic materials [5]. pN level integrin tension generation is found to be essential for the successful phagocytosis of surface bound pathogenic materials, and amount of force is dependent upon the strength of adherence. Overall, the discovery of a new role of integrin force generation at phagocytic cup opens a new area of mechanobiology where integrin can be considered crucial beyond cell adhesion and migration.

Keywords: Phagocytosis, DNA-probe, integrin force, immune cell, force-nanoscopy

References

[1] Buccione R., Orth JO., McNiven MA. **Foot and mouth: podosomes, invadopodia and circular dorsal ruffles**, Nat. Rev. Mol. Cell Biol., 2004, (5): 647. (Journal)
[2] Pal K., Zhao Y., Wang Y., Wang X. **Ubiquitous membrane-bound DNase activity in podosomes and invadopodia,** J. Cell Biol., 2021, (220): e202008079. (Journal)
[3] Zhao Y., Pal K., Tu Y., Wang X. **Cellular force nanoscopy with 50 nm resolution based on integrin molecular tension imaging and localization,** J. Am. Chem. Soc., 2020, (142): 6930. (Journal)
[4] Pal K., Tu Y., Wang X. **Single-Molecule Force Imaging Reveals That Podosome Formation Requires No Extracellular Integrin-Ligand Tensions or Interactions,** ACS Nano, 2022, (16): 2481. (Journal)
[5] Kundu S., Pal K., Pyne A., Wang X. **Force-bearing phagocytic adhesion rings mediate the phagocytosis of surface-bound particles,** Nat. Commun., 2025, (16): 984. (Journal)

Biography:

Name: Kaushik Pal
Designation: Assistant Professor
Affiliation: IIT Tirupati
Email id: *reachkaushik@iittp.ac.in*

Kaushik originally from West Bengal, India. He completed his Bachelor and Master studies from Visva Bharati, Santiniketan in Chemistry honors (2010) and Physical Chemistry (2012) respectively. After completing BSc and MSc he went to IISER Bhopal and joined the lab of Prof. Apurba Lal Koner for his PhD research. He received PhD degree in the field of experimental physical chemistry in 2018. During PhD he got exposure to various interdisciplinary research topics such as supramolecular chemistry, small molecule synthesis, fluorescence spectroscopy, fluorescence microscopy, organelle biophysics etc. After that Kaushik moved to Iowa State University, USA for his first postdoctoral research in the field of molecular cell mechanics in the lab Dr. Xuefeng Wang. Successively, he moved to the east coast of the USA and joined the lab of Dr. Amit Choudhary at Broad Institute of MIT and Harvard. During his second postdoc, his research interest was the use of chemical biology tools to enhance the efficiency of cancer immunotherapy.

In July 2023, Kaushik joined the department of chemistry, IIT Tirupati as assistant professor. In his independent carrier his research interests are understanding the biomechanical aspect of human immune system and development of chemical biology tools for cancer immunotherapy.

Industrial Expert Lecture- IEL

IEL-1
Data-Driven Approaches for Simplifying and Interpreting Molecular Simulation Data

Atreyee BANERJEE*

Freudenberg Technology Innovation SE & Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany

Klüber Lubrication München GmbH & Co. KG, Gmunder Str. 50, 81379 München, Germany

In this talk, I will present a data-driven framework that combines the high-resolution insights from molecular dynamics simulations with the structural information of individual polymer chains. This approach enables accurate identification of the glass transition temperature in polymer melts of semiflexible chains and has recently been extended to model all-atom acrylic polymer systems. I will also discuss its application in detecting the onset of shear thinning in lubricants. Overall, this data-driven framework can extract meaningful states from complex molecular simulation trajectories and can be applied across industries to accelerate the development of new sustainable products, bringing them faster to market.

Keywords: Machine Learning, Unsupervised Learning, Polymer, Glass Transition Temperature, Data Driven Methods

References

[1] Determining glass transition in all-atom acrylic polymeric melts simulations using machine learning. **A. Banerjee**, A. Iscen, K. Kremer, O. Kukharenko. J. Chem. Phys, 2023, 159, 074108.

[2] Data-driven identification and analysis of the glass transition in polymer melts. **A. Banerjee**, H. Hsu, K. Kremer, O. Kukharenko. ACS. Macro. Lett, 2023, *12* (6), 679-684.

Biography

Atreyee Banerjee is a researcher specializing in the structural and dynamical properties of complex systems such as lubricants, greases, supercooled liquids, polymers, polymer gels, and polymorphic organic crystals. She is currently working as a Material Informatics Scientist at Freudenberg Technology Innovation SE & Co and Klüber Lubricant, München, Germany. She earned her B.Sc. and M.Sc. in Chemistry from Visva-Bharati University in India before completing her Ph.D. at CSIR National Chemical Laboratory, Pune. Her postdoctoral work took her to Cambridge University, where she explored energy landscapes in complex materials, and later to the Max Planck Institute for Polymer Research, where she applied machine learning to understand the complex behaviour of polymeric systems. From October 2024 to January 2025, she was an Early Career Fellow at Freiburg Institute of Advanced Studies, FRIAS. Atreyee was also a Freiburg Rising Star Academy Alumni in the 2023-24 cohort.

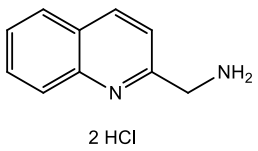
IEL-2
Design of Chemical Processes - Efficiency, Safety & Environment

Sankara Subramanian*

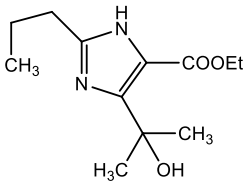
Vishwa-Syntharo PharmaChem Private Limited, India

Development of Chemical Processes for new chemical entities whether it be in the pharmaceutical, specialty chemical, commodity chemical or biotechnology is challenging from several perspectives: a. Cost; b. Efficiency; c. Safety; d. Environment; e. Statutory requirements; f. Non-infringement of existing patents

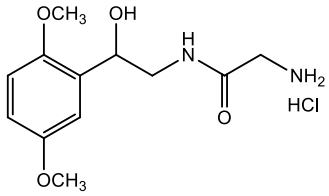
The talk will aim at presenting and discussing first-hand examples in the art of design of chemical processes.



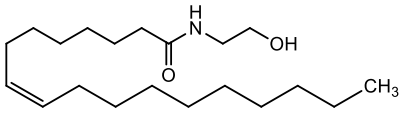
2-Aminomethylquinoline



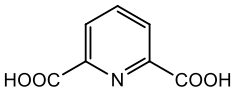
"Imidazole Ester"



Midodrine Hydrochloride



Oleylethanolamide



2,6-Dipicolinic acid

Keywords: Technology Development, Green Chemistry, Patent Infringement,

References

US Patent: US 7,094,928

Vishwa-Syntharo PharmaChem Private Limited, unpublished

Biography:

Sankara Subramanian is a PhD in Chemistry from Indian Institute of Technology, Madras under the supervision of Prof K K Balasubramanian and did his post-doctoral research at the University of Bath with Prof Timothy Gallagher. He is currently the Founder Director of Vishwa-Syntharo PharmaChem involved in the development and scale-up of technologies for New Chemical Entities for the Chemical and Pharmaceutical Industry.

IEL-3
Bridging the Genomic Data Tsunami: From Scientific Discovery to Clinical Action in Personalized Medicine

Parijat Kundu*

Velsera, Pune, India, 411001

The exponential growth of next-generation sequencing (NGS) technologies has created a "data tsunami" in genomics, generating terabytes of molecular information per individual while opening unprecedented opportunities for personalized medicine. However, the true challenge is translating this vast reservoir of research data into actionable clinical insights that directly impact patient care.
Manually curating and interpreting the deluge of genomic variants, scientific literature, and clinical trial updates is unsustainable and a major bottleneck for scaling precision oncology. Addressing this challenge requires a framework that brings together expertise from engineering, bioinformatics, and biology. The journey from raw sequencing reads to personalized treatment includes several critical components:

1. Development of a comprehensive relational knowledgebase linking key biomarkers (genomic, proteomic, transcriptomic) to therapeutic outcomes;
2. Implementation of robust, automated variant interpretation workflows compliant with international standards (e.g., AMP/ASCO/CAP);
3. Adoption of data standardization and process automation to improve accuracy and turnaround time;
4. Deployment of intelligent decision-support systems that empower clinicians without deep bioinformatics expertise;
5. Adherence to regulatory frameworks (ISO13485, CAP/CLIA, FDA).

These elements converge in Velsera's Clinical Genomics Workspace (CGW), an end-to-end platform taming the genomic data deluge through automated variant calling, dynamic evidence-based interpretation, and streamlined reporting. With CGW, healthcare systems can operationalize precision genomics at scale - reducing turnaround from weeks to days and ensuring high-quality, evidence-based clinical decisions.
Real-world use cases, such as the Belgium BALLETT study utilizing CGW and similar platforms, demonstrate rapid identification of 2200+ actionable variants for 750+ patients by processing close to 2TB of genomic data within three days. This highlights how strategic data engineering, scientific leadership, and product innovation collectively address the fundamental challenge of converting overwhelming molecular data into actionable recommendations that advance personalized healthcare.

Keywords: Next-Generation Sequencing, Personalized Medicine, Clinical Genomics, Data Integration, Translational Science

References:

[1] Conway J.R., Warner J.L., et al. Next-Generation Sequencing and the Clinical Oncology Workflow, J. Clin. Oncol., 2019, (37): 2564-2573.
[2] Phillips K.A., Van Bebber S., et al. Challenges To The Translation Of Genomic Information Into Clinical Practice, Health Aff., 2008, (27): 1284-1291.
[3] Mehandziska S., et al. Workflow for the Implementation of Precision Genomics in Healthcare, Front. Genet., 2020, (11): 619.

Biography:

Parijat Kundu is a Senior Scientific Lead at Velsera specializing in translational genomics, clinical knowledgebase development, and precision medicine implementation. With 8+ years of experience bridging molecular disease biology and clinical applications, Parijat leads cross-functional teams in developing scalable data infrastructure and automation strategies that transform genomic discoveries into actionable clinical insights for improved patient care.

Short Invited Lectures- SIL

SIL-1
Application of 3d-transition metal complexes of polypyridyl and Schiff base ligands as potential anticancer agents

Sovan Roy*
Department of Chemistry, School of Advance Sciences, VIT-Vellore, Vellore, Tamilnadu, 632014

Cancer which is the world's second biggest cause of mortality, is a multi-gene illness caused by aberrant cells with altered DNA sequences, known as mutations. [1] At present the drug molecules are used for the treatment of different types of cancer are suffering from multiple drawbacks like non-selectivity towards cancer tissues, emergence of drug resistance and other health issues. [2] To address this issues we, keeping in mind the bioavailability of 3d- transition metal ions like Cu(II), prepared Cu(II) complexes with Schiff base and polypyridyl ligands containing di-keto as well as amines groups and observed their promising interaction with serum protein BSA, binding and cleavage efficacy of DNA, apoptotic cytotoxic effect towards HeLa cell lines with very low IC_{50} values, anti-clonogenic behavior in HeLa cell. We observed the presence of amine group on polypyridyl group enhances the biological activity. [3] Similarly, effect of hard-soft acidity of metal ions towards biological activity was tested by preparing Fe(II) and Fe(III) complexes of same polypyridyl ligands and Schiff ligands. It is observed that softer nature of Fe(II) ion enhances biological activity like DNA interaction, DNA cleavage and anti-cancer activity towards MCF-7 cell lines.

Keywords: Cancer, metal complexes, DNA, BSA, apoptosis.

References

[1] Basu, U., Roy., M, Chakravarty, A.R. **Recent advances in the chemistry of iron-based chemotherapeutic agents**, Coord. Chem. Rev. 2020, (417): 213339.

[2] Rani, J.J., Roy, S. **Recent Development of Copper (II) Complexes of Polypyridyl Ligands in Chemotherapy and Photodynamic Therapy**. Chem.Med.Chem. 2023, 18 (8): e202200652.

[3] Rani, J.J., Roy, S. **DNA and BSA binding, DNA cleavage, anticancer activity and In-Silico drug screening study of novel heteroleptic Cu(II) complexes of polypyridyl ligands.** Eur. J. Med. Chem. Rep., 2025, (15): 100292.

Biography

Dr. Sovan Roy was born in West Bengal, India. He complected B.Sc. with chemistry honors and M.Sc. in Chemistry from Jadavpur University, India. Subsequently, he completed Ph.D. in the field of Bioinorganic chemistry from IISc. Bangalore, India under the supervision of Prof. A.R. Chakravarty. He also gained postdoctoral experience in the field of supramolecular chemistry related to sensing of toxic ions from Florida State University, USA as well as from CSIR-NCL, and CSIR, CSMCRI, India. Presently he is working as an Assistant Professor in the Chemistry Dept. of VIT-Vellore, India. His research area is focused on anticancer activity of transition metal complexes and sensing of metal ions.

SIL-2
Ab initio investigations of zwitterionic polymers and their interactions with water and ice

Tamalika ASH [a], Sara A. TOLBA [b,c], Wenjie XIA [a]*

[a] Department of Aerospace Engineering, Iowa State University, Ames, IA, 50011 USA
[b] Materials and Nanotechnology, North Dakota State University, Fargo, ND 58108, USA
[c] Center for Computationally Assisted Science and Technology, North Dakota State University, Fargo, ND 58108, USA

Preventing ice formation on solid surfaces remains challenging across many technologies. Zwitterionic polymer coatings have shown strong anti-icing potential, yet their molecular interactions with water and ice are not fully understood. Using DFT calculations, we probe how four representative polymers, polySB, polySBi, polyMPC, and polyCBAA interact with water molecules, ice clusters, and model ice surfaces. The polymers exhibit distinct hydration and interfacial behaviors that shape their anti-icing performance. PolyMPC forms strong hydrogen bonds with water, while polyCBAA generates a thicker, more dynamic hydration layer. Both polySB and polyMPC significantly deform ice clusters and promote interfacial lubrication, making ice formation energetically unfavorable. PolyCBAA moderately binds ice but disrupts the ice surface enough to create a quasi-liquid lubricating layer. PolySBi shows the weakest water affinity and poorest anti-icing behavior. These results highlight how the spatial arrangement of charged groups controls polymer-water-ice interactions, guiding the design of next-generation anti-icing materials.

Keywords: Density Functional Theory, Zwitterionic Polymer, Hydration, Anti-icing

References

[1] Tolba S. A., Xia W. **Molecular Insights into the Hydration of Zwitterionic Polymers**, Mol. Syst. Des. Eng., 2023, (8):1040-1048.

[2] Sarker P., Lu T., Liu D., Wu G., Chen H., Jahan Sajib M. S., Jiang S., Chen Z., Wei T., **Hydration Behaviors of Nonfouling Zwitterionic Materials**, Chem. Sci., 2023, (14): 7500-7511.

[3] Chen Z., **Surface Hydration and Antifouling Activity of Zwitterionic Polymers**, Langmuir, 2022, (38): 4483-4489.

Biography

I am Dr. Tamalika Ash, a postdoctoral researcher at Iowa State University working under the supervision of Dr. Wenjie Xia. My current research focuses on studying the hydration and anti-icing behavior of neutral and zwitterionic polymers using computational methods. I completed my Ph.D. from the Indian Association for the Cultivation of Science, Kolkata in 2019. To date, I have published 41 papers in internationally recognized peer-reviewed journals.

SIL-3

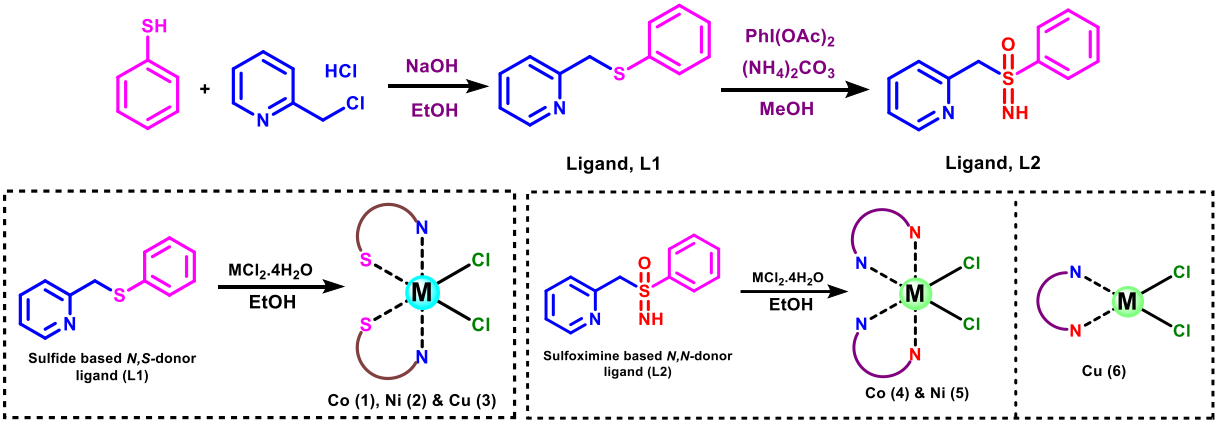
Metal(II) Complexes Derived from NN & NS based Donor Ligands: Synthesis, Structure, electrochemical and biomimitic applications

S. Sabiah & A. Kishore

Department of Chemistry, Pondicherry University, Puducherry, 605014

Over the decades, different classes of sulfur compounds have been described *i.e.,* sulfone, sulfoxides, sulfonates and sulfoximines, etc. A large number of useful procedures for the synthesis of these compounds have been developed. Transition-metal complexes with sulfide and sulfoximine ligands are very rarely reported though they exhibit good catalytic activity in many reactions.[0,0]

Herein, we report Co(II) **1** & **4**, Ni(II) **2** & **5** and Cu(II) **3** & **6** complexes using NN/ *N,S*-donor functionalized ligands. All the complexes were spectrally characterized and structurally determined by SC-XRD. The *N,S*-donor functionalized complexes **1, 2** & **3** were immobilized on graphene sheets and subjected to electrocatalytic studies.[0] The sulfoximine based complexes **4, 5** & **6** were structurally similar to the sulfide complexes. The DFT optimized structure, Frontier Molecular Orbitals and Molecular Electrostatic Potential of all the complexes were obtained by theoretical calculations. All the complexes were investigated for their electrocatalytic efficiency.



Keywords: sulfide, sulfoximine, OER, H_2O_2, biomimcs

References

[1] Kim, J., Ok, J., Kim, S., Choi, W., Lee, P. H. *Org. Lett*. **2014**, 16, 17, 4602–4605, (b) Gupta, S., Baranwal, S., Muniyappan, N., Sabiah, S., & Kandasamy, J. *Synthesis*, **2019**, 51, 2171-2182. (c) Prakash, O., Singh, P., Mukherjee, G., Singh, A. K. *Organometallics*, **2012**, 31, 3379-3388.

[2]Junaid, Q. M., Kumar Singh, D., Ganesan, V., & Sabiah, S. *Chem.: Asian J.*, **2020**, 17(12), e202200160, (b) Ayanarappin, K., Singh, V., Veerakumar, S., Ganesan, V., & Shahulhameed, S. *Polyhedron*, **2025**, 117753.

Biography

Dr. S. Sabiah is a full time Professor in the department of Chemistry, Pondicherry University. Her research interests include Bioinorganic Chemistry and Organometallic Chemistry; Synthesis, structure and applications of metal carbene complexes; Biomimics of hydrolytic enzymes and pyrophosphatase enzymes; Magneto-structural correlation of dinuclear metal complexes with multiple bridges; She teaches Inorganic Chemistry and has been recognized with best teacher award in chemistry by Pondicherry University.

SIL-4

Proton Reduction by Iron Complexes: Impact of Proton Residue Concentration at Catalyst Sites

Bharath M, Srijit Sen, Pankaj Kumar, Munmun Ghosh*

Chemistry Department, Ashoka University, Sonipat Haryana 131029

The microenvironment surrounding a catalyst is pivotal in driving electrocatalytic proton reduction, especially in aqueous systems where multiple proton donors-such as buffer ions, water molecules, and hydronium ions compete for reactivity. Nature elegantly resolves these challenges through the precise architecture of enzyme scaffolds, incorporating features like proton channels, hydrophobic pockets or strategically placed amino acid residues to facilitate efficient proton transfer. Inspired by these biological strategies, we have developed a series of non-heme iron complexes with carefully positioned proton-responsive groups. These synthetic catalysts emulate enzymatic precision, demonstrating that both the presence and concentration of local proton sources significantly influence hydrogen evolution activity. This mirrors the behavior of natural enzymes, where microenvironmental control is key to function. Through comprehensive theoretical modeling and experimental validation, we have elucidated the mechanistic pathways, establishing them as effective catalysts for sustainable hydrogen production.

Keywords: Homogeneous Catalysis, Proton Reduction, Biomimetic hydrogen generation

References

[1] Gora A., Brezovsky J., Damborsky J., **Gates of Enzymes**. Chem. Rev. 2013, 113, 5871-5923

[2] Bharath M., Rana M., Pattanayak S., Kumar P., Tyagi P V., Bommakanti S., Demeshko S., Gupta R., Ghosh A., and Ghosh M. **Accelerating Electrochemical Hydrogen Evolution by Introducing Local Proton Source in Non-Heme Iron (III) Complexes** Chem. Asian. J. DOI: 10.1002/asia.70259

[3] Sen S., Kumar P., Pattanayak S., Das C., Dutta A., Ghosh M. **Proton Reduction by Amino Acid based Iron Complexes: Impact of Proton Residue Concentration at Catalyst Sites**. Chem. Asian. J. DOI: 10.1002/asia.202500827

Biography

Munmun Ghosh is an Assistant Professor in the Department of Chemistry at Ashoka University, Sonipat. She holds a Ph.D. degree in Chemical Science from National Chemical laboratory (NCL) Pune, India. She completed the postdoctoral stint at Göttingen University, Germany as an Alexander Humboldt fellow. She is recognized as Outstanding Early Career Female Investigators in Chemical Engineering-2023.

Her research interests include Bioinorganic Chemistry with a focus on small molecule activation by bioinspired molecular catalysts like Hydrogenase enzymes in nature. We synthesize metal complexes, which are functional mimic of hydrogenase enzymes and thoroughly study the mechanism of the reactions.

SIL-5
AI/ML-Guided Design of Novel Inhibitors Targeting FGFR Tyrosine Kinase and KDM4C for Cancer Therapy

Debasish Mandal*

Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab E-mail: debasish.mandal@thapar.edu

Drug discovery is a long and resource-intensive process, often taking over a decade, with more than 90% of candidates failing during preclinical or clinical trials. Identifying novel drugs requires screening billions of compounds, making the integration of computer-aided drug design (CADD) and AI technologies crucial for accelerating and optimizing discovery.

This presentation highlights two case studies on the design of tyrosine kinase and KDM4C inhibitors. Tyrosine kinase inhibitors are revolutionizing cancer therapy, with FGFR alterations identified as major drivers of cholangiocarcinoma. KDM4C, a histone demethylase regulating gene expression, is frequently overexpressed in several cancers, promoting uncontrolled cell growth. The first study employs a traditional CADD workflow—pharmacophore modeling, virtual screening, docking, ADMET, molecular dynamics, and SAR analysis—while the second combines these methods with advanced AI and machine learning to enhance predictive power and efficiency.

Keywords: AI-ML, CADD, Inhibitor, Cancer,

References

[1] Zhang, K., Yang, X., et.al. **Artificial intelligence in drug development.**, Nat. Med., 2025, (31): 45–59.

[2] Hartmann, T. J., Haap, M., et.el., **Tyrosine Kinase Inhibitors - A Review on Pharmacology, Metabolism and Side Effects, Curr. Drug Metab.**, 2009, (10): 470-481.

[3] Kaur, A., Mandal, D., **Computational identification and exploration of novel FGFR tyrosine kinase inhibitors for the treatment of cholangiocarcinoma**, J. Biomol. Struct. Dyn., 2024, 42: 13153-13164.

[4] Naskar, T., Mandal, D. **AI-ML intensive evaluation and design of novel KDM4C** inhibitors. (Manuscript under preparation)

Biography

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Associate Professor
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Thapar Institute of Engineering & Technology (Deemed to be University)
P.O. Box 32, Bhadson Road, Patiala-147004, Punjab, India
E-mail: debasish.mandal@thapar.edu
Mobile No: 8017296958

Dr. Debasish Mandal is an Associate Professor in the Department of Chemistry and Biochemistry at Thapar Institute of Engineering and Technology, Patiala. He obtained his Ph.D. from the Indian Association for the Cultivation of Science (IACS), Kolkata, and pursued postdoctoral research at the Hebrew University of Jerusalem, Israel. His research interests encompass computational quantum catalysis, organometallic chemistry, and AI/ML-driven drug design. Dr. Mandal has authored around 88 research articles in leading international journals, including JACS and Nature Chemistry, with an h-index of 29 and over 3,100 citations

SIL-6

Engineering Soft Materials via Controlled Catalysis for Smart Health and Sustainability Solutions

Chandan MAITY,* Nikita DAS, Dinesh BHARATHIDASAN, Damini JAGANKAR

(Organic)Material Science and Engineering Lab, Centre for Nanobiotechnology (CNBT), Vellore Institute of Technology (VIT), Vellore-632014

Enzymes in nature catalyze complex reactions with high efficiency and selectivity in aqueous environments, inspiring artificial systems with similar precision. Guided by these principles, we investigate how structural organization and external stimuli can modulate catalysis and drive the formation of functional soft materials. We present an ultrasound-responsive catalytic platform where imidazole moieties switch between 'ON' and 'OFF' states, allowing precise temporal control over ester hydrolysis.[1] Expanding this concept, we design supramolecular hydrogels that respond to chemical inputs like hydrogen peroxide, enabling spatially resolved in-situ gelation.[2] Coupled with enzymatic reactions, these systems exhibit autonomous behavior with biomedical relevance. A hydrazone-based hydrogel also serves as a scaffold for *in-situ* generation of silver nanoparticles, which degrade organic dyes in wastewater, demonstrating environmental potential.[3] Additionally, a coumarin-based hydrogelator is formed *in situ* from non-assembling precursors via acid catalysis, allowing Fe(II) sensing with paper-based devices.[4] Collectively, these systems highlight the potential of catalysis-driven soft materials for biomedical and environmental applications.

Keywords: Smart catalysis, Supramolecular material, Enzyme controlled, Ferrous ion sensing, Dye degradation

References

[1] Das N., Maity C. **Mechanical force-switchable aqueous organocatalysis**, Commun. Mater., 2024, (5): 205. [2] Bharathidasan D., Salvi A. S., Bose S., Maity C. **Biochemical signal-induced supramolecular hydrogelation for structured free-standing soft material formation,** Macromol. Biosci., 2024, (24): 2400419.

[3] Jagankar D., Das N., Mukherjee A., Maity C. **Room-temperature synthesis of silver-based nanoparticleembedded hydrogel material via catalytic crosslinking for recyclable dye degradation applications.** RSC Adv., 2025, (15): 34068.

Biography

Dr. Chandan Maity has received his M. Sc. From IIT Bombay and Ph.D. from Humboldt University of Berlin, Germany. Thereafter, he did his postdoctoral research work in Delft University of Technology, the Netherlands and Technical University of Munich, Germany. Currently he is an Assistant Professor at Centre of Nanobiotechnology (CNBT) in Vellore Institute of Technology (VIT), Vellore campus, India. His research group is interested developing stimuli responsive material in "nature-like" environment using functional organic molecules aiming at catalysis, controlled delivery, and biomedical applications.

SIL-7

Chemical Design Principles for Gene Therapeutic Nanoparticles: Enabling Immune Cell and Extrahepatic Delivery of Nucleic acid

Atanu Chakraborty*
Assistant Professor, Senior Grade 2
Department of Chemistry, School of Advanced Sciences, VIT University, VIT, Vellore Campus, Tiruvalam Rd, Katpadi, Vellore, Tamil Nadu 632014

With the advancement of COVID-19 vaccines genetic programming of immune cells has emerged as a transformative therapeutic technology for the treatment of cancer, infectious diseases, inflammation.[1] However, achieving their full clinical potential requires the development of delivery systems that not only protect and release genetic cargoes efficiently but also induce organ- and cell-specific targeting beyond the liver. The clinical success of mRNA therapeutics relies largely on the development of lipid nanoparticle (LNP).[1,2] Despite of having these successes, other LNP based mRNA therapeutics are still facing some challenges for advancing to the clinical trials. First, like other nanoparticles most of the conventional LNPs also show a predominant hepatic tropism following systemic administration, limiting therapeutic access to extrahepatic organs such as lung, spleen, heart and brains.[3] Second, selective lung transfection by addition of high molar percentage of permanently cationic lipids (e.g. DOTAP), can increase immunogenicity, inflammation and toxicity.[4] My research focuses on leveraging rational chemical design of ionizable polymer nanoparticles to achieve selective delivery of genes and messenger RNA (mRNA) to immune cells and extrahepatic organs.[5] During my whole postdoctoral research career, I worked on designing biodegradable ionizable polymers with tunable functional groups (amine and lipid tails) that mimic ionizable lipids while providing enhanced stability and degradability. By systematically varying polymer composition and branching, we demonstrated that the chemical architecture itself dictates self-assembly of nanoparticle and organ tropism, eliminating the need for permanently cationic "SORT" lipids.[5] These polymeric nanoparticles efficiently transfect "hard-to-transfect" innate immune cells such as macrophages and dendritic cells *in vitro* and mediate lung and spleen selective mRNA expression *in vivo* with minimal toxicity and immune activation.

Keywords: Ionizable Polymer, Mrna Transfection, Targeted *In Vivo* Gene Editing, Immune Cell

References

[1] Hou, X., Zaks, T., Langer, R. et al. Lipid nanoparticles for mRNA delivery. Nat Rev Mater 6, 1078–1094 (2021). [2] Kiaie, S.H., Majidi Zolbanin, N., Ahmadi, A. et al. **Recent advances in mRNA-LNP therapeutics: immunological and pharmacological aspects**. J Nanobiotechnol 20, 276 (2022).

[3] Loughrey, D., Dahlman, J.E., Acc. Chem. Res. 2022, 55, 1, 13–23

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Biography:

I am currently an Assistant Professor in the Department of Chemistry at Vellore Institute of Technology (VIT), India. I received my M.Sc. in Chemistry from the Indian Institute of Technology (IIT) Kanpur in 2011 and completed my Ph.D. in 2017 from the Indian Association for the Cultivation of Science (IACS), Kolkata. My doctoral research focused on the design and synthesis of fluorescent nanoparticles to investigate nano–bio interactions and their subcellular localization. Following my Ph.D., I pursued postdoctoral research at the University of Maryland, Baltimore, where I developed immunomodulatory polymeric nanoparticles for drug and nucleic acid delivery both *in vitro* and *in vivo*. I subsequently secured Keenan Postdoctoral Fellowship and joined the University of Toronto as a postdoctoral research fellow, where my work focused on the synthesis of lipid–polymer hybrid nanoparticles for organ-selective delivery of mRNA, particularly in the context of cancer therapeutics.

I joined VIT in July 2025, where my current research focuses on the design and synthesis of polymer- and lipid-based immunomodulatory nanoparticles for drug and mRNA delivery toward immunotherapeutic applications. My broader research interests lie at the interface of chemistry, materials science, and immunoengineering—aimed at developing next-generation drug delivery platform for targeted genetic and immune modulation.

SIL-8

Copper and Zinc Complexes of Quinoline Based Flexible Amide Receptor as Fluorescent Probe for Dihydrogen Phosphate and Hydrogen Sulphate and Their Biological Application

Dr. Rinku Chakrabarty*
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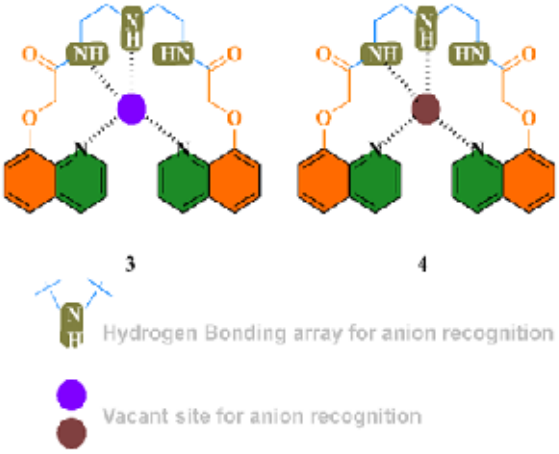
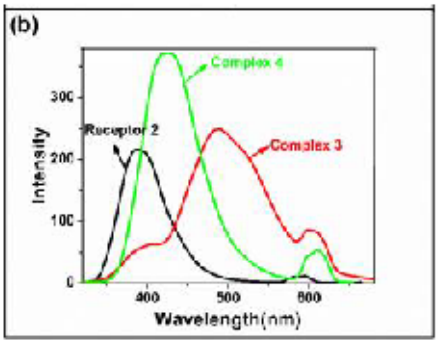
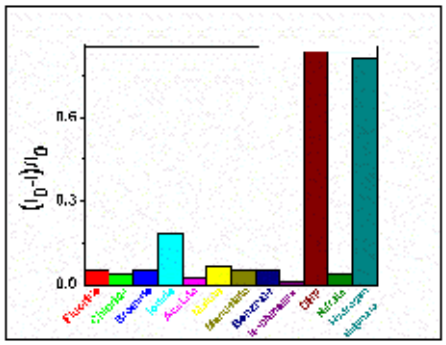
8-hydroxy quinoline-derived amide receptor, in conjunction with its Cu (II) and Zn (II) complexes, has been developed strategically which act as remarkably efficient fluorescent receptors having distinct capability for anion sensing. The comprehensive characterization of the synthesized compounds were achieved through different spectroscopic techniques viz. UV-Vis, IR, NMR, and HRMS. Among the Cu (II) and Zn (II) complexes, the latter exhibits superior selectivity for anions, specifically dihydrogen phosphate and hydrogen sulfate, as their tetrabutylammonium salts in 9:1 acetonitrile-water (v/v) mixture. The Cu (II) complex demonstrates enhanced anion binding compared to that of the precursor amide ligand, with reduced selectivity. Furthermore, the binding affinity was evaluated following the Benesi-Hildebrand plot. The binding constants and Limit of Detection (LOD) for both complexes were precisely quantified. The Job plot illustrates a clear 1:1 binding interaction between the metal complexes and the guest anions. Significantly, both metal-complex receptors display a broad spectrum of antibacterial activity, against both gram-positive and gram-negative bacteria. It is worth highlighting that the Zn (II) complexed receptor outperforms the Cu (II) complexed receptor, as evidenced by its considerably lower Minimum Inhibitory Concentration (MIC) value against both bacterial strains. [1]







Reference:

[1]S Dey, S Ghosh, A Das, R N Yadav, R Chakrabarty, S Pradhan, D Saha, A K Srivastava, M. F. Hossain, J Fluoresc 2024, 34, 1829-1840.

Biography

Dr. Rinku Chakrabarty embarked on her academic journey at Kalyani University, West Bengal, India, followed by her Ph. D. under the guidance of Prof. Shyamaprosad Goswami from the Indian Institute of Engineering Science and Technology, Shibpur, India in 2011, focusing on molecular recognition and supramolecular chemistry. She spent two years at the University of Witwatersrand, Johannesburg, South Africa, for her postdoctoral studies, where she was involved in the synthesis of rare earth-based molecular systems and their extensive application as MRI agents. Her passion for academia led her to assume the role of an Assistant Professor in the Department of Chemistry at Alipurduar University. Her published works encompass an impressive collection of research papers. Her research pursuits are centered on nanomaterials, dye degradation, molecular sensing and bioinorganic chemistry, showcasing her unwavering commitment to the advancement of the field of chemistry.

SIL-9

Versatile Monocopper(II) Catalysts: Design and Application in Oxidative Catalysis

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Copper oxidases are essential redox enzymes that play crucial roles in biological and environmental processes. This study focuses on three representative copper-containing enzymes: ascorbate oxidase, amine oxidase, and catechol oxidase, each possessing distinct copper centers responsible for specific oxidative functions. Drawing inspiration from these natural systems, we investigate the design of biomimetic monocopper(II) complexes to emulate their catalytic activity. Although native enzymes exhibit remarkable efficiency, synthetic analogues often fall short due to structural and electronic constraints. Our work highlights the development of novel ligand architectures that effectively reproduce the coordination environment of native copper sites, enabling efficient and selective oxidation under mild, sustainable conditions. Modeling enzyme active sites not only provides insight into their mechanistic pathways and the role of metal ions in oxygen activation but also guides the design of improved catalysts for green and therapeutic applications, aligning with the principles of sustainable chemical innovation.

Keywords: Monocopper complexes; Ascorbic oxidase; Amine oxidase; Catechol Oxidase; Functional Models.

References

[1] Dey S. K., and Mukherjee A., **Catechol oxidase and phenoxazinone synthase: Biomimetic functional models and mechanistic studies,** Coord. Chem. Rev., 2016 (317): 80-115.
[2] Ravisankar V.C, Selvakumaran B, Ajaykamal T, and Murali M. **Functional biomimetics for copper oxidases: interesting catalytic promiscuity of novel monocopper(ii) complexes.** Dalton Trans., 2025 (54): 7221-7239.

Biography

Dr. M. Murali earned his B.Sc., M.Sc., M.Phil., and Ph.D. degrees in Chemistry from Bharathidasan University, Tiruchirappalli, and received advanced research training in bioinorganic chemistry as a DST-BOYSCAST Visiting Young Scientist under the guidance of Prof. Jan Reedijk at Leiden University, The Netherlands. Since joining National College (Autonomous), Tiruchirappalli, as a lecturer in 2001, he has guided 3 Ph.D. dissertations, 16 M.Phil. dissertations, 36 M.Sc. dissertations, and 6 scholars are currently pursuing their Ph.D. His research focuses on (a) Synthetic Models for Blue Copper Proteins, (b) Ruthenium(II) Complexes Containing Thioether Ligands, (c) Biomimetic Catalytic Oxidations using Ruthenium(III) Complexes, (d) Non-covalent DNA Binding, BSA Interaction, Cytotoxicity and Anticancer mechanisms, and (e) Models for Copper Oxidases. He has published over 30 papers, authored two books, and completed two DST-SERB projects (~80 lakhs). With an h-index of 11, Dr. Murali has participated in 90 conferences, delivered several lectures, and his students have received more than 24 Best Paper Awards. He is a life member of CRSI, RJSF, and RSC, and has organized numerous national and international scientific events.

Awards:

BOYSCAST Fellow - Department of Science and Technology, India
CRSI Best Teacher Award - Chemical Research Society of India
Teacher Fellow - Academies of Sciences, India
RSC Inspiration Committee Award - Royal Society of Chemistry

Oral Presentation- OP

OP1

Smart Alginate Materials: Switchable Aqueous Organocatalysis, Rewritable Ink, and Smart Drug Delivery

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Nature fabricates complex materials by assembling simple molecular building blocks through a bottom-up approach, achieving remarkable precision, adaptability, and efficiency. Inspired by this principle, the design of artificial materials with tunable physicochemical properties has gained significant attention for advancing biomedical and technological frontiers. Stimuli-responsive materials are particularly interesting for their ability to adapt to environmental changes. Alginate, a biocompatible and naturally derived polysaccharide, offers exceptional versatility due to its easy gelation, modifiability, and sustainability, making it an ideal platform for engineering dynamic, responsive systems.[1] In this presentation, we will highlight how strategic chemical modifications impart versatile and adaptive functionalities to alginate-based systems. Alginate hydrogels, formed via divalent cation crosslinking, can be reversibly de-crosslinked using EDTA. Utilizing this, we developed Ca^{2+}-coated paper substrates and formulated a stimuli-responsive alginate ink by coupling it with chromogenic moieties.[2] Next, we will further demonstrate ultrasound-triggered, reversible modulation of aqueous catalysis within alginate gels incorporating organocatalysts.[3] Ultrasound exposure triggers catalytic activation ("ON"), while ceasing it restores the gel network and deactivates catalysis ("OFF"), mimicking enzymatic transformations in aqueous environments. Additionally, dynamic hydrazone crosslinking enables pH-responsive hydrogels with mechanical stability, allowing for controlled release of bioactive such as vitamin B_{12}.[4]

Keywords: Stimuli-responsive materials, biopolymers, switchable catalysis, erasable ink, hydrogels.

References

[1] Maity, C. & Das, N. **Alginate-Based Smart Materials and Their Application: Recent Advances and Perspectives.** Top. Curr. Chem., 2021, 380, 3. (https://doi.org/10.1007/s41061-021-00360-8)

OP2

Functional Duality of Monocopper(II) Complexes: Greener Oxidation Catalysts and ROS-Driven Anticancer Agents

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Oxidation reactions play a crucial role in pharmaceutical and chemical industries; however the activation of molecular oxygen remains a kinetic challenge due to its inert nature and poor selectivity. To address this, biomimetic copper(II) complexes were designed to emulate natural metalloenzymes that efficiently catalyze oxidation using atmospheric oxygen. A series of mixed-ligand monocopper(II) complexes, [Cu(L1-L4)(phen)](ClO_4), where L is condensation of salicylaldehyde or 2-hydroxy-1-naphthaldehyde and 2-(2-aminophenyl) benzimidazole (HL1/HL3) or 2-(2-aminophenyl)benzothiazole (HL2/HL4) and phen is 1,10-phenanthroline, were synthesized and characterized. UV-visible, EPR, and single-crystal X-ray diffraction (τ_5 = 0.31 (1); 0.33 (3)) examinations were used to validate the geometry in solution and solid state as a distorted square-pyramidal with CuN_4O chromophore. DFT calculations reveal a narrow HOMO-LUMO gap, correlating with high catalytic reactivity. Electrochemical studies confirm reversible Cu(II)/Cu(I) redox behavior, and the complexes efficiently catalyze the oxidation of dehydroascorbic acid, benzylamine, 3,5-di-*tert*-butylcatechol, and o-aminophenol. Notably, the complexes exhibited significant cytotoxicity toward cancer cells ($IC_{50} \approx 7$ μM in 24 h) while remaining non-toxic to normal cells, inducing ROS-dependent apoptosis and cell cycle arrest. The enhanced activity is attributed to ligand flexibility, redox tunability, and structural adaptability.

Keywords: Copper(II) complexes; Distorted square-pyramidal geomentry; Redox Behaviour; Biomimietic Oxidase; ROS-dependent apoptosis

References

[1] Zhang, X., Li, J., Ma, C., Zhang, H., Liu, K., **Biomimetic Structural Proteins: Modular Assembly and High Mechanical Performance.** Acc. Chem. Res. 2023**,** 56 (19): 2664-2675.

OP3

Efficient Cobalt-Based Catalyst in Carbon Hollow Nano capsules for Anion-Exchange Membrane Water Electrolysis

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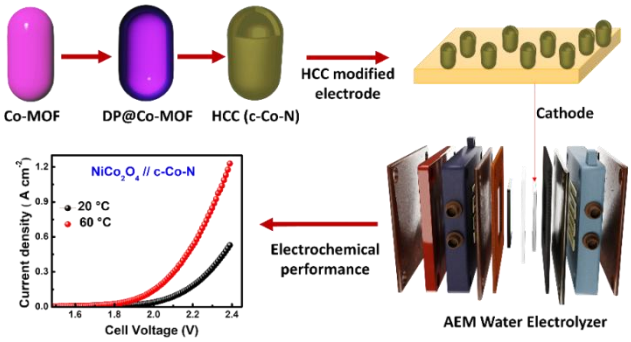
In the present work, a one-dimensional (1-D) nanorod-like Co-MOF was synthesized via a hydrothermal method using cobalt and phenyl phosphonic acid as precursors. These Co-MOF nanorods were then coated with polydopamine and pyrolyzed under nitrogen to fabricate hollow carbon nanorods containing cobalt-based materials (HCC). The resulting 1-D hollow nanorods exhibited excellent electrocatalytic properties for the hydrogen evolution reaction (HER): a low overpotential of 295 mV at 100 mA cm^{-2} and outstanding stability (90.98%) over 150 h. These results were further supported by density functional theory (DFT) calculations. The well-performing catalyst was then used as a cathode material in an anion-exchange membrane water-electrolyser (AEMWE), delivering 500 mA cm^{-2} at 2.19 V and 1000 mA cm^{-2} at 2.33 V in 1.0 M KOH at 60 °C. This non-noble-metal catalyst shows promise for practical AEMWE applications.

Keywords: Cobalt catalyst, Carbon hollow nanorods, Hydrogen evolution, Anion exchange membrane electrolysis, Non noble metal



Schematic illustration of HCC fabrication and AEMWE application.

OP4
Molecular and Enzymatic Characterization of Human SULT1A2 as a Vitamin B_6 Sulfonating Enzyme

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Sulfonation is a key phase II metabolic process that enhances the solubility and excretion of endogenous compounds and xenobiotics via cytosolic sulfotransferases (SULTs). While vitamins D and E are known substrates, the role of sulfonation in vitamin B_6 metabolism remains unclear. Our previous findings identified human SULT1A2 as the enzyme catalyzing pyridoxine and pyridoxal sulfonation. Structural and mutational analyses revealed that Tyr149 within the active site forms a hydrogen bond with pyridoxal's N1 nitrogen, enabling efficient sulfonate transfer from PAPS. In this study, cytosolic fractions from human liver and intestine exhibited strong pyridoxal-sulfonating activity, confirming the physiological relevance of this reaction. Quantitative PCR further showed high SULT1A2 expression in these tissues, consistent with its enzymatic activity. LC–MS analysis verified the formation of pyridoxal sulfate as a specific reaction product. Collectively, these results identify SULT1A2 as a key enzyme mediating vitamin B_6 sulfonation in humans and reveal a tissue-specific mechanism that may regulate pyridoxal bioavailability and metabolic homeostasis.

Keywords: SULT1A2, Sulfonation, Pyridoxal, Vitamin B_6, Human tissues

References

[1] Kauffman, F. C. (2004). Sulfonation in pharmacology and toxicology. *Drug metabolism reviews*, *36*(3-4), 823-843.

[2] Samsel, A., & Seneff, S. (2013). Glyphosate's suppression of cytochrome P450 enzymes and amino acid biosynthesis by the gut microbiome: pathways to modern diseases. *Entropy*, *15*(4), 1416-1463.

OP5
Carbazole-Based COFs: Design, Synthesis and Environmental Adsorption Applications

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Porous covalent organic frameworks (COFs) with heterocyclic units are promising materials for environmental remediation due to their high surface area, tunable porosity, and chemical stability. This study proposes a carbazole–pyrimidine-based COF designed for the adsorption of organic dyes, heavy metals, and gases. The synthesis involves N-protection of carbazole to prevent side reactions, followed by formylation, introducing –CHO linkers. The resulting dialdehyde carbazole condenses with an amine-functionalized pyrimidine under solvothermal conditions to yield an imine (C=N)-linked COF. The framework integrates electron-rich carbazole and nitrogen-bearing pyrimidine units, enhancing π–π stacking and metal coordination. These interactions enable selective and efficient pollutant adsorption. Adsorption kinetics, isotherm models (Langmuir and Freundlich), recyclability, and regeneration will be analysed. Mechanistically, π–π interactions, N–metal coordination, and ordered pore diffusion drive the adsorption process, ensuring high capacity, selectivity, and reusability of the synthesised COF.

Keywords: Carbazole, Covalent Organic Framework (COF), Adsorption, Environmental Remediation, Heterocyclic Polymer, Porous Materials.

References

[1] Gilmanova L., et al., **Chemically Stable Carbazole-Based Imine Covalent Organic Frameworks,** J. Am. Chem. Soc., 143 (2021).
[2] Melhi S., et al., **Novel carbazole-based porous organic frameworks: adsorption, regeneration and recyclability studies,** Mater. Today Commun., 30 (2022).
[3] Zeng W., et al., **A carbazole–porphyrin-based COF: synthesis, characterization, and fluorescence and iodine adsorption properties**, New J. Chem., 49 (2025): 8782-8792.
[4] Xiao Y., et al., **Two-Dimensional Covalent Organic Frameworks with Carbazole units: from design to application,** Mater. Adv. (2024).

OP6

Molecular Insights into Antimicrobial Resistance: Docking Analysis of Antibiotics with *E. coli* β-Lactamase Isolated from Animal-Origin Foods

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Antimicrobial resistance represents a very critical challenge in medicinal chemistry, as drug enzyme interactions which often determines the efficacy of therapeutic agents like antibiotics. In this study the resistance patterns were investigated in Escherichia coli isolates from animal origin food samples, alongside an in-silico analysis of antibiotic binding mechanisms. Thirty fresh chicken and mutton samples were processed to isolate and biochemically confirm E.coli. To explore molecular aspects of resistance , molecular docking was executed between different classes of antibiotics and E.coli beta lactamase using auto docking tool.The docking results revealed variable binding affinities, suggesting reduced drug–target interactions consistent with antimicrobial resistance. This integrative approach links microbial screening with computational chemistry, highlighting how structural insights can support the design of more effective antimicrobial agents.

Keywords: Antimicrobial resistance, *Escherichia coli*, β-lactamase, molecular docking, computational analysis

References

[1] Rahman, M. M., Husna, A., Elshabrawy, H. A., Alam, J., Runa, N. Y., Badruzzaman, A. T. M., ... & Ashour, H. M. (2020). **Isolation and molecular characterization of multidrug-resistant Escherichia coli from chicken meat.** *Scientific Reports*, *10*(1), 21999.

[2] Massella, E. (2020). **Phenotypic and genotypic characterization of antimicrobial resistance in Escherichia coli indicator of animal, food and human origin.**

OP7

Biomimetic nCVTs Hybrids: Bridging the Gap in Targeted Cancer Drug Delivery

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National University of Singapore

Extracellular vesicles (EVs) have emerged as promising cell-derived drug delivery systems (DDSs) due to their intrinsic biocompatibility, low immunogenicity, and natural tissue tropism. However, clinical translation of EV-based formulations remains hindered by laborious isolation, low drug-loading efficiency, and challenges in surface modification. In contrast, synthetic nanocarriers such as liposomes enable scalable production and tuneable physicochemical properties but lack the biological complexity required for efficient targeting. To bridge these gaps, we developed a biomimetic nano Cell Vesicle Technology system (nCVTs), produced through controlled membrane fusion between cell membranes and synthetic liposomes. By adjusting the ratio of cellular to synthetic components, we optimized hybrid formation and surface protein enrichment. Comprehensive characterization confirmed successful membrane fusion, uniform nanoscale morphology, and improved stability. Proteomic profiling verified incorporation of key membrane proteins, while fusion assays and cellular uptake studies demonstrated enhanced internalization compared to conventional liposomes. In vivo biodistribution in healthy mice revealed favourable circulation and organ accumulation profiles, highlighting the biological influence of EV-derived components. Furthermore, nCVTs efficiently encapsulated doxorubicin (DOX) and antisense oligonucleotides (ASOs), validating their suitability for nucleic acid and small-molecule delivery. Altogether, nCVTs represent a versatile biohybrid DDS that combines the structural tunability of synthetic lipids with the biological identity of cell derived DDS. This platform offers a scalable route toward next-generation cancer drug delivery systems while overcoming key challenges that limit traditional EV-based therapeutics.

OP8
Rational Design and BSA-Functionalized Liposomal Encapsulation of Melatonin-based Indole derivatives for Enhanced Neuroprotective Therapy

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Melatonin-imine derivatives (MIDs) were designed and systematically characterized for their potential neuroprotective applications. Nanoscale liposomal vesicles were formulated using a composite lipid system comprising dipalmitoyl phosphatidylcholine (DPPC), cholesterol, Lyso-16PC, cetyltrimethylammonium bromide (CTAB), polyethylene glycol (PEG), and oleic acid, employing thin-film hydration, freeze–thaw cycling, and extrusion techniques. The resulting MID-loaded liposomes demonstrated high encapsulation efficiencies (89.7–94.6%) and sustained release behavior, further modulated through bovine serum albumin (BSA) surface coating. Comprehensive physicochemical characterization confirmed the formation of stable, monodisperse liposomes with favorable particle size, zeta potential, morphology, and thermal stability. In vitro studies using SH-SY5Y neuroblastoma cells revealed that BSA-coated formulations significantly enhanced antioxidant activity, improved cell viability, and attenuated apoptosis compared with uncoated counterparts. The BSA corona imparted biomimetic stealth characteristics, reducing premature clearance and facilitating enhanced cellular uptake.

Overall, the study establishes a robust and multifunctional liposomal platform for the controlled delivery of melatonin derivatives, demonstrating promising neuroprotective efficacy and potential utility in the management of neurodegenerative disorders.

Keywords: Melatonin-based indole derivatives, liposomes, nanoparticle drug delivery, SH-SY5Y cells

References

[1] Anastassova N, Stefanova D, Hristova-Avakumova N, Georgieva I, Kondeva-Burdina M, Rangelov M, Todorova N, Tzoneva R, Yancheva D. **New Indole-3-Propionic Acid and 5-Methoxy-Indole Carboxylic Acid Derived Hydrazone Hybrids as Multifunctional Neuroprotectors**. Antioxidants [Internet]. 2023;12.

OP9
Development and Photophysical Insights into Ru(II) and Ir(III) Benzodipyridophenazine Complexes as Photoresponsive PDT Agents

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The study investigated the impact of benzodipyridophenazine-based Ru(II) and Ir(III) complexes (**Ru1**, **Ru2**, **Ir1**, and **Ir2**) on their anticancer activity. *In vitro*, screening identified that, complex ,**(Ir1)** exhibited the highest potency and selectivity (IC_{50} ~ 2.14 μM, PI > 13) under yellow light irradiation. Biomolecule binding tests using the complexes and ligand showed that attaching with Ru(II)/Ir(III) improved ligand characteristics. Chloro-substituted complexes (**Ir1, Ru1**) are effective for hypoxic tumor treatment, particularly **Ir1** which can generate high amounts of reactive oxygen species (ROS, Type I PDT) in cells under photo irradiation. Colocalisation study and DCFDA studies with **Ir1** revealed that, it can accumulates in the mitochondria, leading to the depolarization of the mitochondrial membrane.

Keywords: DFT, molecular docking, PDT, hypoxia, GSH

References

[1] R. Das, P. Paira, **GSH resistant, luminescent 2-(pyren-1-yl)-1H-imidazo[4,5-f][1,10]phenanthroline-based Ru(ii)/Ir(iii)/Re(i) complexes for phototoxicity in triple-negative breast cancer cells,** *Dalton Transactions* ,**2023**, (*52),*: 15365–15376

[2] S. De, R. Selva Kumar, A. Gauthaman, S. K. Ashok Kumar, P. Paira, A. Moorthy, S. Banerjee, **Luminescent ruthenium(II)-para-cymene complexes of aryl substituted imidazo-1,10-phenanthroline as anticancer agents and the effect of remote substituents on cytotoxic activities,** *Inorganica Chim Acta* ,**2021**, (*515),*:120066.

OP10

Impact of 3-Trimethoxysilyl Propyl Methacrylate on Hydrogels of Nano-MgO/CA_4 Nanocomposite: Synthesis, Characterization and Applications

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In this paper, Citric acid, Triethanolamine, 2-Furoic acid hydrogels (CA_4 hydrogels) are prepared by esterification method, followed by the incorporation of Nano MgO particles, and (3-Trimethoxy silyl propyl methacrylate) TMP is used as a coupling agent. Then, employing the physical cross-linking method, [CA_4 (TMP- MgO)] hydrogels are developed. The prepared [CA_4 (TMP-MgO)] hydrogels has a dense three-dimensional network structure of the hydrogel. Swelling behavior and a pH range of 2.0 to 11.0 were used to closely study the hydrogels properties. As a result, neutral media (pH 7.0) had the highest swelling percentage, compared to acidic and alkaline medium. Swelling equilibrium results significantly improve when nano MgO and TMP concentrations increases. By evaluating the synthesized [CA_4 (TMP- MgO)] nanocomposite hydrogels using a variety of analytical methods, including UV, FTIR, ^{1}H NMR, ^{13}C NMR, TGA and SEM-EDX. It was confirmed that 3-trimethoxysilyl propyl methacrylate (TMP) and nano-Magnesium oxide were incorporated within the CA_4 network. Thermogravimetric analysis (TGA) was also used in this work. Thermal studies showed that the hydrogels of the [CA_4 (TMP- MgO)] nanocomposite were thermally stable up to 270 ^{0}C. The Antibacterial studies were carried out with the gram positive bacteria (*Staphylococcus aureus, Bacillus subtilis),* and Gram negative bacteria *(Klebsiella pneumonia, Escherichia coli)* have been selected for the study. The hydrogel shows excellent results in inhibition percentage. The antifungal studies show the moderate zone of inhibition. The Cytotoxic studies and Antioxidant analysis were also studied which exhibits good zone of inhibition percentage. Thus, the compounds studied in this work might be useful for tissue engineering, wound healing, and other high-performance uses.

Keywords: Hydrogels, pH sensitive, 2-Furoic acid, Citric acid, MgO Nanocomposite, 3-Trimethoxy silyl propyl methacrylate, Antibacterial studies, Cytotoxic studies.

OP11

Design of Eco Friendly Pinacol-Based Hydrogels with Tunable Swelling, Biodegradability, and Antibacterial Efficiency

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Hydrogels are three-dimensional, hydrophilic polymeric networks that absorb and retain enormous amounts of water or biological fluids without disintegrating in their medium. In this study, a pH-sensitive hydrogel was synthesized from citric acid, pinacol, 1,6-hexanediol and 2- furoic acid by employing an eco-friendly melt condensation technique without the use of any external crosslinking agents. The presence of functional groups in the synthesized hydrogels were confirmed by various spectral investigations FT-IR and ^{1}H and ^{13}C NMR .Its thermal stability and morphological characteristics have been studied by TGA and SEM analysis. The equilibrium swelling studies of pinacol-based hydrogels was examined at various pH levels (2.0, 4.0, 7.0, 9.0, and 11.0). The hydrogels exhibited pH-sensitive swelling behavior, demonstrating greater swelling in basic media than acidic. Antibacterial studies were evaluated against two pathogenic microorganism namely *B.subtilis* and *E.coli* by agar well diffusion method. The biodegradability of the hydrogel was studied through **soil burial method,** which provides a realistic evaluation of environmental degradation under natural conditions. Thus, the designed hydrogel acts as a promising material for **drug delivery, wound healing, and environmental remediation** applications.

Keywords: Hydrophilic-pH sensitive- Eco friendly- Swelling – Antibacterial- Biodegradable.

References

1. Franklin, D. S., Guhanathan, S., 2015, **Investigation of citric acid–glycerol based pH-sensitive biopolymeric hydrogels for dye removal applications: A green approach.** Ecotoxicol Environ. Saf.121, 80-86.

OP12

pH sensitive *Insitu* synthesis of silver nanoparticles by almond gum/citric acid and PVA mixture with excellent antibacterial applications and utilization of nancomposite for urea holding applications.

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A pH-sensitive silver nanocomposite hydrogel (SNCH) with intriguing features could be offered for widespread use in environmentally friendly nanomaterial applications. The current study synthesised novel biodegradable and biocompatible hydrogels from citric acid (CA), polyvinyl alcohol (PVA), and almond gum (AG), which were functionalised with silver nanoparticles. Furthermore, Ag nanoparticles were synthesised using an in-situ green synthesis technique. The nanocomposite hydrogels generated showed noteworthy pH-sensitive behaviour, swelling, and urea holding capabilities. As a result, these biomaterials have been used as a non-toxic, biodegradable, and environmentally friendly hydrogel. The silver nanocomposite hydrogel was analysed using FT-IR (functional groups), SEM (surface morphology), and XRD. The FT-IR spectra, XRD patterns, and antibacterial activity of the nanocomposite hydrogels were investigated. The silver nanocomposite hydrogels have outstanding antibacterial action against both gram positive (S. aureus) and gram negative bacteria (E. coli). This hydrogel nanocomposite is suited for agricultural applications due to the exceptional antibacterial activity of silver nanoparticles and the promotion of plant development.

Keywords: 3D network, insitu green synthesis, silver nanoparticles, biodegradation, pH sensing, agricultural applications.

References

1. Sudarsan S., Franklin ,. Sakthivel M., Guhanathan S.∗**Non toxic, antibacterial, biodegradable hydrogels with pH-stimuli sensitivity: Investigation of swelling parameters**,Carbohydr. Polym, 2016, (148) : 206-215.

OP13

Green synthesis of curcumin loaded CeO_2 nanoparticles integrated into CMC-Na/PVA nanocomposites for biomedical applications

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To formulate a sustainable green synthesis approach for curcumin-loaded cerium oxide (CeO_2) nanoparticles incorporated into polyvinyl alcohol (PVA) and carboxymethyl cellulose sodium (CMC-Na) nanocomposites. *Aegle marmelos* leaf extract was used as a natural stabilizing and reducing agent. The phytoconstituents of the leaf extract efficiently mediated the bio-reduction and capping of CeO_2 nanoparticles, while curcumin provided additional antioxidant and medicinal properties. UV-Vis, XRD, FT-IR, FE-SEM, DLS, and zeta-potential analyses were used to systematically characterize the synthesized nanocomposites. These analyses confirmed the nanoscale dimension, uniform dispersion, and excellent colloidal stability. Physicochemical assessments, including swelling behavior, porosity quantification, and water vapor transmission rate, indicated superior fluid absorption and moisture permeability, underscoring the film's appropriateness for biomedical and wound healing applications. The antibacterial investigation demonstrated considerable suppression of both *Staphylococcus epidermidis* and *E-coli* bacterial strains, whereas cytotoxicity experiments validated biocompatibility. The nanocomposite demonstrated significant antioxidant activity, resulting from the synergistic interaction between the redox characteristics of CeO_2 and the radical scavenging capability of curcumin. This study presents an environmentally sustainable, multifunctional CMC-Na/PVA/CeO_2-curcumin nanocomposite produced using extraction of Aegle *marmelos*, demonstrating significant potential for biomedical and therapeutic applications.

Key words: carboxymethyl cellulose sodium, polyvinyl alcohol, Aegle marmelos, CeO_2 NPs

References

1. Sathishkumar, P., Li, Z., Govindan, R., Jayakumar, R., Wang, C., & Gu, F. L. (2021). **Zinc oxide-quercetin nanocomposite as a smart nano-drug delivery system: Molecular-level interaction studies**. *Applied Surface Science*, *536*, 147741.

OP14

Synthesis and characterization of transition metal ion-doped molybdate based inorganic pigments and their heat-reflective coating applications

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In this study, molybdate-based inorganic pigments were synthesized by doping transition metal ions to develop brown-coloured pigments suitable for cool coating applications. The pigments were prepared using a hydrothermal method. Structural, morphological, and optical properties were analyzed using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), and UV–Vis–NIR spectroscopy. The results revealed that transition metal doping effectively modified the electronic structure of the molybdate matrix, resulting in stable brown hues with high near-infrared (NIR) reflectance. The synthesized pigments exhibited excellent thermal stability, chemical resistance, and weather durability, making them promising candidates for eco-friendly and energy-efficient cool coating paints. This study demonstrates the potential of transition-metal-doped molybdate pigments as sustainable alternatives to conventional brown pigments for heat-reflective coating applications.

Keywords: Molybdate pigment, Brown pigment, Cool coating, NIR reflectance, Eco-friendly pigment

References:

[1] Yang Y, Pan Z, Zhang T, Wang Y**. Synthesis of erbium-doped neodymium molybdate based inorganic pigments with high near-infrared reflectance and allochroic effect,** Ceram Int, 2025, (May 28).

[2] George G. **The structural and optical studies of titanium doped rare earth pigments and coloring applications,** Dyes Pigments, 2015, 112: 81–85.

OP15
Integrated In Silico Screening, QSAR, ADME, and Molecular Docking Approach for Liver Cancer Drug Discovery

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Liver cancer is one of the most general and fatal tumors across the globe, this type of cancer distinguished by aggressive disease and low chance of recovery/survival. In spite of the progress in chemotherapy and cell therapy, difficult to achieve anti-tumour drugs. In this work, systematically analyzed a total of 525 reported anticancer compound to recognize promising drug candidates against with liver - cancer with the help of computational drug discovery. By analyzing the ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) this study improves the accuracy of predicting pharmacokinetic properties, toxicity, and therapeutic efficacy. Molecular Docking evaluate the binding affinity, binding pose and different bonding interactions of cancer related compounds with appropriate target protein. The most effective Quantitative Structure-Activity Relationship (QSAR) technique for anti-cancer activity to reveals molecular descriptor. This approach accelerates identification of drug candidates before the costly clinical trial phase, improving the efficiency of developing safer and more effective cancer treatments.

Keywords: Liver cancer, QSAR, ADME, Molecular docking, Computational drug design

References

[1] Alam, S., Nasreen, S., Ahmad, A., Darokar, M. P., & Khan, F. (2021). **Detection of natural inhibitors against human liver cancer cell lines through QSAR, molecular docking and ADMET studies**. *Current Topics in Medicinal Chemistry*, *21*(8), 686-695.

[2] Chen, P. Y., & Han, L. T. (2023). **Study on the molecular mechanism of anti-liver cancer effect of Evodiae fructus by network pharmacology and QSAR model.** *Frontiers in Chemistry*, *10*, 1060500.

OP16
Enhanced Bioactivity, Antimicrobial Efficacy and Biocompatibility of Larnite/Nano Titania Composites for Orthopedic Applications

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Biomaterials dalliance is an immanent vocation in the modern healthcare sector. Multidisciplinary attribute of biomaterials requires scientists to contrive and concoct the material, engineers to design and fabricate the prosthesis and physicians to swot the response of natural tissues on artificial biomaterials implanted in the body. Globally, it has been appraised that about 60% of artificial bone substitutes are mustered for bioceramics. Thus, much enthrallment has been rapted towards use of different bioceramics for bioactive fixation of artificial implants. Most important acmes in the field of biomedical materials for hard tissue engineering applications are biocompatibility and mechanical stability.

The arch factual of this work was to synthesize and characterize larnite/nano titania composite (Ca_3SiO_4/TiO_2) through a facile sol-gel assisted combustion route using l-alanine as fuel. Various relevant analytical techniques such as powder X-ray diffraction, FT-IR spectroscopy and scanning electron microscopy were employed to study the characteristic behaviour of the newly synthesized ceramic/metal composite. FEI-Tecnai G2 20S-TWIN, 200 kV SAED and the nature of the particles were examined using a high-resolution transmission electron microscope. *In-vitro* biomineralization of the synthesized bioceramic composite was examined on the surface of the scaffold for 9 days of immersion in SBF. Using the well diffusion technique, four samples of larnite/nano titania composites were tested for their antibacterial properties against infectious microbial species, including *Staphylococcus aureus, E. coli, Klebsiella pneumonia* and *Bacillus subtilis*. The MTT [3-(4, 5-dimethylthiazolyl-2)- 2, 5-diphenyltetrazolium bromide] test was used to investigate the *in-vitro* cytotoxicity of larnite/nano titania composite.

Keywords: Bioceramic composite, antimicrobial, cytoxicity, biomineralization, sol-gel combustion

References:

1. Su, Y., Yang, H., Gao, J., Qin, Y.X., Zheng, Y., and Zhu, D. (2019**) Interfacial Zinc Phosphate is the Key to Controlling Biocompatibility of Metallic Zinc Implants**. *Advanced Science*, **6** (14).

OP17
Imidazo-Based Ru(II), Ir(III), and Re(I) Complexes as Potent Photodynamic Agents for Targeted Treatment of TNBC

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A selective chemotherapeutic approach calls for the development of photosensitive scaffolds to mitigate the challenges associated with cancer treatment. In this regard, photodynamic therapy (PDT) has emerged as an effective strategy to combat the aggressiveness of triple-negative breast cancer (TNBC). Metal complexes have demonstrated significant potential in targeting the unique cancer cell microenvironment—characterized by elevated GSH levels, low pH, and hypoxic conditions—and have therefore been widely explored for anticancer therapy. Given that TNBC remains one of the most difficult cancers to treat due to its poor prognosis, absence of specific molecular targets, high recurrence rate, and strong metastatic behavior, we have designed phototoxic imidazo-based Ru(II)/Ir(III)/Re(I) complexes to selectively inhibit TNBC progression. The evaluation of [RuL], [IrL], and [ReL] complexes against MDA-MB-231 TNBC cells revealed that these complexes exhibit pronounced cytotoxicity upon visible light irradiation compared to dark conditions, attributed to the generation of abundant singlet oxygen ($^1O_2$) as reactive oxygen species (ROS).[1,2]

Keywords: TNBC triple-negative breast cancer, ROS reactive oxygen species, PDT Photodynamic therapy

References

[1] Das R., Paira P. **GSH resistant, luminescent 2-(pyren-1-yl)-1H-imidazo[4,5-f][1,10]phenanthroline-based Ru(ii)/Ir(iii)/Re(i) complexes for phototoxicity in triple-negative breast cancer cells**, Dalton Trans., 2023, 52, (15365-15376)

[2] Roy N., Sen U, Madaan Y., Muthukumar V., Varddhan S., Sahoo S. K., Panda D., Bose B., and Paira P. **Mitochondria-Targeting Click-Derived Pyridinyltriazolylmethylquinoxaline-Based Y-Shaped Binuclear Luminescent Ruthenium(II) and Iridium(III) Complexes as Cancer Theranostic Agents**, Inorg. Chem., 2020, 59, 23, (17689–17711)

OP18
Anticancer Mechanistic studies of Oxovanadium(IV) Complexes: Structure, DNA Binding and Cleavage, and Cytotoxicity

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Cancer remains a major global health challenge, and cisplatin-based chemotherapy is often limited by resistance and toxicity. Vanadium-based complexes offer a promising alternative due to their cytotoxicity, lower side effects, and unique DNA-binding properties. Here, two oxovanadium(IV) complexes, [VO(L)(diimine)] (HL = Schiff base from N,N-dimethylethylenediamine and salicylaldehyde; diimine = 2,2′-bipyridine or 1,10-phenanthroline), were synthesized and characterized. Single-crystal X-ray analysis confirmed a VO^{2+} center in a distorted octahedral VO_2N_4 geometry, and HOMO-LUMO gaps (2.056 and 2.146 eV) indicated favorable electronic properties. Both complexes showed strong DNA binding and selective cytotoxicity against A549 lung cancer cells, inducing ROS-mediated DNA damage, G1-phase arrest, and apoptosis, while sparing normal L132 cells. The structure-activity relationship (SAR) studies revealed that structural elements, such as metal components, variations in coordination mode, favorable electronic properties with a feasible energy gap, chelated ligands, etc., exert an essential cooperative effect on antitumor activity. These findings highlight oxovanadium(IV) complexes as efficient, selective, and environmentally benign anticancer agents.

Keywords: Oxovanadium(IV) complexes; DNA Binding and Cleavage; Reactive Oxygen Species; Apoptosis; invitro cytotoxicity.

References

[1] Ni, L. Zhao, H. Tao, L. Li, X. Zhou, Z. Sun, Y. Chen, C. Wei, D. Liu, Y. Diao, G. **Synthesis, In Vitro Cytotoxicity, and Structure-Activity Relationships (SAR) of Multidentate Oxidovanadium(IV) Complexes as Anticancer Agents.** Dalton Trans. 2018 (47): 10035-10045.

OP19

Ru (II) *p*-Cymene Complexes of N^N Phenyl Quinazoline-Pyridine ligands: Synthesis, Characterization, and Cytotoxic Properties

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Ruthenium [Ru (II)] complexes have recently garnered substantial attention in medicinal chemistry due to their remarkable anticancer properties. This work describes the synthesis, characterization, and cytotoxic evaluation of a new class of Ru (II) complexes, Ru-1(a-d), which incorporate N^N phenyl-quinazoline-pyridine derivatives. The compounds were characterized using FTIR, NMR, HR-MS and SXRD, UV-Vis absorbance, and fluorescence spectroscopy techniques. The Ru (II) complexes have a unique "piano-stool" shape, with a coordinated p-cymene ligand, two σ-bonded nitrogen atoms from the phenylquinazoline moiety, and a labile chloride ligand, according to structural studies. Binding studies between DNA and bovine serum albumin (BSA) revealed non-covalent interactions with binding constants of 1 × 106 M^{-1} for DNA and 3 × 104 M^{-1} for BSA. Competitive binding experiments with ethidium bromide (EtBr) revealed that Ru (II) complexes successfully displace EtBr via intercalative binding, as verified by viscosity measurements and in silico simulations. In vitro cytotoxicity assays revealed that both the ligands and their corresponding Ru (II) complexes exhibit remarkable anticancer activity against HeLa, MCF-7, and HepG-2 cell lines, with the Ru (II) complexes showing superior potency compared to cisplatin, characterized by lower IC_{50} values. Furthermore, the complexes displayed minimal cytotoxicity toward HEK normal cells, indicating good selectivity toward cancer cells.

Keywords: N^N Phenyl Quinazoline-Pyridine; DNA Binding, BSA binding, MTT Assay.

References

1. De, S. *et al.* New J. Chem. 2019, 43, 3291–3302.
2. Selvam, P. *et al.* Dalton Trans. 2022, 51, 17263–17276.

OP20
Exploring the interactions between Peptides and IL

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Ionic liquids (ILs) have emerged as promising green solvents with unique physicochemical properties that can profoundly influence protein structure, stability, and function. Fundamental impact of IL and peptide is still unclear. From the molecular point of view IL may perturb the protein regulation In this study, the binding interactions between various amino acids and a selected ionic liquid were systematically investigated using first-principles calculations. The binding energies were computed to quantify the strength and nature of the interactions, providing insights into the molecular-level mechanisms governing amino acid–IL affinity. The results reveal that the binding strength varies significantly with the amino acid side-chain polarity and charge, indicating that both hydrogen bonding and electrostatic interactions play crucial roles in stabilizing the complexes. The ionic liquid cation and anion were found to interact preferentially with different functional groups of the amino acids, suggesting a specific pattern of solvation that may contribute to the stabilization of protein conformations in IL environments. These findings enhance the understanding of how ionic liquids modulate biomolecular interactions and provide a theoretical foundation for designing IL-based media for protein preservation, enzyme catalysis, and biotechnological applications.

Keywords: Binding energy, interaction

References:

1.Tietze, Alesia A., Frank Bordusa, Ralf Giernoth, Diana Imhof, Thomas Lenzer, Astrid Maaß, Carmen Mrestani-Klaus, Ines Neundorf, Kawon Oum, Dirk Reith, and Annegret Stark. 2014. "**On the Nature of Interactions between Ionic Liquids and Small Amino-Acid-Based Biomolecules**." ChemPhysChem 15 (2): 305–316

2. Tomé, Luciana I. N., Montserrat Domínguez-Pérez, Ana Filipa M. Cláudio, Mara G. Freire, Isabel M. Marrucho, Oscar Cabeza, and João A. P. Coutinho. 2009. "**On the Interactions between Amino Acids and Ionic Liquids in Aqueous Media**." The Journal of Physical Chemistry B 113 (42): 13971–13979.

Poster Presentation-PP

PP-1

$K_2S_2O_8$-promoted one-pot synthesis of *N*-substituted quinazolinones *via* tandem annulation using DMSO and terminal alkynes.

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A green, metal-free one-pot three-component reaction combining 2-aminobenzamide, phenylacetylene, and DMSO with $K_2S_2O_8$ as the oxidant enables efficient access to *N*-substituted quinazolinones under mild and cost-effective conditions. In this tandem annulation, DMSO plays a dual role-both as the solvent and as a versatile synthon-driving key C–C and C–X bond formations to produce products in moderate to good yields. Mechanistic experiments, including deuterium-labelling studies and control reactions, confirm the involvement of DMSO-derived intermediates and validate the proposed pathway. This scalable, environmentally benign protocol provides a direct route to pharmaceutically relevant heterocycles.

Keywords: One-pot synthesis, Tandem C-C/C-X bond formation, Metal- and base-free conditions, DMSO as solvent and synthon.

References

[1] P. Yadav, S. Yadav, A. Awasthi, et al. **DMSO as a dual carbon synthon in one-pot tandem synthesis of *N*-alkylated quinazolinones from anthranilamides and acetophenones.** New J. Chem., 2022, (46), 16289-16296.

[2] Ajay Uppuluru, Kishor Padala, Annamalai Pratheepkumar, **$K_2S_2O_8$ -promoted one-pot synthesis of N-substituted quinazolinones via tandem annulation using DMSO and terminal alkynes.** Org. Biomol. Chem.,2025,23, 6801-6807.

PP-2
Development of Organellespecific Luminescent Ru (II)/Ir (III)/Re (I) based Pyrene Imidazo Phenanthroline Complexes as Novel Anticancer Therapeutics

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Of late, the worldwide pervasiveness of perilous cancer has created a great menace to the living world after cardiovascular disease. Therefore, researchers are engrossed in profound research to unveil the appropriate medicine for the eradication of cancer. In this regard, many metal complexes have shown greater anticancer efficacy as soon as the discovery of cisplatin. Herein, we have developed Ru (II)/Ir (III)/Re (I) based pyrene imidazophenathroline complexes in order to find out their anticancer potential. These complexes are considerably fluorescent with a high quantum yield value revealing the capability of cellular imaging and have displayed very significant potency against HeLa, Caco-2, and most aggressive HT-29 cancer cell lines. Along with this, they are very competent to bind with DNA, and human serum albumin (HSA) and are very prone to damaging mitochondria through the reduction of the mitochondrial membrane potential (MMP). Not only that, these complexes can restrain proliferation by arresting the cell cycle. In a nutshell, it can be predicted that these complexes may be explored as excellent anticancer agents in near future.

Keywords: Photodynamic Therapy, Anti-cancer agent, Bioinorganic Chemistry

References:

1. N. Roy, U. Sen, Y. Madaan, V. Muthukumar, S. Varddhan, S. K. Sahoo, D. Panda, B. Bose, and P. Paira, *Inorg. Chem.*, **2020**, 59, 23, 17689–17711

PP-3
Novel Triazole Synthesis *via* Azide–Chalcone Cycloaddition Using New Cu-based Polyurethane Foam as a Catalyst

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Triazoles are pharmacologically important heterocycles known for their diverse biological activities. In this study, we present the synthesis of novel triazole derivatives through the cycloaddition reaction between benzyl azide and various chalcones, catalysed by a heterogeneous catalyst associated with copper-loaded polyurethane foam material. This approach offers a metal-mediated pathway that is distinct from conventional azide–alkyne cycloadditions. The performance of copper foam was compared against previously used copper-based systems, including CuO nanoparticles and $[Cu(phen)_2]NO_3$ complex. The copper-loaded polymer catalyst requires less time and exhibits excellent catalytic efficiency, operational simplicity, and reusability, with reduced copper leaching and cleaner product profiles. The synthesized triazoles were purified and fully characterized using NMR and IR spectral data to assess their purity and proposed structural features. Given the known bioactivity of triazole frameworks, the new compounds prepared showed effective anti-cancer activity.

Keywords: Triazoles, Cycloaddition, Anti-cancer activity, Foam catalyst

References

[1] Dey, A., & Biswas, A. (2014). **Regioselective synthesis of β-aryl enaminones and 1,4,5-trisubstituted 1,2,3-triazoles from chalcones and benzyl azides**, Advanced Synthesis & Catalysis, 356(12), 2485–2490.

[2] Paul, S., & Guin, J. (2015). **Regioselective synthesis of 1,4,5-trisubstituted 1,2,3-triazoles from chalcones and benzyl azide under metal- and solvent-free conditions**, RSC Advances, 5(105), 86337–86344.

PP-4
Blue LED-Driven Greener Approach to Access bis(aminothiocarbonyl)disulfides hybrids *via* radical-radical cross coupling

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In this work, we have developed an efficient photoredox-mediated one-pot synthesis of bis(aminothiocarbonyl)disulfides in ethanol as green solvent that provides good to excellent yields. Disulfides, containing sulfur–sulfur (S–S) bonds, play a vital role in both organic and biological systems. Their reversible nature allows them to participate in dynamic covalent chemistry, making them highly versatile. In medicinal chemistry, disulfides are especially important because they can irreversibly inhibit enzymes such as monoglyceride lipase (MGL) by forming covalent bonds with cysteine residues. This selective inhibition makes disulfides promising candidates for drug development. Using our protocol, we were also able to access commercially available compounds like Disulfiram: used for treating chronic alcohol dependence and Thiram: an agrochemical that protects seeds and crops from fungal infections.

Keywords: Disulfides, Photoredox, Drug design, Radical-Radical cross coupling, Disulfiram, Thiram.

References:

1. Wang, M., Song, X., & Ma, N. **Reduced graphene oxide as recyclable catalyst for synthesis of Bis (aminothiocarbonyl) disulfides from secondary amines and carbon disulfide**, Catalysis letters, 2014, (7): 1233-1239.
2. Kapanda, C. N., Muccioli, G. G., Labar, G., Poupaert, J. H., & Lambert, D. M. **Bis (dialkylaminethiocarbonyl) disulfides as potent and selective monoglyceride lipase inhibitors**, Journal of medicinal chemistry, 2009, (22): 7310-7314.

PP-5
Sustainable Iodosulfonylation of internal Alkynes via Metal-Free Visible Light Catalysis.

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We describe a sustainable and metal-free iodosulfonylation of internal alkynes using visible light irradiation. The process utilizes easily accessible sulfonic salts and molecular iodine to obtain regioselective addition over alkynes to give *β*-iodo vinyl sulfones in good to excellent yields. The process operates under mild conditions without the need for metal catalysts or drastic reagents and follows green chemistry principles. Mechanistic studies propose a drastic pathway driven by photo-induced single-electron transfer (SET). This methodology provides a useful and green route for assembling worthy sulfone-containing molecules with promise in pharmaceuticals and materials science.

Keywords: Metal-Free Catalysis, Visible Light Photochemistry, Iodosulfonylation, Green Chemistry

References

[1] R.Kumar, V. Dwivedi, M. S. Reddy, **Metal-Free Iodosulfonylation of Internal Alkynes: Stereodefined Access to Tetrasubstituted Olefins**, Adv. Synth. Catal. 2017, 359, 2847–2856.

[2] R. J. Reddy, J. J. Kumar and A. H. Kumari , **Recent trends in the synthesis and applications of *β*-iodovinyl sulfones: a decade of progress,** Org. Biomol. Chem., 2024, 22 , 2492 -2509.

PP-6
Exploring Photo-responsive Cyclometalated Iridium (III) Complexes for Photodynamic Therapy

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Cyclometalated Iridium (III) complexes have emerged as potent photoactive agents for targeted cancer therapy due to their excellent photophysical characteristics, strong DNA affinity, and tunable electronic structures. In this work, 2,2′-bipyrimidine-based mono- and binuclear cyclometalated Ir(III) complexes were synthesized and evaluated for their potential in photodynamic therapy (PDT). The mononuclear complex and the binuclear complexes were characterized by spectroscopic and crystallographic analyses confirming their stability and photo-responsive behavior. These complexes displayed superior singlet oxygen generation and reactive oxygen species (ROS) production efficiency. Both complexes exhibited strong interactions with DNA and human serum albumin, facilitating efficient cellular uptake. Upon photoactivation, the complexes induced glutathione depletion and oxidative stress, triggering selective cytotoxicity against triple-negative breast cancer (TNBC) cells. Our findings highlight the potential of cyclometalated iridium complexes as next-generation photoactivated chemotherapeutics combining efficiency, selectivity, and photostability for targeted cancer therapy.[1,2]

Keywords: Cyclometalated complexes; Iridium complexes; Photodynamic therapy

References:

[1] S. U, R. Das, I. P. Latha Laxmi, N. Roy, R. Roy, L. Mathivathanan, T. Ramasamy, R. Chakrabarty, P. Paira**, Butterfly-like photo-responsive cyclometalated Ir (III) complex: emergence of a future cancer therapeutic agent**, Dalton Trans.**,** 2025, 54, 14728–14739. DOI: 10.1039/d5dt01164g.

PP-7

A Mild and Efficient Synthesis of Functionalized 2-Fluorobenzamides from 1,2,3-Benzotriazinones via Denitrogenative Fluorination Reactions under Thermal/Visible Light Conditions

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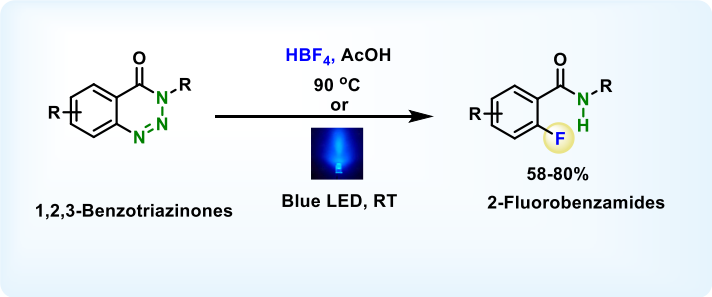
An efficient method for the synthesis of 2-fluorobenzamides is established from 1,2,3-benzotriazinones using tetrafluoroboric acid via denitrogenative fluorination.[1] The reactions proceed under mild thermal conditions, providing a wide range of functionalized 2-fluorobenzamides in 65%–80% yields. On the other hand, the reaction proceeds with 58%–63% yields at room temperature under visible light using blue LED conditions.[1]The developed methodology offers simple operation, metal-free conditions, and a broad substrate scope. In addition, *ortho*-fluoro benzamide structural motifs are found in many drugs and bioactive molecules, which further illustrates the biological utility of the developed methodology.[2]



Keywords: Benzotriazinones, Fluorobenzamides, Tetrafluoroboric acid, Blue LED, Fluorination.

References

[1] Wang, H.; Yu, S. **Synthesis of Isoquinolones Using Visible-Light-Promoted Denitrogenative Alkyne Insertion of 1,2,3-Benzotriazinones**. Org. Lett. 2015, 17 (17), 4272–4275.

[2] Kuriakose, S.; Sundaresan, R.; Kandasamy, J. **A Mild and Efficient Synthesis of Functionalized 2-Fluorobenzamides from 1,2,3-Benzotriazinones via Denitrogenative Fluorination Reactions under Thermal/Visible Light Conditions**. Eur. J. Org. Chem. 2025, 28 (28).

PP-8
Benzimidazole-based Metal Complexes: Emerging Candidates for Anticancer Therapy

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Cancer is the second leading cause of death globally, characterized by uncontrolled cell proliferation and metastasis. Iridium (Ir) and Rhenium (Re) organometallic complexes have emerged as promising chemotherapeutic agents owing to their excellent photoluminescence, versatile coordination chemistry, high oxidation states, and strong stability under tumor conditions. In this study, Ir(III) and Re(I) complexes incorporating a 2-(1H-imidazol-4-yl)-1H-benzo[d]imidazole scaffold was synthesized and characterized by $^{1}H/^{13}C$ NMR, HRMS, and IR spectroscopy, and their photophysical properties were evaluated. The complexes were designed to selectively target cancer cells by exploiting tumor microenvironment features such as hypoxia, high glutathione levels, and acidic pH. Their good aqueous solubility and strong plasma-protein binding further enhance cellular uptake and bioavailability. These results highlight the potential of the synthesized Ir(III) and Re(I) complexes as stable and efficient candidates for targeted anticancer therapy. The interaction of these complexes with biological macromolecules such as DNA and human serum albumin (HSA) demonstrated strong binding affinities, suggesting effective biomolecular recognition. Stability assessments under glutathione (GSH) and PBS environments further highlighted their robustness. Collectively, these results support the potential of the synthesized complexes as stable, photoactive, and biologically relevant candidates for targeted anticancer therapy.

Keywords: Iridium (III) complex, Rhenium (I) Complexes, Anticancer, Chemotherapy, Imidazole-Benzimidazole Scaffold.

References

1 S. U and P. Paira, **2, 3-bis ((4-(pyridin-2-yl)-1H-1, 2, 3-triazol-1-yl) methyl) quinoxaline based Cyclometalated binuclear Ir (III) Complex for Photodynamic therapy in Triple Negative Breast Cancer Cell**. Chemistry, an Asian journal, **2025, e202401047.**

PP-9
Synthesis And Evaluation of Dual Inhibitors: A Multi Targeted Approach in Cancer Drug Discovery

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Cancer has been conventionally presumed to be a genetic disease, orchestrated by successive genetic anomalies that alter gene expression.[1] Tumor progression can also result from aberrations in transcriptional regulations by epigenetic mechanisms. Disruption of the balance between histone acetylases and deacetylases, regulated by HDACs (Histone deacetylases), is often targeted in the development and discovery of anticancer therapeutics.[2] Heat Shock Protein (HSP90), a type of chaperone protein abundantly present in normal, healthy cells, whose role is to ensure proper protein folding. By targeting HSP90, the normal protein-folding mechanism is disrupted, which is normally used by cancer cells for growth and survival**.** Dual inhibitors have shown promising results in targeting cancers due to their high efficacy, low toxicity, ability to overcome drug resistance, and improved selectivity compared with single inhibitors. In this study, we have designed and synthesized a molecule that inhibits both HDAC6 and HSP90, thereby acting as a dual inhibitor. Auto Dock and PyMol was used to evaluate molecular docking and dynamic simulations, providing a detailed understanding of the formation of complexes between hydroxamic acid and the binding pockets of the respective proteins**.** Upon comparison of the binding affinities between SAHA (Vorinostat) and the synthesized drug, the latter exhibited stable, favorable binding conformations. Biological studies will be further evaluated by testing this compound on cancer cell lines.

Keywords: Epigenetic Mechanisms, Histone Acetylase/ Deacetylase, Histone Deacetylases, HSP90, HDAC6, Protein Folding Mechanism, Drug Resistance, Dual Inhibitors, Molecular Docking, Vorinostat

References:

[1] Hillyar, C.; Rallis, K. S.; Varghese, J. Advances in Epigenetic cancer therapeutics. *Cureus* **2020**. https://doi.org/10.7759/cureus.11725.

PP-10
Novel Poly (ADP-ribose) Polymerase 1 (PARP1) Targeting PROTACs for Treating Cancer

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Poly (ADP-ribose) polymerase (PARP) enzyme belongs to the 18-member family, which plays a pivotal role in chromatin remodeling, DNA damage repair, and the induction of apoptosis. The most important enzymes in the PARP family are PARP-1/2 because they are DNA-dependent PARP enzymes and will repair the DNA's single-strand breaks (SSB) using the base excision repair (BER) pathway to maintain genomic stability.[1] Hence, PARP-1/2 is an attractive therapeutic target for cancer treatment. PARP is also overexpressed in various cancers, such as breast cancer, lung cancer, melanoma, glioblastoma, pancreatic cancer, and colon cancer. Currently, the Food and Drug Administration (FDA) has approved six PARP inhibitors for the treatment of various cancers.[2] The approved drugs are available to treat cancer, but many of them suffer from side effects, such as toxicity to normal cells and drug resistance. The alternative strategy to solve this problem is targeted protein degradation (TPD) using proteolysis-targeting chimeras (PROTACs). Here, we proposed to develop PROTACs for the efficient degradation of PARP1, targeting PARP-1/2 with a novel PARP inhibitor conjugated to an E3 ligase ligand, Lenalidomide (CRBN type), using an optimized alkyl linker. All synthesized PARP1-PROTAC degraders were characterized by ^{1}H and ^{13}C NMR and mass spectrometry. The synthesized PARP1-PROTAC exhibited potent cytotoxicity, with an IC_{50} in the nanomolar range, against various cancer cell lines. Our findings highlight that the synthesized PARP1-PROTAC could be a potential candidate for cancer treatment.

Keywords: Cancer, PARP1, DNA repair, Drug resistance, PROTAC

References:

[1] Sulkowski, P. L.; Oeck, S.; Dow, J.; Economos, N. G.; Mirfakhraie, L.; Liu, Y.; Noronha, K.; Bao, X.; Li, J.; Shuch, B. M.; King, M. C.; Bindra, R. S.; Glazer, P. M. **Oncometabolites Suppress DNA Repair by Disrupting Local Chromatin Signalling**. Nature 2020, 582 (7813), 586–591. https://doi.org/10.1038/s41586-020-2363-0.

PP-11
Harnessing Mitochondrial Targeting and Metal Coordination to Enhance Curcumin-Based Phototherapy

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Curcumin, a natural polyphenol from *Curcuma longa*, exhibits broad anticancer activity by modulating multiple signaling pathways and inducing cancer cell death. However, its clinical use is limited by poor bioavailability, rapid metabolism, and lack of subcellular targeting. To address these issues, we developed a mitochondria-targeted curcumin ligand functionalized with triphenylphosphine (TPP), a lipophilic cation that selectively accumulates in mitochondria. The synthesized TPP–curcumin ligand was coordinated with Ir(III), Ru(II), and Re(I) to form photoactive metal complexes. These complexes were characterized using NMR, FTIR, UV–Vis, HRMS, and elemental analysis, and their photophysical properties, including singlet oxygen generation and emission behavior, were evaluated. In vitro studies are expected to show enhanced mitochondrial accumulation, efficient ROS production under light irradiation, and pronounced phototoxicity in cancer cells. This work presents a rational strategy to enhance curcumin-based phototherapy through mitochondrial targeting and metal-assisted photodynamic therapy for effective cancer treatment.

Keywords: Curcumin, Photodynamic therapy (PDT), Mitochondria targeting, Metal complexes

References

[1] Aditya Garai, Ila Pant, Samya Banerjee, Bhabatosh Banik, Paturu Kondaiah, and Akhil R. Chakravarty, **Photorelease and Cellular Delivery of Mitocurcumin from Its Cytotoxic Cobalt(III) Complex in Visible Light,** *Inorganic Chemistry* **2016** *55* (12), 6027-6035

[2] Subin Joseph, Rinku Chakrabarty, and Priyankar Paira, **Advances in nano-drug delivery systems for metallic compounds in cancer therapy: challenges and future perspectives,** Dalton Trans.,2025,54,13820–13850

PP-12

Photobiological Distinction of Imidazophenanthroline-based Ir (III) Cyclometalated complexes in Next-Generation Cancer Therapy

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Imidazophenanthroline-based cyclometalated Iridium(III) complexes have emerged as potent photoactive agents in cancer therapy, owing to their remarkable photostability, tunable electronic properties, and efficient generation of reactive oxygen species (ROS). Upon light activation, these complexes induce oxidative stress that disrupts mitochondrial integrity, triggers caspase-mediated apoptosis, and modulates key signalling pathways involved in cell death. Their ability to localise preferentially within cancerous cells and produce singlet oxygen with high quantum yields enhances selectivity while minimising collateral damage to healthy tissue. This work highlights the structure–activity correlations and mechanistic insights into their light-triggered cytotoxicity, positioning Ir(III) cyclometalated complexes having imidazophennathroline-based ligands as promising next-generation agents for targeted, Photodynamic cancer therapy.[1,2]

Keywords: Photodynamic Therapy (PDT), Iridium (III) complexes, Reactive Oxygen Species (ROS), Oxidative Stress, Cancer Therapy.

References

[1] Ghosh, S., Paira, P. **Instigating Visible Light Inspired DNA Impairment by ROS Harvesting Ir (III)-Cyclometallated Imidazophenanthroline Complexes Against MDA-MB-231 Cells,** European Journal of Inorganic Chemistry, 2025, (10): e202400769. (Journal)

[2] Ghosh, S., Chakrabarty, R., Paira, P**. Harnessing Photodynamic Therapy for Programmed Cell Death: The Central Role and Contributions of Metal Complexes as Next Generation Photosensitizers.** RSC Medicinal Chemistry, 2025.

PP-13
Click-Derived Triazolylmethylquinoxaline-Based Metal Complexes as Photodynamic Therapeutic Agents against Triple Negative Breast Cancer

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Photodynamic therapy (PDT), a light-activated chemotherapeutic approach, has attracted increasing interest due to its higher target specificity and reduced side effects compared to conventional chemotherapy. Cyclometalated and half-sandwich metal complexes have garnered growing attention due to their outstanding photoluminescent properties, high photostability, and large Stokes shift, making them promising candidates for phototherapeutic applications. We have designed and synthesized photodynamically active metal complexes, in which the ligand 2,3-bis((4-(pyridin-2-yl)-1H-1,2,3-triazol-1-yl)methyl)quinoxaline was prepared via a click reaction. This design strategy involves the development of photoactive binuclear Iridium (III) complexes incorporating triazolylmethylquinoxaline ligands that generate reactive oxygen species (ROS) upon light irradiation. These electropositive binuclear complexes are selectively transported to cancer cell membranes through serum albumin, where light-induced ROS production leads to glutathione (GSH) depletion. Consequently, this process disrupts the mitochondrial membrane potential (MMP), induces DNA photocleavage, and ultimately triggers apoptosis.

Keywords: Photodynamic therapy, cyclometalated and half-sandwich complexes, ROS generation, GSH depletion, Apoptosis.

References

[1] S. U and P. Paira, **2, 3-bis ((4-(pyridin-2-yl)-1H-1, 2, 3-triazol-1-yl) methyl) quinoxaline based Cyclometalated binuclear Ir (III) Complex for Photodynamic therapy in Triple Negative Breast Cancer Cell**. Chemistry, an Asian journal, 2025, e202401047.

[2] S. U, U. Basu, P. Paira, **Current Context of Designing Phototheranostic Cyclometalated Iridium (III) Complexes to Open a New Avenue in Cancer Therapy**. ChemMedChem, 2025, *20* (5), e202400649.

PP-14
Synthesis and Characterization of Yellow NIR-Reflective Pigments for Cool Coating Applications

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Pigments play a crucial role in daily life by imparting color to various materials. In recent years, near-infrared (NIR) reflective pigments have gained significant attention due to their ability to mitigate the urban heat island effect and reduce heat-related issues for humans. In this study, praseodymium phosphate-based yellow pigments were developed by doping divalent metal ions, along with vanadium, to achieve an enhanced color hue and high NIR reflectance. The pigments were synthesized via the solid-state method, and the obtained samples were characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), UV–Vis diffuse reflectance spectroscopy (UV–Vis DRS), and X-ray photoelectron spectroscopy (XPS) to analyze their structural, optical, and chemical properties. Additionally, colorimetric parameters (CIE-L*a*b*) were evaluated, and NIR reflectance values were determined. The results confirm the successful formation of yellow pigments with promising NIR reflective properties. Therefore, the obtained compound can be used as a potential yellow pigment with excellent NIR reflective performance for energy-efficient coating applications.

Keywords: Yellow pigment; Vandium; NIR reflectance; Doping; Solid state method

References

[1] Ding C., Tian M., Han A., Ye M., Chen X. **V-doped $LaPO_4$ new solar heat-reflective pigments and its improvement on the aging resistance of poly-methyl methacrylate,** Sol. Energy., 2020 (195): 660–669.

[2] Ianoș R., Rus I., Lazău R., Ciutan R. **Near-infrared reflective coatings based on red-brown $Ce_{1-x}Pr_xO_2$ pigments,** Appl. Mater. Today., 2024, (39): 102301.

[3] Mansour S.A., Farha A.H. **A Review of Near-Infrared Reflective Nanopigments: Aesthetic and Cooling Properties,** Crystals., 2025, (15): 271.

[4] Zou J., Chen Y., Lin H. **Facile fabrication of cool yellow pigment with enhanced NIR reflectance by tailoring oxygen defects and its application in energy-saving building,** Ceram. Int., 2023, (49): 10756-10764.

PP-15

Effect of reagent vibration on the dynamics of the, He + LiH^+ (v = 1-4, j = 0) → $LiHe^+$ + H, reaction

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In the present work the effect of reagent diatom vibrational excitation on the, He + LiH^+ (v = 1,2,3,4, j = 0) → $LiHe^+$ + H, reaction on its electronic ground state is investigated by employing the Coriolis coupled time-dependent quantum mechanical and quasi-classical trajectory methods up to 1.0 eV.[1,2,3,4] collision energy. A recently developed potential energy surface (PES) of Rawat *et. a.l.*[5] is used *for the purpose.* Initial state-selected and state-to-state reaction probabilities and integral cross-sections are calculated to find out the mechanistic details of the reaction in great detail. The results of the investigation provide valuable insight which improves our understanding of Lithium chemistry of the early universe.

Keywords: Time-Dependent Quantum Mechanical, Quasi-Classical Trajectory, State-to-state Reaction Probabilities, Integral Cross-sections, Potential Energy Surface

References

1. S. K. Gray and G. G. Balint-Kurti, J. Chem. Phys. **108**, 950 (1998).
2. M. Hankel, S. C. Smith, R. J. Allan, S. K. Gray, and G. G. Balint-Kurti, J. Chem. Phys. **125**, 164303 (2006).
3. M. Karplus, R. N. Porter, and R. D. Sharma, J. Chem. Phys. **43**, 3259 (1965).
4. J. Sahoo, A. M. S. Rawat, and S. Mahapatra, Phys. Chem. Chem. Phys. **23**, 27327 (2021).
5. A. M. S. Rawat, M. Alamgir, S. Goswami, and S. Mahapatra, J. Chem. Phys. **161**, 124308 (2024).

PP-16
Mitochondrial-Targeting Imidazophenanthroline-Based Bimetallic Complexes as Promising Agents for Synergistic Photodynamic and Chemotherapeutic Cancer Treatment

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Bimetallic complexes have emerged as potent agents for combined photodynamic and chemotherapeutic cancer treatment. However, their efficacy remains limited against aggressive cancers such as triple-negative breast cancer (MDA-MB-231) and human melanoma (A375). In this study, we designed a series of mitochondrial-targeting imidazophenanthroline-based binuclear Ru(II)/Ir(III)/Re(I) complexes capable of generating reactive oxygen species (ROS), inducing mitochondrial dysfunction, causing oxidative DNA damage, and promoting G0/G1 phase cell-cycle arrest. Among the synthesized complexes, the naphthalene-substituted imidazophenanthroline bis-iridium complex (BNS-2) exhibited the most potent cytotoxicity toward MDA-MB-231 and A375 cells. Mechanistic studies revealed that BNS-2 triggered apoptosis by upregulating BAX and cleaved caspase-3, downregulating BCL-2, and activating the caspase-3/9 pathway, effectively shifting the cell-death mechanism from necrosis to apoptosis. In vivo, BNS-2 significantly inhibited tumor growth while preventing body-weight loss and avoiding hepatotoxicity and nephrotoxicity. These findings highlight BNS-2 as a promising bimetallic therapeutic candidate for synergistic photodynamic and chemotherapeutic treatment of resistant cancers.

Keywords:
Bimetallic Complexes; Photodynamic Therapy; Apoptosis; Imidazophenanthroline; Cancer Treatment

References:

1] Yagmurlu, A., Buğday, N., Yaşar, Ş., Boulebd, H., Mansour, L., Koko, W. S., Hamdi, N., & Yaşar, S. (2024). **Synthesis, DFT calculations, and investigation of catalytic and biological activities of back-bond functionalized re-NHC-Cu complexes.** *Applied Organometallic Chemistry*, *38*(7). https://doi.org/10.1002/aoc.7545

PP-17

Microplastic-induced modulation of extracellular polymeric substances in agricultural soil and its impact on seed germination of *Solanum lycopersicum* (tomato)

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This comparative study explores how different microplastics (MPs) polyethylene (PE), polystyrene (PS) and polyvinyl chloride (PVC) affect soil properties, production and the constituents of extracellular polymeric substances (EPS) in agricultural soil (AS) and its impact on seed germination. EPS, made of sugars, proteins, nucleic acids, and lipids, helps microbes survive tough conditions. Agricultural soils were exposed to MPs for 15, 30, and 45 days, and key soil parameters including pH, organic carbon, and nitrogen were monitored. EPS was extracted and the total carbohydrate and protein content were also estimated. Morphological changes in MPs were assessed using field emission scanning electron microscopy (FE-SEM) after 45 days of incubation. Results indicate that PE significantly enhances EPS production in AS compared to PS and PVC, suggesting stronger microbial stimulation. FE-SEM analysis revealed distinct morphological alterations in all MPs, with PE showing pronounced clumping and surface complexity, while PS and PVC exhibited varying degrees of aggregation and texture changes. These interactions between MPs and soil microbes appear to influence nutrient cycling and soil structure. Furthermore, tomato seed germination and early growth of in-situ and ex-situ EPS were affected by the presence of MPs, which shows MPs significantly affect the root and shoot length of tomato seeds. Among the three tested microplastics, PVC exhibited the strongest inhibitory effect on tomato seed root and shoot elongation, particularly when combined with ex-situ EPS at higher concentrations. PE showed moderate phytotoxicity, while PS had the least impact, suggesting that polymer type and EPS origin critically modulate soil plant interaction.[1]

Keywords: - Microplastics, agricultural soil, extracellular polymeric substances, growth, microbes

References

[1] Oliva, R.L., Khadka, U.B., Camenzind, T., Dyckmans, J., Joergensen, R.G. **Constituent of extracellular polymeric substances (EPS) produced by a range of soil bacteria and fungi**. BMC Microbiol., 2025 (25), 298.

PP-18

Hexafluoro isopropanol (HFIP)-Promoted Metal-free chemo selective *O*-Alkylation of 2-Hydroxypyridines with *α*-Halo Hydroxamates at Room Temperature

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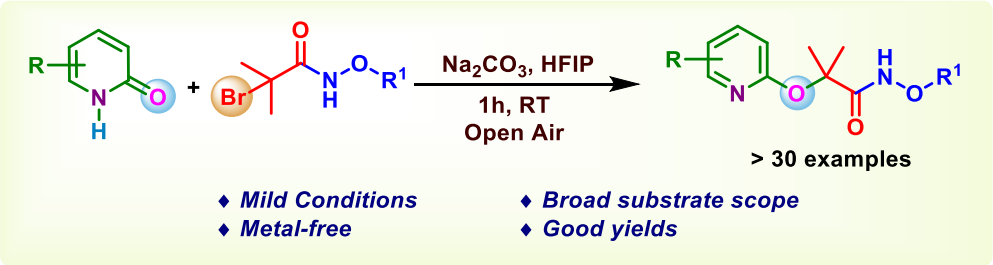
A mild, metal-free, and chemoselective protocol for the *O*-alkylation of 2-hydroxypyridines using α-halo hydroxamates under ambient conditions, using HFIP as the solvent and Sodium Carbonate as the base. The reaction leverages the electrophilic nature of azaoxyallyl intermediates and the nucleophilicity of pyridone oxygen to achieve high *O*-selectivity, overcoming the inherent preference for *N*-functionalization. The method accommodates a broad substrate scope, including diverse hydroxy pyridine derivatives and α-halo hydroxamates with varied substituents. This operationally simple strategy provides streamlined access to pharmacologically relevant heterocycles, offering valuable tools for medicinal chemistry and drug discovery.



Keywords: O-Alkylation, 2-Hydroxypyridines, α-Halo Hydroxamates, Hexafluoro isopropanol (HFIP)

References

[1] Hopkins, G. C.; Jonak, J. P.; Tieckelmann, H.; Minnemeyer, H. J., Alkylation of Heterocyclic Ambident Anions. II. Alkylation of 2-Pyridone Salts, J. Org. Chem. 1967, 32, 12, 4040–4044.

PP-19
Visible Light-Assisted Transesterification of Propylene Carbonate to Afford Octane Booster by Porphyrin Photocatalyst

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In the chemical industry, dimethyl carbonate (DMC) is a significant synthetic intermediate with numerous uses. The present study focuses on a porphyrin photocatalyst that was synthesised and employed for the photocatalytic transesterification of propylene carbonate into dimethyl carbonate. The photocatalyst was characterised using various spectroscopies techniques. Under visible light irradiation, the porphyrin photocatalyst demonstrated conversion of propylene carbonate into dimethyl carbonate using methanol/propylene carbonate 1:10 molar ratio under a 5 W LED at ambient temperature for 24 h. This finding emphasises the utility of porphyrin photocatalysts, furthermore, the results indicate potential applications in sustainable chemical processes, highlighting the significance of utilising renewable energy sources for catalysis.

Keywords: Porphyrin photocatalyst; Transesterification; Visible light; Sustainable; Industrial applications.

References

[1] Gu, S., Marianov, A. N., Lu, T., & Zhong, J. (2023). **A review of the development of porphyrin-based catalysts for electrochemical CO2 reduction**. In *Chemical Engineering Journal* (Vol. 470). Elsevier B.V. https://doi.org/10.1016/j.cej.2023.144249.

[2] Mataghare, B. C., & Bhagat, P. R. (2023). **Construction of porphyrin-based photocatalyst comprising pyridinium ionic liquid moiety for the metal-free visible light-assisted N-arylation of amines: facile approach to afford drug intermediates.** *New Journal of Chemistry*, *47*(47), 21764–21780. https://doi.org/10.1039/d3nj04295b

PP-20

Convergent synthesis of coumarin C3–C4-fused fluorogenic quinoline scaffolds via aldehyde activation using in situ generated hydrazoic acid

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The article describes an efficient route for the construction of diversely substituted coumarin C3-C4 fused quinoline from pre-functionalized 4-azido-3-formylcoumarin using various aromatic/heterocyclic amines in excellent yield with a focus on application-oriented substrates scope. This protocol provides a straightforward synthesis of fluorogenic coumarin-fused quinoline scaffolds through aldehyde activation by 'in-situ' generated HN_3 with excellent atom economy. Our synthetic methodology has been showcased and applied by synthesizing 31 structurally diversified scaffolds, the gram-scale experiment, and structural validation with four single-crystal XRD studies. Also, we have proposed a plausible mechanistic pathway from the control experimental studies. Fascinatingly, the remarkable features of this methodology include, without the intervention of secondary products, excellent yield, chromatography-free isolation, functional group compatibility, and tolerance of electron influence of different substituents, which makes this methodology ideal for the construction of CQ scaffolds.

Keywords: Azido-coumarin, Fluorogenic quinoline, In situ Hydrazoic Acid, Pomeranz–Fritsch–type cyclisation

References

[1] Marshall C. M., Federice J. G., Bell C. N., Cox P. B., Njardarson J. T. **An Update on the Nitrogen Heterocycle Compositions and Properties of U.S. FDA-Approved Pharmaceuticals (2013-2023),** *J. Med. Chem*., 2024, (67), 11622–11655.

[2] Thigulla Y., Kumar T. U., Trivedi P., Ghosh B. **One-Step Synthesis of Fused Chromeno[4,3-*b*]pyrrolo[3,2-h]quinolin-7(1*H*)-One Compounds and their Anticancer Activity Evaluation**, *ChemistrySelect*, 2017, (7), 2718–2721.

[3] Patra P., **A Concise Review on Pyridocoumarin/Azacoumarin Derivatives: Synthesis and Biological Activity**, *ChemistrySelect*, 2019, 4, 2024–2043.

PP-21
ProFA: An Integrated Platform for Protein Structural Characterization and Physicochemical Property Analysis

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Interpreting raw PDB files continues to pose challenges for researchers due to the complex, unorganized nature of these files and limited integrated analysis tools.[1] To address this, we developed a comprehensive web-based platform that streamlines protein structure analysis by combining computational and visualization features into one application. Our tool, built using Streamlit and BioPython libraries, extracts crucial structural details and calculates geometric properties such as bond angles between alpha carbons and pairwise distance matrices.[2] It further evaluates molecular characteristics, including molecular weight and isoelectric point, essential for protein characterization. Advanced analytical modules compute the radius of gyration and surface area using robust computational geometry techniques. The platform supports both ATOM and HETATM records, facilitating multi-chain and quaternary structure analyses. Statistical modules offer descriptive summaries, while interactive graphs and versatile export options (PDB, FASTA, CSV, Excel) enhance user engagement and portability. Evaluations across diverse protein structures demonstrate the tool's scalability and accuracy. By integrating geometric computation with physicochemical property analysis, this accessible web application broadens available bioinformatics resources, supporting applications in drug design, protein engineering, and molecular biology research. Its modular design and reliance on trusted scientific libraries enable efficient protein structure analysis, contributing to advances in structural biology and interdisciplinary chemistry.

Keywords: Protein structure analysis, Structural Bioinformatics, Geometric and physicochemical characterization, Web-based platform

References:

[1] Berman, H. M. The Protein Data Bank. *Nucleic Acids Res.* **2000**, *28* (1), 235–242. DOI: 10.1093/nar/28.1.235.
[2] Kabsch, W.; Sander, C. Dictionary of Protein Secondary Structure: Pattern Recognition of Hydrogen-Bonded and Geometrical Features. *Biopolymers* **1983**, *22* (12), 2577–2637. DOI: 10.1002/bip.360221211.

PP-22
Hub Gene Discovery For Biomarker Development In Parkinson's Disease Using Network Analysis

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Parkinson's disease (PD) is a progressive neurodegenerative disorder marked by bradykinesia and tremors. Despite extensive research, challenges such as early diagnosis, reliable biomarkers, and targeted therapeutic strategies remain unresolved. Identifying novel hub genes and their regulatory elements is crucial for advancing diagnostic and therapeutic approaches. In this study, the expression profiles of GSE135743, GSE181029, and GSE182622 were obtained from the Gene Expression Omnibus, including PD and healthy control samples. The differentially expressed genes were analysed and identified by the GEO2R tool and Venn diagrams. A protein-protein interaction network was created using the Search Tool for the Retrieval of Interacting Genes and visualized in Cytoscape. MCODE was further employed to obtain the hub genes. To find their biological significance, the hub genes are further analysed with the ShinyGO tool for Gene Ontology and Kyoto Encyclopedia of Genes and Genomes pathway enrichment analysis. In addition, using the NetworkAnalyst tool, regulatory elements like microRNAs and transcription factors interacting with the hub genes are identified. The candidate therapeutic molecular drugs were searched for PD using the DGIdb database. The results indicate that a total of 3 genes, HLA-B, B2M, and PSMB9, show differential expression, in which all three genes show downregulation. 132 microRNAs and 11 transcription factors were predicted to interact with these hub genes, suggesting a complex regulatory network. 38 drugs were found to be showing interaction with HLA-B. These findings highlight the novel targets that can be successfully exploited for early diagnosis and targeted therapeutic strategies.[1,]

Keywords: Parkinson's disease, Hub genes, Protein-protein interaction network, Biomarkers, Regulatory network

References:

[1] Zhou, Y., Li, Z., Chi, C., Li, C., Yang, M., & Liu, B. (2023). Identification of Hub Genes and Potential Molecular Pathogenesis in Substantia Nigra in Parkinson's Disease via Bioinformatics Analysis. Parkinson's Disease, 2023. https://doi.org/10.1155/2023/6755569

PP-23
Integrating β-Diketonate Platinum (II) Complexes with Protein Nanocarriers for Advanced Chemotherapeutic Delivery

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Platinum-based chemotherapeutics such as cisplatin and carboplatin remain central to cancer therapy but are limited by toxicity, poor solubility, and drug resistance. To address these challenges, protein nanocarriers, such as bovine serum albumin (BSA) nanoparticles, offer a promising solution due to their biocompatibility and capacity to enhance the pharmacokinetics of hydrophobic drugs [1,2]. A series of Pt (II) complexes, termed AromaPlatins, featuring β-diketonate ligands with extended aromatic rings, was synthesized to modulate reactivity and solubility. HPLC-based studies revealed that increasing aromaticity enhanced reactivity and biomolecular interactions but reduced solubility and formulation stability. Among them, Ant-Platin showed the highest reactivity but poor stability, which was successfully improved by BSA encapsulation. The resulting Ant-Platin-loaded BSA nanoparticles displayed high encapsulation efficiency, colloidal stability, and biphasic drug release exceeding 90% within 72 hours. This strategy effectively overcomes solubility and stability issues of AromaPlatins, establishing a controlled-release system for platinum-based prodrugs and advancing the development of safer, targeted chemotherapeutic platforms.

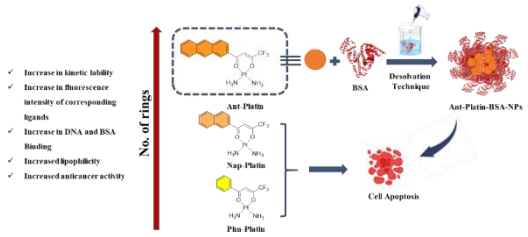

Figure: Schematic showing delivery and apoptotic action of Phn-Platin, Nap-Platin, & Ant-Platin.

Keywords: β-diketonate platinum complexes; BSA nanoparticles; Controlled release; Drug delivery; Encapsulation Efficiency

References

[1] Ji Yeon, J.; Hoang Hai, N.; Sae-Yeol-Rim, P.; Hyang Sook, C.; Byeong-Cheol, K.; Sanghoon, K. *Food Chem*, 2011,127(4),1892-1898.

PP-24

Calixorubicin: Calix[4]arene Appended Upper Rim Modified Hypoxia-Activated Prodrug of Doxorubicin and Its Nanoparticles for Enhanced Retention

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Cancer remains one of the leading causes of death worldwide, accounting for nearly one in six deaths according to the World Health Organization.[1] Among available treatment modalities, chemotherapy is the most prevalent; however, its effectiveness is frequently compromised by severe systemic side effects..[2] Although strategies such as prodrug development and targeted delivery have been explored to address these limitations, their success has often been constrained by biological complexity and insufficient specificity. Supramolecular platforms, characterised by their dynamic non-covalent interactions, offer a versatile foundation for next-generation drug delivery systems.[3] These architectures can be structurally modified to meet therapeutic needs and can accommodate the integration of stimuli-responsive linkers that enable controlled release. Such features allow drugs to remain inactive during systemic circulation and become activated only under specific pathological conditions, thereby preserving the therapeutic potential of the active agent while minimising off-target toxicity. In this study, a calix[4]arene-based supramolecular system was developed as a prodrug carrier for doxorubicin. The drug was covalently attached to the calix[4]arene scaffold through a reduction-sensitive azo linker. Since the core of the tumor generally lacks oxygen, it creates a hypoxic environment. As this hypoxic environment is highly reducing in nature, it can reduce the diazo bond with the help of azo reductase enzyme, releasing the prodrug specifically in the tumor microenvironment.[4] This targeted approach is anticipated to enhance the therapeutic index of doxorubicin while significantly reducing its systemic toxicity.

Keywords: Cancer; Supramolecular drug delivery; Calix[4]arene; Doxorubicin; Stimuli responsive linkers; Prodrug, Targeted drug release; Hypoxic tumor microenvironment.

References

[1] World Health Organization. Cancer – Fact Sheet. 2023

[2] Prieto-Callejero B, Rivera F, Fagundo-Rivera J, et al. **Chemotherapy-induced adverse reactions and quality of life in breast cancer patients.** Medicine (Baltimore). 2020;99(33):e21695. doi:10.1097/MD.0000000000021695.

[3] Langton, M. J. **Engineering of stimuli-responsive lipid-bilayer membranes using supramolecular systems**. Nature Reviews Chemistry, 2021, *5* (1), 46-61. DOI: 10.1038/s41570-020-00233-6.

PP-25
The Synthesis and Characterization of Novel Schiff Bases

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The present work is on the synthesis of Schiff's bases and characterization of the synthesized novel ligand for its confirmation. The empirics are behind the Schiff bases as per the convenience and ease in synthesis, also the work involves byproducts as H_2O and are the solvents used are ecofriendly and have less cost and involves less steps. Here we have synthesized ligand named TA-CL, the aldehyde chosen broadly having biological application and can be even working on metal ion sensing and yet the sensing profile is unexplored, so the potential field to chose that particular chemical. The ligand been confirmed by H^1NMR, C^{13} NMR , HR-MS, FT-IR. HSA binding study is also performed and thereby concluded and hypothesis that the ligand is capable of biological application and also supported by DFT ,and pharmacokinetic profile study (ADME)

Keywords: Novel Schiff base, Chemosensor, Anticancer, Antimicrobial, Pharmacokinetic study

References

[1]. Bayeh, Y.; Mohammed, F.; Gebrezgiabher, M.; Elemo, F.; Getachew, M.; Thomas, M. **Synthesis, Characterization and Antibacterial Activities of Polydentate Schiff Bases, Based on Salicylaldehyde**. *Adv. Biol. Chem.* 2020, *10* (05), 127– 139, DOI: 10.4236/abc.2020.105010

[2]. Ferreira, S. B.; Dantas, T. B.; de Figuerêdo Silva, D.; Ferreira, P. B.; de Melo, T. R.; de Oliveira Lima, E**. In Silico and in Vitro Investigation of the Antifungal Activity of Isoeugenol against Penicillium Citrinum**. *Curr. Top. Med. Chem.* **2019**, *18* (25), 2186– 2196,

[3]. Hassan, A. M.; Said, A. O.; Heakal, B. H.; Younis, A.; Aboulthana, W. M.; Mady, M. F**. Green Synthesis, Characterization, Antimicrobial and Anticancer Screening of New Metal Complexes Incorporating Schiff Base.** *ACS Omega* **2022**, *7* (36), 32418– 32431

[4]. Manjare, S. B.; Mahadik, R. K.; Manval, K. S.; More, P. P.; Dalvi, S. S. **Microwave-Assisted Rapid and Green Synthesis of Schiff Bases Using Cashew Shell Extract as a Natural Acid Catalyst**. *ACS Omega* **2023**, *8*, 473,

PP-26
Mechanically Robust PVA-Incorporated Chitosan-Aminated Starch Films with Shape Memory Effect for Tissue Engineering Applications

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The structural integrity and biocompatibility of polymeric scaffolds are crucial in advanced tissue engineering applications. This study presents the design of biopolymer films composed of chitosan and aminated starch incorporated with polyvinyl alcohol (PVA), fabricated via a casting route to achieve high mechanical robustness and biocompatibility. Mechanical testing using a Universal Testing Machine (UTM) revealed the high tensile strength and flexibility of the PVA-chitosan-aminated starch (PCAS) films. The surface morphology examination highlighted a homogeneous surface, whereas the X-ray diffraction studies indicated the crystalline nature of the films. Thermogravimetry revealed an enhancement in high-temperature resilience with an increase in the polyvinyl alcohol composition of the films. In vitro investigation demonstrated good hemocompatibility and cell viability of 92%, making the developed system suitable for biomedical applications. A shape fixation coefficient of 98.2% and shape recovery of 88.8% for the PCAS films could significantly improve tissue implantation. Additionally, the stable degradation profiles and swelling capacity suggest its potential for sustained functionality, while addressing the different key challenges in tissue engineering.

Keywords: Chitosan; PVA; Starch; Tissue engineering

References

[1] Radhakrishnan A, Panicker UG. **Sustainable Chitosan-Aminated Starch Blends as Innovative Materials for Advanced Optical Applications**, J Polym Environ, 2025, 33(2): 1047-68.

[2] Radhakrishnan A, Panicker UG. **Sustainable chitosan-based biomaterials for the future: a review**, Polymer Bulletin, 2025, 1–49.

PP-27
Development of isocyanate-free Hybrid Polyhydroxyurethane adhesives – Investigating the effects of amines

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The incorporation of urethane linkages into an epoxy backbone is an effective strategy to enhance flexibility through internal crosslinking. In this study, a hybrid monomer containing both epoxy and cyclic carbonate functionalities (EPNCC) was synthesized by partial carbonation of epoxy phenol novolac (EPN) resin. Polyhydroxyurethanes (HPHUs) were then prepared via aminolysis of EPNCC with isophorone diamine, triethylene tetramine, and Gaskamine-328, following a non-isocyanate route that utilizes CO_2 and avoids toxic isocyanates. The influence of different amines on the mechanical, thermal, chemical, and adhesive properties of the HPHUs was investigated. The optimized formulation exhibited high elongation (30–40%) and strong adhesion (15–16 MPa) compared to the parent EPN system. DFT analysis confirmed strong hydrogen-bonding interactions in the Gaskamine-cured system. Overall, the developed hybrid HPHUs show excellent performance and offer a sustainable, environmentally friendly alternative for adhesive and coating applications.[1-5]

Keywords: Cyclic Carbonate, Epoxy Phenol Novolac, Non-isocyanate, DFT, Adhesive, Polyhydroxyurethanes

References

[1] Lambeth R.H., Rizvi A., **Mechanical and adhesive properties of hybrid epoxy–polyhydroxyurethane network polymers**, Polymer, 2019, 183: 121881.
[2] Camara F., Benyahya S., Besse V., Boutevin G., Auvergne R., Boutevin B., Caillol S., **Reactivity of secondary amines for the synthesis of non-isocyanate polyurethanes**, Eur. Polym. J., 2014, 55: 17–26.
[3] Ke J., Li X., Wang F., Jiang S., Kang M., Wang J., Li Q., Wang Z**., Non-isocyanate polyurethane/epoxy hybrid materials with different and controlled architectures prepared from a CO_2-sourced monomer and epoxy via an environmentally friendly route**, RSC Adv., 2017, 7: 28841–28852.

PP-28
Transforming Recycled Microplastic Waste into Conductive Self-Healing Hydrogel for High-Efficiency Energy Harvesting and Real-Time Human Body Detection

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As we all know, microplastics are one of the major global concerns in today's world. Tons of microplastic waste are being generated every year that persists in the environment for decades, which is a serious threat to the environment. Among these, one such unusual kind of microplastic waste is chewing gum waste. Chewing gum residue is non-biodegradable, hard to decompose and easy to cause pollution, which is highly desirable to realize recycling. This study presents synthesis of a self-healing hydrogel derived from waste chewing gum, which is conductive and has good shape memory, for sustainable energy harvesting through Triboelectric Nanogenerator (TENG). Preliminary analyses were performed to evaluate mechanical and electrical characteristics using FTIR, XRD, and SEM. Additionally, Electrochemical Impedance Spectroscopy (EIS) was conducted to assess the ionic conductivity and interfacial resistance of the hydrogel. The hydrogel demonstrates enhanced performance when integrated as an electrode in TENG. The hydrogel-based TENG device shows great potential for use as biomedical sensors, wearable electronics, and other applications. This study directly supports the Sustainable Development Goals by converting waste material into value-added functional materials and utilizing them to generate energy.

Keywords: Microplastic Waste, Self-Healing Hydrogel, Energy Harvesting, Triboelectric Nanogenerator, Recycling Polymer Waste.

References

[1] Zhao J., Li J., Zeng Q., Wang H., Yu J., Ren K., Dai Z., Zhang H., Zheng J., Hu R. **A Chewing Gum Residue- Based Gel with Superior Mechanical Properties and Self-Healability for Flexible Wearable Sensor**, *Macromol. Rapid Commun.*, 2022, *43*(1): 2200234.

PP-29
Flexible, Self-Healing and Lead-Free Nanogenerator based on Natural Rubber -Dextrin Composites for Human Body Stimuli Responsive Applications

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Development of environment-friendly, biocompatible, cost-effective, flexible, self-healing and lead-free piezoelectric materials from sustainable sources is a dynamic research area in view of their potential to transform mechanical energy from the living environment into electrical signals [1,2]. This study explores the modification of an optimized polymer blend system, viz. natural rubber latex/dextrin (NRL/DXT), through the incorporation of nanohydroxyapatite (nHAP) for developing piezoelectric nanogenerators (PENGs). The composite samples exhibited enhanced mechanical capabilities, thermal stability, dielectric properties, and piezoelectric characteristics. The examinations of their conductivity, dielectric loss, and dielectric constant at low frequencies confirm the piezoelectric nature; duly assisted by the observations from dynamic contact electromagnetic force microscopy (DC-EFM). A device prototype was successfully fabricated and subjected to the evaluation of piezoelectric voltage generation through human body motions. The improvements reflected in electrical and static mechanical properties indicate that the developed composite system could be recommended as a promising material for piezoelectric sensors, particularly for detecting human motions.

Keywords: natural rubber, dextrin, nanohydroxyapatite, piezoelectric nanogenerator, self-healing

References

[1] Mankuni A., Varghese S., **High-performance underwater energy harvesting using flexible piezoelectric nanogenerator based on electrospun polyvinylidene fluoride-LiNbO$_3$ fibers**. Nano Energy. 2025, (140):111042. [2] Verma A., Dutta P., Awasthi N., Singh A.K., Karumuthil S.C., **Investigation of the Different WO3 Nanofiller Morphology Influence on the Piezoelectric Properties of WO$_3$-PVDF Nanocomposites for Self-Powered Biomedical Devices and Flexible Wearable Sensors.** ACS Appl. Electron. Mater. 2025, (7): 7149-7159.

PP-30
High-Yielding Regioselective Synthesis of Coumarin/2-Quinolone C3-C4 Fused 5-Substituted-1,4-Benzodiazepine Scaffolds

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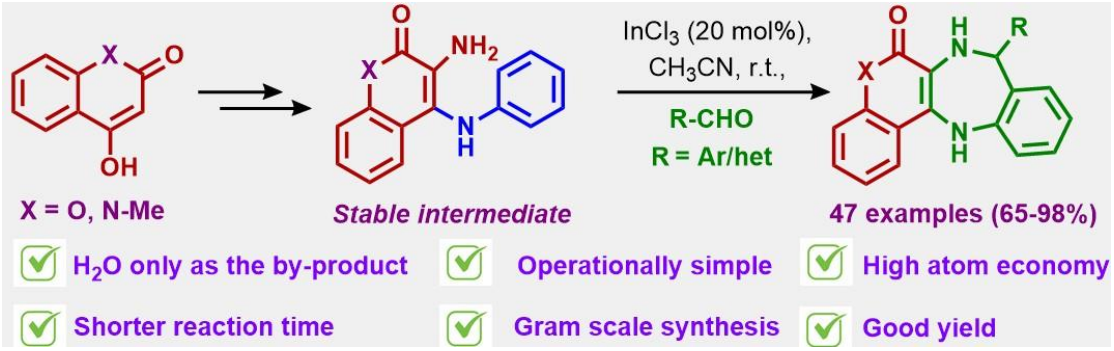
Our research article describes an unprecedented route for the high-yielding regioselective synthesis of coumarin/2-quinolone C3-C4 fused 5-substituted-1,4-benzodiazepine scaffolds *via* indium chloride-mediated Pictet-Spengler type cycloannulation of 3-amino-4-(phenylamino)-coumarin/2-quinolone and aryl/heterocyclic aldehydes through the transitory intermediacy of cyclic diamine-indium complex. Our new synthetic methodology has been successfully applied to synthesize 47 structurally diversified 1,4-benzodiazepine scaffolds, including a gram-scale experiment, structural validation with five single-crystal XRD studies, mechanistic validation with control experiments, and HRMS analysis. This robust protocol eases access to the structurally diversified, privileged seven-membered skeleton with an excellent step economy.



Keywords: Coumarin/2-quinolone, Regioselective synthesis, Indium (III) chloride, Cyclic diamine indium-complex, 1,4-Benzodiazepines

References:

[1] Krishnan A., Kamaraj S. *J. Org. Chem.,* **2023,** *88,* 16315-16329.

[2] Nagamani V., Kamaraj S. *Euro. J. Org. Chem.,* **2024,** *27,* e202400575.

[3] Krishnan, A., Kamaraj, S. *New J. Chem.* **2024,** *48,* 10045-10052.

PP-31
Exploration of Fe and Ru PNP pincer catalysed amide formation from CO and NH_3 'A DFT APPROACH'

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Homogeneous catalysis provides a molecular-level insight into chemical reactivity, especially in the case when catalyst and reactants are present in the same phase. The current study explains how Fe-PNP and Ru-PNP pincer complexes can be used in synthesizing formamide with CO and NH_3 as feedstocks. In this context, Density Functional Theory (DFT) was employed to predict and explain mechanistic pathways for small-molecule activation. All structures, including reactants, intermediates, transition states, and products, were optimized at wB97XD method with conjunction of 6-31++G(d,p) basis for group elements and LANL2DZ for metal centers. Frequency analysis confirmed the nature of a stationary point, where the potential-energy profile was generated for both Fe and Ru systems. Energy profile diagram indicates that Ru–PNP shows a lower activation barrier of ~8 kcal/mol compared with Fe–PNP of ~12–15 kcal/mol for catalytic CO insertion in NH_3($R\text{-}NH_2$) to form amide. The CO ligand serves as a σ-donor and π-acceptor (synergistic effect), through which it can uptake both H^+ and NH_2^- in single (C) center improving catalytic efficiency due to metal–ligand cooperation. Although Ru-PNP shows higher efficiency, Fe-PNP is still an up-and-coming and greener earth-abundant alternative. The work here shows how computational chemistry has connected theory and experiment in catalyst design to aid the development of efficient catalytic systems.

Keywords: Homogeneous catalysis; PNP Pincer complexes; DFT; CO activation; Small-molecule activation.

References:

[1] Dr. Tanay Debnath ., et al., **Exploration of unprecedented catalytic dehydrogenation mechanism of methylamine-water mixture in presence of Ru-pincer complex: A systematic DFT study**, Journal of catalysis, .363, 164-182,2018

[2] Dr.Tanay Debnath ., et al., **Comprehensive Understanding of Bi-functional Behavior of PNP-Pincer Complexes Towards the Conversion of CO into Methanol and CO_2: A DFT Approach**, ChemistrySelect, 4, 10777-10786., 2019

[3] Gupta A., et al., **Computational study on pincer complexes**, Organometallics, 2021.

PP-32
3D/2D layered heterojunction of $NiNb_2O_6$/E-gC_3N_4 as an efficient photocatalyst for pollution abatement

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The major challenge in photocatalysis for environmental remediation is rapid recombination of charge carriers. Recently, the construction of 3D/2D heterojunction is regarded as a viable strategy to overcome this drawback. Towards this objective, 3D $NiNb_2O_6$ − 2D E-gC_3N_4 type-II heterojunction was constructed as a dual catalyst for photo-reduction of Cr^{6+} to Cr^{3+} and photo-oxidation of methylene blue (MB), malachite green (MG) and crystal violet (CV) under visible light. After optimizing the parameters, the photocatalytic activity was studied under direct sunlight. Among the prepared catalysts, NG-20 composite ($NiNb_2O_6$ −80 % & E-gC_3N_4 −20 %) exhibits excellent photocatalytic activity in removing 97 % of Cr (VI) under 120 min and degrading 97.4 %, 96.1 % and 98 % of MB, MG and CV respectively in 20 min under direct sunlight. The superior photocatalytic activity can be attributed to the enhanced charge carrier separation of electron-hole pair due to the construction of 3D/2D heterojunction.

Keywords: 3D/2D heterojunction, photocatalyst, $NiNb_2O_6$, Exfoliated gC_3N_4 and environmental remediation.

References

[1] K. Mishra, N. Devi, S.S. Siwal, V.K. Gupta, V.K. Thakur, **Hybrid semiconductor photocatalyst nanomaterials for energy and environmental applications: fundamentals designing, and prospects**, Adv. Sustain. Syst. 7 (2023) 2300095, https://doi.org/10.1002/adsu.202300095.

[2] S. Shanavas, S. Mohana Roopan, A. Priyadharsan, D. Devipriya, S. Jayapandi, R. Acevedo, P.M. Anbarasan, **Computationally guided synthesis of (2D/3D/2D) rGO/Fe 2 O 3 /g-C 3 N 4 nanostructure with improved charge separation and transportation efficiency for degradation of pharmaceutical molecules,** Appl. Catal. B 255 (2019), https://doi.org/10.1016/j.apcatb.2019.117758.

PP-33

Interactions of Schiff's base complexes of essential bioelements with nucleic acid and protein

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Since time immemorial, azomethine-based coordination compounds have been extensively explored towards various industrial and therapeutic applications. The corresponding metal complexes of such ligands have proven to possess enhanced biological potential due to the perfect synergism that exists between the metal center and the ligand. In the current study, we have synthesized and characterized, hitherto unreported, ligand obtained from 4-Fluoro-o-phenylenediamine and 2-Hydroxy-4-methoxybenzaldehyde and the corresponding copper, zinc, and nickel complexes. The complexes are expected to possess binding interactions with the nucleic acids and proteins. The interaction with nucleic acid provides insight into the cytotoxic potential of the designed compounds, whereas the interaction with BSA sheds light on drug transport and distribution within the biological system. In this context, we have investigated the binding propensities of the designed complexes with DNA and BSA through UV absorption titration and fluorescence quenching assay. The cleaving abilities of the complexes are assessed through gel electrophoresis.

Keywords: Schiff's base, Nucleic acid, Bovine serum albumin, Gel electrophoresis.

References

[1] Islam, M. A., Tasnim, F., Hossain, M. S., Hossen, M. F., Zahan, M. K. E., & Asraf, M. A. (2025). **Experimental and computational insights into antibacterial and antioxidant properties of metal complexes with isoniazid-based Schiff base ligands**. *Journal of Molecular Structure*, *1324*, 140916.

[2] Saravanan, T., Dasgupta, S., Noor, A., & Sheela, A. (2025). **Explorations on antioxidant, enzyme inhibitory, and calf thymus DNA interaction studies of dioxomolybdenum (VI) organo complexes**. *Chemistry & Biodiversity*.

PP-34

Antioxidant, α-amylase inhibition, and DNA/BSA interaction studies of aldimine-based nickel, zinc and copper complexes

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Schiff bases, which coordinate with metal ions, open up wide avenues for enhanced bioactivity and potential therapeutic applications. In the current study, we have designed an aldimine-based ligand, obtained from a 4,5-dimethyl-o-phenylenediamine with 5-chlorosalicylaldehyde, and the corresponding nickel, copper, and zinc complexes. The radical scavenging abilities and antidiabetic potential of the complexes are evaluated. The binding efficacy of the complexes with calf thymus DNA has been monitored using spectroscopic techniques. We have observed a hyperchromic shift in the UV absorption titration, indicating intercalation as the probable mode of interaction of the complexes with DNA. The results of fluorescence quenching assays with DNA and BSA have shown good binding interactions of the complexes with nucleic acid and protein. Besides, the cleavage ability of the complexes on pBR322 DNA is assessed through gel electrophoresis. The experimental observations are supported, computationally, by molecular docking studies. The drug likeness of the complexes is evaluated by ADMET analysis. In conclusion, the results of the studies above indicate that these complexes possess greater potential to be developed as multifunctional drug candidates.

Keywords: Nucleic acid, Aldimine, Antioxidant, Enzyme Inhibition, DNA Binding

References

[1]. Ganesan, S., & Sheela, A. **"Ruthenium and platinum-based anticancer metallotherapeutics from the perspectives of photodynamic therapy and bioimaging applications"**. Chemical Papers, 2024, 78(16), 8531-8561.

[2]. Yusuf, T. L., Akintayo, D. C., Oladipo, S. D., Adeleke, A. A., Olofinsan, K., Vatsha, B., & Mabuba, N. **"The effect of structural configuration on the DNA binding and in vitro antioxidant properties of new copper (II) N_2O_2 Schiff base complexes"**. New Journal of Chemistry, 2022, 46(27): 12968-12980.

PP-35
Computational Studies of Nitrogen-Containing Heterocyclic Chalcones: Molecular Docking and ADMET Evaluation

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Chalcones and their derivatives are significant compounds that have a variety of biological functions including anticancer activity. The present study aims to evaluate the anticancer activity of the designed compounds through computational analysis. EGFR (epidermal growth factor receptor) plays a major role in the development of oncogenes leading to uncontrolled cell division and cell survival. Molecular docking studies were used to determine the binding affinity of the designed compounds with target protein EGFR-a tyrosine kinase (PDB ID:6V6O) obtained from RCSB protein data bank. Compound 10, 14 &16 show binding affinity values -10.3, -10.2 & -10.9 kcal/mol respectively with the inhibition constant shown less than 1μM which represents the stronger binding and better inhibitor towards the target protein. In Silico, studies analyzed the physicochemical properties and pharmacokinetic profile of the designed compounds. All compounds have less than 5 hydrogen bond donors and 10 hydrogen bond acceptors. Among the designed compounds, except compounds (9,10,13,14,15 and16) obeyed Lipinski rule of five without any violations. The gastrointestinal (GI) permeability and blood brain barrier (BBB) both illustrate the absorption and transportation of the pharmaceutical compound. According to the Swiss ADMET predictions, most of the compounds shown high GI absorption and penetrate through blood brain barrier. These results demonstrate that the designed compounds can be synthesized and developed as anticancer agents.

Keywords: Chalcones, Molecular Docking and ADMET, Anticancer

References:

1. Sharma, N., Dhingra, N., & Singh, H. L. (2024). Design, spectral, antibacterial and in-silico studies of new thiosemicarbazones and semi carbazones derived from symmetrical chalcones. *Journal of Molecular Structure*, *1307*, 138000.

PP-36

Oxygen vacancies mediated enhanced photocatalytic activity of band gap engineered $BaSn_{1-x}Cu_xO_3$ towards methylene blue degradation under visible and sunlight

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Photocatalysis, an advanced oxidation process (AOP) has been well explored as a promising and sustainable technology for tackling environmental pollution. While $BaSnO_3$ is a known perovskite photocatalyst, its intrinsic photocatalytic efficiency is limited by poor separation of charge carriers. To overcome this, a proven strategy is to create oxygen vacancies. These defects suppress electron–hole recombination leading to enhanced photocatalytic degradation. The degradation percentages of MB are more than 95% in the doped phase in 30 min in both visible & sunlight whereas the parent phase exhibits it in 3 h. The significantly enhanced activity can be attributed to the oxygen vacancies created due to the substitution of Sn^{4+} by Cu^{2+}. We have also proposed a possible degradation pathway. This study constitutes the first documentation of the photocatalytic activity of $BaSn_{1-x}Cu_xO_3$, thereby opening new avenues for its potential applications in environmental remediation

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Keywords: Photocatalysis, Oxygen vacancies, Charge carrier separation, Environmental remediation.

References:

[1] Mondal I., Halder P., Chatterjee A., Bag N., Sau S., Biswas S., Mondal D., Paul B. K., Paul P. K. and Das S. **Crystal growth mediated physicochemical properties enhancement of $CoMnO_3$ perovskite nanomaterials and its efficient degradation of organic dyes and pathogenic bacteria under mechanical stimuli**, *J. Environ. Chem. Eng.*, 2024, (12): 112385

[2] Rajendran S., and Vijayaraghavan R. Oxygen vacancies mediated enhanced photocatalytic activity of band gap engineered $BaSn_{1-x}Cu_xO_3$ towards methylene blue degradation under visible and sunlight, **RSC Adv.**, 2025, 15(30), 24802–24814.

PP-37
Synthesis, Spectroscopic Characterization, and Biointeraction Studies of Bimetallic Ni(II) and Co(II) Schiff Base Complexes

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The pursuit of novel metal-based therapeutics continues to redefine cancer treatment strategies. In this study, a new class of N^N-donating bimetallic Schiff base complexes of Ni(II) and Co(II), $[Ni_2(L)(PNNI)_2]$ and $[Co_2(L)(PNCO)_2]$, was successfully synthesized and characterized using UV–Vis, FT-IR, and ^1H NMR spectroscopy, confirming the formation of stable coordination frameworks. Biomolecular interaction studies revealed strong affinity toward DNA and human serum albumin (HSA), suggesting efficient intercalative and protein-binding modes. The calculated thermodynamic parameters ($\Delta G°$, $\Delta H°$, $\Delta S°$) indicated spontaneous interactions predominantly governed by hydrophobic and electrostatic forces, confirming excellent stability in biological environments. Cytotoxic assays against A549 lung carcinoma cells demonstrated potent anticancer activity with minimal toxicity toward normal HEK cells, highlighting selective tumor-targeting potential. The synergistic electronic effects of the bimetallic core were found to enhance redox behavior, DNA binding, and overall cytotoxic efficiency. Collectively, these findings position the newly developed Ni(II) and Co(II) bimetallic Schiff base complexes as promising candidates for next-generation chemotherapeutics with improved selectivity and biointeraction profiles.

Keywords: Bimetallic Schiff Base Complexes; Ni(II) and Co(II) Complexes; DNA and HSA Binding; Thermodynamic and Cytotoxic Studies; Anticancer Activity.

References

[1] Kannan S., Devi P. T., Ramesh R. . **Synthesis, Structure, DNA Binding and Cytotoxic Activity of Ni(II) Schiff Base Complexes Containing N,O-Donor Ligands**, *J. Inorg. Biochem.*, 2019, **197**: 110700.

PP-38
Freeze-Dried Larnite-Reinforced PVA/PCL/Silk Fibroin Composite Scaffolds: Biocompatibility and Mechanical Assessment for Hard Tissue Repair"

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Bone tissue engineering (BTE) offers an effective strategy for restoring bone defects through biomimetic scaffolds that promote osteogenic differentiation and tissue regeneration. Among silicate-based biomaterials, larnite (Ca_2SiO_4) has emerged as a promising candidate owing to its superior bioactivity, calcium-rich composition, and ability to support apatite formation. However, its intrinsic brittleness limits its application in load-bearing conditions. To overcome this limitation, a larnite-based composite scaffold was fabricated by incorporating biodegradable polymers such as polyvinyl alcohol (PVA), polycaprolactone (PCL), and silk fibroin (SF) to improve flexibility, biocompatibility, and mechanical integrity. Porous scaffolds (Lap-1, Lap-2, and Lap-3) were prepared via the freeze-drying technique, achieving an optimal balance between porosity and strength. The Lap-2 scaffold exhibited the most favorable characteristics, with a **porosity of 68.93%**, which facilitated nutrient diffusion and cell proliferation. After **nine days of immersion**, the formation of a hydroxyapatite (HAp) layer confirmed its excellent bioactivity. Moreover, Lap-2 showed **59% antibacterial inhibition** and remarkable hemocompatibility with only **1.3% hemolysis**, indicating its safety for biomedical use. Overall, the enhanced bioactivity, antibacterial efficiency, and biocompatibility of the Lap-2 composite scaffold highlight its strong potential for bone tissue engineering applications.

Keywords: polymer ceramic composite, scaffold, bone tissue engineering , polymers.

References:

[1] Donate R., Paz R., Moriche R., et al (full list). **An overview of polymeric composite scaffolds with piezoelectric properties for improved bone regeneration.** *Mater. Des.*, 2022, (231): 112085.

[2] Venkatraman S.K., & Swamiappan S.. **Review on calcium-and magnesium-based silicates for bone tissue engineering applications.** *J. Biomed. Mater. Res. A*, 2020, (108): 1546-1562.

PP-39

Amino acid-triggered activation of double-masked gossyzid–metal conjugates: metal-dependent stability, photophysical properties, and anticancer activity

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Cancer chemotherapy is often limited by systemic toxicity and the emergence of resistance, motivating the design of prodrugs and metal–drug conjugates that are selectively activated in the tumour microenvironment. Gossypol is a polyphenolic natural product with potent anticancer activity but demonstrate aldehyde-linked toxicity. We previously developed gossyzid, an isoniazid-based prodrug of gossypol that masks the aldehyde groups and undergoes pH-responsive activation. In this work, we advance a double-masking strategy by coordinating gossyzid to first-row transition metal ions to generate a family of gossyzid–metal conjugates (GMCs) incorporating Mn, Fe, Co, Ni, Cu and Zn. These GMCs were synthesised and characterised by UV–visible absorption, fluorescence spectroscopy, powder X-ray diffraction and thermogravimetric analysis, consistent with the formation of coordination polymer–like architectures that are stable under physiological conditions. Photophysical titrations established metal-dependent binding modes and relative complex stabilities. We then investigated amino acid–triggered de-chelation using biologically relevant amino acids as model biomolecular stimuli. UV–visible and fluorescence studies revealed that only selected metal–amino acid combinations efficiently unmasked gossyzid, with activation trends correlating with amino acid functional groups and chelation ability, as well as the intrinsic metal–ligand binding strength. Finally, the in vitro anticancer activity of the GMC series was evaluated in triple-negative breast cancer cells and related to their stability and activatability profiles. Conjugates that were sufficiently stable in buffer yet susceptible to amino acid–mediated de-chelation showed the most favourable anticancer performance. Overall, this study demonstrates amino acid–triggered activation of double-masked gossyzid–metal conjugates and highlights metal choice as a key design parameter for next-generation, tumour-selective metal–prodrug systems.

References:

[1]. Rebecca.S . & coworkers , *Cancer Journal for Clinicians*, **2021**,1
[2.] Biswas et al. *Coord. Chem. Rev.* **2024**, 517, 216026
[3]. W. Jiang et al. *Chemico-Biological Interactions,* **2022**, 364,110060
[4]. Biswas et al. *Chem. Eur. J,* **2023**, 29, e202203865

PP-40
2D/2D Z-Scheme $CaCo_2O_4$/g-C_3N_4 heterojunction for the photocatalytic degradation of methylene blue

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One of the major challenges in photocatalysis is the recombination of charge carriers. Constructing composite structures with intimate interfaces and favorable charge transfer routes is an effective way to address this drawback. Herein, a novel 2D/2D Z-Scheme $CaCo_2O_4$/g-C_3N_4 heterojunctions were designed, fabricated, and characterized. The as-prepared $CaCo_2O_4$/g-C_3N_4 catalysts exhibited significant enhancement in the photocatalytic efficiency for the degradation of methylene blue under visible-light irradiation in comparison to the single $CaCo_2O_4$ and g-C_3N_4 components. Among the prepared catalysts, the CCN-30 ($CaCo_2O_4$ (70%), g-C_3N_4 (30%)) had the highest efficiency in removing 95% of methylene blue under 120 mins. The enhanced photocatalytic efficiency can be attributed to the superior charge carrier separation due to the formation of a 2D/2D Z-Scheme heterojunction. Through scavenging studies, superoxide radical anions were found to be the dominant reactive oxygen species (ROS) and based on it, a plausible mechanism for photocatalysis is proposed.

Keywords: Photocatalyst, 2D materials, Z-Scheme, calcium cobalt oxide

References:

[1] Liu, X., Zhang, Q. and Ma, D., 2021. Advances in 2D/2D Z-scheme heterojunctions for photocatalytic applications. *Solar Rrl*, *5*(2), p.2000397.

[2] Tran, H., Mehta, T., Zeller, M. and Jarman, R.H., 2013. Synthesis and characterization of mixed phases in the Ca–Co–O system using the Pechini method. *Materials Research Bulletin*, *48*(7), pp.2450-2456.

PP-41
New Functionalized Terpyridines – Synthesis, Structural Characterization, Chemo sensing and Catalytic Applications

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The structural aspects of tpys prove that they are promising ligand systems with three nitrogen coordination sites. These unique ligands facilitate strong coordination with various metal cations through tight chelation. Notably, the electron-deficient-pyridine cycles make tpys weak σ-donors but very strong π-receptors. Further, remarkably flexible redox properties have led to the development of several catalysts for organic transformations. Perhaps one of the important manifestations is the ability of tpy ligands to achieve very attractive supramolecular coordination polymeric architectures. The analysis of catalytic and biological applications associated with various tpy-based group 8-10 metal complexes revealed a promising contribution of these tpy systems in terms of a wide range of catalytic reactions and potential biological activity.

In this regard, the present study describes a fluorescence-based sensing approach for detecting selective metal ions like thorium (Th^{4+}), zinc (Zn^{2+}), and the anion of the type, fluoride (F^-) using a modified tripodal terpyridine ligand. Also, the usage of tpy-based metal complexes was employed in ethylene oligomerization reactions. The synthesis of selected new terpyridine ligands and the corresponding metal complexes was carried out and the structural evaluation was accomplished by various analytical and spectroscopic data.

Keywords: Terpyridine, complexes, Sensing, Supramolecules, Catalysts

References:

1. Panicker, R. R., Joseph, S., Dharani, S., John, M. L., Kuriappan, A. T., Abraham, J. T., ... & Sivaramakrishna, A. (2025). **A highly lipophilic terpyridine ligand as an efficient fluorescent probe for the selective detection of zinc (II) ions under biological conditions**. *Analytical Methods*, *17*(2), 232-245.
2. Wei, C., He, Y., Shi, X., & Song, Z. (2019). **Terpyridine-metal complexes: Applications in catalysis and supramolecular chemistry**. *Coordination chemistry reviews*, *385*, 1-19.

PP-42

"Synthesis and Characterization of a Novel *Araucaria Heterophylla* Gum - Poly(Acrylic Acid) Hydrogel Silver Nanocomposite for Antibacterial and Antifungal Applications."

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A novel *Araucaria heterophylla* gum – poly(acrylic acid) hydrogel nanocomposite containing silver nanoparticles was successfully synthesized and evaluated for its antibacterial, antifungal effectiveness. The partially interwoven hydrogel framework was developed through a free-radical polymerization of acrylic acid in the presence of *Araucaria heterophylla* gum, where N,N′-methylene bisacrylamide (MBA) functioned as a cross-linking agent and ammonium persulphate (APS), tetramethyl ethylenediamine (TEMED) acted as initiators. The hydrogel network was subsequently infused with silver ions and converted to nanosilver in situ using neem (*Azadirachta indica*) leaf extract as reducing agent, providing a green and sustainable synthetic pathway. The resulting placebo hydrogel and nanocomposite were analyzed using FT–IR, UV–Vis DRS, XRD, SEM and EDX which confirmed the uniform nanosilver formation with altered swelling characteristics due to Ag^0 – polymer interactions. Bioactivity assessments indicated significant antibacterial and antifungal efficiencies, suggesting the release of silver nanoparticles in the culture medium. The findings demonstrate the potential of *Araucaria heterophylla* gum as a renewable and biocompatible polymeric base for eco-friendly hydrogel systems applicable to antibacterial and antifungal fields in biomedical research.

Keywords: *Araucaria heterophylla* gum, acrylic acid, hydrogel nanocomposite, Antibacterial, Antifungal.

References

[1] Hussain I. S. A, Jaisankar V. J. P. T, **An eco-friendly synthesis, characterization and antibacterial applications of novel almond gum–poly(acrylamide) based hydrogel silver nanocomposite**, Polym. Test., 2017, (62): 154–161.

PP-43
Designing Functionalized α-Aminophosphonates for Remarkable Coordination Behaviour, Photophysical, and Biological Applications

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Phosphine oxides are very well-known to exhibit remarkable coordination behaviour, photophysical, catalytic and biological properties including rich structural architectures. Among these interesting organophosphorus family, α-aminophosphonates are unique class of compounds due to the presence of additional N atom(s) responsible for their improved biological and catalytic activities. Since, a subtle change in the electronic and steric properties of remote substituents leads to the hitherto unknown properties, there is a strong demand for the synthesis of new aminophosphonates in search of promising candidates as ligands in coordination chemistry, probes for chemosensors, catalysts for organic transformations including for biological applications. In this regard, the present work is focused on the synthesis of various α-aminophosphonates by a streamlined three-component Kabachnik–Fields synthetic approach under mild conditions driven by a Lewis acid in ethanol at ambient temperature. The products were isolated in high yields (87–95%), accommodating a wide range of ring-substituted substrates and the structural characterization was achieved through various spectroscopic and analytical techniques including single-crystal X-ray diffraction analysis. Cyclic voltammetry revealed that the ferrocene moiety contributes a distinct redox behaviour, modulated by molecular substitutions. A comparison was made among various phosphine oxides and α-aminophosphonates in terms of coordination strength with selected *f*-metals.

Key words: Lewis's catalyst, one-pot synthesis at RT, α- Aminophosphonate, electrochemical studies, coordination behaviour

Reference:

[1] L.D. Quin, A Guide to Organophosphorus Chemistry, John Wiley & Sons, 2000 (book).

[3] Swati Jaydeokara, Vikas G. Yadava, Priyanka V. Bandivadekarb, Ganesh Chaturbhujb, Vijaykumar L. Chavana*, N-(1-hydroxybutan-2-yl)-4-nitrobenzene sulfonamide: A novel organocatalyst for an effective one-pot synthesis of α-amino phosphonates, Results in Chemistry 16 (2025) 102295 (Journal).

PP-44
Visible Light-Assisted Transesterification of Propylene Carbonate to Afford Octane Booster by Porphyrin Photocatalyst

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In the chemical industry, dimethyl carbonate (DMC) is a significant synthetic intermediate with numerous uses. The present study focuses on a porphyrin photocatalyst that was synthesised and employed for the photocatalytic transesterification of propylene carbonate into dimethyl carbonate. The photocatalyst was characterised using various spectroscopies techniques. Under visible light irradiation, the porphyrin photocatalyst demonstrated conversion of propylene carbonate into dimethyl carbonate using methanol/propylene carbonate 1:10 molar ratio under a 5 W LED at ambient temperature for 24 h. This finding emphasises the utility of porphyrin photocatalysts, furthermore, the results indicate potential applications in sustainable chemical processes, highlighting the significance of utilising renewable energy sources for catalysis.

Keywords*:* Porphyrin photocatalyst; Transesterification; Visible light; Sustainable; Industrial applications.

References

[1] Gu, S., Marianov, A. N., Lu, T., & Zhong, J. (2023). **A review of the development of porphyrin-based catalysts for electrochemical CO2 reduction.** In *Chemical Engineering Journal* (Vol. 470). Elsevier B.V. https://doi.org/10.1016/j.cej.2023.144249.

[2] Mataghare, B. C., & Bhagat, P. R. (2023). **Construction of porphyrin-based photocatalyst comprising pyridinium ionic liquid moiety for the metal-free visible light-assisted N-arylation of amines: facile approach to afford drug intermediates**. *New Journal of Chemistry*, *47*(47), 21764–21780. https://doi.org/10.1039/d3nj04295b

PP-45

$ASnO_3$ (A = Ca, Sr, Ba) perovskites as new and efficient photocatalytic Reductants for Cr (VI) remediation: Role of vacancies, pH and D-fructose

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Widespread Cr^{6+} contamination threatens ecosystems and human health due to its toxicity and carcinogenicity. Photocatalysis using perovskite oxides offers an efficient Cr^{6+} reduction route[1]. Their unique structure, electropositive A-site cations, and tunable oxygen vacancies collectively enhance physicochemical properties and photocatalytic activity, enabling effective conversion of Cr^{6+} to non-toxic Cr^{3+}. In this study, oxygen-deficient perovskite oxides $ASnO_3$ (A = Ba, Sr, Ca) were synthesized, characterized, and evaluated for photocatalytic Cr^{6+} reduction. Among them, $BaSnO_3$ exhibited the highest oxygen vacancy concentration due to its electropositive A-site cation, achieving 98.3% Cr^{6+} reduction within 40 minutes under UV light. With fructose as a co-catalyst, reduction extended to 100 ppm Cr^{6+}, marking the first and most efficient undoped $ASnO_3$ perovskite system reported[2].

Keywords: $ASnO_3$, perovskite, chromium, D-fructose, photoreduction, photocatalyst

References

[1] Prasad S., Yadav K.K., Kumar S., Gupta N., Cabral-Pinto M.M., Rezania S., Radwan N. and Alam J., **Chromium contamination and effect on environmental health and its remediation: A sustainable approaches.** Journal of Environmental Management, 2021 (285): 112174.

[2] Rohan T., Harikaran D., and Vijayaraghavan R. **$ASnO_3$ (A= Ca, Sr, Ba) perovskites as new and efficient photocatalytic reductants for Cr (VI) remediation: Role of vacancies, pH and D-fructose. Journal of Environmental** Chemical Engineering, 2025 (13): 118363.

PP-46
Bioactive Copper-Doped S53P4–Polymeric Hydrogel: A Dual-Functional Scaffold for Bone Regeneration and Infection Control

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Bone infections are a serious global threat and it often requires complex, multi-step treatment protocols typically including prolonged antibiotic therapy tailored to the causative organism or surgical debridement and bone grafts. However, with the alarming rise in antimicrobial resistance and the declining approval rate of new antibiotics, there's an urgent need for alternative therapeutic strategies. The goal of this work is to fabricate a dual- functional scaffold that can aid in bone regeneration and also in controlling infection. Copper is well known for its intrinsic antibacterial and osteogenic properties, making it an ideal dopant for this application. Characterization of the fabricated composite was performed to physiochemically assess and confirm the desirable formulation and properties. *In vitro* studies demonstrated that the composite is biocompatible and exhibits strong antibacterial activity against both gram-positive and gram-negative bacteria, highlighting its potential as an effective one-step treatment strategy.

Keywords: Bone infection, copper doped S53P4, scaffolds, bioactive glass, bone regeneration

References

[1] Kandari, Sudipta, Divya, Surbhi Gupta, Simanti Pal, Manisha Yadav, and Sevi Murugavel. **"Copper-Containing Mesoporous Bioactive Glasses with Multifunctional Properties**." *ACS Applied Bio Materials*, 2025, 8, 10, 9285–9298.

[2] Pasqui, Daniela, Paola Torricelli, Milena De Cagna, Milena Fini, and Rolando Barbucci. "**Carboxymethyl cellulose—hydroxyapatite hybrid hydrogel as a composite material for bone tissue engineering applications**." Journal of Biomedical Materials Research Part A 102, no. 5 (2014): 1568-1579.

PP-47

Design and Evaluation of Nitrogen and Oxygen -Based Heterocyclic Framework as Anti-Corrosion Inhibitors on Mild Steel in Acidic Environments

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The persistent challenge of metal degradation in aggressive environments continues to drive interest in synthetic inhibitors, especially those featuring heterocyclic frameworks. The present work focuses on the synthesis and evaluation of novel ((1,3-Diphenyl-1H-pyrazol-4-yl)methylene)benzo[1,3]dioxole-5-carbohydrazide derivatives, PIMFL and PIMNO, as mixed corrosion inhibitors on mild steel in 1M HCl medium. The compound features a methylenedioxy group, a pyrazole ring and an imine bond, which contributes to the corrosion inhibition of steel. The corrosion inhibition efficiency of the compounds was determined by experimental methods such as weight loss, potentiodynamic polarization and electrochemical impedance spectroscopy. Complementary quantum mechanical calculations were done, which corroborates the experimental findings. The novel scaffolds, PIMFL and PIMNO, retarded the degradation of mild steel in acidic media up to 84.17% and 67.55% respectively as per the weight loss experiment. With respect to the corrosion inhibition mechanism and polarization studies, it is inferred that the inhibitor functions as a mixed mode inhibitor.

Keywords: Corrosion, Heterocycles, Pyrazole, Mild steel, acidic medium

References

[1] Ramakrishnan, K., Karthikeyan, S., & Rajagopal, D. (2022). **2-Methoxy-4-(4-(((6-nitrobenzothiazol-2-yl) amino) methyl)-1-phenyl-1H-pyrazol-3-yl) phenol as powerful anti-corrosion inhibitor substantiated by Langmuir adsorption studies.** *Materials Letters*, *313*, 131823.

[2] Ahmed, S. K., Ali, W. B., & Khadom, A. A. (2019). **Synthesis and investigations of heterocyclic compounds as corrosion inhibitors for mild steel in hydrochloric acid.** *International Journal of Industrial Chemistry*, *10*(2), 159-173

PP-48
Synthesis, Characterization and Photophysical Properties of Pyridine-based extended Triazole Moieties

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Click chemistry is a modern and efficient synthetic approach that focuses on reactions which are simple, reliable, and produce high yields with minimal by-products. Among these, the copper(I)-catalyzed azide–alkyne cycloaddition (CuAAC) is the most widely used and is commonly known as the click reaction. This reaction connects an azide and an alkyne to form a stable 1,2,3-triazole ring under mild reaction conditions. Triazole moieties known for their excellent thermal and chemical stability, as well as their ability to coordinate with metals and form hydrogen bonds. Due to these properties, triazole derivatives find wide applications in medicinal chemistry, catalysis, materials science, and coordination chemistry. When triazole rings are combined with aromatic systems such as pyridine, the resulting extended conjugation can lead to interesting electronic and photophysical properties. In this study, pyridine-based extended triazole compounds were synthesized using the Cu(I)-catalyzed click reaction approach and were characterized using different spectroscopic techniques such as UV–Vis, FTIR, NMR, and fluorescence spectroscopy to confirm their structural features and purity. Their photophysical behavior was studied to understand how the presence of both pyridine and triazole units influences their optical properties, including light absorption and emission characteristics. Overall, this work demonstrates the effectiveness of click chemistry in building complex heterocyclic molecules in a simple and efficient manner. It also highlights the versatility of pyridine-based triazole derivatives as promising materials with interesting and adaptable photophysical properties, which could be further explored for practical applications in advanced material design.[1,2]

Keywords: Click Chemistry, Copper(I)-Catalyzed Azide–Alkyne Cycloaddition (CuAAC), Triazole Moieties, Pyridine-Based Compounds, Spectroscopic Characterization

References

[1] S. U and P. Paira, **2, 3-bis ((4-(pyridin-2-yl)-1H-1, 2, 3-triazol-1-yl) methyl) quinoxaline based Cyclometalated binuclear Ir (III) Complex for Photodynamic therapy in Triple Negative Breast Cancer Cell**. Chemistry, an Asian journal, 2025, e202401047.

PP-49
Computational Design and Evaluation of c-MET-Targeted PROTACs for Degradation-Driven Cancer Therapy

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The receptor tyrosine kinase c-MET, a pivotal regulator of cell proliferation, motility, and angiogenesis, is frequently overexpressed or mutated across various cancers, contributing to tumor progression and therapeutic resistance [1], [2]. Targeted Protein Degradation (TPD) through PROteolysis TArgeting Chimeras (PROTACs) offers a next-generation modality to eliminate such oncogenic drivers, overcoming the constraints of conventional inhibition [3], [4]. In this work, a series of novel c-MET-directed PROTACs was rationally designed by conjugating high-affinity c-MET ligands with E3 ligase recruiters (VHL and CRBN) via systematically optimized linkers. An integrated in silico pipeline was employed to assess their pharmacokinetic, physicochemical, and structural attributes. Swiss ADME analyses were conducted to evaluate oral bioavailability and drug-likeness [5]. Molecular docking using AutoDock Vina and SeeSAR revealed stable ternary complex formation among c-MET, the PROTAC, and the recruited E3 ligase, supporting favorable binding orientations and interaction energetics. Among the designed molecules, PROTAC-cMET5 exhibited superior stability and binding energy, indicating efficient target engagement and potential for ubiquitin-mediated degradation. Overall, this computational investigation highlights the promise of structure-guided PROTAC design for selective c-MET degradation, providing a foundation for future experimental validation toward degradation-based cancer therapeutics.

Keywords: c-MET, PROTAC, Targeted Protein Degradation, Molecular Docking, Molecular Dynamics Simulation, Cancer Therapy, E3 Ligase, In Silico Screening.

References

[1] F. Jin *et al.*, "**Recent advances in c-Met-based dual inhibitors in the treatment of cancers,**" *Eur. J. Med. Chem.*, vol. 272, p. 116477, June 2024, doi: 10.1016/j.ejmech.2024.116477.

PP-50
Fibroblast Activation Protein (FAP) ligands for cancer imaging and therapy

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Fibroblast Activation Protein alpha (FAP-α, EC3.4.2. B28) is a type II integral serine protease whose expression is restricted to embryonic mesenchyme and is not observed in normal adult tissues. Interestingly, FAP is highly expressed in cancer-associated fibroblasts and has also been reported in epithelial tumors [1]. Functionally, FAP exhibits the dipeptidyl peptidase and endopeptidase activity, and expression remains scarily noticeable or absent in normal tissues. The overexpression of the FAP in Cancer Associated Fibroblasts (CAFs) (which is located in the tumor microenvironment) across numerous epithelial tumors, including colon, pancreatic, hepatic, and ovarian cancer, has revolutionized tumor imaging and therapy. Various strategies, such as small molecules, peptides, and antibodies, have emerged to harness FAP for tumor imaging and treatment. The discovery of UAMC-1110 by Janson et al paved a new milestone in the small molecule FAP ligands [2].

In this study, we designed a series of novel FAP ligands using in silico methods. The best candidates were synthesized, purified, characterized, and conjugated with imaging agents and therapeutic agents. The selectivity and efficacy of the compounds were studied in vitro using the FAP-expressing U-87 MG cell line.

Reference

[1] M. Bukhari *et al.*, "**Fibroblast activation protein drives tumor metastasis via a protease-independent role in invadopodia stabilization**," *Cell Reports*, vol. 42, no. 10, p. 113302, Oct. 2023, doi: 10.1016/j.celrep.2023.113302.

PP-51
Protein-Polysaccharide Based Composite Hydrogel For Tissue Engineering Application

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Natural polymers are highly valued in biomedical fields for their excellent biocompatibility, biodegradability, and ability to closely mimic the extracellular matrix, facilitating cell growth and tissue regeneration. These sustainable materials are increasingly utilized in biomedical applications, including 3D bioprinting, to precisely fabricate complex, cell-laden structures with tailored mechanical and biological properties, thereby enabling advances in regenerative medicine and personalized therapies. Keratin, a fibrous structural protein extracted from human hair, is particularly attractive for tissue engineering due to its biocompatibility and intrinsic biochemical motifs that promote cell adhesion and proliferation[1]. In this study, we have extracted natural polymers such as keratin from human hair and polysaccharides from fruit. These polymers were characterized with FTIR, NMR, and SDS-PAGE. The fruit polysaccharide was modified with a photo curable group, and a composite hydrogel of keratin and photo curable polysaccharides was fabricated. The hydrogels were then characterized for their swelling properties, protein release, and chemical interactions. In the results, the yield of keratin and polysaccharide was found to be 16 % and 4 %, respectively. Moreover, SDS-PAGE shows a molecular weight of protein ranging from 45-70 kDa, confirming the presence of keratin. Furthermore, composite hydrogels demonstrated good water-holding properties and reduced protein release, suggesting protein retention in the hydrogel that can support cell attachment and proliferation. In conclusion, composite hydrogel can be used as a promising platform for different biomedical applications.

Keywords: Keratin, Bael fruit polysaccharide, Methacrylate polysaccharide, Photocurable hydrogel

References

[1] C.-W. Lin, T.-H. Liu, V. Chen, E.-Y. Chuang, Y.-J. Fan, and J. Yu, “Synergistic potential of gellan gum methacrylate and keratin hydrogel for visceral hemostasis and skin tissue regeneration,” *Mater. Today Bio*, vol. 27, p. 101146, 2024, doi: https://doi.org/10.1016/j.mtbio.2024.101146.

PP-52
Palladium-Catalysed Sonogashira and Suzuki Functionalization of Phenazine: Synthesis, Characterisation, and Photophysical Insights

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The Sonogashira and Suzuki reactions represent cornerstone palladium-catalysed cross-coupling methodologies in modern organic synthesis. In this study, both reactions were employed to functionalize the phenazine core—a redox-active, π-conjugated heterocycle known for its biological and optoelectronic significance. The Sonogashira coupling enabled the introduction of alkynyl substituents, while the Suzuki reaction facilitated aryl functionalization under mild, optimised conditions. The resulting derivatives will be characterised spectroscopically to confirm structural integrity and explored for their photophysical and electronic properties. This dual functionalization approach underscores the versatility of transition-metal catalysis in tailoring the electronic landscape of phenazine, paving the way for its potential applications in drug design, light-emitting materials, and molecular electronics.

Keywords: Suzuki Reaction, Sonogashira Reaction, Phenazine, Palladium catalyst, Photophysical study.

References

[1] Sonogashira, K.; Tohda, Y.; Hagihara, N. **Development of the Sonogashira coupling reaction between terminal alkynes and aryl/vinyl halides**. Tetrahedron Letters, 1975, 16(50), 4467–4470.

[2] Miyaura, N.; Suzuki, A. **Original report on the palladium-catalysed cross-coupling of organoboron compounds with halides**. Chemical Communications, 1979, 19, 866–867.

[3] Negishi, E. **Comprehensive review on palladium-catalysed cross-coupling reactions, including Sonogashira and Suzuki methods**. Angewandte Chemie International Edition, 2011, 50(30), 6738–6764.

PP-53

Valorisation of lignin from agro waste for fabrication of eco-friendly bio composite films with improved physical and functional properties

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Agro waste remains as an underutilised source of lignin, the second most abundant biopolymer on Earth after cellulose. Globally, about 2 billion tons of agro waste is produced every year and most of them are either burnt or improperly dumped. This study utilises lignin from agro waste (coir waste) following the acid precipitation for extraction of lignin. The resulting lignin was used as a functional filler into alginate films to improve their physical and functional properties. SEM analysis confirmed sheet-like morphology and, while FT-IR and 1H NMR analysis further validated its structure. The extracted lignin exhibited a zeta potential of –29.4mV, indicating high colloidal stability. The lignin particles of different concentrations (5-20 w/w %) of were added to the alginate polymeric matrix for the fabrication of bio composite films. The addition of lignin, imparted UV-blocking abilities, enhanced thermal, and mechanical properties of the alginate films. Morphological studies by SEM shows a rough surface and the bio composite films exhibited antibacterial activity against Staphylococcus aureus. As both alginate and lignin are biodegradable in nature, the functionally enhanced alginate-lignin bio composite films exhibit potential for advanced functionalities in sustainable packaging applications.

Keywords: Lignin, Valorisation, agro waste, alginate, biodegradable, bio composites, eco-friendly packaging

References

[1] Steiger, B. G., Zhou, Z., Anisimov, Y. A., Evitts, R. W., & Wilson, L. D. (2023). Valorization of agro-waste biomass as composite adsorbents for sustainable wastewater treatment. Industrial Crops and Products, 191, 115913.

[2] Zadeh, E. M., O'Keefe, S. F., & Kim, Y. T. (2018). Utilization of lignin in biopolymeric packaging films. ACS omega, 3(7), 7388-7398.

PP-54

Phytochemical-Enriched Nano-hydroxyapatite Reinforced into Polymeric Cryogel Scaffolds for Bone Regeneration

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Osteoporosis leads to reduced bone density and strength, increasing fracture risk due to an imbalance in bone formation and resorption. Which risk of fractures and is influenced by aging, lifestyle changes, and nutritional inadequacies. Adverse effects, poor adherence, and costs limit the effectiveness of current treatments, such as autologous bone transplants and bisphosphonates. To handle its increasing burden, safer, more innovative approaches combining cutting-edge regenerative therapies and early diagnostics are vital. The development of polymeric cryogel scaffolds combined with nanocomposites, like phytochemical-loaded nanohydroxyapatite, has grown into an effective strategy for bone regeneration to overcome this challenge. The sponge-like flexibility and highly interconnected macroporous structure of cryogel promote tissue ingrowth, nutrient transport, and cellular penetration. Cryogel are also capable of being precisely sized and shape memory effect to fit bone defects and provide outstanding mechanical stability. By loading plant-based compounds onto eggshell-derived nanohydroxyapatite, the enhancement of biocompatibility combines phytochemicals that possess antibacterial, anti-inflammatory, and antioxidant properties with a natural, porous, and bioactive scaffold closely resembling bone composition. Cell viability is maintained, osteogenic activity is stimulated, and this cooperative integration reduces cytotoxicity. For bone tissue development and healing, the composite material thus provides an ideal environment.

Keywords: Nanohydroxyapatite, Eggshell waste, Polymeric Cryogel, Tissue Engineering, Phyto-therapeutics.

PP-55
Rapid Colorimetric Sensing of Bacterial Contamination in Water Using Polymer-Modified Fe_3O_4 Nanoparticles

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Ensuring the safety of water supplies from bacterial contamination is crucial for protecting public health and the environment. Conventional detection methods often require expensive equipment and trained personnel, limiting their use in resource-limited settings. This study presents a simple, affordable solution using chitosan-coated Fe_3O_4 magnetic nanoparticles as a colorimetric sensor for bacteria detection in water. The chitosan modification improves the nanoparticles' stability and dispersion, and provides functional groups that bind effectively to bacterial cells. When these nanoparticles encounter bacteria, a visible color change occurs that can be recognized instantly without specialized instruments or training. This highly intuitive detection method allows anyone, regardless of scientific background, to easily assess bacterial contamination by just observing the shift in color. Characterization by FTIR, XRD, TGA, SEM/TEM, and XPS verified the successful synthesis and surface modification of the nanoparticles. The approach demonstrates a rapid, user-friendly, and scalable pathway for monitoring water quality, making bacterial detection accessible for both field use and basic community health screening.

Keywords: Nanoparticles, Colorimetric detection, Bacteria

References

[1]Le, T. N., Tran, T. D., & Kim, M. I. (2020). **A Convenient Colorimetric Bacteria Detection Method Utilizing Chitosan-Coated Magnetic Nanoparticles**. *Nanomaterials (Basel, Switzerland)*, *10*(1), 92.

PP-56
Exploring the Synthetic and Photophysical Potential of Benzimidazole-Based Aryl Derivatives through Suzuki Coupling

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The Suzuki cross-coupling reaction serves as a powerful and versatile palladium-catalysed strategy for constructing carbon–carbon bonds in modern organic synthesis. In the present work, benzimidazole—a pharmacologically and photochemically significant heterocyclic scaffold—was utilised as the core framework for designing a new series of aryl-substituted derivatives via the Suzuki coupling approach. Diverse aryl boronic acids were coupled with benzimidazole under optimised palladium-catalysed conditions using a mild base to achieve high efficiency and selectivity. The resulting compounds will be comprehensively characterised by IR and NMR spectroscopy, followed by detailed photophysical investigations to explore their optical properties. This study underscores the synthetic utility of the Suzuki reaction in benzimidazole functionalization and its potential to generate molecules with promising biological applications.

Keywords: Suzuki reaction, Benzimidazole, Palladium catalyst, Boronic acids, Photophysical study.

References

[1] N. Miyaura, A. Suzuki, Chem. Rev. 95 (1995) 2457.

[2] A. Suzuki, in F. Diederich, P.J. Stang (Eds.), **Metal-Catalysed Cross-Coupling Reactions**, VCH, Weinheim, 1998, pp. 49–97.

[3] N R Said, M A Mustakim, N N Md Sani, S N A Baharin, "**Heck reaction using palladium-benzimidazole catalyst: synthesis, characterisation and catalytic activity**," IOP Conf. Ser.: Mater. Sci. Eng. 458 (2018) 012019. doi:10.1088/1757-899X/458/1/012019.

PP-57
Highly Efficient Ternary Composite Adsorbent for Enhanced Dye Removal

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A ternary composite composed of a biopolymer, metal oxide, and a fruit peel biochar was synthesized and evaluated for its capacity to adsorb dyes from aqueous solutions. While the parent and binary composites showed limited effectiveness, the ternary composite demonstrated a substantial improvement, achieving 97.04% dye removal when 20 mg of the adsorbent within 6 hours. Comprehensive characterization techniques such as XRD, FTIR, SEM, and BET confirmed the successful integration and uniform dispersion of components, indicating enhanced surface properties conducive to adsorption. Batch adsorption experiments revealed significant dye uptake, attributed to the synergistic effects of the functional groups, porous structure, and electrostatic interactions of the composite. The enhanced adsorption of further supported by increased surface area and active sites, validated by the characterization techniques. These findings indicate that the composite is highly effective for dye removal from industrial effluents and is suitable for practical wastewater treatment applications, offering scalability and robust performance. Importantly, the use of bio-based components highlights the composite's potential for sustainable wastewater remediation. such materials contribute to environmentally friendly and resource-efficient treatment strategies for dye laden water.

Keywords: Biopolymer, Adsorption, Metal oxide, Dye, Biochar.

References

[1] Yu, Y., Liu, W., Zhang, Y., Zhang, B., Jin, Y., Chen, S., Tang, S., Su, Y., Yu, X., & Chen, G. **Chitosan/magnetic biochar composite with enhanced reusability: Synergistic effect of functional groups and multilayer structure**. *Arabian Journal of Chemistry*., 2024., *17*(5)., 105746.

[2] Ali, S., Dayo, M., Alahmadi, S., & Mohamed, A., **Chitosan-Supported ZnO nanoparticles: Their green synthesis, characterization, and application for the removal of pyridoxine HCl (Vitamin B6) from aqueous media**., *Molecules.*, 2024., *29*(4), 828.

PP-58

Development of the guar gum reinforced injectable calcium magnesium phosphate bone cement

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Bone defects are a common problem caused by fracture, trauma, tumor resection, and infection. Although bones can regenerate and self-repair in young people, bone grafts are needed for large bone defects caused by fracture, trauma, infection, and tumor resection [1]. Polymethyl methacrylate (PMMA) bone cements were used for bone repair; however, their biodegradability, biocompatibility, and limited bone integration limit their use [2]. In this study, we have developed calcium-magnesium-phosphate-based bone cement reinforced with oxidized guar gum and simvastatin-loaded PLGA microparticles to achieve injectability, low setting time, excellent biocompatibility, and local drug release. The bone cement composition was designed to undergo self-setting in a physiological microenvironment. The injectability and setting time of the bone cement were found to be 96% and 10 minutes**,** respectively. The PLGA microparticle with an average diameter of 36.5 µm was fabricated and incorporated in the bone cement for sustained release of simvastatin. Moreover, the FTIR studies confirm the presence of guar gum, PLGA microparticles, and calcium magnesium phosphate cement. In vitro cytocompatibility of bone cement using human dental pulp stem cells demonstrated over 90% cell viability. In conclusion, developed bone cement offers a promising platform for minimally invasive bone defect repair with excellent biocompatibility, injectability, and localized drug delivery.

Keywords: Bone Cement, Injectable Bone Cement, Guar Gum, Calcium Magnesium Phosphate cement

References

1.Wang, W., & Yeung, K. W. (2017). Bone grafts and biomaterials substitutes for bone defect repair: A review. *Bioactive materials*, *2*(4), 224-247.

PP-59
Development of electrospun scaffolds with embedded drug-loaded Chitosan nanoparticles for enhanced tissue regeneration

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Chitosan-based nanoparticles offer a significant potential for controlled and prolonged drug delivery, owing to their biodegradability, biocompatibility, and variable surface properties. This study involved the synthesis of chitosan nanoparticles and the subsequent incorporation of bovine serum albumin (BSA) as a model drug. The encapsulation efficiency of this was quantified, followed by in vitro release studies to assess release kinetics. The physicochemical properties of nanoparticles were analysed using a field emission scanning electron microscope (FESEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR), which confirmed uniform morphology, crystalline behaviour, and drug polymer interaction. To further enhance controlled release, the BSA-loaded chitosan nanoparticles were embedded within an electrospun polymer scaffold. The electrospinning parameters were optimized to obtain stable and continuous fibre morphology and uniform particle distribution within the scaffold. The release of the drug from the electrospun mat was evaluated to determine the efficiency of the hybrid delivery system. Collectively, the finding suggests that the chitosan nanoparticle-electrospun matrix provides a strong dual-layered system capable of achieving a sustained and efficient drug delivery system.

Keywords: Chitosan nanoparticles, BSA, Electrospinning, Smart drug delivery,

References

[1] Vandana, M., & Sahoo, S. K. (2009). **Optimization of physicochemical parameters influencing the fabrication of protein-loaded chitosan nanoparticles**. *Nanomedicine*, *4*(7), 773-785.
[2] Yadav, P., & Yadav, A. B. (2021). **Preparation and characterization of BSA as a model protein loaded chitosan nanoparticles for the development of protein-/peptide-based drug delivery system.** *Future Journal of Pharmaceutical Sciences*, *7*(1), 200.

PP-60
Design, Synthesis, and Characterization of a Metal Oxide–Integrated Biopolymer–Biochar Composite for Sustainable Dye Adsorption

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A novel composite material combining biopolymer, a selected metal oxide, and fruit peel-derived biochar was synthesized and investigated for its potential in the adsorption of a cationic dye from aqueous solutions. The biochar was obtained via pyrolysis of dried fruit peels, while the metal oxide was incorporated into the biopolymer matrix to enhance surface reactivity and stability. The composite underwent comprehensive physicochemical characterization using techniques such as XRD, FTIR, SEM, and BET analysis to assess its structural and functional properties. Batch adsorption studies were conducted under varying conditions to evaluate dye uptake performance. Additionally, adsorption kinetics and equilibrium behavior were examined using established isotherm models. This study was designed to explore the synergistic interaction among the biopolymer, biochar, and metal oxide phases, targeting sustainable wastewater treatment applications. The findings suggest that this composite holds significant potential as a sustainable and economically viable material for efficient dye removal from contaminated water systems.

Keywords: Biopolymer, Metal oxide, Biochar, Cationic dye, Dye adsorption

References

[1] Giraldo, S., Acelas, N. Y., Ocampo-Pérez, R., Padilla-Ortega, E., Flórez, E., Franco, C. A., Cortés, F. B., & Forgionny, A. (2022). **Application of orange peel waste as adsorbent for methylene blue and Cd^{2+} simultaneous remediation**. *Molecules*, 27(16), 5105.

[2] Li, X., Feng, X., et al. (2024). **Construction of Chitosan-biochar/ZnO/NiO composites for efficient photocatalytic removal of Congo red and tetracycline.** *Journal of Hazardous Materials*, 443, 130288.

PP-61
Design and Development of Metal Complexes as Novel Anticancer Therapeutics

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The development of metal-based chemotherapeutics has opened new avenues for cancer treatment beyond traditional platinum-based drugs, offering advantages such as tunable redox behaviour, lower systemic toxicity, and enhanced target specificity [1]. In this study, a new class of half-sandwich ruthenium(II) arene complexes was rationally designed and synthesized employing coumarin–benzimidazole hybrid ligands to achieve synergistic therapeutic and diagnostic potential [2]. The structural integrity and coordination environment of the complexes were confirmed by NMR and UV–Vis-spectroscopy, verifying successful ligand coordination to the ruthenium centre.

The enhanced anticancer efficacy is attributed to strong DNA-binding affinity, reactive oxygen species (ROS) generation, and induction of apoptotic pathways mediated by the synergistic interaction between the metal core and the ligand scaffold [3], [4]. Furthermore, the inherent fluorescence of the coumarin fragment supports its potential use in cellular imaging, establishing a link between therapy and diagnostics. Collectively, highlight the promising potential of ruthenium (II)–coumarin–benzimidazole complexes as next-generation anticancer theragnostic agents, integrating potent cytotoxicity with imaging capability for advanced cancer management.

Keywords: Ruthenium (II) complexes, Anticancer agents, Coumarin–benzimidazole hybrids, Bioinorganic chemistry, Theragnostic

References:

[1] T. Gamberi and M. Hanif, "**Metal-Based Complexes in Cancer Treatment**," *Biomedicines*, vol. 10, no. 10, p. 2573, Oct. 2022, doi: 10.3390/biomedicines10102573.

[2] J. Li *et al.*, "**Half-Sandwich Iridium and Ruthenium Complexes: Effective Tracking in Cells and Anticancer Studies**," *Inorg. Chem.*, vol. 57, no. 21, pp. 13552–13563, Nov. 2018, doi: 10.1021/acs.inorgchem.8b02161.

PP-62
Adsorptive Removal of Heavy Metals Chromium and Copper Using Pomegranate Peel-Reinforced Chitosan Oligosaccharide, Kaolin Clay-Based Hydrogel

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An essential resource for both social and economic advancement is water. Severe water contamination is the outcome of several anthropogenic activities and a sharp rise in industry. Because heavy metals are hazardous, non-biodegradable, and carcinogenic, their discharge contaminates both the aquatic environment and human health. Wastewater treatment is therefore necessary before discharging heavy metals into aquatic bodies. Hydrogels are excellent candidates for removing hazardous heavy metals in wastewater because they are strong adsorbent materials. Hydrogels are soft materials created by creating a three-dimensional network structure by cross-linking natural or synthetic polymers. Adsorption, which offers cost-effectiveness, convenience of use, a wide range of absorbent materials, and sustainability, continues to be the best option despite the adoption of numerous approaches because it permits the use of inexpensive, sustainable, high-efficiency, and environmentally friendly biosorbents. In order to remove wastewater, including the heavy metals chromium and copper, this work optimises a pomegranate peel-enriched chitosan oligosaccharide (COS), Kaolin clay (KC) grafted polyacrylamide (AM) hydrogel without and with pomegranate peel powder (PP) (COS-KC-g-AM-MBA & COS-KC-g-AM/PP-MBA). Grafting was used to fabricate the hydrogels, and their adsorption capacity was assessed. Batch adsorption tests assessed the removal efficiency, obtaining over 97% removal for both Cu (II) and Cr (VI) ions, with a higher removal rate for copper. The adsorbent containing pomegranate peel had a greater adsorption capacity than the other adsorbent. The functional groups from the pomegranate peel, chitosan oligosaccharide, and kaolin clay in the hydrogel with a highly porous structure, because of its three-dimensional network structure, were responsible for the notable adsorption capacity.

Key words: Chitosan oligosaccharide, pomegranate peel hydrogel, adsorption, heavy metals.

References

[1] Sharmila, K., Srinivasan, Latha, Vijayalakshmi, K., Alshalwi, M., Alotaibi, K. M., Sudha, P. N., ... & Deepa, M. (2024). **Evaluation of the efficacy of chitosan oligosaccharide-salicylaldehyde Schiff base to extract copper (II) and chromium (VI) from synthetic wastewater.** *Biomass Conversion and Biorefinery*, 1-16.

[2]Rekha, A., Srinivasan, Latha, Pavithra, S., Gomathi, T., Sudha, P. N., Lavanya, G., ... & Vidhya, A. (2025). **Biosorption efficacy studies of *Sargassum wightii* and its biochar on the removal of chromium from aqueous solution.** *Journal of the Taiwan Institute of Chemical Engineers*, *166*, 105241.

PP-63
Synthesis of nano β-Zeolite possessing hierarchical porosity via Steam-Assisted crystallization of Mesoporous Aluminosilicate

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Hierarchically structured micro-mesoporous nano-zeolites have several advantages in catalyzing reactions involving bulky reactants and products. In this work, hierarchical β-zeolite was synthesized facilely by a steam-assisted dry gel conversion of mesoporous aluminosilicate (Al-SBA-16) using TEAOH as both a structure-directing agent and a mineralizer. Two different Al-SBA-16 precursors were prepared by post-synthetic incorporation of Al into the siliceous SBA-16 using two different aluminium sources, aluminium isopropoxide and sodium aluminate. The effects of varying the amount of TEAOH, crystallization time, and nature of the mesoporous aluminosilicate precursor were studied. The textural characteristics, crystallinity, coordination environment and morphology of the prepared β-zeolites were investigated using nitrogen sorption, powder X-ray diffraction, solid-state NMR spectroscopy, and transmission electron microscopy. The use of Al-SBA-16, obtained from SBA-16 and sodium aluminate, was found to be effective for the synthesis of uniformly nano-sized beta zeolite particles exhibiting intercrystallite mesoporosity. At the same time, the Al-SBA-16 obtained from SBA-16 and aluminium isopropoxide produced larger crystallites of β-zeolite possessing intracrystalline mesoporosity. ^{27}Al MAS NMR spectra of the prepared zeolites indicated the incorporation of Al into the tetrahedral framework of silica. The acidic properties of the prepared zeolites were studied using temperature-programmed NH_3 desorption. The catalytic activity of the prepared zeolites was examined using a standard test reaction between mesitylene and benzyl alcohol, which served as a tool to investigate the hierarchical porosity of the zeolites. The higher catalytic activity of the nano β-zeolite compared to the commercial β-zeolite confirmed the existence of hierarchical micro-mesoporosity in the former. The synthetic strategy reported here eliminates the use of mesopore-directing agents, mineralizers, and alkali hydroxides, producing a meso-microporous hierarchical structure that can be achieved in one pot.

Keywords: zeolite beta, nanoparticles, hierarchical intracrystalline mesoporosity

References

[1] Möller K, Yilmaz B, Jacubinas R. M, Müller U, Bein T, **One-step synthesis of hierarchical zeolite beta via network formation of uniform nanocrystals**, J. Am. Chem. Soc., 2011, (133): 5284–5295.
[2] Sakthivel A, Iida A, Komura K, Sugi Y**, The β-zeolite synthesized by dry-gel conversion method without the use of sodium hydroxide: characterization and catalytic behaviors**, J. Nanosci. Nanotechnol., 2009, (9): 475–483.

PP-64
Bridged Boranoanthracenes: A Facile Generation of Oxoboranes through Aromatisation-Driven Oxidative Extrusion

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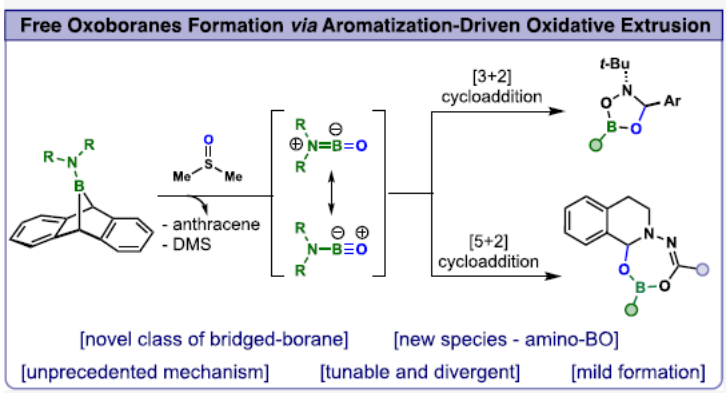
Organoboron compounds have played a central role in organic chemistry for more than 60 years and featured in two Nobel Prize-winning reactions.[1] However, the contemporary strategies mainly rely on the use of a stable boronating agent. The use of transient sub-valent boron species has not been widely studied so far, due to their instability. In this study, we have developed a novel class of boranobornadiene derivatives, termed boranoanthracenes, and provided a detailed investigation of their structures and reactivities. Leveraging these versatile precursors, we propose a fundamentally new mechanism for generating free oxoborane species driven by an oxidative aromatization strategy. We uncovered three distinct reactivity modes of these intermediates: (1) insertion of oxoboranes into B-C bonds, representing, to our knowledge, the first example of such a transformation; (2) a [3 + 2] cycloaddition with nitrones, providing access to new boranoheterocycles; and (3) the first [5 + 2] cycloaddition between oxoboranes and azomethine imines, yielding seven-membered boracycles.[2]



Keywords: Organoboron, boranoanthracenes, oxoboron, aromatization

References:

1. Brown, H. C.; Rao, B. C. S. *J. Am. Chem. Soc.* **1956**, *78*, 5694-5695. (b) Miyaura, N.; Suzuki, A. *Chem. Rev.* **1995**, *95*, 2457-2483.
(2). Deri, S.;# Feller, M.;# Panda, S.;# Batya, B.; Iron, M.; Diskin-Posner, Y.; Avram, L.; Shimon, L. J. W.; Mondal, R.; Gnaim, S. *J. Am. Chem. Soc.* **2025,** *147*, *23*, 19520-19529.

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