30th ISCB International Conference

ISCBC-2025

Current Trends in Chemical, Biological and Pharmaceutical Sciences: Impact on Health and Environment

27th - 29th , January 2025

Department of Chemistry,
University of Lucknow, Lucknow

Abstract Book

Jointly Organized by

Indian Society of Chemists & Biologists (ISCB)
Department of Chemistry, University of Lucknow

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Message

We are delighted to announce that the Indian Society of Chemists and Biologists (ISCB), Lucknow, is hosting the 30th ISCB International Conference (ISCBC-2025). This prestigious event is being jointly organized by Indian Society of Chemists and Biologists and the Department of Chemistry, Lucknow University, and will take place at Lucknow University, Lucknow, India, from January 27 to January 29, 2025.

The central theme of ISCBC-2025 is "Current Trends in Chemical, Biological, and Pharmaceutical Sciences: Impact on Health and Environment." The conference will bring together researchers to discuss ground-breaking advancements in these fields, with a focus on fostering innovation to enhance healthcare practices and environmental sustainability.

Renowned scientists and researchers from across the globe will join as keynote and invited speakers, with over 100 senior scientists and professors presenting insights into cutting-edge developments and innovations in healthcare.

The scientific committee will compile an abstract book showcasing the diverse presentations featured during the conference. We extend our heartfelt gratitude to the organizing committee for their invaluable contributions in making this event possible. The conference aims to facilitate meaningful discussions on emerging trends, opportunities, and future directions in scientific research, creating a vibrant platform for collaboration and knowledge exchange.

The comprehensive program will include plenary lectures, invited talks, and short-gun lectures by eminent scientists from India and abroad. Young researchers will have the opportunity to present oral talks, and poster sessions will highlight the contributions of Ph.D. students and budding scientists.

We warmly welcome national and international delegates from pharmaceutical companies, research organizations, universities, and academic institutions. We hope all participants enjoy a memorable stay in Lucknow. In closing, we extend our sincere thanks to the members and office bearers of the organizing committee for their dedication to the success of ISCBC-2025.

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SCIENTIFIC PROGRAMME

Monday, January 27, 2025

Registration
Venue: Opposite Chemistry Department

9.00 AM onwards	**Registration**

Inaugural Session
Venue: Malviya Hall

10.00 AM - 11.30 AM	**Inaugural Session**

11.30 AM - 12.00 PM	**High Tea** (Venue: Lawn Opposite Malviya Hall)

Session – I
Venue: Malviya Hall
Chairpersons: Prof Anamik Shah and Dr PMS Chauhan

PL-1 12.00 AM - 12.30 PM	**Samir Z. Zard** Laboratoire de Synthèse Organique, Ecole Polytechnique, Palaiseau, France **Radical Alliances. Solutions and Opportunities for Organic Synthesis**
PL-2 12.30 PM - 1.00 PM	**Mukund S. Chorghade** President & Chief Scientific Officer, THINQ Pharma, New Jersey, USA **Science Entrepreneurship**
1.00 PM - 2.00 PM	**Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – II A
Venue: Chemistry Auditorium (S 141)
Chairpersons: Prof Leonid G. Voskressensky and Prof Abbas Ali Mahdi

PL-3 2.00 PM - 2.30 PM	**Rui Moreira** iMed.ULisboa, Department of Pharmaceutical Sciences and Medicines, Faculty of Pharmacy, Universidade of Lisboa, Lisboa, Portugal **Small-Molecule Probes to Target Cell Death Mechanisms and Tumour Microenvironment**

IL-1 2.30 PM - 2.50 PM	**Bapurao B. Shingate** Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, Maharashtra, India **1,2,3-Trizole tethered diversely functionalized heterocyclic compounds as therapeutic agents**
IL-2 2.50 PM - 3.10 PM	**Sartaj Tabassum** Cancer and Bioinorganic Research Lab, Department of Chemistry Aligarh Muslim University, Aligarh, India **Metal-based anti-cancer drug entities as potential ROS-generating species embedded on Graphene oxide as drug carrier**
IL-3 3.10 PM - 3.30 PM	**Indresh Kumar** Professor and Head, Department of Chemistry, Birla Institute of Technology & Sciences (BITS) Pilani, Pilani (Rajasthan), India **Direct Access to C3-Functionalized Pyrrole**
IL-4 3.30 PM - 3.50 PM	**Bhumika Patel** Assistant Professor, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **Two decades of PARP1 Inhibitors in Cancer Research: Success, Challenges and Roadmap Ahead**
IL-5 3.50 PM - 4.10 PM	**Ramendra Pratap singh** Department of Chemistry, University of Delhi, India **Synthesis of new aza-heterocycles from aryl methyl ketone and their antibacterial properties**
4.10 PM - 4.20 PM	**Tea Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – II B

Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Prof Karol Grela and and Prof V.K. Sharma

PL-4 2.00 PM - 2.30 PM	**K.G. Anoja P. Attanayake** Professor in Biochemistry, Department of Biochemistry, Faculty of Medicine, University of Ruhuna, Sri Lanka **Harnessing Herbal Products to Combat Early-Stage Diabetes and Prevent Complications**
IL-6 2.30 PM - 2.50 PM	**Krishna Nand Singh** Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Development of Some New Protocols in Organic Synthesis**

IL-7 2.50 PM - 3.10 PM	**Hitendra M. Patel** Professor, Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **OTBN-1,2,3-triazoles and dihydropyrimido[4,5-b]quinolinones enabling diverse anti-proliferative and anti-invasive activity against glioblastoma cells**
IL-8 3.10 PM - 3.30 PM	**Dalip Kumar** Senior Professor, Department of Chemistry, Associate Dean, International Programmes and Collaboration Division (IPCD), Birla Institute of Technology & Science, Pilani, Pilani Campus, India **Denitrogenative annulation of benzotriazole-appended porphyrins for the rapid and efficient synthesis of diverse heterocycle-fused porphyrins**
IL-9 3.30 PM - 3.50 PM	**Ram Sagar Misra** Professor, School of Physical Sciences, Jawaharlal Nehru University (JNU), New Delhi, India **Synthesis of Chirally Enriched Pyrazolylpyrimidinone and Imidazopyrimidinones based Glycohybrids via Annulation reactions with Glycals**
IL-10 3.50 PM - 4.10 PM	**Divya Vohora** Professor, Department of Pharmacology, School of Pharmaceutical Education and Research (SPER), Jamia Hamdard, New Delhi, India **Beyond Numbers: The Complex Reality of Metrics**
4.10 PM - 4.20 PM	**Tea Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – II C
Venue: Multi Activity Hall

Chairpersons: Prof Sarvesh Paliwal, Prof Sundaram Singh and Dr Narendra Kumar Singh

PL-5 2.00 PM - 2.30 PM	**Diwan S Rawat** Vice Chancellor, Kumaun University, Nainital, India **A ray of hope for Parkinson`s disease treatment: Story of discovery of a clinical candidate**
IL-11 2.30 PM - 2.50 PM	**Dhananjay V Mane** Professor in Chemistry and Regional Director, Yashvantrao Chavan Maharastra Open University, Nashik, Maharashtra, India **RP-HPLC Stability Indicating Method Development and Validation forEstimation of Rivaroxaban in Active Pharmaceuticals Ingredients**
IL-12 2.50 PM - 3.10 PM	**Hitesh D. Patel** Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India **Medicinal Chemistry as multidisciplinary**

IL-13 3.10 PM - 3.30 PM	**Deb Ranjan Banerjee** Assistant Professor, Department of Chemistry, National Institute of Technology Durgapur, Durgapur, West Bengal, India **Towards epigenetic therapeutics of Alzheimer's disease: Discovery of Methyltransferase inhibitor via QSAR screening, *in vitro* and *in vivo* analyses**
IL-14 3.30 PM - 3.50 PM	**Sivapriya Kirubakaran** Professor, Indian Institute of Technology - Gandhinagar, Gandhinagar, Gujarat, India **Targeting *Hp* IMPDH to develop efficient drugs for the infection**
IL-15 3.50 PM - 4.10 PM	**Alok Jain** Assistant Professor and Ramalingaswami Fellow, Department of Bioengineering and Biotechnology, Birla Institute of Technology (BIT), Mesra, Ranchi, India **Deciphering the Atomistic Mechanism of PKM2 Dimerization: Impact of Post-Translational Modifications and Mutation**
4.10 PM - 4.20 PM	**Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – III A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Prof Atul Bapodra, Dr Rachna Sadana and Prof Abhinav Kumar

PL-6 4.20 PM - 4.50 PM	**Chris Farren** Innovation Director, Natara Global Ltd, Hartlepool, United Kingdom **The Magic (and Science!) Behind Flavour and Fragrance**
IL-16 4.50 PM - 5.10 PM	**Ravindra Vikram Singh** Director and Head- India R&D, Technology and Innovation, Sigma-Aldrich Chemicals Pvt. Ltd (Merck KGaA, Darmstadt, Germany), India **Driving Innovation Through R&D Strategies: Emerging Therapeutic Modalities and the Future of Medicine**
IL-17 5.10 PM - 5.30 PM	**Niyati Acharya** Department of Pharmacognosy, Institute of Pharmacy, Nirma University, Ahmedabad, India **NEUROPROTECTIVE EFFECTS OF MYRICETIN NANOFORMULATIONS**
IL-18 5.30 PM - 5.50 PM	**John J. Georrge** Associate Professor, Department of Bioinformatics, University of North Bengal, Darjeeling, West Bengal, India **Identification of novel inhibitors against the endometriosis-associated ovarian cancerous genes: A study based on transcriptomics profiling, docking and molecular dynamics approach**

Parallel Session – III B

Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Prof Erik Van der Eycken and Prof Abha Bishnoi

PL-7 4.20 PM - 4.50 PM	**Virinder S. Parmar** Professor, Department of Chemistry and Environmental Science, Medgar Evers College, The City University of New York, Brooklyn, NY, USA **Microbes *versus* the Environment: Environmental Determinants of Antimicrobial Resistance and Tolerance**
IL-19 4.50 PM - 5.10 PM	**Monalisa Mukherjee** Director, Amity Institute of Click Chemistry Research and Studies, Amity University, Noida, Uttar Pradesh, India **Biogenic Carbon Quantum Dots as a Neoteric Inducer in the Game of Directing Chondrogenesis**
IL-20 5.10 PM - 5.30 PM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **C-H Functionalization of Diazaheterocycles**
IL-21 5.30 PM - 5.50 PM	**Asha Jain** Department of Chemistry, University of Rajasthan, Jaipur, India **New Perspectives, Design and Applications Organotin(IV) Complexes**

Parallel Session – III C

Venue: Multi Activity Hall

Chairpersons: Prof Dipak P. Ramji and Dr Neeraj Kumar Mishra

PL-8 4.20 PM - 4.50 PM	**Athina Athanasios Geronikaki** Professor, Department of Pharmaceutical Chemistry, Aristotle University, Greece **Evaluation of 2-phenylthiazolidin-4-one analogues as inhibitors of the SARS-CoV-2 main protease**
IL-22 4.50 PM - 5.10 PM	**Brajendra K. Singh** Professor, Department of Chemistry, University of Delhi, Delhi, India **Introducing New Class of Selenium-Based Pseudohalides for Cross-Coupling Reactions**
IL-23 5.10 PM - 5.30 PM	**Thirumoorthi Ramalingam** Assistant Professor, Department of Chemistry, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, Bandarsindri, Ajmer, Rajasthan, India **Podium (Oral) Presentation in Organotin Compounds for Organic Synthesis Utilization of Arylmethyl Radicals for C-X (X = C, N, and O) Bond-Forming Reactions**

IL-24 5.30 PM - 5.50 PM	**Siddharth Sharma** Assistant Professor, Department of Chemistry, Mohanlal Sukhadia University, Udaipur, India **Exploring Organic Chemistry of Isocyanide Beyond Conventional Flasks: Our Recent Progress**

Poster Session – I
Venue: Chemistry Department Corridor

Chairpersons: Dr Sergii RUDIUK, Dr Mrunal Ambasana and Dr Pratibha Kumari

5.50 PM – 6.50 PM	**Poster Number P-1 to P-60**

Awadh and Beyond: Uniting Cultures Through Art
Venue: Malviya Hall

7.00 PM – 8.30 PM	**Cultural Programme**

8.30 PM	**Dinner** (Venue: Parking Opposite Chemistry Department)

Tuesday, January 28, 2025

Registration
Venue: Opposite Chemistry Department

9.00 AM onwards	**Registration**

Parallel Session – IV A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Prof Ramrao A. Mane and Prof Anil Mishra

PL-9 9.00 AM - 9.30 AM	**Dipak P. Ramji** Deputy Head, Cardiff School of Biosciences, Professor of Cardiovascular Science, Cardiff University, Cardiff, UK **Harnessing the potential of natural products in the prevention and treatment of atherosclerotic cardiovascular disease and other inflammatory disorders**
IL-25 9.30 AM - 9.50 AM	**Manoj Kumar Gupta** Assistant Professor, Department of Chemistry, Central University of Haryana, Mahendergarh, Haryana, India **Cutting-Edge Applications of Tunable Supramolecular Gels**
IL-26 9.50 AM - 10.10 AM	**Priyankar Paira** Associate Professor, Vellore Institute of Technology, Department of Chemistry, School of Advanced Science, Vellore, Tamilnadu, India **Mitochondria Specific Half-Sandwich and Cyclometallated Ru(II)/Ir(III)/Re(I)-Complexes to Unveil the Dynamic Therapy Against Cancer**
IL-27 10.10 AM - 10.30 AM	**Rinku Chakrabarty** Head, Department of Chemistry, Alipurduar University, Aipurduar, West Bengal, India **Copper and Zinc Complexes of Quinoline Based Flexible Amide Receptor as Fluorescent Probe for Dihydrogen Phosphate and Hydrogen Sulphate and Their Biological Application**
O-1 10.30 AM - 10.40 AM	**Nilam Dilip Bhusare** Somaiya Institute for Research & Consultancy, Somaiya Vidyavihar University, Vidyavihar (East) Mumbai, India **Synthesis, Cytotoxicity Assessment, and Docking Analysis of N^{10}-Substituted Acridone Derivatives as Potential Anticancer Agents**
O-2 10.40 AM - 10.50 AM	**Pratibha Yadav** Centre for Rural Development and Technology, IIT Delhi, Hauz Khas, New Delhi, India **Synthesis of neohesperidose and naringenin from naringin**

O-3 10.50 AM - 11.00 AM	**Asish Bhaumik** School of Pharmaceutical Sciences (GIPS-T), Girijananda Chowdhury University (GCU) Tezpur Campus, Dekargaon, Tezpur, Sonitpur, Assam, India **DESIGN, SYNTHESIS, MOLECULAR CHARACTERIZATION AND EVALUATION OF *IN VIVO* ANTITUMOUR ACTIVITY OF NOVEL OXADIAZOLE SCAFFOLDS**
11.00 AM - 11.20 AM	**High Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – IV B
Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Dr Mohan Prasad and Dr Vinay Kumar Singh

PL-10 9.00 AM - 9.30 AM	**Karol Grela** Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, Poland **The Guard dies but does not surrender!» Olefin metathesis catalysts for challenging cases in pharmaceutical and target oriented synthesis**
IL-28 9.30 AM - 9.50 AM	**Nighat Fahmi** Department of Chemistry, University of Rajasthan, Jaipur, Rajasthan, India **GREEN SYNTHETIC PATHWAYS FOR TRANSITION METAL SCHIFF BASE COMPLEXES: PIONEERING ADVANCES IN SUSTAINABLE COORDINATION CHEMISTRY**
IL -29 9.50 AM - 10.10 AM	**Pratibha Kumari** Associate Professor, Department of Chemistry, Deshbandhu College, University of Delhi, New Delhi, India **Synthesis of bio-based metal-organic frameworks for sustainable environment**
IL -30 10.10 AM - 10.30 AM	**Vikas Tyagi** Associate Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Green Catalysis for Sustainable Organic Synthesis**
O-4 10.30 AM - 10.40 AM	**Shital Panchal** Department of Pharmacology, Institute of Pharmacy, Nirma University, Ahmedabad, India **Evaluation of Protective Effect of C-Phycocyanin against L-Arginine induced Acute Pancreatitis**
O-5 10.40 AM - 10.50 AM	**Nivedita Acharjee** Department of Chemistry, Durgapur Government College, J. N. Avenue, Durgapur, West Bengal, India **UNDERSTANDING THE MECHANISM, REACTIVITY AND SELECTIVITY OF GRIGNARD REAGENT MEDIATED [3+2] CYCLOADDITION REACTIONS FROM THE MOLECULAR ELECTRON DENSITY THEORY PERSPECTIVE**

O-6 10.50 AM - 11.00 AM	**Narendra Dinkar Kharat** Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan, India **Iridium-catalyzed Diacylmethylation of Tyrosine and its Peptides with Sulfoxonium Ylides**
11.00 AM - 11.20 PM	**High Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – IV C
Venue: Multi Activity Hall

Chairpersons: Prof K.G. Anoja P. Attanayake and Dr Shashi Bala

PL-11 9.00 AM - 9.30 AM	**Alam Nur-E-Kamal** Professor, Department of Biology, Medgar Evers College, The City University of New York, Brooklyn, NY, USA **Biology of the Ras GTPases Mediated Signaling in Mammalian Cells: A Potential in Developing Therapy for Cancer**
IL-31 9.30 AM - 9.50 AM	**Kaivalya Kulkarni** Principal Scientist, Emcure Pharmaceuticals Ltd., Pune, India **Challenges in the Process development of simple and complex APIs and overview on the chirality control**
IL -32 9.50 AM - 10.10 AM	**Yashwantsinh Jadeja** Associate Professor, Department of Chemistry, Faculty of Science, Marwadi University, Rajkot, Gujarat, India **Development of Peptide-Heterocycles Conjugates: Synthesis, Characterization, and Biological Studies**
IL -33 10.10 AM - 10.30 AM	**Abhishek Singh** Junior Group Leader, Freie Universität Berlin, Germany **From Molecules to Bio-Materials: The Versatility of Functional Oligo-Glycerol Surfactants**
O-7 10.30 AM - 10.40 AM	**Sushma Naharwal** Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan, India **Rhodium-Catalyzed Synthesis of Functionalized and Fused N-Arylphthalazinediones with Allyl Alcohols**
O-8 10.40 AM - 10.50 AM	**Sudakshina Trivedi** Department of Chemistry, University of Lucknow, Lucknow, India **Potential Applications of Phytofabricated ZnO Nanoparticles**
O-9 10.50 AM - 11.00 AM	**Dhara Vala Jagmalbhai** Center for Research and Development, Dr. Subhash University, Junagadh, Gujarat,

	India **Exploring Bio-Responsive TMP Containing Nitrogen Heterocycles for Urinary Tract Infection Therapy**
11.00 AM - 11.20 PM	**High Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session - V A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Prof Akash Ved and Prof Vijai Kumar Rai

PL-12 11.20 AM - 11.50 AM	**Rachna Sadana** Chair, Department of Natural Sciences, Professor of Biology & Biochemistry, University of Houston-Downtown, Houston, USA **Arylidene-hydrazinyl-thiazoles as Anticancer and Apoptosis-inducing Agents**
IL-34 11.50 AM - 12.10 PM	**Ramesh Kothari** Professor and Head, Department of Biosciences, Saurashtra University, Rajkot, India **Probiotics: The Next Frontier in Health and Wellness**
IL-35 12.10 PM - 12.30 PM	**Neelima Gupta** Department of Chemistry, University of Rajasthan, Jaipur, India **Computational Insight to Stereochemical Aspects of Some Synthetically Important Organic Reactions**
IL-36 12.30 PM - 12.50 PM	**Prachi Singh** Assistant Professor, Department of Environmental Sciences, Hindu College, University of Delhi, New Delhi, India **Sustainable Approaches to Water Purification: Role of Biochar in Photocatalytic Processes**
O-10 12.50 PM - 1.00 PM	**Debnath Palit** Principal, Durgapur Government College, J. N. Avenue, Durgapur, West Bengal, India **IDENTIFICATION OF POLLUTION TOLERANT PLANT SPECIES BY ANALYSIS OF MORPHOLOGICAL AND BIOCHEMICAL PARAMETERS IN THE DURGAPUR INDUSTRIAL REGION**
O-11 1.00 PM - 1.10 PM	**Nagja Tripathi** Dept. of Pharmacognosy, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **Development and Evaluation of Herbal Nano Formulation for Management of Eczema**
O-12 1.10 PM - 1.20 PM	**Harish Chandra Upadhyay** Department of Applied Sciences, Rajkiya Engineering College (Affiliated with Dr. A.P.J. Abdul Kalam Technical University, Lucknow), Churk, Sonbhadra, India

	Integrating Allopathy with Herba and Phytomolecules: The Miraculous Benefits in Dealing with Multidrug-Resistant Infections
1.20 PM - 2.00 PM	**Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – V B
Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Dr Keshav Deo and Dr Prakash Chandra Jha

PL-13 11.20 AM - 11.50 AM	**Virendra N Pandey** Department of Microbiology, Biochemistry and Molecular Genetics, New Jersey Medical School, Rutgers, The State University of New Jersey, USA **Fuse Binding Protein 1 interacts with all the naturally occurring tumor suppressor p53 isoforms, making it a novel target for anti-cancer drug design**
IL-37 11.50 AM - 12.10 PM	**Ravindra Kumar** Senior Scientist, Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Desymmetrization Strategy Towards Stereoselective Construction of Alkaloid-Mimicking Polycyclic Scaffolds and Natural Products**
IL-38 12.10 PM - 12.30 PM	**Lalji Baldaniya** Principal, Faculty of Pharmacy, Marwadi University, Rajkot, Gujarat, India **OPTIMIZING PHARMACEUTICAL PRODUCTION: ADVANCING EFFICIENCY WITH HOT MELT EXTRUSION FOR CONTINUOUS MANUFACTURING**
IL-39 12.30 PM - 12.50 PM	**Farukh Arjmand** Department Of Chemistry, Aligarh Muslim University, Aligarh, India **Molecular design and synthesis of new copper(II) norcraugsodine complexes and their interaction studies with ct-DNA/tRNA and cytotoxicity profile**
O-13 12.50 PM - 1.00 PM	**Nilanjan Dey** Department of Chemistry, Birla Institute of Technology and Science Pilani, Hyderabad campus, India **Hydrogen Bonding-Induced Unique Charge-Transfer Emission from Pyrenylated Terpyridine Derivative: Multifaceted Optical Sensing Applications**
O-14 1.10 PM - 1.10 PM	**Pranab Pathak** Department of Chemistry, School of Science, RK University, Rajkot, India **Design and synthesis of novel 1,3,4-oxadiazole based azaspirocycles catalyzed by NaI under mild condition and evaluated their antidiabetic and antibacterial activities**
O-15 1.10 PM - 1.20 PM	**Dhaneswar Prusty** Department of Biochemistry, Central University of Rajasthan, Ajmer, India **Discovery of new classes of antimalarial compounds by targeting apicoplast Single-Stranded DNA binding protein of *Plasmodium falciparum***

1.20 PM - 2.00 PM	**Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – V C
Venue: Multi Activity Hall

Chairpersons: Dr Vinay Tripathi and Prof Devdutt Chaturvedi

PL-14 11.20 AM - 11.50 AM	**Leonid G. Voskressensky** RAS Professor, Full Professor, Dean of the Faculty of Science, Peoples Friendship University of Russia (RUDN University), Moscow, Russia **ELECTRON–DEFICIENT ALKYNES - UNIVERSAL SYNTHONS FOR THE PRODUCTION OF CONDENSED AZA-HETEROCYCLIC SYSTEMS WITH SIGNIFICANT BIOACTIVITY**
IL-40 11.50 AM - 12.10 PM	**Bichismita Sahu** Associate Professor and HOD, Department of Medicinal Chemistry, NIPER-Ahmedabad, Gandhinagar, Gujarat, India **Investigations of Nucleobases towards development of prospective biomaterials**
IL-41 12.10 PM - 12.30 PM	**Naga Prasad Puvvada** Associate Professor, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Guntur, Andhra Pradesh, India **Melanoma Immunotherapy by Nanosphere-Vaccine Elicited CD4+ and CD8+ T-Cell Response for Tumor Regression**
IL-42 12.30 PM - 12.50 PM	**Gyan Prakash Modi** Associate Professor, Department of Pharmaceutical Engineering & Technology, Indian Institute of Technology (BHU), Varanasi, India **Development of novel theranostic agents for Alzheimer's disease**
O-16 12.50 PM - 1.00 PM	**Afsheen Fatima** Research Analyst, Era Medical University, Lucknow, India **Discoveries in breast cancer treatment from molecular docking and in vitro studies of Adansonia digitata fruit pulp on the receptor tyrosine-protein kinase erbB-2 (ERBB2)**
O-17 1.10 PM - 1.10 PM	**Ram Awatar Maurya** Applied Organic Chemistry Group, Chemical Sciences & Technology Division, CSIR-North East Institute of Science & Technology (NEIST), Jorhat, India **Photo-oxygenation of Furan Tethered α-Azidoketones**
O-18 1.10 PM - 1.20 PM	**Monika Malik** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **A Facile and Regioselective Synthesis of Novel Colchicine Sulfoximine Analogues as Potent Tubulin Inhibitors**
1.20 PM - 2.00 PM	**Lunch** (Venue: Parking Opposite Chemistry Department)

Parallel Session – VI A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Dr Anil Kumar Dwivedi and Prof Shalini Tripathi

PL-15 2.00 PM - 2.30 PM	**Erik Van der Eycken** Full Professor, University of Leuven (KU Leuven), Department of Chemistry, Leuven, Belgium **Synthesis of small complex heterocycles employing post-Ugi transformations**
IL-43 2.30 PM - 2.50 PM	**Sarika Singh** Senior Principal Scientist and Professor of Biology (AcSIR), Toxicology & Experimental Medicine Division, CSIR-Central Drug Research Institute, Lucknow, India **Ubiquitin E3 ligase Pirh2 in Alzheimer's disease**
IL-44 2.50 PM - 3.10 PM	**Suresh E. Kurhade** Principal Scientist, Medicinal Chemistry (STG), Schrodinger Therapeutics, Hyderabad, Telangana, India **In Silico Enabled Discovery of Potent, Selective and Brain-penetrant DLK Inhibitors for the Treatment of Neurodegenerative Diseases**
IL-45 3.10 PM - 3.30 PM	**Debasish Mandal** Assistant Professor, School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Computational Evaluation and Design of Novel FGFR Tyrosine Kinase Inhibitors**
O-19 3.30 PM - 3.40 PM	**Charmy S. Kothari** Department of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **Development and Validation of a Mass-Compatible RP-HPLC Method for Quantification of Berberine Hydrochloride in Plasma**
O-20 3.40 PM - 3.50 PM	**Nagendra Nath Yadav** Department of Chemistry, North Eastern Regional Institute of Science and Technology (NERIST), Nirjuli, Arunachal Pradesh, India **A short and efficient Synthesis of Piperidine and Azepane ring from the Ring expansion of Aziridine**
O-21 3.50 PM - 4.00 PM	**Arvindsinh Bhikhusinh Sisodiya** Institute of Science & Technology for Advanced Studies & Research (ISTAR), Vallabh vidyanagar, Anand, India **Stability study of Aspirin tablet in crush condition stored in plastic container by using Reverse Phase High Performance Liquid Chromatography**
4.00 PM - 4.10 PM	**Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – VI B
Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Prof Athina Athanasios Geronikaki and Dr Rakesh Shukla

PL-16 2.00 PM - 2.30 PM	**Sergii RUDIUK** Associate Professor PSL/ENS, Nanobiosciences and Microsystems, Department of Chemistry, Ecole Normale Supérieure, PSL University, Paris, France **Electrostatic interactions in DNA nanotechnology: from folding of DNA origamis to transfection of DNA nanogels**
IL-46 2.30 PM - 2.50 PM	**Atul Goel** Chief Scientist (CSIR) and Professor (AcSIR), Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Functionalized Fluorescent Probes for Diagnostics and Biomedical Applications**
IL-47 2.50 PM - 3.10 PM	**Deepti Goyal** Assistant Professor, Department of Chemistry, DAV College, Chandigarh, India **Exploring the Synergistic Potential of Phenol–Triazole Derivatives to Attenuate A*β*/ Cu^{2+}–A*β* Aggregation and Reactive Oxygen Species**
IL-48 3.10 PM - 3.30 PM	**Amit Patwa** Associate Professor & Coordinator - Internal Quality Assurance Cell (IQAC), Division of Chemistry, School of Science, Navrachana University, Vadodara, Gujarat, India **Longitudinal in vivo cationic contrast-enhanced computed tomography classifies equine articular cartilage injury and repair**
O-22 3.30 PM - 3.40 PM	**Shiny E.C. Kachhap** Department of Zoology, Marwari College, Ranchi, Jharkhand, India ***In vitro* Anti-cancer efficacy of crude and nanoparticle form of chitosan extracted from carapace of freshwater crab *Sartoriana spinigera* (Wood-Mason, 1871) by MTT assay**
O-23 3.40 PM - 3.50 PM	**Alpesh G. Bhadarka** Department of Industrial Chemistry, Institute of Science and Ttechnology for Advanced Studies and Research (ISTAR), Vallabh Vidyangar, Anand, India **Cyclodextrins Inclusion Complex Formation with Benzimidazole**
O-24 3.50 PM - 4.00 PM	**Sandeep R. Patil** School of Science, Navrachana University Vadodara, Vasna-Bhayli Road, Vadodara, Gujarat, India **HYDROCARBON SOLVENT MEDIATED GEL FORMATION IN AQUEOUS NON-IONIC SURFACTANT MIXTURES**
4.00 PM - 4.10 PM	**Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – VI C
Venue: Multi Activity Hall

Chairpersons: Prof Mukund S. Chorghade and Dr Manisha Shukla

IL-49 2.00 PM - 2.20 PM	**Nisheeth C Desai** Former Professor & Head, Department of Chemistry, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar, Gujarat, India **Perceptions of Scientific Research and Strategies for mapping the Development of Academic Career**
IL-50 2.20 PM - 2.40 PM	**Bhupesh Goyal** Associate Professor, Department of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed to be University), Patiala, Punjab, India **Targeting hIAPP Fibrillation in Type 2 Diabetes by Rationally Designed Peptide Inhibitors: Insights from Molecular Dynamics and Experimental Studies**
IL-51 2.40 PM - 3.00 PM	**Surendra Singh** Professor, Dept. of Chemistry, University of Delhi, Delhi, India **Development of Recoverable Chiral Mn(III) Salen Complexes as Catalysts for Asymmetric Organic Transformations**
IL-52 3.00 PM - 3.20 PM	**Krunalkumar Ramanlal Mehariya** Research and Development Chemist, Natara Global Ltd, Hartlepool, United Kingdom **Exploring Flavour and Fragrance Chemistry in the UK Chemical Industry**
O-25 3.20 PM - 3.30 PM	**Brijesh Kumar Shah** School of Science, Navrachana University, Vasna-Bhayli Road, Vadodara, Gujarat, India **Synthesis and Characterization of Zirconium Titanium amino tris(methylenephosphonic acid) and Its Application in Separation of Metal Ions**
O-26 3.30 PM - 3.40 PM	**Rahul Ravichandran** Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, K1N 6N5, Canada **Machine Learning-Guided Discovery of Small Molecule Inhibitors of SARS-CoV-2 Spike/Human ACE Interaction**
O-27 3.40 PM - 3.50 PM	**Neeti Ashokbhai Patel** Department of Biochemistry, Parul Institute of Medical Sciences and Research, Limda, Waghodiya, Gujarat, India **Evaluation of Diagnostic Efficacy of Anti-Mullerian Hormone in Polycystic Ovarian Syndrome**
O-28 3.50 PM - 4.00 PM	**Denni D Mammen** Division of Chemistry, School of Science, Navrachana University, Vasana-Bhayli Road, Vadodara, India **Aluminium chloride chelation in flavonoid estimation assays: Drawbacks and issues**
4.00 PM - 4.10 PM	**Tea** (Venue: Parking Opposite Chemistry Department)

Parallel Session – VII A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Prof Monalisa Mukherjee, Prof Meenakshi Singh and Dr Seema Mishra

IL-53 4.10 PM - 4.30 PM	**Narender Tadigoppula** Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow, India **Development of Phytopharmaceuticals from the Indian Medicinal Plants**
IL-54 4.30 PM - 4.50 PM	**Murlidhar S. Shingare** Emeritus Scientist, CSIR, Dr. Babasaheb Bhimrao Ambedkar University, Aurangabad, Maharashtra, India **Highly efficient synthetic strategies for bioactive heterocyclic molecules**
IL-55 4.50 PM - 5.10 PM	**Dina Nath Singh** Professor, K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Ayodhya, India **Current Trends of the Search of New Pharmacologically Active Leads from Medicinal Plants**
IL-56 5.10 PM - 5.30 PM	**Neeraj Kumar Mishra** Associate Professor, Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow, Uttar Pradesh, India **Modification and Construction of Late-Stage Drug Candidates *via* C–H bond Functionalization and Annulation**
IL-57 5.30 PM - 5.50 PM	**Amerian Chemical Society** **Abstract Awaited**
O-29 5.50 PM - 6.00 PM	**Kushal Pankajkumar Shah** Department of Industrial Chemistry, Institute of Science & Technology for Advanced Studies & Research, VallabhVidyanagar, Anand, Gujarat, India **An Extensive Analysis Comparing the Non-Steroidal Anti-Inflammatory Drug (NSAID) of Diclofenac Sodium Injection from Branded or Innovator Companies to Generic Companies Drug Products Under Various Stability Conditions**
O-30 6.00 PM - 6.10 PM	**Ruchika Yogesh** Chief Operating Officer, AutoText AI Pvt. Ltd., Dwarka, New Delhi, India **Leveraging Artificial Intelligence and Machine Learning Techniques in Pharmaceutical Research and Development**
O-31 6.10 PM - 6.20 PM	**Priyanka Chaudhary** Department of Chemistry, University of Lucknow, Lucknow, India **Oxidative Coupling of N-Nitrosoanilines with Substituted Allyl Alcohols under Rhodium (III) Catalysis**

O-32 6.20 PM - 6.30 PM	**Akrati Sant** Department of Chemistry, Isabella Thoburn College, University of Lucknow, India **Investigating the Breast Cancer Potential of alkylated 5,7-dihydroxy-2-(4-hydroxyphenyl) chroman-4-one Derivatives: Unveiling In-Silico and In-Vitro Studies**

Parallel Session – VII B
Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Prof Suhas Vyas, Dr Archna Talwar and Dr Ashok Kumar Singh

IL-58 4.10 PM - 4.30 PM	**Sanjeev Kumar Shukla** Senior Principal Scientist (CSIR) and Professor (AcSIR), NMR Lab., SAIF&R Division, CSIR-Central Drug Research Institute, Lucknow, India **Abstract Awaited**
IL-59 4.30 PM - 4.50 PM	**Mahesh C. Sharma** Director, Plants Med Laboratories Pvt. Ltd., Jaipur, India **Toxic Turnaround: The Hidden Goodness of Poisonous Plants**
IL-60 4.50 PM - 5.10 PM	**Anirban Pradhan** Assistant Professor, Department of Chemistry, Birla Institute of Technology (BIT) Mesra, Ranchi, India **Metal Free Porous Carbon Materials Based Electrocatalyst for Green Hydrogen Fuel Production**
IL-61 5.10 PM - 5.30 PM	**Vijai Kumar Rai** Professor, Department of Chemistry, University of Lucknow, Lucknow, India **Design of Nanomaterials Towards Visible-Light-Induced Tandem Reactions**
IL-62 5.30 PM - 5.50 PM	**Amit Rajput** Assistant Professor, Department of Chemistry, J. C. Bose University of Science & Technology, Faridabad, Haryana, India **Neutral, and monocationic forms of copper complex stabilized by redox-active thioether-appended tridentate *o*-aminophenol ligand**
O-33 5.50 PM - 6.00 PM	**Poonam Shukla** Veer Kunwar Singh University, Ara, Bhojpur, Bihar, India **Heterocyclic Natural Products and their Biological Importance**
O-34 6.00 PM - 6.10 PM	**Avni Nayyar** Department of Chemistry, Isabella Thoburn College, Lucknow, India **Enhancing Biocompatibility of Green-Synthesized Nanoparticles through Green Capping Agent**

O-35 6.10 PM - 6.20 PM	**Anupam** Department of Chemistry, University of Lucknow, Lucknow, India **Antioxidant Potential of *Hibiscus rosa-sinensis* Linn: Phenolic and Flavonoid Analysis**
O-36 6.20 PM - 6.30 PM	**Adhish Kumar Jaiswal** Department of Chemistry, University of Lucknow, Lucknow, India **Ultrasmall aqueous starch-capped CuS quantum dots with tunable localized surface plasmon resonance and composition for the selective and sensitive detection of mercury (ii) ions**

Parallel Session – VII C
Venue: Multi Activity Hall

Chairpersons: Prof Sonika Bhatia and Dr Adhish Kumar Jaiswal

IL-63 4.10 PM - 4.30 PM	**Sundaram Singh** Professor and Head, Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, India **Photo-triggered Oxidative Coupling of Indole and Active Methylene Compounds using Eosin Y as a Photocatalyst**
IL-64 4.30 PM - 4.50 PM	**Shashi Bala** Department of Chemistry, University of Lucknow, Lucknow, India **Synthesis and fabrication of metal-oxide nanoparticles & nanocomposites and their role in water remediation**
IL-65 4.50 PM - 5.10 PM	**Mohd Faheem Khan** Associate Professor (Chemistry), Department of Biotechnology, Era University, Lucknow, Uttar Pradesh, India **Electrochemical & Paper-based Wearable Biosensor for the detection of Key Biomarkers: A Non-Invasive Point-of-Care**
IL-66 5.10 PM - 5.30 PM	**Sushil Kumar Maurya** Associate Professor, Department of Chemistry, University of Lucknow, Lucknow, India **Vanadia-Titania Catalyst system for versatile chemical transformation**
IL-67 5.30 PM - 5.50 PM	**Anuj K Yadav** Former Research Associate, University of Illinois Urbana-Champaign, USA **Chemical Tools to Study the Role of Inflammation in Cancer Prognosis by Deep Tissue Imaging**

O-37 5.50 PM - 6.00 PM	**Jeetendra Yuvaraj Salunke** Department of Chemistry, School of Science, Navrachana University, Vadodara, India **Esterification of Phthalic Anhydride with Butanol using Solid Acid Catalyst under Solvent-Less Condition**
O-38 6.00 PM - 6.10 PM	**Manish Arya** CSIR-Central Institute of Medicinal and Aromatic Plants (CSIR-CIMAP), Lucknow, India **Identification and Isolation of Terpenes and Biological Activity**
O-39 6.10 PM - 6.20 PM	**Saurabh Kumar Singh** Department of Chemistry, University of Lucknow, Lucknow, India **Synthesis, in vitro and in silico anti-cancer evaluation of Diosgenin-NSAID's conjugates against SiHa cells**

Poster Session – II
Venue: Chemistry Department Corridor

Chairpersons: Dr Krunalkumar Ramanlal Mehariya, Dr Mohd Faheem Khan, Dr Jaybir Singh and Dr Prachi Singh

6.30 PM – 7.15 PM	**Poster Number P-61 to P-116**

Evening Insights: Engaging Minds Through Workshops and Conversations

Venue: Chemistry Auditorium (S 141)

Workshop 7.15 PM –8.00 PM	**From Passion to Profession: Creating Your Own Career Roadmap** By Prof Rachna Sadana
Panel Discussion 8:00 PM –8.30 PM	**Catalyzing Innovation and Research: Building a Startup Ecosystem to Revolutionize Science and Medicine in India**

8.30 PM	**Dinner** (Venue: Parking Opposite Chemistry Department)

Wednesday, January 29, 2025

Parallel Session – VIII A
Venue: Chemistry Auditorium (S 141)

Chairpersons: Prof Nisheeth C Desai, Dr Jawahar Lal and and Dr Sushil Kumar Maurya

PL-17 9.00 AM - 9.30 AM	**Surya Kant** Professor and Head, Department of Respiratory Medicine, King George's Medical University, Lucknow, India **Abstract Awaited**
IL-68 9.30 AM - 9.50 AM	**Devdutt Chaturvedi** Dean, School of Physical Sciences, Mahatma Gandhi Central University, Motihari (East Champaran), Bihar, India **Synthetic Explorations of Triarylphosphine Based Reagents in Syntheses of Biologically Potent Scaffolds**
IL-69 9.50 AM - 10.10 AM	**Rakesh Kumar Parashar** Bio-Organic Lab, Department of Chemistry, University of Delhi, New Delhi, India **Synthesis and Evaluation of Novel Heterocyclic Scaffolds as quorum Sensing Inhibitors and Possessing Antimicrobial Activity**
IL-70 10.10 AM - 10.30 AM	**Hardik G. Bhatt** Associate Professor & Head, Dept. of Pharmaceutical Chemistry, Institute of Pharmacy, NIRMA University, Ahmedabad, India **Development of Pteridine Derivatives as PI3K/mTOR Dual Inhibitors for the Treatment of Triple Negative Breast Cancer**
O-40 10.30 AM - 10.40 AM	**Sudheer** Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow, India **Energy Dynamics and Mechanistic Insights into Corrosion Inhibition Processes in Corrosive Media**
O-41 10.30 AM - 10.40 AM	**Priyanka Pandey** Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow, India **Co-crystal formation: thermal and crystal structure analysis for their role in pharmaceutical design**
O-42 10.40 AM - 10.50 AM	**Nidhi Mishra** Indian Institute of Information Technology Allahabad, India **In-Silico Exploration of Rutin Derivatives as Potential Inhibitors of Prostate Cancer Signaling Pathways**

Parallel Session – VIII B
Venue: Chemistry Auditorium 2 (S 142)

Chairpersons: Prof Krishna Nand Singh and Prof R N Singh

PL-18 9.00 AM - 9.30 AM	**Anil Kumar Singh** Adjunct Professor, Institute of Chemical Technology, Mumbai, India **Newer Imperatives and Newer Vistas in Designing and Developing Chemicals and Chemical Products for a Sustainable Future: Challenges and Opportunities**
IL-71 9.30 AM - 9.50 AM	**Pushpendra Kumar Tripathi** Director, Institute of Pharmaceutical Sciences, University of Lucknow, Lucknow, India **Engineered PAMAM Dendrimer for Delivery of Bio-actives**
IL-72 9.50 AM - 10.10 AM	**Manaal Zahera** Assistant Professor, Department of Biotechnology, Era University, Lucknow, India **Role of Bio-Fabrication/Bio-conjugation of Metal Nanoparticles for Novel Therapeutic Approaches**
IL-73 10.10 AM - 10.30 AM	**Seema Mishra** Department of Chemistry, University of Lucknow, Lucknow, India **Arsenic fractionation in paddy field soil in relation to physico-chemistry of rhizosphere**
O-43 10.30 AM - 10.40 AM	**Shruti Anand** Department of Chemistry, Isabella Thoburn College, University of Lucknow, Lucknow, Uttar Pradesh, India **Green Synthesis and Stabilization of Zinc Oxide Nanoparticles with Bixa orellana Extract**

Parallel Session – VIII C
Venue: Multi Activity Hall

Chairpersons: Prof Mahesh Sharma, Dr Ranjana Dutta and Dr Sangeeta Srivastava

IL-74 9.00 AM - 9.20 AM	**Farzana Mahdi** Pro Vice Chancellor, Era University, Lucknow, India **Personalized Medicine: How Genomics is shaping the Future of Healthcare**
IL-75 9.20 AM - 9.40 AM	**Namrata Rastogi** Scientist, Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Diazo Umpolung in Hypervalent Iodine Diazo Reagents**
IL-76 9.40 AM - 10.00 AM	**Manisha Shukla** Associate Professor, Department of Chemistry, University of Lucknow, Lucknow, India **Assignment of Structural Anomalies in Milk Oligosaccharides and their Interpretation by 2D NMR Experiments**

IL-77 10.00 AM - 10.20 AM	**Vinod Kumar Vashistha** Assistant Professor, Department of Chemistry, University of Lucknow, Lucknow, India **Enantioresolution of Chiral Pharmaceuticals via High-Performance Liquid Chromatography**
IL-78 10.20 AM - 10.40 AM	**Jaybir Singh** Assistant Professor, Faculty of Pharmacy, Dr. A.P.J. Abdul Kalam Technical University, Lucknow, India **3D Printing of Formulations and Personalize Medicines**

Valedictory Session
Venue: Malviya Hall

11.00 AM – 1.00 PM	**Valedictory Session**

1.00 PM - 2.00 PM	**Lunch** **Venue:** Parking Opposite Chemistry Department

- End of Programme -

PL = Plenary Lecture
IL = Invited Lecture
O = Oral Presentation
P = Poster Presentation


30th ISCB International Conference
ISCBC-2025
Current Trends in Chemical, Biological and Pharmaceutical Sciences: Impact on Health and Environment
27th - 29th, January 2025
Department of Chemistry, University of Lucknow, Lucknow, India
INAUGURAL SESSION
Chief Guest:
Smt. Anandiben Patel
Hon'ble Governor of Uttar Pradesh
Jointly Organized by
Indian Society of Chemists & Biologists (ISCB)
Department of Chemistry, University of Lucknow
Managed By:
SMART CONFERENCE
Gain Knowledge - Expand Network
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30th ISCB International Conference
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PLENARY

PL-1

Radical Alliances. Solutions and Opportunities for Organic Synthesis

Samir Z. Zard

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Radical reactions offer many of the properties desired by synthetic organic chemists, in terms of variety, mildness of conditions, and a selectivity that is often complementary to that of ionic chemistry, making many protection steps superfluous. There is however one major difficulty, which derives from the propensity of radicals tointeract with themselves (dimerisation, disproportionation) with extremely fast rates that are close to diffusion. In order to overcome this complication, it is essential to keep the steady-state concentration of radical species very low. This can be accomplished for example by contriving a chain reaction where the propagating stepsare themselves quite fast, as for example in the typical, and now extremely popular, stannane based processes. While various *unimolecular* cyclisation and fragmentationsteps can be efficiently incorporated into the radical sequence, kinetically slower *bimolecular* transformations, and in particular *intermolecular* additions to un-activatedalkenes, have proven more difficult to implement. In the case of stannanes, the relatively slow addition to the alkene has to compete with premature hydrogen atom abstraction from the organotin hydride, a step that is usually thousands of times faster.

Over the years, we have shown that xanthates and related thiocarbonylthio derivatives allow the generation of radicals under conditions where the radicalspossess a considerably increased effective lifetime even in a concentrated medium. Intermolecular additions to un-activated alkenes, as well as a variety of reputedly difficult radical transformations can now be easily accomplished. No metals, heavy orotherwise, are required, and the starting materials and reagents are cheap andreadily available. Complex, densely functionalized structures can be constructed in a convergent, modular fashion. In the course of our study of the scope and limitationsof this chemistry, we have uncovered a few surprising transformations. Recent results and some mechanistic aspects will be presented and discussed briefly.

PL-2

Science Entrepreneurship

Mukund S. Chorghade

President & Chief Scientific Officer, THINQ Pharma, New Jersey, USA

Abstract

Innovation, Entrepreneurship and Global Collaboration have been pivotally important in transitioning chemistry-based ideas from concept to commercialization, from mind to market and many pharmaceutically relevant chemical entities from bench to bedside and from bedside to bench. Many countries companies and scientists have placed a high premium on the best practices in business establishment allied with entrepreneurship. As a seasoned entrepreneur from academia, industry and one who has also collaborated with government I will present a journey, with trials and tribulations and finally successes that benefitted the Chemical Enterprise, created jobs and provided a new ray of hope for young and old, shy and bold. Some advice and guidance will be presented to young scholars and aspiring entrants into the Chemical Enterprise.

PL-3

Small-Molecule Probes to Target Cell Death Mechanisms and Tumour Microenvironment

Rui Moreira

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Pyroptosis is an active and ordered form of programmed cell death that is highly correlated with the modulation of immunity in the tumor microenvironment. Ultimately, excessive pyroptosis can lead to immune disorders in several pathological conditions [1]. Dipeptidyl peptidases 8 (DPP8) and 9 (DPP9) are intracellular members of the structure homolog sub-family of serine proteases known for their key roles in the immune response, e.g., by controlling inflammasome and pyroptosis activation [2]. Accessing chemical matter able to discriminate DPP8 or DDP9 engagement could significantly illuminate the biology of these proteases and allow further studies on a systems biology context. Using a comprehensive chemical proteomics profiling, we were able to deconvolute the hidden pharmacology of 4-oxo-β-lactams,**1** (Figure 1), showing that these covalent inhibitors potently and distinctively engage DPP8/9 [3]. Our findings enabled, for the first time, the development of specific DPP8 or DPP9 effectors, which may become suitable for forthcoming medicinal chemistry and translational applications. In addition, will also address how modulation of the intrinsic reactivity of bioisosteric covalent warheads such as 3-oxo-β-sultams, **2**,[4] and cyclic phosphonamidates, **3**, is a useful approach to expand the tool box of chemical probes targeting serine proteases involved in several cell death mechanisms.

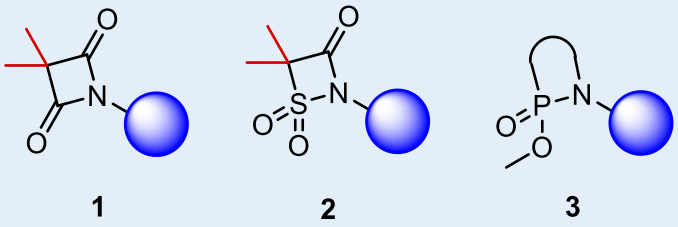

Figure 1: 4- and 5-membered heterocyclic rings developed as covalent warheads to target serine proteases involved in proteases involved in cell death mechanisms.

Acknowledgements: We thank Fundação para a Ciência e a Tecnologia (FCT) for support through projects 2022.07857.PTDC, UIDB/00645/2020 and UIDP/00645/2020.

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2. M C Okondo, D C Johnson, R Sridharan et al. Nat. Chem. Biol 13, 2017, 46.
3. L A R Carvalho, B Ross, L Fehr, O Bolgi et al. Angew. Chem. Int. Ed. 61, 2022, e202210498.
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PL-4

Harnessing Herbal Products to Combat Early-Stage Diabetes and Prevent Complications

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Phytomedicines have evolved from a plethora of medicinal plants with diverse therapeutic potentials. Medicinal plants have been recognized as rich sources of drug leads for the management of diabetes mellitus. *Coccinia grandis* (Linn.) Voigt (Ivy gourd – in English) belonging to the Cucurbitaceae family, is widely used as an ingredient in Sri Lankan traditional herbal medicine preparations for the management of diabetes mellitus from time immemorial. The antidiabetic drug leads isolated from medicinal plants may be scaffolds for new oral hypoglycemic agents. The work present here is the success story of investigating the efficacy and safety of a standardized herbal capsule made from the aqueous freeze-dried extract of *C. grandis* on metabolic profile in newly diagnosed patients with type 2 diabetes mellitus (T2DM) and isolating antidiabetic compounds from the leaves of *C. grandis.* Administration of the herbal capsule *C. grandis* (500 mg/day) for three months (Phase II clinical trial) was able to improve the glycemic state as determined by the percentage of glycated hemoglobin, fasting plasma glucose concentration, fasting serum concentration of fructosamine, insulin, and insulin resistance calculated using homeostasis model assessment with well-tolerated safety (assured through renal, hepatological and hematological parameters) in patients with newly diagnosed T2DM. In addition, administration of the herbal capsule *C. grandis* was able to improve the altered serum lipid profile parameters, atherogenic, cardio-protective, and coronary risk indices, and reduce oxidative stress and inflammation in newly diagnosed patients with T2DM. The α-amylase, α-glucosidase, and DPP-IV inhibitors namely fucosterol and coccinoside C were isolated from the leaves of *C. grandis* following the bioactivity-guided principle. The method of preparation of the herbal capsule *C. grandis* and mechanisms of action in newly diagnosed patients with T2DM have been patented. The successful commercialization of the *C. grandis* capsule has been initiated and will be available in the local market as a dietary supplement at an affordable cost. The development of new herbal products will be able to manage diabetes at the initial stage and to reduce and/or delay the occurrence of diabetic complications. This will aid in reducing the mortality caused by diabetes and its related complications, enhancing the quality of life of patients.

PL-5

A ray of hope for Parkinson`s disease treatment: Story of discovery of a clinical candidate

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Abstract:

To address the drug resistance issue and improve a drug molecule's ADME properties, the concept of molecular hybridization was put forward, wherein two or more distinct pharmacophores are covalently linked into a single molecule. This approach may lead to a molecule with improved efficacy, solve the problem of drug resistance, and reduce undesired side effects [1,2]. Developing such molecular frameworks with synthetic selectivity and economic viability is still challenging for the pharmaceutical industry. Drugs developed through this approach can be used to cure infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamics, and drug resistance. The benefit of using molecular hybrids is that they activate different or the same targets by a single molecule, increase therapeutic efficacy, and improve bioavailability. The molecular hybridization approach has resulted in many drug candidates with improved activity profiles, and some of these compounds are in clinical trials. We have utilized this concept in designing antimalarial molecules, and many molecules with aminiquinoline and pyrimidine pharmacophore showed low nanomolar activity. Later, a massive multi-institutional collaboration was started, and over 700 new molecules were studied for Nurr1 activation, a potential target for the Parkinson's disease model. It identified 15 hits, out of which 3 compounds have cleared pre-clinical trials, and technology has been transferred to NURRON pharmaceuticals for further development [3-10]. These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of α-synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cure the Parkinson-induced mice model at 5 mg/kg body weight without any toxicity, and recently, phase I clinical trials of one of the molecules have begun.

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PL-6

The Magic (and Science!) Behind Flavour and Fragrance

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Abstract:

An introduction to the chemistry of flavours and fragrances – an interactive and entertaining look at the history, application and modern synthesis of some flavour and fragrance molecules.

PL-7

Microbes *versus* the Environment: Environmental Determinants of Antimicrobial Resistance and Tolerance

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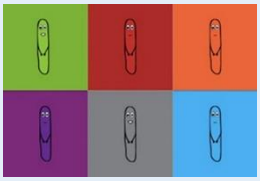

It is easy to forget that bacteria or microorganisms exist until some food item spoils or we get sick, but bacteria do not forget to invade. Easily swept from one place to another by a flushing toilet, prevailing winds, or the movement of their hosts, microbes survive and easily adapt to a constantly changing environment. Bacteria possess a chameleon-like ability to adapt to changes in nutrient availability, osmotic stress, and pH. Growth in nutrient poor conditions leads to accumulation of the small molecule ppGpp [guanosine pentaphosphate or guanosine-3', 5' – bis (diphosphate)] which are implicated in antibiotic tolerance or antimicrobial resistance (AMR). The development of persisted cells that survive for long periods together with the synthesis of novel bactericidal (antimicrobial) compounds are very much desirable, and are active areas of research currently in biology, chemistry, and medicine. We are working on the discovery and development of natural products based novel antimicrobial drugs. Some recent results from our Laboratories shall be presented at the Conference.

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PL-8

Evaluation of 2-phenylthiazolidin-4-one analogues as inhibitors of the SARS-CoV-2 main protease

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In December 2019, a novel virus outbreak was first reported in Wuhan, China. Despite many attempts to contain it, the virus, named Severe Acute Respiratory Syndrome Coronavirus 2 (SARS-CoV-2), spread worldwide, causing a pandemic. This virus belongs to a family of RNA viruses, namely Coronaviruses, responsible for human respiratory tract infections, ranging from a common cold to severe pneumonia. The persistence of SARS-CoV-2 mutations contributed to the COVID-19 epidemic's duration and raised concerns about the efficacy of the available vaccines. Herein, we report the evaluation of several thiazole/benzothiazole based thiazolidinone derivatives selected from 85 designed derivatives through docking studies, as potential inhibitors of the SARS-CoV-2 main protease (MPro). The experimental results revealed that out of the fifteen compounds studied, five displayed inhibitory effects with IC_{50} values ranging from 0.19 to 13.15 μM. The most potent MPro inhibitors were further evaluated for their antiviral efficacy against the delta and omicron variants of SARS-CoV-2. Although certain analogues exhibited antiviral activity, no clear correlation with the MPro inhibition was observed.

PL-9

Harnessing the potential of natural products in the prevention and treatment of atherosclerotic cardiovascular disease and other inflammatory disorders

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Abstract:

Atherosclerotic cardiovascular disease (ACVD) is responsible for a third of all global deaths. Although mortality from ACVD has been reduced recently via lifestyle changes and pharmaceutical intervention, this is expected to reverse in the future because of global increase in risk factors such as hypercholesterolemia, obesity and diabetes. Current pharmacotherapies against ACVD are associated with substantial residual risk for the disease together with other issues such as side effects. In addition, pharmaceutical agents against many promising targets have proved disappointing in clinical trials. It is therefore essential that the molecular basis of ACVD is fully understood, and new therapeutic/preventative agents or targets are identified and validated.

The major focus of recent research in my laboratory is to understand the molecular mechanisms underlying the protective actions of natural products in ACVD using a combination of *in vitro* and *in vivo* model systems together with biochemical, molecular biology, pharmacological and immunological approaches. Our research has provided novel insights into the mechanisms underlying the protective actions of several nutraceuticals, including polyunsaturated fatty acids and polyphenols. In addition to the beneficial effects on ACVD, our studies have revealed protective actions against other inflammatory disorders, particularly non-alcoholic fatty liver disease. Our findings on the mechanisms underlying the beneficial actions of key nutraceuticals will be presented.

PL-10

«The Guard dies but does not surrender!» Olefin metathesis catalysts for challenging cases in pharmaceutical and target oriented synthesis

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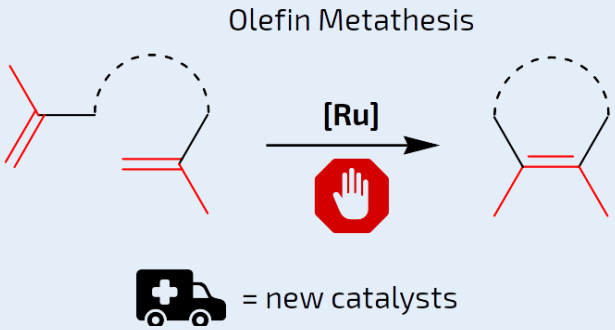
Ruthenium-catalyzed olefin metathesis reactions represent an attractive and powerful transformation for the formation of new carbon-carbon double bonds (1). This area is now quite familiar to most chemists as numerous air and moisture stable ruthenium (2) catalysts are available that enable a plethora of olefin metathesis reactions.

However, formation of substituted and crowded double bonds still remains a challenge, making applications of this methodology difficult (3). This limitation can be solved by designing new, more active and stable catalysts. During the lecture three different very approaches to this problem will be presented (4-6).



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PL-11

Biology of the Ras GTPases Mediated Signaling in Mammalian Cells: A Potential in Developing Therapy for Cancer

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The Ras GTPase superfamily mediates multiple signaling pathways that regulate cell growth, differentiation, movement, and transformation. Ras GTPases have been demonstrated to be associated with development of more than 50% of total human cancer. Not only are oncogenic mutants of Ras associated with the development of many types of cancer, but activation of normal Ras by cellular agonists has also been shown to contribute to the development of this disease. It is important therefore to characterize the Ras signals involved in the control of normal and transformed cell growth as this knowledge could lead to a therapeutic strategy for combating Ras-induced cancer without affecting the normal cellular functions of Ras. Recent studies have shown that the Rho GTPases family (a subfamily of Ras superfamily) is required to transduce Ras signals for transformation and we have found that a member of Rho family, Cdc42, plays an important role in the signaling of oncogenic Ras. Varieties of protein kinases have been reported to be associated in mediating signals from Ras GTPases family. We have found that the Cdc42 effector, activated Cdc42-associated kinase (ACK), is required to transduce Ras signals for transformation. Indeed, our studies indicate that ACK deficiency results in the induction of apoptosis only in v-Ras-transformed NIH 3T3 cells and not the parental NIH 3T3 cells. We also demonstrated that tyrosine kinase inhibitors, which inhibit kinase activity of ACK *in vitro*, also inhibit growth of v-Ras-transformed cells. Collectively, these results indicate a possible role for Ras-Cdc42-ACK in the survival of v-Ras-transformed cells. Based on these observations, our hypothesis is that ACK plays an essential role for survival of v-Ras-transformed cells. Using computer-aided technology we have identified more specific small molecules that inhibit ACK mediated signal transduction and induce apoptosis in v-Ras transformed cells. Various aspects of signaling of the Ras-Cdc42-ACK biology will be discussed.

PL-12

Arylidene-hydrazinyl-thiazoles as Anticancer and Apoptosis-inducing Agents

Rachna Sadana

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Cancer, defined by uncontrolled cell growth, continues to pose a significant global health challenge. Hence, the development of new anti-cancer drugs is crucial for addressing the diverse and evolving challenges associated with cancer treatment, including drug resistance, side effects and the need for personalized and combination therapies. The present research is concerned with the rationale designing, synthesis and anticancer screening of a series of novel functionalized arylidene-hydrazinyl-thiazoles against various human cancer cell lines. All the synthesized novel derivatives were assessed for their cytotoxic potential, ability to induce apoptosis and interference with cell cycle. Among these derivatives, three compounds significantly inhibited cell survival, achieving an approximate 50% reduction across multiple cancer cell lines at a concentration of 10 µM. Furthermore, these three potent compounds demonstrated a marked induction of apoptosis as indicated by loss of mitochondrial membrane potential, increased caspase 3/7 activity, decreased expression of Bcl2 (anti-apoptotic gene) and increased expression of Bax (pro-apototic) mRNA and arrests cell cycle in G2/M phase by inhibiting tubulin polymerization.

PL-13

Fuse Binding Protein 1 interacts with all the naturally occurring tumor suppressor p53 isoforms, making it a novel target for anti-cancer drug design

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Persistent hepatitis C virus (HCV) infection can result in chronic hepatitis C (CHC), which commonly advances to liver cirrhosis (LC) and hepatocellular carcinoma (HCC). However, the molecular mechanisms underlying the progression from CHC to LC and HCC are not fully understood. Our innovative research, based on previous studies, has revealed that FUSE binding protein 1 (FBP1) is significantly overexpressed in CHC, LC, and HCC but is absent in normal liver cells. FBP1 has been found to inhibit the function of the tumor suppressor p53 and may play a role in tumor development. Furthermore, it has been demonstrated that FBP1 physically interacts with p53 and hinders its DNA binding function. A recent study has uncovered that FBP1 interacts with all naturally occurring p53 isoforms carrying large deletions in the N- and C-terminal regions while retaining an intact DNA binding domain (DBD). These exciting findings suggest that the DBD could be the site of FBP1 interaction. Using a recombinant DBD protein of p53, we have verified the interaction of FBP1 with p53-DBD, providing further validation of our research.

PL-14

ELECTRON–DEFICIENT ALKYNES - UNIVERSAL SYNTHONS FOR THE PRODUCTION OF CONDENSED AZA-HETEROCYCLIC SYSTEMS WITH SIGNIFICANT BIOACTIVITY

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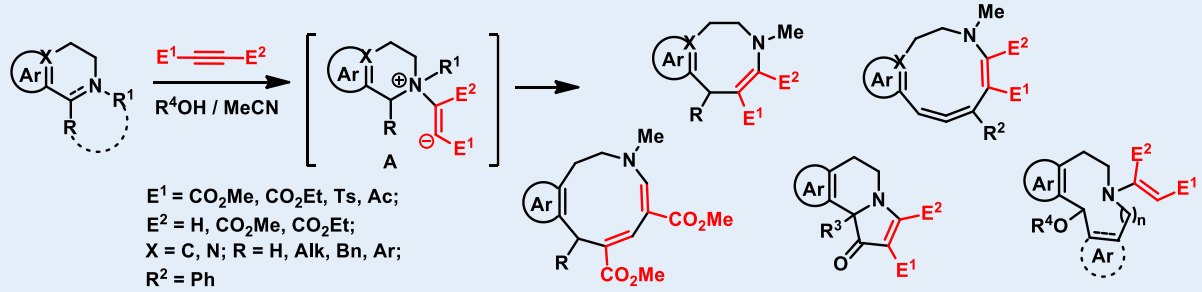
We have developed methods for synthesizing annelated nitrogen-containing 5,6- and medium-sized rings with pharmacophore groups, utilizing electron-deficient alkynes and alkenes. These processes are based on domino and multicomponent reactions and involve a key intermediate, the A [1-4] zwitterion. Many of the resulting compounds exhibit significant bioactivity.



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PL-15

Synthesis of small complex heterocycles employing post-Ugi transformations

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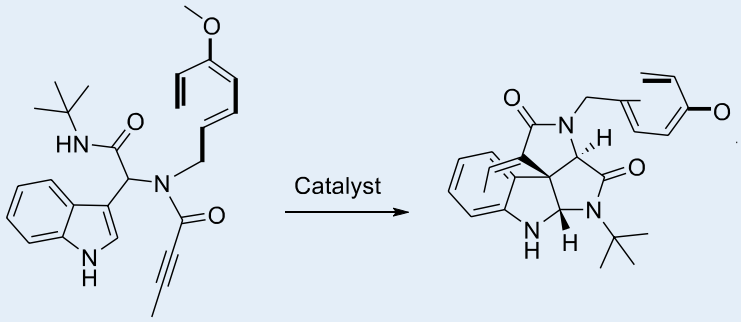
The recent upsurge in the development of mild reaction methodologies for the synthesis of small heterocycles has generated a lot of interest among synthetic organic chemist. To expand this area in organic synthesis, the challenge is to identify novel strategies for the formation of biologically or pharmaceutically important heterocycles under mild conditions as well as continuous flow chemistry to meet up the growing demand for pharmaceuticals as well as agrochemicals. Therefore, in this lecture, an overview will be given about recent synthetic work done in our laboratories regarding this topic. 1) This will include the synthesis of spiroindolines and spiroindoles, which are an important class of spirocyclic compounds present in a wide range of pharmaceuticals and biologically important natural alkaloids. New procedures will be described, including the use of nanoparticles as heterogeneous catalysts. 2) The Ugi-4CR is by far one of the most successful multicomponent reactions leading to high structural diversity and molecular complexity. As the reaction mostly affords a linear peptide backbone, post-Ugi transformations are an elegant solution to rigidify the Ugi-adduct into more drug like species. Not surprisingly, the development of these transformations, leading to new structural frameworks, has expanded rapidly over the last few years. We will comment on the use of homogeneous gold catalysis for performing post Ugi-4CRmodifications (Scheme).



References: see our website https://chem.kuleuven.be/en/research/mds/lomac

PL-16

Electrostatic interactions in DNA nanotechnology: from folding of DNA origamis to transfection of DNA nanogels

Sergii RUDIUK

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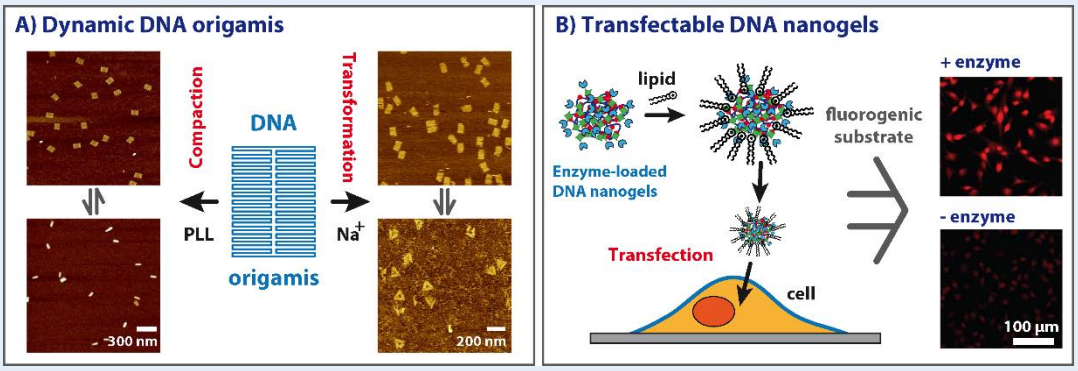
Even though the main biological function of DNA consists in the storage and transmission of genetic information, its biocompatibility combined with highly selective hybridization between complementary strands enabled its applications in material science as a brick for creation of nanobiomaterials. However, up to now in the field of DNA nanotechnology the polyelectrolyte properties of DNA, as negatively charged polyelectrolyte, are yet rather underexploited. In this talk I will demonstrate several examples of what can be achieved either by adjusting electrostatic repulsions between DNA strands, or by full neutralization of DNA charges in such nanostructures as DNA origamis (Figure A) and DNA nanogels (Figure B).

Because of the strong electrostatic repulsions, divalent cations are usually used to stabilize the hybridized DNA network of DNA origamis. I will show that simple adjustment of ionic composition can enable isothermal preparation of various DNA nanostructures at room temperature.[1] Indeed, using "softer" DNA origami stabilizing ions enables thermodynamically driven formation of various nanostructures at room temperature, where the equilibrium state is constituted by properly folded origamis. This approach was used for the first in situ observation of DNA origamis formation, control of the direction of this process, staple competition experiment and even for global morphological transformation of origamis shape from rectangles to triangles. The limits of this approach and its applicability for 3D DNA origamis will also be discussed.

Charge neutralization can induce DNA compaction and promote its transfection through the cell membrane. I will demonstrate that the phenomenon of DNA compaction can also occur for DNA-based nanostructures. 2D DNA origamis and DNA nanogrids could be folded upon their adsorption on positively charged layer-by-layer polyelectrolyte deposits leading to the formation 3D nanostructures.[2] This process was shown to be orthogonal to origami functionalization, and reversible upon treating the folded nanostructures with an excess of competitive negatively charged polyelectrolyte, heparin.

Finally, I will show that cationic lipids can been used to neutralize the surface of enzyme-functionalized DNA nanogels, which we used for successful transfection of a large number of active enzyme molecules embedded in the nanogel, as demonstrated by fluorescence microscopy and flow cytometry analysis of the transfected cells.[3,4] This demonstrates the interest of DNA transfection approaches for the field of DNA nanotechnology.

All these examples we emphasize the interest of tuning electrostatic interactions in DNA nanotechnology for preparation of not only of dynamic, but also transfectable nanobiomaterials.



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PL-17

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Abstract Awaited

PL-18

Newer Imperatives and Newer Vistas in Designing and Developing Chemicals and Chemical Products for a Sustainable Future: Challenges and Opportunities

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Over the years, fossil fuels have been extensively used as the primary source of energy and for development and production of various chemical entities. However, stagnation in petrochemicals and limited availability of petrochemical intermediates now hugely constrains the potential for further development. Hence, a great deal of attention is now towards discovering, developing and promoting alternate strategies for the development and production of chemicals, chemical products, and energy. This talk will uncover a few of these strategies, which are based on renewable and safer sources and processes.

One of the imminent strategies is based on what is now known as the 'Methanol Economy'. This strategy offers great potential for replacing fossil-based fuels and chemical products technology for sustainable production of platform chemicals, and energy security. Essentially aimed at utilization and repurposing of carbon dioxide for the production of CH_3OH and CH_3OCH_3, this strategy is considered to be a promising solution for sustainable fuels requirement and for the production of various kinds of platform chemicals such as hydrocarbons, olefins, propylene, gasoline, aromatics, etc.

More recently, endeavours have been made to devise photoactive core–shell quantum dots-based nano-org microbial bio-factories capable of low-cost carbon sequestration and eco-friendly manufacturing of chemicals. Different core–shell quantum dots, with excitations in UV to near-IR range, could be coupled with targeted enzyme sites in certain bacteria. Such nano-orgs catalyze light-induced air–water–carbon dioxide reduction to biofuels like, isopropanol, 2,3-butanediol, C_{11}–C_{15} methyl ketones, H_2 and chemicals such as formic acid, ammonia, ethylene, bioplastics, polyhydroxybutyrate, etc.

Another new strategy envisions the use of bio-privileged molecules (BMs) for sustainable design and production of chemicals and chemical products. BMs are biotic chemical intermediates, endowed with a diversified group of desirable chemical functionalities beyond those available in the petrochemicals or *via* conventional synthetic means. BMs are abundantly available from bio-resources like the plants and microbes, and can serve as a sustainable and versatile source of various kinds of chemical entities, be it direct replacements for petrochemicals, platform chemicals, or specialty chemicals. This strategy, together with fast-advancing chemical and biochemical technologies greatly facilitates chemical/ biochemical expansion of BMs to almost any molecular framework that one could visualize. This strategy provides a new basis for the diversity oriented synthesis leading to design and development of various kinds of chemical products such as agro-chemicals, antimicrobials, drugs and pharmaceuticals, nutraceuticals, polymers, functional nanobiomaterials, and many others.

Also will be uncovered endeavours of designing photoactive molecular platforms based on the evolutionary and nature-optimized retinal-binding photoreceptor proteins, such as bacteriorhodopsin, which in recent years has received considerable attention owing to its unique photochromic properties and potential utility as smart photoactive element in biosensors and bioelectronic devices such as in optical information processing technology, retinal prosthetic devices, colour-sensitive artificial retina, etc. Since the spectral and photobiological properties of the native photoreceptor may not be entirely suitable for a desired application, successful chemical and biotechnological attempts have been made to tune the molecular properties of the native photoreceptor to produce analogues and variants having desired opto-electronic molecular properties. The chemical method involving substitution of the native retinal chromophore with synthetic analogue chromophores has been successfully employed to develop bR-analogues. In addition, changes effected in the photoreceptor's protein residues by chemical/ genetic modifications have also proved to be of much value in generating functional variants of the photoreceptor. These endeavours have led to designing and developing smart nanobiomaterials, novel molecular phototriggers and photoswitches for dynamic studies in biology, chemistry, physiology and medicine.

Finally, considering the emergence of many new challenges and exciting opportunities, the talk will conclude by emphasizing the essentiality of education and research in chemistry and allied sciences to be progressively integrative, and in alignment with the emerging growth and development trajectories, and technology requirements. Illustrations and examples will be drawn from the research and academic journey of the speaker as well as from the efforts and contributions of other researchers.

INVITED

IL-1

1,2,3-Trizole tethered diversely functionalized heterocyclic compounds as therapeutic agents

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In recent years, click chemistry has emerged as a fast and powerful approach to the synthesis of novel compounds with desired properties. The concept of “click chemistry” was coined by Sharpless to describe a set of “near perfect” bond-forming reactions which were very selective, high yielding, and wide in scope and describes chemistry tailored to generate substances quickly and reliably by joining small units together. In 2022, the Nobel Prize in Chemistry was jointly awarded to Carolyn R. Bertozzi, Morten P. Meldal and K. Barry Sharpless, "for the development of click chemistry and bioorthogonal chemistry". 1,2,3-Triazoles are important class of target molecules due to their interesting biological properties such as anti-allergic, anti-bacterial, and anti-HIV activity. We were encouraged to combine 1,2,3-triazole moieties with pyridine, coumarin, pyrazole, chromenes and many more in a single molecular framework. The synthesized molecules were screened for their antitubercular, antioxidant, antimicrobial, anti-inflammatory and cytotoxic activities and will be discussed.

IL-2

Metal-based anti-cancer drug entities as potential ROS-generating species embedded on Graphene oxide as drug carrier

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Abstract:

A suitable drug delivery system (DDS) based on the graphene oxide nanoparticles (GON) with adequate size and shape to deliver the drug efficiently were established. The Cu(II) based complexes were grafted onto the surface of GON (NCGO-1 and NCGO-2) by simple ultrasonication method. The FT-IR, UV-Vis and powder XRD techniques revealed the successful encapsulation of the complexes onto the surface of GON. In vitro DNA binding interaction studies were carried out by employing various spectroscopic techniques such as absorption, emission, circular dichroism and cyclic voltammetry (CV). The results obtained implicated electrostaic mode of interaction exhibited by both the nano conjugates towards ct-DNA. pBR322 plasmid DNA cleavage activity was performed in the presence of NCGO-1 and NCGO-2 which suggested oxidative cleavage of the DNA by NCG0-1 and NCGO-2 nanoconjugates. The ROS generation concentration inside the cancer cells by NCGO-1 and NCGO-2 was measured and it was observed that both the nanoconjugates was produced high concentration of ROS. One of the most promising documented cell death mechanisms for metal complexes to provide an intrinsic selectivity to cancer cells is the generation of ROS. Cellular uptake and in vitro cytotoxic studies against the lung and breast cancer cell lines have been evaluated and the results obtained demonstrated promising selective cytotoxicity against lung cancer cell line at lower molar concentration in terms of IC 50 value. The release of NC-1 and NC-2 from GON was investigated at 7.4 and 6.5 pH. The fast release of both the drug entities was found at 6.5 pH suggested pH responsive release of drug from GON.

IL-3

Direct Access to C3-Functionalized Pyrrole

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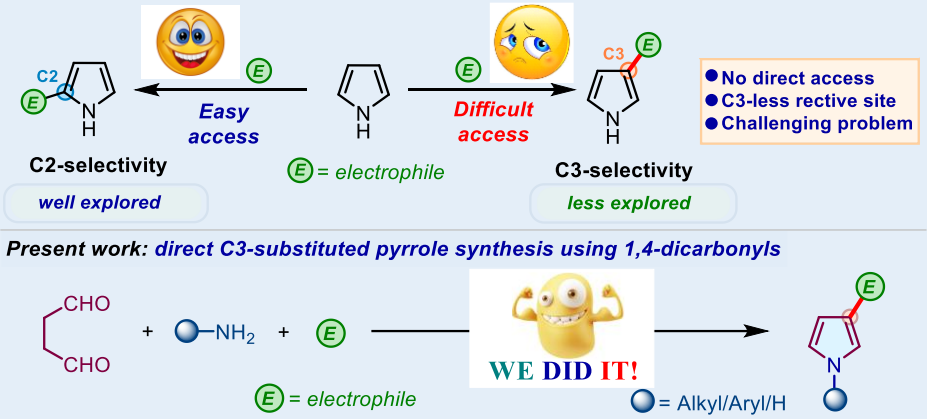
Abstract:

Due to mitigated nucleophilicity, the C3-position of pyrrole is usually considered a non-reactive site in conventional chemistry; thus, the majority of SEAr/Friedel-Craft reactions occur at the C2-(α)-position of pyrrole. Therefore, achieving functionalization at the pyrrole's β-(C3) position is challenging in synthetic chemistry and requires multistep/indirect strategies.[1] These methods can be strictly distributed in two ways: (i) directed functionalization using bulky or electron-withdrawing on pyrrole, and (ii) C3-functionalization-aromatization of N-substituted pyrrolidine. Using amine-catalyzed annulation reactions, we have explored the chemistry of 1,4-dicarbonyls as donor-acceptor (D-A) precursors for synthesizing five-membered N-heterocycles in asymmetric and non-asymmetric fashion.[2] Recently, we have developed a stimulating and straightforward method to access β-(C3)-functionalized pyrrole using mild Lewis acid and catalyst-free conditions.[3] Details of the concept, design, and synthetic strategy for accessing C3-substituted pyrrole in a non-asymmetric/symmetric fashion will be presented here.



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IL-4

Two decades of PARP1 Inhibitors in Cancer Research: Success, Challenges and Roadmap Ahead

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Abstract

Almost twenty years ago, the identification of the synthetic lethality interaction between two essential DNA repair proteins, Poly (ADP-ribose) polymerase 1 (PARP1) and BRCA1/2, encouraged the development of cancer therapies using PARP inhibitors (PARPi) to target tumors with significant genomic instability. Since the USFDA approval of Olaparib in 2014, PARP inhibitors have significantly advanced the treatment of women's cancers, especially BRCA mutant high-grade ovarian cancer and breast cancer. Currently, several more PARP1 targeting drugs, including Rucaparib, Niraparib, Talazoparib, Fluzoparib and Pamiparib have been approved for the treatment of malignant tumors. Over the last decade, the understanding of how PARP1 inhibitors work and how tumors develop resistance to them has greatly expanded. Research has shown that currently marketed PARPi lack selectivity because of their conserved domain, restricting their clinical use and highlighting the necessity for more selective inhibitors. Herein, few design strategies and SARs with the interactions that drive selectivity and offer valuable insights for the development of the next generation of selective PARP inhibitors have been discussed and deliberated which can help medicinal chemists for the rational discovery of selective PARPi.

Acknowledgement: Author are thankful to Gujarat State Biotechnology Mission, Government of Gujarat, India for providing financial support as major research project (Project No. GSBTM/JD(R&D)/663/2023-24/02636697 dated 28/03/2024) to carry out the given work. Authors are also thankful to Nirma University, Ahmedabad, India, for providing necessary facilities and support to carry out the presented work.

IL-5

Synthesis of new aza-heterocycles from aryl methyl ketone and their antibacterial properties

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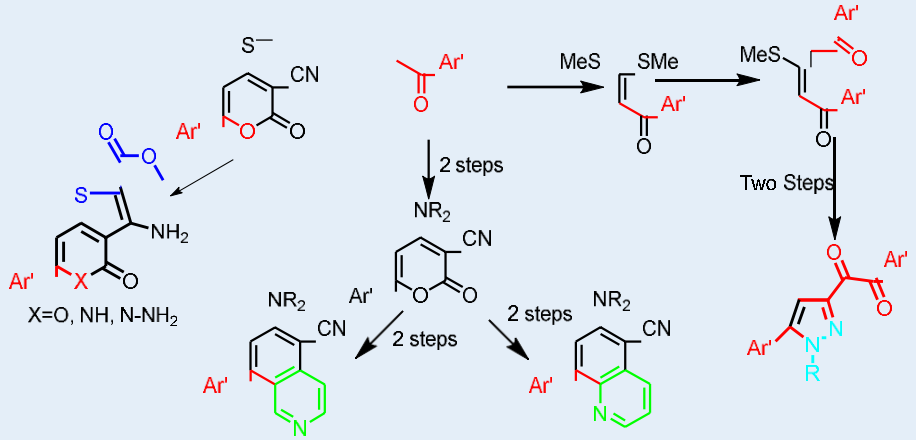
Abstract:



Aryl methyl ketones are very well known primary precursor for the synthesis of a largeclass of molecules. Our group is involved in using ketone for the synthesis of various ketene dithioacetals and pyran and to explore further chemistry.[1] we reported iodine and DMSO-promoted synthesis of multifunctional quinolines and isoquinolines using 6-aryl-4-*sec*.amino-2-oxo-2*H*-pyran-3-carbonitriles and 1-Boc-4-piperidone/1-Boc-3- piperidone as precursors. Synthesis of N-Boc-1,2,3,4-tetrahydroisoquinoline was carried out by ring transformation of suitably functionalized 2-pyranones with 1-Boc- 4-piperidone in DMSO under basic conditions. The N-Boc-1,2,3,4- tetrahydroisoquinoline crude was obtained and treated with iodine and DMSO to affordthe desired isoquinoline. We have also used ketenedithioacetal and synthesized the diketone containing pyrazole at one terminal of diketone in presence of iodine and DMSO.[2] The synthesized 6-aryl-4-methylsulfanyl-2-oxo-2*H*-pyran-3-carbonitriles gives pyranothiophene[3-5] on treatment with methyl thioglycolate, which on further treatment with ammonia or hydrazine provides thienopyridine.[6] Earlier we have achieved a one-pot approach for the synthesis of benzo[h]quinolines[2] and now new azaheterocycles were established ketene dithioacetals.[7]

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IL-6

Development of Some New Protocols in Organic Synthesis

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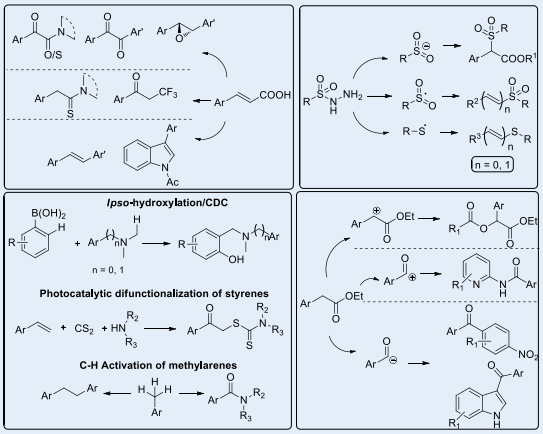
Our current research is focused on the development of some new methodologies in organic synthesis with its medicinal chemistry implications. We have serendipitously discovered the use of sulfonyl hydrazides as a nucleophilic thiol equivalent and Ar-SO_2 source in organic synthesis.[1] Decarboxylative cross-coupling involving *α,β*-unsaturated carboxylic acids/aryl acetic acids, and C-H activation (sp^3 & sp^2) under innovative conditions constitute some other notable contributions from our group.[2] Electrophilic or nucleophilic centre, generated by the activation of benzylic C(sp^3)-H of alkyl arylacetates, has also been explored to construct the C-C/ C-heteroatom bond either via oxidative decarbethoxylation or by cross dehydrogenative coupling.[3] Some other methodologies have also been established using olefins, methylarenes, and *N*-methylated amines to achieve valuable products.[4]



Keywords: Organic synthesis; Sulfonyl hydrazides; Decarboxylative coupling, Alkyl arylacetates.

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IL-7

OTBN-1,2,3-triazoles and dihydropyrimido[4,5-b]quinolinones enabling diverse anti-proliferative and anti-invasive activity against glioblastoma cells

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Abstract:

We explored the synthesis of novel OTBN-1,2,3-triazoles and alkoxy-functionalized dihydropyrimido[4,5-b]quinolinones using room temperature and microwave-assisted multicomponent reaction respectively. The 4k compound of OTBN-1,2,3-triazoles has single-digit micromolar activity against kinase STK33 and exhibits pan-cancer anti-growth activity. It also show potently inhibits cell proliferation, invasion, and 3D neurosphere formation in primary patient-derived glioma cell lines & In silico ADMET and Docking analysis and combination study with clinically relevant brain-penetrant drugs. Analogue 4l of OTBN-1,2,3-triazoles also shows highly specific cytostatic activity against lung cancer cells. Whereas all the synthesized dihydropyrimido[4,5-b]quinolinones analogues show a very good anti-proliferative and anti-invasive activity against glioblastoma cells. In which, 5c shows the most potent anti-proliferative activity with a half maximal effective concentration of less than 3 μM against primary patient-derived glioblastoma cells. It effectively inhibited invasion and tumor growth of 3D primary glioma cultures in a basement membrane matrix. This suggests that the novel compounds could inhibit both the proliferation and invasive spread of glioma and they were selected for further study.

IL-8

Denitrogenative annulation of benzotriazole-appended porphyrins for the rapid and efficient synthesis of diverse heterocycle-fused porphyrins

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Porphyrins are comprised of nitrogen and carbon skeletons, have garnered significant interest in material and biomedicine fields due to their electronic and redox properties. By modifying the core system of porphyrins, intriguing electronic and photophysical properties can be produced.[1] The formation of carbon-nitrogen bond is very important in contemporary organic synthesis. Particularly, the direct formation of carbon-nitrogen bond to aromatic compounds without pre-functionalization is among the emerging and atom-economic strategies. The heteroatom connected porphyrins are of great importance as its presence is expected to alter the optical and electronic properties. For instance, heteroatoms can act as electron-acceptors in the presence of a Lewis acid and an electron-donating unit under basic conditions. They can also provide external coordination sites for forming metal complexes by having an extra pair of electrons or bond pairs. Further, the integration of heteroaromatic systems into the porphyrin ring core increases co-planarity by incorporating the heteroatom into the extension of the π-system.[2-5] Peripheral annulation of heterocycles strongly influence the photophysical properties and often endows the resulting system with a bathochromic shift in the absorption and fluorescence emission spectra.[5] Therefore, in recent years, heterocycle appended and fused (*meso-β*, *β-β* and *meso-β-meso*) porphyrins have been prepared and intensively investigated for their remarkable photophysical properties. In view the immense significance of heterocycle-fused porphyrinoids and our continued in porphyrin-based photosensitizers[6] led us to develop a fairly general approach for heterocycle-fused porphyrins involving denitrogenative annulation of readily available benzotriazole-appended porphyrins. Some of the prepared heterocycle-fused porphyrinoids (*meso-β* and *β-β*) displayed red-shifted absorption spectra and higher singlet oxygen generation ability. The developed protocol and photophysical properties of the prepared heterocycle-fused porphyrins will be discussed during the conference presentation.

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IL-9

Synthesis of Chirally Enriched Pyrazolylpyrimidinone and Imidazopyrimidinones based Glycohybrids via Annulation reactions with Glycals

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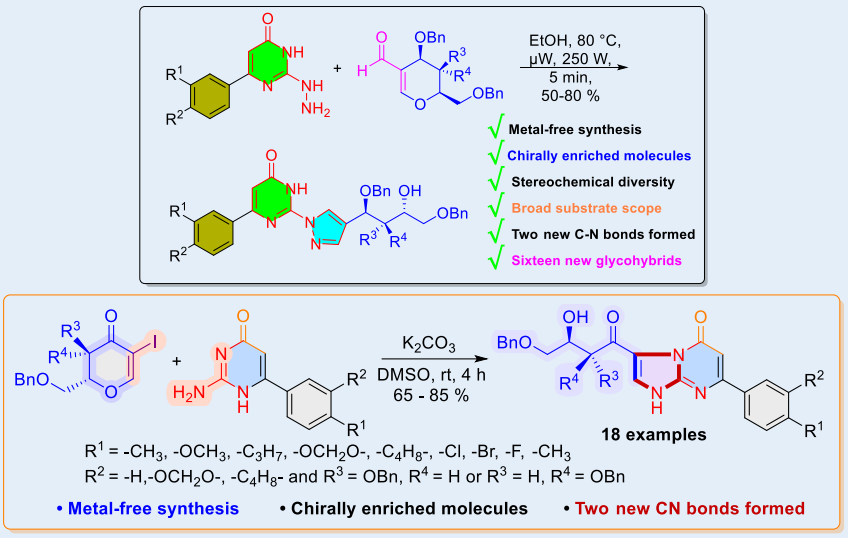

Abstract:

A new strategy for synthesizing chirally enriched pyrazolylpyrimidinone based glycohybrids has been achieved, employing an annulation approach in ethanol without any additives or catalysts under microwave conditions. The designed compounds were obtained within a short reaction time (5 min).[1] Further a simple, environmentally benign and catalyst-free method for the synthesis of chirally enriched imidazo[1,2-*a*]pyrimidinone glycohybrids has been successfully developed. The protocol is based on a base-induced annulation of α-iodo-pyranone with Michael addition of 2-aminopyrimidinones followed by intramolecular nucleophilic substitution reaction.[2] These methods offers several advantages, including mild reaction conditions, a green solvent, and a metal-free approach. Furthermore, the protocol demonstrated a broad substrate scope, successfully incorporating various functional groups with stereochemical diversity, and furnishing chirally enriched molecules.

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IL-10

Beyond Numbers: The Complex Reality of Metrics

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Research metrics have been widely employed as a quantitative tool to evaluate the quality and impact of scholarly research outputs. Among them are journal metrics, author metrics, article metrics and altmetrics. It has become a common practice to evaluate the success of research projects and outputs by employers, research evaluation committees and research funders by using these metrics as a shortcut. Even though several of these are widely used as benchmarks, they are at times deceptive and misleading due to several hidden limitations. Let us introspect the benefits and drawbacks of the popular and widely used metrics in this quickly evolving digital environment, understand their complexity and put an end to their improper use.

Disclaimer – The content presented in the above abstract represent author's personal views.

IL-11

RP-HPLC Stability Indicating Method Development and Validation forEstimation of Rivaroxaban in Active Pharmaceuticals Ingredients

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Abstract:

Rivaroxaban is Anti-hypersensitive drug. In this study RP-HPLC stability indicating method was developed for Rivaroxaban in Active Pharmaceutical Ingredients. Hemochrom Intsil C18 (250 mm X 4.6 mm X 5 µm) HPLCcolumn was used at temperature 35°C.Gradient elution was achieved with 0.01M KH2PO4 Buffer and Acetonitrile-Water(20:80) v/v. The flow rate was 1.0 ml min-1wavelength used was 240 nm. Run time was kept 30 min. The development method was validated according to ICH guideline and found Linear over the range 50 µg ml^{-1} to 500 µg ml^{-1}. The method was studied for force degradation i.e. stress studies parameter and method was capable for separation of degradation product and estimation of Rivaroxaban specifically, selectively, accurately and preciously.

Keywords: Rivaroxaban, HPLC, Force Degradation, Validation.

IL-12

Medicinal Chemistry as multidisciplinary

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ABSTRACT:

Chemistry is the seed of the science. Without chemicals, nothing is in existence.The earth itself is a mixture of chemicals. Chemistry is interlinked with all branches of science. Medicinal chemistry is the field is depending of Chemistry, Pharmaceutical Chemistry, Biochemistry, Microbiology, Computational chemistry and other biological sciences. Drug discovery is possible when chemistry with other branches.

We do in-silico design, organic synthesis, various biological screenings (anticancer, anti-TB, antimalarial, antimicrobial etc…) and toxicity study. Patentsare filed for the promising results with the molecules and then approaches for commercialization.

IL-13

Towards epigenetic therapeutics of Alzheimer's disease: Discovery of Methyltransferase inhibitor via QSAR screening, *in vitro* and *in vivo* analyses

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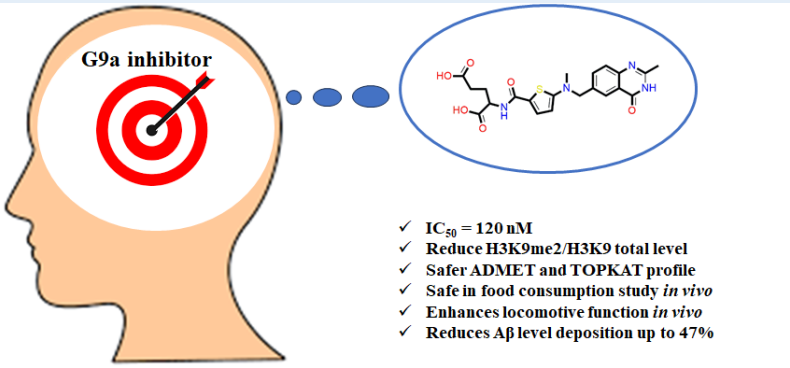
Post-translational modification and epigenetic changes can cause long-term gene silencing or over-expression in a context-dependent manner and are related to various disease conditions, including major diseases such as Cancer and Alzheimer's. Due to high complexities in chromatin architecture and dynamic context-specific cross-talks between chromatin and modifying protein partners, many of these areas are still largely unaddressed (*gap areas*) due to the difficulty in constructing appropriate experimental protocols.

Our target, the G9a, is lysine methyltransferase that mainly di-methylate the H3K9 of chromatin, triggering the repressions of genes epigenetically, leading to various diseased conditions, including Alzheimer's disease (AD). Over the last few decades, considerable inhibitors were reported, such as BIX-01294, UNCO224, UNC0321, UNCO638, UNC0642, E72. However, they have poor pharmacokinetic properties, clinical utility limitations, and side effects (*Bottleneck*).

Therefore, we have ventured to find safer novel leads against G9a by in-depth utilization of QSAR-based database screening, *in vitro*, and *in vivo* analyses. Our lead reduced the Aβ aggregates, an important hallmark in AD, in *C elegans* CL2006 worms up to 47% in a concentration-dependent manner, highlighting its potential in AD treatment. The results of our recently published work will be discussed. [1]



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IL-14

Targeting *Hp* IMPDH to develop efficient drugs for the infection

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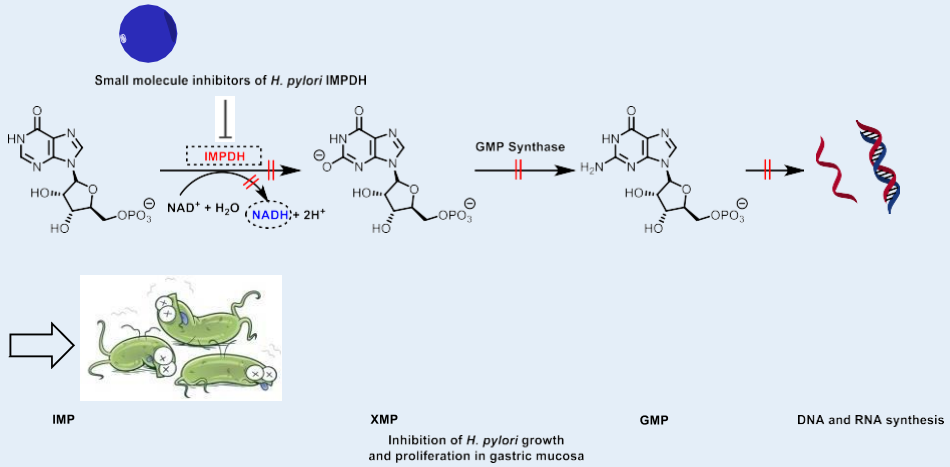
Abstract:

Helicobacter pylori (*H. pylori*) infection is one among many infectious diseases that poses a challenge to the progress of developing nations like India. Anti-bacterial resistance shown by *H. pylori* has affected almost 50% of the total world population and over 80% of the Indian population in the last two decades.[1,2] In order to tackle the infection using efficient therapeutic strategies, many novel drug targets are currently being explored, one among thembeing the crucial metabolic enzyme inosine-5'-monophosphate dehydrogenase (*Hp* IMPDH), involved in the *de novo* nucleotide biosynthesis pathway.

The present study explores the design, synthesis, and biological evaluation of methylpyrazole-substituted benzimidazole derivatives as *Hp*IMPDH inhibitors.The details of *Hp* IMPDH inhibition obtained from the *in vitro* study is beneficial in carrying out further testing directly on the pathogen, which would prove the molecular mechanisms and efficacy of these methylpyrazole-substituted benzimidazole derivatives as potential anti-*H. pylori* agents.[3]

Figure



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IL-15

Deciphering the Atomistic Mechanism of PKM2 Dimerization: Impact of Post-Translational Modifications and Mutation

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[2]*Department of Chemistry, University of Konstanz, Germany*

Abstract

Pyruvate Kinase M2 (PKM2) predominantly operates in its tetrameric configuration, stabilized by the binding of the allosteric regulator fructose-1,6-bisphosphate (FBP). However, post- translational modifications (PTMs) such as Y105 phosphorylation, K305 acetylation, and the R339E mutation can disrupt this structure, leading to a dimeric state. Despite their known effects, the detailed atomic-level mechanisms driving these PTMs and mutations remain elusive. Our molecular dynamics simulations reveal that K305 acetylation increases the distance between the flaps that close over the active site, compromising its integrity and promoting dimerization. Conversely, Y105 phosphorylation induces significant disruptions at the tetramer interface, pulling the dimers apart, reducing hydrogen bonds, and diminishing critical contacts, thereby destabilizing the tetramer. The R339E mutation affects both the active site and tetramer interface, further contributing to instability.

Additionally, notable alterations were observed in the allosteric FBP binding site. The optimal positioning of the FBP molecule was disrupted, leading to altered non-covalent interactions between residues forming the FBP binding pocket compared to the wild type. These structural changes hinder proper FBP binding and drive the transition from a tetrameric to a dimeric form. Our findings provide compelling evidence that PTMs and mutations trigger substantial conformational changes in PKM2, shifting it from an active tetrameric state to a less active dimeric state by obstructing FBP binding. This study offers unprecedented atomistic insights into the modulation of PKM2's structure by PTMs and mutations.

Keywords: Pyruvate Kinase M2 (PKM2), Post-translational modifications (PTMs), Cancer, Computational approaches, Warburg effect, mutation.

IL-16

Driving Innovation Through R&D Strategies: Emerging Therapeutic Modalities and the Future of Medicine

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Propelled by recent unprecedented global healthcare challenges, the landscape of medicine has undergone profound transformations. This evolution, fueled by innovative research and development strategies is unlocking exceptional therapeutic possibilities, and reshaping the future of healthcare through advancements and novel approaches to treatment. The adoption of artificial intelligence (AI), data-driven methodologies, advanced manufacturing technologies coupled with a culture of continuous improvement and learning exemplifies the foundation of robust R&D strategies and innovation. Recent advancements in Proteolysis-Targeting Chimeras (PROTACs), Antibody-Drug Conjugates (ADCs) and mRNA therapies represents promising frontiers in modern medicine, offering groundbreaking approaches for the treatment of a wide range of diseases. PROTACs represent a breakthrough in drug discovery by targeting "undruggable" proteins, offering new therapeutic possibilities for conditions like cancer and neurodegenerative diseases. ADCs, with their ability to deliver cytotoxic agents directly to cancer cells, are enhancing precision medicine by minimizing systemic toxicity, and mRNA-based platforms, propelled into prominence by COVID-19 vaccines, are now being expanded to develop personalized treatments for infectious diseases, cancer, and rare genetic disorders. By leveraging adaptive R&D frameworks, these therapeutic advancements promise to revolutionize medicine, fostering a future of effective, and accessible healthcare. This presentation will highlight the emerging trends in the development of novel therapeutic modalities, mainly development of novel chemical triggers (linkers) and payloads for antibody-drug conjugate (ADC), and their chemistry.

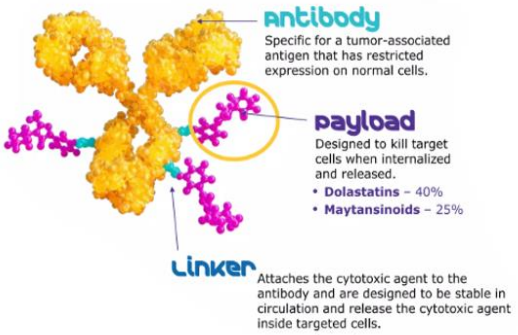

Figure 1. Antibody-Drug Conjugates (ADCs) Composition

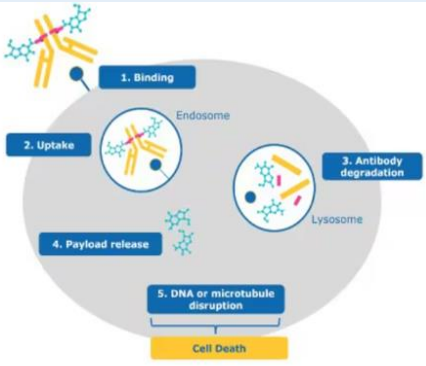

Figure 2. ADC mechanism of action for cancel cell targeting and killing (1) binding, (2) uptake, (3) antibody degradation, (4) payload release, (5) DNA or microtubule disruption, and (6) cell death

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IL-17

NEUROPROTECTIVE EFFECTS OF MYRICETIN NANOFORMULATIONS

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Contributors: Dr. Tripti Halder, Mr. Bharat Patel

ABSTRACT

This study aimed to assess the potential of Myricetin (MY) nanoformulations like MY-loaded nanostructured lipid carriers (MY-NLCs) in improving brain bioavailability and cognitive function in an Alzheimer's model induced by Aβ. MY-NLCs were formulated using precirol ATO 5 (solid lipid), labrafac lipophile WL 1349 (liquid lipid), and tween 80 (surfactant) followed by optimization using a central composite design (CCD) and evaluated based on various parameters.

Cellular toxicity and uptake were studied in SH-SY5Y cells. After intraperitoneal administration of MYS and MY-NLCs (40 mg/kg) to Sprague-Dawley rats (n = 3), MY concentrations in plasma and brain were analyzed. Pharmacodynamic assessments were carried out on an Alzheimer's rat model induced by Aβ1-42 (5 µg/5 µl, ICV, unilateral) (n = 6). Cognitive performance was measured using the Morris water maze, followed by histological and neurotransmitter analyses in the rats' brains.

Key Findings of the study includes optimized method has a desired nanoparticle formulations in terms of particle size of 89.7 ± 26.0 nm, an entrapment efficiency of 80.81 ± 10.39%, and a drug loading capacity of 5.08 ± 1.0%. In vitro release studies showed a biphasic release pattern and demonstrated notable cellular internalization in SH-SY5Y cells. MY-NLCs displayed a 2.77-fold increase in AUC0–24 in plasma, and MY targeting efficiency to the brain was 127.05% higher compared to MYS. The mitigating effects of MY-NLCs (10 mg/kg) were significantly observed in behavioral parameters and in regulating neurotransmitter levels in the brain. **Results conclude that** MY-NLCs show promise as an alternative drug delivery platform for neurodegenerative treatments.

IL-18

Identification of novel inhibitors against the endometriosis-associated ovarian cancerous genes: A study based on transcriptomics profiling, docking and molecular dynamics approach

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Abstract

Endometriosis is a disorder where the tissue identical to the uterine lining, known as endometrial, grows outside the uterus. This tissue is on the ovaries, fallopian tubes, uterine surface, and other pelvic organs. Also, women who are affected with endometriosis have an increased chance of getting Endometriosis-associated ovarian cancer (EAOC), which is a subset of ovarian malignancies that are thought to originate from endometriosis lesions or are strongly related to endometriosis. At present, there is no specific drug available to overcome this. Therefore, this study aims to find crucial genes associated with this infection, their relation to it, and their promising inhibitors. The microarray datasets of endometriosis along with control and endometriosis along with endometriosis-associated ovarian cancer were examined to screen out the differentially expressed genes. Among the differentially expressed genes, the hub genes were identified as having a presence in EAOC. Further, the associated pathways of this gene and their survival rate were also examined. Potential inhibitors for these target genes were identified, and their stability within the molecular connection was examined via the docking and molecular dynamics approach. The overall study suggests that these genes play a major role, and the identified inhibitor can potentially lead to overcoming this.

Keywords: ADME, Docking, Endometriosis, and Endometriosis Associated Ovarian Cancer.

IL-19

Biogenic Carbon Quantum Dots as a Neoteric Inducer in the Game of Directing Chondrogenesis

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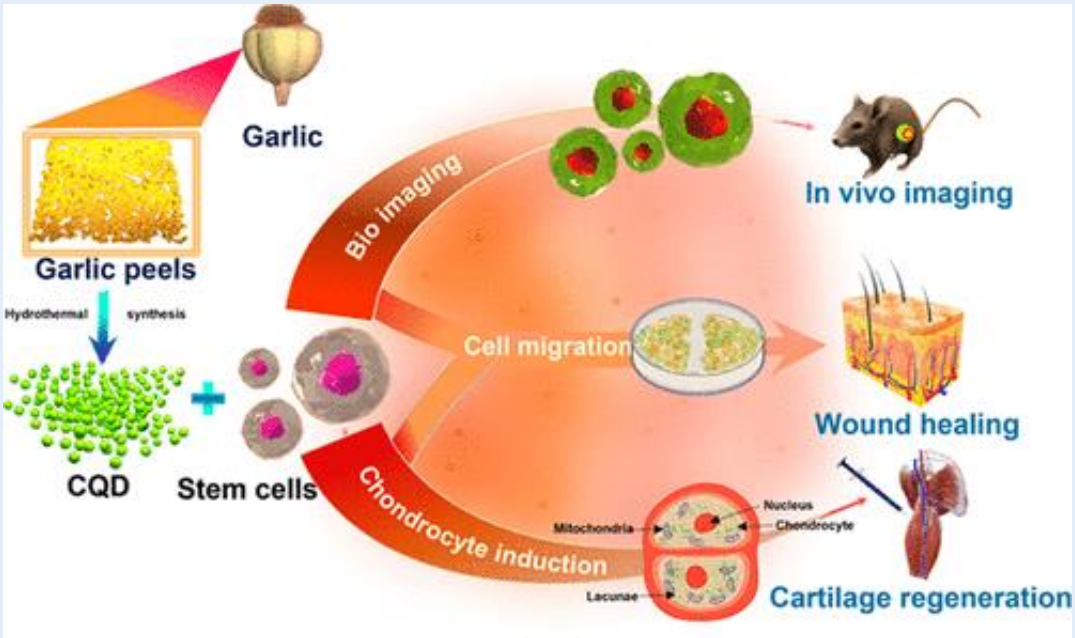
Abstract:

The journey into the field of stem cell biology has been an endeavor of paramount advancement in biomedicine, establishing new horizons in the avenue of materiobiology. The creative drive of the scientific community focuses on ameliorating the utilization of stem cells, which is currently untapped on a large scale. With similar motivation, we present a nascent strategy of maneuvering biogenic carbon quantum dots (CQDs) to eclipse the toxic hurdles of chemical synthesis of carbon allotropes to serve as a biocompatible trident in stem cell biology employing a three-prong action of stem cell differentiation, imaging, and migration. The derivation of CQDs from garlic peels as a biogenic precursor abets in realizing the optophysical features of CQDs to image mesenchymal stem cells without hampering the biological systems with cytotoxicity. We report the versatility of biogenic CQDs to generate reactive oxygen species (ROS) to robustly influence stem cell migration and concomitantly chondrocyte differentiation from human Wharton's jelly mesenchymal stem cells (hWJ-MSCs). This was orchestrated without the use of chondrogenic induction factors, which was confirmed from the expression of chondrogenic markers (Col II, Col X, ACAN). Even the collagen content of cells incubated with CQDs was quite comparable with that of chondrocyte-induced cells. Thus, we empirically propose garlic peel-derived CQDs as a tangible advancement in stem cell biology from a materiobiological frame of reference to hone significant development in this arena.

Graphical Abstract



IL-20

C-H Functionalization of Diazaheterocycles

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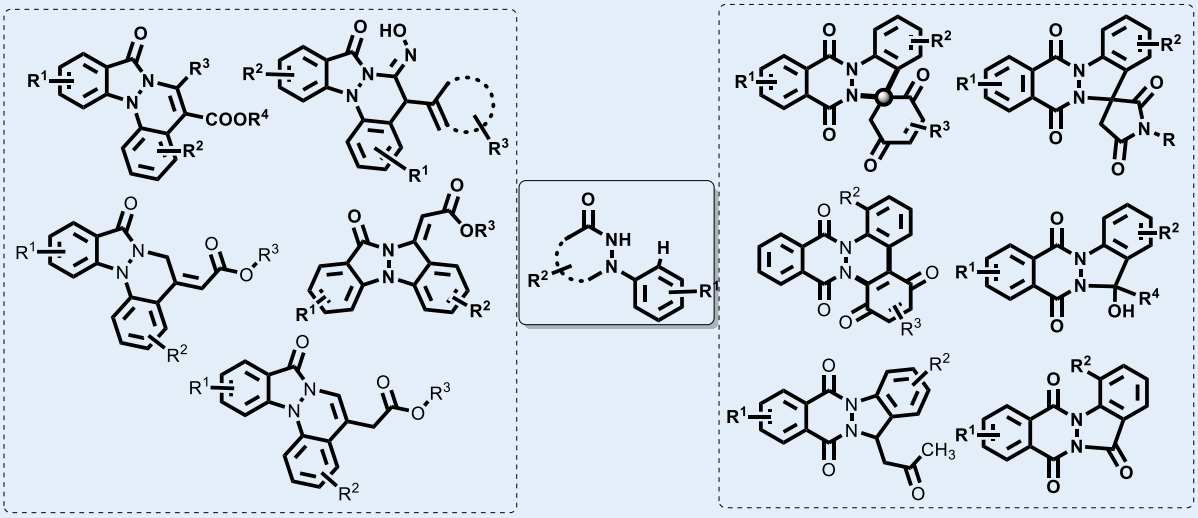
Remarkable advancements in the area of developing transition metal-catalyzed C-H activation strategies have been noticed towards manifesting newer diazaheterocyclic molecular scaffolds due to their occurrence in numerous bioactive natural products and synthetic drug candidates. Among these, indazolone and phthalazine-diones in their fused/functionalized forms have been recognized as valuable synthetic targets due to their wide range of applications in the field of material and medicinal chemistry. Thus, the demand of developing more efficient protocols for synthesizing fused-indazoles and fused-phthalazines in minimum number of steps from readily available precursors continues unabated. In this realm, we have successfully developed interesting transition metal-catalyzed strategies for the synthesis of indazolo-fused indazolylidenes, hydroxy-dihydroindazolo[1,2-*b*]phthalazines, hydroxyimino functionalized indazolo[1,2-*a*]cinnolines & phthalazino[2,3-*a*]cinnolines, 6-arylphthalazino[2,3-*a*]cinnoline-8,13-diones, 5-acyl-5,6-dihydrophthalazino[2,3-*a*]cinnoline-8,13-diones, indazolo[1,2-*b*]phthalazine-triones, indazolo[1,2-*a*]cinnolines and spiro[indazolo[1,2-*b*]phthalazine-13,3'-pyrrolidine]-2′,5′,6,11-tetraones, spiro[cyclohexane-1,13'-indazolo[1,2-*b*]phthalazin]-3-ene-2,5,6',11'-tetraone, benzo[*c*]phthalazino[2,3-*a*]cinnoline-1,4,10,15-tetraones, 13-(2-oxopropyl)-13*H*-indazolo[1,2-*b*]phthalazine-6,11-diones *via* directing group-assisted C-H functionalization.



IL-21

New Perspectives, Design and Applications Organotin(IV) Complexes

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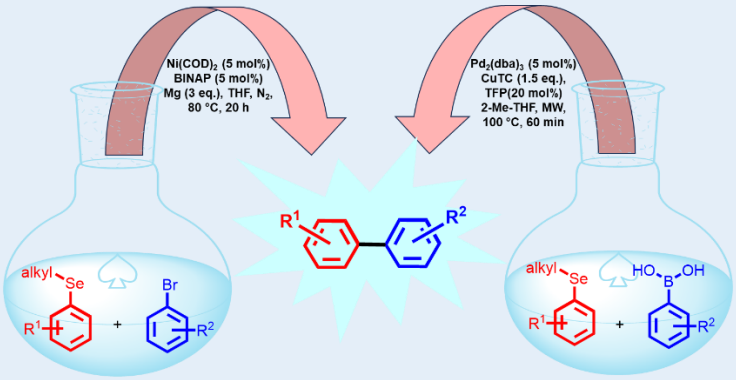
Organotin(IV) complexes are renowned for their structural diversity and broad spectrum of technological and biological applications. Various organic ligands, such as heterocyclic β-diketones, Schiff bases, N-protected amino acids, and oximes, have been utilized in the synthesis of these complexes. The advent of advanced experimental techniques, including multinuclear NMR (^{1}H, ^{13}C, ^{119}Sn NMR), single-crystal X-ray analysis, and density functional theory (DFT/B3LYP method), has provided valuable insights into the structures and stabilities of these complexes. There is a notable synergy between the experimental data and theoretical findings for these complexes. Newly synthesized organotin(IV) complexes have shown a wide range of biological applications. Computational analysis has also been employed to study the optimized molecular structures, geometries, dipole moments, energy gaps, and electronegativity of some of these complexes.

IL-22

Introducing New Class of Selenium-Based Pseudohalides for Cross-Coupling Reactions

Professor BK Singh

Department of Chemistry
University of Delhi



Pseudohalides have transformed synthetic chemistry by enabling efficient C–C bond formation in metal-catalysed cross-coupling reactions. Traditional electrophiles like organohalides and pseudohalides (e.g., triflates, tosylates) have dominated the field, the search of novel pseudohalides is crucial to expand the substrate scope of these transformations. Among these, sulfur-based electrophiles have gained significant attention; however, selenium-based electrophiles (C–Se bonds), despite their inherently weaker bond dissociation energy and unique chemical properties, remain underexplored.

Recently, we have established selenium-based electrophiles as a promising new class of pseudohalides for cross-coupling chemistry which offer complementary advantages to traditional systems. During the meeting, I would be discussing the two innovative methodologies which we have developed. Firstly, the nickel-catalyzed cross-coupling of aryl alkyl selenides with aryl bromides, which eliminates the need for organomagnesium reagents, and secondly, the palladium-catalyzed microwave-assisted protocol that uses copper(I) thiophene-2-carboxylate as a mediator to enable efficient C–Se bond activation, affording biaryls with excellent substrate compatibility and scalability. During the presentation, I would be focusing on the importance of exploring these pseudohalides to unlock broader reactivity profiles, drive sustainable chemical processes, and advance the frontiers of transition-metal catalysis.

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IL-23

Organotin Compounds for Organic Synthesis Utilization of Arylmethyl Radicals for C-X (X = C, N, and O) Bond-Forming Reactions

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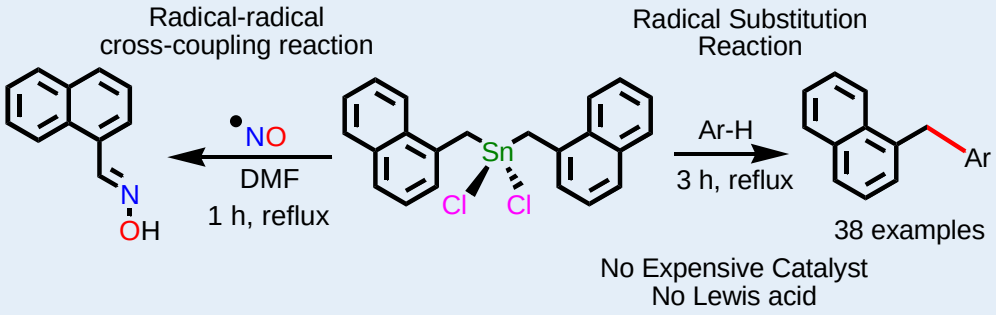
The oxidative-addition reaction between an arylmethyl chloride (RCH_2Cl; R = 1-$C_{10}H_7$, 2,4,6-$Me_3C_6H_2$, 4-MeC_6H_4, 3-MeC_6H_4, C_6H_5, 4-ClC_6H_4) and tin powder in boiling toluene produces bis(arylmethyl)tin dichlorides, [$(RCH_2)_2SnCl_2$] in good yields [1]. At 160 °C in mesitylene bis(1-naphthylmethyl)tin dichloride undergoes Sn-C homolytic cleavage to generate two 1-naphthylmethyl radicals (1-$C_{10}H_7CH_2^{\bullet}$), which were trapped by TEMPO ($C_9H_8NO^{\bullet}$)/**4-hydroxy-TEMPO/4-oxo-TEMPO. We could possibly isolate the inorganic by-product, Sn-O *football-like cages*, with twelve peripheral naphthylmethyl units from the 4-hydroxy-TEMPO reaction. Subsequently, the C-N bond forms eventually result in 1-naphthaldoximes when the 1-naphthylmethyl radicals unite with the toxic pollutant nitric oxide (NO). In contrast, the oxidation instead of the addition reaction happens when nitrogen dioxide is used.** Subsequently, the radicals ($RCH_2^{\bullet}$) produced in this manner were utilized for efficient substitution reactions with electron-rich arenes (R′H; R′ = 2,4,6-$Me_3C_6H_2$, 1,2,4,5-Me_4C_6H, 1,2,3,4,5-Me_5C_6) to obtain a variety of unsymmetrical diarylmethanes ($RR'CH_2$). Functionalized diarylmethanes have been investigated extensively in view of their wide-ranging applications in pharmaceutical, agrochemical and material sciences [2,3]. Adding one iodine equivalent (I_2) to the reaction mixture significantly increased the yields of coupled products. In the case of anisole or xylenes, iodine mediation is necessary to favour the desired diarylmethane derivatives through Friedel-Crafts reaction. Alternative synthetic approaches to this type of organic compounds that avoid using a transition-metal catalyst or a strong Lewis acid are desirable.



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IL-24

Exploring Organic Chemistry of Isocyanide Beyond Conventional Flasks: Our Recent Progress

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Isocyanides, known for their historical importance in the field of organic chemistry, have found applications in both academic research and industrial contexts. Among the various stable divalent carbon nucleophiles, isocyanides stand out due to their exceptional ability to form multiple bonds on the terminal carbon atom. However, the incorporation of isocyanides into diverse areas of organic chemistry offers an exciting opportunity to explore uncharted chemical territory and potentially discover novel lead compounds. Nevertheless, this pursuit remains a significant challenge. In this presentation, I will discuss our recent progress in merging isocyanide chemistry with organic electrosynthesis, resulting in the synthesis of a wide range of medically valuable molecular frameworks.[1-11]

Keywords: Isocyanides, MCRs, Electrochemical, organic synthesis.

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IL-25

Cutting-Edge Applications of Tunable Supramolecular Gels

Dr. Manoj Kumar Gupta

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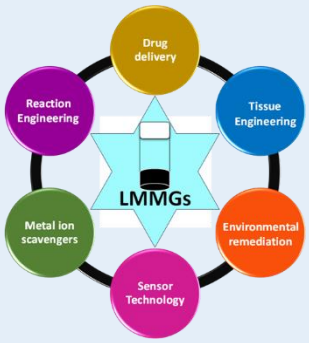
Abstract:

Supramolecular gels represent a highly dynamic class of materials, renowned for their ability to adapt and respond to various stimuli. Among them, low molecular weight gelators (LMWGs) have emerged as a prominent research focus in material science, primarily due to their capacity to form stable, versatile gels through non-covalent interactions such as hydrogen bonding, van der Waals forces, and π-π stacking. These small molecules self-assemble into three-dimensional networks that trap solvents, creating gels with tunable mechanical, chemical, and optical properties. By altering the molecular structure of LMWGs, it can control key properties like gel strength, responsiveness to stimuli, and self-healing capabilities. This adaptability makes supramolecular gels invaluable across a broad spectrum of applications, including controlled drug delivery, tissue engineering, and environmental remediation, such as oil spill recovery and water purification. Additionally, these gels play crucial roles in sensor technology and smart materials, offering innovative solutions in biomedical, industrial, and environmental sectors.



IL-26

Mitochondria Specific Half-Sandwich and Cyclometallated Ru(II)/Ir(III)/Re(I)-Complexes to Unveil the Dynamic Therapy Against Cancer

Dr. Priyankar Paira

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To abate the world-wide rampant prevalence of cancer, recently we have developed mitochondria targeted DNA intercalating Ru(II)/Ir(III)/Re based half-sandwich and cyclometallated complexes for ROS mediated selective dynamic therapy in absence or presence of light (CDT or PDT) enhancing the therapeutic potential against the distinct tumour microenvironment (TME) and elevated GSH level. It has been visualised that these scaffolds are very dexterous to damage DNA, deplete GSH level and increase the oxidative stress through ROS generation. The significant cell cycle arrest, stimulation of p53 genes, upregulation of Bax family proteins and down regulation of Bcl-2 upon administration of these scaffolds against various cancer cell lines, triggers the mitochondrial intrinsic pathway for apoptosis through activation of a cascade of different caspases.[1, 2]

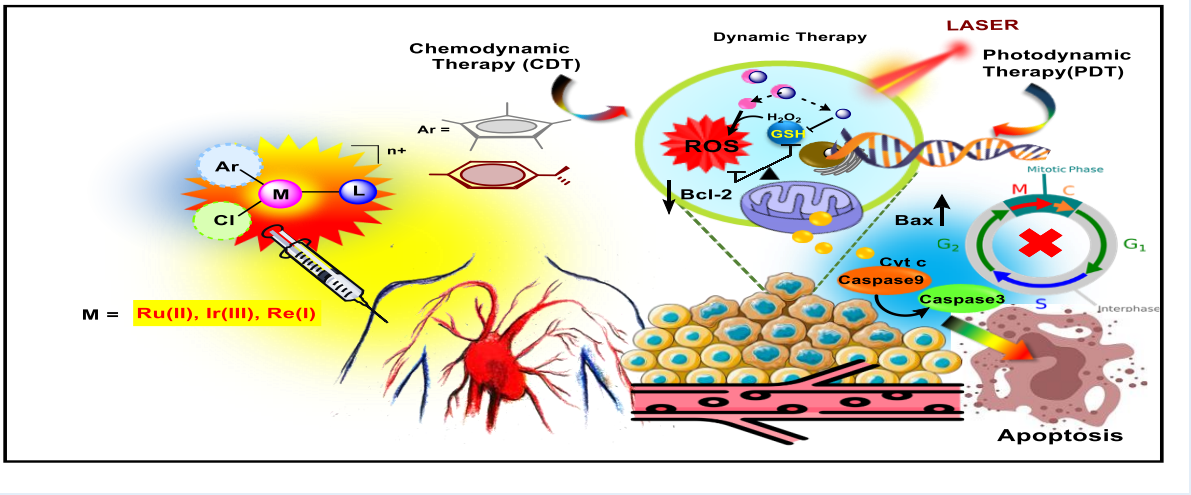

Figure 1: Strategies for destruction of cancer cells

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IL-27

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

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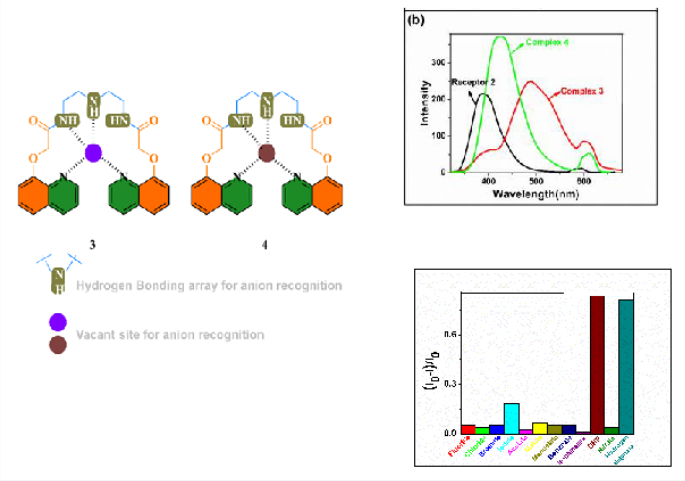
Abstract

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]



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IL-28

GREEN SYNTHETIC PATHWAYS FOR TRANSITION METAL SCHIFF BASE COMPLEXES: PIONEERING ADVANCES IN SUSTAINABLE COORDINATIONCHEMISTRY

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ABSTRACT

Schiff base ligands, renowned for their exceptional versatility, have emerged as pivotal components in modern chemistry due to their ability to form stable complexes with a broad spectrum of metals invarious oxidation states. Their extensive applications, ranging from pharmaceutical development to catalytic processes, continue to captivate the scientific community. The paradigm of inorganic synthesis is progressively shifting towards sustainable methodologies, with microwave-assisted synthesis exemplifying this trend. This avant-garde technique stands out for its eco-friendliness, cost-effectiveness, and energy efficiency. Unlike conventional heating, microwave irradiation ensures uniform energy distribution within the reaction medium, significantly accelerating reaction kinetics and enhancing product yield and purity. This method not only reduces reaction times from hours to mere minutes but also aligns with the principles of green chemistry, fostering more sustainable and efficient chemical processes.

The synthesis, characterization, and biological evaluation of Schiff base coordination complexes involving Cr(III), Ni(II), Co(II), Pd(II) and Pt(II) metals with Schiff base ligands derived from precursors like thiosemicarbazide, semicarbazide, S-benzyldithiocarbazate etc. have been synthesized via both microwave and conventional methods. The structures and formation of the synthesized compounds were confirmed using an extensive array of sophisticated analytical techniques, includingelemental analysis, IR, UV-Vis, ^{1}H NMR, EPR spectroscopy, mass spectrometry, and X-ray diffraction, providing thorough and precise characterization. The synthesized complexes have exhibited significant antimicrobial, antifungal and anti-tubercular activities against variouspathogenic strains. They also act as effective anticancer agents particularly against MCF-7 breast adenocarcinoma cells and HeLa human cervical cancer cells as concluded from their IC_{50} and selectivity index value where a selectivity index value greater than 3 shows good selectivity against cancer cell lines while low toxicity against HEK293 human normal embryonic kidney cell lines. These complexes also show notable DNA cleavage activity.

IL-29

Synthesis of bio-based metal-organic frameworks for sustainable environment

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Abstract:

Bio-based metal-organic frameworks (MOFs) are an emerging class of materials for their potential applications in diverse fields such as environmental science, and medicine. Their unique properties like biocompatibility, high surface area, selectivity, functionalization, tunability, chemical stability, and sensing have made them the most fascinating materials for a sustainable environment. Plastic has been the most widely used food packaging material, however, plastic takes thousands of years to biodegrade. Moreover, recently there has been a growing concern about microplastic in water and food stuffs. Therefore, the development of sustainable packaging material is one of the desirable research areas that has the potential to reduce the environmental impact of hazardous food packaging materials. Gallic acid is a bioactive compound that exhibits anti-oxidant properties. The integration of gallic acid in biopolymer-based packaging film can provide an active material for food safety. Chitosan is a good film-forming material and its combination with cellulose makes the film highly stable with effective UV blocking properties. Herein, we report the synthesis of gallic acid-based MOFs and their application in the development of active food packaging material. A specific combination of chitosan, nanocellulose, and gallic acid-based MOF provides excellent UV protection, and high air and moisture barrier properties which keep the fruits and vegetables fresh for a long duration of time.

IL-30

Green Catalysis for Sustainable Organic Synthesis

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Green catalysis is a crucial strategy in sustainable organic chemistry, focusing on minimizing environmental impact while improving the efficiency of chemical reactions. Enzymes, as biocatalysts, play a crucial role in green catalysis due to their ability to operate under mild conditions, exhibit high specificity, and minimize waste.[1] They facilitate various organic transformations without the need for harsh reagents, making processes cleaner and more efficient. Additionally, using electricity as a sustainable catalytic method has gained momentum, enabling electrochemical reactions that can drive chemical transformations with minimal by-products. By harnessing renewable energy sources, electrochemical catalysis reduces reliance on traditional fossil fuels and hazardous reagents, complementing enzymatic processes and promoting a more sustainable approach to organic synthesis. Together, enzymes and electricity pave the way for innovative green catalysis strategies, driving advancements in sustainable organic synthesis. In our laboratory, we harness the power of enzymes like lipases and amylases as catalysts to facilitate non-natural organic reactions, paving the way for innovative synthetic pathways. These biocatalysts allow us to conduct reactions under mild conditions, enhancing selectivity and minimizing waste.[2-4] Additionally, we have made significant strides in developing chemoenzymatic approaches, which combine chemical and enzymatic methods to synthesize complex organic molecules efficiently. This hybrid strategy leverages the strengths of both paradigms, enabling us to access compounds that may be challenging to produce through traditional methods.[5-6]

On another front, we are exploring the use of electricity to catalyze organic reactions involving N-heterocycles. By employing electrochemical methods, we can drive these reactions precisely while reducing the reliance on hazardous reagents and solvents. Furthermore, we have successfully integrated enzymes with electrochemical processes to enhance the efficiency and sustainability of organic reactions.[7] This innovative merging of enzymatic and electrical catalysis opens new avenues for developing greener synthetic methodologies, contributing to our ongoing efforts to advance sustainable chemistry.

Keywords: Enzyme catalysis, Electrosynthesis, Green organic synthesis, sustainable chemistry

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IL-31

Challenges in the Process development of simple and complex APIs and overview on the chirality control

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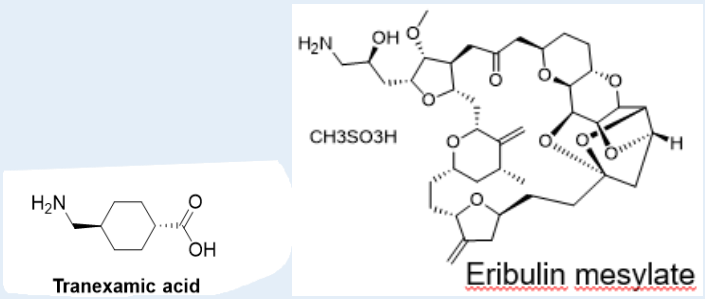
Abstract:

In the generic API market, developing a robust and economic commercially viable manufacturing process is always challenging. Introduction of various small molecules, hormonal and complex API's as well as stringent regulatory guidelines further complicate the process development. Based on the indication of the respective API; scale of production varies leading to challenges in the production and quality compliance.

Process development of a simple API Tranexamic acid and a complex API Eribulin Mesylate (Fig. 1) will be discussed keeping the focus on the strategies involved in the route of synthesis, costing and chiral control.

Figure 1:



IL-32

Development of Peptide-Heterocycles Conjugates: Synthesis, Characterization, and Biological Studies

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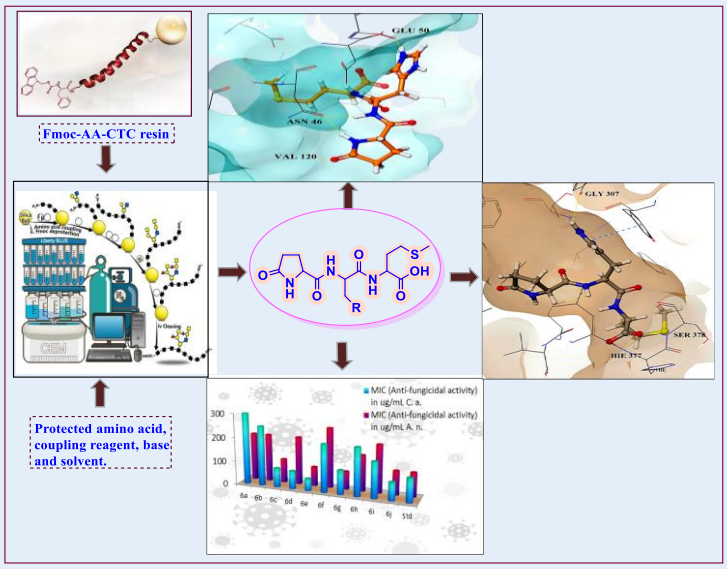
Abstract:

In recent era of the drastic advancements in the field of therapeutics, peptide synthesis is a breakthrough in this developing field. In the present study, the design and synthesis of dipeptide derivatives containing 5-chloro-thiophene-2-carboxylic acid, (S)-5-oxopyrrolidine-2-carboxylic acid, indole-3-carboxylic acid, and tetrahydroisoquinolines, employing solid-phase peptide synthesis and advanced spectroscopic techniques for characterization is presented.

In vitro evaluations of these compounds revealed significant antibacterial activity against Gram-positive (*Streptococcus pyogenes*, *Staphylococcus aureus*) and Gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*), which effectively surpasses the standard antibiotics such as ampicillin and ciprofloxacin. Especially, the Thiophene-Tyr-Arg-OH exhibited exceptional activity against *Escherichia coli* with a minimum inhibitory concentration (MIC) of 15 µg/mL. The antifungal activity against fungi like *Candida albicans* and *Aspergillus Niger* was also noteworthy, with some compounds showcasing superior performance with reference to the standard antifungals like nystatin and fluconazole. *In silico* studies was employed to elucidate the interactions of peptide molecules with specific biological targets, including DNA gyrase and lanosterol-14 alpha demethylase, revealing encouraging binding affinities. These findings underscore the potential of peptide-heterocycle complex compounds as promising candidates for antimicrobial drug development, encouraging the way for innovative therapeutic strategies in combating bacterial and fungal infections.

Key words: -Solid phase peptide synthesis, dipeptides conjugates, heterocycles, biological studies and *in silico* studies.



IL-33

"From Molecules to Bio-Materials: The Versatility of Functional Oligo-Glycerol Surfactants"

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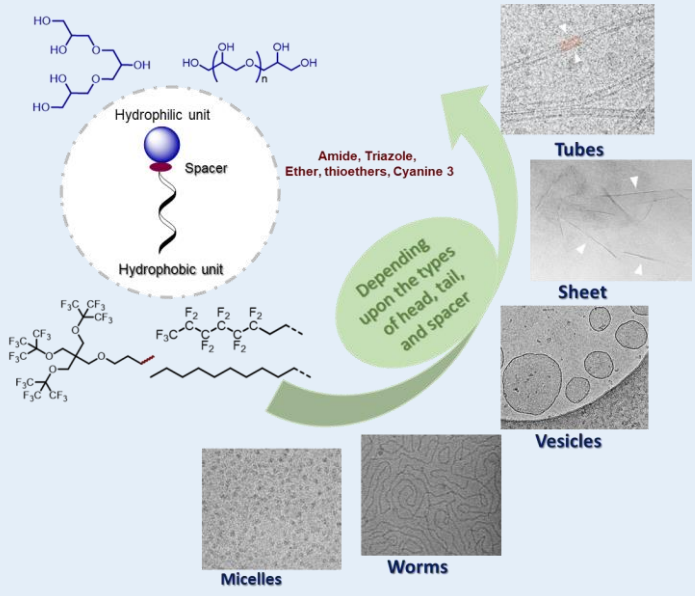
Functional oligo-glycerol (OG) surfactants represent a versatile class of amphiphiles that bridge molecular design and their applications. Their unique structure which provides better hydrophilicity and more possibilities do the post functionalization, these OG can be characterized by tunable hydrophilic oligo-glycerol head groups and customizable hydrophobic tails that linked with different linking chemistry, enables precise control over self-assembly behaviors that directly reflect over their applications. These surfactants can form diverse supramolecular architectures, including micelles, worms, vesicles, sheet, tubes and other nanostructures, which are highly relevant in biomedical and material science applications. This talk will explore the journey from molecular synthesis to material applications, emphasizing various synthetic approach that allows the design of tailored oligo-glycerol surfactants with specific functionalities. Key insights into their physicochemical properties, self-assembly studied using cryo-TEM will be discussed in the context of their structural arrangements of their hydrophilic, hydrophobic and linker. Furthermore, I will present their applications in areas such as antibacterial treatment, 19 FMRI and Protein purifications. This talk aims to highlight the versatility of oligo-glycerol surfactants and their transformative impact, emphasizing their role as a bridge between fundamental chemistry and cutting-edge applications.



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IL-34

Probiotics: The Next Frontier in Health and Wellness

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Abstract:

Probiotics, live microorganisms that confer health benefits when consumed in adequate amounts, have emerged as a promising avenue for promoting human health and well-being. Beyond their traditional role in digestive health, probiotics are increasingly recognized for their potential to influence various aspects of our physiology.

One key area where probiotics have demonstrated significant benefits is immune modulation. By interacting with the gut microbiota, probiotics can help regulate immune responses, reducing inflammation and enhancing the body's ability to fight off infections. Additionally, probiotics have been shown to improve mental health, with studies suggesting their potential to alleviate symptoms of anxiety and depression.

We investigated the isolation, screening and characterisation of probiotic bacteria and the production of antimicrobial peptides from potential probiotic *Lactobacillus* Strain.

While the scientific understanding of probiotics continues to evolve, the growing body of evidence suggests that these microorganisms offer a promising approach to promoting overall health and well-being. As research progresses, it is likely that we will see even more innovative applications of probiotics in various healthcare settings, instilling optimism about future treatments.

IL-35

Computational Insight to Stereochemical Aspects of Some Synthetically Important Organic Reactions

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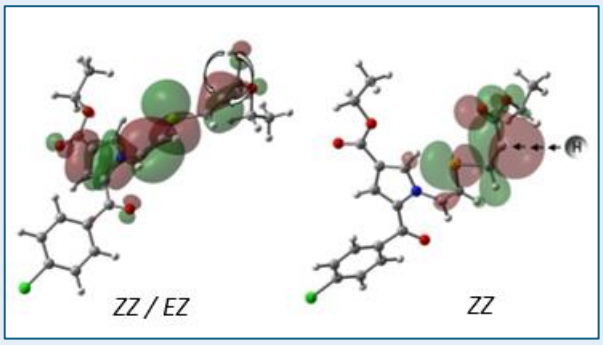
Abstract

N-Cycloimminium ylides serve as versatile synthons for obtaining biologically important *N*-fused heterocyclic compounds through cyclocondensation, electrocyclization and 1,3-dipolar cycloaddition reactions. Wide range of biological and pharmacological activities including antibacterial, antimalerial, anticancer, antiallergic, anti-inflammation, anti-HIV infection and many more shown by naturally occurring and synthetic compounds incorporating *N*-fused heterocylic scaffolds has kept the interest of synthetic chemists alive for obtaining new libraries of molecules with diverse structural features. 1,3-Dipolar cycloaddition of N-cycloiminium ylides constitute an important pathway for construction of fused five-membered heterocycles incorporating a bridgehead nitrogen atom. Additionally, 1,3-dipolar cycloaddition reactions exhibit high regio- and stereoselectivity making them a method of choice for synthesis of biologically important heterocycles. There have been many instances of the reaction proceeding in particular regio- and stereo-selective manner to give varied and unexpected products. Computational chemistry has been advantageous in understanding impact of stereoelectronic effects on progress of a reaction under particular reaction condition. The talk will be focused on the results of computational investigation of mechanistic aspects of competitive pathways pertaining to some interesting cycloaddition/electrocyclization reactions to rationalize the experimental results.



IL-36

Sustainable Approaches to Water Purification: Role of Biochar in Photocatalytic Processes

Dr Prachi Singh*

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Abstract:

Biochar is a carbonaceous material produced from the slow-pyrolysis of biomass. It has recently emerged as a promising support material in photocatalytic degradation processes. This interest is driven by biochar's unique properties, including its high surface area, porosity, and surface functional groups, which enhance the dispersion and stability of photocatalysts. When combined with photocatalytic materials such as titanium dioxide (TiO_2), zinc oxide (ZnO), and other metal oxides, biochar can improve the efficiency of photocatalytic degradation of organic pollutants by facilitating charge separation and reducing electron-hole recombination rates.

The incorporation of biochar into photocatalytic systems has shown considerable promise in the degradation of a variety of contaminants, including dyes, pharmaceuticals, pesticides, and other hazardous organic compounds found in wastewater. Its ability to adsorb pollutants onto its surface provides a pre-concentration effect, enhancing the interaction between the contaminants and the photocatalytic sites. Moreover, the natural carbon structure of biochar can absorb visible light, extending the light absorption range of traditional photocatalysts and improving overall degradation efficiency under solar or visible light conditions.

Future research into the use of biochar in photocatalytic degradation focuses on optimizing its physicochemical properties through methods such as doping with metals, modifying surface functional groups, and adjusting pyrolysis conditions. Additionally, exploring the synergetic effects between biochar and various photocatalysts could lead to the development of novel composites with superior photocatalytic activities. The scalability and economic feasibility of biochar-based photocatalytic systems also present significant areas for further exploration, particularly for large-scale wastewater treatment applications.

Overall, the integration of biochar in photocatalytic degradation presents a sustainable and effective approach to addressing environmental pollution, with potential benefits extending to water purification, air quality improvement, and even energy generation. Continued innovation and interdisciplinary research are key to unlocking the full potential of biochar in photocatalytic applications and establishing its role in advanced environmental technologies.

Keywords: Biochar, Photocatalytic degradation/systems, organic pollutants, metal oxides, interdisciplinary research.

IL-37

Desymmetrization Strategy Towards Stereoselective Construction of Alkaloid-Mimicking Polycyclic Scaffolds and Natural Products

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Stereoselective synthesis of nitrogen-containing complex scaffolds from simple building blocks is important in modern synthetic organic chemistry. Nitrogen-containing ring fused systems in natural products and pharmaceutically important molecules illustrate the need to develop efficient synthetic strategies. Our group is working on desymmetrization strategies that have enabled us to access structurally diverse polycyclic scaffolds with endogenous nitrogen.[1] Strategy was extended to the step-economical total synthesis of natural products, such as Millingtonine and Incargranine. Details of the work will be presented during the conference.

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IL-38

OPTIMIZING PHARMACEUTICAL PRODUCTION: ADVANCING EFFICIENCY WITH HOT MELT EXTRUSION FOR CONTINUOUS MANUFACTURING

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Abstract:

The pharmaceutical industry is undergoing a transformative shift, with increasing demand for diverse dosage forms driving innovation in manufacturing. This study highlights the adoption of continuous manufacturing techniques, particularly hot melt extrusion (HME), as a key solution to enhance operational efficiency, reduce costs, and ensure the consistent production of pharmaceutical products. Our research focuses on the advantages of transitioning from traditional batch processes to continuous manufacturing, emphasizing HME's potential in polymer-drug binding as a flexible and robust method. The study evaluates critical formulation parameters, revealing an average capsule weight of 201 ± 5 mg, a disintegration time of 12 ± 2 seconds, and a drug content of 49 ± 3 mg of Aceclofenac per 100 mg formulation. The dissolution profile indicated a linear release with 76.69 ± 2 %CDR in 60 minutes. These findings offer valuable insights for pharmaceutical manufacturers seeking to optimize production processes through continuous manufacturing and hot melt extrusion technology.

Keywords: Hot Melt Extrusion, Continuous Manufacturing, Pharmaceutical Production, Aceclofenac, Drug Release, Polymer Binding, Process Optimization.

Scan me

IL-39

Molecular design and synthesis of new copper(II) norcraugsodine complexes and their interaction studies with ct-DNA/tRNA and cytotoxicity profile

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Abstract

Amaryllidaceae alkaloid are well known for their myriad pharmacological properties such as Alzheimer's dementia, antimicrobial, and antitumor. The therapeutic potency of this bio-pharmacophore is attributed to the presence of its versatile ring structure and carbon skeleton of alkaloid group. Herein, molecular design, synthesis of new Cu(II) norcraugsodine Schiff base complexes **1** and **2** will be discussed. The interaction studies with therapeutic targets, *ct*-DNA and *t*RNA was studied using complementary biophysical techniques. The corroborative results of binding experiments revealed that both complexes exhibit high propensity against *ct*-DNA (4.98×10^4 M^{-1} and 6.19×10^4 M^{-1}) as compared to *t*RNA (2.00×10^4 M^{-1} and 3.21×10^4 M^{-1}), attenuating the effect of ligand scaffold on therapeutic potency of drug candidates. To gain mechanistic insight in the process of inhibition, DNA cleaving ability of complexes was evaluated by gel electrophoretic assay, the complexes were treated in presence of various activator and scavengers. The complexes and the ligand **SBL** were evaluated for the cytotoxicity response against four resistant cancer cell lines viz.,HeLa, MDA-MB-231, Hep-G2 and MIA-PA-CA-2 by SRB assay., both the complexes showed much enhanced potency as compared to ligand **SBL** against most of the tested cell lines, while complex **2** was more active than **1** towards resistant breast cancer cell line MDA-MB-231. All these studies reconfirmed that on complexation with copper, the therapeutic potency was enhanced multifold as compared to free organic Schiff base.

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IL-40

Investigations of Nucleobases towards development of prospective biomaterials

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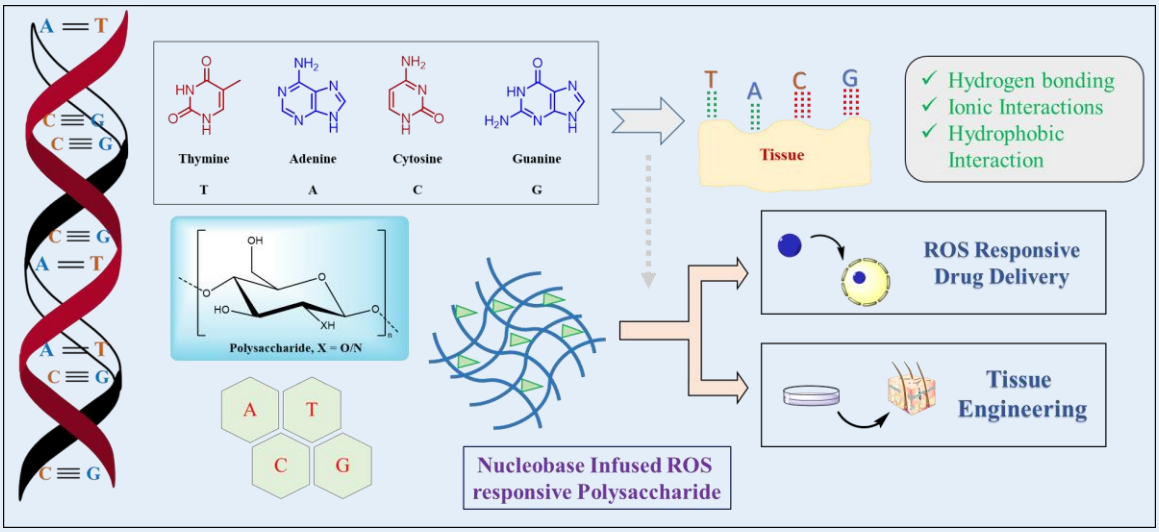
Chitosan is a naturally abundant polysaccharide polymer with wide applications in drug delivery and tissue enginnering. The polymer is having anti-bacterial, hemostatic and tissue adhesive properties. Incorporation of nucleobase and reactive oxygen species responsive (ROS) linker such as thioketal makes the polymer more attractive by infering mucoadhesion and degradation in inflamatory condition. For the first time, we have synthesized four set of polymers, which are conjugated with dithioketal (ROS responsive linker) and nucleobases (A, T, C and G Polymers that are conjugated with A, C and G have shown excellent anti-fungal activity *for Candida albicans, Candida tropicalis* along the anti-microbial properies. The modified polymers are cyto compatible (3T3 and Neuro-2) and hemo-compaticle. Therefore, these modified polymers have hold promise as interesting biomaterials for drug delivery and wound healing.



IL-41

Melanoma Immunotherapy by Nanosphere-Vaccine Elicited CD4+ and CD8+ T-Cell Response for Tumor Regression

Nagaprasad Puvvada*

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Cancer is attributable in part to defective immune surveillance or cancer-cell immune evasion. Solar radiation exposure and delayed diagnosis, amongst an increasingly older global population, is driving up the rate of morbidity and mortality of melanoma. Upon metastasizing, melanoma garners rapid lymphangiogenic and immunosuppressive features that limit effective eradication. Reengaging endogenous immunoreactivity to detect and eradicate metastatic melanoma, even as part of surgical or chemotherapy standard care is a priority to prevent relapse and improve survival.

Here we show that a formulation of lipid-coated glucose nanospheres (LGNP), decorated with ovalbumin (OVA), and containing pCMV-MART-1(MT-1): 'the nLOM vaccine' was capable of eliciting reduction and prevention of metastatic melanoma progression. The effectiveness of the nLOM vaccine was attributed to bone marrow dendritic cell (DC) maturation and specific immune responses by CD4/8+ T-cells targeting MT-1/OVA of melanoma by protected and enhanced antigen presentation via endosomal escape. A resistance to metastasis and direct immunotherapeutic regression of tumor growth was achieved preclinically using orthotopic subcutaneous murine B16-F10 melanoma cells in female C57BL/6J mice. Lymphatic nodes showed robust responses, with elevated cytokines and populations of DCs, MHCII+, CD11c+, and CD4/8+ helper/killer T-cells by cytometry. Tumors were fully penetrated by immunogenic cells with no off-target autoantigenicity nor toxicity in recipients, while melanoma cells were being eradicated. The application of the nLOM vaccine can elicit immunogenicity against metastatic melanoma by enhanced antigen presentation from mature DCs and could be developed for clinical use as immunotherapy.

Keywords: Adjuvant, Immunomodulation, Malignant, Chemotherapy, Autophagy

IL-42

Development of novel theranostic agents for Alzheimer's disease

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Abstract

Alzheimer's disease (AD) is a brain related neurological disorder characterized by gradual loss in memory along with other peripheral and central symptoms. The currently available treatments for AD provide only symptomatic relief without addressing the pathological hallmarks of the disease, therefore, neurodegeneration continues with these therapies.

The development of another series of diagnostic and theranostic probes is also inspired on nature product. The lead probe molecules have shown promising and selective Aβ aggregation detection ability in different AD models including transgenic AD mice model and AD patient autopsy samples. The unique ocular imaging pattern in the AD Drosophila model, strongly suggest that probes hold promise as a dependable indicator for rapid, noninvasive assessment of new therapeutic modulators or inhibitors in AD.

Acknowledgment:(SERB-CRG/2018/007126), the Indian Council of Medical Research (ICMR/EMR/2019-3088), (ICMR/ EMR/2021-10363), and the Indian Institute of Technology (BHU) (SM/2016 – 17/1198/L). GM also thanks Dr. Anita Mahadevan, Coordinator, Human Brain Bank (NIMHANS), for providing the autopsy tissue samples from clinically diagnosed AD patients.

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IL-43

Ubiquitin E3 ligase Pirh2 in Alzheimer's disease

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Pirh2 is an E3 ubiquitin ligase regulates the DNA damage responses through ubiquitylation of various signalling factors, which is one of the key pathological contributor of Alzheimer's disease (AD), therefore the role of Pirh2 was investigated in oligomer $A\beta_{1-42}$ induced rodent experimental model of AD. Augmented level of Pirh2 in AD conditions was observed and transient silencing of Pirh2 inhibited the disease-specific pathological markers like level of p-Tau, β-amyloid, acetylcholinesterase activity and the neuronal death. Biochemically, Pirh2 silencing attenuated the disease related oxidative stress, depleted mitochondrial membrane potential, cytochrome c translocation from mitochondria to cytosol and reinstated the reduced mitochondrial complex-I activity and ATP level. Pirh2 silencing inhibited the altered level of VDAC1, hsp75, hexokinase1, t-Bid, caspase-9 and apoptotic proteins (Bcl-2, Bax). MALDI-TOF/TOF, co-immunoprecipitation and UbcH13-linked ubiquitylation assay confirmed the interaction of Pirh2 with cytochrome c and role of Pirh2 in ubiquitylation of cytochrome-c, along with Pirh2-dependent altered proteasome activity. Additionally, Pirh2 silencing further inhibited the translocation of mitochondrion-specific endonuclease-G and apoptosis inducing factor to the nucleus and DNA damage. Findings suggested the significant role of Pirh2 in disease pathogenesis, predominantly through dysregulted mitochondrial physiology including translocation of cytochrome c, endonuclease-G and apoptosis inducing factor, along with biochemical alterations, DNA damage and neuronal apoptosis.

IL-44

In Silico Enabled Discovery of Potent, Selective and Brain-penetrant DLK Inhibitors for the Treatment of Neurodegenerative Diseases

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**Presenting*
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Dual leucine zipper kinase (DLK) (also known as MAP3K12) is a member of the mixed lineage kinase (MLK) family that contains an N-terminal kinase domain followed by two leucine zipper domains and a glycine/serine/proline rich C-terminal domain. It is expressed primarily in neuronal cells, specifically in the synaptic terminal and axon of neurons. Injury to neurons or other cellular stress leads to DLK dimerization, autophosphorylation, phosphorylation of MKK7 and JNK pathway activation. Recent work has demonstrated that genetic deletion or pharmacological inhibition of DLK results in attenuation of synapse loss, neuronal degeneration, and functional decline in models of both Alzheimer's Disease and Amyotrophic Lateral Sclerosis (ALS), making DLK an attractive therapeutic target for the treatment of neurodegenerative diseases.

The program execution leveraged Schrödinger's free energy perturbation (FEP+) technology to prospectively predict compound binding affinity to hDLK and prioritize design ideas that were either hand drawn or generated by AutoDesigner, our proprietary enumeration algorithm. In the Hit-Finding stage, starting from a minimal hinge binding fragment, monocyclic and bicyclic cores were modeled and evaluated by FEP+ using available DLK co-crystal structure. A focused set of ligands with favorable potency predictions were synthesized, resulting in the identification of multiple novel, nanomolar starting points within the first 2 months of program initiation. Further SAR exploration on the top cores by R-group enumeration allowed for the identification of the most promising lead series as well as multiple backup series. During the lead optimization stage, combining FEP+ technology and predictive ADMET modeling tools, including our recently published energy of solvation method for predicting Kp,uu, the team established an efficient work flow to mitigate multiple challenges such as CNS penetration, hERG inhibition, cytotoxicity and selectivity. This resulted in the identification of potent, selective and brain-penetrant dual leucine zipper kinase (DLK) inhibitors, which showed neuroprotective properties in *ex vivo* axon fragmentation assays and demonstrated dose-dependent p-c-Jun reduction in *in vivo* mouse cerebellum PD models.

IL-45

Computational Evaluation and Design of Novel FGFR Tyrosine Kinase Inhibitors

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Tyrosine kinase inhibitors are a specialized class of drugs transforming cancer treatment. FGFR (Fibroblast Growth Factor Receptor), a member of the receptor tyrosine kinase family, has been implicated in various alterations increasingly recognized as key molecular drivers of cholangiocarcinoma, a malignant tumor arising from bile duct epithelial cells.[1-2]

This presentation outlines a stepwise computational protocol to discover novel FGFR kinase inhibitors. The approach involves pharmacophore modeling, virtual screening, docking, ADMET analysis, molecular dynamics, and a knowledge-based structure-activity relationship (SAR) analysis. The study began with the ZINC 15 database, containing 120,314,868 compounds, and through various filtering steps, four potential inhibitors were identified. Molecular dynamics simulations and MM-GBSA binding free energy analysis confirmed the stability of these compounds within the FGFR protein matrix. Additionally, using insights from knowledge-based SAR and DFT-computed electrostatic potential surfaces, new inhibitor compounds were designed. The results of this work offer promising candidates as potential FGFR inhibitors for treating various cancers.[3]

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IL-46

Functionalized Fluorescent Probes for Diagnostics and Biomedical Applications

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Abstract

The use of small molecule organic fluorescent molecules as emissive materials has become a prominent research field in applied sciences and cutting-edge nanotechnologies. The importance of new efficient fluorescent organic dyes is realized due to their wide applications ranging from labeling of amino acids, peptides, proteins for bioimaging to nano crystal semiconductors and electroluminescent devices like organic light emitting devices (OLEDs). As the demand for fluorescent molecules continues to grow, the need to develop new methodologies for the rapid generation of highly fluorescent materials and evaluation of their optoelectronic and bioorganic properties have become an area of high importance.

Over the last few years, we have pioneered breakthrough innovation of basic building blocks (novel universal quencher and fluorescent dyes) for synthesis of TAQMAN-like probes, and alternate conjugation-chemistry, to develop complete RT-PCR kits for the detection of SARS-CoV-2 and its variants. Our patented platform technology[1] for a novel quencher 'UniQ' and fluorescent dyes was successfully demonstrated for the development of two qRT-PCR Diagnostic Kits INDICoV (SARS-CoV2) and INDICoV-Om (Omicron variant) and validated by the government agencies and institutions.

Furthermore, our group is engaged in the development of new fluorescent materials with absorption and emission at variety of wavelength for biomedical and diagnostics applications.[2] After thorough basic research, we have discovered a new nucleic acid staining dye GreenR to stain nucleic acids like genomic DNA, PCR products, plasmids and RNA. Our indigenous dye GreenR has been launched in the market in India[3]. Innovatively, we have designed and synthesized Donor-Acceptor based Teraryls, Fluoranthene (FLUN-550)[4] and Azafluorene[5] (AF-575) Dye for selective staining of cytoplasmic lipid droplets of 3T3-L1 pre-adipocytes as well as for selective staining of neutral lipid droplets of *Leishmania donovani* parasite and soil nematode C. elegans for live and fixed cell imaging applications. We have discovered[6] 'First' dual colorimetric-ratiometric fluorescent probe for selective and direct visualization of Labile Iron (III) pools in multicellular organisms (Soil nematode C. elegans). We have recently developed non-toxic biocompatible fluorescent nanomaterials Carbon Quantum Dots (CQDs) from Beetroot Extract for non-invasive in vivo Live Imaging in BALB/c Mice and for the FIRST time in C. elegans These results will be discussed during the presentation.

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IL-47

Exploring the Synergistic Potential of Phenol–Triazole Derivatives to Attenuate Aβ/ Cu^{2+}–Aβ Aggregation and Reactive Oxygen Species

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Alzheimer's disease (AD) is a neurological disorder characterized by a spectrum of symptoms such as memory loss and cognitive decline. AD is a multifaceted disease and designing multipotent ligands is an effective stratagem for AD treatment [1]. In this regard, the pharmacophore moiety of clioquinol (CQ, metal chelator) was employed to design the multifunctional phenol–triazole derivatives **4(a–p)**. In particular, **4k** with an *o*-I group on the phenyl ring was as efficient as curcumin in inhibiting Aβ_{42} aggregation (inhibition efficiency **4k**= 90.5%, IC_{50}= 6.51 ± 0.01 μM) (Fig. 1). Furthermore, **4k** significantly disassembled the preformed Aβ_{42} fibrils (Aβf, 92.5%), chelate Cu^{2+} ions, and inhibit Cu^{2+}–mediated Aβ_{42} aggregation. Compound **4k** ceases the production of reactive oxygen species (ROS) as it acts as an antioxidant due to the presence of a phenolic hydroxyl group. Compound **4k** has a sufficient safety–efficacy profile and alleviates the cytotoxicity by Aβ_{42} aggregates in SH–SY5Y cells. In addition, to study the modulation in the fibrillary architecture, hydrodynamic size, and structural transition of Aβ_{42} in the presence of **4k** we resorted to transmission electron microscopy (TEM), dynamic light scattering (DLS), and circular dichroism (CD), respectively. The molecular dynamics (MD) simulations depicted a notable reduction in the conformational transformations in Aβ_{42} monomer (Aβm) and Aβf on the incorporation of **4k**. Compound **4k** modulates Aβ_{42} fibrillation by maintaining helix conformation and simultaneously reduces the sampling of β–sheet structures in Aβm, consistent with the CD results. The MM-PBSA analysis depicted a favourable binding of **4k** to Aβm (–42.12 ± 7.14 kcal/mol) and Aβf (–74.42 ± 4.98 kcal/mol) with a significant contribution of van der Waals interactions to the binding free energy. The deformation in Aβf chains in the presence of **4k** as visualized in the conformational snapshots depicts the destabilization potential of **4k** against Aβf. Finally, our results uncovered the potential of phenol−triazole derivatives as a promiscuous ligand for targeting various pathological conditions in AD.

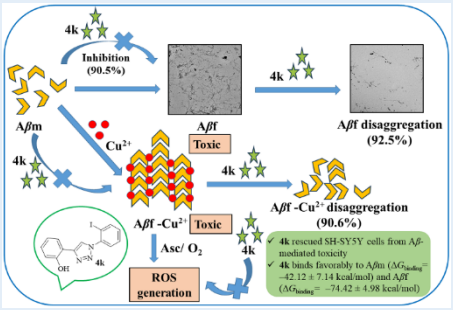

Figure 1: Combined experimental and computational studies in this work unveiled phenol–triazole derivative **4k** as a promising multitarget inhibitor of Aβ_{42} and Cu^{2+}-induced Aβ_{42} fibrillation as well as inhibiting the formation of ROS.

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IL-48

Longitudinal in vivo cationic contrast-enhanced computed tomography classifies equine articular cartilage injury and repair

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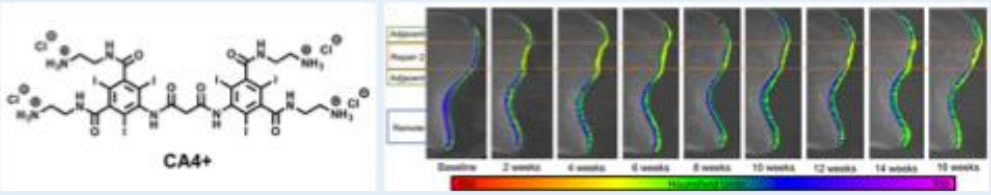
Abstract

Cationic contrast-enhanced computed tomography (CECT) capitalizes on increased contrast agent affinity to the charged proteoglycans in articular cartilage matrix to provide quantitative assessment of proteoglycan content with enhanced images. While high resolution microCT has demonstrated success, we investigate cationic CECT use in longitudinal in vivo imaging at clinical resolution. We hypothesize that repeated administration of CA4+ will have no adverse side effects or complications, and that sequential in vivo imaging assessments will distinguish articular cartilage repair tissue from early degenerative and healthy cartilage in critically sized chondral defects. In an established equine translational preclinical model, lameness and synovial effusion scores are similar to controls after repeated injections of CA4+ (eight injections over 16 weeks) compared to controls. Synovial fluid total protein, leukocyte concentration, and sGAG and PGE2 concentrations and articular cartilage and synovial membrane scores are also equivalent to controls. Longitudinal in vivo cationic CECT attenuation in repair tissue is significantly lower than peripheral to (adjacent) and distantly from defects (remote sites) by 4 weeks ($p < 0.001$), and this difference persists until 16 weeks. At the 6- and 8-week
time points, the adjacent locations exhibit significantly lower cationic CECT attenuation compared with the remote sites, reflecting peri-defect degeneration ($p<0.01$). Cationic CECT attenuation at clinical resolution significantly correlates with cationic CECT (microCT) ($r = 0.69$, $p < 0.0001$), sGAG ($r = 0.48$, $p < 0.0001$), and ICRS II histology score ($r=0.63$, $p < 0.0001$). In vivo cationic CECT imaging at clinical resolution distinguishes fibrous repair tissue from degenerative and healthy hyaline cartilage and correlates with molecular tissue properties of articular cartilage.



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IL-49

Perceptions of Scientific Research and Strategies for mapping the Development of Academic Career

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Abstract:

Perceptions of scientific research and strategies will play a significant role in shaping the career of academicians/scientists in the global perception. Due to this, it is important to deal with this topic. A well-considered publication strategy can help maximize academic impact, support career development, and aid the production of an optimal portfolio of research outputs. For early career academics (ECAs), who are under growing pressure from higher education institutions for greater research output and publications, the adage "publish or perish" is still relevant. With the introduction of the National Education Policy - 2020 and the need for encouraging domestic citation, quality publications are considered to be the height of academic excellence. Research and publications are given utmost importance more than before. Over and above, the government incentivizes publication platforms/hosting for data storage to academic/research institutes. In today's globalized world, research publication strategy is equally crucial, which is why it is still the main topic of discussion on every academic platform. Researchers must write and publish high-quality research papers for a variety of reasons, prominent among them being the promotion of their academic careers and the advancement of empirical knowledge through the dissemination of research findings. Publications are also a gauge of the scholarly output required for advancement. Another reason is that most researchers become authorities in the field in which they work, and when they actively add to the literature and enhance the pool of empirical knowledge, their colleagues acknowledge and validate this expertise. The successful writing of the title, abstract, keywords, literature review, introduction, methods, results and discussion, conclusion, output of the major findings, and references are only a few of the significant components of publications that will be covered in this lecture. Researchers are finding difficulties encountering the issues of plagiarism which is a crucial factor for publishing as well, and this key issue will be discussed with several illustrations.

IL-50

Targeting hIAPP Fibrillation in Type 2 Diabetes by Rationally Designed Peptide Inhibitors: Insights from Molecular Dynamics and Experimental Studies

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The misfolding and aggregation of 37-residue neuropancreatic hormone hIAPP (human islet amyloid polypeptide) to cytotoxic aggregates has been implicated in the pathogenesis of T2D (type 2 diabetes) [1]. Scrocchi et al. identified a fragment peptide SNNFGA (residue 20-25) from the amyloidogenic core region (Ser20-Ser29) of hIAPP as a potential inhibitor of hIAPP fibrillation [2]. Continuing with our efforts to illuminate the inhibitory mechanism of various inhibitors against protein aggregation-derived diseases [3], a library of 863 hexapeptides based on SNNFGA has been computationally designed and evaluated for anti-aggregation activity against hIAPP fibrillation in this work (Figure 1). The MM-PBSA analysis depicted peptides TNNWPL, TQNWAP, and TQNWVP bind to hIAPP with higher affinity than SNNFGA. Notably, TQNWVP displays a more pronounced inhibition effect than other peptides due to its ability to block the conformational transformation of hIAPP from a random coil to aggregation-competent β-sheet conformation. The *in silico* assessment of ADMET values of designed peptides lie within the range for therapeutic candidates and the peptides display higher half-life than SNNFGA. To corroborate the computational findings, the peptides were evaluated for their potential to block hIAPP fibrillation using ThT fluorescence assay, DLS, and TEM. Among the synthesized peptides, TQNWVP exhibited the highest inhibitory activity (Inhibition=75%, IC_{50}=6.19 ± 0.31 μM) against hIAPP fibrillation consistent with the computational results. Importantly, DLS analysis confirmed that TQNWVP reduces the size of hIAPP aggregates. Peptides exhibited a satisfactory safety-efficacy profile and efficiently alleviated the hIAPP aggregates-induced cytotoxicity in human embryonic kidney HEK293 cells. The combined *in silico* and *in vitro* studies in this work identified a new peptide, TQNWVP, as an efficient modulator of hIAPP fibrillation. Furthermore, illumination of the inhibitory mechanism of SNNFGA and top hit peptides against hIAPP aggregation holds significant promise for future therapeutic interventions against hIAPP fibrillation in T2D.

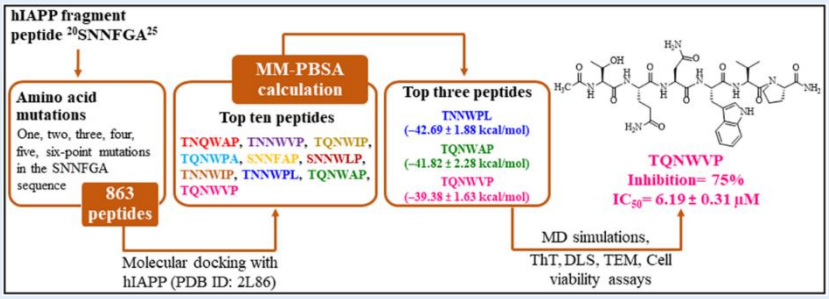

Figure 1: Procedural framework for the computational screening to identify inhibitors of hIAPP aggregation from the designed peptide library based on hIAPP fragment peptide SNNFGA.

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IL-51

Development of Recoverable Chiral Mn(III) Salen Complexes as Catalysts for Asymmetric Organic Transformations

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Metal catalyzed organic transformation is one of the important methods for the synthesis of bulk chemical, fine chemical and pharmaceutical intermediates. Transition metals salts and complexes are mostly used in the organic reactions for generation of the variety of valuable chemicals.[1] We have developed new chiral salen-Mn^{III} complexes **1a-c** and **2a-c** tagged with imidazolium based ionic liquids[2] and their catalytic activities were evaluated in the oxidative kinetic resolution of (±)-1-phenylethanol with *N*-bromosuccinimide (NBS) as an oxidizer in biphasic solvent system [H_2O - organic solvent (2: 1, v/v)] at 0 °C. We also synthesised new chiral Mn(III)-salen complexes **3a-e** and **4a-e** in excellent yields and evaluated in the asymmetric epoxidation of styrene by using NaOCl as an oxidant in ethyl acetate as a green solvent.[3a] The catalysts **3a-e** and **4a-e** were also evaluated in oxidative kinetic resolution of secondary alcohols. The Mn(III) salen complexes of Chiral Covalent Organic Frameworks **5** was synthesized and evaluated in the asymmetric epoxidation of non-functionalised alkenes in acetonitrile as solvent.[3b] The catalysts **1-4** were recovered and reused for oxidative kinetic resolution of 1-phenylethanol and catalysts **1** and **5** were recovered and reused for asymmetric epoxidation of styrene.

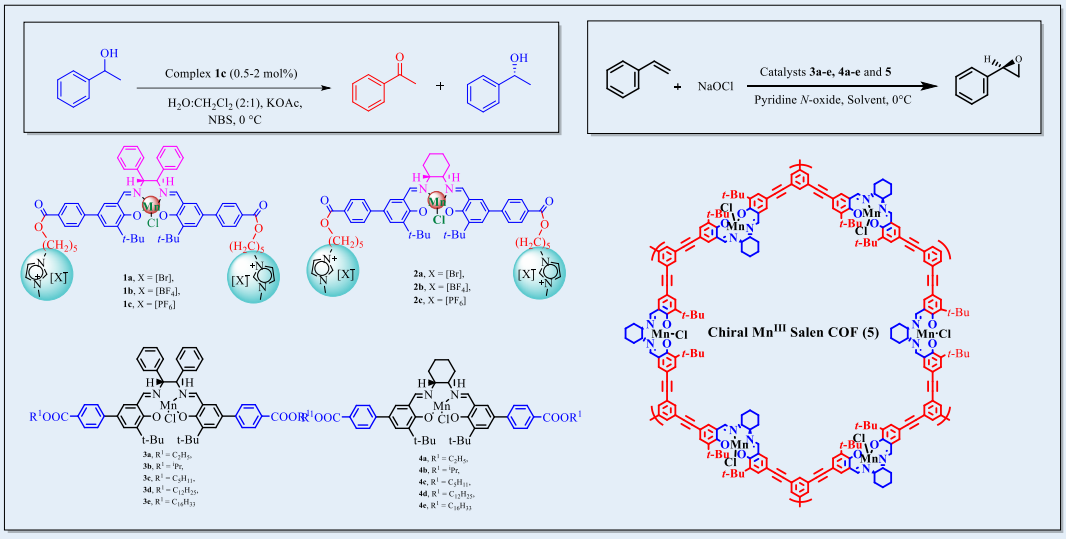

Figure: Chiral Mn (III) Salen complexes for asymmetric oxidation reactions

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IL-52

Exploring Flavour and Fragrance Chemistry in the UK Chemical Industry

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In the UK chemical industry, flavour and fragrance chemistry stands at the intersection of creativity and technical precision. As an organic chemist play a pivotal role, synthesizing novel molecules that meet specific olfactory or taste criteria while adhering to stringent budgetary and project requirements. This process demands expertise in a range of reactions, careful evaluation of each project stage, and close collaboration with various departments to ensure that every formulation aligns with regulatory and consumer standards. Integral to this field is a commitment to health, safety, and regulatory compliance, highlighted by rigorous documentation, such as the Control of Substances Hazardous to Health (COSHH) forms, which assess and mitigate risks associated with chemical exposure. Health and safety protocols are paramount, ensuring that both lab and production environments adhere to industry standards and safeguard personnel. Effective cross-departmental communication spanning Research and Development, Quality Control, Production, and Kilo Labs supports both the troubleshooting of scale-up issues and the seamless transition from laboratory synthesis to large-scale production. By continually reviewing data and producing regular progress reports, chemists contribute to a cohesive, safety-conscious, and innovative environment that drives the development of distinctive flavours and fragrances, supporting the UK chemical industry's reputation for quality and innovation.

IL-53

Development of Phytopharmaceuticals from the Indian Medicinal Plants

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Over 80% of the world population rely on herbal medicine for primary health care. FDA approved new molecular entities also have a large number of contributions from natural products. India is rich in biodiversity has its own traditional medicine system like Ayurveda, Siddha, Unani etc. which uses plants as such or in combination for the treatment of various diseases. These systems rely on traditional knowledge and not much validated by modern scientific studies. Well studied botanical-based drugs like Guggul tablets (for treatment of hypercholesterolemia), *Gingko biloba* tablets (to treat temporary loss of memory), and Silymarin capsules (to treat liver disorders) had taken more than a decade to convince the authority for their approval as drugs by the Central Drugs Standard Control Organization (CDSCO), as there are no provisions for botanical-based drugs in Drugs and Cosmetics Act 1940 and Rules 1945.

The Government of India published a draft amendment to the D&C Act and Rules on 24th October 2013 to add Phytopharmaceutical drugs as a separate category and these new rules came into force on 30th November, 2015 after their publication in the Official Gazette and opened the new dimension to plant based drug discovery will be discussed.

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IL-54

Highly efficient synthetic strategies for bioactive heterocyclic molecules

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The remarkable ability of heterocyclic nuclei has largely contributed to improve the lives of human beings. Though the heterocyclic molecules present in nature are large in numbers, their amount is not sufficient to fulfill the requirements of the overcrowded world of increasing demands. Therefore, the synthetic chemical community has been under increased pressure to produce these myriad of substances following efficient as well as greener synthetic strategies.

The diverse nature of the world of chemical synthesis requires various greener synthetic pathways in our quest towards attaining sustainability. One of the thrust areas for achieving this target is to explore alternative efficient reaction conditions to accomplish the desired chemical transformations with minimized by-products or waste and without the use of conventional volatile organic solvents, wherever possible. Consequently, several newer synthetic strategies have been appeared, such as reactions in greener solvents like water, reactions under solvent-free (dry media) conditions, mechanochemical mixing (grinding), use of solid-supported reagents. Apart from this, utilization of alternate heating and activation methods that employ microwave (MW) and ultrasonic irradiations for the rapid syntheses of organic molecules are also prominent. Availability of these efficient and greener synthetic alternatives, encourage us to explore its applications for achieving large number of organic transformations.

In consideration of the ever increasing biological/pharmaceutical significance of bioactive heterocyclic molecules, there is a need to continue the research for the development of these heterocyclic moieties by developing highly efficient and environmentally benign protocols. From the view point of sustainability, attempts should also be directed towards the exploitation of catalytic applications of easily available and inexpensive reagents for the synthesis of such bioactive heterocyclic molecules.

IL-55

Current Trends of the Search of New Pharmacologically Active Leads from Medicinal Plants

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Drugs derived from plants are biocompatible and generally considered safe compared to synthetic therapeutic agents [1] of diverse activities. Discovery of drugs from medicinal plants continues to provide new and important leads against various pharmacological targets including cancer, HIV/AIDS, Alzheimer's, malaria, and pain. Several natural product drugs of plant origin have either recently been introduced to the United States market, including arteether, galantamine, nitisinone, and tiotropium, or are currently involved in last phase clinical trials. . Lead bioactive molecules obtained from plants have structural diversity and used for the development of new future drug candidates. Due to the increasing of drug resistant strains in parasitic area search of new therapeutic agents are urgently needed. Keeping in view the importance of medicinal plants in the discovery new drugs and our continuous work [1-3] and effort to search the new leads in parasitic area, recently, in our laboratory we have isolated and identified the many bioactive lead molecules from medicinal plants by using various separations and spectral techniques. In this presentation, current trends of the search of new pharmacologically active leads from medicinal plants will be discussed in detailed.

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IL-56

Modification and Construction of Late-Stage Drug Candidates *via* C–H bond Functionalization and Annulation

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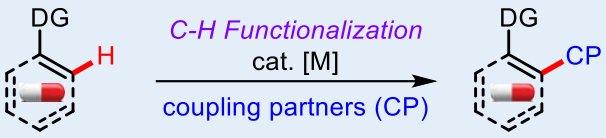
The area of synthetic organic chemistry contributing a key role to hit compounds identification, modification and the construction of late-stage drug candidates. Late-stage modification of drug scaffolds and bioactive compounds have garnered significant interest due to its ability to introduce diverse elements into bioactive compounds promptly. In this context, from last decades, great efforts have been made towards the modification and the construction of late-stage drug candidates via transition-metal-catalyzed and transition-metal free C–H bonds functionalization of various hetero(arenes) as well as a range of drug candidates with various coupling partners. In particular, the direct addition of C–H bonds to π-unsaturates C–X multiple bonds represent a valuable pursuit with profound synthetic potentials for the establishment of N, S, O, and halogens based functional groups into the molecules. In this addition, various groups such as amide, amine, aldehydes, ester, ketone, azo, acids, imines, and etc. not only represent key structural motif found in many natural products, pharmaceuticals, polymers, and biological systems, but they also find application as crucial intermediates for the preparation of various useful compounds and efficiently play the role of directing groups (DG), which coupled with various π-unsaturates to afford the corresponding late-stage drug candidates.

Herein, I will present a brief summary of my research work targeted to the transition-metal-catalyzed and transition-metal free C–H bonds functionalization and annulation of various hetero(arenes) to afford the corresponding late-stage drug candidates. Ultimately, I hope my research work would serve as a valuable resource, facilitating the application of late-stage modification in the construction of novel molecules and inspiring innovative concepts for designing and building of new drugs to the pharmaceutical industries and academia.



IL-57

Amerian Chemical Society

Abstract Awaited

IL-58

Sanjeev Kumar Shukla

Senior Principal Scientist (CSIR) and Professor (AcSIR), NMR Lab., SAIF&R Division, CSIR-Central Drug Research Institute, Lucknow, India

Abstract Awaited

IL-59

Toxic Turnaround: The Hidden Goodness of Poisonous Plants

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Toxic plants have long been recognized within ancient healing traditions such as Ayurveda, Siddha and Traditional Chinese medicine (TCM) as powerful curatives for chronic disease, and as life infusers and bioavailability enhancers (*Yogvah*i). The current presentation is aimed to highlight detoxification techniques and protocols of revered sages of India like *Charaka, Sushruta, Vagbhata* which are still seen to be practiced in exactitude form in present time in sync with green chemistry approach. Even more exciting, we will explore some innovative formulations developed by Plants Med Laboratories that utilized these toxic botanicals.

IL-60

Metal Free Porous Carbon Materials Based Electrocatalyst for Green Hydrogen Fuel Production

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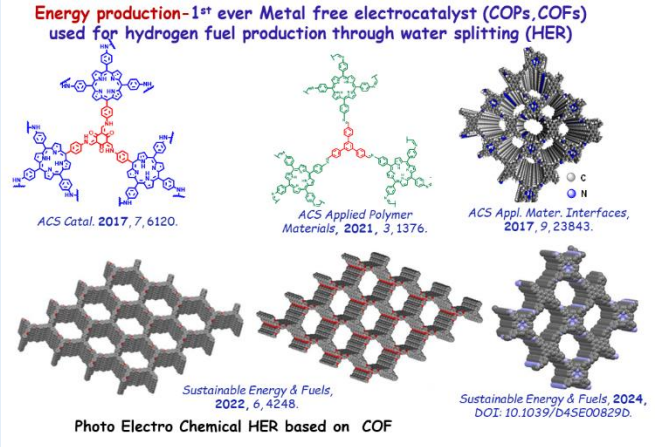
Due to the rise of global warming and climate change, people have started moving away from fossil fuels and leaning towards green, renewable solar and wind energy. Hydrogen, as a renewable and clean energy resource, is a promising future fuel. Hydrogen production through metal-free electrocatalyst water splitting is crucial for obtaining sustainable and clean fuel. Plentiful, economically viable, and easily processed materials are commercially important for green hydrogen production.[1-5] Herein, we are devoted to developing greener energy through the integration of chemistry and materials, optimal utilisation of carbon resources, chemical energy storage and conversion, and commercially viable low-cost carbon material preparation for energy production and storage applications.

Optoelectronic devices such as OLED, Photovoltaic devices, Nano-Graphene, Transistors, storage devices (battery), capacitors are advantageous for countries such as India whose infrastructure is in demand for easy to implement technology.



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IL-61

Design of Nanomaterials Towards Visible-Light-Induced Tandem Reactions

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A catalyst of renewable origin would be in accordance with the green chemistry principle. The polymeric graphitic carbon nitride (g-C_3N_4) has interested earth-abundant elements, which could be obtained by pyrolysis of nitrogen-rich containing precursors, *viz.*, urea, thiourea, cyanamide, dicyandiamide, trithiocyanuric acid, melamine, triazine and heptazine derivatives. Though g-C_3N_4 finds application as a photocatalyst, its photocatalytic behaviour is limited because of low efficiency, mainly due to rapid charge recombination. To overcome this problem, several strategies have been developed including doping of metal/non-metal in the cavity of g-C_3N_4. Metal-doped g-C_3N_4, especially Cu/Co@g-C_3N_4 shows extremely high catalytic activity for organic reactions along with its reusability. To design and develop new catalytic routes for chemical transformations with high activity and selectivity, which is benign to the environment would be most welcome. Due to eco-compatibility, easy availability, safe handling and everlasting abundance as non-conventional energy source for activation of reactions, visible light-induced synthetic strategies, especially photoredox catalysis, have emerged as state-of-art alternative of traditional conventional synthetic methods to advance the green chemistry program. Photoredox catalysis triggers the photo excitation of substrate through single-electron transfer (SET) mechanism and nowadays it has been widely used in organic synthesis. Thus, inexpensive visible light photocatalytic organic transformations have attracted much attention of synthetic chemists in these environmentally cautious days.

IL-62

Neutral, and monocationic forms of copper complex stabilized by redox-active thioether-appended tridentate *o*-aminophenol ligand

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Transition metal complexes with non-innocent ligands got the special attention from almost more than two decades because of the presence multielectron rich behaviour of non-innocent ligands. These metal-coordinated radicals are very important from the perspectives of bio-inorganic chemistry, especially as model systems of various biologically active metalloproteins involved in multifaceted redox reactions in the body.[1-3] From these perspectives we have initiated a program to synthesize and to determine the molecular and electronic structure of such metal-coordinated radical complexes using non-innocent ligands. In this continuing attempt, we have synthesized $[Cu(L)_2]$ using a potentially tridentate thioether appended *o*-aminophenol-based redox-active ligand in its deprotonated form and crystallized as $[Cu(L)_2]\cdot CH_2Cl_2$ ($1\cdot CH_2Cl_2$). Upon oxidation using a stoichiometric amount of $[Fe^{III}(\eta^5\text{-}C_5H_5)_2](PF_6)$, $1\cdot CH_2Cl_2$ yielded $[Cu(L)_2](PF_6)$ (2). Specifically, Structural analysis (100 K) reveals that $1\cdot CH_2Cl_2$ is a four-coordinate bis(iminosemiquinonato)copper(II) complex (CuN_2O_2 coordination), and that the thioethers remain uncoordinated. Crystallographic analysis of 2 both at 100 K and at 293 K reveals that it is effectively a four-coordinate complex with a CuN_2OS coordination. Density Functional Theory (DFT) at the B3LYP level and have attempted to assign the redox level of both the metal ion and the ligand.

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IL-63

Photo-triggered Oxidative Coupling of Indole and Active Methylene Compounds using Eosin Y as a Photocatalyst

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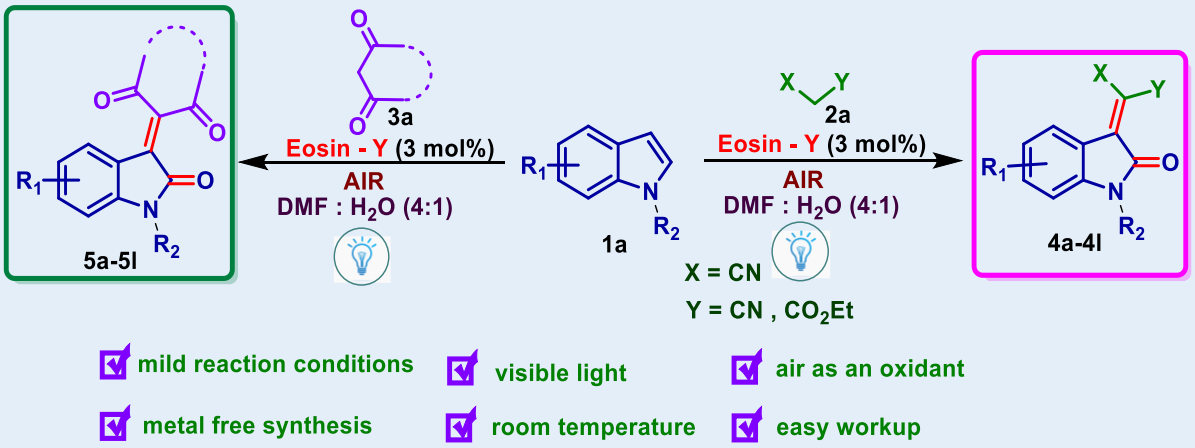
ABSTRACT:

A novel, efficient, mild, and inexpensive photocatalytic approach has been established for visible light initiated oxidative coupling of indole and active methylene compounds using atmospheric air and water as an oxidant in the presence of Eosin Y. An exciting result of our work is that only one molecule of malononitrile, ethyl acetoacetate, and dimedone reacts with one molecule of indole. In contrast, two molecules of barbituric acid react with one molecule of indole. The essential features of this approach are metal-free reaction, high yield of the products, no side product, and use of renewable energy sources.



IL-64

Synthesis and fabrication of metal-oxide nanoparticles & nanocomposites and their role in water remediation

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Green synthesis methods offer a cost-effective and environmentally friendly approach to producing nanoparticles (NPs), particularly metal-based oxides. Nanocomposites have received more attention due to their wide applications in different fields, like catalysts, sensors and other antimicrobial agents. The photocatalytic activity was also added to the utility of the synthesized environment-friendly nanoparticles and nanocomposites. In the textile industry, the most commonly used dye is MB. Textile industries generally discharge a huge amount of MB dye solution in natural water sources, becoming a health issue to humans, animals as well as aquatic life due to toxic and non-biodegradable nature of MB dye, which causes serious diseases such as respiratory distress, abdominal disorders, blindness, and digestive and mental disorders. Malachite green, a water-soluble dye, is another dye which used as an antifungal agent in ponds and lakes. It is cast-off in paper manufacturing, and in the cloth industry for dyeing silks and reported as carcinogenic substance, and can cause chromosome disorders, and skin diseases. In present article, synthesis of nanoparticles of Cu, Fe, La, Sb in their oxide form by various methods like Solvothermal process, Sol-gel method and others, has been discussed and their characterization has done with help of XRD, SET and TEM. The synthesized $LaFe_2O_3$ nanostructure degraded approximately 82% of the MG dye in 80 min only. The photocatalytic activity of $CuFe_2O_4$ NPs was examined against the MB dye, showing 82% degradation of dye under UV-visible light. The photocatalytic activity of B–CuO and B–CuO/rGO binary nanocomposite was tested for Methylene blue (MB) dye degradation under sunlight. The B–CuO/rGO binary nanocomposite exhibited improved photocatalytic competence (98%) as compared to B–CuO (85%) in 90 minutes. The photocatalytic activity of the Graphene Oxide Nanosheet was tested against methylene blue (MB) dye and 63% degradation was obtained in 60 min. a nanocomposite of lanthanum ferrite and antimony oxide heterojunction (LaFe2O3/Sb2O3) was synthesized by facile hydrothermal method for photocatalytic degradation of malachite green (MG) dye under the irradiation of visible light.
It was observed that the composite nanomaterials showed maximum response with 98% degradation of MG in 88 minutes.

Keywords: Metal-oxide nanoparticles, nanocomposite, photocatalytic degradation, methylene blue, malachite green

IL-65

Electrochemical & Paper-based Wearable Biosensor for the detection of Key Biomarkers: A Non-Invasive Point-of-Care

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Abstract:

Over the past decade, the development of electrochemical and paper-based analytical devices (ePADs) for real-time monitoring of important biomarkers has grown exponentially. ePADs offer miniaturisation and on-site capabilities to improve detection limits and selectivity of analytes of interest at the lowest cost. Many ingenious approaches have been used to fabricate ePADs for non-invasive monitoring of various biomarkers in human samples, such as tears, urine, sweat, and saliva. In our lab, we have designed and fabricated some electrochemical and paper-based sensors for measuring L-DOPA, dopamine, vitamin C, lactate, and pH in real human blood, sweat, urine, and tear samples. Our methods are simple, convenient, and cost-effective for easy quantification of the desired biomarkers. For electrochemical sensors, we used the glassy carbon electrode with a nanoparticle-modified surface to achieve high selectivity and specificity of analytes. For paper-based sensors, we developed and produced a unique chromogenic ink that is highly selective for lactate and pH in real human sweat. It was also very stable to variable temperature and pH conditions, which improved durability and colorimetric response compared to the non-functionalized ink. Our work will provide researchers with a logistical platform to work on early disease detection by monitoring several other biomarkers simultaneously.

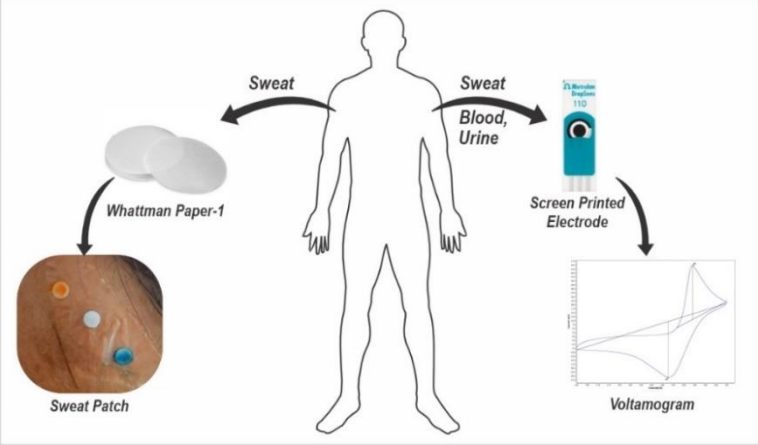

Figure 1: Design and fabrication of electrochemical and paper-based sensors

IL-66

Vanadia-Titania Catalyst system for versatile chemical transformation

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Abstract:

Novel green and sustainable processes to synthesize active pharmaceutical ingredients and key starting materials is a priority for the pharmaceutical industry. Further, the N-alkylation of amines with alcohols using earth-abundant and nonprecious metal catalysts are important for synthesis of range of pharmaceuticals. We have developed TiO_2 and heterogeneous and recyclable V_2O_5/TiO_2 catalyst system and have utilized them for versatile chemical transformation. TiO_2 catalyst have been used for the N-alkylation of amine. Heterogeneous V_2O_5/TiO_2 catalyst used for the oxidative cleavage of the olefins to furnish carboxylic acids. Under photo conditions V_2O_5/TiO_2 successfully utilized for the reduction of nitro compounds to furnish amines at ambient temperature.

IL-67

Chemical Tools to Study the Role of Inflammation in CancerPrognosis by Deep Tissue Imaging

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Abstract:

Small-molecule-based chemical designs are crucial for the development of activity-based sensing (ABS) probes. Unlike binding based probes, ABS probes can directly measure the activity of targeted enzymes or reactive biological analytes. Knowledge of the dynamic reactivities of the bio-analytes will be crucial in deciphering their molecular role in health and diseases. This will be useful in designing suitable diagnostics and treatment strategies. With this goal in mind, I will discuss our advancements towards development of selective imaging probes to study inflammatory responses in tumor microenvironment (TME) at the cellular level and *in vivo*. Thus, BL660-NO was successfully utilized to demonstrate for the first time at molecular level that changes in nitric oxide in TME with diet is responsible for poor prognosis of cancer Yadav et al [1]. Finally, we also developed a strategy to stabilize carboxylate esters from spontaneous and esterases mediated hydrolyses to utilize in ABS probe for hypoxia Yadav et al [2]. This technique will be useful in designing other ABS probes to enable NIR bioluminescence imaging as well as prodrug development for targeted and precise drug delivery by masking free carboxylates.

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IL-68

Synthetic Explorations of Triarylphosphine Based Reagents in Syntheses of Biologically Potent Scaffolds

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Abstract:

Triarylphosphine based reagents plays important role organic and inorganic synthesis and specifically in synthesis of biologically potent scaffolds, synthesis of organometallic complexes&in the generation of potential agrochemicals. Extensive synthetic explorations of these reagents have already been made by various researchers around the globe, through the involvement of a number of reactions such as Mitsunobu's reaction, Wittig reaction, Appel reaction, Deoxygenation, Sulphonation etc. & formation of complexes with transition metal complexes etc.

In search for potential scaffolds, our group have been synthesized various kinds of structurally diverse biologically potent scaffolds starting from various kinds of starting materials employing Triarylphosphine based reagents. In the present talk, I will be discussing some of our efficient and novel synthetic strategies for the syntheses of biologically potent scaffolds such as carbamates, dithiocarbamates, xanthates, *S,S*-dialkyl carbonates, trithiocarbonates, carbazates, dithiocarbazates, substituted ureas &α-amino nitriles employing triarylphosphine based reagents.

IL-69

Synthesis and Evaluation of Novel Heterocyclic Scaffolds as quorum Sensing Inhibitors and Possessing Antimicrobial Activity

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The rise of antibiotic-resistant bacteria and the prevalence of biofilm-associated illnesses present a substantial obstacle to contemporary medicine. This study presents the development and creation of new glyoxamide-based structures that exhibit strong abilities to prevent the formation of biofilms and combat microbial growth. The design of these chemicals was carefully aimed at targeting crucial bacterial activities that are essential in the creation and maintenance of biofilms. The synthesis utilized an efficient, sequential procedure to guarantee optimal production rates and purity levels. The effectiveness of the glyoxamides that were created was tested against several bacterial strains that are clinically important. The results showed that the glyoxamides were able to significantly suppress the development of both individual bacteria and the creation of biofilms. Moreover, these compounds demonstrated less toxicity towards cells, suggesting their suitability as promising candidates for therapeutic advancement. This study emphasizes the potential of glyoxamide scaffolds in addressing the pressing demand for novel antimicrobial drugs that can effectively combat both bacterial growth and biofilm-associated illnesses.
Rhizoctonia solani, a fungal pathogen, poses a substantial risk to worldwide agriculture, resulting in substantial crop damage. We have created a range of benzothiazole-appended bis-triazole structural isomers to address the demand for new antifungal medicines. These compounds were then tested for their ability to inhibit the growth of *R. solani*. The design technique entailed combining benzothiazole, which is recognized for its bioactive characteristics, with triazole rings to augment the effectiveness of the antifungal capabilities. By employing a methodical synthesis procedure, we acquired many structural isomers, each distinguished by distinct spatial configurations of the triazole units. The antifungal efficiency of these compounds was thoroughly evaluated, demonstrating that various isomers displayed potent inhibitory activity against *R. solani*. The investigation of structure-activity relationship (SAR) demonstrated that the effectiveness against fungal infections was strongly associated with specific isomeric configurations. The findings highlight the potential of benzothiazole-appended bis-triazoles as effective antifungal agents, providing new opportunities for controlling fungal diseases in agriculture.

IL-70

Development of Pteridine Derivatives as PI3K/mTOR Dual Inhibitors for the Treatment of Triple Negative Breast Cancer

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Abstract

The most common cancer in the globe by the end of 2024 will breast cancer, which had been diagnosed in approx. 8 million women in the previous years. One of the most prevalent gene mutations that significantly raise the risk of breast cancer is those in the BRCA1, BRCA2, and PALB-2 families of inherited "high penetrance" genomes. Triple-negative breast cancer (TNBC) makes up 20% of all breast cancers and is known for poor treatment outcomes. TNBC is identified by the absence of specific targetable abnormalities, such as the hormone epidermal growth factor receptor 2 (HER2). Breast cancer commonly involves genetic abnormalities that affect the PI3K/AKT/mTOR pathway across all subtypes. This pathway has been identified as a target for therapy in triple-negative breast cancer (TNBC). The pharmacophore models for PI3K and mTOR were developed as ADDRR_1 and DDHRR_1, respectively, and were used to screen the top five virtual hits. Further, 3D-QSAR study was conducted on pyridopyrimidine derivatives, which are dual inhibitors of PI3K and mTOR. The atom-based model exhibited high correlation coefficients (R^2=0.9886 & 0.9228) and standard deviation (SD=0.0871, 0.1871) for PI3K and mTOR, respectively, while the Field-based model also demonstrated high correlation coefficients (R^2=0.9589 & 0.9062) and standard deviation (SD=0.1692, 0.2710) for PI3K and mTOR, respectively. By using pharmacophore-based virtual screening and 3D-QSAR studies, novel 4-hydroxypteridin derivatives were designed with different substitutions that act as PI3K/mTOR dual inhibitors. These designed derivatives showed several interactions in molecular docking when compared to the co-crystal ligand and PI3K/mTOR inhibitor Dactolisib. The docking scores were -9.575 kcal/mol and -9.675 kcal/mol for PI3K and mTOR, respectively for the best-docked molecule, and its stability within a confined pocket was finally evaluated by a 100 ns molecular dynamic (MD) simulation. Therefore, the pharmacophore hypothesis, 3D-QSAR analysis, docking, MD simulation, and QikProp ADME predictions reported in the current study could be helpful for the establishment of various potential pteridine analogues. To treat triple-negative breast cancer, we anticipate that our research will contribute to developing new, effective, yet safe dual PI3K/AKT/mTOR inhibitors.

IL-71

Engineered PAMAM Dendrimer for Delivery of Bio-actives

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Dendrimers, as well-defined and highly branched macromolecules, offer significant potential in drug delivery due to their multifunctionality and specific architecture. Polyamidoamine (PAMAM) dendrimers, comprising a central core, radially extending repeating units, and terminal functional groups, are particularly notable. Dendrimers are promising candidates for designing colloidal drug delivery systems through interactions with anionic surfactants. This study aims to explore the physicochemical properties of colloidal PAMAM/fatty acid complex systems and assess their suitability for sustained drug release.. The research focuses on optimizing PAMAM/fatty acid complexes as vectors, exemplifying efforts in pharmaceutical research to develop dendrimer-based supramolecular delivery systems. The optimized formulation of PAMAM dendrimer and fatty acid nanoparticles was prepared and evaluated for drug entrapment, in-vitro release, and in-vivo studies, demonstrating the potential for controlled delivery of bioactive agents. The formation of PAMAM dendrimer-fatty acid complexes involves the interaction between the dendrimer and fatty acid molecules. This interaction may be driven by various forces, such as hydrogen bonding, hydrophobic interactions, and electrostatic interactions. PAMAM dendrimer-fatty acid complexes represent a versatile and promising platform for the delivery of bioactive compounds. Their ability to enhance solubility, stability, and targeted delivery of therapeutic agents makes them attractive candidates for a wide range of biomedical applications.

IL-72

Role of Bio-Fabrication/Bio-conjugation of Metal Nanoparticles for Novel Therapeutic Approaches

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Nanotechnology is an emerging field of applied science delivering crucial interventions in the biomedical applications. Green synthesis-based metal nanoparticles have received greater attention due to their unique physicochemical properties [1,2]. Natural biogenic nanoparticles have gained popularity recently because of their advantageous effects on the environment and human health. It is possible to produce nanoparticles using various natural products. Green synthesis method is suitable approach for creating nanoparticles with greater stability, clinical adaptability, and biocompatibility [3]. In this context, carbohydrates have attracted extensive attention in the fields of biomedicine and materials due to their unique biocompatibility, biodegradability, and multifunctionality. Among them, the fusion of functional nanoparticles and carbohydrates not only effectively improves the performance, but also expands the related application fields. As one of the most abundant biomolecules in nature, bioconjugation of carbohydrates have shown significant roles in the treatment of various human diseases. Among them, structural polysaccharides and heteropolysaccharides have a long history of application in pharmaceutical science and are used as immunomodulators, anti-tumor adjuvant drugs, and anti-inflammatory drugs. Furthermore, different types of monosaccharides and polysaccharides are of great interest to researchers due to their diverse applications in nanotechnology.

Keywords: Green synthesis, Carbohydrates, Bio fabrication, Natural Products

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IL-73

Arsenic fractionation in paddy field soil in relation to physico-chemistry of rhizosphere

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Arsenic (As) pollution in paddy field through geogenically contaminated irrigation water is a big challenge in many countries. Soil physico-chemistry is crucial in As accumulation in soil as well as its release in soil solution. To assess potential toxic effect of As on crops and to humans it is essential to determine the availability of As in soil solution. In this study, fractionation of As was performed in As contaminated paddy field soils from Uttar Pradesh i.e. Middle Ganga Plain (MGP) and West Bengal i.e. Lower Ganga Plain (LGP) and analyzed in relation to soil properties. The percent of total As extracted was 0.87 to 6.5% as water soluble, 0.13 to 4.8% exchangeable, 6.8 to 14% specifically sorbed and 11 to 21% As in amorphous Fe oxide associated. Most of the As (57 to 79 %) was found in crystalline Fe oxide and residual fraction i.e. incorporated in minerals. The concentration of As in soil and its release in different fractions was strongly correlated to the soil properties. A high content of clay, Fe and Ca and low P and S seems the main factors for accumulation of As in soil of LGP. The primary causes of the more release of As, particularly in water soluble and amorphous Fe oxide associated As in soils of LGP, appeared to be high TOC and EC, and alkaline pH. Conversely, the soils of MGP were more sandy, low in TOC and OM, and have relatively higher level of available P and S causing more release of exchangeable and specifically sorbed As. Although amorphous Fe oxide was the primary As binding fraction in both soils, it would be a substantial source of accessible As in a reducing environment.

Key words: Arsenic, Arsenic Fractionation, Organic Carbon, Paddy Soil, Sequential Extraction

IL-74

Personalized Medicine: How Genomics is shaping the Future of Healthcare

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Abstract

Personalized medicine (PM) is an innovative and rapidly evolving field within the medical and healthcare sectors. It holds the promise of revolutionizing medical interventions by delivering targeted and effective therapeutic strategies, tailored to an individual's unique genomic, epigenomic, and proteomic profile. It aims to reach optimal therapeutics with minimal iatrogenic damage and medical expenses. It has been successfully implemented in oncology to characterize the heterogeneity of the disease, which plays a crucial role in guiding treatment strategies based on patients' genomic profiles and lifestyle factors. In India, we have unique opportunity to explore PM in public health because we have a large population with ethnic diversity and high burden of diseases. India is also working to make its presence in the field of PM by launching various initiatives. PM seems to be the way forward, but there are still challenges that we need to address, such as cost involved, ethics, security of the data, merger of various platforms to integrate data and also availability of trained manpower to manage the data and algorithms. Personalized medicine represents a major breakthrough in healthcare, offering the potential for improved outcomes and greater benefits for both patients and clinicians in the near future.

IL-75

Diazo Umpolung in Hypervalent Iodine Diazo Reagents

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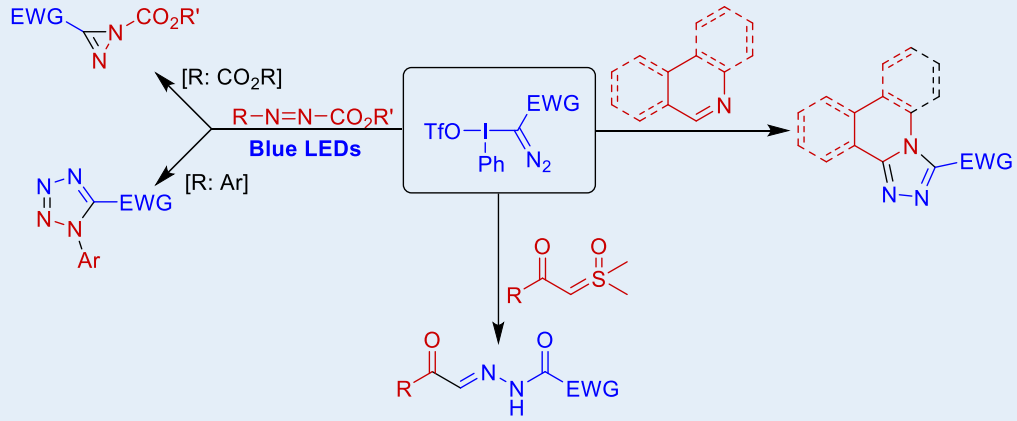
The diazo compounds are among the most valuable building blocks in organic chemistry due to their versatile reactivity pattern.[1] The inherent ambiphilicity of diazo group owing to the nucleophilic diazo-bearing carbon and electrophilic terminal nitrogen atom imparts unique reactivity to diazo-bearing compounds. However, installing a nucleofugal group on the diazo carbon as in Hypervalent Iodine Diazo Reagents (HIDR) **1** leads to the inversion or umpolung of the diazo-polarity. While the HIDR can be employed as electrophilic diazomethylating agents under thermal conditions,[2] they serve as the precursor of diazomethyl radical species under visible light photoredox catalyzed conditions.[3]

We utilized HIDR **1** for the electrophilic diazomethylation of several azaarenes **2** such as isoquinolines, pyridines and phenanthrenes followed by 1,5-cyclization of the resulting ammonium diazonium ylides to prepare corresponding 4,3-fused 1,2,4-triazolyl-azaarenes **3**.[4] On the other hand, nucleophilic attack on the terminal nitrogen of the HIDR by sulfoxonium ylides **4** led to the formation of hydrazineyl moiety-inserted products **5**.[5]

Further, trapping of diazomethyl radicals, generated from Hypervalent Iodine Diazo Reagents under photoredox conditions, with azocarboxylates **6** led to the divergent access to *1H*-diazirines **7** and 1H-tetrazoles **8** depending upon the substituents in the azo-substrate.[6] In the presentation, the observations and conclusions of the abovementioned transformations of Hypervalent Iodine Diazo Reagents will be discussed in detail.



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IL-76

Assignment of Structural Anomalies in Milk Oligosaccharides and their Interpretation by 2D NMR Experiments

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ABSTRACT

Milk oligosaccharides are known for their immunostimulant, brain development and anti-tubercular properties. Their stereoscopic structures are full of intricacies and diversities, caused due to presence of substituted groups at reducing centre and in monosaccharide rings. Mostly these are methoxy groups and substituted aromatic rings. Recently some of the oligosaccharides were isolated where the presence of furanose form of monosaccharides were present causing a rarity in the oligosaccharide structures. The main stereoscopic complexities that are resolved during the structure elucidation of oligosaccharide are configuration, conformation, position of glycosidic linkages and absolute configuration of the monosaccharide present in the constituent monosaccharides in oligosaccharides. All these interpretation along with spectral degeneracy caused by overlapping of ring protons may be sieved and interpreted by 2D NMR experiments. The presence of methoxy group at the reducing end may be fixed by HMBC experiments; position of NHAc group is defined by N-C HSQC experiment. Substitution of aromatic rings in the monosaccharide moiety was confirmed by combining the results of HSQC and HMBC experiments. The loss of cross peaks during the assignment of glycosidic linkages may be re-continued by Reverse HMBC experiments, supported by COSY, TOCSY, HSQC, HMBC, NOESY and C- N HSQC experiments of NMR. This presentation deals in detail with the use of HSQC experiments for confirming the chemical shift of H and C, removal of spectral degeneracy and sieving of ^{1}H signals by TOCSY, sequencing of protons by COSY experiments and use of HMBC and Reverse HMBC for confirming the glycosidic linkages in milk oligosaccharides.

Keywords: NMR, Spectral anomalies, Glycosides, Oligosaccharides

Acknowledgement: Author is thankful to Research and Development grant, Department of Higher Education, UP Government (2023-24) and the Head Department of Chemistry, University of Lucknow for NMR facilities.

IL-77

Enantioresolution of Chiral Pharmaceuticals via High-Performance Liquid Chromatography

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Abstract:

The distinct physiological and chemical properties of enantiomers within biological systems underscore the critical importance of enantiomeric purity in drug synthesis and development. In racemic drugs, enantiomers often display markedly different pharmacological effects, with one enantiomer typically exhibiting higher therapeutic efficacy, while the other may be inactive or potentially harmful. Liquid chromatography methods, particularly high-performance liquid chromatography (HPLC) and thin-layer chromatography (TLC), are widely used in determining enantiomeric purity due to their effectiveness and versatility. Recent research has focused on optimizing these techniques for chiral drug development, with an emphasis on selecting suitable chiral derivatizing reagents (CDRs) to enhance enantiomer separation and detection accuracy. CDRs based on compounds like DFDNB, cyanuric chloride, and naproxen exhibit high sensitivity due to their strong chromophoric properties, making them effective in creating detectable diastereomers. However, there remains significant scope for developing novel CDRs that offer even higher sensitivity and affordability for detection and enantioseparation, especially in pharmaceuticals marketed as racemic mixtures. The demand for such methods will persist until the synthesis of enantiomerically pure compounds becomes both economically feasible and widely adopted. Nevertheless, efficient and cost-effective analytical techniques for monitoring enantiomeric purity will continue to be essential in ensuring the safety and efficacy of chiral drugs.

Keywords: Chiral pharmaceuticals, Enantiomeric purity, Racemic drugs, High-Performance Liquid Chromatography, Chiral derivatizing reagents

IL-78

3D Printing of Formulations and Personalize Medicines

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Abstract

The coming desire for personalized medicines and medical devices has significantly accelerated the impact of alternate manufacturing in recent years. Personalized medicines begin a new route for developing specialized therapeutic formulations that consider an individual's genetic composition, medical history and physiology. Personalized medicines are fetching more popular as they allow the use of patient's genomics and hence help in better drug design with less or fewer side effects. In fact, various doses can be combined into one dosage form which attires the patient's demography. 3 Dimensional (3D) printing technologies for personalized medicine is a modern day treatment method based on genomics of patient. Three-dimensional printing has emerged as a revolutionary and potent tool for the precise manufacturing of custom dosage forms, tissue engineering, and disease modeling. The present accomplishments encompass multifunctional drug delivery systems featuring accelerated release characteristics, customizable and personalized dosage forms, implants and phantoms tailored to specific patient anatomies, in addition to cell-based materials for regenerative medicine. The currently developed techniques of 3D printing are succinctly outlined here. The attributes of printlets, specifically shape and size, are discussed in relation to the manufacturing of personalized dosage forms and medical devices. Current trends in 3D printing of formulation and precision medicines will be discussed.

Keywords: Personalize medicine, 3D Printing, alternate manufacturing, additive manufacturing, medical devices, genomics etc.

ORAL

O-1

Synthesis, Cytotoxicity Assessment, and Docking Analysis of N^{10}-Substituted Acridone Derivatives as Potential Anticancer Agents

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Mode of presentation: Podium
Presenting author: Ms Nilam Bhusare
Date of birth: 28/03/1998

Abstract

One of the most prominent issues facing the globe today is cancer. The number of drugs that are available for therapy is limited since the medication is ineffective at affecting drug resistance. This study focuses on the synthesis and evaluation of N-substituted acetamido derivatives of acridone, where the acetamido group is believed to serve as a crucial linker for the drug's anti-cancer efficacy Bhusare et al. [1]. *In silico* modeling of N-substituted acetamido derivatives was conducted using various software programs, including Biovia Discovery Studio 2024, Molecular Operating Environment (MOE), and Autodock Vina. Compounds displaying the necessary physicochemical properties and pharmacological similarities were selected for synthesis based on the in-silico analysis. A total of 24 derivatives (**AE1-12**, **AF1-12**) were proposed and synthesized, with their structures confirmed through spectroscopic techniques. Additionally, *in vitro* studies were carried out to predict their biological activity. Cytotoxicity assays were conducted to evaluate their effects against several cancer cell lines Yadav et al. [2] Molecular docking studies highlighted that the acridone derivatives are well-positioned in the active binding site of the target protein. According to *in silico* ADME studies, all synthesized compounds exhibited good oral bioavailability and low toxicity, making them promising candidates for further optimization in cancer treatment. Some derivatives showed encouraging results in cancer cell line assays, warranting further investigation into their specific targets. These findings will contribute to future research, offering new ideas, methods, and activities for improving cancer management and treatment Rozycha et al. [3].

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O-2

Synthesis of neohesperidose and naringenin from naringin.

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Abstract

Diglycosidase that transforms naringin into naringenin and neohesperidose, a rare biotransformation, has been purified to homogeneity using a simple procedure involving precipitation of the enzyme from the culture filtrate of the fungal strain. The purified enzyme gives single protein bands of molecular mass 64.6 kDa in SDS-PAGE analysis. Using naringin as the substrate. The specific activity of the purified enzyme using naringin as the natural substrate is 1.018 katal/kg. All results will show in presentation.

The feasibilities of preparing neohesperidose from naringin and rutinose from rutin on milligram scales using the pure enzyme have been demonstrated. These results open the way for developing an enzymatic process for preparation of neohesperidose from naringin. The reported diglycosidase has immense future applications in food and pharmaceutical industries.

Keywords: Disaccharides, Flavonoids, Glycones, Pharmaceuticals, Rhamnose-containing compounds.

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O-3

DESIGN, SYNTHESIS, MOLECULAR CHARACTERIZATION AND EVALUATION OF *IN VIVO* ANTITUMOUR ACTIVITY OF NOVEL OXADIAZOLE SCAFFOLDS

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ABSTRACT

The primary aim of the current research was to synthesize, characterize, and evaluate the in vivo antitumor activity of novel 2, 5-disubstituted 1, 3, 4-oxadiazole derivatives, Giedrute Mekuskiene et al [1]. Molecular docking studies were conducted using Auto Dock to assess binding affinity. *In vivo* antitumor efficacy was tested on HT-29 cell line-induced malignant ascites in a mouse model, A. Brishti et al [4]. Apoptosis in HT-29 cells was evaluated with Gimsa and H33342 staining, and apoptosis ratios were analyzed using flow cytometry with Annexin V-FITC/PI staining, Thummar VR et al [5]. Experimental results showed that the synthesized compounds (AB1-AB8) at a dose of 100 mg/kg significantly improved the post-treatment life span (PILS: percentage increase life span) of the mice, with PILS values ranging from 45.45% to 90.90%. In comparison, 5-FU increased PILS by 97.72%. The apoptosis ratios for the synthesized compounds varied from 24.1% to 63%, whereas the tumor control group showed only 6.1% apoptosis. Among the eight synthesized compounds, AB8 (63%), AB6 (59.2%), AB7=48.2% and AB3=43% induced the highest levels of apoptosis, outperforming the standard drug 5-FU (66.2%). Molecular docking studies revealed that the synthesized compounds exhibited high binding affinities towards the target protein Topoisomerase I, with binding energies ranging from 0.92 to -3.29 kcal/mol. This compares favorably to the standard drug topotecan, which had a binding energy of -2.06 kcal/mol. The data suggests that the novel 2, 5-disubstituted 1, 3, 4-oxadiazole derivatives effectively inhibit Topoisomerase I and exhibit significant antitumor potential.

Keywords: Antitumour activity; malignant ascites; apoptosis; flow cytometry and percentage increase life span etc.

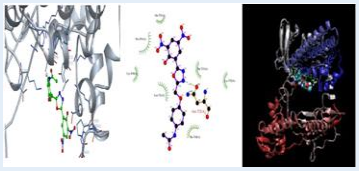

Fig-1: Molecular Docking studies

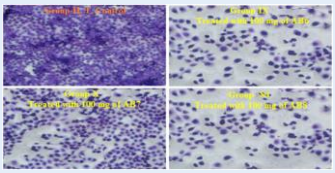

Fig-2: Morphological changes of HT-29 cells

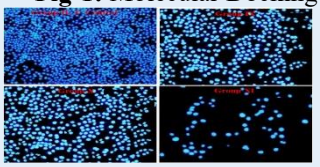

Fig-3: Morphological changes of HT-29 cells

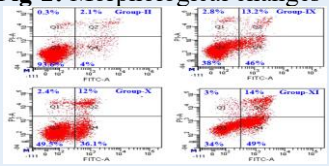

Fig-4: Apoptosis ratios analysis by FCM

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O-4

Evaluation of Protective Effect of C-Phycocyanin against L-Arginine induced Acute Pancreatitis

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Abstract

Acute pancreatitis is an inflammatory disease with high necrosis of acinar cells. The available treatment of pancreatitis is for symptomatic relief such as use of anti-inflammatory, surgical treatment, alcohol use abduction, fluid therapy to provide balance in the nutrient Sing Et al. [1] C-phycocyanin is a blue colored, bilin protein derived from algae spirulina platensis, with prominent anti-inflammatory, anti-oxidant and neuroprotective effect Romay et al. [2] The present study was designed with the aim to evaluate effect of C-phycocyanin against L-arginine induced acute pancreatitis and its mechanism of action.

Healthy male 36 SD rats were divided in 6 groups: Normal Control, Disease Control, Disease with Standard drug treated (indomethacin; 10mg/kg; I.P.), Disease Treated-1 (50mg/kg C-Phycocyanin), Disease Treated-2 (100mg/kg C-phycocyanin) and Disease Treated-3 (200mg/kg C-phycocyanin). Animals were induced acute pancreatitis with L-arginine (I.P.; 500mg/kg 1st day; 250mg/kg on 4th, 7th and 10th day) Dawra et al [3], C-phycocyanin was given to animals 30 mins before injection of L-arginine. After 14 days animals were sacrificed. Blood and pancreas were collected. Serum biochemical parameters such as amylase activity, lipase activity, SGPT, SGOT, inflammatory, oxidative stress and Nitrosative stress parameters, and histopathology were carried out. The results indicated improvements in physical, biochemical, oxidative and nitrosative stress parameters and histopathology due to C-phycocyanin treatment in a dose dependent manner. The beneficial effect of C-phycocyanin might be due to anti-oxidant, anti- Nitrosative and anti-inflammatory effect which was reflected as reduced necrosis of acinar cells. Future studies can be planned to explore molecular mechanism of C-phycocyanin as well as its effect in chronic pancreatitis.

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O-5

UNDERSTANDING THE MECHANISM, REACTIVITY AND SELECTIVITY OF GRIGNARD REAGENT MEDIATED [3+2] CYCLOADDITION REACTIONS FROM THE MOLECULAR ELECTRON DENSITY THEORY PERSPECTIVE

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Keywords: Cycloaddition, Molecular Electron Density Theory, Density Functional Theory, Selectivity

The [3+2] cycloaddition (32CA) reactions serve as one of the promising synthetic strategies for the regio- and stereochemical synthesis of several five membered heterocycles of pharmacological significance [1]. The mechanism, reactivity and selectivity of these reactions require special mention and has been studied in terms of diverse theoretical models. With the advent of advanced computational tools since the last two decades, the density functional theory (DFT) [2] has been successfully applied to predict and outline the mechanism, reactivity and selectivity of chemical reactions. The molecular electron density theory (MEDT) proposed by Domingo [3] in 2016 establishes that changes in electron density dictate the molecular reactivity by using diverse set of quantum chemical tools [4]. Herein, we present the application of MEDT to analyze the Grignard reagent mediated 32CA reactions leading to the generation of 1,5-disubstituted 1,2,3 triazole [5] and isoxazole derivatives [6]. The regioselective synthesis of 1,5-disubstiuted 1,2,3-triazoles takes place through a one-step mechanism, with the reduction of 2 kcalmol^{-1} in presence of Grignard reagent and total regioselectivity unlike the uncatalyzed process in complete agreement with the experimental findings. This computational model involves coordination of two ether molecules to the magnesium cation. For the 32CA reaction of mesitonitrile oxide to Baylis-Hilman adduct, the diastereoselectivity is reversed in the absence and the presence of Mg(II) cation and shows decrease in the activation Gibbs free energy by 3.1 kcalmol^{-1} for the Mg(II) mediated process as observed experimentally. Although the presence of Mg(II) cation shows unappreciable acceleration, remarkable change in regio- and stereoselectivity is observed in the Grignard mediated process for the studied reactions. The intertomic interactions at the located transition states have been studied by analysis of the Quantum Theory of atoms-in-molecules (QTAIM) parameters [7] and the non-covalent interaction (NCI) [8] plots, and the electron density changes along the reaction path and at the TSs have been predicted in terms of the topological analysis of the electron localization function (ELF) [9,10].

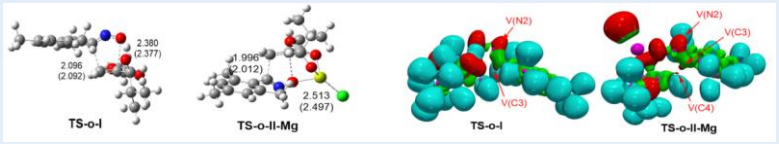

Fig. 1. Optimized geometries and ELF localization domains of the located TSs in absence and in presence of Mg(II) cation for the 32CA reaction of mesitonitrile oxide and Baylis-Hilman adduct

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O-6

Iridium-catalyzed Diacylmethylation of Tyrosine and its Peptides with Sulfoxonium Ylides.

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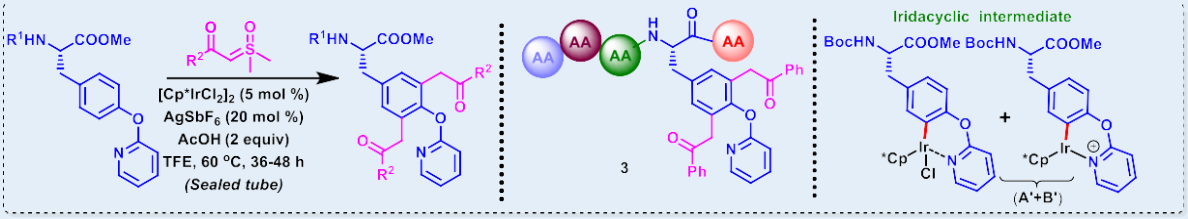
Unnatural amino acids (UAAs) prepared by site selective manipulation or conjugation of an amino acid with bioactive molecules have demonstrated remarkable applications in drug optimization and drug delivery studies. Such designer amino acids possess unique structural features that foster peptide interactions with biological targets, leading to the discovery of new therapeutic modalities.[1] Among all amino acids, tyrosine (Tyr) is a proteinogenic amino acid that is ubiquitous in both natural and synthetic bioactive molecules, including endomorphine, levothyroxine, KN-62, OF4949-I, mycocyclosin. In recent years, eminent scientists have intensified their efforts towards the selective functionalization of tyrosine and tyrosine-containing oligopeptides by employing a variety of directing groups (DGs), such as pyridyloxy, carbamate,[2-4] Interestingly, sulfoxonium ylides that are often employed for *o*-acylmethylation, and annulation of variedly decorated (hetero)arenes, have not been explored for the CAr-H acylmethylation of any aromatic amino acids. We have developed a Ir(III)- catalyzed strategy for C3Ar/C5Ar-difunctionalization of N-protected O-pyridyloxy tyrosines with electron-rich and deficient sulfoxonium ylides to furnish a series of diacylmethylated tyrosine-based unnatural amino acids in moderate-to-good yields.[5] The strategy was successfully employed for the late-stage difunctionalization of tyrosine-containing dipeptides, tripeptides, and tetrapeptides in reasonable reactivity. Isolation of a stable iridacyclic intermediate and the successful deprotection of the C- and N-side protecting groups are the added highlights of the presented work.



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O-7

Rhodium-Catalyzed Synthesis of Functionalized and Fused N-Arylphthalazinediones with Allyl Alcohols

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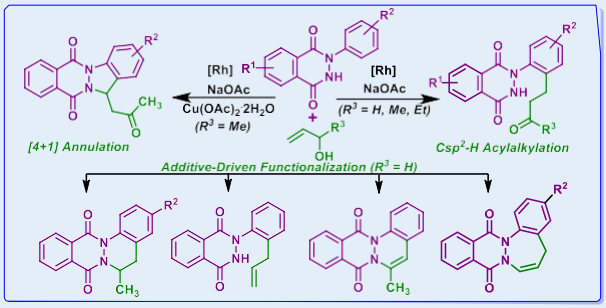
Abstract:

Transition phthalazine are ubiquitous diazaheterocycles found in a number of natural products, and established therapeutic drugs and exhibit diverse biological activities such as antitumor, anticonvulsant, antihypertensive, anti-inflammatory, cardiotonic, and antimicrobial activities[1].

Accordingly, focused efforts have been devoted towards the synthesis of aforementioned diazaheterocycles by conventional acid/base-mediated cyclization or multi-component reactions. In this regard *N*-aryl-2,3- dihydrophthalazine-1,4-diones creates more interest towards its synthesis with various coupling partners including isocyanates,[2] nitroolefins,[3] alkynes,[4] sulfoxonium ylides[5] , α-diazo compounds[6] 1,4-benzoquinones,[7] and diaryl iodonium salt[8] for the synthesis of indazolo-phthalazines by C-C and C-N bond coupling through transition metals such as Rh(III), Ru(II), Ir(I)[8].

We herein describe a Rh(III)-catalyzed C-H oxidative strategy for Csp2-H acylalkylation of N-aryl 2,3- dihydrophthalazine-1,4-diones with unsubstituted and substituted allyl alcohols. In addition, a [4+1] oxidative annulation of N-aryl -2,3-dihydrophthalazine-1,4-diones with but-3-en-2-ol was achieved by additionally employing Cu(OAc)2.2H2O as an oxidant in moderate reactivity. The substrate scope of N-aryl-2,3- dihydrophthalazine-1,4-diones as well as allyl alcohols were studied in detail.



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O-8

Potential Applications of Phytofabricated ZnO Nanoparticles

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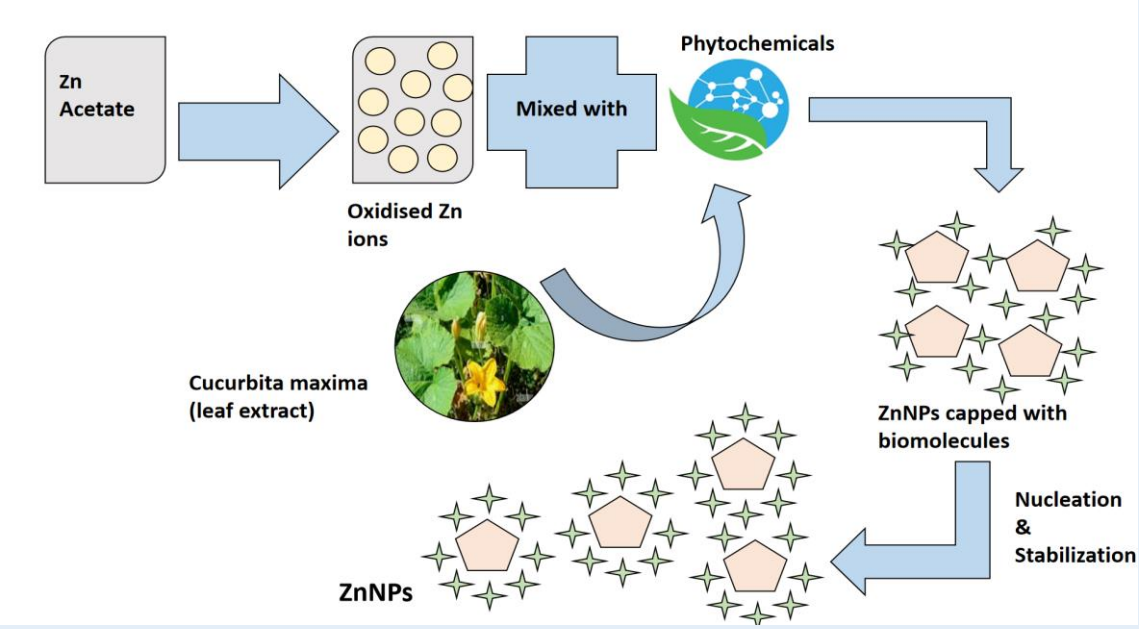
Abstract-

Nanotechnology is an integrative method of research that flourishingly hooks up with other branches of science as agriculture, biotechnology, engineering and medicine. Nanoparticles fabrication has also been shifted to green methods from chemical or physical synthesis. Non hazardous method of preparation and cost friendliness are two basic perks of green synthesis method. While approaching for green fabrication method, impact of phytochemical constituents is a bit critical. *Cucurbita maxima* is an edible species of Cucurbitaceae family and is very popularly been consumed in North India. This plant has also own antioxidant properties and plays vital role in preventing chronic heart diseases and cancer disease. Current research focuses on synthesizing Zinc oxide nanoparticles employing *Cucurbita maxima* leaves extract. Characterization methods like FTIR, SEM and others were involved to detect properties of synthesized nanoparticles. UV spectra was observed in range of 250-400 nm. FTIR data showed bands at 3298cm^{-1}, 2937cm^{-1}, 1409cm^{-1}, 1001cm^{-1}, 428cm^{-1}.

Keywords: Zinc Oxide Nanoparticles, *Cucurbita maxima* , FTIR, SEM, UV, Cucurbitaceae

GRAPHICAL ABSTRACT



O-9

"Exploring Bio-Responsive TMP Containing Nitrogen Heterocycles for Urinary Tract Infection Therapy"

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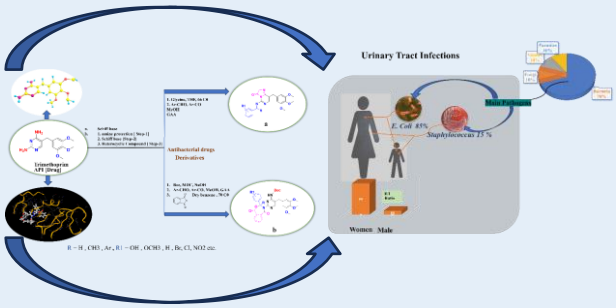
Abstract:

The most prevalent bacterial infection is a Urinary Tract Infection (UTI), accounting for 150–250 million cases annually. UTIs are prevalent infections, more commonly in women than in men, with an 8:1 ratio and affecting different age groups. The primary common cause of UTIs is bacteria but also infected fungi, viruses and parasites. Clinically, UTIs are classified as lower or upper urinary tract infections and are either uncomplicated or complicated. which can involve the kidney [pyelonephritis], ureters, bladder [cystitis] and urethra and are caused by gram-negative bacteria followed by gram-positive bacteria. Escherichia coli makes up 80%–85% of infection-causing bacterial species, while Staphylococcus species make up 10%–15%. UTIs are caused by uropathogenic E. coli (UPEC), which can be multidrug-resistant. this study investigates the synthesis and biological evaluation of bio-responsive nitrogen-containing heterocycles derived from trimethoprim (TMP) as potential therapeutic agents for UTI treatment. TMP, a well-known antibacterial agent, was chemically modified to incorporate nitrogen heterocycles, aiming to enhance its efficacy and selectivity against UTI-causing pathogens. The synthesized TMP derivatives were characterized using spectroscopic techniques and subjected to in vitro assays to assess their antimicrobial properties against common UTI pathogens. Several TMP-derived nitrogen heterocycles exhibited significant antibacterial activity, with minimum inhibitory concentrations (MICs) comparable to or better than standard UTI treatments. These results highlight the promise of TMP-derived as a novel class of UTI therapeutics. This research contributes to the development of targeted, responsive treatments for UTIs, providing a foundation for future advancements in infectious disease therapy.



Keywords: Urinary Tract Infection, *E. coli*, UTI Treatment, Trimethoprim Antibiotic Drugs, Structure-Activity Relationships (SARs), Multidrug Resistance (MDR).

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O-10

IDENTIFICATION OF POLLUTION TOLERANT PLANT SPECIES BY ANALYSIS OF MORPHOLOGICAL AND BIOCHEMICAL PARAMETERS IN THE DURGAPUR INDUSTRIAL REGION

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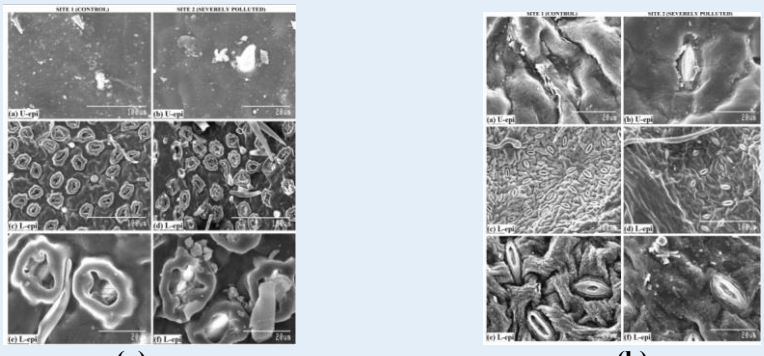
Keywords: Green belt, Morphology, Biochemistry, Air Pollution, Epicuticular wax

Physiological, biochemical, macro- and micro-morphological adaptations in plant species are evidenced in response to the changing environmental conditions [1]. The morphological and biochemical attributes of plant species can be analyzed as the bioindicators for air pollution assessment of a particular region. Herein, we present detailed analysis of a total of 21 morphological and biochemical parameters of two plant species *Ficus benghalensis (FIBE)* and *Terminalia arjuna (TEAR*) in two sites of Durgapur industrial region, designated as the control site and the severely polluted site respectively[2]. The variation of SO_2, NO_x and suspended particulate matter (SPM) in different regions have been studied and the intensity of air pollution assessed from the Air Pollution Index (API) [3], followed by cuticular, morphological and biochemical evaluation. Scanning Electron Microscopy (SEM) studies revealed different deposition patterns of the epicuticular wax. This study reveals that leaf length (LL), leaf breadth (LB), size of leaf (LS), stomatal length/stomatal breadth (SB/SL), Air Pollution Tolerance Index (APTI) [4], petiole length (PL), stomatal frequency (SF),amino acid (AA), pH, relative water content (RWC) and total soluble sugar (TSS) are the most affected variables of the studied plant species under air pollution stress. The predicted correlation was justified through Principal Component Analysis (PCA). This study can be applied for the development of an effective Green Belt as a control measure for air pollution in urban industrial regions.



(a) **(b)**

Fig. 1. (a) Comparative leaf cuticular study of *FIBE* in light air pollution and severely polluted sites. **(b)** Comparative leaf cuticular study of *TEAR* in light air pollution and severely polluted sites

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O-11

Development and Evaluation of Herbal Nano Formulation for Management of Eczema

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Eczema, also known as atopic dermatitis, is a persistent inflammatory skin disorder that is characterized by dry, itchy and inflammatory skin. Current treatments like topical corticosteroids, calcineurin inhibitors, immunosuppressants and anti-histamines have adverse effects like erythema, skin thinning, skin burning and hypertension and pharmacokinetic issue like low bioavailability, low solubility and low absorption.

There are many herbal drugs reported in ancient text for their usage in treatment of skin disorder like *Cuscuta* species, *Matricaria* species, *Rubia cordifolia*, *Bauhinia variegata*, *Hemidesmus indicus*, etc. Since herbal drugs are comparatively safer than synthetics drugs, have fewer side effects and are inexpensive it was thought worthwhile to explore the possibility of developing herbal nano formulation using such reported herbal drugs for the treatment of eczema. Nano-sized drug products can be employed at lower concentrations, have a faster onset of bioactivity and pharmacokinetic issues like low absorption, low solubility and low bioavailability can also be resolved.

After extensive literature review, *Cuscuta reflexa* plant was selected as it contained high amount of flavonoids and phenolics which are mainly responsible for the therapeutic effect in management of eczema. Hydroalcoholic extract of *Cuscuta reflexa* dried plant material was prepared by maceration technique. Total flavonoid content, total phenolic content, Apigenin and Quercetin content were determined in the herbal extract. Nanoemulgel of the extract was prepared and characterized for globule size, zeta potential, pH, viscosity, thermodynamic stability, drug content and *in-vitro* drug release study.

O-12

Integrating Allopathy with Herba and Phytomolecules: The Miraculous Benefits in Dealing with Multidrug-Resistant Infections

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ABSTRACT

Global health is facing a significant danger from the increasing prevalence of multidrug-resistant (MDR) infections, necessitating creative and comprehensive methods for treatment. Conventional Western medicine, known as allopathy, has traditionally been the primary approach to fighting infections using antibiotics. Nevertheless, the excessive and improper use of these antibiotics has resulted in the development of MDR bacteria strains. WHO identified the "dirty dozen," consisting of 12 human pathogenic bacteria urgently in need of novel antibiotics due to drug resistance and a lack of available treatments. These bacteria, including *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacteriaceae*, contribute to increased cost, duration, and severity of infections as a result of limited treatment options. The current rate of emergence and spread of anti-microbial resistance (AMR) is projected to result in over 10 million deaths by 2050, with an approximate annual economic burden of $100 trillion [1]. Notably, the present antibiotic pipeline is insufficient to meet current and foreseeable clinical needs. Several highly efficient antibiotics of the time have now become inactive due to the continuous rise in drug-resistant strains of pathogenic microbes.

Since the dawn of humanity, India has been a rich source of medicinal and aromatic plants and herbs utilized in countless medical operations. The field of Indian traditional medicine, known as "AYUSH," includes Ayurveda, Unani, Siddha, and folk (tribal) remedies. Referred to as the "Science of Life," Ayurveda is among the most ancient holistic healing systems globally and has its origins in India over 5,000 years ago. Recent research has shown that herbs, herbal extracts, or phytomolecules (generally named Bioenhancers), when coupled with an antibiotic, increase the drug's bioavailability and bioefficacy, reducing the dose [2], [3]. These bioenhancers promote the biological activity, bioavailability, or uptake of drugs when combined with a drug. In our studies, the extracts and phytomolecules have reduced the dose of antibiotics up to 512 folds [4]. Our research suggests that integrating allopathy with Ayurveda or traditional medicines may lead to miraculous benefits in dealing with multidrug-resistant infections, reducing the dose and cost burden on the common people.

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O-13

Hydrogen Bonding-Induced Unique Charge-Transfer Emission from Pyrenylated Terpyridine Derivative: Multifaceted Optical Sensing Applications

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Abstract

A multichromophoric pyrenylated terpyridine (Pytpy) conjugate has been synthesized and its emission behavior has thoroughly been investigated.[1-2] The twisted geometry of the probe molecules in both the solid state and aprotic solvents significantly curtails the electronic communication between the aryl moiety and pyridyl ligand. Since the excited-state hydrogen bonding interactions with methanol could result in the formation of a nearly planar conformation with larger charge separation, the probe could be utilized for the detection of methanol impurity in soy-based biodiesel samples.[3] At the same time, the probe showed formation of nanoscopic aggregates with distinct red-shifted emission maxima both in the aqueous medium and bilayer membrane.[4] The nature of the aggregates in bulk medium was found to be very distinct than that observed in bilayer membrane. This unique membrane-driven self-assembly of Pytpy was utilized for ratiometric probing of vesicle to micelle phase transition,[5] while the fluorescent nanoaggregates formed in the aqueous medium was utilized for selective detection of Cu^{2+} ions.[6]

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O-14

Design and synthesis of novel 1,3,4-oxadiazole based azaspirocycles catalyzed by NaI under mild condition and evaluated their antidiabetic and antibacterial activities

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Abstract

A modest, efficient, and mild synthetic procedure has been developed for the synthesis of novel series of 1,3,4-oxadiazole containing azaspirocycles derivatives.[1] The reaction of 1,3,4-oxadiazole derivative with diverse azaspiro compounds under room temperature condition with helps of sodium iodide catalyst and polar aprotic solvent. Numerous compensations of this strategy embrace less time required, yield increment, consumption of all reactants, and mild condition. All synthesized compounds evaluated for in vitro antidiabetic and antibacterial screening. Among them some compounds show significant biological response.

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O-15

Discovery of new classes of antimalarial compounds by targeting apicoplast Single-Stranded DNA binding protein of *Plasmodium falciparum*

Dhaneswar Prusty

Abstract

Resistance to frontline antimalarials by malaria parasites presents a significant challenge, necessitating the discovery of new antimalarial compounds that target novel drug targets. In this context, the Single-Stranded DNA Binding Protein (PfSSB) of Plasmodium falciparum stands out due to its crucial role in the DNA replication process of the apicoplast, an essential organelle for malaria parasite survival. We employed an integrative approach, combining computational, biochemical, and parasite growth inhibition studies, to search for potential inhibitors targeting PfSSB. Molecular docking, dynamics simulation, and ADMET prediction revealed that two compounds, PPG and 9-HPF, showed a strong binding affinity with the ssDNA binding pocket of PfSSB and exhibited favourable drug-likeness properties. In the gel retardation assay, both compounds disrupted the ssDNA binding property of PfSSB. Real-time bio-layer interferometry analysis confirmed the stronger binding affinity of 9-HPF with PfSSB. Additionally, PPG and 9-HPF effectively killed Plasmodium falciparum with an IC_{50} in the low micromolar range. Notably, the MTT assay demonstrated the non-cytotoxic effect of both compounds. A structural diversity investigation, utilising the Tanimoto coefficient (Tc) and distance matrix score, revealed that both compounds have distinct structures compared to existing known antimalarial drugs, reducing cross-resistance likelihood. In summary, this study has identified a new class of antimalarial compounds that can help to combat antimalarial drug resistance.

Keywords: Plasmodium falciparum, drug resistance, SSB, Molecular Docking and Dynamics, EMSA, Parasite growth inhibition

O-16

Discoveries in breast cancer treatment from molecular docking and in vitro studies of Adansonia digitata fruit pulp on the receptor tyrosine-protein kinase erbB-2 (ERBB2)

Afsheen Fatima

Abstract:

A significant challenge in pharmaceutical development is the safe distribution of medication. Because of their involvement in breast cancer cell development and progression, the receptor tyrosine-protein kinase erbB-2 has emerged as a promising therapeutic target for the disease. The fruit pulp extract of the *Adansonia digitata* tree has been found to contain a high concentration of phenolic compounds and to exhibit antioxidant properties. The fruits of the *Adansonia digitata* tree have a long history of medical use, which is believed to be due to the high polyphenol content of these fruits. Investigating how the bioactive components and antioxidant activity of baobab fruit pulp affect erbB-2 was the primary aim of the study. Bioactive compounds that potentially target erbB-2 were the focus of this in silico study. Using drug-likeness criteria from Lipinski's rule of five, 21 bioactive compounds derived from different plants were assessed for their potential as anticancer treatments targeting the receptor tyrosine-protein kinase erbB-2. Docking with the receptor tyrosine-protein kinase erbB-2 allowed phytochemicals to be studied. In order to determine their pharmacokinetic effects, ligands were further tested if they were drug-like and had binding energies comparable to those of traditional drugs. The phytochemicals found in this study had binding energies that were on par with those of traditional medications; more information about these compounds' efficacy as anticancer agents was gleaned from analyses of ADME, bioactivity score, and bioavailability radar.

Keywords: Molecular docking, ADMET, ERBB-2, *Adansonia digitata*, Breast cancer, Anticancer agent, Pharmacological property, Invitro analysis

O-17

Photo-oxygenation of Furan Tethered α-Azidoketones

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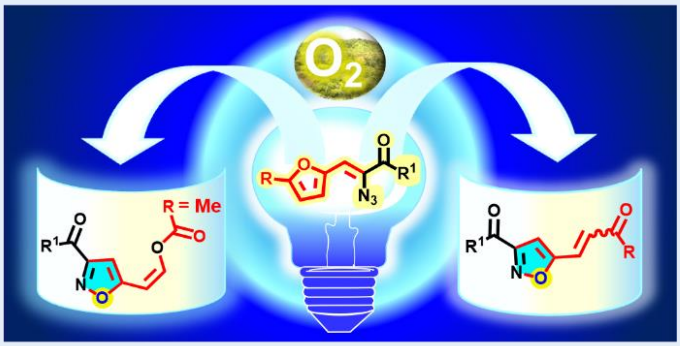
ABSTRACT:

Visible light-enabled photocatalyst-free direct oxygenation of furan-tethered α-azidoketones was studied. The reaction yielded a number of products depending on the substituents, with isoxazoles forming as the major products. The findings suggest that singlet oxygen was generated during the reaction and reacted with α-azidoketones in a [4+2] fashion to yield endoperoxides, which rearranged in multiple ways to generate isoxazoles.



O-18

A Facile and Regioselective Synthesis of Novel Colchicine Sulfoximine Analogues as Potent Tubulin Inhibitors

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Microtubule cytoskeletons are composed of α and β tubulin heterodimers [1]. They play key role in numerous biological functions such as intracellular transport of cellular components during interphase, developing the mitotic spindle throughout the cell division as well as maintaining the cell motility. For this reason, chemical agents that interfere with microtubule cytoskeleton functions are found to have broad spectrum of anticancer activity [2]. Colchicine binding site has been continuously attracting the attention of researchers and has become a dynamic area of research due to its better pharmacological properties, particularly its potent antimitotic effects, making colchicine a promising candidate for cancer treatment [3]. However, its clinical application is limited by inherent toxicity and the development of multidrug resistance. To overcome these challenges, extensive research has focused towards the structural modification of colchicine to reduce its adverse effects while maintaining its therapeutic efficacy [4]. The structural modifications of methoxy(C-10) and N-acetyl moieties along with incorporation of a halogen atom have been described to enhance molecular stability and tubulin-binding affinity [5]. In recent years, sulfoximines have emerged as a promising class of compounds in cancer therapy owing to their unique structural features and favorable pharmacokinetic properties, such as better solubility in protic solvents, and high stability [6]. The combination of colchicine and sulfoximine moieties offers an unique opportunity to develop novel colchicine derivative with potentially enhanced biological activities and therapeutic applications. As a part of our ongoing efforts to develop novel anticancer agents, in the present work, we successfully synthesized colchicine-sulfoximine derivatives by treating thiocolchicine with a combination of iodobenzenediacetate and ammonium carbamate high yields up to 87%. The synthesized colchicine derivatives exhibited a broad spectrum of cytotoxic and tubulin activity against tested cancer cell lines (with >80 % inhibition). Our findings suggest that colchicine analogues, particularly those combined with sulfoximine moieties, hold promise as potent anticancer agents. The synthesis and biological results of colchicine-sulfoximines will be delivered during the conference.

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O-19

Development and Validation of a Mass-Compatible RP-HPLC Method for Quantification of Berberine Hydrochloride in Plasma

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Berberine hydrochloride (BH) exhibits a broad spectrum of pharmacological activities, such as antibacterial, antiviral, antihypertensive, hypoglycaemic, antiarrhythmic, and anticancer effects. The study of its pharmacokinetics is essential for understanding its therapeutic potential and interactions in clinical settings. To facilitate this, a robust and mass compatible reverse phase high-performance liquid chromatography method with UV detection was developed and fully validated for estimation of Berberine hydrochloride in human plasma. Dimethylamino benzaldehyde was employed as an internal standard, and Liquid-Liquid Extraction (LLE) was optimized for efficient sample clean-up, achieving high extraction efficiency and minimizing matrix effects. Chromatographic separation was achieved with Phenomenex C18 column (250 x 4.6, 5 µm) with a mobile phase composed of ACN: 10 mM Ammonium acetate buffer (40:60, v/v), adjusted to pH 3.5 with formic acid, at a flow rate of 1.0 mL/min and detection at 350 nm. The method was validated in compliance with US-FDA guidelines for selectivity, recovery, accuracy, precision, matrix effect, dilution integrity and stability. The analyte demonstrated extraction recovery above 85%, with reproducible and consistent results. Stability studies confirmed the long-term stability of the samples, ensuring reliability from collection through analysis. The validated RP-HPLC/UV method is mass compatible and adaptable for LC-MS/MS applications. It offers a valuable tool for pharmacokinetic studies, therapeutic drug monitoring, and investigating drug-drug interactions, supporting future clinical applications of Berberine hydrochloride.

O-20

A short and efficient Synthesis of Piperidine and Azepane ring from the Ring expansion of Aziridine

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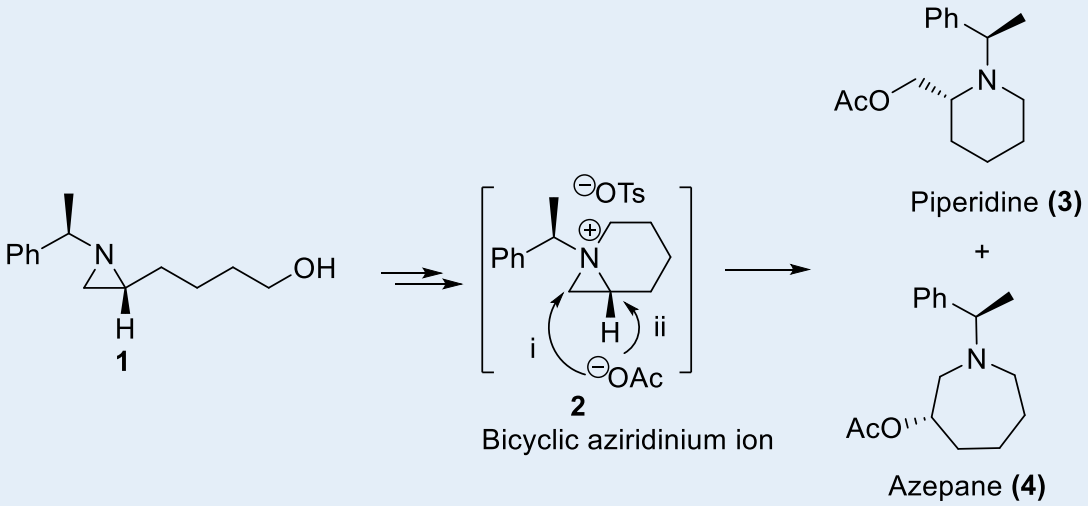
Abstract:

Ring expansion of substituted aziridine (1) via the formation of bicyclic aziridinium (2) resulted the ring expanded products piperidine and azepane in good yields. The ring openings of bicyclic aziridinum ion with several nucleophiles proceeded in highly regio- and stereoselective manner with release of the ring-strain of the three-member aziridine ring through the breakage of either C-N bond. This ring expansion apprach of aziridine provides a short route for asymmetric synthesis of biologically active natural alkaloid such as *R*-Pipecolic acid.

Keywords: Aziridine, Ring expansion, Piperidine, Azepane, Ring strain



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O-21

Stability study of Aspirin tablet in crush condition stored in glass and plastic container by using the Reverse Phase High Performance Liquid Chromatography.

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Abstract:

The objective of the present to research work is to provide the detailed analytical stability study of anti-inflammatory drug product i.e. Aspirin tablet on its different physical condition and storage container. In crush condition the surface area of drug product increased which lead to increase in impurity levels. And by using the different storage container, compatibility of packaging materials can be evaluated. Aspirin is available in the form of tablet with aluminium wrapped blister pack. In this study, tablets were crushed and stored in plastic container which kept in different stability stations (30°C/65%RH and 40°C/75%RH). The samples kept in plastic container at different stability time points were analysed by using the Reverse Phase-High Performance Liquid Chromatography (RP-HPLC) as per Indian Pharmacopeia (IP). Based on the analytical data, the Assay of tablet found more than 95.0% while related impurities were found less than 1.0% as per specification of Indian Pharmacopeia. The data shows the molecule stability in crush condition and null impact of packaging material on crushed tablets.

O-22

In vitro Anti-cancer efficacy of crude and nanoparticle form of chitosan extracted from carapace of freshwater crab *Sartoriana spinigera* (Wood-Mason, 1871) by MTT assay

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ABSTRACT

Presently, Cancer is one of the biggest health issues faced by human population and a leading cause of death, cancer fact sheet [1]. Keeping in view the side effects of synthetic medicines, society is considering medicines of natural origin that are not only cost effective but also sustainable to the environment. In the present study, one such molecule known as chitosan and its nanoparticle form has been extracted from the carapace of a freshwater edible crab *Sartoriana spinigera* , locally found in Jharkhand. *In vitro* anti-cancer activity of chitosan (both crude and nanoparticle form) was studied by MTT assay. 4µg/ml Doxorubicin was used as standard. After incubation at 24 ,48 and 72 hours, samples showed highest cell cytotoxicity at 72 hours. Crude chitosan showed cell viability of MCF-7 cells by 64.90±0.0049 %, 55.07±0.0007%, 45.96±0.0021%, 38.29±0.0049%, and 32.88±0.0007% at concentration 100µg/ml, 150 µg/ml, 200µg/ml, 250 µg/ml and 300 µg/ml respectively, when treated for 72 hours. Chitosan nanoparticle was able to show cell viability by 54.30±0.002%, 4.29±0.0041%, 38.06±0.001%,29.40±0.002 % and 25.52±0.004% at same concentrations after treatment for 72 hours. Results of present study indicate significant dose dependent anti cancer efficacy of both crude and nanoparticle form of chitosan obtained from *Sartoriana spinigera* against MCF-7 cell line.

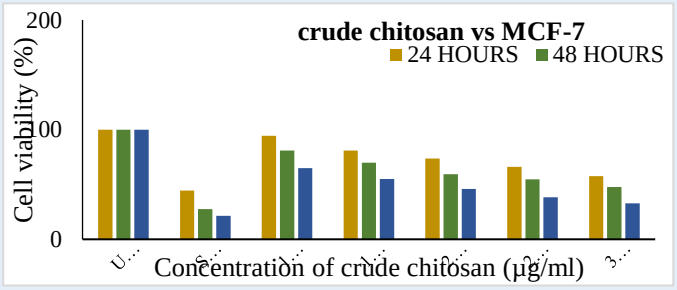

Figure 1: Plot depicting the cytotoxic effect of crude chitosan compared to the untreated
Figure 2: Plot depicting the cytotoxic effect of chitosan nanoparticle compared to the untreated

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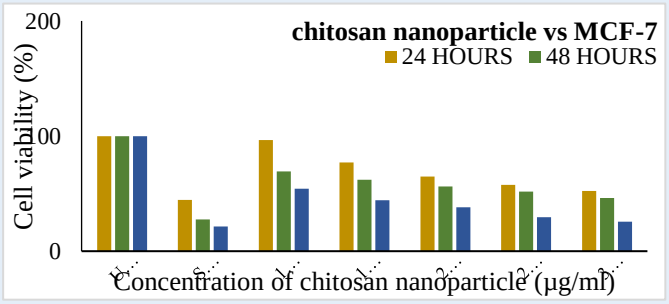

Cancer fact sheet, world health organization;2022

O-23

Cyclodextrins Inclusion Complex Formation with Benzimidazole

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A major component of cashewnut shell liquid (CNSL), benzimidazole (BNZ) has been shown to have antibacterial activity against a variety of bacterial species; however, because of its poor physicochemical stability and water solubility, it has limited bioactivity and clinical relevance. The current study aimed to enhance the aqueous solubility and antibacterial activity of BNZ by creating an inclusion complex including two distinct cyclodextrins, namely β-Cyclodextrin (β-CD) and Hydroxy propyl β-cyclodextrin HP-β-CD. Using the co-evaporation approach, the inclusion complex was made with perfect molar ratios in mind, or 1:1. FT-IR, SEM, and 1H NMR were used to describe the prepared inclusion complex, and these methods offered sufficient evidence to validate the creation of the inclusion complex. The produced inclusion complex showed an improvement in aqueous solubility of around 2009 times. When used against microbiological strains, the generated complex preserved the antibacterial action of pure BNZ. For practically all of the strains under investigation, BNZ and both cyclodextrin complexes showed outstanding %Reduction values and MIC values. In conclusion, the poor water solubility of benzimdazole (1:1) can be efficiently overcome by the created inclusion complexes, enhancing the therapeutic efficacy for numerous different indications.

O-24

HYDROCARBON SOLVENT MEDIATED GEL FORMATION IN AQUEOUS NON-IONIC SURFACTANT MIXTURES

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A ternary systems consisting of Water/ Non-ionic surfactant/hydrocarbon solvent (oil) as well as Water/Non-ionic surfactant mixture/hydrocarbon solvent (oil) were formulated. Phase transitions were observed as a function of temperature and microstructure was observed using Polarization microscopy. The following ternary systems were investigated for hydrocarbon mediated gel formation: 1) Water/ Plantacare-810:Triton X-100,1:1/Hexane, 2) Water/ Plantacare-810:Triton X-100,1:1/Octane, 3) Water/ Plantacare-810:Triton X-100,1:1/Decane, 4) Water/ Plantacare-810:Triton X-100, 1:1/Dodecane and 5) Water/ Plantacare-810:Triton X-100, 1:1/Tetradecane. Hydrocarbon solvent mediated clear isotropic gel formation was observed at a particular mass fraction of surfactant in the above formulations. T_{gel} determination and rheological study (frequency sweep test, amplitude sweep test) was carried out to ascertain structure-property correlations, corroborate the factors responsible for the phenomenon of gel formation. The potential applications of these formulations have been explored.

O-25

Synthesis and Characterization of Zirconium Titanium amino tris(methylenephosphonic acid) and Its Application in Separation of Metal Ions

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Abstract:

In the present study, a novel hybrid ion exchanger, zirconium titanium amino tris (methylenephosphonic acid) (ZTATMP), of the class of tetravalent bimetallic acid (TBMA) salt has been synthesized by the sol gel route. ZTATMP has been characterized for ICP-AES, TGA, FTIR, and XRD. Chemical resistivity of ZTATMP in various media—acids, bases, and organic solvents have been assessed. Ion exchange capacity (IEC) and the effect of calcination (100°C to 500°C) on IEC has also been studied. The distribution behavior of metal ions Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+} (d-block), Cd^{2+}, Hg^{2+}, Pb^{2+} (heavy) and La^{3+}, Ce^{3+}, Pr^{3+}, Nd^{3+} and Sm^{3+} (f-block) towards ZTATMP has been studied and the distribution coefficient (K_d) evaluated in aqueous as well as various electrolyte media/concentrations. Based on differential selectivity, the breakthrough capacity (BTC) and elution behavior of various metal ions towards ZTATMP, have been carried out. Based on the studies it is observed that ZTATMP exhibits good selectivity for Cu^{2+} among transition metal ions, Pb^{2+} heavy metal ions and Nd^{3+} among the lanthanides metal ion suggesting their selective removal from the wastewater effluents. A study on regeneration and reuse of the ion exchanger ZTATMP shows that it is effective upto six cycles without much decline in performance.

O-26

Machine Learning-Guided Discovery of Small Molecule Inhibitors of SARS-CoV-2 Spike/Human ACE Interaction

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Choice of mode: Podium

Traditional drug discovery and development pipelines require significant economical and time investments and are associated with high failure rate for translating discoveries from bench to clinic. In recent years, machine learning (ML) approaches have emerged as promising methods to improve and expand the hit identification process in early-stage drug discovery, contingent to the availability of high-quality training data. Thus, employing ML techniques prior to preclinical evaluation can reduce the cost and expand the search for novel drugs to unexplored chemical spaces [1,2]. In this work, we utilized data derived from a biosensor-based high throughput screening (HTS) of a large chemical library to develop an efficient ML framework for the identification of synthetic small molecule disruptors of the SARS-CoV-2 Spike/human ACE interaction, a central player of SARS-CoV-2 infection mechanism. By representing molecules with their RDKit molecular descriptors and ECFP4 fingerprints, we trained and evaluated a series of Random Forest, RF [5] and Multi-Layer Perceptron, MLP [6] models for the classification of interaction inhibitors. To mitigate data leakage issues, we implemented a rigorous, strict scaffold splitting strategy combined with 5-fold cross-validation and we adopted an ensemble based approach, demonstrating promising performance in retrospective virtual screening experiments. Prospectively, both models returned significantly higher hit rates (RF: 14.65%, MLP: 8.97%) than the original random screen (1.30%), demonstrating at the same time significant exploration of new chemistry. Our results suggest that the combination of highly complementary HTS and ligand-based ML approaches can significantly expedite therapeutic discovery over large regions of the chemical space.

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O-27

Evaluation of Diagnostic Efficacy of Anti-Mullerian Hormone in Polycystic Ovarian Syndrome.

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Introduction: Polycystic ovary syndrome (PCOS) is a group of endocrine disorders that commonly affect reproductive women, characterized by irregular, anovulatory menstrual cycles, hyperandrogenism and polycystic ovaries with a prevalence of 8.2 to 22.5% in India. Hypothesized mechanism for hyperandrogenism is follicle maturation abnormalities due to altered levels of serum Follicle Stimulating Hormone (FSH) and Serum Luteinizing Hormone (LH). Concurrently Anti-Mullerian Hormone (AMH) levels are also observed to be higher in PCOS patients, but the exact mechanism is still under grey area and postulated that obesity, insulin resistance and hyperandrogenism play major roles in increasing its level. This study was conducted to investigate the association between AMH and hormonal parameters to assess predictive value of Serum AMH levels in the clinical diagnosis of PCOS.

Material and Methods: A Cross-sectional study was conducted where 90 newly diagnosed PCOS patients were categorized into four PCOS phenotypes using Rotterdam criteria and 90 healthy women as controls. Fasting blood samples collected were analysed for Serum AMH, Serum LH, Serum FSH, Serum Fasting Insulin and Serum Testosterone. LH:FSH ratio and HOMA-IR were calculated. ANOVA test and Spearman correlation analysis were conducted to investigate associations using MedCalc 22.009 software.

Results: All 4 PCOS phenotype groups presented a significant difference (p value < 0.05) on comparison with control group. Diverse and appreciable correlation was observed between serum AMH and other hormonal parameters across all four PCOS phenotypes; with highest values observed in patients with phenotype A.

Conclusion: AMH is directly correlated with the LH/FSH ratio, HOMA-IR and Serum Testosterone, highlighting its significance in the neuroendocrinology of PCOS. AMH can also act as an intermediary variable between HOMA-IR and Serum Testosterone, influencing the LH/FSH ratio. Management of Serum AMH levels can lead to better prognosis of PCOS patients.

Keywords: AMH, Hormones, Hyperandrogenism, Insulin, PCOS, Phenotype.

O-28

Aluminium chloride chelation in flavonoid estimation assays: Drawbacks and issues

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Abstract:

Colorimetric methods have been used rampantly for rapid and convenient estimation of certain classes of flavonoids in fruits, vegetables, grains, raw herbal material, herbal formulations, and nutraceuticals. However, these methods are not selective since several factors influence color development. Chelation using $AlCl_3$ is used to develop deep yellow-colored complexes of the flavonoids and absorbance subsequently measured at 420 nm, using quercetin as standard. In a modification, potassium acetate is added after the addition of $AlCl_3$, and the absorbance was measured at 415 nm, again against standard quercetin solutions, wherein only flavones and flavonols were estimated. A study conducted by our team proves that all flavonoids do not form complexes that absorb at 420 nm, and each flavonoid shows variation in λ_{max}. Only flavonoids with *o*-dihydroxy systems show good results, while others absorb at either higher or lower wavelengths. Catechins, flavanones, and anthocyanins cannot be estimated using this method, due to either inability to bind with $AlCl_3$ in an appropriate manner or due to differences in λ_{max} of the complex formed. Many flavonoid compounds occur in the form of glycosides, where the presence of sugar molecules like glucose, rhamnose, galactose, etc. can hamper complex formation responsible for color development. Hydrolysis can yield better results by removing the sugar moieties, and the aglycones can be estimated. Therefore, the term 'Total Flavonoid Content' using the $AlCl_3$ chelation method cannot be used as a parameter indicating the total amount of flavonoids in the samples, as stated in thousands of research articles.

O-29

An Extensive Analysis Comparing the Non-Steroidal Anti-Inflammatory Drug (NSAID) of Diclofenac Sodium Injection from Branded or Innovator Companies to Generic Companies Drug Products Under Various Stability Conditions

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Abstract:

The objective of this research work is to provide detailed comparative analytical data of stability studies for Non Steroidal Anti Inflammatory Drug (NSAID) i.e. Diclofenac sodium injection. The drug products of different manufacturers were purchased from medical store at maximum retail price (MRP). Every selected drug products were analyzed by checking their physical appearance and by keeping them at different stability conditions. Diclofenac injection is available in the form of ampoule and it is used to treat the adults having mild to moderate pain. In this study, injections were stored at different stability conditions at 30°C/65%RH and 40°C/75%RH. The samples were kept as such in containers provided by the manufacturers and analyzed at different stability time points. The samples were analyzed qualitatively and quantitatively by using Reverse Phase-High Performance Liquid Chromatography (RP-HPLC) as per Indian Pharmacopeia (IP) methods. Based on the analytical data, the assay and related impurities of all drug products were found within limit as per the specification of Indian Pharmacopeia. The analyzed data shows that all manufacturers' medicines are stable in both the stability conditions and can be consumed by patients irrespective of the price.

O-30

Leveraging Artificial Intelligence and Machine Learning Techniques in Pharmaceutical Research and Development

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Pharmaceutical research aims to find new active molecules for the currently incurable ailments; increase the safety profile of existing drugs; repurpose medicines, combat drug resistance and minimize therapeutic failures [1]. There is huge scope of using artificial intelligence (AI) and machine learning (ML) techniques in optimizing innovation processes, increasing the efficiency of research/clinical trials and improving decision-making to create better medicines [2]. The future of AI is promising in precision medicine, where integrating emerging technologies like multi-omics can be utilized for linking molecular mechanisms and diseases [3].

Molecular modeling software enabled with AI algorithms and trained ML models can analyze vast biomedical data to identify potential drug candidates and target proteins, and predict possible drug-target interactions for drug efficacy and possible toxicity. Other aspects such as *in silico* activity scoring and ADMET (absorption, distribution, metabolism, excretion, and toxicity) evaluation of a drug molecule can be enhanced by using by AI/ML algorithms. AI can aid in patient selection, study design, and real-time data analysis during clinical trials, leading to enhanced drug safety and efficacy. Further, AI-based systems can be utilized to monitor adverse events and support pharmacovigilance efforts in post-marketing phases [5].

Although, AI and ML techniques can be very beneficial, the key for their successful utilization is availability of appropriate datasets with large number of datapoints well represented by appropriate sample population. Adopting AI in pharmaceutical research would raise ethical considerations ensuring data privacy and security which can be ensured by a successful collaboration among academia, industry, and regulatory bodies [6].

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O-31

Oxidative Coupling of *N*-Nitrosoanilines with Substituted Allyl Alcohols under Rhodium (III) Catalysis

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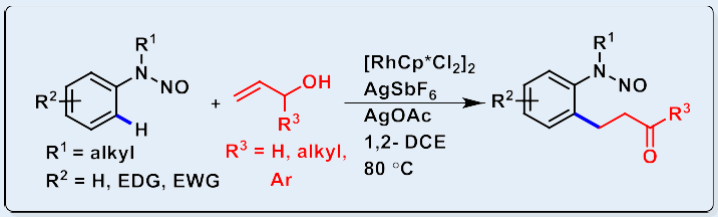
Abstract

C-H activation of *N*-nitrosoanilines was accomplished by employing rhodium(III) catalysis with substituted allyl alcohols (Scheme 1). This method provides an efficient synthesis of the functional *N*-nitroso *ortho* β-aryl aldehydes and ketones with low catalyst loading, high functional group tolerance, and superior reactivity of allyl alcohols towards *N*-nitrosoanilines[1]. We demonstrated that reaction also proceeds through the one-pot synthesis of *N*-nitrosoaniline followed by subsequent C-H activation. The protocol was also feasible with acyrlaldehyde and methyl vinyl ketone which furnished the same oxidative *N*-nitroso coupling product.



Scheme 1. Rh (III) catalyzed C-H activation of *N*-nitrosoanilines using substituted allyl alcohols.

Keywords: C-H functionalization, N-nitrosoanilines, Allyl alcohols, Rhodium catalysis, Mechanistic Studies.

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O-32

"Investigating the Breast Cancer Potential of alkylated 5,7-dihydroxy-2-(4-hydroxyphenyl) chroman-4-one Derivatives: Unveiling In-Silico and In-Vitro Studies"

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Abstract:

Citrus fruit contain a flavanone glycoside called naringenin(Chen et al., 2023; Najmanová et al., 2020; Shah and Smith, 2020), which has attracted a lot of attention due to its possible therapeutic use in the treatment of hormone-related cancers(Motallebi et al., 2022; Stabrauskiene et al., 2022), especially breast cancer. In this study, various alkyl derivatives of naringenin were synthesized and characterized. The pharmacokinetic profiles and molecular docking studies of the compounds were evaluated against multiple hormonal targets implicated in breast cancer, including Epidermal Growth Factor Receptor (EGFR), Estrogen Receptors (ESR-α and ESR-β), Human Epidermal Growth Factor Receptor 2 (HER2), and Progesterone Receptor (PR), with binding energies ranging from -6 to -10 kcal/mol. The docked complex's stability was evaluated using molecular dynamic simulation for 20 nanoseconds. The results indicate that ligand RMSD values varied marginally, suggesting they all stayed stable within the binding pocket, most fitting within ~1 nm. NMR spectroscopy and Mass spectrometry were used to characterize the derivatives, one unique chalcone derivative of naringenin was obtained during alkylation. SWISS-ADME tool was utilized to evaluate the compounds' physicochemical attributes and drug-likeness. Using MTT assay on MCF-7 breast cancer cells, the derivative's anticancer activity was investigated, revealing significant inhibition of cell viability. The derivatized naringenin compounds showed notable drug-likeness, binding affinity, stability, and IC50 values when compared to the parent molecule. This study improves our knowledge of the effects of derivatizing naringenin on its pharmacokinetics and anti-breast cancer characteristics, highlighting the potential of computer-aided drug design in creating novel scaffolds that serve as effective cancer therapeutics.

Keywords: Naringenin, Breast Cancer, MCF-7, Molecular docking, MD simulation

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O-33

Heterocyclic Natural Products and their Biological Importance

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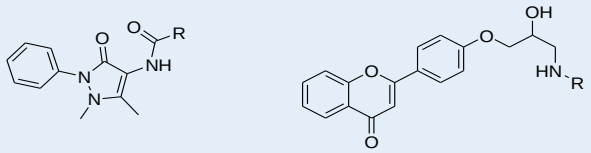
Abstract

Heterocyclic natural products (HNPs) are primary or secondary metabolites which have heterocyclic (N-heterocyclic) skeletons are containing high biological potential.1 Chalcones have α, β-unsaturated ketone are an important natural product, antecedent for isoflavonoids and flavonoids.2 Its derivatives have shown active biological properties, which are useful for designing and discovery of different types of therapeutic drugs with high potency.3 A number of biological activities are found in HNPs such as antimicrobial,4 antihelminthic,5 antithrombotic, anti-platelet and anticoagulant,6 anti-inflammatory,7 antiulcer,8 antifungal and acetycholinesterase,9 anti-tubercular, antiviral, anti-HIV.10
On knowing about the bioactive properties of heterocyclic natural products, we have decided to synthesize several prototypes of heterocyclic natural product derivatives which are shown below:



R= Picolinic acid,cinnamic acid, Pyrrole-2-carboxylic acid, Pyridine-2-carboxylic acid, etc.

R= Imidazole compounds

After synthesizing several natural products as discussed above, we have evaluated for several biological properties, are shown result from good to moderate bioactive potential.

Keyword: Heterocyclic, chalcone, flavones, benzimidazole, 4-aminoantipyrine.

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O-34

Enhancing Biocompatibility of Green-Synthesized Nanoparticles through Green Capping Agent

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The biocompatibility of nanoparticles is a critical consideration for their application in biomedicine. This study explores the enhancement of biocompatibility in green-synthesized nanoparticles through the use of a green capping agent [1] like aqueous leaf extract of *Solanum nigrum*. The synthesis of nanoparticles using plant-based extracts is gaining attention due to its eco-friendliness and potential for biomedical applications. Plants, rich in bioactive compounds, serve as a reducing agent stabilizing the nanoparticles and improving their interaction with biological systems [2]. These bioactive components donate electrons to metal ions, reducing them from a higher oxidation state to a lower one, resulting in the formation of stable nanoparticles [3]. The synthesized nanoparticles were characterized by various analytical techniques confirming their nanoscale size, shape, and crystalline nature [4]. The biocompatibility of green-synthesized nanoparticles is evaluated through comprehensive in vitro studies. Therefore, the research elucidates the potential of green synthesis approaches coupled with green capping agents to address the biocompatibility challenges associated with nanoparticle-based applications. The findings underscore the importance of sustainable and eco-friendly strategies in nanoparticle synthesis, paving the way for safer and more efficacious nanotechnology-enabled solutions in diverse fields.

Keywords: Green Nanoparticles, Biocompatibility, Capping agent.

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O-35

Antioxidant Potential of *Hibiscus rosa-sinensis* Linn: Phenolic and Flavonoid Analysis

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ABSTRACT

Extracts from *Hibiscus rosa-sinensis* L. have become of attention due to their potentially therapeutic bioactivity. The potential health benefits of *Hibiscus rosa-sinensis* Linn. ethyl acetate extract and ethanolic extract of leaves have been examined for their total phenolic content (TPC), flavonoid constituents via HPLC, further antioxidant, anti-inflammatory, and anti-cancer activities have been evaluated in vitro. The free radical scavenging activity of *Hibiscus rosa-sinensis* L. leaves extract using the 1,1-diphenyl-2-picrylhydrazyl assay (DPPH) method have been evaluated. This finding demonstrated the existence of phytochemical components including phytosterols, gum and mucilage, phenolic compounds, tannins, glycosides, terpenoids, and triterpenoids. Additionally, the extract contained significant levels of four flavonoids—rutin, quercetin, kaempferol, and myricetin which are identified as major contributors to its antioxidant potential. The study concludes by highlighting the leaves of *Hibiscus rosa-sinensis* L.'s significant antioxidant, anti-inflammatory, and anticancer properties. Phenolic compounds may prove to be a good substitute for the treatment of specific ailments since they have demonstrated a high bioactive potential against a variety of illnesses, including breast cancer cell line.

Keywords: *Hibiscus rosa-sinensis* L., Total phenolics, Flavonoids, Antioxidant etc.

O-36

Ultrasmall aqueous starch-capped CuS quantum dots with tunable localized surface plasmon resonance and composition for the selective and sensitive detection of mercury (ii) ions.

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Ultrasmall starch-capped CuS quantum dots (QDs) with controllable size were chemically fabricated in an aqueous medium. The phase of the CuS QDs was confirmed via X-ray diffraction (XRD), whereas the characteristic localized surface plasmon resonance (LSPR) peak in the near-infrared (NIR) region was measured using UV-Vis spectroscopy. Transmission electron microscopy and high bandgap analysis confirmed the formation of ultrasmall CuS QDs in the size range of 4–8 nm. CuS QDs have been used for the selective and sensitive detection of Hg^{2+} ions through colorimetric and spectroscopic techniques. The selective sensing of Hg^{2+} ions from various metal ions was detected via a remarkable change in color, damping in LSPR intensity, significant change in the Fourier-transform infrared spectra and X-ray photoelectron spectroscopic measurements. The mechanism of interaction between the CuS QDs and Hg^{2+} ions has been deeply explored in terms of the role played by the starch and the reorganization of sulfide and disulfide bonds to facilitate the access of Hg^{2+} ions into the CuS lattice. Finally, an intermediate $Cu_{2-x}Hg_xS$ nanostructure resulted in the leaching of Cu+ ions into the solution, which were further recovered and reused for the formation of fluorescent Cu_2S nanoparticles. Thus, the entire process of synthesis, sensing and reuse paves the way for sustainable nanotechnology.

O-37

Esterification of Phthalic Anhydride with Butanol using Solid Acid Catalyst under Solvent-Less Condition

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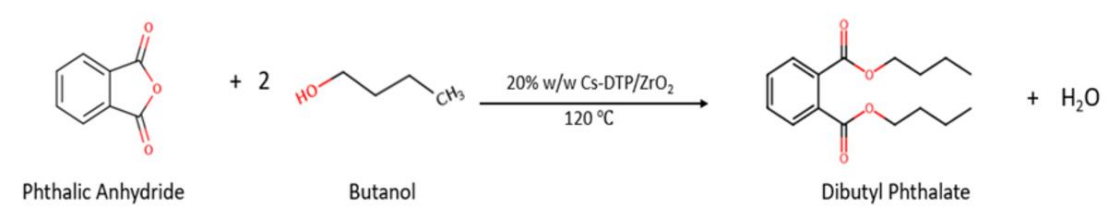
Abstract

The heterogeneous active and selective Cs-DTP/ZrO_2 catalyst was prepared and used for the esterification reaction. A set of catalysts was prepared, consisting of different DTP loadings on zirconia. The highest yield was achieved in the esterification reaction between phthalic anhydride and butanol using a 1:10 molar ratio and 20% w/w Cs-DTP/ZrO_2 catalyst at 120 °C temperature. The catalyst employed in this process effectively provided the necessary acidity, facilitating the formation of the desired ester. Upon completion of the reaction, the catalyst was recovered by simple filtration without any significant loss in quantity. The recovered catalyst was then reused in subsequent batches, demonstrating consistent product formation and indicating the stability of the catalyst. This stability underscores the potential of 20% w/w Cs-DTP/ZrO_2 as a reusable catalyst in esterification reactions. The synthesized catalyst has been characterized by using different characterization techniques and the product was confirmed by using NMR analysis.

Reaction Scheme:



Scheme 1. Esterification of phthalic anhydride with butanol using Cs-DTP/ZrO_2

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O-38

Identification and Isolation of Terpenes and Biological Activity

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Natural products are small molecules produced naturally by any organism including primary and secondary metabolites.The nature products mayhave isolated from the plant source and in these plants some are aromatic plants which have a very rich source of essential oils and the essential oils has aroma, essence, fragrance, flavour and odour or smell. Essential oils are aromatic substances present in the specialized cells or glands of certain plants used by them to protect themselves from predators and pests, but also to attract pollinators. These volatile liquids are very complex molecular substances, extremely potent and precise as action. Essential oil is not actually an oil because it contains no fatty substance. It is obtained from the essence rich in natural flavours and active ingredients that it secretes the cells of certain parts of the plant. Precious liquids are obtained by distilling or pressing the secretory organs.

The secondary metabolites are terpenes biomolecules isolated from essential oils of aromatic plants which have biological activities such as antioxidant, anticancer, antiprotozoal, antifungal, antibacterial and anti-inflammatory. The natural products from Some aromatic plants have bioactive terpenes biomolecules and it may have specific important properties and enormous application potential research study in term of bioactivity.

Keywords: antioxidant, anticancer, antiprotozoal, antifungal, antibacterial and anti-inflammatory

O-39

Synthesis, in vitro and in silico anti-cancer evaluation of Diosgenin-NSAID's conjugates against SiHa cells

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Abstract:

All classes of steroids have great biological activities such as antimicrobial, anti- Alzheimer's disease, anti-inflammatory, hypoglycemic and anti-cancer. Many studies shows that different steroids and their derivatives can be used as a template to develop new anti-cancer agents. Steroidal sapogenins are one of the important classes of steroid which shows good anti-cancer activity individually and as well as in conjugation with other bioactive materials. Modern experimental and clinical studies have suggested that nonsteroidal anti-inflammatory drugs (NSAID's) may be developed as anticancer agents. In the present study, we have synthesized two novel diosgenin-NSAID's conjugates. Column chromatography was used to purify the synthesized compounds. Some modern spectroscopic techniques like ^{1}H, ^{13}C NMR, FT-IR, UV-Visible spectroscopy and mass spectrometry were used to establish the structure of synthesized compounds. The geometries of both the compounds were optimized in the ground state by density function theory at the B3LYP/6-31G(d,p) level. Both the synthesized compounds were evaluated *in vitro* for anti-cancer activity against SiHa cells which demonstrated an appreciable activity as indicated by the IC_{50} values. Molecular docking studies were also performed for the investigation of the inhibitory action of steroidal derivative against the HPV protein. The result of molecular docking study shows that the synthesized compounds have better binding energies than the parent compound with the selected HPV protein.

Keywords: Diosgenin, Human cervical carcinoma, Anti-cancer activity, Molecular Docking, DFT, HPV.

O-40

Energy Dynamics and Mechanistic Insights into Corrosion Inhibition Processes in Corrosive Media

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Abstract

In developing countries, materials are vital building blocks for a variety of applications that drive economic growth and social progress. However, many of these materials, particularly metals like carbon steel, are highly vulnerable to corrosion, which presents significant challenges. Corrosion results in substantial financial losses, with global economic costs estimated at 3-4% of GDP. This underscores the urgent need for effective corrosion control strategies. Traditional corrosion control methods often carry environmental and health risks. Therefore, it is essential to develop suitable and efficient approaches for corrosion management. **Heterocyclic compounds** have emerged as promising corrosion inhibitors due to their conjugated π-electron systems, heteroatomic centers, and high molecular weights, which enhance their adsorption on metal surfaces. Specifically, nitrogen (N) and sulfur (S)-containing heterocyclic derivatives, such as triazoles and pyrimidines, have proven particularly effective in protecting carbon steels in acidic environments. Our approach focuses on developing new derivatives of triazoles and pyrimidines that achieve maximum corrosion efficiency at very low concentrations. The study will take a comprehensive approach to evaluate the effectiveness of these inhibitors.

O-41

Co-crystal formation: thermal and crystal structure analysis for their role in pharmaceutical design

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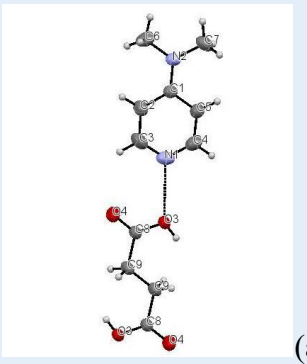
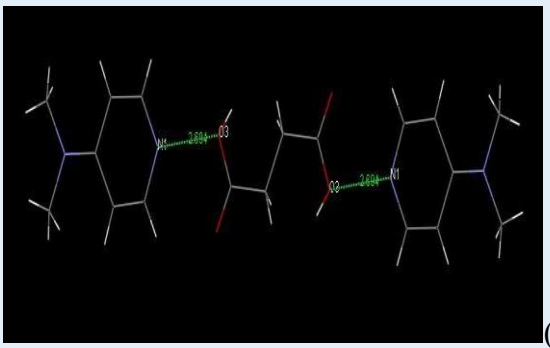
Nowadays, Co-crystal engineering strategy is gaining a lot of interest in modifying the existing drugs with enhanced physico-chemical and therapeutic properties. The novel organic co-crystal (DMAPSA) has been synthesized using the phase diagram analysis of 4-Dimethylaminopyridine and Succinic acid (an API). The stoichiometric ratio of the co-formers was found to be 1:1 with melting point of the co-crystal be 135 ºC and it's heat of fusion value was 31.47 kJ/mole. The single crystal of DMAPSA was grown by slow solvent evaporation technique from saturated solution of the compound in acetonitrile at 302 K. The structure of DMAPSA, its atomic packing and functional groups have been confirmed by single crystal X-ray diffraction techniques. The single crystal structure reveals the carboxylic acid...pyridine hydrogen bonding interactions between co-formers in formation of cocrystal.



(a)



(b)

(a) ORTEP view and numbering scheme, **(b)** hydrogen bonding pattern

Keywords: Co-crystal, API, Phase diagram, DSC, crystal structure

O-42

In-Silico Exploration of Rutin Derivatives as Potential Inhibitors of Prostate Cancer Signaling Pathways

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Abstract

Prostate Cancer (PCa) is a global health issue and a major malignancy among men. The development of the disease results from a complex interplay between genetic, epigenetic, environmental, chronological, and behavioral factors. Thus, understanding complex molecular pathways associated with the second leading cause of death from cancer in men requires elucidation. The present research focuses on targeting crucial pathways that are known to have significant involvement in the progression of PCa, namely AKT, EGFR, and ERK. Rutin derivatives were screened for their therapeutic efficacy against different pathways by molecular docking to find the favorable interactions, therefore the most promising molecules have been selected. The comprehensive analyses include metabolites predication, density functional theory pharmacokinetics, molecular dynamics simulation, principal component analysis, free energy landscape evaluation, and Molecular Mechanics Poisson–Boltzmann Surface Area on candidate selection. Of all the compounds, RU4b1 showed potent inhibitory activity and favorable drug-like properties, which included significant antioxidant activity. Predictive metabolic site study of RU4b1 provided information about its biotransformation. Comparing standard drugs, RU4b1 showed better effectiveness, and this compound was shown to be very promising as a targeted therapy for prostate cancer. This work thus underlines the potentiality of rutin derivatives in enhancing the therapy of PCa, thus greatly providing insights for developing some effective anti-cancer drugs.

O-43

Green Synthesis and Stabilization of Zinc Oxide Nanoparticles with *Bixa orellana* Extract

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The green synthesis of zinc oxide (ZnO) nanoparticles offers a promising and sustainable alternative to conventional chemical methods, addressing critical challenges such as toxicity, agglomeration, and biocompatibility. In this study, a novel approach utilizes the aqueous seed extract of *Bixa orellana* as a green- reducing agent to synthesize ZnO nanoparticles. The rich phytochemical content of *Bixa orellana*, including flavonoids and carotenoids [1,2] plays a pivotal role in the reduction process [3], contributing to the formation of nanoparticles with enhanced properties. To further improve the stability and prevent agglomeration, a carefully selected capping agent is employed during the synthesis [4]. This dual-function approach ensures that the ZnO nanoparticles remain well-dispersed, stable, and biocompatible, making them suitable for various applications. The ZnO nanoparticles have the potential to exhibit significant biological activities, including antioxidant, anticancer, and antidiabetic effects, due to their unique physicochemical properties. These multifunctional nanoparticles hold great promise for applications in biomedicine [5], where their antioxidant properties could be harnessed to combat oxidative stress-related diseases, their anticancer potential could be explored in targeted cancer therapies, and their antidiabetic effects could offer new avenues for managing diabetes. Moreover, the environmentally friendly synthesis process aligns with the growing demand for sustainable and scalable nanomaterial production methods. The innovative use of *Bixa orellana* seed extract and the capping agent addresses key challenges in nanoparticle synthesis and paves the way for expanding the practical applications of ZnO nanoparticles in various industries, particularly in biomedicine and environmental science.

Keywords: Green synthesis, *Bixa orellana*, Capping agent, Agglomeration, Biocompatibility

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POSTER

P-1

Indolin-2-one linked 1,2,3-triazoles as EGFR (6P8Q) inhibitor

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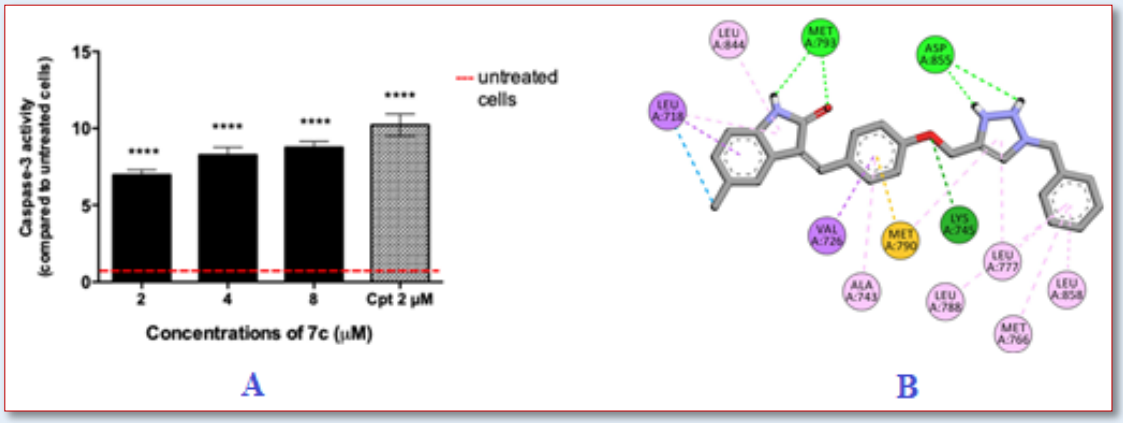
A series of twenty-four 1,2,3-triazoles were screened for *in-vitro* cytotoxicity and EGFR 6P8Q binding affinity. Most of the analogs exhibited cytotoxicity in the micromolar range. Molecule **AD-3 (7c)** found to be most active against L1210 (IC_{50}: 3.0 ± 0.9 µM), CEM (IC_{50}: 1.5 ± 0.6 µM) and HeLa (IC_{50}: 3.4 ± 0.6 µM) cells. Caspase-dependent apoptosis in Jurkat cells observed by activating intrinsic and extrinsic apoptotic pathways involving cell-cycle perturbation. No genotoxicity observed. Molecular docking showed that, derivatives AD-3, AD-15 and AD-22 bind to EGFR-6P8Q with residue MET793, MET790, LEU788, and ALA743 residues [1, 2].



Keywords: Indolin-2-one, 1,2,3-triazole, cytotoxicity, apoptosis, cell cycle, molecular docking, EGFR 6P8Q.

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P-2

Design and Synthesis of Some New Series of Polysubstituted Fused Pyrimidine Derivatives for their Biological Activity

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The development of the drug resistant parasitic strains in parasitic area has been recently immersed as a big problem as existing drugs has their limited therapeutic potential, hence, drug discovery research industries recently mainly focus on the design and synthesis of new drugs in parasitic area which are having significant therapeutic potential and least side effect. The pyrimidine derivatives have attracted much attention in pharmaceutical industries due to its diverse pharmacological activities viz. CNS depressant, anti-HIV, antitumor, antimalarial, antihypertensive, antifungal, anti-inflammatory, analgesic, anti-convulsant, antihelmentic, antioxidant and anti-bacterial. SAR studies of various pyrimidines based drugs either derived from natural products or synthetic revealed that pharmaceutical activities are due to the presence of pyrimidine nucleus. Keeping in view the above facts and importance of pyrimidine nucleus in various therapeutic targets and continuous of our work[1,2], recently, we have designed, synthesized and characterized some new series of polysubstituted fused pyrimidines for their biological activity. All the synthesized compounds were characterized by using of various spectroscopic techniques. In this presentation, the detailed synthetic procedure, mechanisms of the reactions and characterizations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

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P-3

Biomimmitic Catalysis for Environment Friendly One pot Multicomponent Synthesis of Chromeno[4,3-b]chromene-6,8,13-triones in aqueous micellar CTAB

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Abstract

The catalytic activity of biomimitic CTAB was studied for the synthesis of chromeno[4,3-b]chromene-6,8,13- triones (**4a-n**) by the cyclocondensation of benzaldehydes, 4-hydroxy coumarine and 2-hydroxy-1,4- napthaquinone in aqueous media. This green and eco-safe domino approach revealed simplicity, use of biodegradable and highly efficient catalyst, avoidance of toxic organic solvents, excellent yields, easy work-up procedures. The reusability of the catalyst and being in agreement with the green chemistry protocols, and time- saving aspects of the reaction suggest that this method presents real alternatives over conventional reaction protocols.

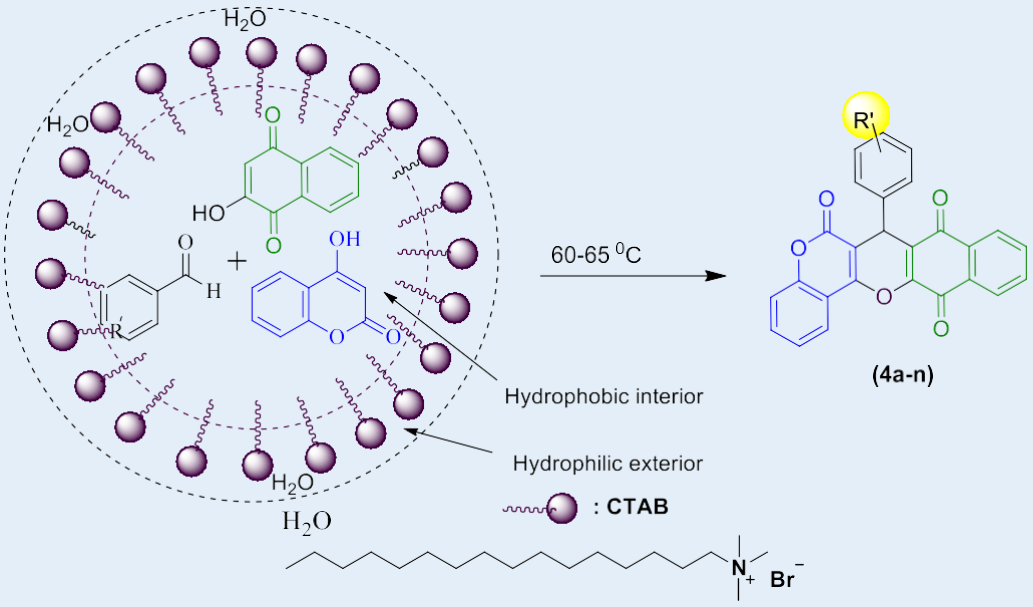

Figure 1. Graphical abstract for the synthesis of chromeno[4,3-b]chromene-6,8,13-triones (**4a-n**)

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P-4

Indanone-Benzimidazole hybrids as potential anti-Alzheimer's agents: Design, synthesis, biological evaluation, DFT, molecular docking and molecular dynamics study

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Abstract:

The growing concern of Alzheimer's disease underscores the urgent requirement for the development of novel therapeutic agents. In this study, a series of 15 hybrid molecules containing Indanone-Benzimidazole heterocycles were designed utilizing the molecular hybridization approach. The synthesized molecules were characterized by spectroscopic techniques and their anti-Alzheimer's behaviour were examined. Biological assessment demonstrated that compounds **14** and **15** exhibited significant reduction of "human" amyloid beta (Aβ) peptide aggregation, expressing on transgenic *Caenorhabditis elegans* (*C. elegans*) strain CL4176. These compounds were further evaluated for their AChE inhibitory effects in transgenic *C. elegans* strain CL2006 and found significant activity. Molecular docking investigations have elucidated the commendable affinity exhibited by the studied ligands towards the Aβ pentamer (PDB: 2BEG) and acetylcholinesterase (AChE) (PDB: 4EG7). Subsequent to these docking studies, molecular dynamics simulations were conducted, affirming the stability of both ligands in association with the Aβ pentamer and ACh. Additionally, Density functional theory (DFT) calculations were performed by using B3LYP energy level with the basis set 6–311 G (d,p) basis set to correlate with experimental results. Taken together, all these findings evidenced the experimental results and this study sheds light on the anti-Alzheimer's potential of Indanone-Benzimidazole hybrids.

P-5

In Silico and *In Vitro* Assessment of Dashmool for SARS-CoV-2 Drug Discovery

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Abstract

The COVID-19 pandemic has prompted research into potential therapeutic agents from traditional medicine. This study investigated the Dashmool Ayurvedic formulation, comprising ten plants, for its inhibitory effects against SARS-CoV-2 proteins and Cathepsin L. We employed both in silico molecular docking and in vitro assays to evaluate the formulation's efficacy. Molecular docking was performed using PyRx with AutoDock Vina against three targets: Omicron protease (7TOB), Spike protein (7XO5), and Cathepsin L (8A4W). In vitro assays included SARS-CoV-2 Spike Protein Inhibition, Main Protease Inhibition, and Cathepsin L Inhibition assays using BPS Bioscience kits. Docking studies revealed promising compounds, with Psychotridine showing strong binding affinities across all targets (binding energies: -11.3 kcal/mol for 7TOB, -9.1 kcal/mol for 7XO5, -11.2 kcal/mol for 8A4W). Other notable compounds included Xanthoaphin, Cadabicine, and various steroidal saponins. In vitro assays demonstrated varying inhibition levels among Dashmool plants. Spike Protein inhibition ranged from 35.3% to 87.2%, with the complete Dashmool formulation showing 90.1% inhibition. Protease assay inhibition reached up to 98% for some plants, while Cathepsin L inhibition peaked at 83.8%. This comprehensive study identified several compounds and extracts from the Dashmool formulation with potential inhibitory activity against key SARS-CoV-2 proteins and Cathepsin L. The complete formulation showed notable activity against the Spike protein. These findings provide a foundation for further investigation into Dashmool compounds as potential therapeutic agents against COVID-19, warranting additional in vivo studies to validate results and explore pharmacological properties.

Keywords: Dashmool, SARS-CoV-2, Molecular Docking, In Vitro Assays, Ayurvedic Medicine

P-6

In Silico Evaluation of *Morinda* Anthraquinones as BACE1 Inhibitors: Potential Therapeutic Applications for Alzheimer's Disease Treatment

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Abstract

Alzheimer's disease is a neurodegenerative disorder that severely affects memory and cognitive functions. It is the primary cause of dementia, accounting for 60-80% of all cases, and is characterized by the accumulation of abnormal protein deposits, specifically amyloid beta plaques, in the brain. This leads to nerve cell death and a gradual decline in brain tissue. Currently, there is no cure for Alzheimer's disease, and existing treatments only provide temporary relief from symptoms (Yiannopoulou et al. [1]). Natural anthraquinones and their derivatives have attracted considerable attention for their potential to target various molecular pathways involved in Alzheimer's disease (Campora et al. [2]). The present study focuses on inhibiting the enzyme β-site amyloid precursor protein cleaving enzyme 1 (BACE1), which plays a key role in the formation of amyloid beta plaques. To this end, 104 anthraquinones from the *Morinda* genus were analyzed using Biovia Discovery Studio 2024 software in *in silico* studies. The research involved generating a structure-based pharmacophore model based on interactions between BACE1 (PDB ID: 2ZHV) (Shimizu et al. [3]) and Resveratrol. A virtual screening of an anthraquinone database was then conducted against this model. The top hit molecules, after secondary filtering using ADME, Lipinski's rule of five, and Veber's rule, were subjected to docking studies and validated through a 100ns molecular dynamics simulation. These identified compounds may contribute to the rational design of new BACE1 inhibitors for Alzheimer's disease treatment (Coimbra et al. [4]).

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Mode of Presentation – Poster presentation
Name of presenter – Pratima Parshuram Pandey
Date of Birth – 29th August 1999

P-7

β-Oxodithioester-Based Multicomponent Synthesis of Thiochromenes via Heterogeneous Catalysis

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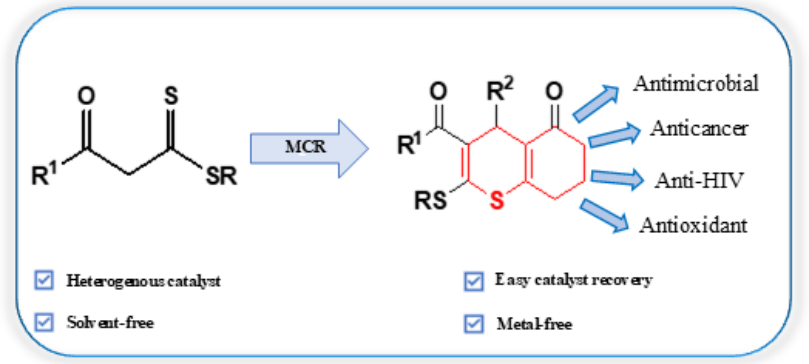
Thiochromenes are an important class of sulfur-containing heterocycles known for their diverse biological activities, including antimicrobial, anti-HIV, anticancer, and antioxidant properties, making them valuable in drug development[1]. Multicomponent reactions (MCRs) have emerged as powerful tools for the efficient synthesis of complex molecules, including thiochromenes, due to their ability to combine multiple reactants in a single step[2]. While several MCR approaches for thiochromene synthesis have been developed, methods involving β-oxodithioesters remain scarce[3].

β-Oxodithioesters are versatile building blocks in organic synthesis due to their unique reactivity, possessing both electrophilic and nucleophilic centers[4]. This dual functionality makes them highly valuable in the construction of a wide variety of sulfur-containing heterocycles[5].

In this study, we report the use of a heterogeneous catalyst to promote the multicomponent synthesis of thiochromen-5-ones derivatives from β-oxodithioesters, aromatic aldehydes, and dimedone. The reaction proceeds under solvent-free conditions, offering high yields, and a simple work-up process. The catalyst was easily recovered and reused for five times without any significant loss of activity. This protocol not only provides an efficient and sustainable approach for synthesizing thiochromenes but also highlights the potential of β-oxodithioesters in MCR chemistry.



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P-8

From Nature to Therapeutics: *In Silico* Molecular Docking of Bisindole Alkaloids as VEGFR2 Inhibitors for Melanoma Treatment

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Abstract:

Melanoma is a highly metastatic cancer originating from melanocytes, the primary pigment-producing cells in the body. The VEGF/VEGFR axis has been extensively investigated for its potential as a biomarker for diagnosing and predicting melanoma, as noted by Malekan et al. [1]. Advances in understanding the disease's pathophysiology have led to the development of new treatment modalities, including small molecule kinase inhibitors and immune checkpoint inhibitors, according to Lopes et al. [2]. Recently, there has been growing interest in the therapeutic potential of natural bisindole alkaloids, sourced from marine and terrestrial environments, for treating melanoma, as highlighted by Xu et al. [3]. This study focuses on evaluating various natural bisindole alkaloids as potential VEGFR2 inhibitors for melanoma treatment. Using Biovia Discovery Studio 2024, we generated a structure-based pharmacophore model to screen these compounds. Molecular docking studies were performed with the VEGFR2 receptor (PDB ID: 2OH4*)* [Hasegawa et al. [4]] to assess their binding affinity. The compounds that passed the pharmacophore filter were further analyzed through ADMET filtering to predict drug-like properties. The selected compounds underwent molecular dynamics simulations to evaluate the stability of their complexes with VEGFR2. These *in silico* results helped identify potential inhibitors that interact with VEGFR2, which will be validated through bioactivity-based testing.

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Choice of mode of presentation: Poster
Name of the presenter: Aditi Pawankumar Agarwal
Date of birth: 27/09/1999

P-9

"Design and modification of leelamine derivatives for their chemotherapeutic interest"

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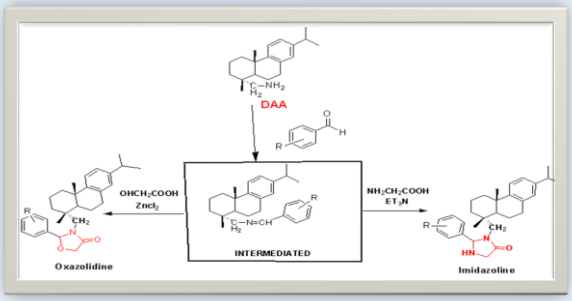
Abstract:

Cancer emerges as a significant global public health issue, with millions of occurrences and deaths annually as per the 2014 WHO cancer report, where 8.2 million cancer-related deaths were documented showing an upward trend. Dehydroabietylamine, which is a natural substance extracted from coniferous trees, possesses various biological activities such as anti-inflammatory, antimicrobial, and anti-tumor effects.) Research has shown that derivatives of DAA exhibit inhibitory effects on different cancer cell lines like MCF-7 (breast cancer), A549 (lung cancer), HepG2 (liver cancer), and HCT116 (colon cancer), indicating a wide-ranging potential for anticancer properties. However, further investigation is necessary to comprehend the mechanisms of action and to potentially improve the growth inhibition activity on cancer cell lines The structural modification of DAA using heterocyclic derivatization has been studied to enhance its effectiveness against cancer. Incorporation of heterocyclic compounds like thiophene, pyrazine, and imidazole into the DAA structure has resulted in the creation of new compounds with better pharmacological characteristics. DAA derivatives with altered heterocyclic rings demonstrate potential as agents for combating cancer. integrating heterocycles into the DAA framework, new compounds with increased cytotoxic effects against various cancer cell lines have been developed.



Keywords: cytotoxic effects, various cancer cell line, Structure-Activity Relationships (SARs), leelamine anticancer drug.

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P-10

Removal of Surfactants onto modified activated carbon derived from agriculture waste as Absorbent

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Abstract

Surfactants, commonly found in industrial, household, and agricultural waste, are a prevalent pollutant in wastewater. The amphiphilic nature of surfactants allows them to accumulate at interfaces (such as air-water or oil-water), disrupting biological membranes and aquatic ecosystems. They are responsible for causing foams in rivers and effluent treatment plants and affect water quality. Their accumulation in water bodies disrupts aquatic life, reduces water quality, and poses a risk to human health. Consequently, treatment process is necessary in order to remove or reduce surfactants from industrial and domestic wastes.This study focuses on the development of a modified eco-friendly and low-cost adsorbent derived from agricultural waste such as orange peel, rice husk, water chestnut , walnut shell etc for the efficient removal of surfactants from wastewater. The adsorbent material is abundant, renewable, and inexpensive, making it a sustainable alternative to conventional adsorbents like activated carbon, which are costly and not biodegradable.The adsorbent was chemically modified to enhance its surface area, porosity, and functional groups, thereby improving its adsorption capacity for surfactants. A series of batch experiments were conducted to investigate the performance of the adsorbent under various conditions, such as different initial surfactant concentrations, pH levels, adsorbent dosages, and contact times.The results demonstrated that the modified adsorbent achieved high removal efficiencies, under optimal conditions.This eco-friendly adsorbent not only provides an efficient solution for surfactant removal but also offers economic and environmental benefits due to its low production cost, biodegradability, and reusability. The study emphasizes the potential for scaling up this technology for industrial applications in wastewater treatment, contributing to sustainable water management practices.

Keywords: Eco-friendly adsorbent, surfactant removal, wastewater treatment, adsorption kinetics, agricultural waste.

P-11

Modified Eco-friendly and Low Cost Adsorbent for Efficient Removal of Dyes from Wastewater

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Abstract

Water pollution caused by environmental wastes such as dyes, polyphenols, pesticides, polycyclic hydrocarbons and heavy metal ions is a serious problem for the environment and living beings due to the severe toxicity and carcinogenic nature of these pollutants. Modifying the adsorbent surface of these adsorbent materials to enhance their adsorption capacity is important for removing pollutants. The raw material used for production of the new eco-friendly adsorbent is widely available across the world in the form of agricultural waste, forest waste and marine waste which makes it industrially produced and its cost is much lower than other commercial adsorbents. It is based on an attempt to replace the high cost-ineffectiveness of activated carbon and other commercial adsorbents. In this study, the removal of organic pollutants such as dye from wastewater using various modified eco-friendly adsorbents by chemical treatment processes. Among these, adsorbent is considered to be the most effective due to its high removal capacity, cost effectiveness, high availability, easy operation, biodegradability and recyclability. The influences of several factors such as initial dye concentration, pH of the solution, temperature, amount of adsorbent on dye adsorption capacity and adsorption mechanisms responsible for dye removal based electrostatic attraction, ion exchange and surface complexation are described.

Key word: Eco-friendly adsorbent, organic pollutants, water treatment,

P-12

Design, Synthesis, In silico and In vitro studies on 1,4-Naphthoquinone Tethered Hybrid Molecules as Anticancer Agents

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Abstract

Hybrid molecules offer an innovative approach to the treatment of multifactorial diseases like cancer that involve several biological pathways and targets. Cancer is one of the most dreaded diseases in the world, characterized by the rapid and uncontrolled growth of abnormal cells beyond typical limits. Female breast cancer is one of the most common cancers across the globe, ranking top among 36 types of cancer, including lung, colorectal, prostate, and stomach cancers. In silico docking and ADMET-based screening were applied to an in-house library of virtual hybrids of 1,4-naphthoquinone with natural terpinols and amines. The designed hybrid molecules were docked with anticancer targets, EGFR containing the T790M Resistance Mutation (PDB: 4RJ3) and 4,5-diarylisoxazole Hsp90 chaperone (PDB: 4RJ3) on AutoDock vina. The top hits were screened on the parameters of physicochemical and absorption, distribution, metabolism, excretion and toxicity (ADMET) on SwissADME and pkCSM online servers. Finally, ten compounds were synthesized and evaluated for their in vitro anticancer activity against the human breast carcinoma cell line MCF-7. The 1,4-naphthoquinone-thymol hybrid exhibited the highest anticancer activity (IC50= 4.59 µg/mL), while the rest showed IC50 values in the range of 12.28- 62.98 µg/mL. Our study suggests that may be a suitable drug candidate for the treatment of human breast cancer.

Keywords: Hybrid molecules, docking, 1,4-naphthoquinone, anticancer

P-13

Enhanced Neuroprotective Potential of Marine Dietary Polyphenols: *In Vitro* Biotransformation and Evaluation of Acetylcholinesterase Inhibition for Alzheimer's Disease Treatment

Anushree Gade[1], Maushmi S. Kumar[1*]

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Mode of presentation: Poster
Name of presenter: Anushree Gade
Date of birth: 28/04/1998

Abstract

The gut microbiome plays a crucial role in regulating the pathophysiology of Alzheimer's disease (AD), influencing neuroinflammation and metabolic homeostasis. Dietary polyphenols from brown macroalgae are known for their ability to cross the blood-brain barrier and help prevent the progression of AD (Figueira et al. [1]). When ingested, polyphenols that are not immediately absorbed into the bloodstream undergo transformation by the gut microbiota, leading to the formation of various low-molecular-weight (LMW) metabolites (Marques et al. [2]; Corona et al. [3]). In this study, we conducted *in vitro* biotransformation of polyphenols and examined the inhibitory effects of the resulting LMW polyphenols on acetylcholinesterase, a key enzyme in AD pathology. The polyphenols were characterized using FT-IR, HPLC, and LC-MS/MS before and after biotransformation. Post-biotransformation, we observed a significant enhancement in both acetylcholinesterase inhibitory activity and antioxidant potential. The acetylcholinesterase inhibitory activity of the LMW polyphenols was further investigated through molecular docking, which provided insights into the binding patterns of these compounds to the enzyme. Additionally, we assessed the ADME properties (absorption, distribution, metabolism, and excretion) of these compounds. All *in silico* studies were performed using Biovia Discovery Studio 2024 software. This study underscores the potential of marine dietary polyphenols for neuroprotection against AD.

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P-14

Optimization and Pharmacological Evaluation for the Development of a Novel Combinational Oleoresin Capsicum based Riot Control Formulation.

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Abstract:

Oleoresin capsicum (OC) spray, widely used as a riot control agent (RCA) globally, has been associated with numerous fatal outcomes when used at higher concentrations or for extended periods [1,2]. This has led to severe inflammation and, in some cases, life-threatening effects [3]. Considering the above, a combinational riot control formulation was designed by incorporating an optimized concentration of OC as irritant to incapacitate rioters temporarily, skatole as foul-smelling agent to create disturbances, and a color (triarylmethane) to identify rioters [4]. For this study, all the ingredients were optimized using Box–Behnken design (response surface methodology) by Design expert software (version 13). Which used the dependant variables like Irritation reversibility time by the formulation (minute), color retention time (hrs), tidal volume (ml/kg) and independent variables are triarylmethane (gm), skatole (%w/v), OC (%v/v), surfactant (%v/v). For the evaluation of dependant variable responses *in vivo* experiments using Wistar albino rats were conducted and assigned randomly as test and control group. Text group animals were exposed dermally for colour retention and irritation reversibility study with the triarylmethane and OC respectively, while skatole was given through inhalation exposure for tidal volume measurement using whole body plethysmograph. A total of twenty-nine nano emulsions have been predicted using the Design Expert. Out of which one nanoemulsion with independent variables like triarylmethane (0.5 gm), skatole (2%w/v), OC (1.5%v/v), surfactant (6%v/v Tween 80) and dependent responses 30 minutes of irritation reversibility, 36 hours of color retention time and 0.011345 ml/kg tidal volume, reported the desired and satisfactory outcomes.

Key words: Riot control formulation, Oleoresin capsicum, Box–Behnken design, Optimization, *Invivo* study.

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P-15

"Synthesis, Spectral Studies and Anti-microbial screening of New Pyrazoline Derivatives"

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ABSTRACT:

A series of new 3-{4-[3-(methyl)-4-(2, 2, 2-trifluoroethoxy) pyridin-2-yl]methylamino phenyl}-4,5-dihydro-5-aryl 1-H-pyrazol) (4a-4k) have been articulated by the reaction of 3-aryl-{4-[3-(methyl)-4-(2, 2, 2-trifluoroethoxy) pyridin-2- yl]methylamino phenyl}prop-2-en-1-one(3a-3k) with hydrazine hydrate. The structural elucidation has been made by using Mass Spectrometry, Infrared Spectroscopy and 1H Nuclear Magnetic Resonance Spectroscopy. All lately synthesized derivatives were recognized for their anti-bacterial and anti- fungal activities against two Gram positive, two Gram negative bacteria and one fungi. Anti-microbial evolution of above compounds compared with known standard drugs.

SUMMARY: Synthesis of heterocyclic compound to target the micro-organism.

Keywords: Pyrazol ; Pyridine; Anti- bacterial ; Anti-fungal ; Trifluoroethoxy pyridine

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Development of 7-chloroquinolinyl hydrazone based thiazolidine-4-one analogues as anti-cancer agents by attenuating TLR4 activation

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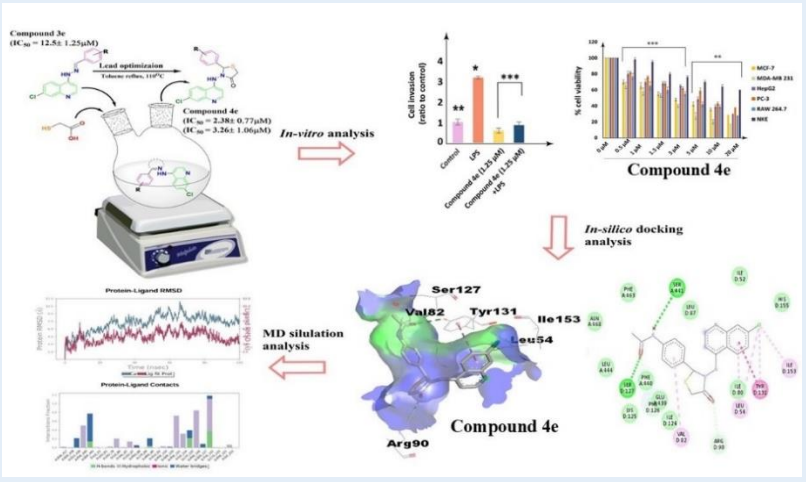
Abstract:

A series of 7-chloroquinolinyl hydrazone based thiazolidine-4-one analogues (**4a-m**) have been synthesized to explore the anti-cancer activity by reducing TLR4 activation. All newly synthesized compounds were evaluated for their anti-inflammatory activities based on their capability to inhibit pro-inflammatory cytokine secretion from the macrophages after stimulation with lipopolysaccharide (LPS). In addition, *in vitro* anti-cancer activities were also searched for these compounds to find a new lead. Six compounds appeared as promising agents for anti-inflammatory as well as anti-cancer activities. Among them **compound 4e** revealed the most promising anti-inflammatory activity at lower micromolar level (**IC_{50} = 2.35µM**). Also, it showed excellent anti-cancer property against triple negative breast cancer cell line (**IC_{50} = 1.54µM**). The mechanism of anti-cancer activity of the potent **compound 4e** was further investigated by using a series of biochemical, molecular and microscopic techniques. Further structure activity relationship (SAR) study followed by MD simulation study was carried out to identify probable binding residues which may play a significant role in developing anti-inflammatory activity for promoting cell apoptosis in cancer cells. Our experimental data revealed that the active moiety i.e. **compound 4e** majorly causes apoptosis in cancer cells by inhibiting TLR4 signaling pathway, and this appears to be the novel functional attribute of this compound.



Keywords: 7-quinolinyl hydrazone derivatives; anti-inflammatory agents; toll-like receptor 4; anti-cancer activity; structure- activity relationship (SAR); MD simulation**.**

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Investigating the Antimicrobial Properties of a Probiotic-Derived Biosurfactant

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Abstract

Microorganisms produce amphiphilic compounds known as biosurfactants, which are increasingly recognized for their unique surface-active properties and potential applications across various industries (Miao, et al [1]). *Lactobacillus* species are commonly used in biosurfactant production due to their Generally Recognized as Safe (GRAS) status (Kachrimanidou, et al [2]). The primary objective of this research is to isolate and characterize a biosurfactant obtained from Greek yogurt produced with *Lactobacillus delbrueckii* subsp. *bulgaricus*. The study outlines the steps involved in isolating the probiotic strain and provides an in-depth description of the subsequent extraction process. This research evaluates the antibacterial and antifungal efficacy of the biosurfactant against pathogenic microorganisms, including *Staphylococcus aureus*, *Aspergillus niger*, and *Escherichia coli*, as well as its emulsifying and detergent capabilities. The isolated biosurfactant exhibits excellent antibacterial and detergent properties, particularly against human pathogens like *Staphylococcus aureus* and *Escherichia coli*. The biosurfactant's characteristics were analysed through foaming tests, emulsifying index, and oil displacement assays (Ewida, et.al [3]). The study highlights the environmental advantages of using probiotics for biosurfactant production over conventional surfactants. The findings suggest that *Lactobacillus delbrueckii* subsp. *bulgaricus* is a promising source of environmentally friendly biosurfactants with strong antimicrobial properties, contributing to the growing evidence supporting probiotics for both health benefits and the generation of valuable bioproducts, marking a significant advancement in microbiology and biotechnology.

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Mode of presentation- Poster presentation
Name of presenter- Ms. Shruti Sandeep Gawde
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P-18

A Paradigm Shift in Platinum Chemotherapy: Unveiling Kinetically Inert Agents

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The quest for improved chemotherapeutic agents to address the deficiencies of the current Pt-based drugs has gained momentum in the new millennium. There has been a disparate effort to develop superior and safer Pt drugs to combat the issues of deactivation, resistance and toxic side-effects. However, the achievements in this area is constrained by sub-optimal pharmacological profiles of the designed drug candidates. [1] Considering the strong correlation between the kinetic lability of the Pt drugs and their limitations, our group has endeavored to address this challenge by methodologically designing substitutionally inert Pt (II) drug candidate (compound **4**). [2] Compound **4** exhibits excellent anti-proliferative activity in a panel of different cancer cell lines, lacks multi-factorial Pt cross resistance and demonstrates notable plasma stability. Noteworthy, compound **4** exhibits remarkable efficacy in both Pt-sensitive and Pt-resistant xenograft models *in vivo* without inducing nephrotoxicity. Mechanistic investigations suggest multi-targeting ability of compound **4** including QDNA and causes oxidative stress in cancer cells. [3]

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P-19

Optimizing IR detection assay condition in cell culture to save time and money

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Abstract:

Insulin resistance (IR) is characterized by the diminished ability of cells to respond to insulin, leading to impaired glucose uptake and altered metabolic homeostasis. IR is associated with number of non-communicable diseases including type 2 diabetes, cardiovascular diseases (CVD), metabolic syndrome, cancers, non-alcoholic fatty liver disease (NASH) and polycystic ovary syndrome (PCOS) which leads to millions of death worldwide. To study IR various cell culture and pre-clinical animal models are available. Sophisticated techniques and instruments are required to study IR in animal/human based models. Thus cell culture based IR studies are majorly used model and has been reported to be carried out by using diverse assays including fluorescence, radiolabelled and colorimetric. For fluorescence and radiolabelled assays not only costly and specialized equipment are required but also they may pose potential threats to health and environment. The colorimetric assay (i.e. Glucose consumption assay) is the only reported method which is simple, effective and efficient to study IR in cell culture model. But this assay itself has number of variabilities such as - a) insulin concentration; b) time of incubation of cells with insulin etc reported in the literature. Therefore, in the present article we addressed these issues and re-standardized the assay conditions by using C2C12 skeletal muscle cell line. Our findings depict that significant glucose consumption occurs either after 6h of incubation with a 200 nM concentration of insulin or after 24h with a 10 nM concentration of insulin. These results of optimized experimental conditions suggest that future studies in the IR using cell culture can be benefitted either to reduce time (by a factor of 4) or decrease costs (by reducing insulin concentration by a factor of 20) depending upon experimental model and avialable resources.

Key words: IR, Glucose Consumption assay, C2C12 cell lines

P-20

Organic framework-based sensors for organophosphorus/phosphate ions used in chemical warfare agents (OP CWAs)

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Abstract

Organic scaffolds have been widely proved to be an excellent chemo-sensors for ions and molecules of importance in human health, safety and environment. They show an incredible potency in sensing inorganic ions which play role in chemical warfare agents (CWA) [1] as well as environmental pollution such as phosphate [2], Hg^{2+}, Pb^{2+} Zn^{2+} and Cd^{2+} [3] with high sensitivity. In addition to this, they are also employed for sensing toxic molecules [4]. Phosphate ion/organophosphorus group is found in various classes of chemical warfare agents such as Tabun (GA), Sarin (GB), Soman (GD) and VX [5]. Therefore, identification of phosphate ion especially in toxic compounds is of utmost importance. Various classes of organic scaffolds have been tested for phosphate ion/organophosphorus binding with high selectivity [6-10]. Supramolecular forces play an important role behind the sensing procedure which include electrostatic interactions, hydrogen bonding and inter-molecular interactions. "Supramolecular/Host-Guest Complexes" are formed during the process. The organic frameworks are designed in such a way that they contain the necessary sensing/signaling/recognizing moiety in their chemical structure which can bind to the target.

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P-21

Exploring Electronic Effect on ESIPT-Driven pH Sensing: Mechanistic Insights and Amines sensing.

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Abstract:

For the excited state-induced photon transfer (ESIPT) phenomenon, the intra-molecular hydrogen bonding strength affects their photophysical properties. Here in this work, we have synthesized substituted 2-(2-hydroxyphenyl) benzothiazole and tuned their electronic structures with different Hammett substituent constants (σ) in the para position of the phenol ring. Theoretical calculation and crystal structure explain the large σ constant, intra-molecular solid hydrogen bonding, and more ESIPT. These probes further employed for amine and the limit of detection (LOD) was found for ammonia and hydrazine to be 28.6 µM and 61.34 nM, respectively. In addition, strip-based detection of spoilage of chicken meat was studied for real-world applications via both contact and non-contact mode.

Figure/Scheme:

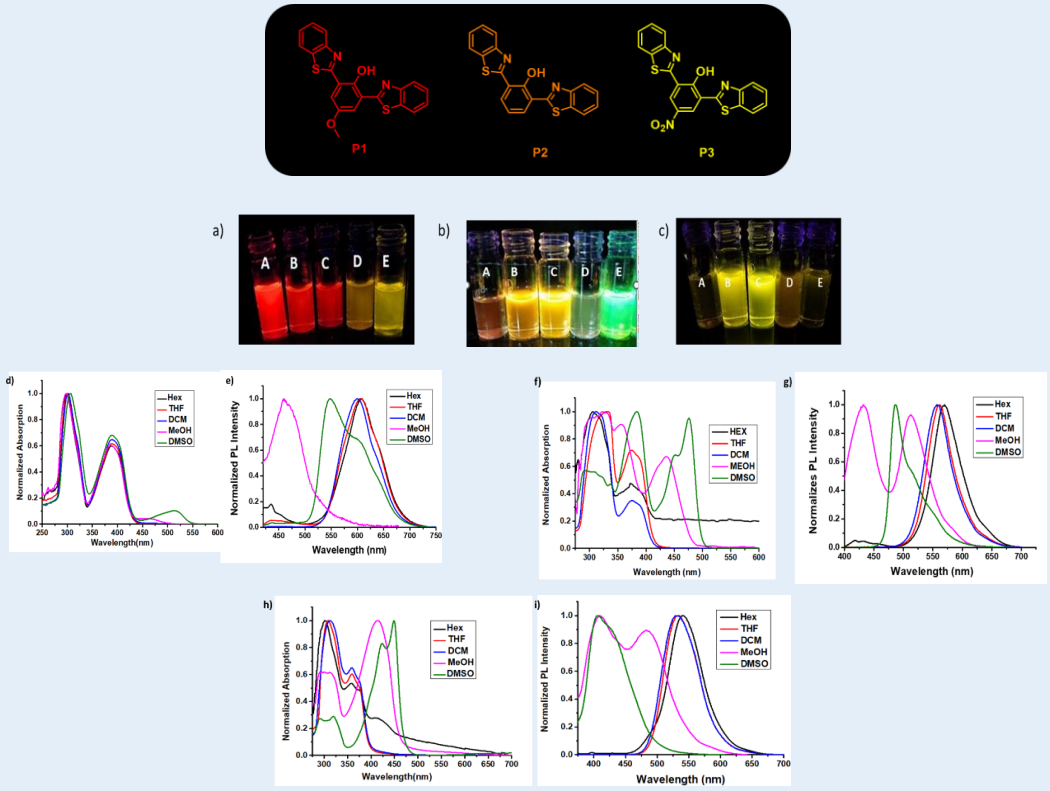

Figure - Photograph of emissions in different solvents A. Hexane, B. THF, C. DCM, D. methanol, E. DMSO, for compound P1 a), P2 b), and P3 c) under UV-lamp (λ_{ex}= 365 nm), absorption spectra d), f) and h); and emission spectra e), g), and i) of P1, P2 and P3 respectively.

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P-22

Application of Computational Chemistry in Drug Discovery

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This research presents an in-depth exploration of molecular filters as essential computational techniques in medicinal chemistry, significantly contributing to drug discovery and development.

The main objective of this research was to make a computational tool with the help of Python programming so that we could screen extensive libraries of compounds, identifying those with desirable drug-like and lead-like properties, such as molecular weight, number of hydrogen donors, number of hydrogen acceptors, topological polar surface area (T.P.S.A.), and LogP. Essential criteria, including Lipinski's" Rule of Five [2], "Mozziconacci Filter [3]," "Van der Waterbeemd Filter [4]," and many other Filters, help in reducing the vast number of potential drug candidates to a manageable subset suitable for further detailed analysis. Our research begins by introducing the concept of molecular properties and filters. And their role in narrowing down the chemical space of large libraries toward predetermined goals by removing unwanted chemical structures and properties.

Using Python programming, a computational model incorporating various molecular properties and filters was developed using multiple libraries, such as RDKit, etc., to facilitate the manipulation of chemical data and the generation of predictive models, streamlining the drug discovery process. We demonstrate the integration of these tools to establish filters for selecting lead compounds, thereby reducing time and cost in the early stages of drug development. This research underscores the transformative potential of computational chemistry in modern drug discovery, showcasing how systematic analysis of molecular properties, enhanced by Python's capabilities, can significantly improve the efficiency and accuracy of drug design efforts.

In future research, I would focus on predicting more accurate B.B.B. permeability and improving B.B.B. scoring. Additionally, developing more advanced computational tools will enhance research quality and effectiveness.

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P-23

Design, synthesis, and biological studies of novel indolyl-keto-acrylonitriles as potent anti-cancer agents

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Cancer is one of the leading causes of death worldwide [1]. A noticeable success rate in cancer research is observed, with diverse groups of antimitotic drugs containing indole moiety, as they are target specific to various cancerous cell lines [2]. Indole and it's derived compounds have been found to display a wide range of biological activities such as; antioxidant, antidepressant, anti-HIV, antiviral, antimicrobial, antituberculosis, anti-cancer, *etc*. Particularly, microtubule targeting agents (MTAs) work primarily by blocking mitotic activity leading to apoptosis in cells [3]. As the search for better MTAs continues over the years, it is observed that colchicine binding site inhibitors (CBSIs) have superior success rate in multi-drug therapy over its contemporaries because they have high therapeutic index and better water solubility [4, 5]. Indole based CBSIs, such as Indibulin, Dragmacidin, Topsentins amongst others have also gained importace over the years, in cancer treatment. Eudistomin K, a indole based marine alkaloid, with antiproliferative activity against the P-388 tumor cell line (IC_{50} = 0.01 µg/mL) has been considered as a lead compound for the design of anticancer agents [6]. Acrylonitrile scaffold has significant chemical importance, and is the center of attention to researchers due to the flexible properties of its conjugated system. The common methods for the preparation of keto-acrylonitriles utilizes Knoevenagel condensation in presence of different bases, involving conventional heating as well as under Microwave irradiation. Yangjie Li *et al*. carried out a series of reactions to provide evidence that glass surfaces accelerate various base-catalyzed chemical reactions like Knoevenagel condensation [7]. The silanolate group not only affect base-catalyzed chemical reactions but also act as base catalysts. Following this analogy, we have devised a green protocol for the successful preparation of various indolyl-keto-acrylonitriles in good to excellent yields, by grinding its precursor indolyl-acrylonitrile with varoius substituted aldehydes in a glass mortar and pestle under solvent-free conditions. Some of the indolyl-keto-acrylonitriles were found to exhibit IC_{50} < 10 µM against selected cancer cell lines. The poster presentation will include design, synthesis and anticancer activity studies of various indolyl-keto-acrylonitriles.

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P-24

Organocatalytic [4+2] annulation between enals and nitro-olefins for the direct synthesis of highly substituted 2-nitro-1,1'-biphenyl: Scope and applications

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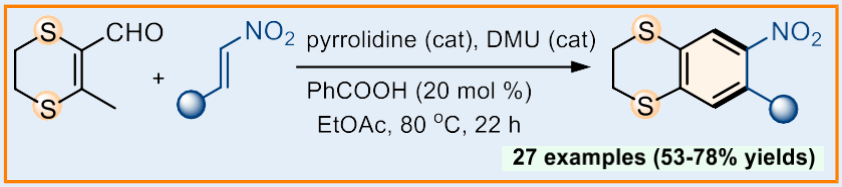
A new strategy for the construction of unsymmetrical biaryls and highly substituted carbazoles. This is an efficient one-pot synthesis of 6-nitro-7-phenyl-2,3-dihydrobenzo[b][1,4]dithiine (1,4-dithiane-fused but-2-enal) was achieved *via* pyrrolidine catalyzed [4+2] benzannulation of in situ generated fused azadiene from 3-methyl-5,6-dihydro-1,4-dithiine-2-carbaldehyde and nito-olefins. Utilizing 1,4-dithiane-fused but-2-enal in this way provided rapid access to various scaffolds. This is a unique metal-free approach for constructing unsymmetrical biaryls and highly substituted carbazoles. This protocol is characterized by mild conditions, excellent functional group tolerance, complete regioselectivity, and atom economy. The successful scale-up synthesis proved the practicality and reliability of this reaction. The details of the method development will be presented.



Scheme 1: Organocatalytic [4+2] annulation between enals and nitro-olefins.

Keywords: 1,4-dithiane-fused but-2-enal, highly substituted carbazoles, nito-olefins.

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P-25

A multifunctional approach for Alzheimer's disease therapy: Novel cholinesterase inhibitors as a neuroprotective agent.

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AD is a neurodegenerative disorder which shows gradual loss of neurons and synapses, mainly within the brains cholinergic system, resulting in loss of memory and other cognitive functions. Nearly 7 million Americans are suffering from AD and about 6.9 million Americans age 65 and older are living with AD in 2024. A multifunctional approach can be used to treat AD by targeting reactive oxygen species, metal chelation, Aβ aggregation, Cholinergic neuron damage. Compounds from natural origin plays pivotal role in multifunctional cure of Alzheimer disease. Design of novel ferulic acid analogues have been done. cholinesterase inhibition studies, AChE,BChE inhibition kinetic studies, measurement of propidium iodide displacement from the peripheral anionic site (PAS) of AChE, evaluation of antioxidant activity have been performed. Evaluation of in-vivo efficiency involves scopolamine induced AD mouse model. Solubility enhancement for drug to cross blood brain barrier and toxicity reduction are main challenges.

P-26

Palladium-Catalyzed Oxidative Alkenylation of 2-Arylindolizines using Allyl Alcohols

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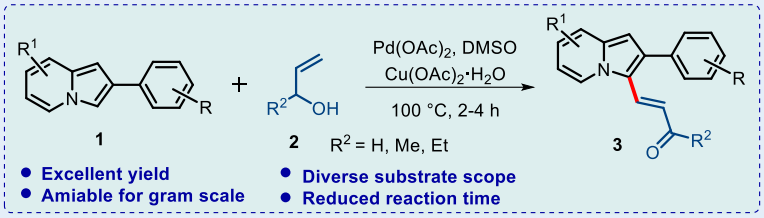
Indolizines are a class of heterocyclic compounds with promising applications in organic electronics, pharmaceuticals, and materials science due to their unique structural properties. The indolizine framework contributes extensively to various medical applications including anti-cancer,[1] anti-viral, anti-inflammatory,[2] and anti-diabetic.[3] Despite their potential, the functionalization of indolizines remains challenging, with conventional methods often requiring prolonged reaction times and harsh conditions.[4] Addressing this limitation, we have developed a novel and efficient Pd-catalyzed method for the C3-functionalization of indolizines using allyl alcohol. Oxidative coupling of 2-arylindolizines (**1**) with allyl alcohols (**2**) in the presence of $Pd(OAc)_2$ and $Cu(OAc)_2 \cdot 5H_2O$ in DMSO produced β-(3-indolizinyl) ketones and aldehydes (**3**) (Scheme 1). Our approach is notable due to its mild reaction conditions and significantly reduced reaction time towards achieving cross-dehydrogenative coupling. The method was applied to diverse substrates, demonstrating good yields and excellent regioselectivity across a range of functional groups. Additionally, the use of allyl alcohol as a reactant provides a versatile platform for further functionalization, enabling the synthesis of a variety of substituted indolizines with potential applications in multiple fields. These findings equip us for further development of indolizines in drug chemistry. Our study emphasizes the utility of palladium-catalyzed reactions in modern organic synthesis, offering a robust tool for the development of heterocycles. Details of the reaction conditions, mechanism, and substrate scope will be presented.



Scheme 1

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P-27

Kinetic and Physicochemical Studies of the Silver Nanoparticles synthesized by Nicotinamide as a Reducing and Stabilizing Agent

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Abstract

In present evaluation silver nanoparticles (SNPs) were synthesized using nicotinamide (NTA) as a reducing agent and cetyltrimethylammonium bromide (CTAB), as a good stabilizing agent by the chemical reduction method. The kinetic study on the formation of SNPs have been performed spectrophotometrically at 410 nm (SPR) in aqueous medium as a function of [$AgNO_3$], [NTA], [NaOH], and [CTAB]. The plot of $\ln(A_\infty - A_t)$ versus time exhibited a straight line and the value of rate pseudo-first-order of different reaction variables. Based on experimental findings a most plausible mechanism was proposed for the formation of SNPs. From the mechanism, it is proved that the reduction of silver ions proceeded through the formation of silver oxide in colloidal form by its reaction with hydroxide ions and nicotinamideafter performing its function, readily undergo hydrolysis to form nicotinic acid as a hydrolysis product with the release of ammonia gas. The preliminary characterization of the silver nanoparticles was done by using UV–Visible spectrophotometer. The detailed characterization of SNPswas also performed using other experimental techniques such asFourier transformed infrared spectroscopy (FTIR), field-emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM), and powder X-ray diffraction (XRD) respectively.

Keywords: Silver nanoparticles, Nicotinamide, Growth kinetics, Transmission electron microscopy

P-28

Microwave-assisted Green Synthesis of Sustainable Zinc Oxide Composites for Effective Sequestration of Crystal Violet

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Cationic dyes such as Crystal Violet, Methyl Violet, Malachite Green, and Methylene Blue may add vibrant colors to industrial products, but their toxicity are alarming. These dyes are carcinogenic, toxic, and persist in the environment, leading to long-lasting contamination in water, soil, and agricultural systems. Their persistent resistance to degradation disrupts plant growth, alters soil chemistry, and throws microbial ecosystems into disarray, resulting in significant ecological harm.

In response to this pressing issue, the process of adsorption has emerged as a powerful and eco-friendly method for depolluting wastewater. This study introduces an innovative approach: preparing zinc oxide nanoparticles using a microwave-assisted biosynthesis method with extracts from the *Annona squamosa* plant. These nanoparticles are then transformed into a nanocomposite designed for superior dye adsorption.

This study involved detailed characterization of prepared nanostructures for structural, chemical, and morphological features. We focused on understanding how Crystal Violet interacts with the nanocomposite, examining variables such as pH, adsorption kinetics, and isotherm models.

Results demonstrated notable adsorption capacities of 151.47 mg g^{-1} and 272.68 mg g^{-1} for crystal violet at an initial concentration of 1000 mg L^{-1}. These findings highlight remarkable potential of this approach for effectively removing toxic dyes for a more sustainable future.

P-29

N1 neuraminidase inhibitor from nature: A computational approach

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Influenza or flu is an infectious respiratory disease that causes approximately 300,000 human deaths globally per year. Different strains of influenza A can infect large number of people and through antigenic shift and antigenic drift, it can lead to a pandemic situation. Though synthetic drugs and vaccines are available for flu treatment, owing to mutation most of the inhibitors attain resistance with time. Various studies revealed that natural compounds become promising antivirals [1,2]. Neuraminidase a surface protein is crucial for viral entry into host cell, making it one of the most promising anti-influenza target for the control and treatment of influenza infection. Hence aim of our research is to identify influenza A inhibitor from natural compounds. We selected diosmin polyphenol determine its inhibitory potential and also compare with FDA drug oseltamivir. In this regard, we performed ADMET prediction, molecular docking, MD simulation and MMGBSA calculation of diosmin and oseltamivir with H1N1 neuraminidase protein. Interestingly, diosmin showed better interaction and stability than oseltamivir.

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P-30

One-Pot, Three-Component Synthesis and Anti-tubercular Activity of New 3-(1-acetyl-2-isonicotinoyl-5-phenyl-2,3-dihydro-1H-pyrazol- 3-yl)-2H-chromen-2-one Derivatives Catalyzed by β-Cyclodextrin for Green Catalysis in Water

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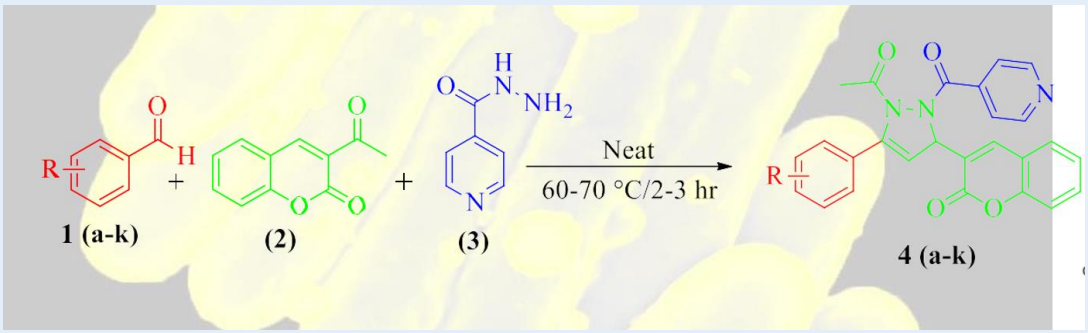
To increase the antitubercular potency, we synthesized a series of novel 3-(1-acetyl-2-isonicotinoyl-5-phenyl-2,3-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one **4 (a-k)** using the one-pot multicomponent reaction of the substituted aldehydes **1 (a-k),** 3-acetyl-2H-chromen-2-one **(2)**, and isonicotinohydrazide **(3)** in the presence of β-cyclodextrin as a supramolecular catalyst in water as the green solvent at 60-70 ºC temperature. The salient features of the green protocol are the one-pot reaction, shorter reaction time, and straightforward workup procedure.



- No toxic catalyst
- No hazardous/toxic solvent
- No tedious reaction set-up
- No chromatographic purification
- Highly atom economic
- Broad substrate scope and yield up to 92%
- Promising anti-tubercular activity

P-31

Biodegradation of Imidacloprid by *Bacillus altitudinis* DG4: A Sustainable Solution

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Mode of Presentation: Poster

Abstract:

Imidacloprid, a neonicotinoid insecticide extensively utilized in agriculture, has elicited concerns over its environmental persistence and potential detrimental effects on non-target creatures. This abstract examines the microbial breakdown of imidacloprid by bacteria as a viable approach to reduce its environmental impact. Bacterial strains proficient in degrading imidacloprid have been identified and characterized, demonstrating various pathways involved in the degradation of this herbicide. Numerous studies have identified essential enzymes, including esterases, glutathione S-transferases (GSTs), and cytochrome P450, that are pivotal in the earliest stages of imidacloprid breakdown. The genetic routes and metabolic intermediates implicated in bacterial degradation processes have been clarified, offering significant insights into the mechanisms facilitating imidacloprid decomposition. Sample sites exhibit distinctive faunal richness, as evidenced by the isolation of 20 bacterial species using BH medium. *Bacillus altitudinis DG4* strain, obtained from contaminated sea sediments, is capable of removing 74% of imidacloprid after 10 days. The biochemical results indicate that all isolates tested positive for catalase, nitrate reduction, and citrate utilization, while exhibiting negative results for urease activity and demonstrating the ability to ferment all carbohydrates. Moreover, the impact of environmental variables such as temperature, pH, and substrate concentration on the efficacy of bacterial-mediated degradation has been examined to enhance degradation conditions. The capacity of the *Bacillus altitudinis DG4* bacterial strain to restore habitats contaminated with imidacloprid is highlighted by its efficacy in diminishing pesticide residues and mitigating related ecological hazards. In summary, comprehending the bacterial-mediated breakdown of imidacloprid establishes a basis for formulating eco-friendly and sustainable strategies to alleviate the environmental repercussions of this extensively utilized pesticide.

Keywords: Imidacloprid, Microbial Degradation, Environment

P-32

Demethylated lignin derived from biorefinery-sourced rice straw spent cake using chemical and microbial methods and its applications

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Choice of mode: Poster presentation

Abstract:

Lignin, being the most abundant naturally available aromatic biopolymer provides a promising alternate, sustainable source for phenolic resins. However, in its current form it cannot be utilized as such and needs modification. Demethylation of lignin to replace methoxy group with more reactive hydroxyl group increases lignin's reactivity and applicability [1]. Rice straw spent cake which is rich in lignin was obtained from 2G bio-refinery. Lignin from rice straw spent cake was extracted by charging the spent cake in pressure reaction vessel with sodium hydroxide, magnesium oxide and water followed by separation of the dissolved lignin in the liquid stream from the solid cake. Action of chemical demethylating agents such as sodium sulfite and hydrogen iodide as well as microbial agents like *Pseudomonas putida*, *Pseudomonas fluorescens* (bacterial) and *Trametes versicolor* (fungal) on lignin was compared. In addition to the above studies, an analysis of physical-chemical and morphologictal properties of all respective demethylated lignins was done using thermogravimetric graph, FTIR, and GPC. The demethylated lignin finds its prospective application in area of thermosetting polymer and fillers.

Keywords: Lignin, demethylation, bio-refinery

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P-33

Renewable phosphine ligands for homogeneous catalysis

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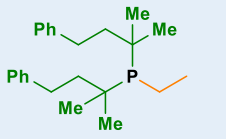
In the pursuit of sustainable catalysis, homogeneous catalysis featuring first-row transition metals has emerged as a prominent avenue. Despite inherent challenges in recycling and reusability, the reliability and comprehensive understanding of the mechanisms underlying homogeneous catalysts make them a compelling choice. Contemporary catalysts employed in organic synthesis often comprise a combination of metals and ligands, necessitating a holistic approach to sustainability that extends to both the metal and the ligand.

This presentation delves into the quest for a truly sustainable homogeneous catalyst, wherein the ligand is sourced from renewable building blocks. Recent investigations have illuminated the potential of biomass-derived molecules as viable precursors for crafting renewable analogues of well-established phosphine ligands, such as those pioneered by Beller.[1]

To address the stereoelectronic requirements crucial for effective phosphine tuning, we have introduced renewable analogues of Stradiotto's phosphine ligands.[2] These analogues are characterized by di-tertiary alkyl substituents and an aryl moiety and are derived from renewable starting materials.

Our research demonstrates that ligands derived from renewable biomass are effective with catalysts based on palladium (Pd), nickel (Ni), copper (Cu), and platinum (Pt), achieving high yields in various reactions and matching the performance of traditional ligands. This approach not only reduces reliance on non-renewable resources but also enhances the sustainability of the chemical industry, aligning with the principles of green chemistry which emphasize minimizing environmental impact through innovative processes and products. This multifaceted approach to sustainable homogeneous catalysis represents a significant stride towards greener synthetic methodologies.



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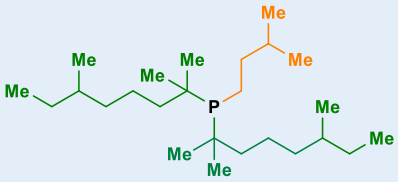

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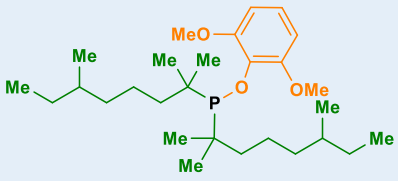

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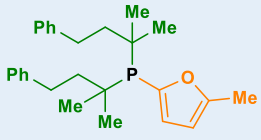

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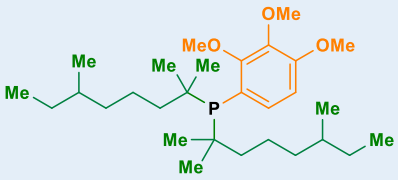

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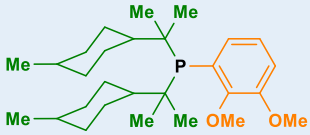

From (−)-α-Terpineol and Guaiacol

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P-34

Paper Sludge waste material For Ethanol Production & their application

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Abstract

The utilization of paper sludge (PS), which is waste from the pulp and paper industry, is described in this review. The advantages of PS make it the cellulosic biomass with the most potential for bio-refinery research and applicability for industrial scale.[i] The selection of yeast strains suitable for simultaneous saccharification and fermentation of waste paper is the aim of this work. The waste paper, as a lignocellulosic material, is represented as an unconventional source for the production of ethanol, which is considered a promising alternative fuel . [ii] Waste paper can be served as a feedstock for ethanol production due to its richness in cellulose and the lack of requirement for energy-intensive thermophysical pretreatment. An efficient process to convert waste paper to ethanol was developed in this study. [iii] A preferred process for the efficient bioconversion of waste paper to ethanol is described. A short saccharification was given to the paper by cellulase enzymes at 45 °C, followed by fermentation in the continued presence of the enzymes at 37 °C. [iv] Ethanol produced from lignocellulosic biomass is viewed as a renewable alternative to diminishing petroleum-based liquid fuels. Two types of waste paper materials, newspaper and office paper, were evaluated for their potential to be used as a renewable feedstock for the production of fermentable sugars via enzymatic hydrolysis of their cellulose fractions.[v]

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5. **Enhanced Enzymatic Hydrolysis of Waste Paper for Ethanol Production Using Separate Saccharification and Fermentation** Published: 20 September 2014 Volume 175, pages 25–42, (2015

P-35

Antipyrine Derivatives and its Biological Activities.

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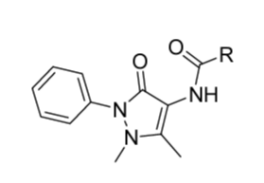
Abstract

4-Aminoantipyrine (4-AAP) or Benzopyrane is a heterocyclic compound containing a ring with two N- atoms and a carbonyl group, which contains an active amine group.[1] A number of researchers found that 4- AAP derivatives are the most valuable due to it is biologically important molecule.[2] There are so many biological activities found in this molecule such as analgesic,[3,4] anti-inflammatory,[5] antimicrobial,[6,7,8] and anticancer activity,[9] anti-tuberculosis, antihelmintic[10].

On the basis above biological activities, we have decided to synthesize several ligands with the help of 4-AAP and several derivatives of aromatic acids. The motifs of synthesized molecule are shown below:-



R= Picolinic acid,cinnamic acid, Pyrrole-2-carboxylic acid, Pyridine-2-carboxylic acid, etc.

After synthesizing several ligands as discussed shown above, we have evaluated for several biological activities and they have shown good to moderate activity.

Keywords: 4-Aminoantipyrine, analgesic, anti-inflammatory, anti-microbial, anticancer.

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P-36

Flavones based imidazole motifs and its Biological Potential

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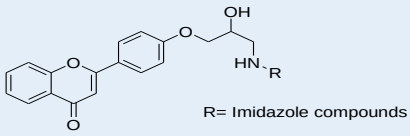
Abstract

Flavones are important class of natural product, found in various plant, fungi, and vegetables having potential pharmacological activities.1 Benzimidazole is a heterocyclic compound which has two N-atoms.2 In recent studies reporting that compound which containing benzimidazole motifs having high potential and have a number of biological activities including antimicrobial ,3 antihelminthic,4 antithrombotic, anti-platelet and anticoagulant,5 anti-inflammatory,6 antiulcer,7 antifungal and acetycholinesterase,8 anti-tubercular,9 antiviral, anti-HIV,10 and antitumour. The β3-adrenoceptor (β3-AR) having several physiologic and metabolic activities that why the involvement of β3-ARs is important in derived molecules.11

On the basis of such effective biological potential, we have decided to synthesize prototypes of flavones derivatives which contain β3-AR linkage, and then the derived ligands were evaluated for their biological activities (cardiovascular disease, diabetes). They have shown result from good to moderate.



R= Imidazole compounds

Keyword: Flavone, benzimidazole, β3-adrenoceptor, cardiovascular disease, diabetes.

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P-37

Phytochemical Investigation and Biological Activity Profiling of *Solanum nigrum* Extracts.

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Background: *Solanum nigrum*, a medicinal plant known for its widespread use in traditional medicine, has been reported to possess a wide range of therapeutic effects. However, systematic isolation and evaluation of its phytochemical components remain understudied, especially concerning their potential anti-inflammatory, antioxidant, and anticancer properties.

Aim of the study: This study was designed to isolate and characterize phytochemicals from *Solanum nigrum* and evaluate their biological activities to explore their therapeutic potential.

Methodology: The plant material was subjected to sequential extraction using hexane, ethyl acetate, and methanol. Phytochemical screening was carried out, followed by the isolation of bioactive compounds through column chromatography. Structural elucidation of the compounds was achieved using UV, IR, NMR, and MS techniques. Biological activities, including antioxidant, anti-inflammatory, and anticancer effects, were assessed using DPPH radical scavenging assay, COX-2 inhibition assay, and MTT assay, respectively.

Results: The study identified key bioactive compounds, including solanine, quercetin, and beta-sitosterol. Methanolic extracts exhibited notable antioxidant activity (IC50 = 25.7 µg/mL), while quercetin-rich fractions showed significant COX-2 inhibition (65% at 50 µg/mL). Additionally, solanine demonstrated cytotoxic effects against MCF-7 breast cancer cells with an IC50 value of 38.2 µg/mL, suggesting its potential as an anticancer agent.

Conclusion: The isolated compounds from *Solanum nigrum* demonstrated promising antioxidant, anti-inflammatory, and anticancer properties, indicating the plant's potential for use in pharmaceutical applications. Further studies are required for in vivo validation and mechanism elucidation.

Keywords: *Solanum nigrum*, solanine, quercetin, antioxidant, anti-inflammatory, anticancer

P-38

Synthesis and Spectroscopic Characterization of Zinc-Carboxylate Metal-Organic Frameworks

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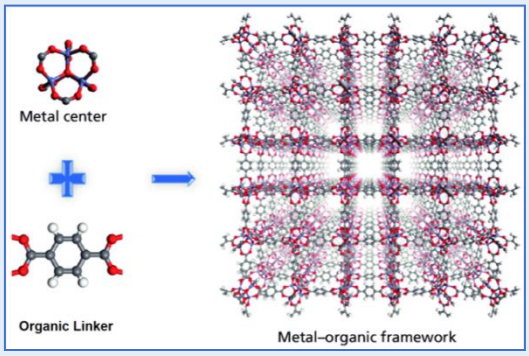
Abstract:

Metal-Organic Frameworks (MOFs) represent a class of crystalline porous materials constructed from metal centers and organic linkers. Their unique architectures and tunable properties have enabled diverse applications in gas storage, separation, catalysis, magnetism, luminescence, and drug delivery. The synthesis of MOFs is significantly influenced by factors such as the choice of metal ions, organic ligands, solvent systems, and molecular interactions like hydrogen bonding and π-π stacking, which direct the self-assembly process. In this study, a zinc-based MOF was synthesized using 1,4-benzenedicarboxylic acid as the organic linker in N,N-dimethylformamide (DMF) under ambient conditions. The synthesized material was analyzed using Fourier Transform Infrared Spectroscopy (FTIR) to identify functional groups, Scanning Electron Microscopy (SEM) to study surface morphology, and X-Ray Diffraction (XRD) to determine its crystalline structure. The structural and spectroscopic data will be presented, highlighting the material's potential for advanced functional applications.



Keywords: Metal-Organic Frameworks, Zinc MOFs, FTIR, SEM, XRD, Crystalline Porous Materials.

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P-39

Pharmacognostical Evaluation of *Cassia occidentalis* and Comparative Phytochemical Analysis with *Cassia floribunda*

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The study examines the pharmacognostical features of *Cassia occidentalis*, a medicinally significant plant, and comparative phytochemical analysis with *Cassia floribunda* to develop quality standards for development of authentic drug i.e. Ayurvedic, Siddha, Unani, and Homoeopathic (ASU&H) drug formulations. *C. occidentalis* is traditionally employed in managing fractures, inflammation, and hepatotoxicity, due to its bioactive constituents such as flavonoids and anthraquinones. The plant extract has been patented by CSIR-CDRI for osteoporosis treatment, owing to the presence of flavonoids such as isovitexin. Therefore, this study focuses on the morphological and microscopic evaluations of its leaves, stems, and seeds, revealing diagnostic features like dorsiventral leaf architecture, xylem vessel patterns, and calcium oxalate crystals, stone cells, which aid in its identification and standardization. Furthermore, comparative phytochemical analysis of different plant parts of *C. occidentalis* and *C. floribunda* was done using thin layer chromatography (TLC) to assess the marker compounds namely Dihydroxyflavone, Trihydroxyflavone, Tetrahydroxyflavone, and Isovitexin (Apigenin-6-C-glucoside) & emodin. The research aligns with the principles of pharmacognosy, emphasizing the botanical standardization and development of pharmacopoeial parameters for ASU&H drugs. The Botanical Reference Standards (BRS) repository plays a crucial role in ensuring the authenticity and quality of plant-derived raw materials. This study supports the development of reference standards for ASU&H drug formulations and contributes to the repository of Botanical Reference Standards, ensuring the reliability of traditional medicine practices. It also underscores the value of pharmacognostic training for stakeholders, enhancing the standardization of herbal drugs.

Keywords: Pharmacognostical Evaluation; Isovitexin; Ayurvedic, Siddha, Unani, Homoeopathic (ASU&H), Thin Layer Chromatography (TLC), Microscopic Evaluation, Herbal Drug Standardization

P-40

Design, Synthesis, and Computational Analysis of a Novel Progesterone Oxadiazole Derivative with Anticancer Potential

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Abstract:

A derivative of progesterone oxadiazole was synthesized through the substitution of the α-hydrogen of acetyl progesterone. The compound was characterized using advanced spectroscopic techniques, including FT-IR, ^{1}HNMR, ^{13}CNMR, UV-vis, and mass spectrometry, along with elemental analysis. Quantum chemical calculations were conducted using the **DFT-B3LYP** method with the **6-311G(d,p)** basis set. The FT-IR spectrum was extensively interpreted through normal coordinate analysis, revealing vibrational absorptions at 1520 and 1505 cm^{-1}, which correspond to theoretical values of 1539 and 1513 cm^{-1}, confirming the formation of the oxadiazole ring. In the ^{1}HNMR spectrum, two methyl group peaks at 0.67 and 1.84 ppm, along with the absence of the acetyl methyl peak at 2.40 ppm, indicate the participation of the acetyl methyl group in forming the oxadiazole ring. This is further supported by ^{13}CNMR peaks at 167 and 171 ppm. Experimental data showed minimal deviation from theoretical predictions in most cases. The calculated electronic transitions within the molecule were identified as $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$. The rotational barrier between conformers I and II in the gas phase was determined to be 3.6474 kcal/mol. The compound exhibited a static hyperpolarizability (β_0) of 6.46×10^{-30} esu, highlighting its potential for non-linear optical (NLO) applications. ADME-based toxicity parameters were assessed, and anticancer activity was evaluated against **MDA-MB-231**, **MCF-7**, and **DU145** cell lines. The results revealed cytotoxicity, apoptosis induction, and effects on cell cycle progression, providing valuable insights for future clinical trials.

P-41

Comprehensive Exploration of Ampicillin-Schiff Base Complexes: Synthesis, DFT Insights, Molecular Docking, and Biotherapeutic Applications

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Abstract

The studies investigate the synthesis, characterization, and biotherapeutic potential of ampicillin-derived Schiff base metal complexes. Schiff bases were synthesized via condensation reactions with ampicillin and coordinated with transition metals to form mixed-ligand complexes. The structures were confirmed through FTIR, UV-Vis spectroscopy, NMR, and elemental analysis. Density Functional Theory (DFT) studies revealed optimized molecular geometries and electronic properties, including HOMO-LUMO energy gaps of 7.08 eV, 6.72 eV, and 6.05 eV for LM1, LM2, and LM3, respectively, suggesting varied reactivity and stability among the complexes. Molecular Electrostatic Potential (MEP) analysis further identified regions of potential electrophilic and nucleophilic interactions. Biological evaluations highlighted significant antimicrobial and anticancer activities. Antimicrobial screening against *Mycobacterium tuberculosis* H37Ra demonstrated over 90% inhibition for specific complexes at 100 µM, with MIC values supporting their potency. Cytotoxicity studies on SiHa cervical cancer cells indicated dose-dependent activity, with IC50 values of 80 µM and 100 µM for the most active complexes. Ex vivo macrophage studies showed substantial bacterial reduction over 72 hours, corroborating their antimicrobial efficacy. Molecular docking against AKT kinase revealed strong binding affinities, with binding energies as low as -7.08 kcal/mol, underscoring their anticancer potential. This integrative study establishes ampicillin-Schiff base metal complexes as promising candidates for dual antimicrobial and anticancer therapies. The integration of experimental techniques with computational insights provides a solid foundation for advancing their development in biotherapeutic applications.

Keywords: Ampicillin-Schiff Base Complexes, HOMO-LUMO Energy Gap, Antimicrobial Activity, Molecular Docking, DFT Analysis

P-42

Metal-free α-alkynylation of α-Fluoroacetoacetamides employing alkynyliodonium salt

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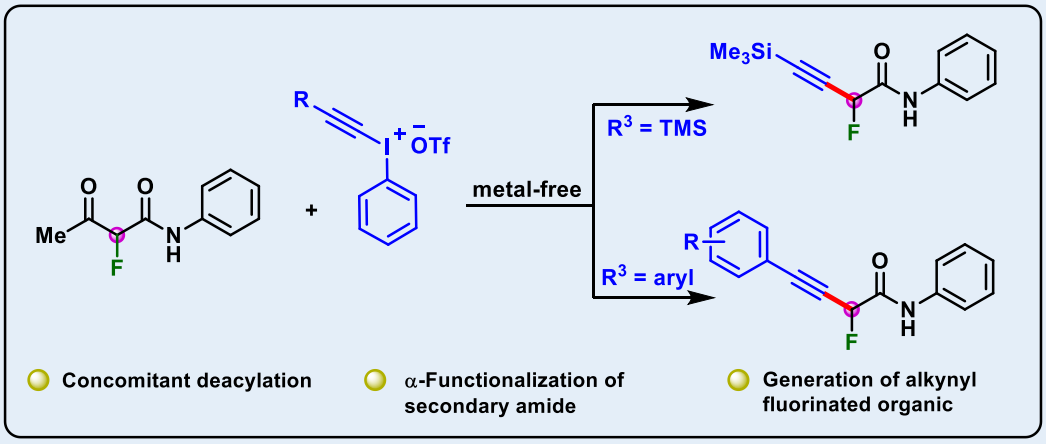
Abstract

A mild and efficient metal-free electrophilic α-alkynylation of α-fluoroacetoacetamide was developed using versatile class of alkynylating agent alkynyl hypervalent iodonium salts (AHIs). Nonetheless, the fluorine has found a pivotal role in both pharmaceutical and agrochemical industries with approved drugs containing at least one fluorine atom. The protocol provides a convenient metal-free method of trimethylsilyl protected α-alkynylated fluoroacetamides were obtained via concomitant deacylation process to yield the α-fluoro-propargyl amides in good yields. In addition, this direct α-alkynylation protocol works efficiently with arylethynyl(mesityl)iodonium salts thereby widening the scope even further.



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P-43

Designing of Metal-Organic Frameworks for their Promising Applications

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Metal-Organic Frameworks (MOFs), owing to their wide-ranging applications have emerged as versatile materials over the past few decades, in industries. These materials consist of crystalline structures built from metal nodes and organic linkers, designed using the “node-and-spacer” and “secondary building unit” concepts. In hybrid porous MOFs, solvents act as primary templates, promoting the formation of neutral frameworks and equilibrated structures. This review provides a comprehensive understanding of MOF structures, focusing on their organic and inorganic building blocks. Various conventional and non-conventional synthetic strategies for MOF development are discussed, highlighting the advancements in tailoring their properties for specific applications. A key aspect of MOFs is their ability to customize pore sizes, enabling compatibility between the material's surface and guest molecules. This adaptability is crucial for their use in adsorption processes and other industrial applications. MOFs' exceptional gas storage capabilities, presenting them as promising candidates for renewable energy solutions. Their ability to store gases like hydrogen and methane makes them potential alternatives to traditional energy sources. Moreover, the strong adsorption capacities of MOFs position them as effective materials for environmental remediation and toxicological research. Overall, this study emphasizes the significant role of MOFs in advancing sustainable technologies. By exploring their structural features, synthetic routes, and applications, this review offers valuable insights that will aid future research and development in energy, environmental, and chemical sectors.

Keywords: Secondary Building Unit (SBUs), Porous Materials, Adsorption, Tunability.

P-44

Study of Some Biologically active Bismuth-Based Mixed-Ligand Complexes

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Abstract

Thiosemicarbazones (TSCs) are versatile ligands in coordination chemistry, known for their ability to form stable complexes with various metal ions due to their multiple binding sites. These sites include sulfur atoms, primary amine nitrogens, and imine nitrogens, enabling TSCs to adopt diverse geometries and structures. This flexibility results in a wide range of chemical and biological properties, making them valuable for medicinal and catalytic applications. The coordination behavior of TSCs often enhances the bioactivity of their metal complexes compared to the free ligands. Bismuth complexes containing TSCs have gained attention due to their promising medicinal potential. Bismuth and its compounds are recognized for their biological safety and low toxicity, which have made them suitable for use in pharmaceuticals, catalysis, and chemical synthesis. The biological activity of bismuth complexes is often influenced by the choice of ligands, and the unique properties of TSCs contribute significantly to this effect. Review of existing studies reveal a significant gap in research on mixed-ligand bismuth(III) complexes containing TSCs. Addressing this gap, we synthesized a series of mixed-ligand bismuth complexes by incorporating thiosemicarbazone as the primary ligand in along with hetero co-ligands. These complexes were thoroughly characterized using molar conductivity measurements, UV-Vis spectroscopy, FT-IR spectroscopy, and ^{1}H-NMR spectroscopy to explore their structural and functional properties and they were evaluated for their biological applications. The present paper describes the synthesis and characterization of some mixed-ligand bismuth(III) complexes containing thiosemicarbazone ligand and hetero co-ligands, along with an evaluation of their structural, functional, and biological properties.

Key words: bismuth complexes, thiosemicarbazone, geometry, synthesis, biological activity

P-45

Green Synthesis of Coupled Metal Oxide ZnO/SnO_2 Nanocomposite for Wastewater Treatment

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Abstract

Water contamination is health alarming and life-threatening problem for aquatic eco-system and human health as well.[1,2] Therefore, it is prime concern to treat the wastewater and remove off the water contamination before discharge them into main stream of water. For the remediation of wastewater, advanced oxidation process (AOP) has become an important chemical treatment method for mineralization of organic contaminants into smaller fragments or inorganic mineral ions.[1,2] Due to p-n junction formation, low band gap, high thermal and chemical stability of $ZnO\text{-}SnO_2$ nanocomposite, coupled metal oxide $ZnO\text{-}SnO_2$ nanocomposites have been synthesized via greener approach by varying the mole ration of Zn:Sn i.e. 1:1, 2:8, 4:6, 6:4, 8:2 and nanocomposites identified as ZS-A, ZS-B, ZS-C, ZS-D and ZS-E, respectively. Crystallinity and phase purity of all five synthesized nanocomposites was ensured by powder x-ray diffraction (PXRD) analysis. Optical properties of synthesized samples were analyzed by ultraviolet diffuse reflectance spectroscopy (UV-DRS) and textural properties were confirmed by BET analysis. Morphological analysis was examined by scanning electron microscopy (SEM) and transmission electron microscopic (TEM) analysis.

Further, $ZnO\text{-}SnO_2$ nanocomposites were employed as an efficient photocatalysts for the degradation of methylene blue under UV-visible halogen lamp (500 W) irradiation. It has been found that ZS-E nanocomposite exhibits maximum photodegradation efficiency (60%) as compared to ZS-A, ZS-B, ZS-C, ZS-D nanocomposites. Furthermore, degradation efficiency, recyclability, degradation mechanism and kinetics also have been discussed.

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P-46

Development of novel TSPO ligands for the treatment of psychiatric disorders

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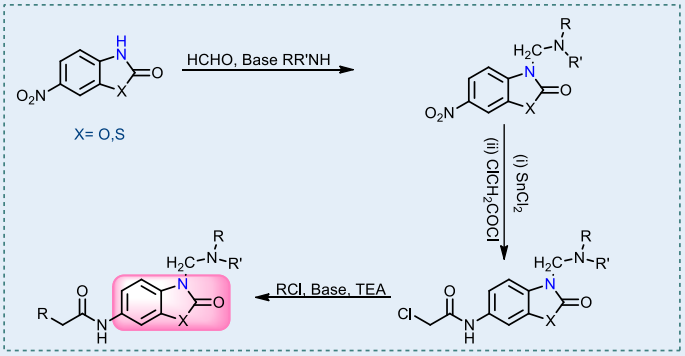
The 18kDa translocator protein (TSPO) plays a role in various physiological and pathological conditions, such as anxiety, depression, and neurodegenerative diseases. Consequently, TSPO ligands are being investigated as potential treatments for these conditions. However, the current TSPO ligands face limitations, including poor pharmacokinetic properties and undesirable side effects. To address these issues, the researchers set out to design and synthesize novel benzoxazolone derivatives as TSPO ligands with enhanced pharmacokinetics and fewer side effects.

The goal of this work is to develop potential therapeutic agents for psychiatric disorders with fewer side effects. The research approach involved the design, synthesis, and structure-activity relationship (SAR) analysis of novel benzoxazolone derivatives as TSPO ligands. A series of 5-phenyl benzoxazolone derivatives were synthesized, incorporating various substituents at the amide group and the C-5 position of the benzoxazolone ring. The binding affinity of these compounds to TSPO was evaluated through a radioligand binding assay. Additionally, a pharmacophore model study was conducted to identify the key structural features necessary for effective TSPO binding.

We synthesized and evaluated a series of benzoxazolone derivatives as a new class of potent TSPO ligands, with potential therapeutic benefits for psychiatric disorders. The pharmacophore model study revealed that effective binding to TSPO requires three hydrophobic groups and a hydrogen bond acceptor within the ligand molecule. Overall, the findings of this research offer a promising pathway for developing novel TSPO ligands that exhibit improved pharmacokinetic properties and fewer side effects, paving the way for their use in treating psychiatric disorders.

Keywords: Psychiatric disorders, TSPO ligands, Benzoxazolone, Anxiety.



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P-47

Regioselective synthesis of polycyclic heteroarenes as carcinoma cells growth inhibitor

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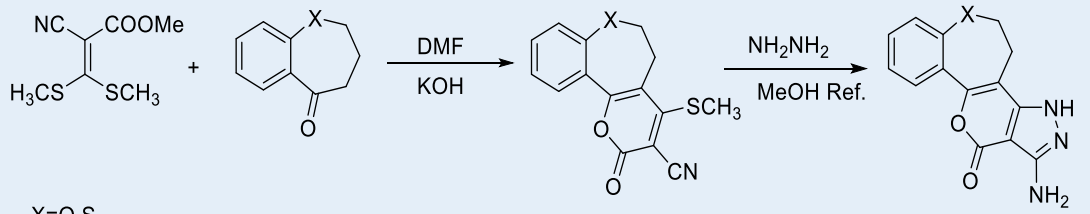
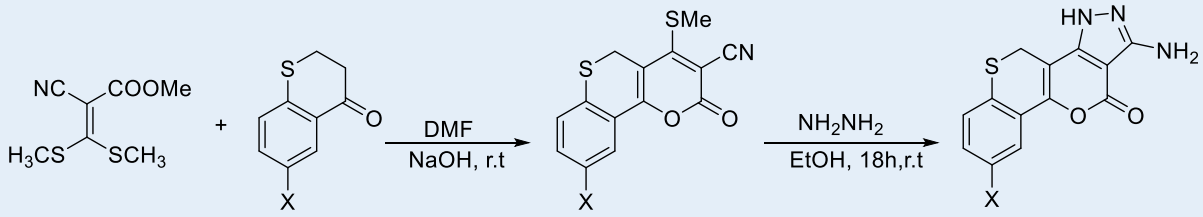
Abstract

An efficient regioselective synthesis of polycyclic diheteroaryl[b,d]diazepines has been reported through ring transformation reaction of 2-oxo-2,5-dihydrothiochromino[4,3-b]pyranes(3,4),2-oxo-5,6-dihydro-2H-benzo[b]pyrano[2,3-d]oxepine and 6-oxo-3,6-dihydro-2H-benzo[1,2-b]pyran [2,3-d]oxepine by hydrazine, at ambident and reflux temperature. None of the compound showed cytotoxicity in normal IEC-6 cells and resulted in killing of colo-205 cells. Further, caused apoptosis through a cascade of mitochondrial pathway in colo-205 cells indicating anti-cancerous potential against intestinal cancer.



Scheme-1



Scheme-2

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P-48

1,1′-Bis-(diphenylphosphino) ferrocene appended d^8- and d^{10}-configuration based thiosquarates: the molecular and electronic configurational insights into their sensitization and co-sensitization properties for dye sensitized solar cells

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A typical DSSC setup involves a photo-anode with a light harvester on a semiconducting material (such as nanocrystalline TiO_2), a counter electrode, and a redox mediator [1]. Amongst all these components, the photosensitizer, a crucial component, plays a key role in the overall efficiency of the DSSC [1,2]. Several ways have been proposed to improve photovoltaic efficiency in DSSCs, with co-sensitization being one of them [3]. Three new d^8- and d^{10}-configuration based 1,1′-bis-(diphenylphosphino) ferrocene (dppf) appended thiosquarates complexes with general composition $[M(mtsq)_2dppf]$ (M = Ni^{2+} (**NiL₂**); Zn^{2+} (**ZnL₂**) and Cd^{2+} (**CdL₂**)) (mtsq = 3-ethoxycyclobutenedione-4-thiolate) have been synthesized and characterized spectroscopically as well as in case of **NiL₂** by single crystal X-ray diffraction technique. The single crystal X-ray analysis reveals square planar geometry around Ni(II) in **NiL₂**, where Ni(II) coordinates with two sulfur centres of two mtsq ligands in monodentate fashion and two phosphorus of a dppf ligand in chelating mode. The supramolecular architecture of **NiL₂** is sustained by intermolecular C–H···O interactions to form one-dimensional chain. Further, the application of these newly synthesized complexes as sensitizers and co-sensitizers/co-absorbents with ruthenium based N719 sensitizer in dye-sensitized solar cells (DSSCs) have been explored. The DSSC set-up based on **NiL₂** offers best photovoltaic performance with photovoltaic efficiency (η) 5.12%, short-circuit current (J_{sc}) 11.60 mA cm^{-2}, open circuit potential (V_{oc}) 0.690 V and incident photon to current conversion efficiency (IPCE) 63%. In co-sensitized DSSC set-up, **ZnL₂** along with state-of-the-art N719 dye displays best photovoltaic performance with η 6.65%, J_{sc} 14.47 mA cm^{-2}, V_{oc} 0.729 V and IPCE 69%, thereby showing an improvement by 15.25% in photovoltaic efficiency in comparison to the photovoltaic efficiency of N719 sensitized DSSC set-up. Variation in co-sensitization behaviour have been ascribed to the differences in the excited state energy level of co-sensitizers. The **ZnL₂** and **CdL₂** have a higher energy level position than N719 dye, allowing efficient electron transfer to N719 during light irradiation, while excited state of **NiL₂** is lower than N719 dye, preventing photoexcited electron transfer to N719, resulting in its lowest overall efficiency among the three co-sensitized DSSC setups.

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P-49

C–H Allylation and Tandem Cyclization of Late-Stage Drug Candidate 2-Aryl Quinazolinones with Cyclic Carbonate

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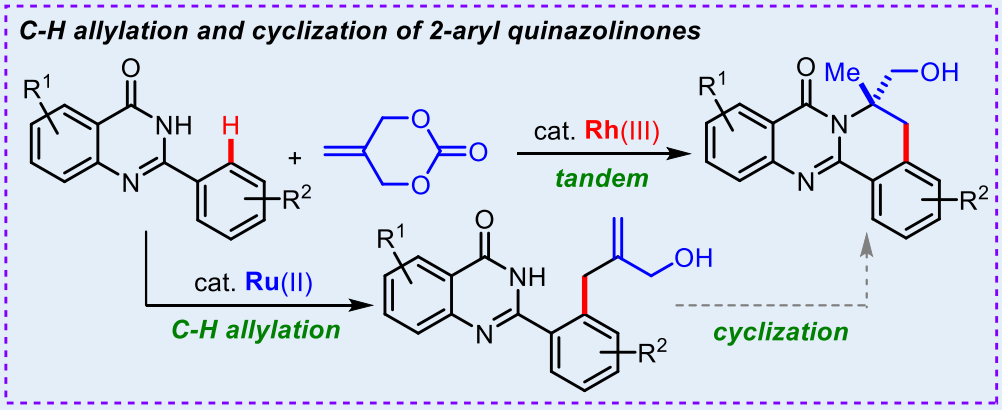
Quinazolinone motif is a prevalent nitrogen-heterocyclic scaffold present in various biologically active natural products and pharmaceuticals, that exhibit anti-inflammatory, antidiabetic, antitumor, antimalarial, and anticonvulsant, activities. The applicability of quinazolinone is also emphasized by using quinazolinone-based metallacycle as a photoredox catalyst. Thus, site-selective variation of quinazolinone framework still remain on demand in organic synthesis and material chemistry. Based on directing group capability and nucleophilic feature of unmasked quinazolin-4(3*H*)-one motif, recent efforts have been made in the C–H functionalization and tandem cyclization of 2-aryl quinazolinones with range of coupling partners under various transition metal catalysts such as Co(III), Pd(II), Ru(II), Ir (III), and Rh(III) catalysis. With a rational design on tandem allylation[1] and cyclization, in this poster, I will present the ruthenium(II)-catalyzed C–H allylation and rhodium(III)-catalyzed C–H/N–H cyclization of 2-aryl quinazolinones with 2-methylidene cyclic carbonate.[2] Notably, intramolecular cyclization under rhodium(III) catalysis was successfully achieved in the presence of organic acids to delivered a tertiary carbon center with primary alcohol, that can be employed into various synthetic transformations.



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P-50

Advanced Exploration of Schiff Base Metal Complex: Synthesis, Computational Studies, and Therapeutic Potential

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Abstract

This research delves into the synthesis, structural characterization, and biomedical potential of Schiff base metal complexes derived from ampicillin. These complexes were formed through condensation reactions involving ampicillin and transition metals, resulting in mixed-ligand frameworks. Structural confirmation was achieved using FTIR, UV-Vis spectroscopy, NMR, and elemental analysis. Computational approaches employing Density Functional Theory (DFT) provided insights into molecular geometry and electronic properties. The evaluation of HOMO-LUMO energy gaps revealed variations in reactivity and stability among the complexes. Additionally, Molecular Electrostatic Potential (MEP) analysis identified regions prone to electrophilic and nucleophilic interactions, offering a deeper understanding of their chemical profiles.Molecular docking studies targeting the AKT kinase demonstrated robust binding interactions and favorable binding energy values, highlighting significant anticancer potential. Biological evaluations further confirmed the dual-action capabilities of these complexes, with notable antimicrobial and anticancer activities.This integrative study combines experimental techniques with advanced computational analyses, paving the way for the development of Schiff base metal complex as innovative therapeutic agents. The findings establish a strong basis for their future applications in combating microbial infections and cancer.

Keywords: Schiff base metal complexes, therapeutic applications, HOMO-LUMO energy gaps, molecular docking, DFT analysis, MEP mapping.

P-51

New isomeric phenylmercury(II)-dithiocarbamates: Influence of positional isomeric phenolic group on supramolecular framework

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Abstract

The positional isomeric phenolic -OH functionalized phenylmercury(II) dithiocarbamates with general compositions [PhHgdtc] (dtc = N- benzyl-N-2-hydroxybenzyl (Hg-1); N- benzyl-N-3- hydroxybenzyl (Hg-2) and N- benzyl-N-4-hydroxybenzyl (Hg-3)) have been synthesized and characterized spectroscopically as well as by single crystal X- ray diffraction technique. The immediate geometry around Hg(II) in all the three isomeric complexes are distorted linear satisfied by one sulfur of the dithiocarbamate ligand and phenyl carbon. Another doubly bonded sulfur of dtc ligand exhibits intramolecular Hg···S Spodium bonding (SpB) interaction and is responsible for the distortion in the linear geometry around Hg(II). The supramolecular framework of all three complexes are stabilized by weak intermolecular Hg···S SpB interactions along with S···H, C···H and O···H intermolecular interactions. The isomeric positions of –OH group affects the supramolecular frameworks engendering single helical motifs held by O-H···C(Ar) and pair of O-H···S and C-H···S interactions in Hg-1 and Hg-3 respectively. While, Hg-2 displays two dimensional sheet like motif sustained by (Ar)C-H···O interactions. These interactions further have been investigated and correlated using Hirshfeld surface analyses and computational studies. The QTAIM and NBO analyses indicate that for Hg-2, the computed intermolecular Hg···S SpB bonding interaction energy is highest (3.64 kcal·mol^{-1}).

Keywords: Dithiocarbamate, Hirshfeld Surface, Single crystal X-ray Diffraction

P-52

Development of a Benzimidazole-Based Compound for Non-Melanoma Skin Cancer Treatment: Computational and Synthetic Approaches

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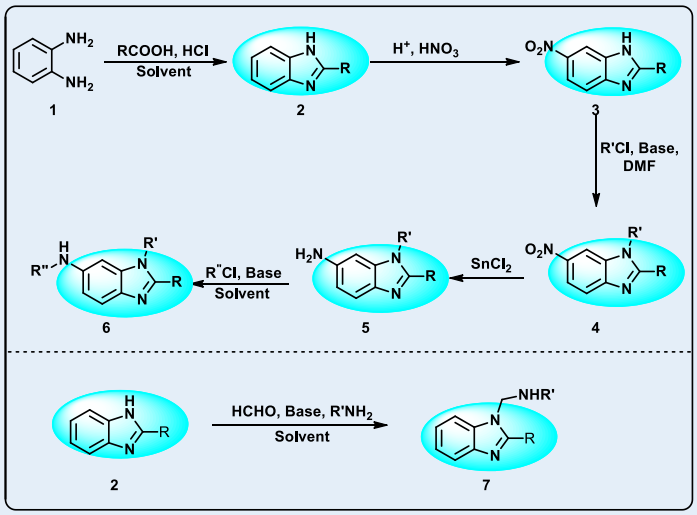
Benzimidazole have wide property pharmaceutical industry. Many of the benzimidazole derivatives are synthesized which show their presence in various drugs having distinct pharmaceutical properties such as Candesartan cilexitil, Telmisartan (AT1 receptor antagonists), Azilsartan, Aedoxomil, and Mibefradil, are used as antihypertensives drugs, Benoxaprofen and Timegadine are used as anti-inflammatory drugs, Bendamustine as antitumor drug, Astemizole and Emedastine are used as antihistaminic analogous, Mizolastine used for treatment of allergic rhinitis, Albendazole, Oxibendazole, and Mebendazole to treat parasitosis, bis-benzimidazole derivatives are active compounds in interfering with DNA topoisomerase, cytotoxic against breast adenocarcinoma (MCF7) and skin epidermoid carcinoma (A431), Methyl-2-benzimidazole carbamate (carbendazim, FB642) is an anticancer agent induces apoptosis of cancer cells, Omeprazole(proton pump inhibitor) and Rabeprazole for the treatment of gastric ulcer, 2-mercaptobenzimidazole derivatives for anticonvulsant activity, Hoechst 33258 and Netropsin for antioxidant activity, Albendazole for antimicrobial treatment, Enviradine as antiviral, 2-mercapto benzimidazole 4-thiazolidinone and 2-mercapto benzimidazole 1,3,4-oxadiazoles are used as antidiabetic analogous etc. Some Benzimidazole such as 5-chloro and 5,6-dichloro-2-substituted derivatives exhibit specific activity against several viruses such as influenza, human cytomegalovirus, hepatitis B virus (HBV), hepatitis C virus (HCV) and (HIV-1). Cancer is the most common disease created by Apoptosis cause death. The most critical problem tries to solve by the Benzimidazole derivative and we decide that, developed new path reaction and design Novel diaryl Benzimidazole derivative and molecule contain vinyl or allyl position because in other previous work this type of derivative has very anticancer property and low cytotoxicity.



P-53

Nanotized Tungsten metal: OER electrocatalysis and Energy Storage applications

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The use of nano-sized metals for electrochemical applications is widespread. Au (El-Sayed et al. [1]), Ag (Zahran et al. [2]) and Cu (Barreto et al. [3]) nanoparticles (NPs) commonly find electrochemical applications. Herein, we report low-temperature nanotized tungsten (W NPs) that can act as an oxygen evolution reaction (OER) electrocatalyst and electrochemical energy storage material. The W NPs were physicochemically characterized via PXRD (Powder X-ray Diffraction), FTIR (Fourier Transform Infrared) Spectroscopy and Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy (SEM-EDS). The Gamry Reference 600 ZRA electrochemical impedance workstation was used to carry out the electrochemical characterization. The electrochemical evaluation was performed through Cyclic Voltammetry (CV), Tafel Anodic Polarization and Electrochemical Impedance Spectroscopy (EIS). The CV analysis revealed a quasi-reversible redox process. Tafel anodic polarization showed a Tafel slope of 71 $mVdec^{-1}$ and a current density of 50 $mAcm^{-2}$ was achieved at an overpotential of 332 mV. Through the electrochemical impedance Bode analysis, double-layer capacitance (C_{dl}), impedance (log |Z|) and roughness factor (R_F) were calculated. Nyquist plot showed no charge-transfer resistance (R_{CT}) and a small solution resistance (R_S) of 420.6 mΩ. The W NPs displayed appreciable OER behaviour and good energy storage properties.

Keywords: Electrocatalyst, OER, Energy storage

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P-54

Electrochemical insight of hydrothermally synthesized $CuCo_2S_4$ microstructures

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The need for advanced electrocatalysts for enhanced electrocatalytic behaviour sparked intense research in this field. Transition metal sulfides are the compounds that show good electrocatalytic properties for various electrochemical applications Wang et al. [1]. Advanced research on transition metal compounds for their electrocatalytic behaviour has been witnessed in the recent past as reported by Yan et al. [2] and Zhang et al. [3]. In this work, $CuCo_2S_4$ has been electrochemically evaluated as electrocatalysts for oxygen evolution reaction (OER). The $CuCo_2S_4$ was synthesized via hydrothermal route. The synthesized material was characterized physicochemically via FTIR (Fourier Transform Infrared) spectroscopy, PXRD (Powder X-Ray Diffraction) Analysis and SEM-EDX (Scanning Electron Microscopy with Energy Dispersive X-ray). PXRD pattern confirms the successful synthesis of the material. The electrochemical characterization of the synthesized material was done by employing standard electrochemical techniques, viz., cyclic voltammetry (CV), Tafel and Electrochemical Impedance Spectroscopy (EIS) on the Gamry Reference 600 ZRA electrochemical impedance system. The outcomes of the electrochemical characterization support that the material can act as an efficient OER electrocatalyst.

Keywords: Transition metal sulfides, OER, Electrochemical.

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P-55

Solid Forms Screening of Antineoplastic Drug Hydroxyurea

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Hydroxyurea (Trade Name: Hydrea) was approved by the Food and Drug Administration (FDA) in 1967 as an antineoplastic agent.[1] Further, hydroxyurea (HU) has been recommended in conjunction with other antitumor drugs to treat neoplastic diseases,[2] which prompted us to screen various cocrystal formers (CCFs) to identify a potential synthon for cocrystal preparation.[3] Virtual cocrystal screening of hydroxyurea was done using CCFs with different functionalities. First of all, HU and CCFs were optimized using density functional theory (DFT) and molecular electrostatic potential surfaces (MESPs) were generated. Surface site interaction points (SSIPs) and energy difference (ΔE) were calculated for all HU and CCFs combinations (as mentioned in equation 1). A hierarchy of HU-CCFs combinations were prepared on the basis of ΔE. The experimental screening of feasible combinations was performed using solvent drop mechanochemical grinding and solid phase changes were characterized by Powder X-ray Diffraction (PXRD). Synthon interaction analysis was done using computational and experimental Fourier transform infra-red (FTIR) spectroscopy.

$$\boldsymbol{\Delta E} = E_{cc} - nE_a - mE_b \qquad \text{eq.1}$$

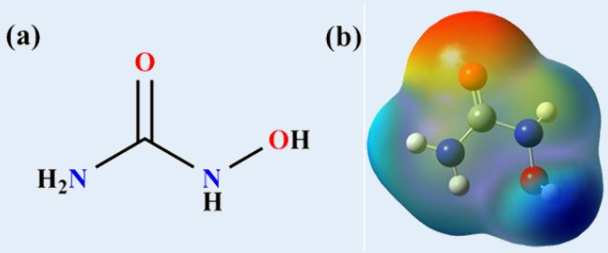

Figure (a) Chemical structure of hydroxyurea, and (b) electrostatic potential surface diagram.

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P-56

Improving Dissolution, Solubility and Permeability of Diclofenac by Preparing Primary Alkyl Ammonium Salts

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The preparation of salts of diclofenac (DCF) with alkyl amines is an important pharmaceutical formulation in terms of improving its skin permeability.[1][2] However, no trend in permeability changes has been reported in case of primary alkyl ammonium salts of DCF. Herein, we have prepared diclofenac (DCF) salts with primary alkyl amines (n-butylamine, iso-amylamine, n-hexylamine, and 2-phenylethylamine).[3][4] The salts were characterized by single crystal X-ray diffraction, DSC and TGA analysis that showed good thermal stability of salt forms. The solubility and permeability tests revealed that n-butyl ammonium salt of diclofenac had the highest solubility and permeability, with 1000 times higher bioavailability compared to DCF free acid. This study establishes a correlation between the salt's molecular properties and its membrane permeability.

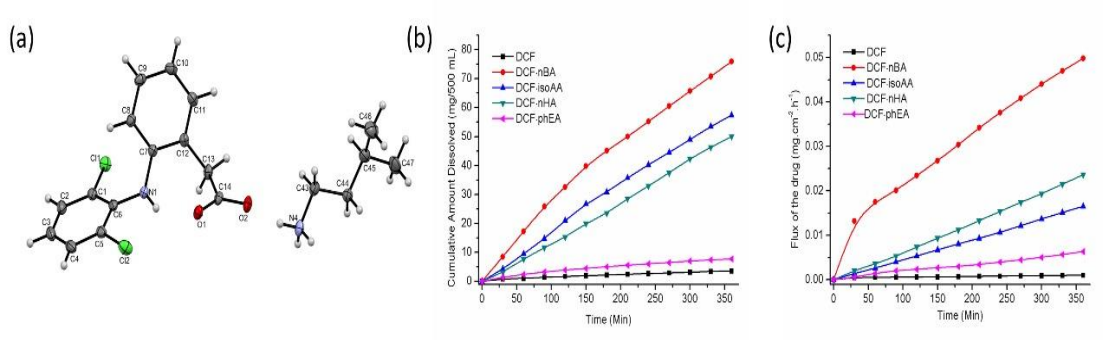

Figure (a) ORTEP diagram of Ammonium salt of Diclofenac, (b) *The dissolution profile of DCF and its alkyl ammonium salts, (c) flux of DCF free acid and alkyl ammonium salts across the dialysis membrane at different time intervals.*

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P-57

Facile Synthesis of ZnO/SnO_2 Nanocomposite and it's Application for Wastewater Remediation

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Abstract

Due to rapid industrialization, a million ton of waste generates which is offloaded by landfilling causes the toxicity, preferably, water contamination is health alarming and life threatening for aquatic eco eco system and human as well.[1] Therefore, before discharge of contaminated water into water bodies, it is prime concern to treat the wastewater and remove off the contamination. For the wastewater treatment, advanced oxidation process (AOP) has become an important chemical treatment method for mineralization of organic contaminants into smaller fragments or inorganic mineral ions.[1] Owing to p n junction formation of ZnO-SnO_2 nanocomposite material, coupled metal oxide ZnO-SnO_2 nanocomposites have been synthesized via sol-gel method by varying the mole ration of Zn:Sn i.e. 1:1, 2:8, 4:6, 6:4, 8:2 and nanocomposites identified as ZS-11, ZS-28, ZS-46, and ZS -64, and ZS-82, respectively. Powder X-ray diffraction (PXRD) pattern was ensured the crystallinity and phase of all five synthesized nanocomposites. Textural, optical and morphological properties of synthesized materials were confirmed by BET, ultraviolet diffuse reflectance spectroscopy (UV-DRS), scanning electron microscopy (SEM) and transmission electron microscopic analysis, respectively. Further, XPS analysis has also been studied to validate the stochiometric ration of ZnO and SnO_2 NPs within ZnO SnO_2 nanocomposite. Moreover, ZnO-SnO_2 nanocomposites have been utilized as an efficient photocatalysts for the degradation of methylene blue under UV-visible halogen lamp (500 W) irradiation. It has been found that 8:2 molar ratio of ZnO-SnO_2 nanocomposite (ZS-82) exhibits the maximum photodegradation i.e. 50% toward 0.5×10^{-5} M MB dye solution at pH 7.89. Further, degradation efficiency, recyclability, degradation mechanism and kinetics also have been discussed.

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P-58

Investigation of corrosion mitigation by organic inhibitors in an acidic medium

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ABSTRACT

For the development of the developing country the society are lived around the material based environment. Due to many uses of these materials these are main building blocks of any infrastructure. These materials used as very susceptible to corrosion.

The reported documents ensure that 3-4% of GDP loss as the result of about corrosion processes. It is very demanding to control the corrosion. There are several techniques to control but they impose the burden on the environment, health also. So it is very necessary to develop the most suitable and easy way to control the corrosion.Our goal is to create corrosion inhibitors that are both environmentally benign and extremely effective by investigating the synergistic effects of several chemicals and refining the formulation. By lessening the influence on the environment and advancing industrial sustainability, this research aids in the development of sustainable corrosion prevention techniques.

There are some heterocyclic compounds as corrosion inhibitors. These heterocyclic contains pi electron more conjugate hetero center and high molecular weight to adsorb on the metal surface easily. In this regards N and S contains heterocyclic are very useful and eco-friendly that can prevent carbon steel from corroding in acidic solutions. So that we are focusing to develop some new derivatives of triazole, Pyrimidine, for their best inhibitor efficiency results.

A major problem in many industries, corrosion poses a risk to safety and causes large financial losses. Because of their toxicity and lack of biodegradability, traditional corrosion inhibitors can present environmental risks. The goal of this research is to create new corrosion inhibitors that are safe for the environment using plant extracts and biopolymers.

The primary goal of the study is to determine whether certain chemicals can prevent mild steel from corroding in acidic environments. The effectiveness of these compounds' corrosion inhibition will be assessed using electrochemical methods such as electrochemical impedance spectroscopy, potentiodynamicpolarization; and adsorption isotherm. Computational studies like DFT and molecular dynamic stimulations.

In today's world, human societies are deeply dependent on materials, forming the foundation of modern living.In developing countries, materials serve as the essential building blocks for various applications, which underpin economic growth and social advancement.However, these materials, especially metals like carbon steel, are highly susceptible to corrosion, posing significant challenges. Corrosion leads to extensive financial losses, with reported global economic costs amounting to 3-4% of GDP. This highlights the urgent need for effective corrosion control methods.Traditional methods for corrosion control often impose environmental and health burdens.Therefore, it is very necessary to develop the most suitable and easy method to control corrosion.Heterocyclic compounds have shown promise as corrosion inhibitors due to their conjugated π-electron systems, heteroatomic centers, and high molecular weights, which facilitate strong adsorption on metal surfaces. Focusing on nitrogen (N) and sulfur (S)-containing heterocyclic derivatives, such as triazoles and pyrimidines, they are particularly effective in protecting carbon steels in acidic environments.[] Our approach emphasizes the development of new derivatives of triazoles and pyrimidines that have maximum corrosion efficiency at very low concentrations.The study will adopt a comprehensive approach to assess the effectiveness of these inhibitors. Electrochemical techniques such as electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) will be employed to determine the inhibitors inhibition efficiency. Additionally, computational methods including density functional theory (DFT) and molecular dynamics simulations will be utilized to further understand the mechanisms of inhibition. Our findings will contribute to advancing industrial sustainability by providing innovative strategies for corrosion prevention that align with environmental conservation efforts.

P-59

C–H Allylation and exo [3+2] Cycloaddition for the synthesis of Tetrahydro Methanobenzo Pyrazolo Diazepinones under Ruthenium(II) Catalyst

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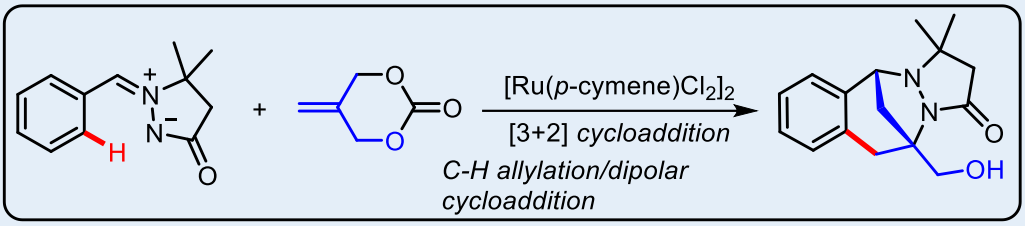
C–H allylation reaction has paid attention due to its capability to expedite the incorporation of allyl functionality into heteroaromatics over the traditional allylations. The directing group-mediated C–H bond allylation has proved as a useful method due to the regioselective formation of allylarenes without prefunctionalization.[1] Till now, very few allylating sources, e.g., allyl carbonates, allyl ethers, allyl halides, allyl alcohols, allyl acetates, 1,3-dienes, allenes, and unactivated alkenes, have been successfully applied under different transition-metal catalysis.

C–H bond functionalization and subsequent cyclization has been found as a better approach for the synthesis of various heterocycles. To extend this approach, cyclization route involving the electrophilic addition of π-unsaturates or the nucleophilic addition of C–M intermediates with directing groups have been intensively reported.

Azomethine imines having 1,3-diple structure, have used as a starting synthon in the dipolar cycloaddition reaction. Thus, inspired by our previous reported works on the Ru(II)-catalyzed C–H allylation and dipolar cycloaddition between azomethine imines and 2-methylidenetrimethylene carbonate is described herein. Initially generated β-substituted allyl species could promote the exo-type [3+2] cycloaddition with polar azomethine, generating the bridged tetracycles having a hydroxymethylene group at the bridgehead carbon.[2]



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P-60

Emerging Contaminants: Transformation and Fate in the Environment

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Abstract:

Emerging contaminants in water pose a significant challenge to environmental and public health. This study explores transformation and fate of these pollutants in aquatic ecosystems. Emerging contaminants including pharmaceuticals, personal care products, micro plastics, industrial chemicals, and nanoparticles enter water bodies through various pathways such as wastewater discharge, agricultural runoff, and atmospheric deposition. According to the U.S. Geological Survey (USGS) and the U.S. Environmental Protection Agency (EPA), ECs lack established regulatory status, and their effects on the environment and health are not yet fully understood. These contaminants have been detected in surface water, groundwater, and even drinking water with concentrations typically ranging from nanograms per litre (ng/L) to significantly high levels Kümmerer et al. [1]. Effluents from pharmaceutical manufacturing such as those in Patancheru near Hyderabad, have recorded highest global levels of pharmaceutical pollution about 2500 ng/L. Also nanoparticles like ZnO and TiO_2 used as UV filters along with compounds like parabens, triclosan in personal care products are prominent contaminants with their levels detected in the river water ranging from 1.1 to 9.65 μg/L.Their transformation in the environment is influenced by processes such as photodegradation, biodegradation etc. Schwarzenbach et al. [2]. Understanding these processes is crucial for assessing ecological and human health risks and implementing appropriate regulatory measures. This synthesizes current knowledge on the transformation products and environmental fate of emerging contaminants in water, highlighting the need for continued monitoring, advanced analytical techniques, and approach to address this growing environmental concern.

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P-61

Interactive Effect of Trace and Toxic Elements on Nutrient Acquisition and Distribution

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Abstract

The toxicity of trace elements in plants is a significant concern in environmental science and agriculture. Trace elements are categorized as essential and non-essential based on their biological importance while essential for plant growth in minute quantities, can become toxic when present in excess. With particular emphasis on nickel (Ni), essential for certain plant functions, elevated levels can cause severe physiological and biochemical disturbances. Excessive Ni concentrations inhibit root elongation, reduce chlorophyll content, disrupt nutrient uptake and induces the production of reactive oxygen species (ROS) which leads to oxidative damage in plant tissues. Plants absorb these elements from soil, water, and air, accumulating them in various tissues. Common toxic trace elements include arsenic, cadmium, lead, and mercury. The trace elements can exhibit both synergistic as well as antagonistic effects depending on their concentration and exposure conditions. However, this relation between As and Ni is unclear. Plants have evolved various defence mechanisms to cope with trace element toxicity, including sequestration, complexation, and exclusion. Understanding the dynamics of trace element uptake, translocation, compartmentation, and toxicity in plants is crucial for developing strategies to mitigate environmental contamination, ensure food safety, and improve phytoremediation techniques for contaminated soils.

P-62

DFT directed vibrational and electronic investigation, thermodynamic parameters, non-covalent interactions analysis, Molecular Docking as well as anti-inflammatory activity of the novel synthesized steroidal Schiff base

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Abstract

In the present study, the detailed molecular structure and spectroscopic analysis of newly synthesized compound 2 has been performed using experimental techniques like ^{1}H, ^{13}C NMR, FT-IR, UV spectroscopy and high resolution mass spectrometry as well as theoretical calculations. The energy, geometrical parameters and vibrational wavenumbers of compound 2 were calculated by using B3LYP with 6-31G (d, p) basis set. Detailed interpretations on vibrational modes have been made on the observed and theoretical spectra and PED for each mode was also reported precisely. The electronic structures and the assignment of absorption bands in the electronic spectra are also discussed. The strength and nature of weak intramolecular interactions have been studied by AIM and NCI approach. Global and local reactivity descriptors have been computed to predict reactivity and reactive sites present in compound 2. First hyperpolarizability values have been calculated to describe the nonlinear optical (NLO) property of compound 2. HOMO- LUMO energy gap and MEP analysis has also been carried out. Moreover, Compound-2 has also been analysed to show good anti-inflammatory activity via docking and *in-vitro* analysis.

Keywords: DFT, FT-IR, Conformation, MEP, NLO, anti-inflammatory activity.

P-63

Synthesis, characterization ZnS and ZnO/ZnS and their OER application

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Abstract

The requirement of more sustainable and cleaner energy is an ever-growing worldwide interest due to global warming and increasing population. Oxygen evolution reaction (OER) is one of the key electrocatalysis technologies for the development of renewable energy conversion and storage systems like water splitting, metal-air batteries, and fuel cells. In this work, zinc sulphide and ZnO/ZnS composites were synthesised by hydrothermal method adapting a green route. Zhao, J. G.et al [1] Modern analytical techniques like powder X-Ray Diffraction (XRD), Fourier transform infrared (FT-IR) have been employed to characterize ZnS and ZnO/ZnS. We fabricated the electrode of synthesised ZnS and ZnO/ZnS composites and investigated electrochemical oxygen evolution reaction. Ramachandran, et al [2]

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P-64

Efficient synthesis of danazol derivatives via palladium catalyzed Sonogashira cross coupling with evaluation of in vitro anti-oxidant activity and computational analysis.

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Novel derivatives of danazol (compound **1**) have been synthesized through sonogashira cross coupling reaction yielding the (1S,10aR,12aS)-1-((4-fluorophenyl)ethynyl)-10a,12a-dimethyl-2,3,3a,3b,4,5,10,10a,10b,11,12,12a-dodecahydro-1H-cyclopenta [7,8] phenanthrol [3,2-d] isoxazole-1-ol (compound **2**) and (1S,10aR,12aS)-1-((6-aminopyridin-3-yl)ethynyl)-10a,12a-dimethyl-2,3,3a,3b,4,5,10,10a,10b,11,12,12a-dodecahydro-1H-cyclopenta[7,8] phenanthrol [3,2-d]isoxazol-1-ol (compound **3**). Characterization of synthesized compounds were carried out with the help of UV-visible, FT-IR, ^{1}H NMR, ^{13}C NMR and HRMS analysis. Synthesized compounds were investigated for *in vitro* anti-oxidant activity showing significant result. Molecular geometry of compounds was optimized using B3LYP hybrid functional and 6-31G (d, p) basis set and compared with experimental data. Lower value of HOMO-LUMO gap for compound **3** indicates high chemical reactivity of compound **3** in comparison to compound **2**. Electrophilic and nucleophilic sites within molecules were obtained by molecular electrostatic potential surfaces. Molecular docking was performed with Oxidoreductase target protein having PDB ID 3F9P. The docking results showed binding energy values for **1, 2** and **3** against protein 3F9P were **-8.81, -9.47** and **-9.66 kcal/mol** respectively, indicates that compound **3** has high affinity to bind with oxidoreductase protein. Pharmacokinetic properties were evaluated through ADMET analysis.

P-65

Innovative Insights into Schiff Base Metal Complex: Synthesis, Computational Modeling, and Applications

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Abstract

This study explores the design, characterization, and therapeutic potential of Schiff base metal complexes derived from ampicillin. These complexes were synthesized through condensation reactions involving ampicillin and transition metals, resulting in mixed-ligand compounds. Structural properties were confirmed using FTIR, UV-Vis spectroscopy, NMR, and elemental analysis. Computational analyses with Density Functional Theory (DFT) revealed optimized molecular structures and electronic characteristics. HOMO-LUMO energy gap evaluations highlighted differences in stability and reactivity among the complexes. Molecular Electrostatic Potential (MEP) mapping identified regions favorable for electrophilic and nucleophilic interactions, providing deeper insights into their chemical behaviour. Molecular docking studies against AKT kinase revealed strong binding interactions, supported by favorable binding energy values, indicating significant anticancer potential. Biological assessments confirmed robust antimicrobial and anticancer activities, positioning these complexes as promising agents for dual therapeutic purposes.This comprehensive investigation combines experimental techniques with computational methods to advance the understanding and application of Schiff base metal complexes. The findings lay a strong foundation for their potential use in developing innovative antimicrobial and anticancer therapies.

Keywords: Schiff base metal complexes, dual therapeutic agents, HOMO-LUMO gap, molecular docking, DFT modeling, MEP analysis.

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Regioselective Synthesis of Phenanthridines via Pd(II)-Catalyzed Annulative C(sp2)−H Activation

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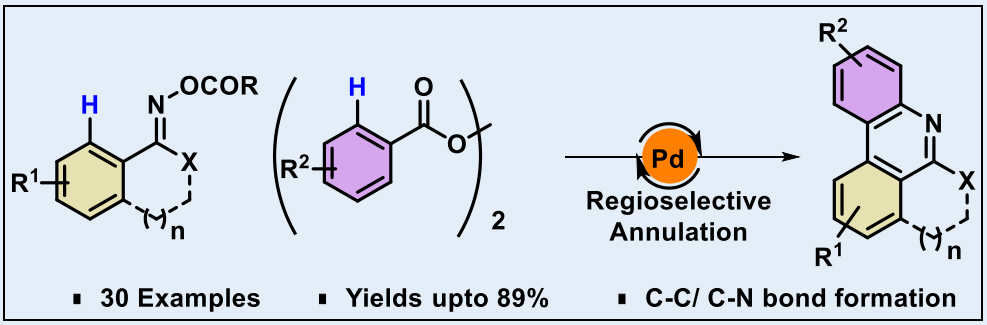

Abstract

Traditionally, phenanthridines have been synthesized *via* intra-molecular cyclization of biphenyl-derived oximes Okamura *et.al.*, Jiang,H.*et.al* [1][2], while in 2014, Li improvised the same reaction using copper as the co-catalyst to construct diverse phenanthridines.Tang *et.al.*[3]. Using oxime esters with aryl acyl peroxides, a highly regioselective domino C(sp2)−H activation/N-arylation process catalysed by Pd(II) has been reported to produce phenanthridines in a robust manner. The modular construction of functionalised phenanthridines with a broad tolerance of electronic functionality is made possible by this protocol, which is compatible with acetophenone and oxime esters derived from benzophenone. Control experiments were carried out to investigate the plausible reaction mechanism, and additional transformations were carried out to synthesize essential building blocks. Upadhyay *et.al.* [4]

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P-67

"Construction of diversified indole/hetero-fused indole frameworks *via* Ugi-multicomponent approach: A Review"

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Indoles constitute one of the most significant classes of structure in organic chemistry, being ubiquitous in biologically active natural products and pharmacophoric molecules. The synthesis of indoles and the advancement of innovative synthetic methods related to indoles remain pivotal in organic chemistry research. A novel and efficient method for constructing indoles has been developed using the Ugi-multicomponent reaction. This approach enables the rapid construction of complex indole structures from simple building blocks, including an array of amines, aldehydes, isocyanides, and acids. The review highlights the potential of the Ugi multicomponent reaction as a valuable tool for the synthesis of complex indole-based compounds, covering the scope, key advances, limitations, and applications of the methodology and thereby, aims to serve as a useful resource for researchers involved in indole synthesis and to inspire further advancements in this field.

Keywords -: Multicomponent synthesis, indole.

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Transition Metal Catalyzed Reduction of Nitroarenes

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Amines and their derivatives are industrially relevant molecules spanning pharmaceuticals and agrochemicals. Their primary synthesis method is the reduction of nitro compounds [1] which conventionally requires precious, costly noble metals, harsh reaction conditions and toxic reagents. To overcome these problems the use of earth abundant transition metal mediated photocatalytic methods have emerged as potential rescuers [2]. These methods employ cheap affordable transition metals as heterogeneous photocatalytic material and use green solvents with mild reaction conditions that enables fruitful conversions of nitro compounds into corresponding amines under visible light [3],[4]. The simplistic approach efficiently utilises semiconductor properties of photoredox metals to facilitate electron transfer and induce the reduction process. Working along the same lines newer catalytic protocols comprising of different transition metals could be proposed that have higher economic viability and scalability for nitro-reduction.

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V_2O_5 Catalyzed *N*-alkylation of aromatic amines with alcohols

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Abstract:

Amines are one of the most important compounds that have huge applications in medicines, surfactants and agrochemicals [1]. The formation of amines through reduction of nitro groups represents a fundamental transformation in organic chemistry. Synthesis of secondary amine by constructing a C-N bond is a challenging task [2]. We have developed an effective method for the *N*-alkylation of amines following the borrowing hydrogen methodology [3]. The approach utilizes V_2O_5 as a catalyst, $ZnBr_2$ as an additive, and KOH as a base to add *N*-alkylation to furnish secondary amine. From the perspectives of stability and sustainability, alcohols are among the most desirable choices for this method [4]. V_2O_5 serves as a robust and versatile catalyst due to its ability to facilitate both oxidation and reduction. The method eliminates the need for hazardous alkylating agents or external H_2 gas, making it safer and more environmentally friendly [5]. Moreover, the heterogeneous nature of catalyst allows for easy catalyst recovery and reuse, further enhancing its economic and ecological appeal [6]. Additionally, synthesizing the product on a gram scale significantly broadens the applicability of the established protocol.

Keywords: Amine alkylation, Heterogeneous catalysis, Nitroarenes, Nitro reduction

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Mode: Poster Presentation
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P-70

Synthesis of Novel Ciprofloxacin-Lipophilic Conjugates

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Abstract:

To overcome the ever-growing global threat of antibacterial resistance, we synthesized a series of Ciprofloxacin-Lipophilic conjugates, The synthesis was accomplished by using a carbodiimide reagent. Vitamin E, known for its lipophilic character and fat-soluble and antioxidant properties was used as a coupling partner. The strategy resulted in 17- novel conjugates. These conjugates hold huge potential for the development of novel antibacterial agents particularly combating the formidable *S. aureus* pathogen.

Keywords: Ciprofloxacin, Drug Conjugates, Antimicrobial resistance

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"Fluorescent Probes for Explosive Detection: A Review"

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ABSTRACT

The detection of explosives is an essential priority for global security and public safety. In recent years, imidazole- and benzimidazole-based fluorescent sensors have emerged as highly effective solutions for explosive detection. These sensors are renowned for their exceptional sensitivity, selectivity, and ease of synthesis. This review delves into the sophisticated mechanisms underlying these sensing technologies and presents innovative strategies for their development. It also rigorously evaluates the performance characteristics of these sensors, showcasing their robust potential for real-time monitoring and field detection applications. This comprehensive analysis highlights the remarkable capabilities of these advanced sensors to significantly enhance explosive detection efforts, reinforcing their crucial role in bolstering national security measures and ensuring public safety.

Keywords: Fluorescent sensors, explosive detection.

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P-72

Co (II) and Cu(II) Porphyrins Catalysed Synthesis of Quinoline and Naphthoxazine *via* Degydrogenative Reactions

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Abstract:

This research focuses on developing a simple and efficient catalytic system using cobalt (II) and copper (II) porphyrins to facilitate dehydrogenative coupling reactions. This method enables the synthesis of quinolines through the coupling of benzyl alcohol with acetophenone derivatives, and naphthoxazines through the intramolecular cyclization of Betti base. To achieve this, we synthesized novel porphyrins functionalized with ester and quinoline rings, namely CoTPPBenzo(NPh) and CuTPPBenzo(NPh). These porphyrin catalysts were then employed to catalyze the dehydrogenative coupling reactions, demonstrating excellent catalytic activity and a wide substrate scope. Furthermore, a series of controlled experiments were conducted to validate the proposed reaction mechanism and the role of the porphyrin catalysts in these transformations.

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Evaluation of comparative biological potency of Michael addition conjugate of (1E,6E) 1,7 bis(4-hydroxy-3-methoxyphenyl) hepta-1,6-diene-3,5-dione via *in silico* and *in vitro investigation*, ADMET and DFT studies

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Abstract-

In the present work, Michael addition reaction was utilized to synthesize a novel scaffold from (1E,6E) 1,7 bis(4-hydroxy-3-methoxyphenyl) hepta-1,6-diene-3,5-dione. The synthesized compound was characterized by using experimental methods viz FT-IR, ^{1}H, ^{13}C NMR, UV visible spectroscopy and theoretical calculations as well. A comparative biological activity exploration was done against lung cancer and liver cancer in which it showed higher efficacy for lung cancer than liver cancer. ADMET studies to identify the drug like characteristics has been performed. Theoretical calculations were performed utilizing the B3LYP/6-31G (d, p) basis set at the DFT level of theory. The time dependent density functional theory (TD-DFT) has been used to compute the electronic characteristics, including frontier orbitals and band gap energy. The AIM technique has been used to study the nature and intensity of weak intramolecular interactions. To forecast the molecule's reactivity and reactive sites, global and local reactivity descriptors have been calculated. The first hyperpolarizability values have been computed to characterize the synthetic substances' nonlinear optical (NLO) feature. Analysis of the molecular electrostatic potential (MEP) to explore the electrophilic and nucleophilic sites has also been done.

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Multicomponent reactions: A Versatile approach for an economic synthesis

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Abstract:-

Multicomponent reactions (MCRs) have gained much significance over the past decades because of their huge versatility to synthesize complex materials by using simple starting materials which hardly requires any separation or purification of the intermediates [1]. Multicomponent synthesis an approach to bring all reactants together in one pot, thus, reducing the time of reaction as well as wastage of chemicals. Multicomponent reactions have a growing application in drug development, materials chemistry, and catalysis as well [2]. Multicomponent reactions have also succeeded in achieving the twelve principles of "Green Chemistry" that were formulated in early 1990s [3]. The eco-friendly synthesis through MCRs has drawn much attention of the researchers in both the academia as well as industries all over the world [4]. Some of the well-known multicomponent reactions such as Ugi reaction, Passerini, Hantzsch, Biginelli, Staudinger etc. are very widely used nowadays to synthesize various novel heterocyclic scaffolds such as pyrroles, indoles, pyrazoles, pyrrolidines, chromenes, oxazines, pyrimidines etc. Several drugs, which have been synthesized using multicomponent reactions, have also been modified through various methods to generate complexity in the structures so that it can serve biological as well as pharmacological purposes.

Keywords- Multicomponent reactions, Ugi, Passerini, Biginelli, Heterocycles

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P-75

Micellar Behaviour of SDS And CTAB With the Aid of Clopidogrel, A Cardiovascular Antiplatelet Drug, Using Physical and Computational Techniques

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Abstract

Cardiovascular diseases stand out prominently, demanding complex medication regimes often associated with adverse effects. Addressing this challenge, this work delves into a promising avenue: the interaction between surfactants and cardiovascular drugs. In this work, we provide a short study on the effect of micellization (critical micelle concentration) with aided cardiovascular antiplatelet drug Clopidogrel [1-2]. Surfactants are chemical compounds that decrease the surface tension or interfacial tension between two liquids. The word "Surfactant" is a blend of surface-active agents, are amphiphilic molecules and are responsible for concentration at the interfaces or aggregate (undergoing aggregation) i.e. micellization [3-4]. The phenomenon of aggregation results due to attractive and repulsive forces (electrostatic forces) present in the solution. To reflect these two properties surfactant must have a chemical structure with different functional groups with different affinity in the same molecule [5-7]. Physical findings reveal the increase in critical micelle concentration (CMC) value of SDS from 8mmol – 13.9 mmol and increased molecular binding energies from -0.94 kcal to -2.42 kcal concluding the synergistic molecular interactions between SDS and clopidogrel are attractive. As depicted from micellization and molecular docking analysis, the enhanced solubilization of clopidogrel in the presence of SDS, as supported by CMC values, underscores the potential molecular attraction between anionic surfactant SDS and clopidogrel.

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Metal-Free Green Synthesis of Vicinal Diamines via Regioselective Ring-Opening of Aziridines

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Abstract –

Nucleophilic ring-opening of aziridines, facilitated by C-N bond cleavage, is an essential strategy for the synthesis of β-functionalized amines and 1,2-diamines, typically involving catalytic assistance. These diamines are precursors for the formation of aza-heterocycles, which can undergo cyclization or cycloaddition reactions (ring closing) to generate various aza-heterocyclic compounds. Traditional methods for synthesizing these compounds often rely on high temperatures or hazardous catalysts, which posed significant environmental and safety concerns. In recent years, numerous simple, efficient, and sustainable green chemistry approaches have been developed to synthesize these compounds, replacing traditional toxic metal catalysts and emphasizing environmentally friendly methods.

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P-77

Selective and sensitive cation exchange reactions in the aqueous starch capped ZnS nanoparticles with tunable composition, band gap and color for the detection and estimation of Pb^{2+}, Cu^{2+} and Hg^{2+}

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ABSTRACT

Cation exchange reactions (CER) at room temperature are a flexible method that can be used in place of laborious conventional techniques for colorimetrically detecting heavy metal ions in water samples. Here, we provide a colorimetric sensor for the detection and measurement of Pb^{2+}, Cu^{2+}, and Hg^{2+} and their corresponding converted products in water samples: selective and sensitive CER in aqueous starch-capped ZnS nanoparticles (NPs). Other heavy metal ions that are not involved in CER include Sn^{2+}, Cr^{3+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+},and Cd^{2+}. Composition, band gap, and color are the three time-dependent signals that the sensor displays to identify the corresponding metals. The partially converted products $Zn_{1-x}Pb_xS$, $Zn_{1-x}Cu_xS$, and $Zn_{1-x}Hg_xS$ were immediately recognized based on their spectroscopic data and orange, pale brown, and light-yellow colors in the presence of the corresponding metal ions. PbS, Cu_xS, and HgS were all completely changed, but they could still be recognized by their distinct colors, which were brown, pale brown, and bright yellow, respectively. Because of the advantageous room temperature nanoscale CER, the suggested ZnS NPs-based approach may be used to track Pb^{2+}, Cu^{2+}, and Hg^{2+} qualitatively and quantitatively in a variety of actual water samples without the need for any instruments.

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P-78

Novel cost-effective Hibiscus flower based colorimetric paper sensor containing anthocyanins to monitoring the quality and freshness of raw fish

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ABSTRACT

This article described the low-cost hibiscus flower based colorimetric paper sensor to monitor the quality and freshness of raw fish. The extract of hibiscus flower was used to develop pH sensing paper strips for qualitative analysis. The sensitivity of paper sensor was checked by colorimetric detection of ammonia gas and then it was implemented to monitor the freshness of fish visually. The extract of hibiscus flower containing anthocyanin molecules are the key molecule for visual detection of spoiled food. The above molecule was spectroscopically analyzed with change in pH of the solution before and after the interaction of food products. We also studied the variation of both color and shade of paper sensor with change in pH at natural and artificial light conditions. The color information extracted from images and their relationship with pH was explored in red, green, blue (RGB) and hue, saturation, and value (HSV) color spaces by the image-J software for qualitative monitoring of food. Anthocyanin based paper sensor is used as a convenient and real time smart food sensor in packaging application.

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P-79

Molecular docking studies and *in vitro* evaluation of newly synthesized steroidal derivatives as anti-cancer agents

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Abstract

Steroids exhibit a broad range of physiological functions and biological activities such as antimicrobial, anti-Alzheimer's disease, anti-inflammatory, anti-cancer. Structural modifications of steroids require great synthetic efforts. In the current study, some novel steroidal derivatives have been synthesized using two different methodologies. The synthesized compounds were purified by using column chromatography and characterized with the help of modern spectroscopic techniques like ^{1}H, ^{13}C NMR, FT-IR spectroscopy and Mass spectrometry. The synthesized compounds were evaluated for anti-cancer activity against cervical cancer cell line, SiHa *in vitro* which demonstrated an appreciable activity as indicated by the IC_{50} values. Molecular docking studies were carried out to investigate the inhibitory action of steroidal derivative against the HPV protein. The result of molecular docking study reveals that the synthesized compounds have better binding energies than the parent compound with the selected HPV protein.

Keywords: Steroidal derivatives, Human cervical carcinoma, Anti-cancer activity, Molecular Docking, HPV.

P-80

Synthesis, Molecular study and Spectral Evaluation of Pyrrole 4- imidazole derivatives

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Abstract

In this work Ethyl 4-formyl-3,5-dimethyl-1H-pyrrole carboxylate and phenylene diamine derivatives/ethylene diamine were condensed, cyclized, and oxidized to create pyrrole 4-imidazole derivatives, benzimidazoles, and pyrrole 4-imidazoline. Theoretical research and elemental and spectroscopic investigation, including IR, UV, MS, ^{1}H, and ^{13}C NMR, have been used to determine the structure of these bi-heterocyclic compounds. For pyrrole 4-imidazole derivatives, the static initial hyperpolarizability, or β0 values, have been determined to be 10.901 x 10^{-31}, 19.607 x 10^{-31}, 40.323 x 10^{-31}, and 5.686 x 10^{-31} esu, respectively. The synthesized pyrrole-imidazoles are suitable as non-linear optical (NLO) materials, as evidenced by the high β0 values and experimental absorption spectra that were found to be in the UV region.

Keywords: Benzimidazoles, Pyrrole-benzimidazole derivatives Hyperpolarizability, non–linear optical (NLO).

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P-81

Finely tuning Cobalt Valence in Co_3O_4 Lattice through Chromium Substitution: Regulating the charge transfer and oxygen vacancies for Oxygen Evolution and Methanol Oxidation Reaction

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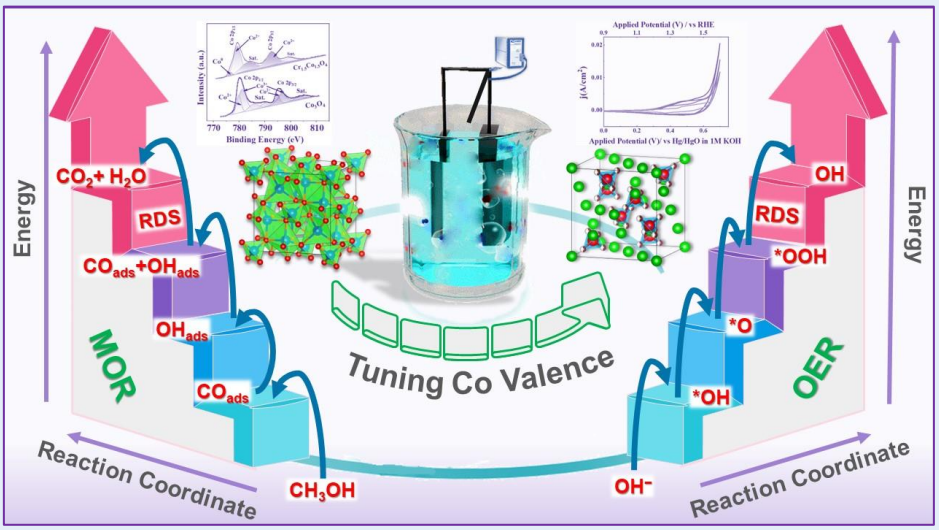
Abstract

In this intriguing study, our central focus revolves around efficiency of the Oxygen Evolution Reaction (OER) and methanol oxidation Reaction (MOR) through a captivating approach: harnessing the power of cobalt valence modulation in Cobaltite (Co_3O_4), achieved by the enchanting substitution of chromium (Cr). By seamlessly integrating chromium atoms into the crystal lattice of Co_3O_4, our ultimate aim is to orchestrate a remarkable transformation in the potential-determining step of the OER, resulting in a symphony of improved catalytic performance. This substitution is done by utilising simple sol-gel method at low temperatures. This gentle adjustment of cation valence states creates oxygen vacancies on the spinel surface, achieving an ideal ion ratio of Co^{2+}/Co^{3+}. The formation of spinel oxides has been confirmed by a comprehensive range of precise physicochemical techniques including, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction analysis (XRD), X-ray photoelectron spectroscopy (XPS), High Resolution Transmission Electron Microscopy (HRTEM), scanning electron microscopy (SEM) coupled with energy dispersive X-ray spectroscopy (EDS), Brunauer–Emmett–Teller (BET) technique and Raman spectroscopy. The presence of oxygen vacancy has been verified with Electron Paramagnetic Resonance (EPR) spectroscopy. The spinel oxide, $Cr_{1.5}Co_{1.5}O_4$ displays superior activity for OER with current density of 100mA/cm^2 at the overpotential of only 413mV. Our findings highlight the significance of cobalt valence control in promoting OER/MOR activity, paving the way for advanced electrocatalytic systems with enhanced energy conversion capabilities.



P-82

Capsicum annum Extract Mediated Green Synthesis of Fe-Zn Nanocomposite for Remediation of Tetracycline Antibiotics in Aqueous Medium

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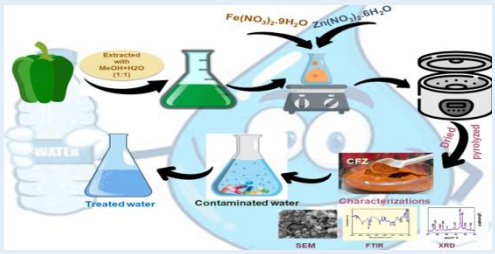
ABSTRACT

The presence of antibiotics in the aquatic environment has been a major reason to worry because there is Antimicrobial Resistance (AMR) in various microbial communities. To overcome the raising AMR concerns, antibiotic decontamination of the aquatic environmental matrices is required. The present study investigates the use of capsicum annuum mediated Fe-Zn nanocomposite (CFZ) for the remediation of five antibiotics (belonging to Tetracyclines class) from wastewater. The adsorption capacities of nanoparticle for the concurrent removal of the tested antibiotics were investigated at different contact times, temperature, pH values, initial concentrations of the adsorbate and adsorbent doses. Green synthesized nanocomposite demonstrated high adsorption capacity of (~95%), (~87%), (~93%), (~98%), (~93%) for minocycline, oxytetracycline, demeclocycline, chlortetracycline, doxycycline hydrate respectively in 30 min.. Further, amongst the applied isotherm models Freundlich, Temkin and Langmuir, The Langmuir model fitted well for all antibiotics. Adsorption kinetic data followed pseudo-second order kinetics, indicating chemisorption as the favoured adsorption mechanism. Adsorption studies at various temperatures were carried out in order to establish thermodynamic characteristics which indicated a spontaneous exothermic adsorption phenomenon. The instrumental techniques, Fourier transformed infrared (FTIR) spectroscopy, XRD were used to determine the structural and chemical composition of CFZ nanocomposite and Dynamic light scattering (DLS) was used to determine the hydrodynamic size of the nanocomposite and its zeta potential.

Keywords: Fe-Zn nanocomposite, tetracyclines, antimicrobial resistance, remediation

Graphical abstract



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P-83

Fabrication of silver-cobalt alloy nanoparticles for catalytic reduction of nitrophenol derivatives in wastewater treatment applications

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Abstract:

The purpose of this work is to support the efficacy of the immiscible alloy Ag-Co nanoparticles (NPs) synthesis. For it to be effectively applied topically as a catalyst in nitrophenol derivatives reductions for wastewater remediation.

Keywords: Alloy nanoparticles; Chemical reduction; Nitrophenol derivatives; Catalytic reduction

Design/methodology/approach-

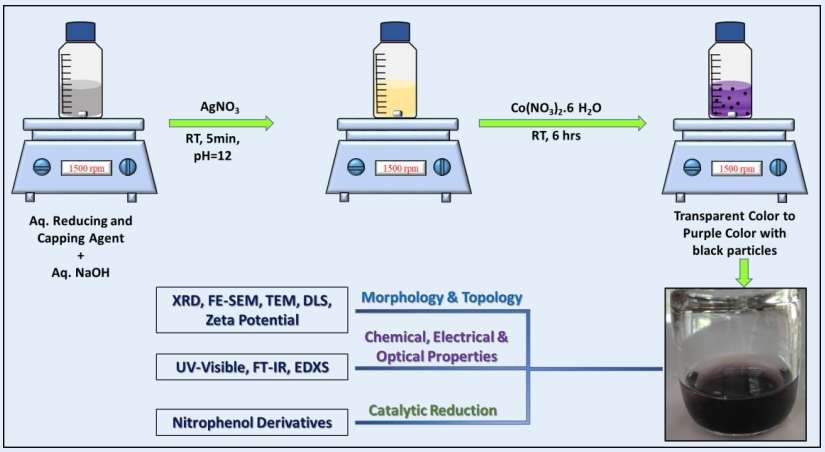

Figure 1. Cartoon representation of the synthesis of immiscible alloy Ag-Co NPs

Results and discussions- The morphological and other properties were analyzed by using various analytical tools such as UV-visible spectroscopy, FT-IR, DLS, PXRD, EDAX, FE-SEM, and TEM. It was proven that the synthesized Ag-Co NPs are immiscible and consist core-shell structure [1,2]. From the TEM analysis, it was found that Ag-Co NPs have an average diameter that ranges from 9-21 nm. The catalytic efficiency was calculated by recording absorption spectra at specific time intervals.

Conclusions- This study corroborates the synthesis of immiscible alloy Ag-Co NPs synthesized by the chemical reduction method. The catalytic reduction of nitrophenol derivatives was successfully investigated.

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P-84

Investigating the Acoustic Interactions, Molecular Dynamics and Biodegradation of HPMC Blended Polyethylene Glycol (PEG): A Sustainable Approach to Environmental Innovation

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Abstract

This study investigates the acoustic interactions and biodegradation behaviour of a polyethylene glycol (PEG) and hydroxypropyl methylcellulose (HPMC) blend. The research involves creating biodegradable films with a PEG/HPMC blend and then analyzing their biodegradation behaviour in both open and soil settings. The acoustic properties of the blend were examined to gain a better understanding of PEG and HPMC interactions. As a probing technique, we used ultrasonic velocity measurement to carefully examine these blends' acoustic landscape. The precise calculations of parameters including adiabatic compressibility, acoustic impedance, free length, and relaxation time provided insight into the complex dynamics present in the blends. The biodegradable films were subjected to various environmental conditions, and their breakdown was tracked over time. The findings demonstrate a significant difference in biodegradation rates, with soil degradation being substantially more pronounced than in the open environment. Additionally, we examined the molecular interactions in the PVA-starch blends using molecular docking techniques, revealing their binding affinities and possible uses. Our results highlight how starch-blend PVA, driven by its improved acoustical qualities and molecular complexities, has emerged as a promising environmentally friendly material with a wide range of applications. This study provides a road towards significant environmental innovation in addition to deepening our grasp of sustainable material science.

Keywords- Biodegradable Polymers, PEG, HPMC, Blending, Acoustical parameters, Biodegradation, Molecular Docking

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P-85

Molecular engineering in Carbon Nitride/mesoporous $Ni_{0.5}Co_{2.5}O_4$ nanocomposite as bifunctional electrocatalyst for alkaline water splitting

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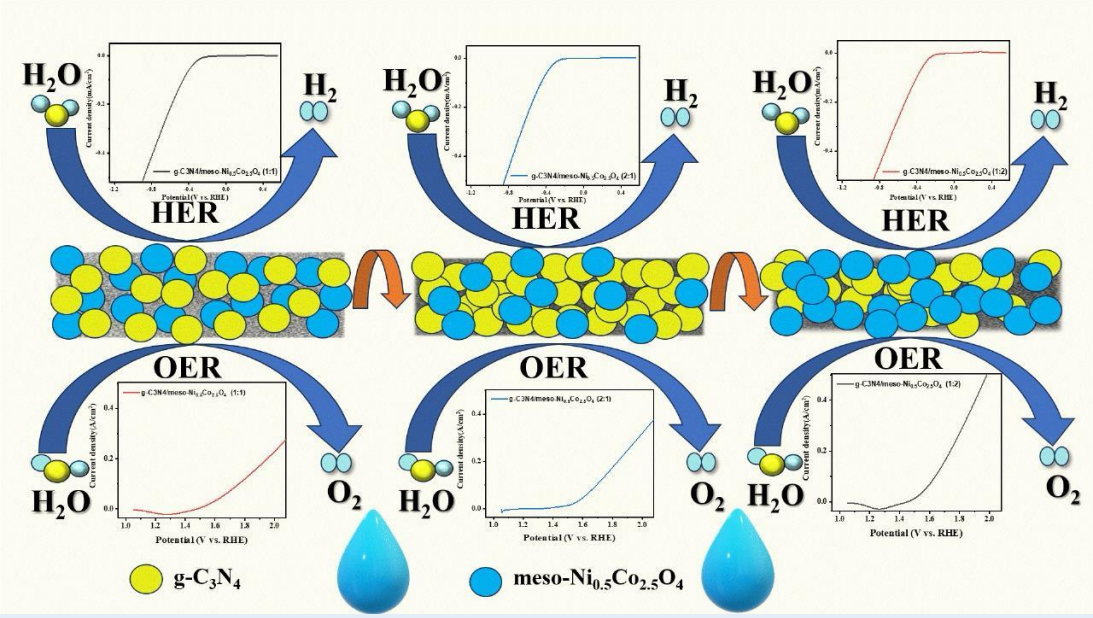
Abstract

This research explores the effect of optimizing molar ratios in a series of innovative nanocomposites to enhance their electrocatalytic performance for both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in alkaline environments using molecular engineering of the two components. The study involved the synthesis of a novel nanocomposite consisting of carbon nitride (C_3N_4) and meso-$Ni_{0.5}Co_{2.5}O_4$ using the simplest feasible route with systematic variations in their molar ratios. Comprehensive physicochemical characterization, including Rietveld refinement, provided detailed insights into the crystal structure, phase purity, morphology, and electronic properties. The robust electrochemical analysis provides evidence in favour of the nanocomposite with a 1:2 molar ratio for its outstanding electrocatalytic activity, requiring only 253 mV overpotential for 10 mA/cm^2 during OER and 198 mV for 10 mA/cm^2 during HER in 1M KOH at 25°C. Thermodynamic and kinetic analyses were conducted to determine the enthalpy of activation and reaction order to substantiate the electrochemical performance. The results highlight the significance of precise molar ratio optimization in developing high-performance electrocatalysts. This investigation demonstrates superior catalytic activity and provides a comprehensive understanding of the thermodynamic and kinetic factors influencing electrocatalytic performance, laying the groundwork for more efficient hydrogen generation technologies.



P-86

New Heteroleptic bis-(diphenylphosphino)ethane appended dialkyldithiophosphatecobalt(III) cations: Apt electrocatalysts for heterogeneous Oxygen Evolution Reaction and homogeneous Hydrogen Evolution Reaction

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Hydrogen is considered a viable fuel to address energy scarcity issue [1]. Although the hydrogen evolution reaction (HER) appears to be a very simple reaction, it is in fact a sluggish process that must be accelerated [2]. Hence, like the oxygen evolution reaction (OER), the HER also requires appropriate catalysts. In the same quest, two new heteroleptic cobalt(III)diakyldithiophosphate complex cations with 1,2-bis(diphenylphosphino)ethane (dppe) ancillary ligand having formula $[Co\{S_2P(OR)_2\}_2(dppe)](B(C_6H_5)_4)$ (R = $-C_2H_5$ (**Co-Et**); $-CH(CH_3)_2$ (**Co-Pr**)) have been synthesized and characterized spectroscopically as well as by single crystal X-ray diffraction. The single crystal X-ray diffraction analyses reveals that the immediate geometry around Co(III) in both the complexes are distorted octahedral which are satisfied by four sulfur atoms of two diakyldithiophosphate ligands and two phosphorus centers of dppe ligand. These complex cations are neutralized by tetraphenyl borate $B(C_6H_5)_4$ anions. The solid-state framework of both the complexes have been stabilized by C-H$\cdots\pi$ and C-H$\cdots$C interactions. The nature of these interactions have been addressed with the help of Hirshfeld surface analyses and the percent contributions of the pertinent interactions in the crystal structure of these complexes have been addressed using fingerprint plots. Both complexes have been used as heterogeneous electrocatalysts for oxygen evolution reaction (OER) and results suggest that **Co-Et** is better electrocatalyst for OER displaying onset potential of 1.68 V and Tafel slope of 114 $mV\cdot dec^{-1}$. Further, in homogeneous electrocatalysis of hydrogen evolution reaction (HER) using trifluoroacetic acid the overpotential for **Co-Et** and **Co-Pr** comes out to be 1.05 V and 0.92 V, respectively with turnover frequencies of 1518 s^{-1} and 287.5 s^{-1}. Overall, both heterogeneous OER and homogenous HER results suggest that **Co-Et** can be used as efficient molecular electrocatalyst for oxygen/hydrogen evolution reactions.

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P-87

Molecular Docking Studies of Optimized 7-(4-nitrophenyl)-5,7-dihydro-6H-benzo[6,7] chromeno[3,2-c][1,8] naphthyridin-6-one against *Mycobacterium Tuberculosis*

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Abstract:

Molecular docking is a time-saving and cost-effective approach in the field of computational chemistry. The compound 7-(4-nitrophenyl)-5,7-dihydro-6H-benzo[6,7] chromeno[3,2-c][1,8] naphthyridin-6-one was optimized by DFT/B3LYP/6-311++G(d,p) and its potential was assessed against *Mycobacterium tuberculosis* by using AutoDock 4.2 software. The results were analyzed with the help of Gauss View 6.0, PyMol 1.5.7 and PLIP visualization softwares.

P-88

Design, Synthesis, and Evaluation of Coumarin Hydrazone Derivatives as Potential Antidiabetic Agents: *In-vitro* and *In-silico* Analysis of α-glucosidase Inhibition.

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Abstract

This study focused on the design and synthesis of new coumarin hydrazone derivatives, NCEBHZ (**3a**) and DNCEBHZ (**3b**), to evaluate their potential as α-glucosidase inhibitors for antidiabetic therapy. The chemical structures of these derivatives were confirmed using a range of spectroscopic methods, including FTIR, ^{1}HNMR, ^{13}CNMR, and elemental analysis. Both compounds showed significant α-glucosidase inhibitory activity with IC50 values of 130.30 ± 2.53 µM for NCEBHZ (**3a**) and 145.26 ± 1.18 µM for DNCEBHZ (**3b**), outperforming the parent 3-acetyl coumarin (IC50: 1.5 x 10^{5} µM) and the positive control, acarbose (IC50: 259.90 ± 1.06 µM). Kinetic assays indicated that both derivatives act as mixed-type inhibitors of α-glucosidase, with inhibition constants (KI and KIS) of 18.82 µM and 59.99 µM, respectively. Computational studies of electronic transitions revealed π→π* behavior, and isotropic chemical shifts were calculated using the GIAO method in DMSO-d6. The electronic descriptor analysis suggested that these compounds could serve as building blocks for new heterocyclic compounds. First static hyperpolarizability values (β0) of 22.64 and 21.30 × 10–30 esu for NCEBHZ (**3a**) and DNCEBHZ (**3b**) at the B3LYP/6-31G(d,p) basis set indicated their potential as nonlinear optical materials. Molecular docking revealed strong binding affinity to the α-glucosidase active site, with docking scores of -8.82 and -8.86 kcal/mol. The study also includes ADMET, molecular electrostatic potential surfaces (MEPS), NLO, and NBO analyses, highlighting the need for further optimization to enhance their efficacy for diabetes treatment.

Keyword: α-glucosidase inhibition, *in silico*, pharmacophore, NLO, ADMET, MEPS.

P-89

Graphitic Carbon Nitride based Nanocomposites for Electrochemical sensing of Environmental Contaminants: A Review

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ABSTRACT:

Uncontrolled population growth, excess use of chemicals like pesticides, herbicides, dyes from industry, pharmacological wastage from anthropogenic activities leads to serious issue of contamination that need real time monitoring to avoid hazardous impact on human as well as aquatic environment. Electrochemical Sensors are the most effective, economical, balanced, sensitive, selective, and least time-consuming for this purpose. Graphitic Carbon Nitride (g-C_3N_4) based nanomaterials are the most promising for the electrochemical sensing devices as they are cost effective, chemically stable, biocompatible, provides fast charge transfer. Despite these advantages, g-C_3N_4 suffers with limitation of low conductivity, reluctant active sites and combination of electron hole. Tailoring the surface of g-C_3N_4 by forming nanocomposites with transition metal oxides, carbon conducting materials and MOF that enhance its active sites, reduce ion transport path, tunable band gap and improved transportation efficacy.

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P-90

Structure Elucidation of Novel tetrasaccharide having pentose sugar from A2 cow colostrum by 2D NMR

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ABSTRACT

Recently numerous variety of cow species are being developed whereas the Desi cow, often referred as A2 cow, is important and has its own significance. The importance of cow milk is well defined and described in Ayurveda and Charak Samhita. *Colostrum* is the milk produced by mammals during the first few days after they gave birth .We have collected (10 litres) of A2 cow colostrum and then processed it by modified method of Kobata and Ginsburg incorporating deproteination, microfiltration and lyophilisation which gave 165 gm. of oligosaccharide mixture. Further we have acetylated the oligosaccharide mixture by acetic anhydride and pyridine. The acetylation was done for conversion of polar oligosaccharide into their non-polar derivatives. It was purified on silica gel column chromatography. Structural analysis of pure oligosaccharide "Inditose" was performed by using various spectroscopic techniques including 1D and 2D NMR. The HSQC spectrum of "Inditose" showed five cross peaks at 90.13x6.17, 91.18x5.40, 95.29x4.74, 101.00x4.50 and 114.07x4.97 suggested it to be a tetrasaccharide in its reducing form. Further the TOCSY spectrum of "Inditose" sieved the ring protons of each anomeric proton which suggested the position of glycosidic linkages in each of the monosaccharide. The sequence of the ring protons were confirmed by COSY spectrum. Further the glycosidic linkages were confirmed by HMBC spectrum of "Inditose".The configuration of glycosidic linkages were confirmed by the splitting pattern (J values) of anomeric protons. Moreover the absolute configuration of monosaccharides were also discussed. In light of the results obtained from 1D and 2D NMR experiments, the structure of the novel tetrasaccharide "Inditose" was deduced having a pentose sugar at the non-reducing end.

Keywords: A2 cow, Milk oligosaccharide, Inditose, 1D NMR, 2D NMR.

Acknowledgement: Authors are thankful to Research and Development grant, Department of Higher Education, UP Government.

P-91

Extensive Analysis of Schiff Base Complex: Fabrication, Quantum Chemical Investigations, Molecular Interactions

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Abstract

This research explores the creation, analysis, and therapeutic potential of Schiff base metal complexes derived from ampicillin. The Schiff bases were synthesized through condensation reactions with ampicillin and were further complexed with transition metals to form mixed-ligand compounds. Structural confirmation was achieved using FTIR, UV-Vis spectroscopy, NMR, and elemental analysis. Computational studies employing Density Functional Theory (DFT) revealed optimized molecular geometries and electronic properties, including a HOMO-LUMO energy gap, indicating variable stability and reactivity among the complexes. Molecular Electrostatic Potential (MEP) mapping identified regions prone to electrophilic and nucleophilic interactions, enhancing the understanding of their chemical behavior. Molecular docking studies targeting AKT kinase revealed strong binding interactions, with promising binding energy values, emphasizing the complexes' potential in anticancer applications. These findings suggest that ampicillin-Schiff base metal complexes can serve as effective agents for dual-purpose therapeutic strategies, addressing microbial infections and cancer.This comprehensive approach, combining experimental techniques with computational analyses, offers a robust framework for further exploration of these complexes in biomedicine. The study underscores their potential for innovation in antimicrobial and anticancer therapy development.

Keywords: Schiff Base Complexes, HOMO-LUMO Energy Gap, Molecular Docking, DFT Analysis, Molecular Electrostatic Potential (MEP)

P-92

Mechanistic Insight into Epoxide-Based Ring Transformation

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Abstract –

Epoxides, a three-membered strained cyclic ring containing oxygen atom, are pivotal intermediates in organic synthesis. Highly strained ring structures are facile for various ring opening and closing reactions. Epoxides have been synthesized through various routes, a few of them are – photoelectrochemical epoxidation of alkenes on α-Fe_2O_3 including some organo-metallic compounds such as Rhodium complexes. Ring-opening of epoxides has been reported by multiple methodologies *viz.*, nucleophilic via OH^- [1], OOH^- [2], electrophilic reaction pathways *via* Zn-complex [3], metal-catalyzed reactions employing Al-complexes [4], and the most efficient green approaches via organocatalysts [5]. Along with the emphasis on regio- and stereoselectivity by diversifying the reaction conditions, these reactions afforded diols, amino alcohols and cyclic carbonates as valued products that could serve as potential scaffolds in pharmaceuticals, material science and environmental sustainability.

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P-93

Isolation and structure elucidation hexasaccharide “pakose” isolated from tharparker cow

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Abstract

Structure diversities are found in milk oligosaccharides which depend on food, flora and fauna around the animal. The structure of oligosaccharides. that is a particular milk depends on the habitat around the animal and fodder the take. The cow species belonging to arid region that is Rajasthan and Gujarat of India have different fooding. That’s why it was found that the oligosaccharide. Put in their milk are not free sugars instead they are present their in the milk are present as their methyl glycosides. Some other diversity like of pentose in their milk. Oligosaccharides containing pentose sugar simultaneously. They were also having reducing oligosaccharides. in our present study on Tharparkar cow milk, we isolated another novel hexasaccharides name as Parkose. The HSQC spectrum of parkose showed seven cross peak of anomeric proton and carbon at 89.12×6.228, 90.17×5.397, 91.57×5.66, 95.27×4.672, 101.8×4.52 concluding it to be a hexasaccharides into its reducing form further 2D NMR studies of Parkose involving TOCSY, COSY, HMBC and HSQC concluded its structure.

Keywords- Milk, Oligosaccharides, 1D and 2D NMR Spectroscopy.

P-94

Evaluation of fluorescence properties of novel Lophine Derivatives

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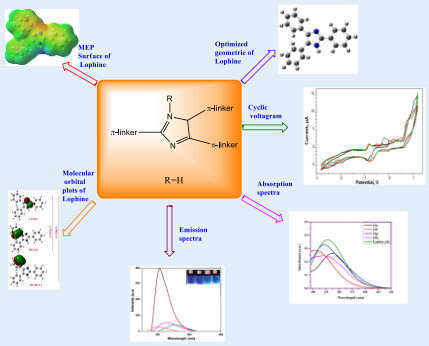
Abstract:

Heterocyclic imidazole derivatives have attracted considerable attention because of their unique optical properties. These compounds play a very important role in chemistry as mediators for synthetic reactions, primarily as a means for preparing functionalized materials. Therefore novel lophine (2,4,5-triphenylimidazole) derivatives, have been synthesized and their physicochemical properties were determined. All derivatives have been characterized by FT-IR, UV–Vis, ^{1}H-NMR, ^{13}CNMR Mass spectrometry and elemental analysis. Additionally, the fluorescence behavior and physicochemical characteristics of produced compounds in DMSO at various pH levels have been ascertained. The electrochemical characteristics were also evaluated with cyclic voltammetry. The optical band gap and quantum yield of imidazole derivatives were found to be between 3.13 and 3.55 eV and between 0.016 and 0.269, respectively. The highest and lowest occupied molecular orbitals, as well as associated energy gaps, were measured using cyclic voltammetry measurements, and the findings indicated that they ranged from 2.04 to 2.26 eV. The calculated band gaps were discovered to be between 4.014 and 4.216 eV. To gain a better understanding of these derivatives and their relationship to their photophysical properties, computational studies have been conducted. The results of theoretical and experimental absorption are well supported by one another. The results show that the synthesized imidazole derivatives can be employed as luminous materials.



Keywords: Lophine Derivatives, Cyclic Voltammetry, Physicochemical Properties, Optical band gap and Quantum yield

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P-95

Triazole-pyrrole hybrids as antimicrobial agents: Synthesis, spectroscopic evaluation, molecular docking and ADMET

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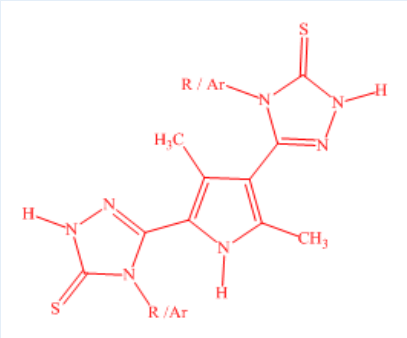
Abstract

In the present investigation, a series of triazole-pyrrole hybrids have been synthesized in good yields and structures of these compounds were established by IR, ^{1}H NMR, ^{13}C NMR, mass spectral and elemental analysis. The newly synthesized compounds were evaluated for their antimicrobial activities. The tested compounds, displayed promising antimicrobial activity. Further, some compounds were also assessed for their cytotoxic activity (IC_{50}) against mammalian cell lines using the MTT assay method. The results revealed that these compounds exhibit antimicrobial activity at non-cytotoxic concentrations. The docking of inhibitors revealed the vital interactions and binding conformation of the inhibitors. Finally, the prediction of ADMET properties suggests that almost all hybrid compounds possess good pharmacokinetic profiles and no signs of observed toxicity.

Keywords: Triazole-pyrrole hybrids, Antimicrobial activity, cytotoxic activity, docking



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P-96

Impacts of Arsenic-Contaminated Soil and Water on Rice Quality and Safety

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Arsenic contamination in rice is a growing global health concern, particularly in regions like South Asia due to use of As contaminated ground water for irrigation. This is especially more pronounced in developing countries such as Bangladesh and India where groundwater contamination levels of As far exceeds the WHO's safety threshold of 10 μgl^{-1}. In many part of India the agricultural soil is often exceeding the normal level of As i.e. 5mg/kg, further in West Bengal and Eastern districts of Uttar Pradesh, the level of As in soil is frequently exceeding the FAO threshold limit of 20 mg/kg for agricultural soils. It has been scientifically proven that irrigation with arsenic water significantly increases arsenic concentration in the rice plant tissues. The Codex Alimentarius Commission, a global authority on food standards, recommends limiting total arsenic in rice to 300 µg/kg and inorganic arsenic to 200 µg/kg. In recent years, it has been observed that As accumulation in rice not only compromise yield but it significantly hamper the nutritional and cooking quality of rice. Arsenic toxicity affects key components like amylose, lipids, proteins, vitamins, and amino acids. Farmers in eastern Uttar Pradesh widely cultivate short-grain aromatic varieties, such as Kanak Jeera, Shakkar Chini, Vishnu Bhog, Chini Kapoor, and Kalanamak. It has been noticed that the aroma quality of these rice varieties is reducing in recent years, however, the underlying reason is yet unknown. The climatic and environmental factors may be the potential cause. Since in these regions, paddy soil has been shown the have significant level of As contamination, thus, it is worthwhile to understand if As also hamper the aroma quality of rice similar to other quality traits. This understanding will add to improved agricultural practices in As contaminated areas.

Keywords: arsenic contamination, rice quality, aromatic rice varieties, nutritional traits, agricultural practices

P-97

New –OH positional isomeric 1,1′-bis(diphenylphosphino)ferrocene appended Ni(II) dithiocarbamates as sensitizers in dye sensitized solar cells

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Abstract

The global energy demand, currently at 13 terawatts (TW), is projected to rise to 23 TW by 2050 [1]. With 80% of world's energy requirements met by rapidly depleting fossil fuels [2], their use contributes significantly carbon dioxide emissions, exacerbating global warming. Consequently, clean and renewable energy technologies are urgently needed to address these challenges [3].

Three new –OH positional isomeric heteroleptic Ni(II) dithiocarbamates with general formula [Ni(dppf)(L)][PF_6] (dppf = 1,1′-bis-(diphenylphosphino)ferrocene and L = N-benzyl-1-(2-hydroxyphenyl)dithiocarbamate (L_1) (1), N-benzyl-1-(3-hydroxyphenyl)dithiocarbamate (L_2) (2), and N-benzyl-1-(4-hydroxyphenyl) dithiocarbamate (L_3) (3)) have been synthesized and characterized by spectroscopic methods and microanalyses. The optimized molecular geometries for all the three ferrocene-based complexes reveal that the coordination geometries around Ni(II) is distorted square planar that is satisfied by two sulfur centers of dithiocarbamate ligand and two phosphorus of dppf. The application of these complexes as sensitizers have been assessed in DSSCs. Amongst these three sensitizers based the DSSC set-ups, the assembly fabricated using 3 displayed superior performance.

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P-98

Ultrasonic Investigation of Molecular Interactions in Polymethylmethacrylate-Toluene Binary Liquid Mixture

Preeti Yadav*, Indu Saxena

Abstract-

Understanding molecular interactions in liquid mixtures is crucial for various industrial and scientific applications. In this study, ultrasonic technology was employed to investigate the nature and power of molecular interactions in a binary liquid mixture of polymethylmethacrylate (PMMA) and toluene at two different temperatures (308.15K and 298.15K) using a 2 MHz frequency. Acoustical characteristics including adiabatic compressibility (βad), intermolecular free length (L_f), acoustic impedance (ƶ), relaxation time (τ), free volume (V_f), and surface tension (S) were evaluated based on measured values of density (ρ), ultrasonic velocity (u), viscosity (η), and specific conductance. The results revealed significant variations in these parameters with temperature, indicating temperature-dependent molecular interactions. The calculated specific conductance provided additional insights into the conductivity of the liquid mixture. Overall, this study elucidates the complex molecular interactions in the PMMA-toluene binary system, providing valuable information for understanding its behavior and potential applications in various fields.

Keywords- Ultrasonic technology, Molecular interactions, Binary liquid mixture, Polymethylmethacrylate (PMMA), Toluene, Temperature-dependent analysis

P-99

Iodobenzene-Catalyzed Synthesis of Fully Functionalized NH-Pyrazoles and Isoxazoles from *α,β*-Unsaturated Hydrazones and Oximes via 1,2-Aryl Shift

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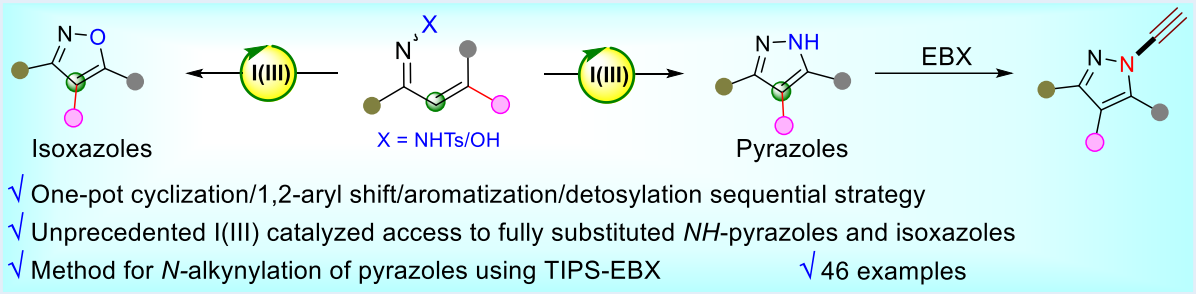
Hypervalent iodine catalysts have recently garnered increasing attention for the oxidative functionalization of π-bonds, enabling access to complex molecular scaffolds from simple and widely available substrates. Pyrazoles and isoxazoles are the privileged motifs found in numerous marketed drugs and natural products possessing vital properties like antidepressant, anti-inflammatory, antiviral, antibacterial, etc. Editing them with a heteroatom(s) often improves/expands the clinical efficacy of the parent molecules and opens new domains for applications through easy manipulations of these functionalities. Our group has recently developed highly efficient I(III) catalyzed methods for the preparation of pyrazoles and isoxazoles.



Keywords: Hypervalent iodine catalyst, Pyrazoles, Isoxazoles,, 1,2-Aryl migration, anti-Baldwin 5-endo-trig cyclization

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P-100

Bio-inspired Nanoparticle Synthesis from Oligosaccharides: A Pathway to Green Technology

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Abstract

Carbohydrates are natural compounds which are present in the form of oligosaccharide chains which are responsible for various medicinal properties like immuno-stimulant, anticancer, anti-tuberculosis etc. Nanoparticles are used to speedup chemical reaction as catalysts as well as they are also used for biomedical purpose to fight against viral and bacterial diseases. It may be used for targeted drug delivery. Goat milk reported for treatment in tuberculosis as well as increase numbers of platelets in Dengue suffered patients. In present article Nanotization of goat milk oligosaccharide mixture with metal precursor has been used to enhance their medicinal values. Co and Zn precursor were homogenized at 40ºC and resultant precipation so obtained was dried by established methods and was analyzed by UV-Vis, FTIR, SEM and EDX techniques. These nanoparticles of oligosaccharides may also be used as anti-inflammatory and anti-tuberculosis with other therapeutic significance.

Keywords: Milk, Oligosaccharide, UV-Vis, FTIR, SEM, EDX.

P-101

Mixed-Ligand Complexes of Vanadium as Potential Biomolecules

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Abstract

Vanadium is an important transition metal. The medicinal and diagnostic applications of vanadium complexes with minimum toxicity, have been extensively reported in the past [1]. Vanadium complexes have been reported to exhibit antidiabetic, tissue regeneration, anticancer, anti-inflammatory and antibacterial activities [2]. Thiosemicarbazones (TSCs) are one of the important Schiff-based ligands and exhibited remarkable chelating property due to their polydentate nature. TSCs containing metal complexes have been reported and have garnered significant interest among researchers due to their potential antibacterial, anticancer, and antineoplastic activities [3]. This study, present synthesis of novel mixed-ligand complexes of vanadium containing substituted thiosemicarbazone as primary ligand along with hetero-co-ligand. Molar conductivity and spectroscopic techniques like FT-IR, ^{1}H-NMR, UV–Vis, XRD and Elemental analysis reported in this paper have been used to characterize these complexes. Antibacterial activity evaluation of synthesized ligand and vanadium complexes against two Gram-positive (*B. subtilis, S. aureus)* and two Gram-negative bacteria (*E. coli, and S. abony*), establishes that these mixed ligand complexes can be considered as potential bio molecules in search of new generation drugs.

Keywords: Thiosemicarbazone, synthesis, vanadium, mixed-ligand complexes, antibacterial activity

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P-102

Molecular docking based studies of the steroidal derivatives as anti-cancer agents

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Cancer results in a large number of fatalities worldwide, due to which a lot of research is going on centered on this particular disease. Cancer is a condition where cells start growing uncontrollably, which is not seen in normal cells Hanahan et al. [1]. Previously, many molecules have been synthesized by introducing modifications in the steroids, like pregnanes, sapogenins and cholestanes which are reported to show anti-cancer activity against prostrate, cervical, and breast cancer, respectively Silva-Ortiz et al., Sethi et al., Carrasco-Carballo et al. [2-4]. Here, molecular docking of the steroidal derivatives is performed by using AutoDockTools-1.5.6., intended to find out what would be their probable effects on the actual cancerous cells. Molecular docking studies are serving as an excellent tool for predicting biological activities of the compounds computationally without actually performing *in vitro* experiments Fan et al. [5]. The activity of the compound is judged on the basis of the binding energy of that compound with the selected protein. The protein can be selected from the different databases like PDB (Protein Data Bank) and good biological activity is indicated by the large negative value Berman et al.[6].

Keywords: Anti-cancer, Molecular Docking, Steroidal Derivatives, AutoDock, Binding Energy

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P-103

Synthesis, characterization and Biological Studies of zinc and ruthenium complexes of thiosemicarbazones schiff's base derived from 4-(cholro-phenyl)-(5-flouro-2-hydroxy-phenyl)-methanone

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Abstract

This study focuses on the synthesis, characterization, and biological evaluation of zinc and ruthenium complexes derived from thiosemicarbazones Schiff bases, based on 4-(chlorophenyl)-(5-fluoro-2-hydroxyphenyl)-methanone. The synthesized ligands and complexes were characterized using FTIR, 1H NMR, 13C NMR, UV-Vis spectroscopy, mass spectrometry, and elemental analysis. Optimized geometries were calculated using Gaussian-09 with the B3LYP method. The biological activity of these compounds was evaluated against breast cancer (MDA-MB-231) and lung cancer (A549) cell lines using the MTT assay.The study highlights the anticancer potential of these metal complexes, with cytotoxic effects observed in a dose-dependent manner. Among the tested compounds, the ruthenium complex RHB1 demonstrated the highest activity against MDA-MB-231 cells, achieving an IC50 value of 115 µM. The zinc complexes ZHB1 and ZHB2 also exhibited significant cytotoxicity, with lower IC50 values compared to the free ligands. Spectroscopic studies confirmed the bidentate coordination mode of the thiosemicarbazone ligands through sulfur and azomethine nitrogen.These findings suggest that zinc and ruthenium complexes of thiosemicarbazones could serve as promising candidates for further development as anticancer agents, offering new insights into the design of metal-based therapeutics with enhanced biological activity.

Keywords: Thiosemicarbazones, Zinc complexes, Ruthenium complexes, Schiff base, Cytotoxicity, MTT assay, Breast cancer, Lung cancer, Spectroscopic analysis, Gaussian-09, IC50.

P-104

Design, Synthesis and Biological Evaluation of New Quinazolinone-Tetrazole Derivatives as Anticancer Agents

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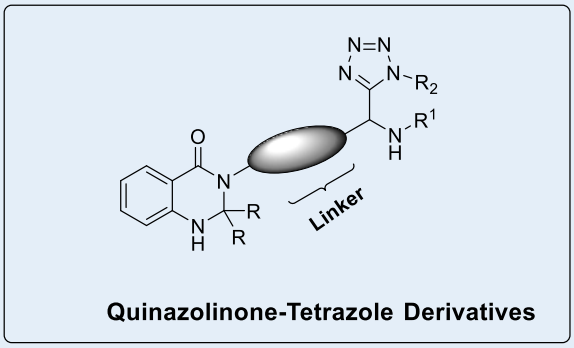
Cancer is a major public health and economic issue in the 21st century, causing almost one in six deaths (16.8%) worldwide and one in four deaths (22.8%) from noncommunicable diseases (NCDs). The number of new cancer cases per year is expected to rise to 29.5 million and the number of cancer-related deaths to 16.4 million by 2040, hence is a major health issue around the world [1]. Owing to the multifactorial nature of cancer, the cell develops resistance by resorting the compensatory factors or switching the signal pathway that promotes proliferation. In this regard, the synthesis of hybrid molecules with different pharmacophores emerged as an attractive strategy[2]. Notably, Quinazolinone is a privileged pharmacophore present in a plethora of natural products and displays diverse biological activities, including anticancer activities. There are many synthetic and natural product-based drugs, containing quinazoline and quinazolinone moiety, which are used clinically for treating various disease conditions [3]. Furthermore, tetrazoles are remarkably 10 times more lipophilic than the corresponding carboxylic acid, which increases the bioavailability of the drug. Research has recently focused on designing efficient tetrazole-based anticancer drugs due to their drug-like properties, targeting mechanisms like microtubulin polymerization inhibition, COX-2 angiogenesis, and efflux pumps.[4]. On the basis of the above observation, we designed novel Quinazolinone-Tetrazole derivatives and synthesized their analogues in order to discover a new class of potent anticancer agents.

Keywords -: Cancer, Quinazolinone, Tetrazole, isocyanide, Multicomponent reaction



Quinazolinone-Tetrazole Derivatives

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P-105

Pentafluoropyridine-mediated one-pot Strategy for the construction of biologically relevant 2,3-dihydroquinazolin-4(1*H*)-ones

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Dihydroquinazolin-4(1*H*)-ones have been recognized as a promising bioactive scaffold showing a broad range of physiological, pharmacological, and biological activities, including anti-inflammatory, antitumor, antibacterial, antimalarial, antiviral, anti-fungal, etc. Given the widespread use, researchers have directed their efforts towards developing various synthetic procedures for substituted dihydroquinazolinones[1].

In this regard, recently, we have reported the employment of commercially available, cheap pentafluoropyridine (PFPy) for a simple and straightforward one-pot synthetic protocol for the construction of 2, 3-Dihydroquinazolin-4(1H)-one derivatives. The reported protocol involves a PFPy-mediated multicomponent condensation reaction of aldehyde, amine and isatoic anhydride at elevated temperatures. This new chemical approach provides both mono- and di-substituted 2,3-dihydroquinazolin-4(1*H*)-ones in high yields. This research work exploited the electron-withdrawing nature of fluorine atoms in PFPy for the nucleophilic substitution at *para* to the *N*-atom to produce fluoride ions that assisted the synthesis of the 2,3-Dihydroquinazolin-4(*1H*)-ones in excellent yield. The broad substrate scope, easy purification, short reaction times, high yields and ease of operation enhance the versatility of the protocol [2].

Keywords: Pentafluoropyridine (PFPy), Multicomponent condensation, Isatoic anhydride, 2,3-Dihydroquinazolin-4(1H)-ones

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P-106

NMR and Mass Spectral Interpretation of Cusose - A Novel Pentasaccharide Isolated from Goat Milk and Its DFT Studies

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Abstract

Carbohydrates are one of the four major classes of biomolecules; they play important roles in various biological processes, including inflammation and immune response, angiogenesis and metastasis of cancer cells, viral and bacterial infections, and many other cell-cell communications. Oligosaccharides are the carbohydrate that contains 2-10 units of monosaccharides and have varied biological activities such as biological recognition, anti-complementary, anti-coagulant, anti-inflammatory, anti-viral, anti-bacterial, anti-tumor, anti-oxidant, lipid lowering, immunological, prebiotic and hypoglycemic activities. Goat milk oligosaccharides have anti-inflammatory properties and are involved in the repairing process after a dextran sodium sulphate-induced colitis. Keeping in mind the biological importance of goat milk oligosaccharides, in the present studies, goat milk was analyzed for its oligosaccharide content which led to the isolation of a novel oligosaccharide, cusose, $C_{36}H_{61}O_{26}N_3$. The HSQC spectrum of acetylated compound Cusose **'c'** at 300 MHz in $CDCl_3$ showed presence of four cross peaks of six anomeric protons and carbons in their respective region at δ6.25x88.97, δ5.67x91.53, δ4.47x100.95 and δ4.45x101.21 suggesting that compound Cusose **'C'** must be a pentasaccharide in its reducing form. Further, the ring protons of each anomeric proton were sepated using TOCSY spectrum. The sequencing of ring protons of each of the monosaccharides were carried out by COSY spectrum which gave an insight of the position of glycosidic linkages in the monosaccharides. Further the glycosidic linkages were confirmed by HMBC experiments. The configuration of the glycosidic linkages were ascertained by the splitting pattern of the respective anomeric proton signals. The absolute configuration of each monosaccharide were also ascertained by J values of anomeric protons. The structure of the isolated oligosaccharide was elucidated by chemical transformation, chemical degradation, ^1H, ^{13}C, 2D-NMR (COSY, TOCSY, HMBC and HSQC) and mass spectrometry as under.

β-D-GalNHAc(1→4)-β-D-Glc(1→3)-β-D-GalNHAc(1→3)-β-D-GalNHAc(1→4)Glc
CUSOSE

Keywords: Goat milk, oligosaccharides, cusose, NMR, Mass spectrometry, DFT studies.

Acknowledgement: Authors are thankful to Research and Development grant, Department of Higher Education, UP Government (2023-24)

P-107

Isolation and structure elucidation of a resembling trisaccharide core unit from Friesian cow milk

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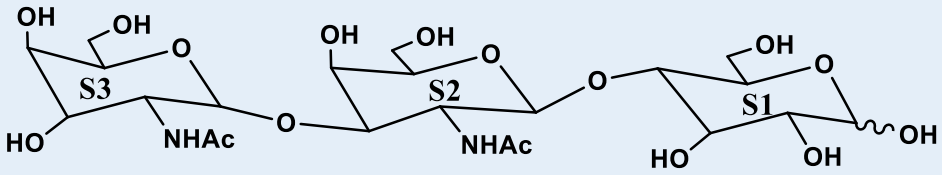
Abstract-

Structure of milk oligosaccharide is made up monosaccharides; Glucose, Galactose, GlcNHAc, GalNHAc, and Fucose. These monomers are linked together by varied glycosidic linkage having $^4C_1$ and $^1C_4$ conformations. The most commonly available core unit in oligosaccharides is lactose i, e. Gal β 4→1 Glc, further the enhancement of this core chain is elongated by addition of other monosaccharides to lactose moiety, relating it to the cow milk oligosaccharides. In our present studies, we have investigated an unexplored milk of Friesian cow. On processing it with modified method of Kobata and Ginsburg that incorporated de-proteination, micro filteration and lyophilisation and further, followed by its acetylation there after purification over silica column chromatography. A new trisaccharide 'Friuose' was isolated and its structure was elucidated by 2D NMR experiments of COSY, TOCSY, HSQC and HMBC besides this, basic NMR of ^1H and ^{13}C were also involved. Since the HSQC experiment showed 4 cross-peaks of anomeric carbon × proton at **δ88.9×6.25, δ91.50×5.68, δ100.93×4.48,δ100.93×4.48** confirming it to be a trisaccharide in its reducing form. The specificity of this novel trisaccharide was garneted by a ɑ glycosidic linkage between reducing Glc and GalNHAc where an ɑ glycosidic linkage was found instead of a β glycosidic linkage found in lactose, further the chain elongation was also garnished by another ɑ glycosidic linkage between S2 and S3 i. e. GalNHAc. All the assignment was confirmed by 2D NMR experiments of COSY, TOCSY, HSQC and HMBC. Further to remove the spectral degeneracy in ^1H NMR signals by sieving it using TOCSY experiment, which was further correlated by COSY experiment and confirmation of glycosidic linkages were performed by HMBC experiment., Configuration of glycosidic linkages were configured by splitting pattern of respective anomeric proton, more over the absolute conformation of monosaccharides were ascertained by J value of the respective anomeric proton. In the light of foregoing evidences the structure of a new trisaccharide 'Friuose' was elucidated as under.



FRIUOSE

Keywords: Friesian cow milk, 1D NMR, 2D NMR experiments, Friuose.

Acknowledgement: Authors are thankful to Research and Development grant, Department of Higher Education, UP Government.

P-108

Catalytic Synthesis of 1H-benzoxazolo[3,2-a]pyridin-1-ones via Formal [3 + 3] Annulations of NHC-generated Alkynyl Acylazoliums with Benzoxazolyl acetates and their Photophysical Studies

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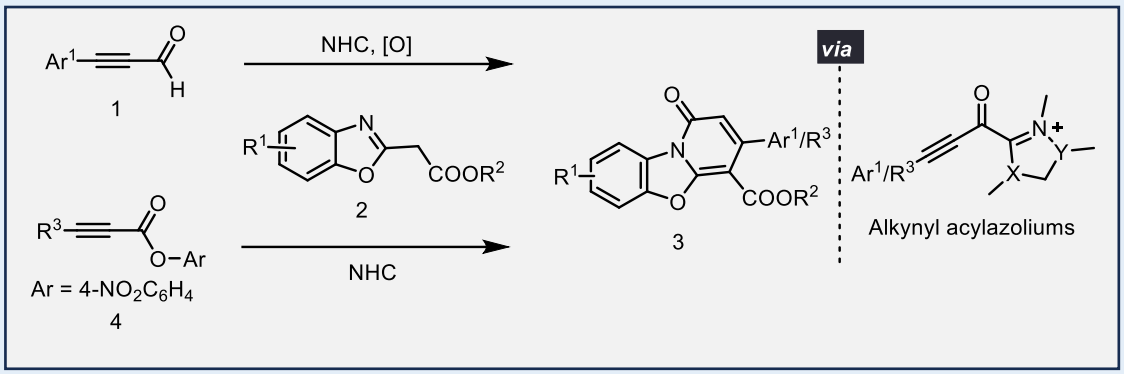
Abstract:

We have carried out synthesis of a tricyclic fused N-heterocycle via the NHC-catalysed annulation of either a ynal or an alkynyl ester with readily accessible benzoxazolyl acetate. Alkynyl acylazolium intermediates are formed directly with an NHC in the reaction with alkynyl esters, but the annulation with ynals necessitates the use of an oxidant. The lack of catalytic ways to obtain 1H-benzoxazolo[3,2-a]pyridin-1-ones from simple starting materials makes this procedure especially important. Furthermore, photophysical properties of the product have been assessed.



Keywords: N-heterocyclic carbene, alkynyl acyl azolium, polycyclic fused heterocycles.

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P-109

Hyperbaric Oxygen Therapy for Cancer

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As tumors grow, they start getting deprived of nutrients and oxygen, resulting in development of hypoxia and acidosis. Tumors have known to be adapted to hypoxic conditions, tumors increase glycolysis, angiogenesis in response to hypoxia as survival mechanism. Hpoxia induces multiple alterations in cancer cells such as upregulation of survival factors, enhanced invasive potential, genetic instability, preservation of undifferentiated state. Tumors shift to ischemic and low nutrient environments by three mechanism: 1) Angiogenic switch, resulting from change in balance between pro-angiogenic and anti-angiogenic factors, the secretion of cytokine VEGF is increased resulting in development of tortous and highly permeable blood vessels, the blood flow becomes highly chaotic in these vessels , further resulting in development of hypoxia, the increased permeability of blood vessels further cause development of invasive cancer phenotype resulting from enhanced migration of cancer cells, 2) Hypoxia helps tumors evade apoptosis by deregulating tumor suppressor p53 and increasing expression of telomerase enzyme 3) Glycolytic shift. Hyperbaric oxygen therapy involves administration of oxygen at pressures greater than atmospheric pressure intermittently. At normal pressure haemoglobin is 97% saturated with oxygen, any further increase in pressure has minimal impact on oxygen saturation of haemoglobin, but increases the oxygen concentration of plasma. Hyperbaric Oxygen therapy greatly increases oxygen pressure of tumor, altering hypoxic microenvironment. HBO therapy may have implications for angiogenesis and apoptosis and may push ROS levels beyond the threshold that can be handled by tumors, thus resulting in induction of apoptosis, this has been shown in colon, leukemic & ovarian cell lines. Many chemotherapies and radiotherapies work by increasing oxygen pressure in tumors, so combining radiotherapy with chemotherapy is proposed for better therapeutic outcome [1,2, 3]

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P-110

Synthesis, computational characterization, and Docking studies of 2,5-thiazole derivatives: insights into biological interactions and ADMET profiles.

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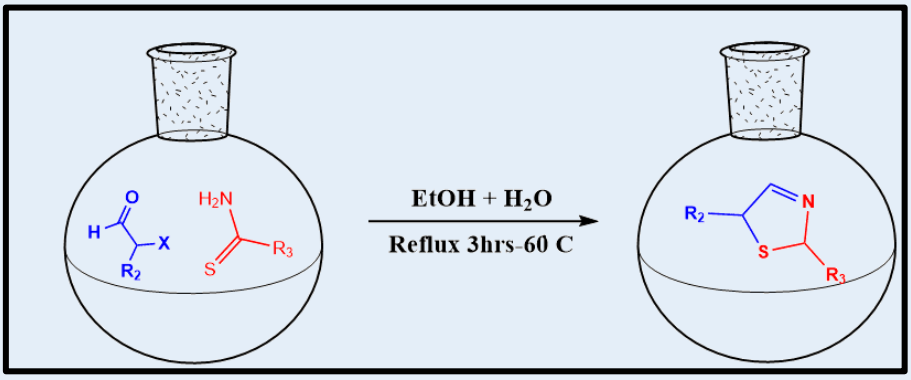
Abstract

This study focuses on the synthesis and computational evaluation of 2,5-thiazole derivatives, aiming to explore their potential as anti-fungal and anti-bacterial via in-silico study. The synthesized compounds were subjected to computational optimization using the 6-311G+ basis set within the framework of density functional theory (DFT). The docking analysis was conducted to investigate the binding interactions of the synthesized derivatives with three significant biological targets: *Escherichia coli* (PDB ID: 2CCZ), *Aspergillus fumigatus* (PDB ID: 6IDY), and *Streptococcus thermophilus* (PDB ID: 6W1E). These targets were selected based on their relevance to bacterial and fungal infections. The docking results revealed key interactions between the ligands and active sites of the target proteins, highlighting the compounds' potential inhibitory activities. Furthermore, ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) studies were performed to evaluate the pharmacokinetic profiles of the synthesized derivatives. This analysis provided critical information regarding their drug-likeness, bioavailability, and toxicity, offering insights into their suitability as drug candidates. The comprehensive integration of synthetic, computational, and pharmacokinetic studies underscores the potential of 2,5-thiazole derivatives as promising scaffolds for future drug discovery and development.



Scheme 1: systematic route for syntheses of 2,5-thiazole derivatives.

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Keywords: Thiazole derivatives, DFT, ADMET, Docking.

P-111

Synthesis, Spectroscopic Analysis and Computational Studies of 4-hydroxy-1,8-naphthyridin-2(1H)-one

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Abstract

Malignant tumours of many kinds have been identified to carry the BRAF-V600E mutation. It is believed that the development of potent BRAF-V600E inhibitors is an essential step in the treatment of several malignancies. This study employed *in-silico* techniques, including molecular docking analysis, ADMET assessment, and Density Functional Theory (DFT) computations, to test and determine the most effective BRAF-V600E inhibitor. The characteristics of 4-hydroxy-1,8-naphthyridin-2(1H)-one was investigated using different spectroscopic methods, including FT-IR, 1H-NMR, 13C-NMR, and UV-Vis spectroscopy. The DFT technique was used to do the theoretical calculations using the 6-311 ++ G (d, p) basis set and the B3LYP functional. The gap between the energy levels, LUMO (Lowest Unoccupied Molecular Orbital) and HOMO (Highest Occupied Molecular Orbital) values were calculated using the DFT approach. The Molecular Electrostatic Potential (MEP) was investigated in order to demonstrate the charge density patterns that could be connected to the biological activities. With the help of these findings, the development of a new anticancer drug is possible.

P-112

9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(*2H*,*5H*)-dione: Crystal Structure, In-silico studies and Anti-lung Cancer Activity

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Abstract

In this study, the synthesis, characterization and anti- lung cancer properties of 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8(*2H*,*5H*)-dione are presented. The formation of product was observed in a one-pot synthesis from 1,8-naphthyridine-2,4(1H,3H)-dione, dimedone, p-chloro benzaldehyde and ammonium acetate. The plausible mechanism of this multi-component reaction includes the initial formation of a chalcone derivative followed by Michael addition and finally, the product was formed by nucleophilic attack of ammonium acetate with elimination of water. The structure was assigned on the basis of detailed spectral analysis and also confirmed by X-ray crystal studies. The most significant interaction was found to be O···H/H···O (13.3%) with the help of Hirshfeld surface analysis and 2D fingerprint plot. The cytotoxicity value was found to be 316 µM in 48 h as compared to the reference (control). The results of biological activity and *in-silico* analysis indicated that the synthesized molecule could act as a precursor for the synthesis of certain other moieties of medicinal importance.

P-113

Synthesis, Characterization, and in-silico analysis of 2H pyrido[1,2-a]pyrimidine-2,4(3H)-dione

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Abstract

This research focuses on the synthesis, spectroscopic characterization, and computational analysis of 2H-pyrido[1,2-a]pyrimidine-2,4(3H)-dione. Advanced spectroscopic methods, such as FT-IR, UV-Vis, and ^{1}H and ^{13}C NMR, have been employed for the structure elucidation of the synthesized molecule. All the DFT calculations were performed using the B3LYP functional with a 6-311G+(d,p) basis set. A strong correlation was observed between the theoretical and experimental spectroscopic data. The time-dependent density functional theory was used to analyze its electrical properties and composition. The computational analysis of 2H-pyrido[1,2-a]pyrimidine-2,4(3H)-dione involves calculations of the electric dipole moment, Mulliken atomic charges, polarizability, and initial static hyperpolarizability values. Additionally, hyperconjugative interactions were investigated through NBO analysis, and the thermodynamic properties were assessed at various temperatures. Molecular docking results indicate significant anti-cervical cancer activity against HeLa cells, with a binding energy of -6.17 kcal/mol.

P-114

Synthesis, single crystal X-ray explication biological evaluation, and hirshfeld surface analysis, 2D fingerprint plot and 3D energy framework calculations of a malonamide derivative

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Abstract

The crystals of malonamide derivative were grown using slow evaporation solution technique. The molecule was investigated utilizing a variety of physiochemical and contemporary spectroscopic techniques. The unit cell Volume of 1182.5 (4) Å3 with dimensions of 13.009 (3) Å, 9.357 (2) Å, and 9.745 (2) Å were crystallized in P121/C1 space group of monoclinic crystal system and investigated using void mapping and Hirshfeld surface analysis. Other significant intermolecular interactions include N/H H/N (17.7), N/C C/N (2.4), C/C C/C (1.6), O/C C/O (1.0), and O/N N/O (0.4). Their influence on crystal packing is obvious in 2D fingerprint plots. The 3D structure of crystal packing was explored using 3D energy framework analysis.

P-115

Computational Studies of Benzoxazolone Derivatives as Translocator Protein Marker

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Abstract:

Translocator Protein (18 kDa) TSPO, is widely distributed in the outer mitochondrial membrane and highly expressed during microglia activation in neuroinflammatory diseases.
The translocator protein (TSPO, 18 kDa) is a highly promising biomarker for studying the role of neuroinflammation in humans as well as in various animal species. The binding data of first- and second-generation PET radioligands has revealed that TSPO binding sites varies with different affinities and they were differentiated as HABs, LABs and MABs. We have also studied a series of TSPO molecules through docking and MD simulation analysis (PDB: 2MGY). Computational data analysis showed pattern of variable binding profile of known diagnostic ligands and our screened ligands via interactions with conserved residues in the binding pocket. These findings suggested that benzoxazolone derivatives may become a promising marker for visualization of neuroinflammation via TSPO targeting.

Fluorescent probes have become valuable tool in protein research as well as protein binding ligand, carried out through docking studies to gain better insight of its interaction with TSPO as compared to other known TSPO probes.

This study seeks to investigate the potential of benzoxazolone derivatives as TSPO imaging agents using advanced computational techniques. Through molecular docking simulations, DFT calculations, and molecular dynamics simulations, we examine the interactions between these compounds and the TSPO binding site. Quantum mechanical calculations are utilized to assess the electronic properties and reactivity of the benzoxazolone derivatives, offering insights into their potential as effective TSPO ligands. The results provide a comprehensive molecular understanding of the binding mechanisms between these derivatives and TSPO, highlighting their promise as potential TSPO markers for neuroimaging and diagnostic purposes. However, further experimental validation is necessary to confirm the clinical applicability of these computational predictions.

Key Words: Docking, Benzoxazolone, Neuroinflammation, TSPO, DFT.

P-116

Synthetic approaches towards Imidazo-Fused Heterocycles

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Abstract:

Imidazole moiety when fused with other heterocyclic system form numerous compounds with different types of pharmacological and biological activities. In this review we discussed a comprehensive analysis of the synthesis methodologies and reaction mechanisms for imidazo-fused heterocyclic molecules. These molecules represent a crucial class of compounds due to their significant applications and versatile chemical reactivity. This article meticulously examined various synthetic routes for the construction of imidazo-fused heterocycles, ranging from traditional methods to modern approaches such as microwave assisted, NPs catalyzed, light mediated, electrochemical reactions, transition metal free synthesis routes. By consolidating the current knowledge and highlighting future directions, this review aims to serve as a treasure for research community in the fields of organic chemistry, medicinal chemistry and material science.

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