31st ISCB International Conference ISCBC 2025-2026

Innovations in Interdisciplinary Areas of Sciences Towards Global Health and Sustainability

19-21 December, 2025
Kalinga Institute of Industrial Technology (KIIT)
Bhubaneswar, Odisha, India

ABSTRACT BOOK

Jointly Organized by:
Indian Society of Chemists & Biologists (ISCB)
School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT)

www.iscbindia.com | www.iscbconference.com

ISCBC 2025-2026

Jointly Organised by

Sapphire Sponsor

MAHANADI COALFIELDS LIMITED
(A Govt. of India Undertaking & Subsidiary of Coal India Limited)

Crystal Sponsor

CAS
A division of the
American Chemical Society

Sponsors

Rhodium MASTER
Mines to Medicine

GaloreTx
Transformative Medicines

DEEPALI

TCG Lifesciences | CHEMBIOTEK

STAR DMC
WORLD FAMOUS TOURS

HOTEL SUDHA REGENCY

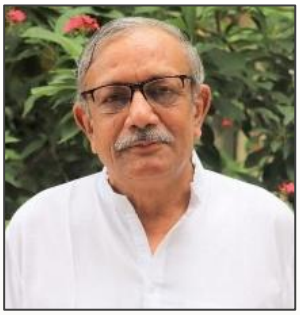
RANI SATI ENTERPRISES

Knowledge Partner

ISCB RESEARCH FOUNDATION

Digital Partner

Webgrade TECHNOLOGIES



Prof. (Dr.) Anamik Shah
President, ISCB

Prof. (Dr.) PMS Chauhan
General Secretary, ISCB

Message

We are delighted to announce that the Indian Society of Chemists and Biologists (ISCB), Lucknow, is hosting the **31st ISCB International Conference (ISCBC 2025-2026)**. This prestigious event is being jointly organized by **Indian Society of Chemists and Biologists** and the **School of Applied Sciences, Kalinga Institute of Industrial Technology (KIIT), Bhubaneswar, Odisha**, and will take place at **KIIT, Bhubaneswar, Odisha, India, from December 19 to 21, 2025**.

The central theme of ISCBC 2025-2026 is "**Innovations in Interdisciplinary Areas of Sciences Towards Global Health and Sustainability**." 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 panel discussions 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 research organizations, universities, academic institutions, and pharmaceutical companies. We hope all participants enjoy a memorable stay in Bhubaneshwar. 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 2025-2026.

Organizing Committee ISCBC 2025-2026

Chief Patron
Prof. Achyuta Samanta, Founder KIIT, KISS & KIMS

Patron:
Prof. Saranjit Singh, Vice Chancellor, KIIT DU, Bhubaneswar
Prof. Jnyana Ranjan Mohanty, Registrar, KIIT DU, Bhubaneswar

National Advisors:
Prof. Anamik Shah, President, ISCB, Lucknow
Dr. Prem Man Singh Chauhan, General Secretary, ISCB, Lucknow
Dr. Mahesh C. Sharma, Director, Plants Med Laboratories, Jaipur
Prof Prasanta Rath, Dean, School of Applied Sciences
Prof. Mrutyunjay Suar, Director General R&D, KIIT,Bhubaneswar
Prof. Gopal C. Kundu, Director R&D, KIIT, Bhubaneswar
Dr. Suresh Chandra Satapathy, Director Doctoral Research & Publications, KIIT, Bhubaneswar
Dr. Debasis Dash, Director, DBT-ILS, Bhubaneswar
Dr. Sanghamitra Pati, Director of ICMR-Regional Medical Research Centre (RMRC)
Prof. Jagneshwar Dandapat, Vice-Chancellor, Utkal University

Convener:
Dr. Chandana Mohanty, Associate Dean Biology, School of Applied Sciences, KIIT DU, Bhubaneswar

Co Conveners:
Dr. Sarbari Acharya, School of Applied Sciences, KIIT DU, Bhubaneswar
Dr. Nikita Mahapatra, School of Applied Sciences, KIIT DU, Bhubaneswar

Organizing Secretaries:
Dr. Ch. Vinod, School of Applied Sciences, KIIT DU, Bhubaneswar

Joint Secretaries:
Dr. Sutanu Satpathy, School of Applied Sciences, KIIT DU, Bhubaneswar
Dr. Jagnyaseni Tripathy, School of Applied Sciences, KIIT DU, Bhubaneswar

Local Organizing Committee:
Dr. Tapan Kumar Bastia, Associate Dean, SAS, KIIT DU, Bhubaneswar
Dr. Mrutyunjaya Das, Associate Dean, SAS, KIIT DU, Bhubaneswar
Dr. Dibyaranjan Rout, Associate Dean, SAS, KIIT DU, Bhubaneswar
Dr. Kajal Parashar, Dy. Director-CEC, KIIT DU, Bhubaneswar
Dr. Bhavya Bhusan, SAS, KIIT DU, Bhubaneswar
Dr. Gopal Pradhan, SAS, KIIT DU, Bhubaneswar
Dr. Jashashree Ray, SAS, KIIT DU, Bhubaneswar
Dr. Pratap Kumar Deheri, SAS, KIIT DU, Bhubaneswar
Dr. Rakesh Mohan Das, SAS, KIIT DU, Bhubaneswar
Dr. Supriya Roy, SAS, KIIT DU, Bhubaneswar

Dr. Biswadeep Das, School of Biotechnology, KIIT DU, Bhubaneswar
Dr. Rahul Modak, School of Biotechnology, KIIT DU, Bhubaneswar
Dr. Rambabu Dandela, ICT Mumbai (IOC Bhubaneswar campus)
Dr. Kruthi Doriya, ICT Mumbai (IOC Bhubaneswar campus)
Dr. Swagat Mohapatra, ICT Mumbai (IOC Bhubaneswar campus)
Dr. Ramakanta Naik, ICT Mumbai (IOC Bhubaneswar campus)
Dr. Sangram Keshari Samal, RMRC-ICMR, Bhubaneswar
Dr. Tushar Kant Beuria, Institute of Life Sciences, Bhubaneswar

International Advisory Board ISCBC 2025-2026

- **Prof Jyoti Chattopadhyaya,** Chair of Chemical Biology, Uppsala University, Uppsala, **Sweden**
- **Prof Mike Threadgill,** University of Bath, Claverton Down, Bath, **UK**
- **Prof Dr. Stefan Brase,** Karlsruhe Institute of Technology, **Karlsruhe, Germany**
- **Prof Kazuaki Matsumura,** Japan Advanced Institute Science and Technology, **Japan**
- **Prof Kwang-Soo Kim,** Professor and Director, Molecular Neurobiology Laboratory, McLean Hospital/Harvard Medical School, Boston, **USA**
- **Prof Athina Geronikaki,** University of Thessaloniki, Thessaloniki, **Greece**
- **Prof Colin J Suckling,** Research Professor of Chemistry, Department of Pure & Applied Chemistry, University of Strathclyde, Glasgow, **Scotland**
- **Prof A. Ganesan,** School of Pharmacy, University of East Anglia, **United Kindgom**
- **Prof Om Prakash,** Kansas State University, Manhattan, **USA**
- **Prof Binghe Wang,** Georgia State University, Atlanta, Georgia, **USA**
- **Dr Ute Schepers,** KIT, Institut for Toxikologie und Genetik, **Germany**
- **Prof Dr. Erik Van der Eycken,** Katholieke Universiteit Leuven, **Belgium**
- **Prof Alvarez Mercedes,** University of Barcelona, **Spain**
- **Dr Mukund S. Chorghade,** President & Chief Scientific Officer, THINQ Pharma, **USA**
- **Prof Mahesh K. Lakshman,** The City College and The City University of New York, **USA**
- **Prof Rachna Sadana,** University of Houston-Downtown, Houston, **USA**
- **Prof Karol Grela,** Polish Academy of Sciences, Warsaw, **Poland**
- **Prof Christophe LEN,** Universit de Technologie de Compigne, **France**
- **Prof Rui Moreira,** University of Lisbon, **Portugal**
- **Prof Sun CHOI,** College of Pharmacy & Graduate School of Pharmaceutical Sciences, EwhaWomans University, Seoul, **Korea**
- **Prof Girolamo Cirrincione,** Emeritus Professor of Medicinal Chemistry, University of Palermo, Via Archirafi, 32 - 90123 Palermo, **Italy**
- **Prof To Ngai, Dept.** of Chemistry, The Chinese University of, **Hong Kong**
- **Prof Anoja Attanayake,** Department of Biochemistry, Faculty of Medicine, University of Ruhuna, **Sri Lanka**
- **Prof Barbara Zajc,** Department of Chemistry and Biochemistry, The City College of New York, **USA**
- **Prof Dipak P. Ramji,** Cardiff School of Biosciences, Cardiff University, Cardiff, **UK**
- **Dr Edmond Differding,** Managing Director, Differding Consulting, **Luxembourg**
- **Dr Harsha Rajapakse,** Department of Chemistry and Environmental Science, Medgar Evers College, The City University of New York, Brooklyn, New York, **USA**
- **Prof Marco L. Lolli,** Assistant Professor in Medicinal Chemistry, Dept. Science and Drug Technology - University of Turin (UniTO), **Italy**
- **Prof Michele Vittadello,** Professor of Chemistry and Nanoscience, Medgar Evers College of the City University of New York, Energy Nanotechnology and Materials Chemistry Team, 1638 Bedford Avenue, Brooklyn, NY, **USA**
- **Prof Nigel G. J. Richards,** Department of Chemistry, Cardiff University,

Cardiff, **UK**

- **Prof Ramaiah Muthyala,** Centre for orphan drug development, University of Minneapolis, MN, **USA**
- **Prof Premysl Mladenka,** Faculty of Pharmacy in Hradec Králové, Akademika Heyrovskeho 1203, 500 05 Hradec Kralove, **Czech Republic**
- **Prof Katsuhiko Ariga,** World Premier International (WPI) Research Center for Materials Nanoarchitectonics National Institute for Materials Science 1-1 Namiki, Tsukuba, Ibaraki, **Japan**
- **Dr Anna Kajetanowicz,** Biological and Chemical Research Centre, Faculty of Chemistry, University of Warsaw, Warsaw, **Poland**
- **Prof Krishna Kumar,** Department of Chemistry, Tufts University, Medford, MA, **USA**

SCIENTIFIC PROGRAMME

Friday, December 19, 2025

Registration
Venue: Campus 5

9.00 AM onwards	**Registration**

Inaugural Session
Venue: Campus 5 Auditorium

10.00 AM - 11.30 AM	**Inaugural Session**

11.30 AM – 12.00 PM	**High Tea**

Session – I
Venue: Campus 5 Auditorium

Chairpersons: Prof Anamik Shah and Dr PMS Chauhan

PL-1 12.00 AM - 12.35 PM	**M.V. Raghavendra Rao** Professor of Microbiology and Senior Executive Vice President, World Academy of Medical Sciences, Netherlands **Is Interdisciplinary technology the future of Medicine?**
IL-1 12.35 PM - 1.00 PM	**Bapurao B. Shingate** Professor in Organic Chemistry, Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, (Formerly Aurangabad), Maharashtra, India **Monocarbonyl Analogues of Curcumin (MACs): Development towards new therapeutic agents**
1.00 PM - 2.00 PM	**Lunch**

Poster Session
Venue: Kunjaban Area at Campus-6

Chairpersons: Dr Rohit Jain, Dr Hardik Bhatt, Dr Alok Panda

2.30 PM – 3.30 PM	**Poster Number P-1 to P-50**

Parallel Session – II A
Venue: Conference Hall-1 at Campus-6

Thematic Area: - Life sciences and Health care

Chairpersons: Prof Murlidhar S. Shingare, Dr Sanjeeb K. Sahoo

IL-2 3.30 PM - 3.55 PM	**Alok Jain** Assistant Professor and Ramalingaswami Fellow, Birla Institute of Technology Mesra, Ranchi, India **Accelerating Alzheimer's Drug Discovery: Machine Learning–Driven Design and Prediction of Amyloid-β Aggregation Inhibitors**

IL-3 3.55 PM - 4.20 PM	**Sanjay Kumar** Professor of Practice, Department of Chemistry, BITS Pilani, K K Birla Goa Campus, Goa, India **Drug discovery research in India: Current trends and analysis of Industry-Academia and Government collaborations**
IL-4 4.20 PM - 4.45 PM	**Niyati Acharya** Assistant Professor & Head, Department of Pharmacognosy, Institute of Pharmacy, Nirma University, Ahmedabad, India **Neuroprotective Natural Products: Emerging Strategies for Alzheimer's Disease Management**
IL-5 4.45 PM - 5.10 PM	**Raghuvir Ramakant Pissurlenkar** Professor, Department of Pharmaceutical Chemistry, Goa College of Pharmacy, Panaji, Goa **TARGETING DPP-IV FOR ANTI-DIABETIC THERAPY: COMPREHENSIVE COMPUTATIONAL EXPLORATION OF NOVEL AND PROMISING INHIBITORS**
IL-6 5:10 PM - 5.35 PM	**Bhumika Patel** Assistant Professor, Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad, India **Next-Generation Selective PARP1 Inhibitors: Enhancing Therapeutic Index Through Reduced Toxicity in Oncologic Applications**
5:35 PM - 5.45 PM	**Tea**

Parallel Session – II B
Venue: Conference Hall-2 at Campus-6

Thematic Area: - Material Sciences and Technology/Life sciences and Health care

Chairpersons: Prof Devdutt Chaturvedi, Dr Tushar Kant Beuria, Dr Srinivas Patnaik

IL-7 3.30 PM - 3.55 PM	**Soumen Basu** Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Development of a Portable Microcontroller-Based Fluorescence Sensing Module for Dual Detection of Hexavalent Chromium and Ascorbic Acid Using Banana Peel-Derived Carbon Quantum Dots**
IL-8 3.55 PM - 4.20 PM	**Hardik G. Bhatt** Associate Professor and Head, Dept. of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University and Head, Centre for Advanced Instrumentation, Nirma University, Ahmedabad, India **HIT to LEAD Optimisation of *N*-Substituted Acridine-9-Amino Derivatives as Telomerase Inhibitors for the Treatment of Lung Cancer**
IL-9 4.20 PM - 4.45 PM	**Priyankar Paira** Associate Professor, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore, Tamilnadu, India **Stimuli-responsive Prodrug Activation in Mitochondria for Cancer Therapy**

IL-10 4.45 PM - 5.10 PM	**Saravanan Matheshwaran** Associate Professor, Microbial Adaptation and Chromatin Remodeling Laboratory, Department of Biological Sciences and Bio-engineering, Environmental Microbiology Laboratory, Center for Environmental Sciences and Engineering, Indian Institute of Technology, Kanpur, Uttar Pradesh, India **Targeting Mycobacterial "SOS" Response- a strategy to toggle Antimicrobial Resistance (AMR)**
IL-11 5:10 PM - 5.35 PM	**John J Georrge** Associate Professor, Department of Bioinformatics, University of North Bengal, Raja Rammohunpur, Darjeeling, West Bengal, India **Decoding Monkeypox–HIV Crosstalk: FDA-Approved Therapeutic Leads**
4:35 PM - 4.45 PM	**Tea**

Parallel Session – II C
Venue: Conference Hall-5 at Campus-6

Thematic Area: - Synthetic Inorganic and Organic Chemistry

Chairpersons: Dr Rahul Shrivastava, Dr Samaresh Jana

IL-12 3.30 PM - 3.55 PM	**Asha Jain** Professor, Department of Chemistry, University of Rajasthan, Jaipur, India **Design and Synthesis of Organotin(IV) Complexes: Structural Insights and Potential Applications**
IL-13 3.55 PM - 4.20 PM	**Ram Sagar Misra** Professor, School of Physical Sciences, Jawaharlal Nehru University (JNU), New Delhi, India **Synthesis of 2-Deoxy Sugars, Chirally Pure 3-Bisindolyl-C-Glycosides, Pyrazolyl-pyrimidinone and Imidazopyrimidinonesbased Glycohybrids from Glycals**
IL-14 4.20 PM - 4.45 PM	**Debasish Mandal** Associate Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, India **The Effect of Ligand Environment on the C–H Activation Properties of Bio-inspired Metal–Oxo Complexes**
IL-15 4.45 PM - 5.10 PM	**Shovan Mondal** Assistant Professor in Chemistry, Syamsundar College, Shyamsundar, Burdwan, India **A thorough investigation of the synthesis of TAM and MET receptor kinases inhibitor's core (R)-2-((4-(4-amino-2-fluorophenoxy)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)amino)propan-1-ol**
IL-16 5:10 PM - 5.35 PM	**Bhupendra Goswami** Assistant Professor, Department of Chemistry, Central University of Rajasthan, Bandarsindri, Rajasthan, India **NPN Coordination Complexes: From Ligand Design to Applications**

5:35 PM - 5.45 PM	**Tea**

Parallel Session – II D
Venue: Conference Hall-8 at Campus-6

Thematic Area: - Sustainable and Green Chemistry

Chairpersons: Prof Sundaram Singh, Dr Nibedita Jena (ILS)

IL-17 3.30 PM - 3.55 PM	**Hitendra M. Patel** Professor, Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Sustainable synthesis of imidazo[2,1-*b*]quinazolin-1(2*H*)-ones as PDGFRA inhibitors**
IL-18 3.55 PM - 4.20 PM	**Dalip Kumar** Senior Professor, Department of Chemistry, Birla Institute of Technology & Science, Pilani, Pilani Campus, Rajasthan, India **Abstract Awaited**
IL-19 4.20 PM - 4.45 PM	**Banibrata Maity** Assistant Professor, Department of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology, Patiala, Punjab, India **Sustainable Synthesis of Biomass-Derived Carbon Quantum Dots for Nanosensing Applications**
IL-20 4.45 PM - 5.10 PM	**Rinku Chakrabarty** Head, Department of Chemistry, Alipurduar University, Aipurduar, West Bengal, India **Biotemplated Synthesis of Perovskite oxide: Waste to Wealth Conversion and its Potential Application in Bioremediation**
IL-21 5.10 PM- 5.35PM	**Vikas Tyagi** S Associate Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, India **Green Catalysis for Sustainable Organic Synthesis**
4:35 PM - 4.45 PM	**Tea**

Cultural Evening
Venue: Rose Garden (Campus 12)

7.00 PM – 8.00 PM	**Cultural Programme**
8.00 PM	**Dinner**

Saturday, December 20, 2025

Registration
Venue: Campus 6

9.00 AM onwards	**Registration**

Parallel Session – III A
Venue: Conference Hall-1 at Campus-6

Thematic Area: - Life Sciences and Health care

Chairpersons: Dr Keshav Deo, Dr Gopal Kundu, Dr SKS Parashar

PL-2 9.00 AM - 9.35 AM	**Om Prakash** Professor, Biochemistry & Mol. Biophysics, Dept. of Biochemistry and Molecular Biophysics, Kansas State University, Manhattan, USA **How Staph Bacteria Blocks Host Immune Enzymes: New Structural Insights**
IL-22 9.35 AM - 10.00 AM	**Amit Shard** NIPER-Ahmedabad, India **Orchestrating Metabolic-Microbial Synergy: A New Frontier with Thiazole-Based PKM2 Inhibitors in Colorectal Cancer**
IL-23 10.00 AM - 10.25 AM	**Sonu Gandhi** Scientist-E, Biosensor and NanoBioengineering Laboratory (BNBL), National Institute of Animal Biotechnology, Hyderabad **Endemic Flaviviruses: A Persistent Challenge for India's Healthcare?**
O-1 10.25 AM - 10.40 AM	**Shital Panchal** Department of Pharmacology, Institute of Pharmacy, Nirma University, S.G. Highway, Ahmedabad, India **Mechanistic Insights into the Protective Role of a Novel Metallic Curcumin Complex in Acute Pancreatitis**
O-2 10.40 AM - 10.55 AM	**Nandini Roy** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, India **Design, Synthesis, Biological Evaluation, and In Silico Studies of Novel Indolyl Acrylonitriles as Potential Anti-cancer Agents**
O-3 10.55 AM - 11.10 AM	**Advait Pramod Dubey** Department of Clinical Pharmacology, Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Kharghar, Navi-Mumbai – 410210, India **Discovery and Development of Drugs against Transplant Associated Thrombotic Microangiopathy (TA-TMA)**
11.10 AM – 11.25 AM	**Tea Break**

IL-24 11.25 AM - 11.50 AM	**Dina Nath Singh** Professor, K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Ayodhya, India **Current Sequential Stages for the Search of New Pharmacologically Active Agents from Medicinal Plants**
IL-25 11.50 AM – 12.15 PM	**Priya Ranjan Debata** Assistant Professor, Department of Zoology, Maharaja Sriram Chandra Bhanja Deo University (Erstwhile North Orissa University), Takatpur, Baripada, Mayurbhanj, Odisha, India **Reprogramming of Carbohydrate Metabolism Pathways by Mutant Isocitrate Dehydrogenase in Glioma**
O-4 12.15 PM – 12.30 AM	**Ashutosh Sahoo** Metabolic Systems Biology Lab, School of Biosciences and Bioengineering, Indian Institute of Technology Mandi, Kamand 175075, Himachal Pradesh, India **Discovery of promising metabolic pathway targets and essential oil phytochemicals against *Mycobacterium sp.***
O-5 12.30 PM – 12.45 PM	**Siri Chandana Gampa** Department of Life Sciences, School of Science, GITAM (Deemed to be University), Visakhapatnam, Andhra Pradesh, India **LMTK3 as a regulator of TRAIL-induced apoptosis in breast cancer: Mechanistic insights**
1.00 PM - 2.00 PM	**Lunch**

Parallel Session – III B
Venue: Conference Hall 2 at Campus-6

Thematic Area: - Material Sciences and Technology

Chairpersons: Dr Mahesh Sharma, Dr Snehasish Mishra, Dr Dibya Ranjan Rout

IL-26 9.00 AM - 9.25 AM	**Dhananjay V Mane** Associate Professor, Department of Chemistry, Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat, Gujarat, India **Process Validation of Anti-Fungal Drug Product -Immediate Release Oral Solid Dosage Form by Wet granulation approach : Itraconazole Capsules**
IL-27 9.25 AM - 9.50 AM	**Brajendra K. Singh** Professor, Department of Chemistry, University of Delhi, Delhi, India **Photophysical Insights into Base-Modified Fluorescent Nucleosides**
IL-28 9.50 AM - 10.15 AM	**Sunil K. Sharma** Senior Professor, Department of Chemistry, University of Delhi, Delhi, India **Synthesis of Amphiphilic Nano-architectures for Targeted Drug Delivery**

IL-29 10.15 AM – 10.40 AM	**Monochura Saha** Assistant Professor, Birla Institute of Technology, Mesra (BIT Mesra), Ranchi, India **Magnetically Actuated Nanoantennas for Wireless Glioblastoma Therapy**
O-6 10.40 AM - 10.55 AM	**Ashlesha Arjun Jadhav** Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University Chhatrapati Sambhaji Nagar-Maharashtra, 431004, India **MOF-Derived NiO/SrO Nanocatalyst Enabled Multicomponent Synthesis of Novel AIPDs with Promising Anticancer Potential**
O-7 10.55 AM - 11.10 AM	**ISHANKI BHARDWAJ** Department of Chemistry, Sir PT Sarvajanik College of Science, MTB College Campus, Jawaharlal Nehru Marg, Opp. Chaupati, Athwalines, Surat, Gujarat, India **Organic framework-based sensors for environment and chemical security**
11.10 AM – 11.25 AM	**Tea Break**
IL-30 11.25 AM – 11.50 AM	**Soma Chattopadhyay** Scientist-F, Infectious Disease Biology, Institute of Life Sciences, Bhubaneswar, India **Abstract Awaited**
O-8 11.50 AM – 12.05 PM	**Shital Butani** Department of Pharmaceutics, Institute of Pharmacy, Nirma University, Gujarat, India **Protective Role of Quercetin Nano-suspension Delivered via Inhalation in Experimental Pulmonary Fibrosis**
1.00 PM - 2.00 PM	**Lunch**

Parallel Session – III C
Venue: Conference Hall-5 at Campus-6
Thematic Area: - Synthetic Inorganic and Organic Chemistry

Chairpersons: Prof Nisheeth Desai, Dr Tapas R. Sahoo

IL-31 9.00 AM - 9.25 AM	**Ravindra Kumar** Principal Scientist, Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute (CDRI), Lucknow, India **Modular Approaches for the Synthesis of Boron-Heterocycles and BN-Isosteres**
IL-32 9.25 AM - 9.50 AM	**Ajay Kumar Srivastava** Senior Principal Scientist/ Professor (AcSIR), Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Post-Ugi Cyclizations: A Magical Tool to Molecular Diversity**
IL-33 9.50 AM - 10.15 AM	**Neelima Gupta** Professor, Department of Chemistry, University of Rajasthan, Jaipur, India **Unraveling Stereochemical Control in Cycloaddition Reactions of Thiazolium Ylide: A Computational Perspective**

O-9 10.15 AM - 10.30 AM	**Nivedita Acharjee** Department of Chemistry, Durgapur Government College, Durgapur, West Bengal, India **Understanding the Tether Length Effects on Nitrone Intramolecular [3+2] Cycloadditions: Insights from Molecular Electron Density Theory (MEDT)**
O-10 10.30 AM - 10.45 AM	**Rapti Goswami** Biophysical Chemistry Laboratory, Physical Chemistry Section, Department of Chemistry, Jadavpur University, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India **Insights into the Binding of Phenothiazinium Dye Methylene Blue with Triple and Double Helical Forms of RNA: A Multispectroscopic Approach**
O-11 10.45 AM – 11.00 AM	**Apeksha Hiru Naik** School of Chemical Sciences, Goa University, Taleigao Plateau, Goa, 403206, India **Synthesis of novel analogues of fused angular and linear π-extension of Acridones from quinoxalinones and benzoxazinones**
11.00 AM – 11.15 AM	**Tea Break**
IL-34 11.15 AM - 11.40 AM	**Indresh Kumar** Professor, Department of Chemistry, Birla Institute of Technology & Science Pilani, Pilani, Rajasthan, India **Direct Access to C3-Functionalized Pyrrole**
O-12 11.40 AM – 11.55 AM	**Shivam Kumar** Department of Chemistry Birla Institute of Technology, Mesra, Ranchi, India **Synthesis, characterization, and Mosquiticidal Studies of Isoxazoleoxadiazole analogs**
1.00 PM - 2.00 PM	**Lunch**

Parallel Session – III D
Venue: Conference Hall- 8 at Campus-6

Thematic Area: - Sustainable and Green Chemistry

Chairpersons: Prof Okram Mukherjee Singh, Dr Amiya Priyam, Dr Ashok k. Sahoo

IL-35 9.00 AM - 9.25 AM	**Ramesh Kothari** Professor (Direct), Head, Department of Biosciences, Coordinator (Institute of Biotechnology), Saurashtra University, Rajkot, Gujarat, India **Functional Traits of Peanut-Associated Rhizobacteria: Unlocking Biofertilizer Potential for Enhanced Productivity and Sustainable Agricultural Practices**
IL-36 9.25 AM - 9.50 AM	**Surendra Singh** Professor, Department of Chemistry, University of Delhi, Delhi, India **Development of Recoverable Chiral Mn(III) Salen Complexes as Catalysts for Oxidative Kinetic Resolution of secondary alcohols**

IL-37 9.50 AM - 10.15 AM	**Pratibha Kumari** Department of Chemistry, Deshbnadhu College, University of Delhi, New Delhi, India **Heterogeneous and homogeneous catalytic approaches for the conversion of carbon dioxide into cyclic carbonates**
IL-38 10.15 AM - 10.40 AM	**Anirban Pradhan** Assistant Professor, Department of Chemistry, Birla Institute of Technology (BIT) Mesra, Ranchi, India **Porous Carbon Materials based Green and Renewable Hydrogen Fuel Production**
O-13 10.40 AM - 10.55 AM	**Amit Kisan Bhosale** Centre for research and development, Dr. Subhash University, Junagadh (362001), Gujarat, India **Synthetic Strategies for Adenine-Derived Acyclic Nucleoside Phosphonates: Toward Greener and Scalable Manufacturing Solutions**
10.55 AM – 11.10 AM	**Tea Break**
IL-39 11.10 AM – 11.35 AM	**Sundaram Singh** Professor and Head, Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh, India **Visible light-induced C-N bond formation: A green and Sustainable approach**
IL-40 11.35 AM – 12.00 PM	**Ramendra Pratap** Professor, AvH and JSPS Fellow, Department of Chemistry, University of Delhi, North Campus, Delhi, India **Green approach for the synthesis of various functionalized isolated and fused thiophenes and their biological and photophysical properties**
IL-41 12.00 AM – 12.25 PM	**Hitesh D. Patel** Professor & Head, Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India **Collaborative Research - The Key to Success**
O-14 12.25 PM - 12.40 PM	**Sibangini Misra** Lecturer in Botany. Maharishi College of Natural Law, Bhubaneswar, India **ORGANIC FARMING FOR SUSTAINABLE AGRICULTURE: A REVIEW**
1.00 PM - 2.00 PM	**Lunch**

Parallel Session – IV A
Venue: Conference Hall-1 at Campus-6

Thematic Area: - Life sciences and Health care

Chairpersons: Prof M.V. Raghavendra Rao, Dr Luna samanta, Dr Naresh Chandra Bal

IL-42 2.00 PM - 2.25 PM	**Dinesh Kumar** Assistant Professor and Ramanujan Fellow, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education & Research (NIPER), Ahmedabad, Gandhinagar, Gujarat, India **Discovery of a Novel Hit Candidate for Oral Cancer *via* Dual (Distal) C-H Bond Activation Relay Protocol**
IL-43 2.25 PM - 2.50 PM	**Partha Sarathi Addy** Assistant Professor, Department of Chemistry, Birla Institute of Technology and Science (BITS), Pilani, Rajasthan, India **Rationally Engineered Non-Canonical Peptidyl Optical Probes (nCPOPs) Targeting Cancer Microenvironment Detection**
IL-44 2.50 PM – 3.15 PM	**Prem Tripathi** Senior Scientist, Cell Biology & Physiology **Biochemistry, Molecular Biology, and Cell Biology Research**
O-15 3.15 PM - 3.30 PM	**Dwipen Kakati** Department of Chemistry, Rajiv Gandhi University, Rono Hills, Doimukh, Arunachal Pradesh, India **Targeted Phytochemical Investigation of *Calamus leptospadix Griff***
O-16 3.30 PM - 3.45 PM	**Hitesh Mansukhlal Tank** Department of Chemistry, School of Science, Dr. Subhash University, Junagadh (362001), Gujarat, India **Chromatographic Method Development, Validation and Analytical Studies of Ceftazidime and Avibactam in its Bulk and Pharmaceutical Formulation**
O-17 3.45 PM – 4.00 PM	**Rohit Maurya** Department Food and nutrition Biotechnology, BRIC-National Agri-Food Biomanufacturing Institute Mohali, India **Valorization of Food Bioprocess Waste for Production of Prebiotic Oligosaccharides**
4.00 PM - 4.10 PM	**Tea Break**
IL-45 4.10 PM - 4.35 PM	**Bijay Kumar Barik** Assistant Professor, Department of Biochemistry, Cell Biology and Genetics, American University of Antigua, College of Medicine, Coolidge, Antigua **Shedding Light on Cancer Metabolism: Insights from Fluorescence Spectroscopy in Cervical and Renal Carcinomas**
IL-46 4.35 PM – 5.00 PM	**Soumya Mishra** Physiologist, MBBS, MD **Abstract awaited**

O-18 5.00 PM – 5.15 PM	**Saurabh Chandra Saxena** Department of Biochemistry, Central University of Haryana, Mahendergarh, Haryana, India **Caffeic acid O-methyltransferases (COMTs) from *Eleusine coracana*: A key melatonin biosynthetic enzyme confers salinity and drought stress tolerance**
O-19 5.15 PM – 5.30 PM	**Shruti Saini** BRIC-National Agri-food and Bio-manufacturing Institute, SAS Nagar, Punjab, India **Comparative Study Of Endo-β-1,4-Mannanases From Novel Bacterial Strains For The Production Of Galactomannooligosaccharides**

Parallel Session – IV B
Venue: Conference Hall-2 at Campus-6

Thematic Area: - Material Sciences and Technology

Chairpersons: Prof Bapurao B. Shingate, Dr Puspalata Pattajoshi, Dr Rosalin Sahu

IL-47 2.00 PM - 2.25 PM	**Devdutt Chaturvedi** Head, Department of Chemistry, Dean, School of Physical Sciences, Mahatma Gandhi Central University, Motihari (East Champaran), Bihar, India **Syntheses of biologically potent scaffolds involving novel CO/CS bond forming reactions**
IL-48 2.25 PM - 2.50 PM	**Mayank K. Pandya** School of Science, Dr. Subhash University, Junagadh, Gujarat, India **Exploring Bio-Responsive TMP Containing Nitrogen Heterocycles for Urinary Tract Infection Therapy**
IL-49 2.50 PM - 3.15 PM	**Pravinkumar M. Patel** Head & Associate Professor, Industrial Chemistry Department. V. P. & R. P. T. P. Science College, Affiliated to Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Advantages of Nanoscale Dendritic Macromolecules for Active Pharmaceutical Ingredient (API) Formulation**
IL-50 3.15 PM – 3.40 PM	**Dillip Kumar Bishi** Assistant Professor, Department of Biotechnology, Rama Devi Women's University, Bhubaneswar, India **PHYTONANOMEDICINE EMBEDED NANOFIBROUS MESH FOR LIVER CANCER TREATMENT**
O-20 3.40 PM – 3.55 PM	**Charmy S. Kothari** Department of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **Development and Validation of Analytical Device for rapid Iron determination**
3.55 PM - 4.05 PM	**Tea Break**

IL-51 4.05 PM – 4.30 PM	**Namrata Rastogi** Principal Scientist, Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India, India **Organophotocatalytic Ring Opening Reactions of 2*H*-Azirines**
IL-52 4.30 PM – 4.55 PM	**Bandita Rath** Assistant Professor and HOD, Rajdhani College **Abstract Awaited**
IL-53 4.55 PM - 5.20 PM	**Shailendra Vyas** Director, Deepali United Mfg. Pvt. Ltd, Mumbai, India **Affordable Indegenised Lab Automation**
O-21 5.20 PM - 5.35 PM	**Giribala M Bondle** Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University Chhatrapati Sambhaji Nagar-Maharashtra, India **MOF-Derived NiO/SrO Nanocatalyst Enabled Multicomponent Synthesis of Novel AIPDs with Promising Anticancer Potential**

Parallel Session – IV C
Venue: Conference Hall-5 at Campus-6

Thematic Area: - Synthetic Inorganic and Organic Chemistry

Chairpersons: Dr Ravindra Kumar, Dr Swagat Mohapatra

IL-54 2.00 PM - 2.25 PM	**Suresh Kumar Kalangi** Scientist, MMI Division, CSIR-Central Drug Research Institute (CDRI), Lucknow, India **Alternative to Radiolabeled Probes in Drug Discovery and Diagnosis**

Parallel Session – IV D
Venue: Conference Hall- 8 at Campus-6

Thematic Area: - Sustainable and Green Chemistry

Chairpersons: Prof Ramesh Kothari, Dr Surya k. Mishra

IL-55 2.00 PM - 2.25 PM	**Ravi Prakash Singh** Professor, Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, India **New Endeavours in Asymmetric Vinylogous Reactions: Towards Functionally Rich Synthon**

Poster Session
Venue: Kunjabana at Campus 6

Chairpersons: Dr Namrata Rastogi, Dr Mayank Pandya, Dr Gopal K. Pradhan

5.30 PM – 6.30 PM	**Poster Number P-51 to P-90**

Panel Discussion
Venue:

Chairpersons:

6.30 PM – 7.30 PM	**Panel Discussion**

Sunday, December 21, 2025

Breakfast: Banquet Hall at Campus 6

Parallel Session – V A
Venue: Conference Hall-1 at Campus-6

Thematic Area: - Life sciences and Health care

Chairpersons: Prof Dina Nath Singh, Dr Madan Mohan Sharma

IL-56 9.00 AM - 9.25 AM	**Sarita Jena** Scientist-E (Scientist- in-Charge of Laboratory Animal Facility), Institute of Life Sciences, Bhubaneswar, India **Preclinical Animal Models**
IL-57 9.25 AM - 9.50 AM	**Anshuman Dixit** Scientist-F, BRIC-Institute of Life Sciences, Nalco Square, Chandrasekharpur, Bhubaneswar, India **Ultra large scale screening of chemical libraries to explore new kinase inhibitors**
IL-58 9.50 AM - 10.15 AM	**R Selvi Bharathavikru** RNP Biology Laboratory, Department of Biological Sciences, Indian Institute of Science Education and Research, Berhampur, India **RNA Methylation Dynamics regulates Cancer Stem Cell Maintenance through cell cycle modulation in spheroidal models of TNBC cells**
IL-59 10.15 AM - 10.40 AM	**Cuckoo Mahapatra** Asst Professor. Department of Zoology, Maharaja Sriram Chandra Bhanja Deo University (erstwhile North Orissa University). Takatpur, Baripada, Odisha, India **Implications of amphibian regeneration research for regenerative medicine: A study on limb regeneration in the Indian tree frog, Polypedates maculatus**
IL-60 10.40 AM - 11.05 AM	**Chandan Goswami** Professor, NISER, BBSR **How do cells sense temperature? The regulation of cellular thermal homeostasis by TRP channels**
11.05 AM – 11.15 AM	**Tea Break**
IL-61 11.15 AM – 11.40 AM	**Bhaskar C. Dash** Division Head, Division of Drug and Biotherapeutic Discovery and Professor, Department of Pharmaceutical Sciences, University at Buffalo, New York, USA **Abstract Awaited**

Parallel Session – V B
Venue: Conference Hall-2 at Campus-6

Thematic Area: - Material Sciences and Technology

Chairpersons: Dr Babita Malik, Dr Chaitali Pattanayak

IL-62 9.00 AM - 9.25 AM	**Amiya Priyam** Professor and Head, Department of Chemistry, Dean, School of Physical and Chemical Sciences, Central University of South Bihar, Gaya, Bihar, India **Soft Chemical Routes to Tunable Quantum Dots and Plasmonic Nanoshells for Catalytic and Therapeutic Applications**
IL-63 9.25 AM - 9.50 AM	**Okram Mukherjee Singh** Chemistry Department, Manipur University, Canchipur, Imphal, Manipur, India **Synthesis of functionalized imidazoles with applications as antioxidants, antidibetics, and functional organic materials**
IL-64 9.50 AM - 10.15 AM	**Sandip Kumar Dash** Assistant Professor (Stage-II), Berhampur University, Ganjam, Odisha, India **Solanum tuberosum-based Biogenic Hollandite Ag2Mn8O16 Nanocomposite for Inhibition of Indian Critical and High-Priority Pathogen-Listed Bacteria**
IL-65 10.15 AM - 10.40 AM	**Deepak Kumar** Senior Scientist, Organic & Medicinal Chemistry, CSIR-IICB, Kolkata, India **Drawing Inspiration from Mother Nature: Natural Product Scaffolds in Drug Discovery**
O-22 10.40 AM – 10.55 AM	**Shikha Singh** Bhubaneshwar, India **Design and Development of a Thermo-Mechanical Leaf Processing System for Sustainable Biodegradable Material Production**
10.55 AM – 11.05 AM	**Tea Break**
IL-66 11.05 AM - 11.30 AM	**Aliva Patnaik** Assistant Professor, School of Life Sciences, Sambalpur University, India **Vermitechnology with special reference to vermifiltration**
O-23 11.30 AM – 11.45 AM	**Ranjan C Khunt** Department of Chemistry, Saurashtra University, Rajkot, India Triazole-Linked Heterocyclic Hybrids via Click Chemistry: Structure–Activity Insights Toward Potent Anticancer Agents

Valedictory Session
Venue: Seminar Hall at Campus 6

11.45 AM – 1.00 PM	**Valedictory Session**

1.00 PM	**Lunch**

- End of Programme -

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

ISCBC 2025-2026

PLENARY

PL-1

Is Interdisciplinary technology the future of Medicine?

Prof. Dr. M V Raghavendra Rao

M.D (Medicine) (Hon) (USA), D.Sc, Ph.D (ANU), Ph.D (London)
FRCP(Edin), FWAMS(Netherlands),FRSTMH(UK), FIBMS(UK),FIMSA
Professor of Microbiology and Senior Executive Vice President, World Academy of Medical Sciences, Netherlands (Europe)
Former Scientist and Director Apollo Institute of Medical Sciences and Research, Hyderabad
Former Prof and Dean, Avalon University School of Medicine, Curacao (Central America)
email--reachdrmvrrao@gmail.com
Phone--9959817484
Website: The World Academy of Medical Sciences

ABSTRACT

The healthcare sector is growing vigorously as the global population is increasing with ages. Research in medicine has a great scope. Clinical research, field research, trials, and pharmaceutical companies would help them contribute to newer science with good discoveries and inventions in drugs for treatment or diagnostic tools. Multidisciplinary Science is the combination of different scientific disciplines to handle some of the world's most pressing challenges. It is driving innovation among individuals in the 21st century. Cross disciplinary Science is the combination of different scientific disciplines to handle some of the world's most significant challenges. Interdisciplinary sciences combine courses in biology, chemistry, physics, geology, math, computer science, and psychology. Integration of scientific and technological breakthroughs with new and emerging care pathways will bring exceptional opportunities to improve clinical outcomes. The role of clinicians will continue to evolve into a broader team, to engage with a wide range of different disciplines and play leading roles in the healthcare of the future. Interdisciplinary promotes innovation by mixing diverse knowledge and perspectives. Technological advancements, such as Artificial Intelligence (AI), often arise from the convergence of computer science, Organ-on-chips (OCC), and Genome Editing. Engineering and Medical sciences are closely related fields that are highly interdependent. Future trials would be based on artificial intelligence (AI) and Machine learning. Interpretation of images improves precision medicine and immunology. Bioengineering, translation medicine, Biotechnology, Genetic engineering, Medical electronics, artificial organs, Biosensors, Biomedical robotics.MRN technology, Neurotechnology,3D Printing, and CRISPR will change the healthcare system. Specialist surgeons will use remote robots to operate on patients on different continents. Babies will have their DNA sequenced before they are even born. Patients will be able to generate new blood inside their bodies without the need for a blood donor.

New technology in healthcare continues to improve, and it is difficult to forecast what medical advances will come next

PL-2

How Staph Bacteria Blocks Host Immune Enzymes: New Structural Insights

Om Prakash

Department of Biochemistry and Molecular Biophysics, Kansas State University, Manhattan, KS 66506, USA

Abstract:

Due to host-pathogen coevolution, *Staphylococcal aureus* expresses a diverse arsenal of innate immune evasion proteins that target many aspects of the neutrophil antibacterial responses. Over the past decade, our collaborator Dr. Geisbrecht's laboratory has identified two classes of Extracellular Adherence Proteins (EAPs), which are expressed and secreted by the Staph bacteria. These proteins specifically target immune proteases found exclusively in human neutrophils The EAPs and their smaller homologues EapH1 and EapH2 are high affinity, selective inhibitors of neutrophil serine proteases (NSP) including cathepsin-G (CG) and neutrophil elastase (NE). Notably, NE also plays an important role in selectively killing tumor cell and reducing primary tumor growth by promoting an anti-tumor immune response. In this presentation, I will discuss and summarize recent advances in our understanding of the structural and functional properties of these proteins, as well as the mechanism by which they inhibit NSPs.

ISCBC 2025-2026

INVITED

IL-1

Monocarbonyl Analogues of Curcumin (MACs): Development towards new therapeutic agents

Dr. Bapurao B. Shingate

Professor in Organic Chemistry
Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University,Chhatrapati Sambhajinagar-431 004, Maharashtra (India)
E-mail: bapushingate@gmail.com

Monocarbonyl Analogues of Curcumin (MACs) is a class of synthetic organic compounds inspired from the structure of Curcumin. Recent literature suggests that MACs displayed promising biological potential as antioxidant, anticancer and anti-inflammatory agent. Structural diversity to the MACs can be imparted by embedding aromatic heterocycles in the side chain of MACs. In our continuous research on design and therapeutic potential of MACs in last decade, we have reported hundreds of new MACs with pyrazole, quinoline and 1,2,3-triaozle scaffolds. These MACs were well characterized for their structure elucidation using ^{1}H NMR, ^{13}C NMR, FT-IR and Mass spectrometry. These synthetic MACs were screened for their potential as anti-oxidant, anticancer, antifungal and antitubercular agent. Furthermore, in silico molecular docking and DFT study strengthen the outcome of therapeutic results and will be discussed.

IL-2

Accelerating Alzheimer's Drug Discovery: Machine Learning–Driven Design and Prediction of Amyloid-β Aggregation Inhibitors

Avantika Bansal1 , Akshat Raj Sharma1 , Arya Chakraborty2 , Aditya Sunkaria3 and Alok Jain*

[1]*Advanced BioComputing Lab, Department of Bioengineering and Biotechnology, Birla Institute of Technology Mesra, Ranchi-835215, Jharkhand, India*
[2]*Department of Computer Science and Engineering, Birla Institute of Technology Mesra, Ranchi-835215, Jharkhand, India*
[3]*Department of Biotechnology, Guru Nanak Dev University, Amritsar-143005, Punjab, India*

Abstract

Alzheimer's disease is a devastating neurodegenerative disorder, with amyloid-β (Aβ) aggregation being a central factor in its onset and progression. Designing inhibitors against Aβ aggregation is particularly challenging due to its disordered structure and conformational flexibility, which limits both experimental and computational approaches. To address these challenges and expedite the discovery process, we developed a machine learning based, freely accessible web server for virtual screening and rational design of Aβ aggregation inhibitors. The platform integrates two classification models and one regression model trained on a curated dataset of 584 biologically validated compounds. The Random Forest classifier achieved 100% accuracy in distinguishing inhibitors from decoys, while Histogram-based Gradient Boosting effectively categorized compounds by potency (81% accuracy). The IC_{50} regression model demonstrated robust predictive capability with an R^2 value of 0.93. Key molecular descriptors, hydrophobicity, molecular shape, charge distribution, and symmetry were identified as major determinants influencing aggregation inhibition. These insights enhance the interpretability of model predictions and provide a framework for structure-guided drug design. The web server represents a valuable tool for accelerating AD therapeutic discovery, offering researchers a practical solution to streamline early-stage inhibitor development.

IL-3

Drug discovery research in India: Current trends and analysis of Industry-Academia and Government collaborations

Sanjay Kumar

Department of Chemistry, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, NH17 B, Zuarinagar, Sancoale, GOA 403726, India
Email: sanjaykumar@goa.bits-pilani.ac.in;
Ph. (office): 0832-2580463

Abstract:

India has long been recognized as the "pharmacy of the world," owing to its stronghold in the generics and biosimilars market. However, its contributions to innovative drug discovery, particularly in the development of new chemical entities (NCEs), have been relatively modest. This talk will provide a critical overview of the current trends in drug discovery research in India, highlighting both the scientific advancements and systemic challenges that define the landscape. Recent years have witnessed a growing emphasis on next-generation drug delivery strategies, including antibody–drug conjugates (ADCs), nanoparticle-based formulations, bioconjugates designed to enhance therapeutic efficacy and reduce systemic toxicity. One such innovation is our Exa-HSA-Nanoparticle, which demonstrates promising potential as a novel delivery system for oncology applications. These advances underscore the importance of multidisciplinary collaboration among industry, academia, and government agencies.

Despite these scientific strides, India's NCE output remains limited. A key reason lies in the industry's preference for low-risk, high-reward generics, coupled with fragmented collaboration frameworks and limited translational funding. This presentation will analyze the evolving role of government initiatives such as the Anusandhan National Research Foundation (ANRF) and explore how academia–industry partnerships can be restructured to incentivize innovation.

By presenting a comprehensive analysis that blends technical progress with policy insights, this talk aims to foster dialogue on how India can transition from a generics-dominated ecosystem to a globally competitive hub for innovative drug discovery.

IL-4

Neuroprotective Natural Products: Emerging Strategies for Alzheimer's Disease Management

Dr. Niyati Acharya

Institute of Pharmacy, Nirma University, Ahmedabad

Abstract

Alzheimer's disease is the most prevalent form of dementia, is characterized by multifactorial pathological hallmarks like progressive cognitive decline, amyloid-β aggregation, tau hyperphosphorylation, neuroinflammation, oxidative stress, and synaptic dysfunction. Despite extensive research, current pharmacological interventions remain largely symptomatic, underscoring the urgent need for safe, effective, and multi-targeted therapeutic strategies. Natural products holds great potential with their structural diversity and multitarget pharmacology and explored as the most promising reservoir of neuroprotective agents for AD management. Natural neuroprotectives from well known traditional plants like brahmi, withania, turmeric, giloy have been explored a lot for their potential. Among this, asiaticosides (from Centella asiatica) demonstrated potent antioxidant, anti-inflammatory, and neuroregenerative properties, supporting synaptic plasticity and memory enhancement. Bacosides (from Bacopa monnieri) have been widely recognized for their nootropic potential, exerting effects through cholinergic modulation, reduction of β-amyloid toxicity, and promotion of neuronal repair. Bergenin, a polyphenolic compound, exhibits significant anti-amyloidogenic, antioxidant, and mitochondrial protective actions, making it a candidate for slowing neurodegenerative progression. Cannabidiol (CBD), a non-psychoactive phytocannabinoid, offers broadspectrum neuroprotection by modulating endocannabinoid signaling, reducing neuroinflammation, and improving neuronal survival without psychotropic side effects. This talk will highlight emerging insights into the molecular mechanisms of these bioactives, and translational perspectives in AD therapy. By integrating evidence from preclinical models and clinical observations, the talk aims to present natural products not merely as adjuncts but as emerging neuroprotective strategies for holistic Alzheimer's disease management.

IL-5

TARGETING DPP-IV FOR ANTI-DIABETIC THERAPY: COMPREHENSIVE COMPUTATIONAL EXPLORATION OF NOVEL AND PROMISING INHIBITORS

[1] Raghuvir Ramakant Pissurlenkar and [2] Deepika Maliwal

[1]Department of Pharmaceutical Chemistry, Goa College of Pharmacy, Panaji Goa 403001. INDIA
[2] In Silico Chemist, Mumbai 400101, INDIA
Email. raghuvir@pissurlenkars.net

Diabetes mellitus remains a major global health burden, necessitating novel and affordable therapeutic strategies. Dipeptidyl peptidase-IV (DPP-IV) inhibition is a clinically validated approach that prolongs incretin activity and improves glycemic control. Although several gliptins are approved, the search for next-generation inhibitors is hindered by high development costs and time constraints, making computational drug repurposing an efficient alternative.

In this study, FDA-approved DPP-IV inhibitors were employed as templates to screen a vast chemical library (~33.8 million compounds) using 1024-bit Morgan fingerprints and Tanimoto similarity for rapid large-scale structural comparison. A machine learning pipeline was subsequently developed using 1,863 curated DPP-IV inhibitors from BindingDB, filtered for drug-likeness and safety. Molecular descriptors and fingerprints were generated and clustered via K-means to ensure chemical diversity. A Random Forest Regressor trained on this dataset exhibited strong predictive performance (high R^2, low MAE/RMSE) across training, validation, and external test sets.

The validated model was benchmarked against known gliptins and applied to prioritize compounds with predicted pIC50 > 8.0. These hits underwent ADME and toxicity screening, followed by docking using AutoDock Vina against the DPP4–Linagliptin complex, identifying ligands with binding affinities ≤ –9.0 kcal/mol. Subsequent shape and electrostatic potential (ESP) Tanimoto analyses refined the set to ~100 candidates, which were further evaluated via molecular dynamics simulations and MM- GBSA free-energy calculations.

Finally, density functional theory (DFT) calculations elucidated frontier molecular orbitals and reactivity descriptors, providing quantum-level insight into binding preferences. This integrative workflow combining ligand-based (similarity search, ML) and structure-based (docking, MD, DFT) approaches yielded several promising DPP-IV inhibitor candidates, offering a rational framework for antidiabetic drug discovery and future experimental validation.

IL-6

Next-Generation Selective PARP1 Inhibitors: Enhancing Therapeutic Index Through Reduced Toxicity in Oncologic Applications

Patel Bhumika*[1], Shaikh Jahara[1], Saini Nidhi[1], Acharya Niyati[2], Rawal Rakesh[3]

[1]Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, SG Highway, Ahmedabad 382481, Gujarat, India
[2]Department of Pharmacognosy, Institute of Pharmacy, Nirma University, SG Highway, Ahmedabad 382481, Gujarat, India
[3]Department of Medical Biotechnology, Gujarat Biotechnology University, Gujarat International Finance Tec-City, Gandhinagar, Gujarat 382355
bhumika.patel@nirmauni.ac.in

Abstract

Poly (ADP–ribose) Polymerase1 (PARP1) inhibitors are in clinical use and have proven their efficacy in BRCA-mutated high grade ovarian cancer, breast cancers and pancreatic cancer. Cancers having deficiency in homologous recombination repair (HRR) pathway have been found sensitive towards PARP1i treatment. Current clinically approved PARP1i; Olaparib, Rucaparib, Niraparib, Talazoparib, Pamiparib etc. are non-selective molecules which inhibit both, PARP1 and PARP2 as both share a high degree of sequence homology (69%) at the catalytic domain. Their clinical applications are limited due to their haematological toxicity associated with PARP2 inhibition and due to development of monotherapy resistance. These demand for the development of next generation selective PARP1i with reduced toxicity which can show promise for improving the survival and outcomes of cancer patients. Present review summarizes the structural insights and promising results of such next generation selective PARP1i which currently are under various stages of development; NMS-P118, NMS-293, AZD5305 (Saruparib), EIK1003, HRS-1167 (M9466) and IMP1734. Although it is too early to conclude the positive and impactful clinical promise of these inhibitors at this stage, improved toxicity profile of these new agents will permit newer combination strategies to improve efficacy, tolerability and patient outcomes. 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-7

Development of a Portable Microcontroller-Based Fluorescence Sensing Module for Dual Detection of Hexavalent Chromium and Ascorbic Acid Using Banana Peel-Derived Carbon Quantum Dots

Aayushi Kundu and Soumen Basu

Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, 147004, India.
E-mail: *soumen.basu@thapar.edu*

Carbon quantum dots (CQDs), distinctive zero-dimensional nanomaterials, have garnered significant attention due to their exceptional fluorescent properties. The CQDs with intense fluorescence were synthesized from banana peel waste through a simple, one-step, and chemical-free approach. The as-prepared CQDs were thoroughly characterized using TEM, FT-IR, XRD, and XPS analyses, confirming their structural and chemical features. Exhibiting bright green fluorescence under UV illumination and a quantum yield of 41%, the CQDs served as efficient on–off fluorescent probes for the selective and sensitive determination of toxic Cr(VI) ions, driven by the inner filter effect (IFE) and static quenching phenomena. The detection limit for Cr(VI) was as low as 60.5 nM. Furthermore, the CQDs–Cr(VI) ensemble demonstrated an off–on sensing behavior toward ascorbic acid (AA) with a detection limit of 86 nM, owing to the reduction of Cr(VI) to Cr(III) by AA, which suppressed the IFE and reinstated fluorescence. In addition, a cost-effective, portable microcontroller-enabled spectroscopy module was developed for real-time monitoring of heavy metal ions in environmental samples. The results validate its applicability for on-site detection of Cr(VI). Overall, this work highlights the potential of banana peel-derived CQDs as sustainable nanoprobes for fluorescence-based detection and portable sensing of environmental pollutants and biomolecules.

References:

1. Aayushi *et al. Mater. Adv.*, 2025, 6, 743–755.
2. Aayushi *et al. ACS Omega* 2023, 8, 22178−22189.
3. Neeraj *et al. ACS Appl. Bio Mater.* 2023, 6, 4846−4855.

IL-8

HIT to LEAD Optimisation of *N*-Substituted Acridine-9-Amino Derivatives as Telomerase Inhibitors for the Treatment of Lung Cancer

Hardik Bhatt, Ph.D

Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad 382 481. India.
Email. hardikbhatt23@nirmauni.ac.in, drhgbhatt@hotmail.com

Abstract

Lung cancer is one of the deadliest cancers, among all types of cancer. An exponential increase in deaths related to cancer has led development and identification of newer targets and molecules to cure the disease. Telomerase is an attractive anti-cancer target, as 85-90% of malignant tumors including lung cancer, show telomerase-mediated proliferation and apoptosis. However, none of the small molecules for targeting telomerase has been successful in getting FDA approval, either due to lower potency, lower selectivity or toxicity constraints. This research emphasizes finding novel anticancer agents for targeting telomerase enzyme that can provide a broad-spectrum activity with a significant reduction of toxicity. During the research, by utilizing knowledge-based approaches, thiadiazole bearing acridine derivatives were designed, synthesized and evaluated as telomerase inhibitors for the treatment of lung cancer by performing various in vitro assays like MTT, colony forming, apoptosis and TRAP assay in comparison with standard drug BIBR-1532. In vivo lung cancer model demonstrated potency of 4 HIT compounds (HB-KV-A1-102, HB-KV-A2-101, HB-KV-A2-102, and HB-KV-A3-101).

Based on outcome of this study, a novel *N*-substituted acridine-9-amino derivatives incorporating -NH- linker were designed and synthesised to transform HIT to LEAD strategy. To evaluate their anticancer potential, MTT assays were conducted to assess cytotoxicity, while TRAP assays confirmed their ability to inhibit telomerase activity. Further, colony forming and Apoptosis assays were performed to determine the compounds' impact on cancer cell proliferation. The most promising LEAD candidates, HB-3Aq-02 and HB-BPh-03, showed exceptionally high Cq values and strong fold reductions in telomerase activity, indicating potent suppression even at low concentrations, and further selected for in vivo evaluation using a chemically induced lung cancer model, providing insights into their therapeutic efficacy. Histopathology revealed near-normal lung architecture and minimal inflammation in treated animals.

Overall, this research establishes a strong foundation for the development of novel telomerase inhibitors with potential clinical applications in lung cancer therapy.

Stimuli-responsive Prodrug Activation in Mitochondria for Cancer Therapy

Priyankar Paira*

Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014, India
*priyankar.paira@vit.ac.in

Mitochondria, the 'powerhouse of the cell' or 'local energy gradients' serve as highly dynamic organelles and arbitrators of cell's life and death. Incessant proliferation and undaunted growth of cancer cells are nourished by the immensely exploitation of the mitochondria. The design of mitochondria-demolishing anticancer agents can, therefore, be the significant weapons for efficiently treating the cancer. But chemoresistance and systemic toxicity are inexorable issues associated with the traditional chemotherapy. To securely cut-off the energy source of the cancer cells, contriving of the mitochondria-targeting prodrugs will be "kill of two birds with one stone" strategy, where prodrugs remain inactive at the outset and liberate active form of the drugs either by internal stimuli like copious thiols, acidic pH, and reactive oxygen species (ROS) in tumour tissue microenvironment or by external stimuli like localised light, ultrasound, electric impulse, magnetic field and radiation after reaching at the target-site. To abate the world-wide rampant prevalence of cancer, recently we have developed organelle targeted Ru(II)/Ir(III)/Re based half-sandwich and cyclometallated complexes for ROS mediated selective dynamic therapy with or without visible light irradiation (CDT or PDT) enhancing the therapeutic potential against the distinct tumour microenvironment (TME) (**Figure 1**).[1-3]

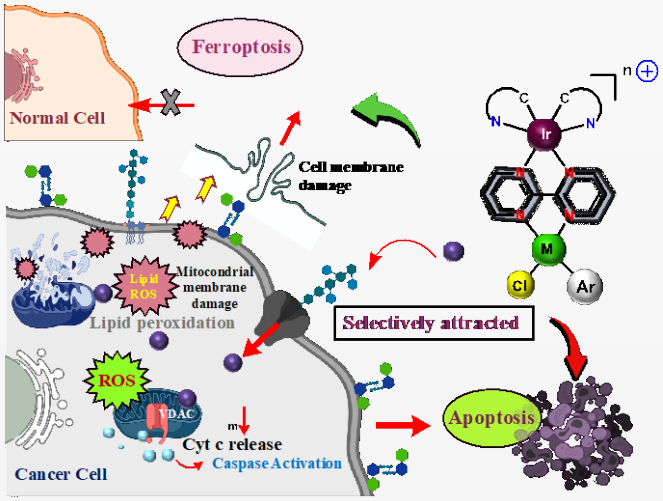


Figure 1: Mechanistic pathway of metal complexes in mitochondria for cell death

Reference

1. N. Roy, U. Sen, Y. Madaan, V. Muthukumar, S. Varddhan, S. K. Sahoo, D. Panda, B. Bose and P. Paira Inorg. Chem., 59, 2020, 17689-17711.
2. B. Kar, S. Shanavas, A. Karmakar, A. H. Nagendra, S. Vardhan, S. K. Sahoo, B. Bose, S. Kundu and P. Paira, J. Med. Chem. 67, 2024, 10928-10945.
3. N. Roy, T. Dasgupta, S. Ghosh, M. Jayaprakash, M. Pal, S. Shanavas, S. K. Pal, V. Muthukumar, A. Senthil Kumar, R. Tamizhselvi, M. Roy, B. Bose, D. Panda, R. Chakrabarty and P. Paira, Sialic Acid-Targeted Ru(II)/Ir(III)/Re(I) Complexes for Ferroptosis Induction in Triple-Negative Breast Cancer, Langmuir 40, 2024, 25390-25404.

IL-10

Targeting Mycobacterial "SOS" Response-a strategy to toggle Antimicrobial Resistance (AMR)

Saravanan Matheshwaran, PhD

Associate Professor
Microbial Adaptation and Chromatin Dynamics Laboratory, Department of Biological Sciences and Bio-engineering, Environmental Microbiology Laboratory, Centre for Environmental Sciences and Engineering, Mehta Family Centre for Engineering in Medicine, Kotak School of Sustainability, Indian Institute of Technology Kanpur, Uttar Pradesh -208016.
Email: saran@iitk.ac.in

Abstract

The "SOS" response is an essential systematic mechanism against DNA damage in bacteria. It is indispensable for its regulatory role in maintaining genome integrity and in gaining fitness advantage by developing useful mutations to tolerate genotoxic stress, leading to the development of antimicrobial resistance. LexA and RecA are the key players regulating the global network of stress-responsive and damage-repair genes involved in this pathway. In an era of expanding drug resistance, targeting such non-traditional yet non-compromising pathways can provide useful answers in tackling global health hazards such as Tuberculosis (TB). The potential of targeting the "SOS" response is gathering increasing support to strengthen therapeutic efficacy. RecA inhibitors have been reported from chemical screening assays conducted in *E.coli* and *Mycobacterium tuberculosis* (Mtb), the latter being the causative agent of TB. However, RecA bears homologs not only across prokaryotic but also eukaryotic organisms, posing a challenge for specific action. Consequently, a shift in gears has taken place with scientists switching to the other master regulator, LexA, which does not possess any eukaryotic counterpart. An academic-industry partnership successfully delivered the first-of-its-kind inhibitors targeting *E.coli* LexA autoproteolysis. Such efforts have not yet been extended to Mtb and addressing this gap forms a major objective of our study. Here, we report potential inhibitors of Mtb LexA. We have elucidated the kinetic parameters of interaction and generated a homology model to obtain an idea of possible drug-binding sites in Mtb LexA. Our studies involve characterizing such compounds with the broader aim of improving the existing arsenal of anti-TB therapeutics. Characterizing such inhibitors of Mtb LexA autoproteolysis can be effective in stalling "SOS" induced mutagenesis and AMR in mycobacteria.

IL-11

Decoding Monkeypox–HIV Crosstalk: FDA-Approved Therapeutic Leads

John J. Georrge[1*], Suraksha Rana[1], Saurav Kumar Mishra[1]

[1]Department of Bioinformatics, University of North Bengal, District-Darjeeling, West Bengal-734013, India
Presenting author Email: johnjgeorrge@gmail.com

Abstract

Mpox (Monkeypox virus, MPXV) and Human Immunodeficiency Virus (HIV) are significant viral pathogens with global health implications. Mpox, a zoonotic orthopoxvirus, has re-emerged as a public health concern, often co-occurring in immunocompromised individuals, particularly those with HIV. Understanding host gene expression changes is critical for identifying therapeutic targets. This study employed transcriptomic profiling, protein interaction analysis, and molecular docking to uncover key molecular signatures and potential inhibitors. Two transcriptome datasets were analysed: one for Mpox (9 infected and 3 control colon organoid samples across clades I, IIa, and IIb) and one for HIV (50 HIV-infected and 7 uninfected blood samples). Differential expression analysis identified 298 DEGs in Mpox (228 upregulated, 70 downregulated) and 3070 DEGs in HIV (1294 upregulated, 1776 downregulated). Venn analysis revealed common DEGs, which were subjected to STRING-based protein–protein interaction (PPI) network construction. CytoHubba analysis in Cytoscape identified 15 shared genes and 7 key hub genes (NTRK3, TFF1, NFIA, XAF1, FOS, EGR1, and CXCL10). Functional enrichment revealed significant immune-related pathways, including IL signalling, TNF signalling, and Toll-like receptor pathways. To explore therapeutic opportunities, molecular docking of FDA-approved drugs against the hub genes was performed, leading to the identification of five promising candidates with strong binding affinities. This integrative bioinformatics approach highlights critical genes driving Mpox–HIV crosstalk and identifies potential FDA-approved inhibitors for therapeutic repurposing. These findings provide a foundation for targeted drug development; however, further experimental validation is essential to confirm their clinical applicability.

Keywords: Mpox, HIV, Differentially Expressed Genes, FDA-Approved Drug, Molecular Docking.

IL-12

Design and Synthesis of Organotin(IV) Complexes: Structural Insights and Potential Applications

Asha Jain

Department of Chemistry, University of Rajasthan, Jaipur- 302004, India
Email: aashajain27@gmail.com, ashajain@uniraj.ac.in

Abstract:

Organotin (IV) complexes continue to attract significant research interest owing to their remarkable coordination versatility, structural diversity, and wide-ranging applications. The ability of tin compounds to adopt variable coordination numbers allows the formation of geometries ranging from tetrahedral to octahedral. The generation and structural characterization of organotin(IV) complexes with potentially biologically active ligands remains an active area of research in medicinal, pharmaceutical, and organometallic chemistry. Organotin(IV) compounds/ complexes have demonstrated diverse applications in industrial, agricultural, and health care fields. They have been reported as potential biologically active metallopharmaceuticals exhibiting anticancer activity against various tumor cell lines. The biological activity of these complexes is influenced by several factors, including the type of metal, coordination geometry, presence or absence of halogen, and the nature of the ligands. The ligand containing hetero donor atoms such as O, N, and/or S , when coordinated to the tin(IV), plays a crucial role in modulating the biological activity of the complexes. Moreover, their interaction with biomolecules such as DNA, proteins, enzymes and lipids further governs their pharmacological potential. Thus, the selection of organic ligands is of paramount importance for the design of pharmaceutically useful complexes. In our Research group, novel organotin (IV) complexes were synthesized employing Schiff bases, N-protected amino acids, semicarbazones, thiosemicarbazones, substituted pyrazolones, and β-diketones as chelating ligands. The complexes were systematically characterized by elemental analysis, melting point determination, FT-IR, and NMR(^{1}H, ^{13}C, and ^{119}Sn) spectroscopy. Spectral studies revealed the presence of penta- and/or hexa-coordinated tin(IV) centers, adopting distorted geometries influenced by the steric and electronic properties of the ligands. These structural features are closely associated with their reactivity and potential applications. The synthesized complexes exhibit considerable promise as bioactive agents with antimicrobial, anticancer, and anti-inflammatory activities, alongside prospective uses in catalysis and material science.

References:

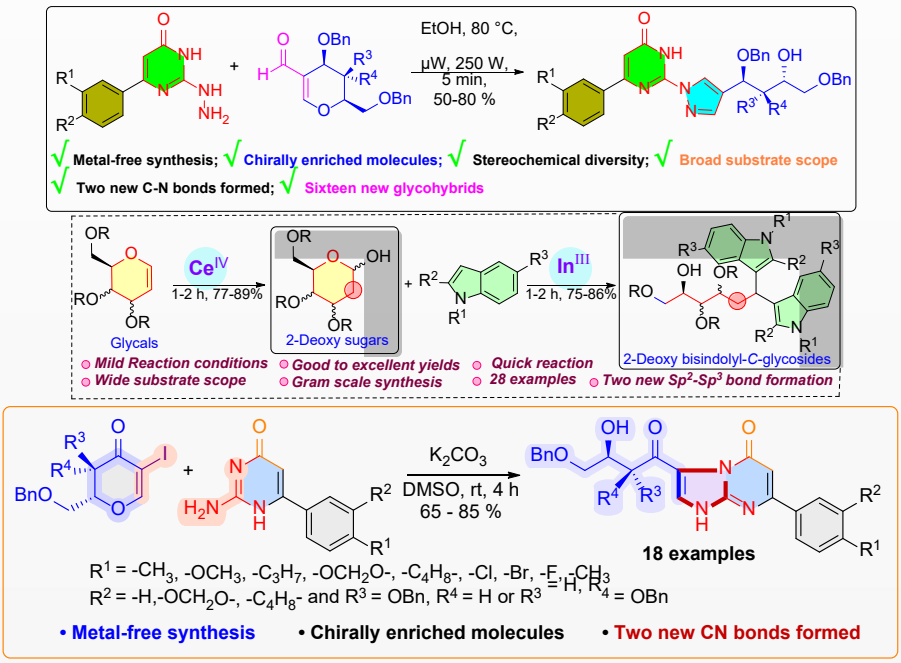
1. Komal Soni; Anita Kumawat; Sanjiv Saxena & Asha Jain;, Dibutyltin(IV) formulations as potential antitubercular scaffold: DFT-assisted emerging advances and mechanism of antitubercular action, *Bull. Chem. Soc. Jpn.* **2024**, *97*, uoae056.
2. Ankur M. Kumar**;** Suchitra Budania &Asha Jain;**,** Novel organic–inorganic hybrid dimethyltin(IV) complexes of heterocyclic carboxylic acid and N-phthaloyl amino acids: Design, synthesis, spectroscopic characterization, DFT calculations and their anti-oxidant potential, *Synthetic Communications*,**2024**,54, 390-405**.**
3. Anita Kumawat; Komal Soni; Sanjiv Saxena&Asha Jain, De novo unified robust antidiabetic pharmacophores based on biopotent hybrid material: DFT-assisted design, optimized molecular structure, and understanding mechanism of antidiabetic bioassay, *Applied Organometallic Chemistry*,**2023**, 37, e7205
4. Komal Soni; Sanjiv Saxena& Asha Jain, Deciphering mechanistic implications of antimicrobial and antioxidant potentials of certain new dibutyltin(IV) formulations as possible therapeutic options based on DFT and hybrid materials paradigm. *J. Biochem. Mol. Toxicol.* **2022**, 37, e23276.
5. Komal Soni; Sanjiv Saxena& Asha Jain, Recent advances in DFT assisted optimized energy, stability and distortion of optimized topologies of certain biopotent dimethyltin(IV) complexes. *J. Indian Chem. Soc.* **2022**, 99, 100332.

IL-13

Synthesis of 2-Deoxy Sugars, Chirally Pure 3-Bisindolyl-C-Glycosides, Pyrazolyl-pyrimidinone and Imidazopyrimidinonesbased Glycohybrids from Glycals

Ram Sagar Misra*

Glycochemistry Laboratory, School of Physical Sciences, Jawaharlal Nehru University, New Delhi – 110067
**E-mail (Corresponding author): ram.sagar@jnu.ac.in*



Abstract:

A new strategy for synthesizing chirally enriched 2-deoxysugars and their application in the synthesis of bisindolyl[1] and 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).[2] 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.[3] 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.

References:

1. Yogesh Yadav, **Ram Sagar*** *Org. Lett,* **2025***, 27*, 4006-4012, https://doi.org/10.1021/acs.orglett.5c00976
2. Ghanshyam Tiwari, Vinay Kumar Mishra, Ashish Khanna, Rajdeep Tyagi and **Ram Sagar*** *J. Org. Chem.* **2024**, 89, 5000–5009. https://doi.org/10.1021/acs.joc.4c00211.
3. Vinay Kumar Mishra, Ghanshyam Tiwari, Ashish Khanna, Yogesh Yadav and **Ram Sagar*** *Eur. J. Org. Chem.* **2024**, 27, e202301301. https://doi.org/10.1002/ejoc.202301301.

IL-14

The Effect of Ligand Environment on the C–H Activation Properties of Bio-inspired Metal–Oxo Complexes

Debasish Mandal*

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

Bio-inspired Fe(IV)=O complexes play a crucial role in efficient C–H bond activation. Their reactivity is governed by multiple interconnected factors, including axial and equatorial ligand coordination around the metal center, the overall ligand framework, acceptor orbital energies, spin-state distribution, electrophilic character, and quantum mechanical tunneling effects.[1-4]

In this presentation, we will discuss several representative cases illustrating how variations in ligand frameworks, as well as systematic axial and equatorial atom substitutions, influence the reactivity of both heme and non-heme bio-inspired metal–oxo complexes. These comparative studies provide valuable mechanistic insight into how subtle electronic and structural modifications govern their catalytic efficiency and selectivity in C–H bond activation processes.[3-7]

Keyword: C-H activation, Bio-inspired, **Metal**-oxo, Non-heme and heme, DFT

References:

1. Que, L.. Acc. Chem. Res., **2007**, 40, 493.
2. W. Nam, Acc. Chem. Res., **2007**, 40, 522.
3. Kaur, L., Mandal, D. Inorg. Chem. **2022**, 61, 14582.
4. Kaur, L., Mandal, D. Dalton Trans., **2024**, 53, 7527.
5. Kaur, L., Mandal, D. ChemPhysChem 2024, e202400765 (1 of 9)
6. Katoch, A., Mandal, D. Dalton Trans., **2024**, 53, 15264.
7. Katoch, A.; Mandal, D. J. Phys. Chem. B 2025, 129, 1, 88–95

IL-15

A thorough investigation of the synthesis of TAM and MET receptor kinases inhibitor's core (R)-2-((4-(4-amino-2-fluorophenoxy)-1-(4-methoxybenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)amino)propan-1-ol

Dr. Shovan Mondal*

Assistant Professor of Chemistry, Syamsundar College, Shyamsundar, Purba Bardhaman -713424, West Bengal, India.
**Corresponding Author E-mail: shovanku@gmail.com*

ABSTRACT

Important signalling hubs that control vital cellular functions like growth, survival, migration, and differentiation are receptor tyrosine kinases (RTKs). Many aggressive malignancies are characterised by the dysregulation of particular RTK families, including the MET receptor (c-MET/HGFR) and the TAM receptors (Tyro3, Axl, MerTK), which aid in tumour initiation, development, metastasis, resistance to therapy, and immune evasion. Therefore, creating inhibitors that target these receptors is a significant advancement in precision oncology.

In 2023, Beijing Anshi Biotechnology Co., Ltd. discovered that structural analogues with the coremotif(R)-2-((4-(4-amino-2-fluorophenoxy)-1H-pyrazolo[3,4-b]pyridin-3yl)amino)propan-1-ol exhibited inhibitory action. Kinases linked to c-Met, VEGFR-2, Axl, TAM receptors, NTRK, and RET are targeted by these compounds.

Pfizer revealed a ten-step synthesis of the aforementioned compound, starting with ethyl 2-cyano-3-(dimethylamino)acrylate, with an overall yield of about 25% during their initial attempts. An improved five-step synthesis procedure to obtain the deprotected analogue was developed later; it began with 2,4-dichloronicotinic acid and progressed with a 49% overall yield. On the other hand, Beijing Anshi Biotechnology created a short six-step process that starts with 4-chloro-1H-pyrazolo[3,4-b]pyridine, but the total yield was not revealed. In order to further optimize, the method for the synthesis of the targeted molecule, we have conducted a thorough analysis of this patented procedure. At the conference, the specific findings will be shared.

Keywords: TAM inhibitor; Selective S_NAr reaction; Pyrazolo[3,4-*b*]pyridine; Ullmann reaction.

Reference:

1. X. Zhu, B. Liu, B. Li, S. Mondal, S. Debnath *Org. Process Res. Dev.* **2025**, 29, 2116-2123.

IL-16

NPN Coordination Complexes: From Ligand Design to Applications

Dr. Bhupendra Goswami*

[a]*Department of Chemistry, Central University of Rajasthan, Bandarsindri, Rajasthan*
Email – bhupendra.goswami@curaj.ac.in

In the area of coordination chemistry, the reactivity and coordination pattern with the metal center can be exploited by carefully designing the coordination pocket of the ligand. In this regard, there has been immense interest among chemists in designing new ligand frameworks. In this context, the achiral heteroatomic ligand, the Iminophosphonamide (NPN) ligand, has been extensively studied, unlike its chiral counterpart.[1] This work introduces the design of novel chiral iminophosphonamide ligands and their diverse metal complexes.[2] Investigation of the photophysical properties revealed that these metal complexes exhibit intriguing photoluminescence characterized by thermally activated delayed fluorescence (TADF).[1,2,3] Notably, the alkali metal complexes, present in dimeric forms, displayed TADF above 150 K. To explore the impact of substituents on photoluminescence, a range of iminophosphonamide ligands was designed. The case study was further extended to other elements of the periodic table, such as calcium, group-4 metals: Zr and Hf,[4] d^{10}-configured metal centers (*i.e.*, Cu, Zn), and lanthanide metals,[5] coordinated with a variety of iminophosphonamide ligands. The study revealed that the photoluminescence and TADF of these metal complexes are influenced by the metal centers, the ligand arrangement around them, and the observation temperature.

References:

1. **B. Goswami**,‡ T. J. Feuerstein,‡ (‡equal contribution), P. Rauthe, R. Köppe, S. Lebedkin, M. M. Kappes, P. W. Roesky. *Chem. Sci.*, **2018**, *10*, 4742-4749.
2. **B. Goswami**, T. J. Feuerstein, R. Yadav, R. Köppe, S. Lebedkin, M. M. Kappes, P. W. Roesky, *Chem. Eur. J.*, **2021**, *27*, 4401 –4411.
3. **B. Goswami**,‡ T. J. Feuerstein,‡ (‡equal contribution), R. Yadav, S. Lebedkin, P. J Boden, S. T Steiger, G. N.-Schatteburg, M. Gerhards, M. M Kappes, P. W Roesky, *Chem. Eur. J.*, **2021**, *27*,15110 –15119
4. **B. Goswami***, R. Yadav, H. Joshi, P. Roy, *Eur. J. Inorg. Chem.*, **2025**, *28*, e202400627.
5. **B. Goswami**, X. Sun, T. J. Feuerstein, M. T. Gamer, P. W. Roesky, *organometallics*, **2023**, *42,* 1317□1323.
6. **B. Goswami***, P. W. Roesky, *Inorg. Chem. Front.,* **2025**, *12*, 3555-3581.

Sustainable synthesis of imidazo[2,1-*b*]quinazolin-1(2*H*)-ones as PDGFRA inhibitors

Hitendra M. Patel

Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar-388120, Gujarat, India,;
Email: hm_patel@spuvvn.edu

Abstract

Herein, we report the synthesis of novel imidazo[2,1-b]quinazolin-1(2H)-one derivatives as potential kinase inhibitors. These analogues were designed and synthesized via a one-pot, three-component reaction involving 2-aminobenzimidazole, aryl/heteroaryl aldehydes, and 5-phenyl-cyclohexane-1,3-dione in ethanol — a green and recyclable solvent — under reflux conditions. The reaction is highly cost-effective and atom-efficient, affording pure products in moderate to excellent yields (up to 99%) without the need for chromatographic purification. Kinase profiling against a panel of 137 kinases identified one lead scaffold exhibiting potent inhibitory activity against platelet-derived growth factor receptor A (PDGFRA) with an IC_{50} value of 1.25 μM. **In silico** molecular docking, molecular dynamics simulations, and ADMET predictions revealed that this lead compound binds to the same site on PDGFRA as imatinib, with favourable brain bioavailability. Elevated PDGFRA RNA expression is strongly correlated with both low- and high-grade gliomas, underscoring its oncogenic significance in brain cancer. Consistent with this, the lead compound demonstrated potent cytotoxicity across multiple glioma cell lines, including patient-derived primary cells, exhibiting superior efficacy compared to the clinical PDGFRA inhibitor imatinib. These findings suggest that the imidazo[2,1-b]quinazolin-1(2H)-one scaffold represents a promising chemical backbone for the development of next-generation PDGFRA inhibitors with potential applications in glioma therapy.

Keywords: Sustainable synthesis, Onepot Synthesis, imidazo[2,1-b]quinazolin-1(2H)-ones , glioma cell lines, PDGFRA inhibitors.

IL-18

Efficient Synthesis of *N*-Heterocycle-Fused Porphyrins with Enhanced Absorption as Singlet Oxygen Generators

Dalip Kumar

Department of Chemistry, Birla Institute of Technology and Science, Pilani-333031, India
E-mail: dalipk@pilani.bits-pilani.ac.in

Over several decades, π-extension of porphyrinoids and other aromatic molecules *via* intramolecular carbon-carbon or carbon-nitrogen coupling has been of keen interest to many researchers because of its potential applications in near-IR (NIR) electroluminescence displays, photovoltaic solar cells, non-linear optical materials, photodynamic therapy, and molecular electronics [1]. The carbon-carbon or carbon-nitrogen bond fusion forces the aromatic core and the aromatic substituent to be co-planar, which promotes enhanced electronic communication between both fragments. These π-extended molecules demonstrate changes in their optical as well as electronic properties, such as bathochromic shift in their absorption/emission spectrum, large absorption and fluorescence in the NIR range, increase in the two-photon absorption cross section, decrease in their HOMO-LUMO gap in comparison with the non-fused non planar parent aromatic core. The functionalization of porphyrin with various heteroatoms has become an important milestone in porphyrin chemistry due to their advantageous features such as availability of nitrogen containing heterocyclic compounds can greatly influence the electronic properties of porphyrin core. Heteroatoms can act as functional units such as Lewis acid-base, hydrogen-bond acceptors, and provide external coordination sites. Another application of heteroatom is that they can be easily set up and undergo functional group transformations *via* electrophilic substitution and transition-metal catalysed cross coupling reaction [1]. In general, formation of expanded porphyrins with π-conjugated electronic system involves direct fusion of a co-planar aromatic segment onto the periphery of the porphyrin. In recent years, intramolecular carbon-carbon or carbon-nitrogen coupling reactions have been utilized as one of the important strategies for the construction of π-extended porphyrins to be useful in molecular electronics, photodynamic therapy, nonlinear optical materials, near-IR electroluminescence, and photovoltaic cells [2-6]. Given the interesting photophysical properties and applications of N-heterocycle-fused porphyrins [7] we developed a facile and efficient synthesis of six and seven-membered N-heterocycle fused porphyrins from readily available precursors. The synthetic details, photophysical properties and applications of the prepared N-heterocycle-fused porphyrins will be discussed in the conference presentation.

REFERENCES

1. I. G. Denisov, T. M. Makris, S. G. Sligar, I. Schlichting, *Chem. Rev.* **2005**, *105*, 2253. (b) N. Fukui, K. Fujimoto, H. Yorimitsu, A. Osuka, *Dalton Trans.* **2017**, *46*, 13322. (c) J. Barber, *Chem. Soc. Rev.* **2009**, *38*, 185. (d) M. Pawlicki, H. A. Collins, R. G. Denning, H. L. Anderson, *Angew. Chem. Int. Ed.* **2009**, *48*, 3244.M. O. Senge, *The Porphyrin Handbook* **2000**, *1*, 239. (d) J. P. Lewtak, D. T. Gryko, *Chem. Commun.*. **2012**, *48*, 10069.
2. (a) A. Singh, M. Nath, *Org. Lett.* **2025**, *27*, 9007. (b) P. Singh, M. Nath, *Org. Lett.* **2022**, *24*, 8586.
3. M. Berthelot, G. Hoffmann, A. Bousfiha, J. Echaubard, J. Roger, H. Cattey, A. Romieu, D. Lucas, P. Fleurat-Lessard, C. H. Devillers, *Chem. Commun.* **2018**, *54*, 5414.
4. N. Fukui, W. Cha, D. Shimizu, J. Oh, K. Furukawa, H. Yorimitsu, D. Kim, A. Osuka, *Chem. Sci.* **2017**, *8*, 189.
5. A. Nowak-Król, D. T. Gryko, *Org. Lett.* **2013**, *15*, 5618.
6. A. Pereira, C. Alonso, M. Neves, A. Tomé, A. Silva, *J. Org. Chem* **2008**, *73*, 7353.
7. P. P. Taur, N. Verma, D. Sharma, D. Kumar, J. Org. Chem. **2025**, 90 (10), 3570.

IL-19

Sustainable Synthesis of Biomass-Derived Carbon Quantum Dots for Nanosensing Applications

Dr. Banibrata Maity

Assistant Professor
Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab

Abstract

Carbon quantum dots (CQDs) have emerged as a promising class of fluorescent carbon nanomaterials owing to their exceptional properties, including high aqueous solubility, low cytotoxicity, tunable photoluminescence, chemical stability, and environmental compatibility. A wide range of synthetic strategies and carbon precursors have been explored for CQD fabrication; among these, the conversion of biomass waste into value-added CQDs offers a sustainable and eco-friendly route. The present work focuses on the sustainable synthesis of highly fluorescent CQDs from biomass-derived precursors and their application as efficient nanosensors. The use of renewable biomass feedstocks not only minimizes chemical waste and production costs but also contributes to sustainable waste management and resource utilization. Furthermore, the surface chemistry and particle size of the as-synthesized CQDs can be precisely tuned to enhance their quantum yield and sensing performance. This study underscores the potential of biomass-derived CQDs as versatile, green nanomaterials for next-generation sensing and environmental monitoring applications.

IL-20

Biotemplated Synthesis of Perovskite oxide: Waste to Wealth Conversion and its Potential Application in Bioremediation

Dr. Rinku Chakrabarty

Assistant Professor, Department of Chemistry, Alipurduar University, Alipurduar-736122, West Bengal.
Email: rinkuapduchem@gmail.com

Abstract:

Mushrooming research is going on in recent decades for the biogenic synthesis of inorganic nanoparticles due to reduced toxicity, simplified synthesis technique, and eco-friendliness. Water pollution has become one of the major concerns of the scientists worldwide, which is mainly originated from the dye present in the wastewater of the industries like textile, cosmetics, pharmaceuticals, ink, etc. Carcinogenic as well as mutagenic effect of these dyes throws a serious challenge to the scientists for their removal technique. Complex organic structure and costly removal technique makes the process more difficult. In the present study we will discuss about the synthesis of metal/metal oxide nanoparticles using the plant extracts, their characterization and application as catalyst for the degradation of noxious organic dyes present in the effluents of industrial wastewater.

References:

1. N. Roy, N. T, P. Paira,* Rinku Chakrabarty* RSC Advances 15, 2025, 3008.
2. B. Lakshmi M, A. Akbar, T. Chatterjee, P. Sarkar, Rinku Chakrabarty,* Q. A. Islam, M. Ghosh ChemistrySelect 9, 2024, e202401578.
3. P. Sarkar, S. K. Paul, K. Sahu, S. Mandal, Q. A. Islam, Rinku Chakrabarty* ChemistrySelect 8, 2023, e202301906.

IL-21

Green Catalysis for Sustainable Organic Synthesis

Vikas Tyagi*

Thapar Institute of Engineering and Technology, Patiala, Punjab, India
Email: vikas.tyagi@thapar.edu,

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.

References:

1. Dutt S., Mohapatra A., Pandey S., Tyagi V., *Tetrahedron*, **2024**, 155, 133905.
2. Kambojm P., Mohapatra, A., Mandal, D., Tyagi, V., *Org. Biomol. Chem*., **2024**, 22, 1839-1849.
3. Kamboj, P., Tyagi, V., *ChemBioChem*, **2024**, e202300824.
4. Kamboj, P., Tyagi, V., *Green Chem*., **2024**, 26, 1990-1999.
5. Kaur, P., Tyagi, V., *ChemNanoMat*, **2023**, e202300441.
6. Kamboj, P., Tyagi, V., *Tetrahedron*, **2023**, 148, 133679.
7. Soam, P., Tyagi, V., J. Org. Chem., 2024, https://doi.org/10.1021/acs.joc.4c01384

IL-22

Orchestrating Metabolic-Microbial Synergy: A New Frontier with Thiazole-Based PKM2 Inhibitors in Colorectal Cancer

Moumita Ghosh Chowdhury, Saumya Kapoor and Amit Shard*,!

Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research Ahmedabad (NIPER A), Gandhinagar, Gujarat, India 382355
**Corresponding and !Presenting author Email id: amit@niperahm.res.in*

Colorectal cancer (CRC) remains a major global health challenge, with conventional therapies largely focused on eradicating tumor cells. However, chemotherapy-induced gut dysbiosis often aggravates inflammation and accelerates disease progression, highlighting the need for integrative therapeutic strategies. Although metabolic inhibition and microbiome modulation have been investigated independently, no agent to date has been shown to concurrently target cancer metabolism and gut microbial homeostasis. In this study, we designed and synthesized thiazole- based tumor pyruvate kinase M2 (PKM2) inhibitors, hypothesizing that selective PKM2 modulation could suppress tumor proliferation while restoring microbial balance. Among these, compound **10j** demonstrated potent and selective PKM2 inhibition both in cell-free assays (IC_{50} = 0.01 ± 0.0009 µM) and CRC cells (IC_{50} = 4.21 ± 0.04 µM), effectively disrupting key oncogenic metabolic pathways. Remarkably, metagenomic analysis revealed that 10j reinstated gut microbiota equilibrium disrupted during CRC progression. These findings unveil a dual-function therapeutic paradigm wherein thiazole-based PKM2 inhibitors not only impede tumor metabolism but also restore gut microbial homeostasis-pioneering a novel, metabolism–microbiome-integrated strategy for colorectal cancer treatment. This study will be discussed in the talk.

IL-23

Endemic Flaviviruses: A Persistent Challenge for India's Healthcare?

Akanksha ROBERTS,[1] Sonu GANDHI*,[1]

[a]*DBT-National Institute of Animal Biotechnology (NIAB), Hyderabad-500032, Telangana, India*
[b]*DBT-Regional Centre for Biotechnology (RCB), Faridabad-121001, Haryana, India*

ABSTRACT:

Japanese Encephalitis Virus (JEV) is the leading cause of mosquito-borne encephalitis in South-East Asia and Western Pacific and is often misdiagnosed as Dengue. JEV belongs to the family Flaviviridae genus Flavivirus and exists in a zoonotic cycle. Since there is no cure or fool proof vaccine available for JEV, early detection is essential to mitigate a breakout. Hence, in this research work, we have developed an electrochemical based immunosensor for the rapid, sensitive and specific detection of the Non-Structural 1 (NS1) secretory protein, which is suitable biomarker for JEV found circulating in the blood and has been reported to elicit an immune response. Since the conventional methods for JEV diagnosis are expensive, more hazardous and time-consuming diagnostic techniques which require an elaborate laboratory set up and trained expertise, the developed biosensor may be able to overcome these limitations. The JEV NS1 protein and its antibody (Ab) were initially studied through *in-silico* analysis epitopes and paratopes were identified. Later docking studies helped identify the specificity of the epitopes of different flaviviral NS1 with JEV NS1 antibody paratopes. Furthermore, JEV NS1 sequence was amplified and cloned, followed by transformation. The NS1 protein was expressed in *E. coli*, characterised, and immunized in rabbits to raise polyclonal antibodies. The NS1 Ab were purified from serum, characterized, and used as the bioreceptor to fabricate electrochemical and colorimetric sensors for the detection of JEV NS1 antigen (Ag). Fabrication steps were characterised and the sensor was optimised by CV, DPV and optical phenomenon in clinical samples as tested in other flaviviral infections. The fabricated immunosensor was also specific towards JEV NS1 Ag as compared to other flaviviral NS1 Ag. Hence, the proposed platforms may be a promising candidate for the development of accurate and rapid diagnostic kits for specific and sensitive detection of JEV from clinical samples.

IL-24

Current Sequential Stages for the Search of New Pharmacologically Active Agents from Medicinal Plants

D. N. Singh

Department of Chemistry, K. S. Saket PG College, Dr. R.M.L. Avadh University, Ayodhya-224001, India
E-mail: *dnsinghsaket@yahoo.com*

Photochemistry plays a pivotal role in understanding the chemical constituents from medicinal plants and bioassay guided phytochemical screening provides insights about the biological activities of the isolated bioactive compounds leading to the discovery of new therapeutic agent in pharmaceutical industries by the using various recent analytical techniques. Drugs derived from plants are biocompatible and generally considered safe compared to synthetic therapeutic agents [1] of diverse activities. Bioassay monitored technique serves as a bridge between traditional knowledge and modern pharmacological evaluation. Phytopharmaceuticals, derived from medicinal plants have emerged as a vital frontier in modern therapeutics and play a central role in medicinal chemistry. Several plant-derived drugs on the market have been developed to treat various diseases *viz.* apomorphine is made semisynthetically from morphine isolated *from Papaver somniferum* acting as a dopamine receptor agonist and it is now approved for the treatment of Parkinson's disease. Arteether is a semisynthetic drug derived from artemisinin from *Artemisia annua* and is used to treat malaria. Arteether is oil soluble, has a long elimination half-life, and is more stable than artemisinin. Galantamine is an Amaryllidaceae alkaloid from *Galanthus woronowii* and an acetylcholinesterase inhibitor used in Alzheimer's treatments. Tiotropium is a muscarinic receptor antagonist from Atropa belladonna that has been used to treat asthma and chronic obstructive pulmonary disease. Even in recent times, natural products play a significant role in drug development, with 6 of 53 new products approved by the FDA in 2023 has been inspired from natural products. Keeping in view the importance of medicinal plants in the discovery new drugs and our continuous work and effort to search the new leads in parasitic area, recently, in our laboratory we have isolated and identified the many bioactive lead molecules viz. anthraquinones, spirostan saponins and triterpenoids from medicinal plants by using various separations and spectral techniques [2-4]. Recent trends leading to the search of novel pharmacologically active leads from medicinal plants will be discussed in detail during the presentation.

REFERENCES

1. DN Singh, N Verma, Bentham Science, Frontiers in Medicinal Chemistry, 10, **2023**,81.
2. DN Singh, N Verma, S Raghuwanshi, PK Shukla and DK Kulshreshtha, *Bioorg. Med. Chem. Lett.,* 16**, 2006**, 4512.
3. DN Singh**,** N Verma, DK. Kulshreshtha and AK Agrawal , *Journal of Natural Remedies,* 12, **2012,** 68**.**
4. DN Singh, N Verma, Indian. J. Chem. 56B, **2017**, 993.

P-25

Reprogramming of Carbohydrate Metabolism Pathways by Mutant Isocitrate Dehydrogenase in Glioma

Subhalaxmi Pattanayak[1], Sutapa Biswas[2], Amrita Sahoo, Swati Sucharita Panda[1], and Priya Ranjan Debata[1*]

[1]Department of Zoology, Maharaja Sriram Chandra Bhanja Deo University [2] Department of Pathology, SPARSH Hospital, Bhubaneswar,
[*] Corresponding author's email: prdebata@gmail.com

Abstract

Mutations in *Isocitrate dehydrogenase* (IDH1 and IDH2) are among the most common genetic alterations in gliomas and have been closely associated with metabolic reprogramming during gliomagenesis. These neomorphic mutations impair normal oxidative metabolism and drive the accumulation of oncometabolites, altering cellular redox balance and energy flux. In this study, we investigate the role of IDH1/2 mutations in modulating carbohydrate metabolism using a combined approach of mammalian cell culture and *Drosophila melanogaster* models. Biochemical analyses focused on quantifying key metabolites, including lactate, pyruvate, glucose, NADH, and NAD^+, to unravel the extent of glycolytic shift and altered mitochondrial function. Our findings suggest that IDH1/2 mutations promote a dysregulated balance between glycolysis and oxidative phosphorylation, accompanied by changes in lactate–pyruvate dynamics and NADH/NAD^+ homeostasis. By integrating in vitro and in vivo models, this work provides mechanistic insights into how IDH mutations rewire carbohydrate metabolism to support glioma initiation and progression. These results may open avenues for identifying metabolic vulnerabilities as potential therapeutic targets in glioma.

Keywords: Gliomagenesis; IDH1 mutation; IDH2 mutation; Carbohydrate metabolism; Redox balance; *Drosophila melanogaster*

IL-26

Process Validation of Anti-Fungal Drug Product -Immediate Release Oral Solid Dosage Form by Wet granulation approach: Itraconazole Capsules

Shinde N.K.*and Mane D. V.**

***Corresponding Author Email: dvmane11@gmail.com*
***PG and Research Center, Shri ChhtrapatiShivaji College, Omerga, Tal: Omerga, Dist. Dharashiv- 413 606. Maharashtra, India.*
***dvmane11@gmail.com*

ABSTRACT:

Validation is a very crucial step involved in achieving and maintaining the quality of any Pharmaceutical Drug Products. Validation of drug product establishes the documented evidence which provides a high degree of assurance that a manufacturing process will consistently produce a product of predetermined specifications and quality attributes. The main objective of my research was to study the process performance qualification of Drug Product Itraconazole Capsules 100 mg Immediate Release Capsule dosage form. The study untaken here provides the assurance that the manufacturing procedure is suitable for intended purpose and the product consistently meets predetermined specifications and quality attributes.

It gives the detailed information of various steps involved in the manufacturing process like Sifting, Dry Mixing, Wet granulation, Drying, Sizing, Blending, Lubrication, Capsule filling, Packing and analysis of in-process tests and finished product.

During this study, Critical Process Parameters (CPPs) involved in Sifting, Dry Mixing, Wet granulation, Drying, Sizing, Blending and Capsule filling were identified with the help of developmental study and evaluated during process validation study. During this process, all the Critical Quality Attributes (Critical Control Parameters) were observed such as Blend Uniformity (BU), Water content, Physical characteristics of blend, physical parameters of Capsules, Description, Water content (Finished product) Dissolution, Uniformity of Dosage Unit, Assay, Degradation products and Microbial examination.

After the evaluation of analytical results and discussion, it can be concluded that this manufacturing process is capable of producing the product consistently meeting with quality attributes and its predetermined specification. Hence the manufacturing process of drug product is validated and can be used for routine manufacturing of Itraconazole Capsules 100 mg.

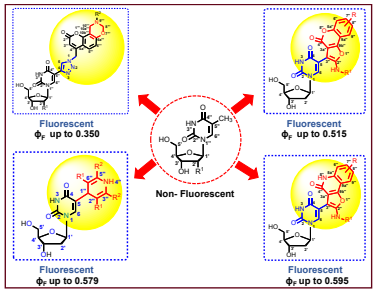
Keywords: Process Validation, Itraconazole Capsules 100 mg, Critical Process Parameters (CPPs), Critical Quality Attributes (CQAs), Sampling plan, and Testing plan, Acceptance criteria, finished product

IL-27

Photophysical Insights into Base-Modified Fluorescent Nucleosides

Brajendra K. Singh

Department of Chemistry, University of Delhi, Delhi, India 110007
singhbk@chemistry.du.ac.in



Fluorescent nucleosides, created by replacing natural nucleobases with luminescent analogues, have become indispensable tools for probing the structure, dynamics, and interactions of nucleic acids. By introducing targeted chemical modifications that impart optimal photophysical properties, these probes retain the crucial base-pairing attributes of DNA and RNA, while enabling real-time monitoring of molecular processes. Their sensitivity to subtle environmental changes—ranging from polarity shifts to protein binding—has played a pivotal role in advancing diagnostic assays, high-throughput screening, and live-cell imaging, underscoring their broad significance in both biomedical research and materials science.

In this context, a series of systematic studies has been conducted to design novel fluorescent nucleosides with enhanced emission characteristics and practical synthetic accessibility, focusing on diverse heterocyclic scaffolds at the C-5 position of uridine. We employed an efficient, catalyst-free, and atom-economical multicomponent approach to incorporate oxazine-coumarin triazoles, furo[3,2-c]coumarins, 1,4-dihydropyridines, and furo[3,2-c]quinolones into nucleoside frameworks. Comprehensive exploration of their photophysical properties revealed that precise incorporation of heteroaromatic units not only significantly enhances fluorescence but also opens new avenues for applications in nucleic acid chemistry and molecular diagnostics.

Keywords: Base-Modified, Nucleosides, Fluorescent, Photophysical, Uyridine/Thymine

References:

1. Arora, S. Kumar, S. Kumar, A. Dua, and B.K. Singh, Synthesis,characterization and photophysical studies of dual-emissive base-modified fluorescent nucleosides. *Org. Biomol. Chem.,* **2024**, *22*, 4922.
2. S. Kumar, A. Arora, S. Kumar, A. Dua, J. Maity, and B.K. Singh, Synthesis of Base-Modified Fluorescent Furo[3,2-c]coumarin Nucleosides and their Photophysical Studies *J. Mol. Struct.*, **2025**, *1321*, 139915.
3. A. Arora, S. Kumar, J. Maity, and B.K. Singh, Microwave-Assisted Synthesis of Base-Modified Fluorescent 1,4-Dihydropyridine Nucleosides: Photophysical Characterization and Insights *RSC Adv.*, **2024**, *14*, 39833.
4. S. Kumar, A. Arora, G. Deo, M. Tiwari, J. Maity, and B.K. Singh, Microwave-Assisted Synthesis of Base Modified Furo[3,2-c]quinolone Nucleosides and Insights into Their Photophysical Properties *Dyes Pigm.*, **2025**, *240*, 112826.

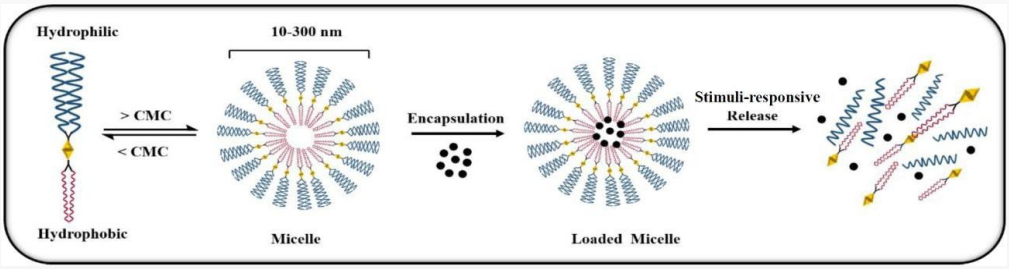
Synthesis of Amphiphilic Nano-architectures for Targeted Drug Delivery

Sunil K. Sharma

Department of Chemistry, University of Delhi, Delhi 110007
sksharma@chemistry.du.ac.in

The global pharmaceutical industry has been developing compounds for over a century, but many of these never get to market. Many drugs fail clinical trials because the compound cannot be delivered to the desired site where without having some interaction with the human body on the way. The result can range from triggering a severe immune system response to toxic side effects. Getting the active compound at the target site in an effective manner is one of the holy grails in the treatment of diseases ranging from inflammations to cancer.

Nanotechnology-enabled drug delivery systems (DDS) are considered to address the challenges of drug delivery and are forecast to dramatically reshape the way existing drugs are delivered. We have designed and developed stimuli-responsive amphiphilic polymeric architectures using easily available biocompatible starting materials that aggregate in aqueous medium to form nanospheres. The synthesised nano-architectures exhibit good chemical stability and inertness under biological conditions. Molecular encapsulation of small hydrophobic drugs using these polymeric / dendritic architectures followed by stimuli-responsive release has been studied. An overview of this research will be shared during the conference.



Representative Publications: SK Sharma *et al.*

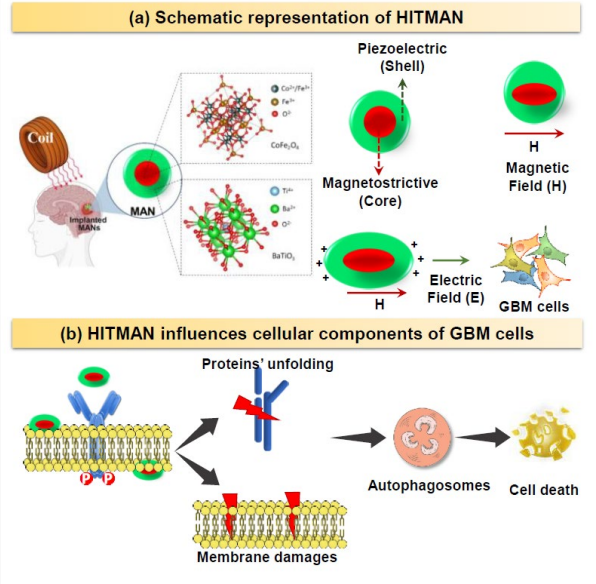
a) ***ACS Appl. Polym. Materials*** **7**, 8699-8707 (2025);
b) ***ACS Polym. Sci. Technol.*** **1**, 144-154 (2025);
c) ***European Polymer Journal***, **213**, 113127 (2024);
d) ***Soft Matter*** **20**, 1282-92 (2024);
e) ***Polym Adv. Technol.*** e6223 (2023);
f) ***ACS Applied Polymer Materials***. **4**, 8269-8276 (2022);
g) ***RSC Advances*** **12**, 23566-23577 (2022); ***ChemistrySelect***, 7, e202203274 (2022);
h) ***Macromol. Rapid Commun.***, 2100914 (2022);
i) ***ChemMedChem***, ISSN: 1860 - 7179 16, 1–11, (2021);
j) ***Int. J. Pharmaceutics*** **580**, 119212 (2020);
k) ***Advanced Materials*** 22, 190 – 218 (2010).

IL-29

Magnetically Actuated Nanoantennas for Wireless Glioblastoma Therapy

Monochura Saha[1,2], Ishaq N. Khan[1], Baju Joy[1], Preet Patel[1], Faheem Azeemi[1], Deblina Sarkar[1*]

[1]MIT Media Lab, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA.
[2]Birla Institute of Technology, Mesra, Ranchi, 835215, INDIA
**deblina@mit.edu*



Glioblastoma (GBM) is one of the deadliest brain cancers. It grows aggressively, resists standard treatments, and leaves patients with very poor survival chances. In our work, we introduce a new approach we call **HITMAN** (short for *Highly-localized-electric-field Induced Tumor-therapy using Magnetically Actuated Nanoantennas*). In simple terms, HITMAN uses tiny "nanoantennas" that can be placed inside a brain tumor. When exposed to harmless, low-frequency magnetic fields from outside the body, these antennas create highly focused electric fields right on the surface of cancer cells. This electric shock at the microscopic level causes the tumor cells' proteins to misfold, their membranes to rupture, and their internal machinery to fail leading to cancer cell death. In lab studies, HITMAN killed more than half of drug-resistant glioblastoma cells, while the standard chemotherapy drug (temozolomide) only reduced their growth by about 10%. Importantly, HITMAN did not harm healthy brain cells. We also tested it in mouse models of human glioblastoma, where it dramatically slowed tumor growth, extended survival by more than 50%, and showed no signs of damage to normal tissues. Unlike other electric-field therapies that require wires or electrodes, HITMAN works **wirelessly, non-invasively, and with pinpoint precision** delivering powerful electric effects deep inside the brain without heating, mechanical damage, or toxic drugs. We believe this technology opens a completely new way to treat brain tumors that don't respond to current therapies, combining strength, safety, and the possibility of real- world translation into future clinical care.

IL-30

Soma Chattopadhyay

Scientist-F, Infectious Disease Biology, Institute of Life Sciences, Bhubaneswar, India

Abstract Awaited

IL-31

Modular Approaches for the Synthesis of Boron-Heterocycles and BN-Isosteres

Ravindra Kumar

CSIR-Central Drug Research Institute (CDRI), Lucknow, India
Email: ravindra.kumar1@cdri.res.in

Drugs and materials are typically built from carbon and other elements like hydrogen, nitrogen, and oxygen. When chemists swap a carbon-carbon pair with a boron–nitrogen pair, the resulting BN "isosteres" may behave like the original carbon compounds—but with unique benefits due to the inherent property of elemental boron, next to carbon in periodic table. In addition, diversification of privileged molecular scaffolds for improving properties is key in drug design and the development of novel pharmaceutical candidates.[1] Recently, bioisosteric replacement chemistry has emerged as an important tool for modifying existing biologically active compounds, potentially influencing the overall pharmacological activity of related compounds.[2] Moreover, the formation of covalent B-N bonds (isoelectronic with C=C) for the generation of novel boron-containing heterocycles drew much attention of the wide research community, comprised of synthetic, medicinal and materials chemists.[3] They often exhibit better therapeutic features, such as improved metabolic stability and aqueous solubility, than the parent molecules, probably because the NH groups of the azaborines can act as hydrogen-bond donors for better binding to proteins.[4]

We developed a simple and sustainable method for constructing such high-valued BN-isosteres, commonly named **BN-2,1-azaboranaphthalenes**, from inert feedstock materials, by an organo-catalyzed **three-component reaction**.[5] The developed transformation followed unprecedented Wolff-type rearrangement with the concomitant formation of Carbon–Carbon, Carbon–Nitrogen, and Boron–Nitrogen bonds in a single go at ambient temperature or with mild heating. The reaction tolerates a broad range of substituents, allowing chemists to incorporate electron-rich or electron-poor groups without sacrificing yield or selectivity. The methodology has also been adapted to tune privileged scaffolds, drug molecules, and natural products to BN-congeners. Its modular nature and benign reaction conditions makes the method **scalable** and ideal for generating boron-based diverse chemical libraries for medicinal chemistry or materials science. Detail of the work will be presented during the conference.

References:

1. J. Kim, H. Kim, S. B. Park, *J. Am. Chem. Soc.* 2014, **136**, 14629−14638.
2. P. Zhao, D. O. Nettleton, R. G. Karki, F. J. Zécri, S.-Y. Liu, *Chem. Med. Chem.* 2017, **12**, 358–361.
3. D. Diaz, A. Yudin, *Nature Chem.* 2017, **9**, 731–742.
4. H. Lee, M. Fischer, B. K. Shoichet, S.-Y., Liu, *J. Am. Chem. Soc.* **138**, 12021–12024 (2016).
5. A. Singh, R. Kant, M. Grellier, R. Kumar, *Nature Chem.* 2025, *https://doi.org/10.1038/s41557-025-01938-1*

Post-Ugi Cyclizations: A Magical Tool to Molecular Diversity

Ajay K. Srivastava

Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Sector 10, Jankipuram Extension, Lucknow-226031, India
Academy of Scientific and Innovative Research (AcSIR), New Delhi-110025, India
ajayk.srivsatava@cdri.res.in

Abstract:

Efficient construction of novel molecular scaffolds is pivotal in modern drug discovery, where speed, scalability, and purity govern the transition of small-molecule drugs to clinical applications. This work emphasizes the strategic use of isocyanide-based multicomponent reactions (IMCRs) combined with intelligent post-IMCR functionalizations to achieve atom-economical synthesis of diverse scaffolds. We report the development of one-pot post-IMCR methodologies enabling the synthesis of alkaloid-mimicking tricyclic azaspiroenones, fused quinolines, 2,5-pyrrolidinediones, and functionalized 1,2,3,4-tetrahydroisoquinolines (THIQs). These novel scaffolds have been instrumental in identifying potent drug candidates highlighting the potential of IMCR-based approaches in accelerating drug discovery.

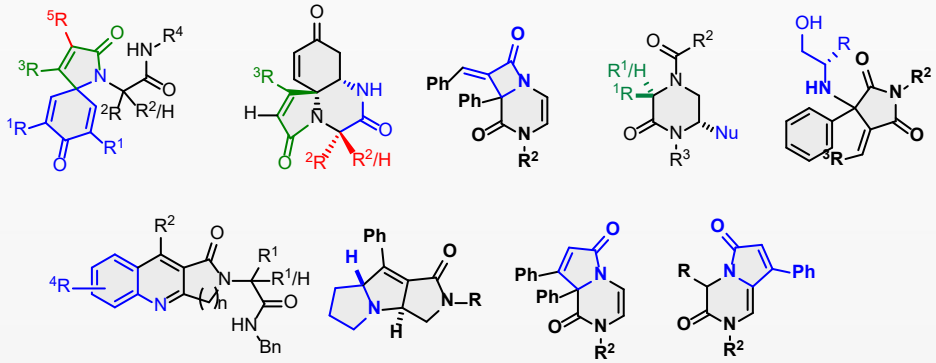


Figure 1. Scaffolds generated by post-IMCR modifications.

References:

1. M. Bhumij, R. Ahamed, R. Kant, S. K. Mudedla and A. K. Srivastava, *Chem. Commun. (Cambridge, U. K.)*, 2025, **61**, 12757.
2. M. Bhumij, M. D. Ambule, S. Sinha, S. Prabhat, R. Kant and A. K. Srivastava, *J. Org. Chem* 2024, **89**, 16679
3. A. Yadav, S. Upadhyay, R. Kant and A. K. Srivastava, *J. Org. Chem* 2023, **88**, 13568
4. S. P. Singh, A. Kumar, R. Kant and A. K. Srivastava, *J. Org. Chem.*, 2022, **87**, 12799
5. M. D. Ambule, S. Tripathi, A. Ghoshal and A. K. Srivastava, *Chem Commun*, 2019, **55**, 10872
6. A. Ghoshal, A. Kumar, D. Yugandhar, C. Sona, S. Kuriakose, K. Nagesh, M. Rashid, S. K. Singh, M. Wahajuddin, P. N. Yadav and A. K. Srivastava, *Eur J Med Chem*, 2018, **152**, 148
7. D. Yugandhar, S. Kuriakose, J. B. Nanubolu and A. K. Srivastava, *Org. Lett.*, 2016, **18**, 1040

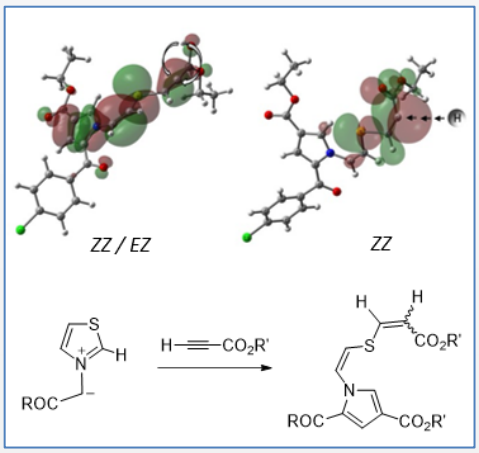
Unraveling Stereochemical Control in Cycloaddition Reactions of Thiazolium Ylide: A Computational Perspective

Neelima Gupta

Professor, Department of Chemistry, University of Rajasthan, Jaipur-302004
guptaniilima@gmail.com

Abstract

Thiazole-based scaffolds constitute an important class of heterocycles exhibiting diverse biological and pharmacological activities, including antibacterial, antimalarial, anticancer, antiallergic, anti-inflammatory, and anti-HIV effects. The 1,3-dipolar cycloaddition of cyclic nitrogen ylides offers a versatile strategy for constructing fused five-membered heterocycles incorporating a bridgehead nitrogen atom. Consequently, numerous *N*-fused heterocycles have been synthesized via [3+2] cycloaddition reactions employing cycloiminium ylides as reactive intermediates. Owing to their inherent regio- and stereoselectivity, such reactions have become a preferred route for the synthesis of bioactive heterocyclic frameworks. Thiazolium ylides, in particular, have attracted significant attention in [3+2] cycloaddition chemistry due to their unusual reactivity patterns. Utilization of thiazolium ylides in synthesis of heterocyclic compounds has been attempted repeatedly to give varied and unexpected results. [3+2] Cycloaddition reaction of thiazolium ylides has been often found to undergo subsequent ring opening resulting in interesting product depending on the reaction conditions. The mechanistic aspects of the competitive pathways involving cycloaddition, ring opening, and rearrangement mediated by nucleophilic addition of the dipolarophile under varying molar ratios explored through a combination of experimental and computational approaches has provided valuable insight into the influence of reaction conditions on product distribution. The combined results offer a comprehensive mechanistic rationale for the experimentally observed outcomes and underscore the utility of computational chemistry in elucidating reaction pathways in heterocyclic synthesis. Advantageous application of computational chemistry in understanding progress of a reaction under different reaction conditions by identifying the stabilization of reaction intermediates and location of transition structures on competitive pathways to rationalize the experimental results will be highlighted.



IL-34

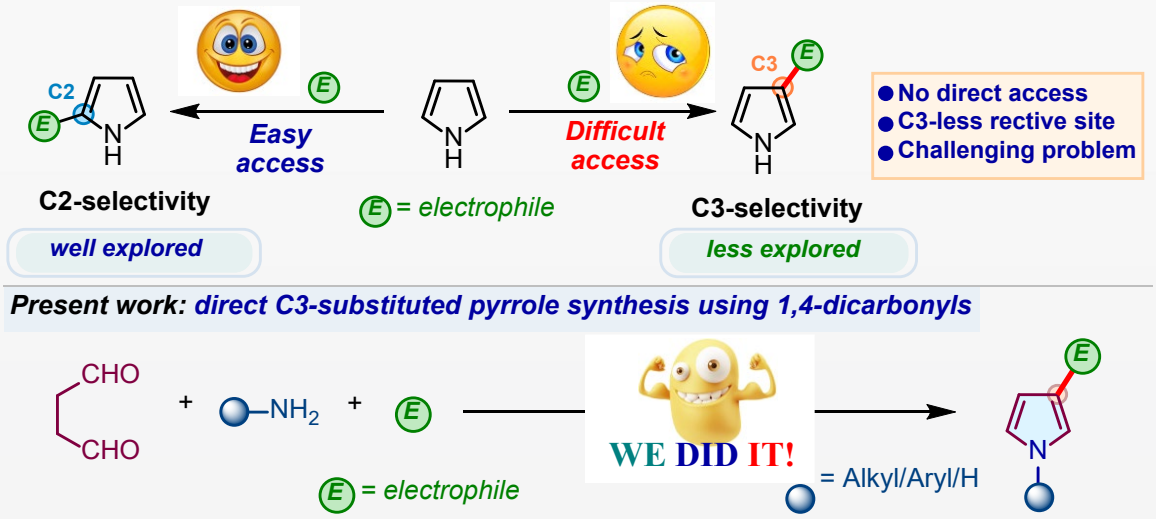
Direct Access to C3-Functionalized Pyrrole

Indresh Kumar

Department of Chemistry, Birla Institute of Technology and Science, Pilani-campus 333 031 (Rajasthan) India
Email: indresh.kumar@pilani.bits-pilani.ac.in, indresh.chemistry@gmail.com

Abstract:

Due to mitigated nucleophilicity, the C3-position of pyrrole is usually considered a non-reactive site in conventional chemistry; thus, most 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 groups 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 straightforward and stimulating method to access β-(C3)-functionalized pyrrole under 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.



References:

1. T. Tsuchimoto, *Chem. Eur. J.* **2011**, 17, 4064.
2. (*a*) I. Kumar, N. A. Mir, V. K. Gupta, Rajnikant, *Chem. Comm.* **2012**, 48, 6975. (*b*) I. Kumar, N. A. Mir, P. Ramaraju, B. P. Wakhloo, *RSC Adv.* **2012**, 2, 8922. (*c*) N. A. Mir, S. Choudhary, P. Ramaraju, D. Singh and I. Kumar *RSC Adv.*, **2016**, 6, 39741. (*j*) P. Ramaraju, N. A. Mir, D. Singh, and I. Kumar; *RSC Adv.*, **2016**, 6, 60422. (*d*) S. Choudhary, A. Singh, J. Yadav, N. A. Mir, S. Anthal, R. Kant, I. Kumar; *New J. Chem.*, **2019**, 43, 953. (*n*) A. Singh, S. Vanaparthi, S. Choudhary, R. Krishnan, I. Kumar; *RSC Adv.*, **2019**, 9, 24050.
3. (a) A. P. Pawar, J. Yadav, N. A. Mir, E. Iype, K. Rangan, S. Anthal, R. Kant, I. Kumar, *Chem. Commun.*, **2021**, 57, 251. (b) A. P. Pawar, J. Yadav, A. J. Dolas, E. Iype, K. Rangan, I. Kumar, *Org. Biomol. Chem.*, **2022**, 20, 5747. (c) A. P. Pawar, J. Yadav, A. J. Dolas, Y. K. Nagare, E. Iype, K. Rangan, Indresh Kumar, *Org. Lett.*, **2022**, 24, 7549.

IL-35

Functional Traits of Peanut-Associated Rhizobacteria: Unlocking Biofertilizer Potential for Enhanced Productivity and Sustainable Agricultural Practices

Ramesh K. Kothari* and Krunal R. Hirpara

Department of Biosciences, Saurashtra University, Rajkot 360005
**Email: kothari1971@gmail.com*

Abstract

Sustainable agricultural practices are eco-friendly farming methods that maintain soil health, conserve resources, and support long-term productivity while minimizing environmental harm. Bioformulations are products made by formulating beneficial microorganisms with carriers to enhance plant growth, protect crops, and reduce reliance on synthetic chemicals, promoting sustainable farming.

The rhizosphere microbiome, particularly the bacterial community known as rhizobacteria, plays a vital role in enhancing plant nutrition through both symbiotic and nonsymbiotic interactions. Among these, plant growth-promoting rhizobacteria (PGPR) are especially important, as they improve nutrient availability through mechanisms such as nitrogen fixation, phosphate solubilization, and phytohormone production.

Our study focused on isolating and identifying indigenous PGPR from peanut plants to develop an effective biofertilizer for sustainable agriculture. Out of 435 native bacterial isolates, 11 strains demonstrated multiple growth-promoting traits, including nitrogen fixation, phosphate and potassium solubilization, indole-3-acetic acid (IAA) production, ACC deaminase activity, and siderophore production. Notably, KR-60 showed the highest phosphate solubilization (120 ± 0.75 µg ml^{-1}), KR-29 exhibited the highest IAA production (54 ± 1.74 µg ml^{-1} at 2 mM tryptophan), and KR-15 was most effective in siderophore production (94.52% psu). Peanut seeds treated with these PGPR strains achieved significantly higher germination rates, seedling vigor, and growth parameters compared to untreated controls under sterile soil conditions. The PGPR consortium also improved nutrient uptake and soil health. Overall, the findings indicate that indigenous PGPR hold strong potential as biofertilizers to enhance peanut productivity while supporting sustainable soil management.

Development of Recoverable Chiral Mn(III) Salen Complexes as Catalysts for Oxidative Kinetic Resolution of secondary alcohols

Surendra Singh

Department of Chemistry, University of Delhi, Delhi-110007
Email: ssingh1@chemistry.du.ac.in

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-d** 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-d** were also evaluated in oxidative kinetic resolution of secondary alcohols. The catalysts **1-3** were recovered and reused for oxidative kinetic resolution of 1-phenylethanol and catalysts and catalyst **3** was successfully reused up to seven recycles with significant loss in activity after 5th recycle.

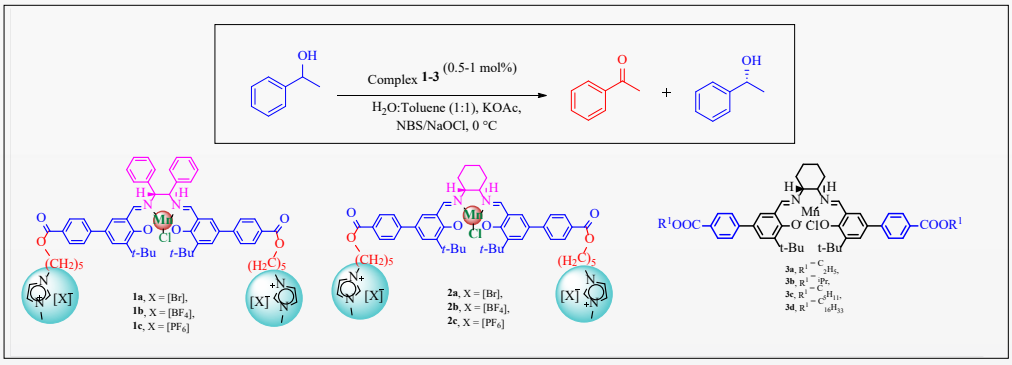


Figure: Chiral Mn (III) Salen complexes for asymmetric oxidative kinetic resolution of secondary alcohols

References

1. V. Schurig, F. Betschinger, Chem. Rev., **1992**, 92, 873-888; (b) K. Sato, M. Aoki, M. Ogawa, T. Hashimoto, R. Noyori, J. Org. Chem., **1996**, 61, 8310-8311; (b) M. Wills, Angew. Chem. Int. Ed. **2008**, 47, 4264-4267; (c) V. K. Singh, Synthesis, **1992**, 7, 605-617
2. (a) P. Chaudhary, C. Len, S. Singh, Molecular Catalysis, **2023**, 542, 2023, 113127; (b) P. Chaudhary, Geeta D. Yadav, K. K. Damodaran, S. Singh, New J. Chem., **2022**, 46, 1308.

IL-37

Heterogeneous and homogeneous catalytic approaches for the conversion of carbon dioxide into cyclic carbonates

Pratibha Kumari

Department of Chemistry, Deshbandhu College, University of Delhi, Kalkaji, New Delhi-110019, India.
***Email**: pkumarichemistry@gmail.com; pkumari@db.du.ac.in*

Abstract:

With the steady increase in atmospheric CO_2 contributing to global warming, its transformation into high-value chemicals offers a practical strategy for carbon capture and utilization. Converting carbon dioxide into cyclic carbonates provides an effective approach to addressing both environmental and economic challenges. Cyclic carbonates are particularly important products, finding use as green solvents, electrolyte components in batteries, and precursors in the development of pharmaceuticals and polymers. Such an approach not only reduces reliance on fossil-derived resources but also supports the advancement of cleaner and more sustainable chemical manufacturing.

The choice of catalytic system plays a crucial role in the efficiency of the cycloaddition reaction between carbon dioxide and epoxides to produce cyclic carbonates. Homogeneous catalysis using ionic liquids offers significant advantages, including high tunability of structure, excellent solubility, and the ability to simultaneously activate both CO_2 and epoxides under mild conditions, resulting in high selectivity and yield. On the other hand, heterogeneous catalysis based on porphyrin-linked covalent organic frameworks (COFs) offers a stable, recyclable, and porous platform that combines the intrinsic catalytic activity of porphyrins with the structural robustness and large surface area of COFs. Herein, we report the synthesis of functionalized ionic liquids and porphyrin-based COFs to catalyze the cycloaddition reaction of CO_2 with different epoxides. This dual approach not only addresses the challenge of catalyst recovery and reusability but also ensures high efficiency and sustainability, making it a promising strategy for large-scale CO_2 utilization.

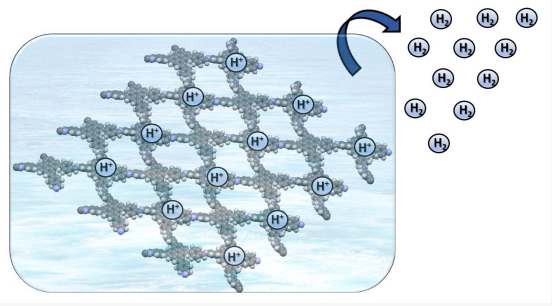
IL-38

Porous Carbon Materials based Green and Renewable Hydrogen Fuel Production

Nitesh Singh, Satadal Sahoo and Dr. Anirban Pradhan*

Department of Chemistry, Birla Institute of Technology (BIT) – Mesra, Ranchi
Jharkhand, 835215, India,
Mob- +91 7003322012,
Email: anirbanpradhan@bitmesra.ac.in

Extensive energy consumption of fossil fuels has caused a global energy crisis1, climate change, and environmental pollution, which has prompted us to explore renewable green energy. Fuels such as hydrogen, which have high specific energy density (143 kJ g-1), have been suggested as suitable and eco-friendly alternatives to diminish fossil fuels. Steam methane reforming, coal gasification, and water splitting are the most cost-effective and widely used processes to produce hydrogen. Herein, we devoted to various porous carbon materials, including COFs/COPs[1-7] and graphene-based materials, and investigate their applications in areas like: Hydrogen fuel production: Developing efficient and sustainable methods for generating hydrogen fuel using these porous materials as electrocatalysts.



This work has a direct impact in our modern society where extreme demand for green and sustainable energy is the biggest concern. In this regard, it is conspicuous to say that the outcome of this research work slowly but surely will be an integral part of our "***Make in India***" project.

References:

1. Electrochemical Stimuli-Driven Facile Metal-Free Hydrogen Evolution from Pyrene-Porphyrin-Based Crystalline Covalent Organic Framework. S. Bhunia, S. K. Das, R. Jana, S. C. Peter, S. Bhattacharya, M. Addicoat, A. Bhaumik, **A. Pradhan*,** *ACS Appl. Mater. Interfaces* **2017**, *9*, 23843.
2. A Metal-Free Covalent Organic Polymer for Electrocatalytic Hydrogen Evolution. B. C. Patra, S. Khilari, R. N. Manna, S. Mondal, D. Pradhan, **A. Pradhan*,** A. Bhaumik, *ACS Catal*. **2017**, *7*, 6120.
3. Efficacious Electrochemical Oxygen Evolution from Novel Co (II) Porphyrin-Pyrene based Conjugated Microporous Polymer, S. Bhunia, K. Bhunia, B. C. Patra, S. K. Das, D. Pradhan, A. Bhaumik, **A. Pradhan*,** S. Bhattacharya. *ACS Appl. Mater. Interfaces*, **2019**, 11, 1520.
4. Surface Modified Porous Organic Polymer for Metal-Free Electrocatalytic Hydrogen Evolution Reaction, **A. Pradhan*,** R. Manna, *ACS Applied Polymer Materials*. **2021**, *3*, 1376.
5. Photoelectrochemical water splitting by triazine based covalent organic framework. **A. Pradhan*,** M. A. Addicoat, *Sustainable Energy Fuels*, **2022**, *6*, 4248-4255.
6. A metal-free perylene-porphyrin based covalent organic framework for electrocatalytic hydrogen evolution. S. Samanta, S. Khatun, I. Mukherjee, S. Maity, M. A. Addicoat, and **A. Pradhan, *** *Sustainable Energy & Fuels*, **2024**, 8, 4183-4191.
7. Metal-free Carbon-based Porous Materials, a Promising Electrocatalyst for Hydrogen Fuel Production, S. Samanta, and **A. Pradhan, *** *Chemical Communications*, **2025**, 61, 8108 - 8119.

Visible light-induced C-N bond formation: A green and Sustainable approach

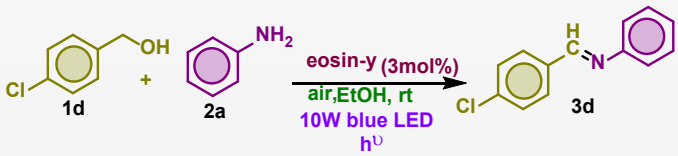
Sundaram Singh

Department of Chemistry, IIT(BHU), Varanasi-221005
sundaram.apc@itbhu.ac.in

Photocatalyst-initiated organic transformations are becoming increasingly powerful tools for forming new chemical bonds in organic synthesis, offering greater environmental sustainability and milder operating conditions.[1-3] In modern synthetic chemistry, developing green and mild methods for forming various C–N bonds to replace older, harsher protocols is a key focus. These newer methods are typically less toxic and easier to manage. In contrast, photocatalysts based on transition metals like iridium, ruthenium, and polypyridyl complexes have several drawbacks, including high cost, low sustainability, potential toxicity, and difficulty in separation.[4-7] Eosin Y photochemistry under visible light has been widely researched, revealing that eosin Y rapidly undergoes intersystem crossing to the lowest energy triplet state[8]. Instead of metal-based photo redox catalysts, metal-free organic dyes like eosin Y are preferred due to their cost-effectiveness and environmental friendliness.[9] Recently, visible light-mediated photo redox catalysis for single electron transfer (SET) has gained recognition as a versatile, economical, and eco-friendly approach for key chemical transformations.

As a continuous work in the field of green synthetic chemistry, wherein we would like to report a facile, metal-free, and visible light-mediated approach for the C-N bond formation using a photocatalyst (Scheme 1 and 2).

Scheme1



Scheme 2

References:

1. Kudo, A.; Miseki, Y., Heterogeneous photocatalyst materials for water splitting. *Chem. Soc. Rev.* **2009,** *38*, 253-278.
2. Xuan, J.; Xiao, W. J., Visible-light photoredox catalysis. *Angew. Chem. Int. Ed.* **2012,** *51*, 6828-6838.
3. Schultz, D. M.; Yoon, T. P., Solar synthesis: prospects in visible light photocatalysis. *Sci.* **2014,** *343*, 1239176.
4. Tambe, S. D.; Rohokale, R. S.; Kshirsagar, U. A., Visible-Light-Mediated Eosin Y Photoredox-Catalyzed Vicinal Thioamination of Alkynes: Radical Cascade Annulation Strategy for 2-Substituted-3-sulfenylindoles. *Eur. J. Org. Chem.* **2018,** *2018*, 2117-2121.

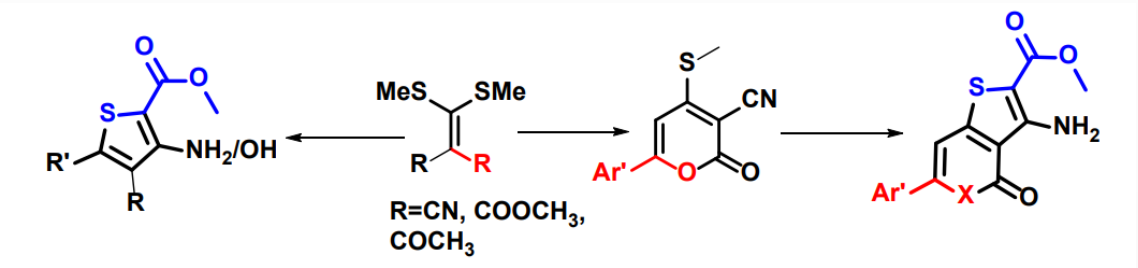
IL-40

Green approach for the synthesis of various functionalized isolated and fused thiophenes and their biological and photophysical properties

Ramendra Pratap*

Department of Chemistry, University of Delhi, North campus, New Delhi-110007
Email: rpratap@chemistry.du.ac.in; ramendrapratap@gmail.com

ABSTRACT:



Ketene dithioacetals are very well-known primary precursors for the synthesis of a large class of molecules. Our group is involved in using these molecules for the synthesis of various pyran and exploring further chemistry.[1,2] As we talk about sustainability, we are working on the green synthetic approaches. In this connection, we have developed a green synthetic approach for the synthesis of pyranothiophene in water from functionalized 2-pyranones, and these compounds were studied for antibacterial, anticancer, and photophysical properties.[3] Additionally, further synthetic application of these compounds are also carried out.

Ketenedithioacetal was also used for the synthesis of aminated thiophenes in one pot in water under mild reaction conditions.[3]

1. Singh, S.; Yadav, P.; Sahu, S. N.; Althagafi, I.; Kumar, A.; Kumar, B; Ram, V. J.; Pratap, R. *Org. Biomol. Chem.* **2014**, 12, 4730; Singh, S.; Althagafi, I.; Yadav, P.; Panwar, R.; Kumar, A.; Pratap, R. *Tetrahedron* **2014**, 70, 8879.
2. Singh, S.; Yadav, P.; Sahu, S.N.; Sharon, A.; Kumar, B.; Ram, V.J.; Pratap, R., *Synlett,* **2014**, 2599. Singh, S.; Panwar, R.; Yadav, P.; Sahu, S. N.; Pratap, R. *RSC Adv.* 2015,**5**, 18335-18341.
3. Sahu, SN; Shaw, R,; Yadav, S.; Althagafi, I.; Upadhyay, MK; **Pratap, R** *RSC Adv.* 2025,**15**, 12117; Gompper, R.; Topfl, W. *Chem. Ber.* **1962**, *95*, 2861.

IL-41

Collaborative Research - The Key to Success

Prof. Hitesh D. Patel

Professor & Head
Department of Chemistry, Gujarat University, Ahmedabad – 380009, Gujarat, INDIA
hdpatel@gujaratuniversity.ac.in, drhiteshpatel1@gmail.com

Abstract:

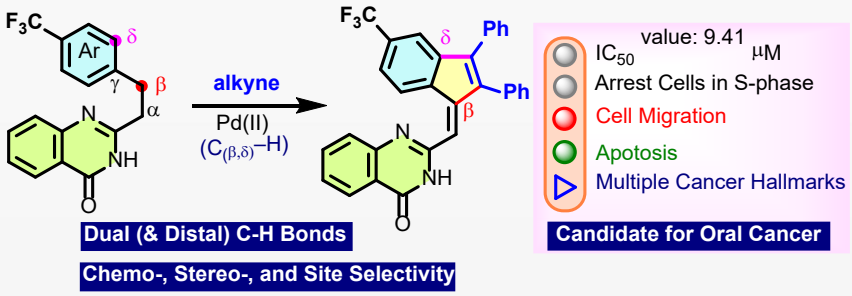
In an increasingly interconnected and interdisciplinary world, collaborative research has emerged as a cornerstone of innovation and progress. The partnerships among researchers, institutions, and industries contribute to the success of scientific and academic endeavours. By combining diverse perspectives, skill sets, and resources, collaborative research enhances problem-solving capabilities, accelerates discovery, and improves the quality and impact of outcomes. The collaborative mindset is not only beneficial but essential in addressing complex global challenges and achieving sustainable research success.

Discovery of a Novel Hit Candidate for Oral Cancer *via* Dual (Distal) C-H Bond Activation Relay Protocol

Dinesh Kumar*

Department of Medicinal Chemistry
National Institute of Pharmaceutical Education and Research (NIPER) – Ahmadabad, Palaj, Gandhinagar-382355, Gujarat, India
Email: dineshk@niperahm.res.in, dkchem79@gmail.com

Oral cancer remains a major global health concern, particularly in India, where its incidence and mortality are alarmingly high. Current chemotherapeutic strategies are limited by poor selectivity and the emergence of chemoresistance, underscoring the urgent need for new drug candidates capable of targeting multiple cancer hallmarks simultaneously. In this context, the present talk highlights the discovery of a novel quinazolone-tethered benzofulvene hit candidate synthesized through a dual (distal) β-C(benzylic)-H and δ-C(aryl)-H bond activation relay protocol. This strategy enables the chemo-, regio-, and stereoselective construction of heterocycle-tethered benzofulvenes via [3 + 2] C-H/C-H alkyne annulation under palladium catalysis. The resulting new chemical entities (NCEs) represent a unique molecular scaffold exhibiting potent anticancer activity against oral squamous cell carcinoma (OSCC). Comprehensive biomolecular analyses, including RNA sequencing, reveal that these compounds induce S-phase cell cycle arrest and modulate multiple oncogenic pathways, collectively demonstrating their promise as multifunctional chemotherapeutic leads for oral cancer.



References:

1. Lombardino, J. G.; Lowe, J. A. The role of the medicinal chemist in drug discovery-then and now. *Nat. Rev. Drug Discovery* **2004**, *3*, 853-862.
2. Sinha, S. K.; Guin, S.; Maiti, S.; Biswas, J. P.; Porey, S.; Maiti, D. Toolbox for distal C-H bond functionalizations in organic molecules. *Chem. Rev.* **2022**, *122*, 5682-5841.
3. Satpute, D. P.; Narang, G.; Rohit, H.; Manjhi, J.; Kumar, D.; Shinde, S. D.; Lokhande, S. K.; Vatsa, P. P.; Upadhyay, V. Selective [3 + 2] C-H/C-H Alkyne Annulation via Dual (Distal) $C_{(\beta,\ \delta)}$-H Bond Activation Relay: A Novel Therapeutic Quinazolone-Tethered Benzofulvenes for Oral Cancer. *JACS Au* **2025**, *5*, 1234-1245.

IL-43

Rationally Engineered Non-Canonical Peptidyl Optical Probes (nCPOPs) Targeting Cancer Microenvironment Detection

Saurajit Ghosh[a] & Partha Sarathi Addy*[a]

Department of Chemistry, Birla Institute of Technology and Science Pilani, Pilani Campus, Pilani, Rajasthan 333031, India.[a]
**E-mail: partha.sarathi@pilani.bits-pilani.ac.in*

Keywords: Peptide, Fluorescence, Cathepsin-B, Cancer, Biomarker, Detection

Abstract

Development of autonomous decision-making synthetic molecular templates that undergo trigger recognition induced chemical and photo-physical changes in complex environments is a grand challenge in synthetic chemistry. We aim to create a standard toolbox for generating chemical systems that are capable of autonomous operations. Such fundamental design tools will enable next-generation smart materials targeting advanced biomedical sensing. In the enzyme family, proteases are an important class of enzymes that regulate several biological functions. In the protease family, Cathepsin-B (Cat-B) is one of the endopeptidases that have a crucial role in cell tissue digestion and cell autolysis.[1] Although the overexpressed Cat-B could be a potential biomarker for several diseases, including cancer.[2] So, based upon the Cat-B target, we developed a panel of Cat-B cleavable non-canonical amino acid based dark non-canonical peptidyl-probes (nCPOPs) which can detect the cellular Cat-B, as well as gave positive results in 3D-spheroid tumour model, which depicts the beauty of our synthesized probe towards Cat-B detection (Figure-1).

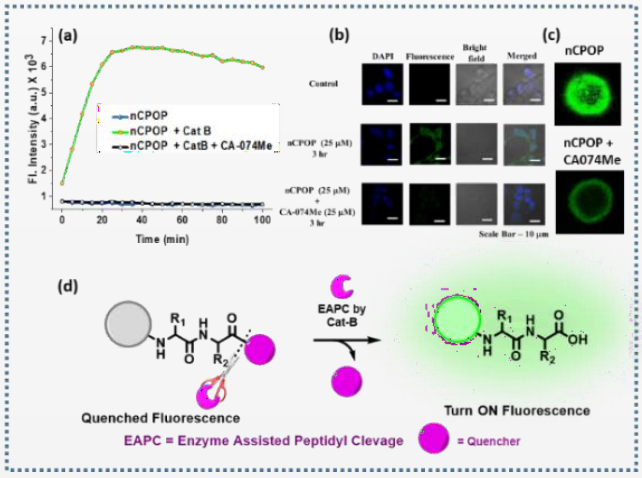


Figure 1: Schematic representation of (a) End point fluorescence detection assay of nCPOP in the presence of Cat- B and inhibitor CA-074OMe (b) Cellular Cathepsin-B detection in MCF-7 cell line (c) Cathepsin-B detection in 3D-spheroid tumour model (d) working mechanism of the probe. (Unpublished)

References

1. S. Ghosh, S. Adhikari, P. S. Addy*, *Chem. – An Asian J.* **2025**, *20*, DOI 10.1002/asia.202401096.
2. S. Adhikari, S. Ghosh, P. S. Addy*, *Chem. – An Asian J.* **2025**, DOI 10.1002/asia.202500211.

P-44

Hippocampal Neurodegeneration Triggers Transient Regeneration Followed by Long-Term Exhaustion of the Neurogenic Niche

Prem Tripathi

Senior Scientist, CSIR- Indian Institute of Chemical Biology (IICB), Kolkata, India

Abstract:

Hippocampal neurodegeneration is commonly associated with cognitive decline, yet the dynamic response of the endogenous neurogenic niche to injury remains insufficiently understood. In this study, we investigated the temporal regulation of adult hippocampal neurogenesis following experimentally induced neurodegeneration. Our findings reveal a biphasic response within the dentate gyrus: an early surge in proliferation of neural progenitor cells, followed by a progressive decline that culminates in long-term exhaustion of the neurogenic pool. This transient regenerative attempt is characterized by enhanced activation of $Sox2^{+}$ and DCX^{+} progenitors; however, sustained inflammation, altered microglial states, and niche remodeling impair the long-term maintenance of stemness. Ultimately, the neurogenic niche becomes structurally and functionally compromised, limiting its capacity for regeneration during chronic stages of damage. These results highlight the inherent, but short-lived, compensatory potential of endogenous hippocampal progenitors and underscore the need for therapeutic strategies aimed at preserving niche integrity to support long-term neuronal replacement. Our study provides conceptual and mechanistic insights relevant to neurodegenerative disorders such as epilepsy, Alzheimer's disease, and age-associated cognitive decline.

P-45

Shedding Light on Cancer Metabolism: Insights from Fluorescence Spectroscopy in Cervical and Renal Carcinomas

Bijay Kumar Barik[1,2], Sanoop Pavithran M[1], Ajaya kumar Barik[1], Arun Chawla[3] , Rekha Upadhya[4], Santhosh Chidangil[1]

1. Centre of Excellence for Biophotonics, Manipal Institute of Applied Physics, Manipal Academy of Higher Education, Manipal
2. Department of Biochemistry, Cell Biology and Genetics, College of Medicine, American University of Antigua, Antigua and Barbuda
3. Department of Urology, Kasturba Medical College Manipal, Manipal Academy of Higher Education, Manipal
4. Department of OBG, Kasturba Medical College Manipal, Manipal Academy of Higher Education, Manipal

Abstract

Autofluorescence spectroscopy provides a non-invasive optical probe into cellular metabolism by capturing fluorescence signatures of endogenous fluorophores such as collagen and NADH in its bound and free forms. This study demonstrates the diagnostic potential of laser induced fluorescence (excitation 325 nm) with curve resolved spectral analysis for distinguishing normal, inflamed, and malignant tissues in both cervix and kidney by probing these metabolic markers. In cervical tissue, progression from normal, cervicitis to cervical cancer is characterized by a progressive decline in bound NADH fluorescence (~440nm), a marked reduction of collagen fluorescence in cancer versus both normal and cervicitis, and a steady increase in free NADH fluorescence (~465nm). These opposing trends directly reflect the metabolic shift from oxidative phosphorylation (OXPHOS) dominant energy production in healthy cells, which consumes free NADH, to aerobic glycolysis (Warburg effect) in cancer cells, which occurs in the cytosol and leads to accumulation of free NADH.

Extending to renal tissue, this study reveals distinct metabolic phenotypes between the two major subtypes of kidney cancer. Clear cell renal cell carcinoma (ccRCC) exhibited significantly elevated free NADH emission at ~465 nm compared to normal renal tissue, confirming its heavy reliance on aerobic glycolysis. In contrast, chromophobe renal cell carcinoma (chRCC) showed diminished bound NADH fluorescence at ~440 nm relative to normal tissue, consistent with maximized dependence on OXPHOS. These studies highlight the ability of 325nm excited autofluorescence to objectively discriminate normal, precancerous, and cancerous states in cervix, as well as differentiate ccRCC from chRCC in kidney. The results support the future development of fluorescence guided endoscopic probes for real-time, label-free optical diagnosis and subtyping of gynaecological and renal malignancies.

References

1. Y. Fu, S. Liu, S. Yin, W. Niu, W. Xiong, M. Tan, G. Li, and M. Zhou, The reverse Warburg effect is likely to be an Achilles' heel of cancer that can be exploited for cancer therapy, Oncotarget 8, 57813 (2017).
2. S. R. Alam, H. Wallrabe, Z. Svindrych, A. K. Chaudhary, K. G. Christopher, D. Chandra, and A. Periasamy, Investigation of mitochondrial metabolic response to doxorubicin in prostate cancer cells: an NADH, FAD and tryptophan FLIM assay, Scientific reports 7, 1 (2017).
3. D.J. Parekh, W.-C. Lin, S.D. Herrell, Optical spectroscopy characteristics can differentiate benign and malignant renal tissues: a potentially useful modality, The Journal of urology, 174 (2005) 1754-1758.
4. J.P. Couapel, L. Senhadji, N. Rioux-Leclercq, G. Verhoest, O. Lavastre, R. De Crevoisier, K. Bensalah, Optical spectroscopy techniques can accurately distinguish benign and malignant renal tumours, BJU international, 111 (2013) 865-871.
5. H. Nilsson, D. Lindgren, A.M. Forsberg, H. Mulder, H. Axelson, M. Johansson, Primary clear cell renal carcinoma cells display minimal mitochondrial respiratory capacity resulting in pronounced sensitivity to glycolytic inhibition by 3-Bromopyruvate, Cell death & disease, 6 (2015) e1585-e1585.
6. A.U. Rehman, A.G. Anwer, M.E. Gosnell, S.B. Mahbub, G. Liu, E.M. Goldys, Fluorescence quenching of free and bound NADH in HeLa cells determined by hyperspectral imaging and unmixing of cell autofluorescence, Biomedical optics express, 8 (2017) 1488-1498.
7. K. Kessenbrock, V. Plaks, and Z. Werb, Matrix metalloproteinases: regulators of the tumor microenvironment, Cell 141, 52 (2010

IL-46

Soumya Mishra

Physiologist, MBBS, MD

Abstract awaited

IL-47

Syntheses of biologically potent scaffolds involving novel CO/CS bond forming reactions

Prof. (Dr.) Devdutt Chaturvedi*

Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University, Motihari-845401(East Champaran), Bihar, India.
E-mails: devduttchaturvedi@gmail.com; devduttchaturvedi@mgcub.ac.in

Abstract:

In recent years, development of novel synthetic methodologies have been attracted a great deal of attention for organic chemists around the globe, for the synthesis of structurally diverse biologically potent molecules. The advantages associated with these synthetic methodologies are lesser synthetic steps, use of cheaper and safer new alternatives, involves overall lesser reaction time, milder reaction conditions, and afforded high yields. Extensive efforts have been made by organic chemists around the globe and thus developed several kinds of new and highly efficient methods for the generation of various kinds of structurally diverse molecules of biological significance.

In recent years, carbon dioxide/carbon disulfide/carbonyl sulfide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and $COCl_2$. Recently, carbon dioxide/carbon disulfide/carbonyl sulfide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, we will focus some of our novel and efficient methods for the synthesis of biologically potent scaffolds.

IL-48

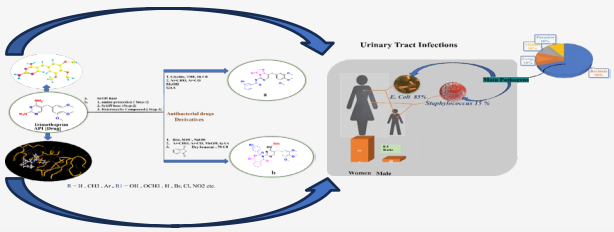
"Exploring Bio-Responsive TMP Containing Nitrogen Heterocycles for Urinary Tract Infection Therapy"

Dhara Vala Dr. Mayank Pandya*

Center for Research and Development, Dr. Subhash University, Junagadh (362001), Gujarat, India.
Email: mayank.pandya3010@gmail.com

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.



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

1. Obayes AK, Hasan F, et al., The forgotten role of methenamine to prevent recurrent urinary tract infection: urgency for reuse 100 years after discovery. Pharmaceutical and Biomedical Research. 2020 Sep 10;6(4):247-50.
2. Khdir KA, Sidiq AS, et al., Prevalence of Multi-Drugs Resistant Escherichia coli Implicated in Urinary Tract Infection in Sulaimaniyah, Iraq. Prevalence. 2023 Apr;63(04).
3. Smilack JD. et al., Trimethoprim-sulfamethoxazole. In Mayo clinic proceedings 1999 Jul 1 (Vol. 74, No. 7, pp. 730-734). Elsevier.
4. Ghany LM, Ryad N, et al., Design, synthesis, antimicrobial evaluation, and molecular modeling of new sulfamethoxazole and trimethoprim analogs as potential DHPS/DHFR inhibitors. Journal of Molecular Structure. 2024 Aug 5; 1309:138170.

IL-49

Advantages of Nanoscale Dendritic Macromolecules For Active Pharmaceutical Ingredient (API) Formulation

PRAVIN KUMAR M. PATEL, Ph.D.

Head, Associate Professor, Industrial Chemistry Department, V. P. & R. P. T. P. Science College (Autonomous) Sardar Patel University, Vallabh Vidyanagar 388120, Gujarat, India.
Email id: drpmpatel73@gmail.com
Contact number: 09428437109

Abstract:

Dendrimers are nanoscale macromolecules with unique properties that make them promising candidates for pharmaceutical applications, particularly as drug delivery systems and solubility of API. Their controlled synthesis allows for modifications in size, shape, and surface properties, enabling the encapsulation of bioactive agents. It is also enhancing the solubility of poorly water-soluble drugs. There are many other advantages like reduce drug toxicity and improve drug efficacy. The ability to host guest molecules in their internal voids is a key advantage for non-covalent drug encapsulation. Their unique characteristics, such as uniform size, high degree of branching, and biocompatibility, make them ideal candidates for active excipients in various pharmaceutical formulations. Potential nanoscale triazine based dendritic macromolecules G1, G2 and G3 are developed as solubility enhancers of API and investigated. Many API were encapsulated by inclusion complex method and also characterized by spectroscopy methods. Sustained release study of API from API loaded dendrimer was carried out and compared with free API. Hemolytic potential and Cytotoxicity assay revealed that synthesized triazine based dendritic macromolecules having more potential that commercially available Poly(amidoamine) (PAMAM) dendrimer.

PHYTONANOMEDICINE EMBEDED NANOFIBROUS MESH FOR LIVER CANCER TREATMENT

Dillip Kumar Bishi, Ph.D.

Department of Biotechnology, Rama Devi Women's University, Bhubaneswar-751022, India
E-mail: dillipkumarbishi@rdwu.ac.in

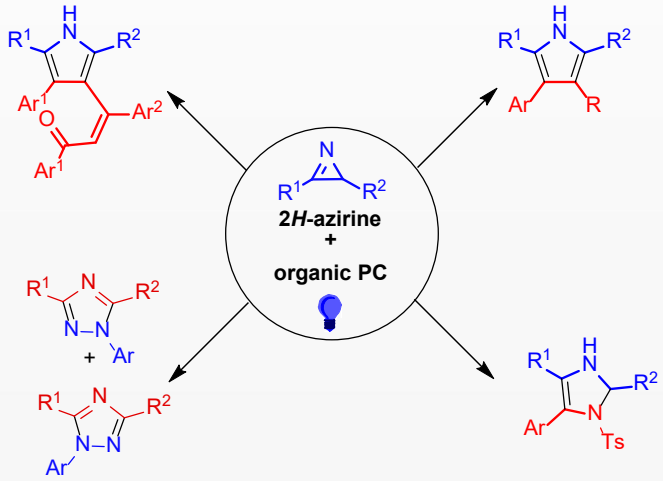
Hepatocellular carcinoma (HCC) is the third most cause of cancer-related deaths worldwide and chemotherapy is the only treatment modality. Due to poor response with conventional chemotherapy, there is a dire need to develop natural anti-HCC drugs with therapeutic potential and less systemic toxicity. Potential traditional anti-cancer phytoformulations combined with advanced nanotechnology offers to be natural alternatives to chemotherapy, when using a potent drug delivery platform. Annona Muricata (Graviola) well-known for its diverse medicinal uses and is one of the richest known sources of phytocompounds, predominantly known as Annonaceous acetogenins. Zinc oxide nanoparticle (ZnO NP), an FDA-approved pharmaceutical nanocarrier for delivery of drugs, is widely used in drug formulations due to their biocompatibility, stability and safety. This report presents fabrication of biogenic zinc oxide nanoparticles (ZnO NPs) with the aqueous leaf extract of Annona muricata (Am) plant collected from semi-evergreen forests of Odisha, India. The synthesized Am-ZnO NPs were physicochemically characterized and were found to be biocompatible and hemocompatible. Furthermore, Am-ZnO NPs displayed strong anticancer effects on both 2D and 3D tumor models. We observed a dose-dependent toxicity on both A549 and MOLT4 cells and observed a size reduction in the A549 tumor spheroids. Subsequently, we observed a depolarization in mitochondrial membrane potential of Am-ZnO NP-treated cancer cells leading to the apoptosis induction in cancer cells. Annonacin, a lipophilic acetogenin and an active component extracted from Annona Muricata is reported to have anti-cancer activity on prostate, ovary, colon, pancreatic, breast and cervical cancers. Anti-proliferative effects of Annonacin in liver cancer is explored in this study using HepG2 spheroids. Since naked Annonacin is poorly soluble in aqueous extracellular environment with limited bioavailability and pharmacokinetic profile, we hypothesize that nano-formulations of Annonacin embedded with ZnO may enhance its anti-proliferative effects. Poly-L-Lactic acid (PLLA), an FDA approved polymer, with excellent attributes such as biodegradability, biocompatibility was used to fabricate nanofibrous scaffold by electrospinning. PLLA-based nanofibrous scaffold, loaded with Annonacin-ZnO nanocomposite have been tested on HepG2 spheroid to assess anti-proliferative properties, which may have tremendous future therapeutic applications in liver cancer.

Organophotocatalytic Ring Opening Reactions of 2*H*-Azirines

Namrata Rastogi

Medicinal & Process Chemistry Division, CSIR-CDRI, Lucknow, India

The use of visible light for carrying out chemical transformations has helped discovering unexplored activities of organic compounds using sustainable source of energy. In this context, visible light-mediated ring opening reactions of small organic molecules generate reactive intermediates, which could be trapped with suitable agents to afford valuable heterocyclic/carbocyclic scaffolds. For instance, the ring opening reactions of three-membered azaheterocycle 2*H*-azirine led to the direct access to pyrroles,[1-3] imidazolines,[4] triazoles[5] etc through intermediate azaallenyl radical cation. Notably, the reactions employed organic dyes or small organic molecules as photocatalysts, making these protocols environment-friendly and sustainable.



1. Karki, B. S.; Devi, L.; Pokhriyal, A.; Rastogi, N. *Chem-Asian J.* **2019**, *14*, 4793-4797.
2. Pokhriyal, A.; Karki, B. S. ; Kant, R.; Rastogi, N. *J. Org. Chem.* **2021**, *86*, 4661-4670.
3. Devi, L.; Mishra, P.; Pokhriyal, A.; Rastogi, N. *SynOpen* **2022**, *6*, 198-207.
4. Mishra, P.; Shruti, I.; Kant, R.; Thakur, T. S.; Kumar, A.; Rastogi, N. *Eur. J. Org. Chem.* **2022**, e202201079.
5. Mishra, P.; Kumar, P.; Srivastava, O. S.; Rastogi, N. *Chem. Asian J.* **2023**, *18*, e202300007.

IL-52

Bandita Rath

Assistant Professor and HOD, Rajdhani College

Abstract Awaited

IL-53

Affordable Indegenised Lab Automation

Shailendra Vyas

Director, Deepali United Mfg. Pvt. Ltd, Mumbai, India

Abstract Awaited

Alternative to Radiolabeled Probes in Drug Discovery and Diagnosis

Suresh K. Kalangi

Scientist, MMI Division, CSIR- Central Drug Research Institute (CDRI) Lucknow, India
suresh.kalangi.cdri@csir.res.in

Abstract

Currently, most of the disorders especially like cancer are challenging to cure as they are not diagnosed at an early stage. These diseases can be treated effectively if, they are diagnosed in the initial phases. Along with diagnosis, the other factors such as bio-distribution, action, and kinetics of the therapeutic molecules are crucial and can only be elucidated by the available imaging techniques during the lengthy, costly and tedious process of drug discovery. Earlier to nanotechnology applications in Pharmacology field, radiolabeled isotopes are the only option to either image/diagnose or to study the distribution and kinetics of therapeutic molecules. Later with the arrival of nanoparticles and nano tubes, quantum dots (QDs) etc., have appeared as promising options of nanotheranostics. Being in tunable size to color, Quantum dots have emerged as promising single molecule tracers with multi-tasking probes in theranostics. On the other hand, though metal toxicity of these nano probes became one of major road blocker, with advancements in chemical synthesis and optical technology, Biodegradable nanoparticles and nano clusters, and various other less toxic nanotheranostic probes have bloomed with a new hope in the field. Recent advances in understanding supramolecular chemistry led to the synthesis of molecules that could aggregate or self-assemble as nanoparticle (aggregated induced emission) enabling the field to address many challenged thrust aspects of metal Nanotoxicity associated with earlier nanotheranostics. Though, an alternative to radiolabel isotope probes with less toxicity is yet to be served on pharmacology table, to allow frequent cyclic experiments of diagnosis and therapy at pre-clinical stage in labs, all the above directions of field are still competing with their own merits and demerits to serve better in theranostics.at this juncture Quantum dots with highly tunable and engineering option to conjugate drugs with out losing the selectivity and efficacy can be one of suitable option to stand as alternative to radiolabeled probes in pharmacology.

IL-55

New Endeavours in Asymmetric Vinylogous Reactions: Towards Functionally Rich Synthon

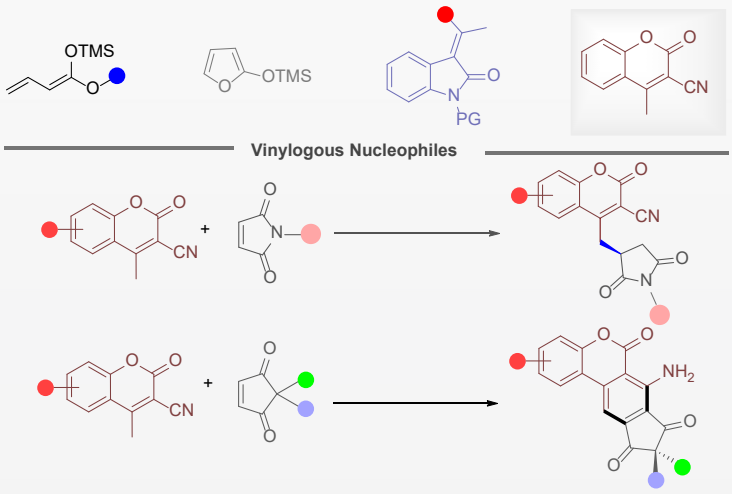
Ravi P Singh*

Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, Delhi 110016
e-mail: ravips@chemistry.iitd.ac.in

The relay of electronic effects through a conjugated organic bonding system, such as those in a vinylogous system provides opportunity to achieve transformation at a remote place. The vinylogous nucleophile after reaction with carbonyl and carbonyl derived compounds (aldehydes, ketones, aldimines, ketimines, enals, enones, and heteroatom-stabilized carbenium ions) offer a multitude of highly functionalized structures. [1],[2],[3] It grants a synthetic track, where a number of functional group and selected stereochemistry can be established. In this presentation, a highly diastereo- and enantioselective organo catalytic asymmetric vinylogous Mukaiyama-Michael addition of various silyoxyfurans to enones,[4] and vinylogous aldol reaction of 2-silyloxyindoles to ketones, which proceeds through the bifunctional catalysis,[5] will be presented.[6]

Also, an asymmetric vinylogous Michael addition reaction between 3-cyano-4-methylcoumarins and biologically active maleimides, developed *via* non-covalent organocatalysis and enantioselective desymmetrization of cyclopentene-1,3-diones *via* [4+2] annulation will be discussed.

Figure: Vinylogous nucleophiles and representattive reactions involving these nucleophiles



1. Casiraghi, G.; Battistini, L.; Curti, C.; Rassu, G.; Zanardi, F. *Chem.Rev*. **2011**, *111*, 3076.
2. Gupta, V.; Sudhir, V. S.; Mandal, T.; Schneider, C. *Angew. Chem. Int. Ed*. **2012**, *51*, 12609.
3. Huang, H.; Yu, F.; Jin, Z.; Li, W.; Wu, W.; Liang, X.; Ye, J. *Chem. Commun*. **2010**, *46*, 5957.
4. Jadhav A.P.; Rao, V. U. B.; Singh P.; Gonnade R. G.; Singh R. P. *Chem. Commun*. **2015**, *51*, 13941.
5. Kumar, K.; Jaiswal, M. K.; Singh R. P. *Adv. Synth. Catal*. **2017**, *359,* 4136.
6. Kumar, K.; Singh, B.; Singh R. P. *Chem. Commun*. **2020**, *56*, 15153.

The Backbone of Preclinical Research: Laboratory Animal Models

Dr.Sarita Jena

Scientist-F
BRIC-Institute of Life Sciences, Bhubaneswar-751023, Odisha
Email:saritajena@ils.res.in

Animal research has played a vital role in nearly every major medical advance in both human and animal health. Studies using animal systems provide invaluable and often irreplaceable insights into biomedical science. Practically every procedure for preventing, treating, curing, or controlling disease, pain, and suffering is rooted in knowledge gained through animal research. Many scientific questions simply cannot be answered without examining the integrated functions of a whole living organism.

Disease processes are inherently complex, often involving multiple physiological pathways and organ systems. Because of the anatomical and physiological similarities between humans and many animal species, researchers rely on animal models to investigate disease mechanisms and to evaluate new therapies before progressing to human trials. These models have been essential for addressing a broad spectrum of scientific inquiries, from fundamental biological research to the development and assessment of innovative medical interventions. By providing a complete organism context, they enable scientists to understand disease mechanisms, test therapeutic strategies, and refine medical and surgical techniques. As a result, animal research has saved lives, extended life expectancy, and improved quality of life across species.

Progress in vaccines, antibiotics, surgical innovations, cancer treatments, and numerous veterinary interventions has depended heavily on studies conducted in experimental animals. Laboratory species—from mice to non-human primate's offer integrated physiological, developmental, immunological, and behavioral systems that cannot be fully replicated through in-vitro or in-silico methods. Because of their indispensable contributions, these animals are often regarded as the "BACKBONE" of biomedical and preclinical research.

Ultra large scale screening of chemical libraries to explore new kinase inhibitors

Baddipadige Raju, Bineet K. Mohanta, Gera Narendra, Anshuman Dixit*

Computational Biology and Bioinformatics Lab, Institute of Life Sciences, Bhubaneswar, 751023, India,
Corresponding authors E-mail: anshumandixit@gmail.com

Abstract:

Janus kinase 1 (JAK1) is a non-receptor tyrosine kinase critically involved in cytokine-mediated signaling pathways associated with autoimmune, inflammatory, and oncological disorders. The therapeutic potential of existing JAK inhibitors, such as Tofacitinib and Ruxolitinib, is limited by their shared pyrrolo[2,3-d] pyrimidine scaffold, which leads to poor isoform selectivity, cross-binding to JAK3, and consequent toxicity. To address these limitations, we developed a scalable AI-guided virtual screening strategy to discover chemically novel and selective JAK1 inhibitors. Uniquely, the deep neural network (DNN) model was trained for the first time using docking scores derived from an ensemble of eight distinct JAK1 crystal structures, capturing protein flexibility and providing a more robust activity landscape. Average docking scores across the eight structures were used to label actives and inactives, enabling the model to learn from a structurally diverse dataset while maintaining chemical realism. Screening of over 1 billion compounds yielded approximately 13,000 top candidates based on enrichment factor analysis. Bemis-Murcko scaffold analysis revealed approximately 8000 unique scaffolds, with minimal overlap with known JAK1 inhibitors. Clustering using UMAP and HDBSCAN identified 3 chemotypes, from which 66 diverse representatives were shortlisted. Ensemble docking confirmed robust binding predictions, and 13,000 compounds passed stringent drug-likeness and ADME filters. This study represents the first application of a machine learning model trained on ensemble docking scores across multiple protein conformations, enabling billion-scale virtual screening to uncover chemically novel scaffolds for selective JAK1 inhibition. These results highlight a new paradigm for integrating protein flexibility into AI-guided drug discovery and expanding unexplored chemical space. Experimental validation confirmed the biological activity of some of the identified molecules.

IL-58

RNA Methylation Dynamics regulates Cancer Stem Cell Maintenance through cell cycle modulation in spheroidal models of TNBC cells

Ruthrotha Selvi Bharathavikru

RNP Biology Laboratory, Department of Biological Sciences, Indian Institute of Science Education and Research, Berhampur
Email: brselvi@iiserbpr.ac.in

m6A methylation is one of the most abundant and reversible RNA modification, catalysed by the writer complex proteins that methylate and erasers that remove the m6A mark. The readers recognise these modifications and play a major role in regulating the functional outcome [1]. The m6A RNA methylation has been shown to play a very crucial and diverse role in physiological processes and also involved in disease progression including cancer [2], However, there is limited information regarding the role of the m6A RNA methylation in cancer stem cell (CSC) maintenance. Recent studies have looked at the effect of m6A RNA modification in cancer by looking at either the writers or erasers separately, which have led to contradicting evidence. We decided to investigate the role of RNA methylation dynamics by modulating the erasers and writers in similar cell types and understand their effects on a comparative basis. Using TNBC cell line, MDA-MB 468 and MDA_MB 231, monolayer and 3D spheroidal models, we have identified a role for m6A RNA modification on cancer stem cell maintenance. We observe that the m6A modification on key cell cycle regulators is essential for the cancer cell proliferation as well as the spheroid formation, evidenced through CSC marker expression. We also observe that additionally, the m6A writer complex protein WTAP contributes to CSC maintenance through alternative splicing of CSC marker gene expression thus influencing cell migration [3]. Thus, the RNA methylation dynamics regulates the CSC maintenance implicating alternative mechanisms to target aggressive and metastatic cancers.

References:

1. Roy A, Padhi SS, Khyriem I, Nikose S, Sankar S H H, Bharathavikru RS. Resetting the epigenome: Methylation dynamics in cancer stem cells. Front Cell Dev Biol. 2022 Sep 26;10:909424.
2. Chen XY, Zhang J, Zhu JS. The role of m6A RNA methylation in human cancer. Mol Cancer. 2019 May 29;18(1):103.
3. Dey S, Padhi SS, Behera RR, Lala S, Arshida MM, Das P, Bharathavikru R, bioRxiv 2025.07.22.666067;

P-59

Implications of amphibian regeneration research for regenerative medicine: A study on limb regeneration in the Indian tree frog, *Polypedates maculatus*

Cuckoo Mahapatra

P. G. Department of Zoology, Maharaja Sriram Chandra Bhanja Deo University, Baripada-757003, Odisha, India

ABSTRACT

Amphibians possess a remarkable capacity to regenerate nearly all of their organs. Salamanders and *Xenopus* are key models for studying complete tissue and limb regeneration, offering insights directly relevant to regenerative medicine and the development of new therapies for humans. Recent advances in genomic resources, genetic tools, and molecular research have revealed cellular programmes, mechanisms of positional memory, and signalling feedback loops that govern precise patterning during regeneration. Studies on tissue integration and skeletal reformation in salamander limbs show both the accuracy and the constraints of natural regeneration, guiding translational efforts and engineering strategies. Interdisciplinary approaches can help transform amphibian biology into progress in regenerative medicine, sustainable biomaterials, and global health solutions. Understanding how animals re-establish pattern, scale, and function after major injury will speed up the development of therapies for limb, spinal cord, and organ repair. Gaining insight into both the successes and failures of amphibian regeneration will help refine translational priorities and ethical considerations for human applications.

Amphibians beyond the standard models also regenerate, and their species-specific differences in regeneration mechanisms are becoming increasingly significant for research on regeneration. Such studies can offer insights into alternative strategies for limb regeneration, potentially leading to new approaches in regenerative medicine and engineering. In this study, we present information on the species-specific novel regulators of limb regeneration in the Indian tree frog, *Polypedates maculatus*. The study reports the upregulation of proteoglycans, such as epiphycan, chondroadherin, hyaluronan, and proteoglycan link protein 1, alongside collagens, as well as several tumour suppressors and methyltransferases in the *P. maculatus* tadpole blastemas. Comparing gene expression between tadpole and froglet limbs showed that the upregulation of cysteine and serine protease inhibitors, coupled with the downregulation of serine proteases, antioxidants, collagenases, and inflammatory genes in tadpole limbs, was vital for creating an environment conducive to regeneration. Dermal myeloid cells were GAG+, EPYC+, INMT+, LEF1+, and SALL4+, and appeared to migrate from unamputated regions of the tadpole limb to the blastema. Conversely, myeloid cells in the froglet limb blastemas were scarce and likely contributed to sustained inflammation, which ultimately led to the healing process.

Insights from *P. maculatus* demonstrate a coordinated approach to limb regeneration that involves a supportive ECM profile, regulated proteolysis, and controlled inflammation; applying these principles to mammalian regenerative medicine will require targeted validation, precise spatiotemporal management of interventions, and thorough safety assessments.

P-60

How do cells sense temperature? The regulation of cellular thermal homeostasis by TRP channels

Chandan Goswami*

School of Biological Sciences, National Institute of Science Education and Research, An OCC of Homi Bhabha National Institute, Khordha, Jatni, Odisha, 752050, India
** Correspondence: chandan@niser.ac.in*

Temperature is an integral part of the biological systems that govern almost all biological functions. Yet, how cells as a unit "sense" temperature and "regulate thermal homeostasis", that remains poorly understood. In this context, Transient Receptor Potential (TRP) ion channels are important as some of these channel members are thermosensitive in nature and are known to be activated by different temperatures that range from high heat to noxious cold. Recently we have used a series of thermosensitive fluoresce probes that are targeted to different subcellular organelles such as to the mitochondria, ER, lysosome, nucleus, lipid droplets and also to the nucleus. Using such probes, we have measured the relative changes in the subcellular organelle temperatures in different experimental conditions. In my talk, we will share some of these examples that high-lights the changes in the subcellular organelle temperature in conditions that mimic rare genetic disorders, obesity, chemotherapeutics-induced neuropathic pain, infection or even ion channel modulation. Our work suggests a complex process of thermal homeostasis regulated by different TRP ion channels.

IL-61

Bhaskar C. Dash

Division Head, Division of Drug and Biotherapeutic Discovery and Professor, Department of Pharmaceutical Sciences, University at Buffalo, New York, USA

Abstract Awaited

P-62

Soft Chemical Routes to Tunable Quantum Dots and Plasmonic Nanoshells for Catalytic and Therapeutic Applications

Amiya Priyam

Dept. of Chemistry, School of Physical and Chemical Sciences, Central University of South Bihar, Gaya-824236
Email: apriyam@cub.ac.in

Abstract

The advent of nanotechnology has brought new solutions to the pressing problems in the society and is improving the quality of life for the mankind. However, most of the nano-syntheses utilize capping agents, reducing agents and solvents that are damaging to the environment. There is a need to make the processes greener and cleaner. The talk describes the aqueous syntheses routes for plasmonic nanomaterials using mild reagents and under normal temperature and pressures. In the first part, synthesis of hollow plasmonic nanoshells of silver is described which have tunable size, shape and structure. Application of such nansostructures in solar-catalysis and chemo-photothermal therapy will also be discussed. The choice of silver stems from the fact that it has highest quality factor for surface plasmons and greater photothermal efficiency in the spectral region of 400-1200 nm. Thus, it presents an opportunity to study the plasmonic properties over wide wavelength region and harness them for suitable applications.

Hollow silver nanoshells (HAgNS) with tunable plasmon bands were synthesized by employing a combination of mild reductant (hydrazine hydrate) and a mild stabilizer (sodium citrate). The plasmon peak was tuned in a wide range from 460 nm to 630 nm. In the second part, we also developed a method using folic acid as stabilizer. A peculiar folate-directed shape transformation from solid nanospheres to hollow silver nanocubes (HAgNCs) has also been discovered and temporal evolution was spectroscopically followed.

The cube-shaped hollow silver nanoshells were found to be very good solar photocatalyst in the entire visible range at sub-picomolar level. Furthermore, the anisotropic Silver NCs vis-à-vis spherical have been found to act as an excellent SERS tool for the detection of metal ion contaminants such as of As (III), Cr(III) and Cr(VI).

Our work also challenges the preconception that if the solutions are not stirred well, the outcome would not be good. We have developed a unique zero-rpm synthesis (i.e, no stirring) to obtain hollow silver nanoshells with versatile tunability of SPR wavelength from visible to the NIR-II region (1000-1350 region). The reaction mixture is neither shaken nor stirred, yet we could obtain hollow plasmonic nanoshells having small size (34-62 nm), and highly tunable, intense, and narrow SPR extinction spectra. As no magnetic sitrrers are used, the process becomes greener, cleaner, and simpler as no electricity is consumed and carbon footprints are minimized.

References:

1. B.K. Dadhich, P. Gupta, S. Ballav, B. Bhushan, P.K. Datta, A. Priyam, ***ACS Applied Nano Materials***, 2024, 7, 1212-1221.
2. B.K.Dadhich, S. Bhattacharya, S. Ballav, B. Bhushan, P.K. Datta, A. Priyam, ***ACS Applied Nano Materials***, 2020, 3, 11620.
3. P. Bose, A. Priyam, R. Kar, S.P. Pattanayak, **RSC Advances**, 2020. 10, 31961
4. B. K. Dadhich, B.Bhushan, A.Saha & A.Priyam ***ACS Applied Nano Materials***, 2018, *1*,4294.
5. S. Patra, B.Bhushan & A. Priyam, ***Dalton Trans.***, 2016, 45, 3918.
6. S. Pattanayak, A. Swarnkar, A. Priyam and GM Bhalerao, ***Dalton Trans.***, 2014, *43*, 11826
7. S. Pattanayak, P. Paik and A. Priyam, ***Dalton Trans.***, 2013, *42*, 10597.

Acknowledgements: The authors thank DST, Govt. of India for the research funding through Fast-Track (grant no.SB/FT/CS-84/2011) and Nano-Mission (grant no. SR/NM/NS-1047/2012) schemes. We also thank UGC-DAE CSR, Kolkata Centre, for funding under the CRS scheme

Synthesis of functionalized imidazoles with applications as antioxidants, antidibetics, and functional organic materials

Okram Mukherjee Singh

Chemistry Department, Manipur University, Canchipur-795003, Imphal, Manipur, India
Email: ok_mukherjee@yahoo.co.in

Abstract

The research findings presented in this article highlight the common assertion in scientific research that chemistry is a central science bridging the gap between physical and life sciences.[1-2] The study reports a one-pot synthesis of 2,4,5-triphenyl-1H-imidazole (lophine) derivatives using eco-friendly deep eutectic solvents (DES). These derivatives show significant in vitro inhibitory activity against α-glucosidase, with six compounds identified as promising candidates for further anti-diabetic research. Molecular docking simulations assessed their binding affinity, while density functional theory (DFT) calculations analyzed their electronic properties. Additionally, a new series of (4H)-imidazol-4-ones were synthesized from phenylalanine and tyrosine via derivatization with phenylacetyl chloride and cyclocondensation using PCl3 and DES. These compounds demonstrated antioxidant activities in assays such as DPPH, ABTS, FRAP, and CUPRAC, with one compound showing superior activity compared to ascorbic acid and Trolox. Some indole-conjugated imidazolone compounds were also identified as π-conjugated analogs of green fluorescent protein.

References:

1. M Maneeta Devi, K Subharani Devi, T Linda Devi, T Prasanta Singh, Okram Mukherjee Singh, Synthesis of (4*H*)-Imidazol-4-ones from α-Amino Acids, and their Antioxidant Activities using Electron Transfer Methods, *Eur. J. Org. Chem.* 2025, e202401449.
2. M Maneeta Devi, T Linda Devi , Francis A S Chipem, Okram Mukherjee Singh, S Sureshkumar Singh, Synthesis of lophines as potent *α*- glucosidase inhibitors with molecular docking and DFT studies, *Journal of Molecular Structure*, **2025,** *1351*, 144088.

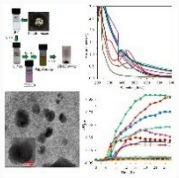
P-64

Solanum tuberosum-based Biogenic Hollandite $Ag_2Mn_8O_{16}$ Nanocomposite for Inhibition of Indian Critical and High-Priority Pathogen-Listed Bacteria

Sandip Kumar Dash, Bandita Panda

P.G. Department of Zoology, Berhampur University, Berhampur, Odisha-760007, India
E-mail: dashsandipkumar@gmail.com

The critical and high-priority bacteria from the Indian Priority-Pathogen List, as well as common waterborne disease-causing antibiotic-resistant bacteria, are of major concern today due to their virulence and rapid transmission. Improper/overuse of antibiotics or antibiotic-coated nanomaterials (NM) may promote antimicrobial resistance and may also affect beneficial microbes. Silver or equivalent NMs with established antimicrobial properties are poorly biocompatible. Metal oxides, such as manganese, would not only enhance the antimicrobial efficiency but also the biocompatibility of the NM.



The contamination of water bodies with methylene blue (MB) and hydrogen peroxide (H_2O_2) demands an effective and eco-friendly treatment. The physicochemical approaches used in the past focused on the phase transformation of the dye rather than the degradation. An effective alternative would be a nano-catalyst. However, the majority of the nano-catalysts used in the past are difficult to synthesise, inefficient, require high-energy UV rays, or a specific environment. A biogenic MnO_2 nano-catalyst would be a simple, eco-friendly, and effective method for degrading MB and H_2O_2.

Sheet-like, hydrophilic, polyhedral crystalline δ-MnO_2 NMs of average thickness, diameter, and crystallite size, 1-3 nm, 25-27 nm, and 15 nm, respectively, Ag_2O NPs (4-18 nm), and hollandite $Ag_2Mn_8O_{16}$ nanocomposite (6-24 nm) were biosynthesised from $KMnO_4$ and $AgNO_3$ as precursors and tuber extracts of solanum tuberosum containing starch as bio-reducing as well as a stabilizing agent at a temperature of 80°C.

The chemical composition of the synthesised NMs was characterised using energy-dispersive X-ray spectroscopy and Fourier transform infrared spectroscopy. At the same time, the crystalline nature and grain size of the NMs were detected using an X-ray diffraction study. The size and shape of the NMs were determined using field-emission scanning electron microscopy and high-resolution transmission electron microscopy (Karthik et al., 2024, and Vasanthavel et al., 2024).

The antimicrobial properties of the NMs were assessed using a disc diffusion assay (Bauer et al., 1966), a growth curve assay (Krishnaraj et al., 2016), and the calculation of MIC and MBC values. Disc-diffusion and growth-curve assays were conducted against *Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Enterococcus faecalis*, *Bacillus cereus*, *Vibrio cholerae*, *Streptococcus pyogenes*, and *Proteus mirabilis*. MnO_2 NPs didn't exhibit antimicrobial properties, while Ag_2O inhibited six strains, except *S. pyogenes* and *P. mirabilis*, with the highest zone of inhibition (ZOI) 5.33±0.57 mm against *S. aureus*. In contrast, $Ag_2Mn_8O_{16}$ nanocomposite inhibited all eight strains with an efficiency higher than the Ag_2O NMs and the highest ZOI 6.66±0.57 mm against *P. aeruginosa*. The MIC and MBC values were found to be 10 ng/µL for both the NM against *B. cereus*, while the MBC for Ag_2O NM was 20 ng/µL. The non-haemolytic concentrations for Ag_2O, MnO_2, and $Ag_2Mn_8O_{16}$ NMs were found to be 0.01, 1, and 0.1 µg/µL, respectively (Stumpf et al., 2016).

The MnO_2 NMs were found to be stable for 75 days at room temperature and could withstand temperatures of up to 500°C for up to 3 hours. However, at ≥ 600ºC, transformed into Mn_3O_4. The oxidative catalytic assay of the NMs demonstrated that they could effectively degrade up to 89.27% of methylene blue at pH 3 ± 0.2 in water within 55 min at a temperature of 55 °C. An electrospray ionisation mass spectrometry study was conducted to confirm the catalytic degradation of MB. The reusability test of the NM showed a loss of ~5.50% catalytic degradability after five recycles. Additionally, those NMs could decompose H_2O_2 both catalytically and electrocatalytically into H_2O and O_2. The O_2 bubbles thus generated were visible even to the naked eye. The synthesised NM could detect as low as 1 nM of H_2O_2 in water, using the naked eye through catalytic degradation-based detection.

References

1. Bauer AW, Kirby WMM, Sherris JC, et al (1966). Antibiotic susceptibility testing by a standardised single disk method. Am J Clin Pathol 45:493-496.
2. Karthik P, Jose PA, Chellakannu A, et al (2024). Green synthesis of MnO2 nanoparticles from Psidium guajava leaf extract: morphological characterisation, photocatalytic, and DNA/BSA interaction studies. Int J Biol Macromol 258:128869.
3. Krishnaraj C, Ji B-J, Harper SL, et al (2016). Plant extract-mediated biogenic synthesis of silver, manganese dioxide, silver-doped manganese dioxide nanoparticles, and their antibacterial activity against food- and water-borne pathogens. Bioprocess Biosyst Eng 39:759-772.
4. Stumpf S, Hostnik G, Primozic M, et al (2020). The effect of growth medium strength on minimum inhibitory concentrations of tannins and tannin extracts against *E. coli*. Molecules. 25:2947.
5. Vasanthavel S, Ezhilan M, Rella AK, et al (2024). Structural and morphological analysis of $ZrSiO_4$ formation induced by the simultaneous additions of cerium and manganese in ZrO_2-SiO_2 binary system. J Solid State Chem 335:124694.

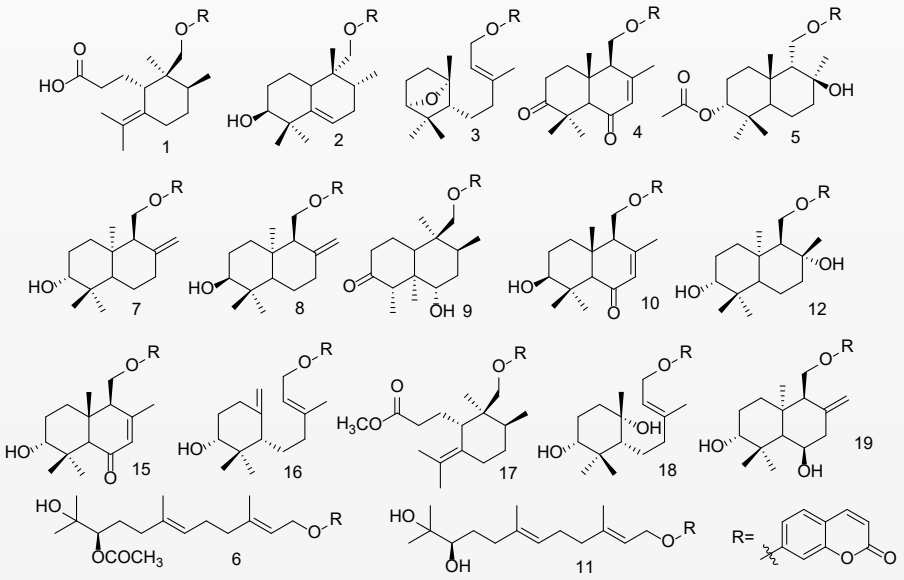
P-65

Discovery and Development of a Phytopharmaceutical Drug Candidate for Parkinson's Disease

Dr. Deepak Kumar

Senior Scientist, CSIR-Indian Institute of Chemical Biology, Kolkata
E-mail: deepak@iicb.res.in

Natural products continue to be a vital source of bioactive molecules for the development of new therapeutics. Traditional medicines have increasingly gained the attention of regulatory agencies and are now officially recognised. In alignment with Indian drug regulatory reforms, a new drug category, phytopharmaceutical drug, has been introduced to enhance the global acceptability of Indian medicinal plant–based drugs by implementing stringent guidelines. Following this framework, we successfully identified naturally occurring coumarin–terpene hybrid molecules substituted at the 7-position using a bioactivity-guided approach against the MAO enzyme from oleo-gum-resin of *Ferula assa-foetida*. This led to the identification of 19 molecules, among which two showed notably strong activity in in vitro assays. These lead molecules were isolated on a gram scale and further evaluated in both in vitro and in vivo models. This work has culminated in the development of a phytopharmaceutical candidate standardised with six constituent molecules, and additional assessments are currently underway.



References:

Banerjee C, Yatham P, Mukherjee S, Chakraborty J*, Kumar D*. Activity-guided isolation of sesquiterpene coumarins from Ferula assa-foetida as Monoamine oxidase inhibitors: Investigation on their therapeutic implications in a mice model of Parkinson's disease. J. Ethnopharmacol. 2025. 120608. https://doi.org/10.1016/j.jep.2025.120608

IL-66

Vermitechnology with special reference to vermifiltration

Dr. Aliva Patnaik

Assistant Professor
School of Life Sciences, Sambalpur University
alivapatnaik@gmail.com

Soil physical, biological and ecological properties play an important role in soil health. Soil organisms are defined as 'Organisms that spend at least part of their lifecycle in the soil or on the soil' (Hendrix, 1900). Soil fauna are categorized into four classes: microfauna (100µ-200µ), mesofauna (0.1mm-2mm), macrofauna (0.5mm-5cm), and megafauna (more than 5cm) according to their body size.

Soil biota plays a crucial role in beneficiation for the resistance and resilience of agro ecosystems against biotic disruptions and stress. As per their service fauna, especially earthworms are called as ecosystem engineers. Among the macrofauna, earthworms are the mechanical blenders as they disrupt plant materials, make the availability of organic matter to microbes, distribute fragments and bacteria-rich excreta all around as they work as homogenizers of soil strata.

Earthworms are ecologically categorized into three groups based up on their body size, colour, shape, feeding habit, and habitat: epigeic, anecic, and endogeic. Epigeic are otherwise called as soil surface dwellers. They are small, live in 0-20 cm in soil, coloured and they are the decomposers. For example *Perionyx excavates*. Anecic species such as *Octochaetina surensis*, *Lampeto marutii* live in vertical burrows at 1-2 m in soil profile. Endogeic like *Pontoscolex corethurus* live in horizontal burrows within the soil. Earthworms help in vermicomposting, vermifiltration for wastewater treatment, vermiremeadiation of contaminated soil, vermiprotection to prevent, cure diseases and protect human health and used as nutritive feed material (vermimeal) for poultry dairy and fishery industries.

Exploiting environmental conditions lead to fluctuations in temperature, moisture, and water holding capacity, that in turn make the soil impotent for growth of its biota. The regular ploughing and management practices like tillage may detrimentally affect the biomass, density and diversity of earthworms.

Dyes are coloured and aromatic compounds which are used in many industries like paper, cosmetics, textile, leather, paints etc. In recent times textile industry is rapidly advancing. The state of Odisha is famous for its "Sambalpuri Handloom" which has unique designs and patterns crafted through tie and dye technique. During the dyeing process a large amount of effluent is generated. This highly coloured, acidic effluent containing chemicals and high organic matter, suspended and dissolved solids, and heavy metals is discharged directly into the soil causing pollution and impacting the fauna of soil. The present study focused on the effect of textile dye effluent on earthworm growth, respiration, feeding and excretion. The earthworm used for the study is *Perionyx excavates* which was exposed sub lethal doses of the effluent i.e. 0% (control), 4%, 8% and 10%, above which it could not survive. The result showed significant reduction by 30th day in parameters like growth by 12.89% in 10%, 11.28% in 8% and 9.91% in 4%; feeding by 70.19% in 10%, 58.86% in 8% and 51.13% in 4% and excretion by 81.11% in 10%, 63.38% in 8% and 51.58% in 4% whereas a significant increase in respiration rate by 83.16% in 10%, 54.59% in 8% and 29.39% in 4% was seen. The increased demand for more energy for survivability and recovery of the earthworm reduced the available energy for growth and development.

ORAL

O-1

Mechanistic Insights into the Protective Role of a Novel Metallic Curcumin Complex in Acute Pancreatitis

Panchal Shital*, Singh Ekta, Kalra Amanpreet Kaur, Saini Sakshi, Gandhi Pallav

Department of Pharmacology, Institute of Pharmacy, Nirma University, S.G. Highway, Ahmedabad, 382481

Acute pancreatitis is an inflammatory disorder of the exocrine pancreas characterized by oxidative stress and systemic inflammation, often progressing to multi-organ dysfunction. Despite existing treatment options, effective prevention and complete recovery remain challenging. A novel metallic complex of Curcumin has been reported to exhibit potent antioxidant and anti-inflammatory properties, suggesting its potential as a preventive intervention. The present study aimed to evaluate the protective effects of a metallic Curcumin complex in an L-arginine-induced acute pancreatitis model in Wistar rats. Acute pancreatitis was induced by intraperitoneal administration of L-arginine (250 mg/100 g). Experimental groups were treated with the metallic Curcumin complex (25 mg/kg, p.o.), Curcumin (25 mg/kg, p.o.), or Indomethacin (10 mg/kg, p.o.) as a standard drug. Biochemical, oxidative stress, inflammatory, and histopathological parameters were evaluated at 24, 48, and 72 hours. Treatment with the metallic Curcumin complex significantly attenuated disease-associated alterations, including disturbances in physical parameters, liver enzyme markers, lipid profile, and oxidative stress indicators. Levels of pro-inflammatory cytokines were markedly reduced, and antioxidant defenses were restored. Histological analysis demonstrated reduced acinar cell degeneration, necrosis, and edema, indicating protection against pancreatic injury. The most pronounced effects were observed at 72 hours. In conclusion, the metallic Curcumin complex demonstrated significant antioxidant, anti-inflammatory, and tissue-protective properties in L-arginine-induced acute pancreatitis. These findings highlight its preventive potential in mitigating pancreatic and intestinal damage. Future investigations should focus on elucidating molecular mechanisms, optimizing dosing strategies, and assessing long-term effects in chronic pancreatitis models.

Keywords: Acute Pancreatitis, Curcumin, Metallic complex, Oxidative stress, Inflammation

O-2

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

Nandini Roy, Monika Malik, Rajeev Sakhuja and Dalip Kumar

Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, India
E-mail: p20200437@pilani.bits-pilani.ac.in

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 nuclei, 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, Topsentin 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 exposure. A series of twelve α, β-unsaturated indolyl acrylonitriles (**6a-l**) was synthesized from the reaction of 2-cyano acetyl-indoles **4** and appropriate aldehydes **5**, in good to excellent yields (79-93%). L-proline was used as a catalyst to establish a greener protocol in the synthetic procedure. Six compounds showed selective cytotoxicity (IC_{50} <10 µM) against four cancer cell lines, i.e., MDA-MB-231, PC3, C4-2, and 22Rv1.The oral presentation will include design, synthesis and anticancer activity studies of various indolyl-keto-acrylonitriles.

References:

1. Lasser, S. A.; Ozbay Kurt, F. G.; Arkhypov, I.; Utikal, J.; Umansky, V., Myeloid-derived suppressor cells in cancer and cancer therapy. Nat. Rev. Clin. 2024, 21, 147-164.
2. Dadashpour, S.; Emami, S., Indole in the target-based design of anticancer agents: A versatile scaffold with diverse mechanisms. Eur. J. Med. Chem. 2018, 150, 9-29.
3. Chen, L.; Hu, Y.; Lu, Z.; Lin, Z.; Li, L.; Wu, J.-Q.; Yu, Z.-L.; Wang, C.; Chen, W.-H.; Hu, J., Design, Synthesis, and Antitumor Efficacy of Substituted 2-Amino[1,2,4]triazolopyrimidines and Related Heterocycles as Dual Inhibitors for Microtubule Polymerization and Janus Kinase 2. J. Med. Chem 2023, 66, 15006-15024.
4. Horgan, M. J.; Zell, L.; Siewert, B.; Stuppner, H.; Schuster, D.; Temml, V., Identification of Novel β-Tubulin Inhibitors Using a Combined In Silico/In Vitro Approach. J Chem Inf Model. 2023, 63, 6396-6411.
5. Lu, Y.; Chen, J.; Xiao, M.; Li, W.; Miller, D. D., An Overview of Tubulin Inhibitors That Interact with the Colchicine Binding Site. Pharm. Res. 2012, 29, 2943-2971.
6. Roggero, C. M.; Giulietti, J. M.; Mulcahy, S. P., Efficient synthesis of eudistomin U and evaluation of its cytotoxicity. Bioorg. Med. Chem. Lett. 2014, 24, 3549-3551.

O-3

Discovery and Development of Drugs against Transplant-Associated Thrombotic Microangiopathy (TA-TMA)

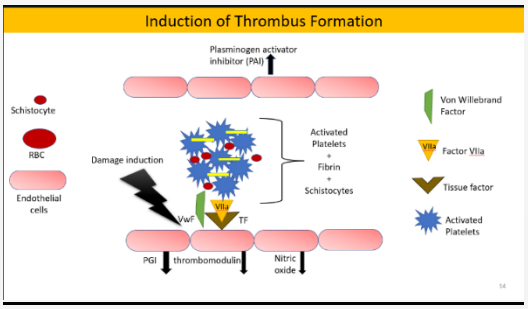
Advait P. Dubey[1,2] and Vikram Gota[1,2]*

[1]Department of Clinical Pharmacology, Advanced Centre for Treatment, Research and Education in Cancer (ACTREC), Kharghar, Navi-Mumbai – 410210
[2]Homi Bhabha National Institute, Mumbai, India

Transplant Associated thrombotic Microangiopathy (TA-TMA) is the most severe complication of Hematopoietic Stem Cell Transplant (HSCT) and is characterized by endothelial activation & dysfunction, microvascular thrombosis and end organ damage [1]. The incidence and mortality rates range from 10%-30% and 40%-90% respectively [2]. Due to the orphan status of the disease, TA-TMA lacks pharma investment resulting in lack of drugs against it. Phytochemicals can be likely drug candidates as they contain bio-actives exhibiting both anti-thrombotic and anti-inflammatory properties leading to alleviation of endothelial dysfunction and treatment of the disorder [3]. We aim to screen phytochemicals against TA-TMA models & markers to identify Hits stabilizing cascades and mitigating endothelial dysfunction.

A phytochemical library was curated by in-silico docking against 20 proteins involved in pathophysiology of TA-TMA using commercially and publicly available compound repositories constituting nearly 2500 compounds. Around 200 hits were found, out of which 52 were chosen based on their predicted ADME characteristics, for invitro screening. In-vitro screen comprised of Human Umbilical Venous Endothelial cells (HUVECs) being exposed to Cyclosporine A (CsA), a known dysfunction inducer in transplant setting. Dysregulation was confirmed with viability assays, Increase in cell surface markers like ICAM-1, VCAM-1 & E-selectin, secretory markers and oxidative stress.

During preliminary screening, out of 52, ICAM-1 expression was decreased by 8 compounds in cotreatment intervention. More stringent invitro screens would be set up against Oxidative stress and membrane damage alleviation. Based on readouts hits would be identified, further proceeding to organ on chip and in-vivo models for selection of robust Drug candidate.



References:

1. Lazana , "Transplant-Associated Thrombotic Microangiopathy in the context of allogenic Hematopoietic Stem cell Transplantation: Where we Stand," *International Journal of Molecular Sciences* , 2023.
2. S. Punatar and N. Khattry, "Pre-transplant use of tyrosine kinase inhibitors and transplant associated thrombotic microangiopathy - a single centre analysis of incidence, risk factors and outcomes," *Bone Marrow Transplantation,* 2021.
3. P. Chihomvu, A. Ganesan and M. A. Hayes , "Phytochemicals in Drug Discovery - A Confluence of Tradition and Innovation," *International journal of Molecular Sciences,* 2024.

O-4

Discovery of promising metabolic pathway targets and essential oil phytochemicals against *Mycobacterium sp.*

Ashutosh Sahoo[1], Shagun Shagun[1], Nidhi Yadav[2], Rithika Pai[1#], Amay Sandilya[1#], Ranjan Kumar Nanda[2*], Shyam K. Masakapalli*[1]

[1] Metabolic Systems Biology Lab, School of Biosciences and Bioengineering, Indian Institute of Technology Mandi, Kamand 175075, Himachal Pradesh, India
[2] Translational Health Group, International Centre for Genetic Engineering and Biotechnology, New Delhi, 110067, India
 # Interns at MSBL
**Corresponding author email – shyam@iitmandi.ac.in*
Presenter email – ashutosh.msbl.iitmandi@gmail.com

Abstract

The emergence of multidrug-resistant *Mycobacterium tuberculosis* (MDR-Mtb) poses a major challenge to global tuberculosis control, underscoring the urgent need for novel drug targets and alternative therapeutic strategies. This study employed comparative genome and metabolic pathway analyses of six clinical MDR-Mtb strains from North-East India, alongside twenty reference strains representing diverse Mtb lineages, to identify conserved metabolic vulnerabilities suitable for drug discovery. Single nucleotide polymorphism (SNP)-based conservation analyses were carried for validation of the targets across the MDR strains. The study identified the methylerythritol phosphate (MEP) and biofilm biosynthesis pathways as conserved and could be promising drug targets across Mtb lineages.

Further, selected Essential oils (EOs) catalogued in an inhouse repository of Himalayan Medicinal & Aromatic Plant and Phytochemical (HMAP²) database were screened against *Mycobacterium smegmatis* to assess antimycobacterial and antibiofilm activities. Phytochemical profiling using GC-MS and NMR ($^{1}H/^{13}C$) was carried as well as ADMET properties of the identified small molecules were predicted. Among the tested oils, *Trachyspermum ammi* (Ajowan) oil demonstrated potent antimycobacterial and biofilm inhibitory activity, highlighting its phytochemicals as promising candidates for anti-Mycobcaterial drug development. Ongoing efforts focus on isolating and characterizing the active components and assessing their effects on MDR-Mtb strains to advance lead optimization for therapeutic applications.

Keywords: Comparative genome analysis, Metabolic pathway comparison, Anti-mycobacterial, Antibiofilm, Essential oils, Phytochemicals, Drug discovery, HAMP² Database

References:

1. Sahoo, A., Mohapatra, A. K., Priyadarsini, H., Pemmadi, R. V., Das, A., Choedon, T., Nikam, C., Behera, R. K., Masakapalli, S. K., & Nanda, R. K. (2022). Whole genome sequencing and global metabolome profiling of clinical Mycobacterium tuberculosis isolates provide insights to their drug resistance status. *MedRxiv*, 2022.09.30.22279918. https://doi.org/10.1101/2022.09.30.22279918 (Currently under review)

O-5

LMTK3 as a regulator of TRAIL-induced apoptosis in breast cancer: Mechanistic insights

Siri Chandana Gampa* and Sireesha V Garimella**

Department of Life Sciences, School of Science, GITAM (Deemed to be University), Visakhapatnam, Andhra Pradesh, India
***Corresponding author: Dr Sireesha V Garimella, email: sgarimel@gitam.edu*
**Presenting author: Siri Chandana Gampa, email: sgampa@gitam.in*
Choice of Mode: Podium

Tumor Necrosis Factor-Related Apoptosis-Inducing Ligand also called Apo-2 Ligand (TRAIL/Apo-2L) is a cytokine that selectively triggers apoptosis in cancer cells by binding to TRAIL-R1 (DR4) and TRAIL-R2 (DR5) receptors. Administration of recombinant human TRAIL (rhTRAIL) or TRAIL-receptor (TRAIL-R) agonists promotes apoptosis preferentially in cancerous cells over normal cells. However, its application in the clinic is limited due to the negative regulation of the TRAIL pathway by several intracellular molecules. In this study, we investigate the role of Lemur Tail Kinase 3 (LMTK3) in the regulation of TRAIL pathway. Knockdown with gene-specific siRNA or inhibition of LMTK3 with a small molecule inhibitor, C28, decreased the viability of MCF7 cells in the presence of TRAIL (55.4%±2.2) compared to the control (93.7%±8.9). Inhibition of LMTK3 alone increased cell death, decreased cell migration and caused cell cycle arrest in G2/M phase in breast cancer cells. Enhanced apoptosis in MCF7 cells by C28 and TRAIL could be attributed to the elevated expression of death receptors, which was observed to be significantly upregulated in LMTK3-inhibited cells. Studies pertaining to the regulation of death receptors in LMTK3-inhibited cells is further being explored.

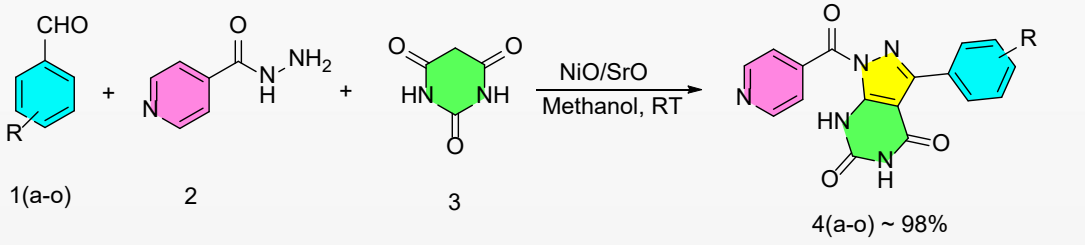
MOF-Derived NiO/SrO Nanocatalyst Enabled Multicomponent Synthesis of Novel AIPDs with Promising Anticancer Potential

Mueataz G. Thabet, Ashlesha Jadhav, Giribala M. Bondle*

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University Chhatrapati Sambhaji Nagar-Maharashtra, 431004, India.
Email: gmbondle@gmail.com

Abstract

A sustainable nanocatalyst approach was developed for the efficient synthesis of aryl-isonicotinoyl-pyrazolopyrimidine-dione (AIPD) derivatives using a MOF-derived NiO/SrO (75:25 wt%) nanocomposite. The catalyst achieved up to 98% yield within 60 minutes under mild conditions and was recyclable for multiple cycles without loss of activity. Structural characterization confirmed its crystalline and hierarchical morphology, enhancing catalytic performance. Density Functional Theory (DFT) and molecular docking studies revealed compound 4i as a potent binder to the cancer target 5IVE (−10.4 kcal/mol) and compound 4m as highly reactive (ΔE = 0.104 Hartree). ADMET analysis indicated favorable pharmacokinetics, and in vitro studies against HeLa cells showed significant cytotoxicity (IC50 = 94.5 µg/mL). This work demonstrates how integrating nanocatalysis, synthetic methodology, computational modeling, and biological screening can accelerate the development of new anticancer scaffolds.



Keywords: NiO/SrO Nanocomposite, Molecular Docking, DFT, ADMET Profiling, HeLa Cell Line

References

1. A.V. Sadybekov, V. Katritch, Computational approaches streamlining drug discovery, Nature 2023, 616 .
2. D.C. Onwudiwe, N.H. Seheri, L. Hlungwani, H. Ferjani, R. Rikhotso-Mbungela, NiO nanoparticles by thermal decomposition of complex and evaluation of the structural, morphological, and optical properties, J. Mol. Struct.,2024.
3. A.K. Shimi, C. Parvathiraj, S. Kumari, J. Dalal, V. Kumar, S.M. Wabaidur, Z. Alothman, Green synthesis of SrO nanoparticles using leaf extract of Albizia julibrissin and its recyclable photocatalytic activity: an eco-friendly approach for treatment of industrial wastewater, Environ. Sci.*: Adv.* 1, 2022.
4. Z. Yang, Z.Y. Liu, M. Ablise, A. Maimaiti, Z. Mutalipu, Y. Alimujiang, A. Aihaiti, Design, synthesis, and anti-cervical cancer and reversal of tumor multidrug resistance activity of novel nitrogen-containing heterocyclic chalcone derivatives, Molecule*s* 28, 2023.

O-7

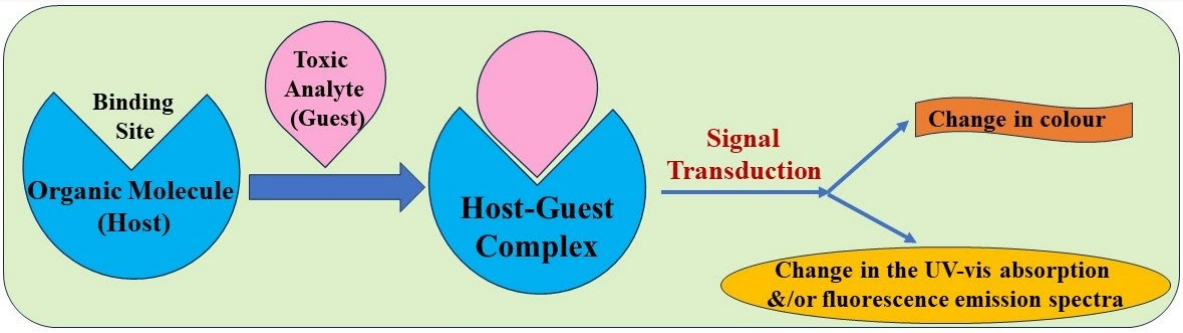
Organic framework-based sensors for environment and chemical security

Dr. Ishanki Bhardwaj

Department of Chemistry, Sir PT Sarvajanik College of Science, MTB College Campus, Jawaharlal Nehru Marg, Opp. Chaupati, Athwalines, Surat-395001, Gujarat, India.
ib@ptscience.ac.in

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) as well as environmental pollution such as phosphate, Hg^{2+}, Pb^{2+} Zn^{2+} and Cd^{2+} with high sensitivity. In addition to this, they are also employed for sensing toxic molecules. Supramolecular forces play an important role behind the sensing procedure which include electrostatic interactions, hydrogen bonding and inter-molecular interactions. "Supramolecular Complexes" are formed during the process which is observed in the form of change in excitation and/or emission spectra of the sensor. The changes are measured with the aid of different spectroscopic techniques. Supramolecular complexes can be regarded as "Host-Guest" complexes, the "sensor" acting as "Host" and the "toxic analyte" acting as the "Guest". The organic frameworks are designed in such a way that they contain the necessary sensing/signalling/recognising moiety in their chemical structure which can bind to the target.



References:

1. Butera, E.; Zammataro, A.; Pappalardo, A.; Trusso Sfrazzetto, G. Supramolecular Sensing of Chemical Warfare Agents, *ChemPlusChem* 2021, 86, 681.
2. Zheng, Q.; Fu, Y.; Xu, J. Advances in the chemical sensors for the detection of DMMP- A simulant for nerve agent sarin, *Procedia Engineering* 2010, 7, 179-184.
3. **Kumar, V.** Chromo-fluorogenic sensors for chemical warfare agents in real-time analysis: journey towards accurate detection and differentiation, ***Chem. Commun.*** 2021,**57**, 3430-3444.
4. Sekhar, P. K.; Brosha, E. L.; Mukundan, R.; Garzon, F. Chemical Sensors for Environmental Monitoring and Homeland Security, *Electrochem. Soc. Interface* 2010, 19, 35.
5. Bhardwaj, I. Design and Synthesis of Disulfide-based Macrocycles and their Heavy Metal Ion Complexation and Self-assembly Studies, *Ind J Adv Chem Sci*, 2023, 11 (2), 97-101.

O-8

Protective Role of Quercetin Nano-suspension Delivered via Inhalation in Experimental Pulmonary Fibrosis

Shital Butani, Nikita Gupta, Mitali Paryani, Srashti Verma, and Snehal Patel

Department of Pharmaceutics, Institute of Pharmacy, Nirma University, Gujarat, 382481, India,
shital.butani@nirmauni.ac.in

Background:

Pulmonary fibrosis (PF) is a progressive, irreversible, and life-threatening interstitial lung disease characterized by excessive fibrotic remodeling and loss of lung elasticity. Currently available therapeutic options are limited, with oral formulations showing restricted efficacy and significant adverse effects. Quercetin, a plant-derived flavonoid, possesses anti-inflammatory, anti-fibrotic, and mast cell-stabilizing properties, making it a promising candidate for pulmonary fibrosis therapy.

Objective: The present study aimed to develop and evaluate an inhalable quercetin dihydrate nano-suspension (QD-NS) as a targeted pulmonary delivery system to enhance therapeutic efficacy and reduce systemic side effects in silica-induced pulmonary fibrosis in rats.

Methods: QD-NS was prepared using a top-down approach involving high-pressure homogenization. The formulation parameters, including stabilizer type, homogenization pressure, and number of cycles, were optimized. The developed nano-suspension was characterized for particle size analysis (PSA), FTIR, DSC, P-XRD, TEM, osmolarity, in vitro drug release, and stability. Aerosolization and aerodynamic properties were assessed, and pharmacodynamic studies were conducted in silica-induced pulmonary fibrosis rat models.

Results: The optimized QD-NS exhibited a fine particle fraction of 69.07 ± 0.135%**,** confirming efficient aerosol deposition in the lower respiratory tract. The formulation demonstrated sustained drug release and remained stable under refrigerated conditions (2–8°C). Pharmacodynamic evaluation revealed that inhaled QD-NS significantly reduced levels of TGF-β, LDH, and ALP, and decreased infiltration of inflammatory cells (lymphocytes, granulocytes, monocytes, leukocytes, and eosinophils) compared to the silica-induced disease control group. Moreover, inhalation therapy showed superior therapeutic efficacy over oral administration, indicating improved local targeting and bioavailability.

Conclusion: The inhalable quercetin dihydrate nano-suspension (QD-NS) represents a promising and effective pulmonary delivery approach for the management of silica-induced pulmonary fibrosis. The formulation enhances drug deposition, reduces inflammatory and fibrotic markers, and demonstrates improved therapeutic performance compared to oral delivery.

References:

1. Feng, F., Cheng, P., Xu, S., Li, N., Wang, H., Zhang, Y. and Wang, W., 2020. Tanshinone IIA attenuates silica-induced pulmonary fibrosis via Nrf2-mediated inhibition of EMT and TGF-β1/Smad signaling. Chemico-Biological Interactions, 319, p.109024.
2. Gupta N, Paryani M, Patel S, Bariya A, Srivastava A, Pathak Y, Butani S. *Therapeutic Strategies for Idiopathic Pulmonary Fibrosis – Thriving Present and Promising Tomorrow.* J Clin Pharmacol. 2024 Jul;64(7):779-798. DOI: 10.1002/jcph.2408

O-9

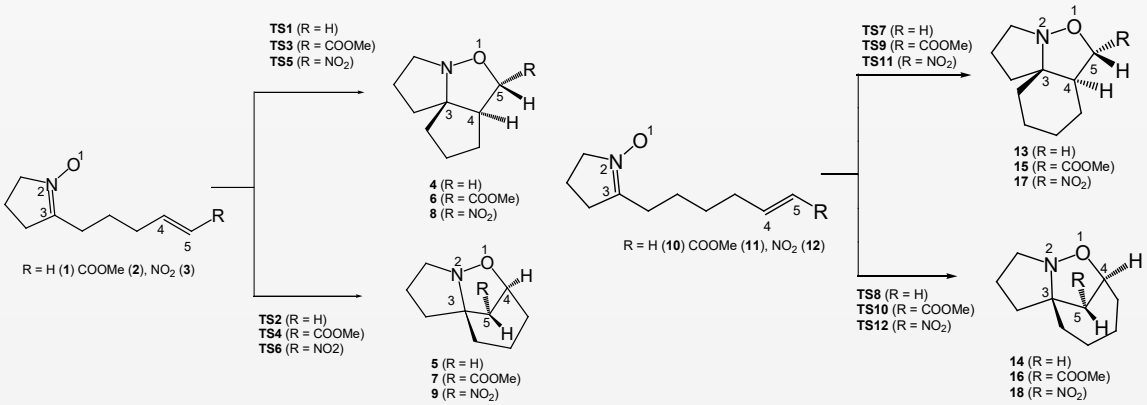
Understanding the Tether Length Effects on Nitrone Intramolecular [3+2] Cycloadditions: Insights from Molecular Electron Density Theory (MEDT)

Nivedita Acharjee[1]*, Luis R Domingo,[2] Asmita Mondal[1]

[1]*Department of Chemistry, Durgapur Government College, Durgapur-713214, West Bengal, India.*
[2]*Department of Organic Chemistry, University of Valencia, Dr. Moliner 50, Burjassot, 46100 Valencia, Spain*

Abstract

The impact of ethylene substitution and tether length between the reacting centers on the selectivity and reactivity of intramolecular [3+2] cycloaddition (IM32CA) reactions of cyclic nitrones leading to tricyclic isoxazolidines has been examined within the Molecular Electron Density Theory (MEDT) framework at the MPWB1K/6-311G(d,p) level of theory. These *zw*-type IM32CA reactions proceed via a one-step mechanism, with activation barriers lowered by the introduction of electron-withdrawing (EW) substituents at the alkene unit in both intra- and intermolecular cases. Reactions involving unsubstituted alkenes display a non-polar character with negligible electron density transfer, consistent with the null electron density flux (NEDF) type, while those involving nitro-substituted alkenes are significantly more favourable, characterized by strong forward electron density flux (FEDF) from the nitrone to the alkene. Increasing polarity reduces the activation Gibbs free energies in intramolecular reactions, though highly polar IM32CA processes are less favored compared to their intermolecular counterparts. Notably, regioselectivity trends shift: low-polar IM32CA reactions with three methylene units between the nitrone and alkene frameworks show opposite preferences compared to those with four methylene units, consistent with experimental observations. Furthermore, electron localization function (ELF) and quantum theory of atoms in molecules (QTAIM) analyses confirm that these IM32CA reactions generally proceed through early transition states in which the formation of new C–C and C–O bonds has not yet commenced.



Scheme 1. Studied reaction paths for the IM32CA reactions of nitrones **1-3** and **10-12.**

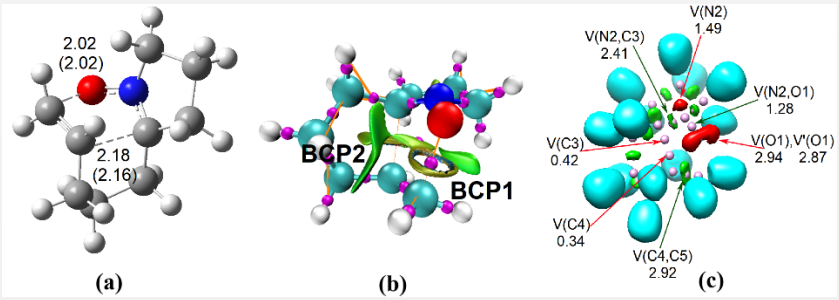


Figure 1. (a) MPWB1K/6-311G(d,p) optimized geometry, **(b)** NCI isosurface, and **(c)** ELF domain of **TS1.**

O-10

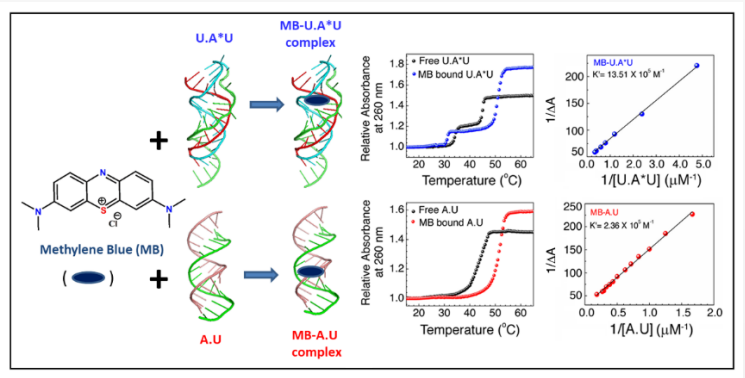
Insights into the Binding of Phenothiazinium Dye Methylene Blue with Triple and Double Helical Forms of RNA: A Multispectroscopic Approach

Rapti Goswami, Lopa Paul, Himal Das, Amar Ghosh, Susmita Chowdhury and Suman Das*

Biophysical Chemistry Laboratory, Physical Chemistry Section, Department of Chemistry, Jadavpur University, Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, India
E-mail: raptirai6@gmail.com
Choice of mode: Oral (podium)

Abstract:

In recent times, higher-ordered nucleic acid structures like triplex, quadruplex forms are relevant in the current research field of medicinal chemistry. In this study, we have focused on RNA triplex, (U.A*U) because of its various biological significance including telomerase activity, movement of ribosomal template in mRNA coding regions, etc. [1, 2]. Methylene Blue (MB), a cationic dye of phenothiazine families, exerts diverse pharmacological and clinical applications [3]. Considering the wide range of medicinal usages of MB and the biological importance of higher-ordered structures of RNA, our present study has focused on the elucidation of the comparative binding interaction of Methylene Blue (MB) with RNA triplex (U.A*U) and duplex (A.U) structures employing various spectroscopic tools. MB has been found to show comparably greater binding affinity towards the triplex form than the parent duplex form. The thermal melting profile revealed that MB substantially stabilized the Watson-Crick base-paired strands of both the RNA triplex and duplex structures; however, it destabilized the Hoogsteen base-paired strand of triple helical RNA. Fluorescence quenching, steady-state anisotropy, and circular dichroic studies all together supported intercalative mode of binding. Thermodynamic data revealed that the interactions of MB with both RNA triplex and duplex forms were characterized by both negative enthalpy and entropy changes. Ionic strength-dependent study showed that the non-polyelectrolytic forces are the predominating factors in the binding process although a minor but certain extent of polyelectrolytic contribution is present [4].



References:

1. G Felsenfeld, D R Davies and A Rich, J. Am. Chem. Soc. 79, 1957, 2023.
2. S Bhuiya, L Haque, R Goswami and S Das, J Phys Chem B 121, 2017, 11037.
3. P O Vardevanyan, A P Antonyan, M A Parsadanyan, M A Shahinyan and N H Petrosyan, J. Biomol Struct Dyn. 40, 2022, 7779.
4. R Goswami, L Paul, H Das, A Ghosh, S Chowdhury and S Das, J Phys Chem B 129, 2025, 9068.

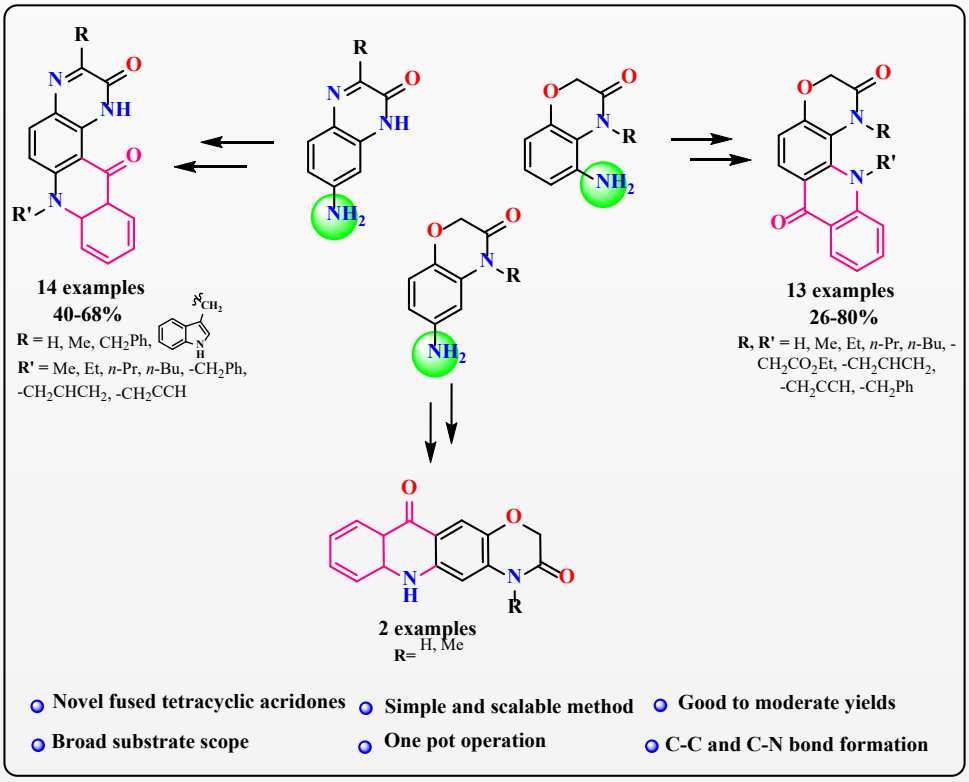
O-11

Synthesis of novel analogues of fused angular and linear π-extension of Acridones from quinoxalinones and benzoxazinones

Apeksha H. Naik and Dr. Bidhan A. Shinkre*

School of Chemical Sciences, Goa University, Taleigao Plateau, Goa, 403206
chem.apeksha@unigoa.ac.in

Polycyclic fused heterocycles such as acridones/acridines have been studied extensively for their application as anti-cancer agents. We herein report an efficient diphenyliodonium-2-carboxylate (DPIC) assisted copper catalysed cyclization of substituted quinoxalinones and benzoxazinones to a variety of tetra substituted acridones. This one pot reaction proceeds through C-N bond formation followed by acid mediated intramolecular cyclization/dehydration sequence leading to formation of novel acridone derivatives in good to moderate yields. To combat the issue of drug resistance to the diseases in humans, the angular and linear acridones have the potential to serve as new pharmaceutical agents due to their unique structural features enabling quick SAR expansion of the tetracyclic core. The biological activities of the novel targets is currently being pursued.



References

1. Chen, C. H.; Lin, Y. W.; Kakadiya, R.; Kumar, A.; Chen, Y. T.; Lee, T. C.; Su, T. L.,*Tetrahedron,* **2011**, *67* (33), 5883–5893.
2. Yadav, T. T.; Murahari, M.; Peters, G. J.; YC, M.,*Eur. J. of Med. Chem.*, **2022**, 114527
3. Gao, C.; Jiang, Y.; Tan, C.; Zu, X.; Liu, H.; Cao, D., *Bioorg Med Chem,* **2008**, *16* (18), 8670–8675.

O-12

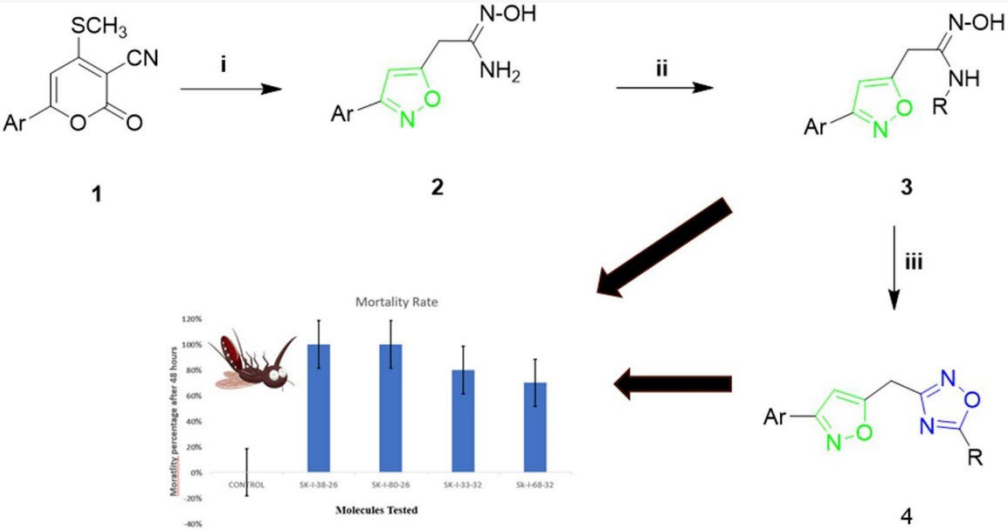
Synthesis, characterization, and Mosquiticidal Studies of Isoxazole-oxadiazole analogs

Shivam Kumar, Ashoke Sharon*

Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, 835215
Email: asharon@bitmesra.ac.in

Five-membered heterocycles, such as isoxazoles and oxadiazoles, are well known for their wide range of biological activity in agrochemical and medical research. These scaffolds are useful because they have been shown to have antiviral, anticancer, antibacterial, anti-inflammatory, insecticide, and mosquitocidal properties. Based on binding affinity and protein stability, twenty candidate compounds were selected for synthesis using in silico screening and molecular dynamics simulations on the acetylcholinesterase protein. DFT calculations for the HOMO-LUMO gap and ESP were used for the stability of the compounds. Mild bases were used to synthesise the target isoxazole–1,2,4-oxadiazole analogues under reflux conditions in ethanol at 80 °C, utilizing both traditional heating and microwave irradiation techniques. Four analogues with notable mosquitocidal activity were found during the biological assessment of the target compounds, indicating that they may serve as primary leads for the development of novel mosquitocidal.

Keywords: Isoxazole-Oxadiazole, Molecular Dynamics, mosquitocidal, acetylcholinesterase



O-13

"Synthetic Strategies for Adenine-Derived Acyclic Nucleoside Phosphonates: Toward Greener and Scalable Manufacturing Solutions"

Amit Kisan Bhosale[1]* Dr Mayank Pandya[2]

Centre for research and development, Dr. Subhash University, Junagadh (362001), Gujarat, India.

Abstract

Adenine derivatives bearing acyclic nucleoside phosphonates (ANPs) represent a critical class of antiviral agents with demonstrated efficacy against a range of viral infections, including cytomegalovirus (CMV), HIV and hepatitis B (HBV). Clinically approved drugs such as adefovir and tenofovir, along with advanced clinical candidates like GS-9148, GS-0840, GS-9131, GS-0577 and GS-7340, exemplify the therapeutic potential of this scaffold. These compounds typically consist of an adenine nucleobase connected to a phosphonate side chain, with structure–activity relationship (SAR) studies guiding extensive modifications to enhance potency, selectivity, and pharmacokinetics.

This review provides a comprehensive summary of the synthetic strategies employed in the development of ANP-based analogues, highlighting opportunities for improvement in terms of reagent selection, reaction conditions, and cost-effectiveness. Emphasis is placed on optimizing synthetic routes to minimize waste, reduce environmental impact, and improve overall yield. Traditional batch manufacturing processes, currently used by most pharmaceutical producers, are associated with several drawbacks, including high energy consumption, generation of hazardous waste, and limited scalability.

To address these limitations, the adoption of continuous flow manufacturing is explored as a transformative alternative. This advanced approach offers several advantages—such as enhanced reaction control, reduced production costs, and improved safety—making it highly suitable for the sustainable and efficient synthesis of adenine phosphonate analogues. By integrating modern process technologies with innovative chemistry, continuous flow methods hold great promise for the future of large-scale antiviral drug production.

Keywords: Adenine derivatives, Acyclic nucleoside phosphonates (ANPs), Antiviral agents, Tenofovir, Adefovir, Phosphonate side chain, Synthetic strategies, Analog development, Reagent selection, Reaction conditions, market study, Process innovation, Flow chemistry, Large-scale production, pharmaceutical manufacturing, Advanced manufacturing technologies

References

1. Development and Clinical Application of Phosphorus-Containing Drugs:Medicine in Drug Discovery 8 (2020) 100063
2. Karaman R. Prodrugs Design: A New Era (Pharmacology- Research, Safety Testing and Reaction). 1th ed.. Nova Biomedical, New York: Nova Science Publisher, Inc; 2014;112–5 ISBN: 9781631177019
3. Schwolow, S.; Neumuller, A.; Abahmane, L.; Kockmann, N.; Roder, T. Design and application of a millistructured heat exchanger reactor for an energy-efficient process. Chem. Eng. Process. 2016, 108, 109−116.
4. Schwolow, S.; Hollmann, J.; Schenkel, B.; Roder, T. Application oriented analysis of mixing performance in microreactors. Org. Process Res. Dev. 2012, 16, 1513−1522.
5. Reckamp, J. M.; Bindels, A.; Duffield, S.; Liu, Y. C.; Bradford, E.; Ricci, E.; Susanne, F.; Rutter, A. Mixing Performance Evaluation for Commercially Available Micromixers Using Villermaux−Dushman Reaction Scheme with the Interaction by Exchange with the Mean Model. Org. Process Res. Dev. 2017, 21, 816−820
6. REVIEW article Front. Chem., 20 May 2022 Sec. Medicinal and Pharmaceutical Chemistry Volume 10 - 2022 | https://doi.org/10.3389/fchem.2022.889737
7. Bronson, J.J.; Kim, C.U.; Ghazzouli, I.; Hitchcock, M.J.M.; Kern, E.; Martin, J.C. In Nucleotides as Antiviral Agents, Martin, J.C., Ed, American Chemical Society, Washington DC, 1989, pp. 72-87.
8. Balzarini, J.; Naesens. L.; Slachmuylders, J.; Niphius, H.; Rosenberg, I.; Holy, A.; Schellenkens, H.; De Clercq, E. AIDS, 1991, 5, 21.
9. De Clercq, E.; Holy, A.; Rosenberg, I. Antimicrob. Agents Chemother., 1989, 33, 185
10. Egerbrink, A.; Borst, M.; Niphuis, H.; Balzarini, J.; Neu, H.; Schellenkens, H.; De Clercq, E.; Horzinek, M.; Koolen, M. Proc. Natl. Acad. Sci. USA, 1990, 87, 3087.
11. Bronson, J.J.; Ghazzouli, I.; Hitchcock, M.J.M.; Russell, J.W.; Klunk, L.J.; Kern, E.; Martin, J.C. 1989, 5th International Conference on AIDS, Abstract No. M.C.P. 74, Montreal, Canada.
12. Shen, Y.; Zhukovskaya, N.L.; Zimmer, M.I.; Soelaiman, S.; Bergson, P.; Wang, C-R.; Gibbs, C.S.; Tang, W-J. PNAS, 2004, 101, 3242.

O-14

ORGANIC FARMING FOR SUSTAINABLE AGRICULTURE: A REVIEW

Dr Sibangini Misra

Lecturer in Botany
Maharishi College of Natural Law, Bhubaneswar
EMAIL: loni.misra@gmail.com

Abstract:

Organic farming is an agricultural production system that avoid synthetic inputs like pesticides and fertilizers instead relying on methods such as crop rotation, animal manure and biological systems to maintain soil health and manage pests. Organic farming reduces the risk of adverse environmental effects compared to conventional farming methods; in terms of soil fertility and nutrient management. Comparative studies on biodiversity demonstrate that organic farming has a greater impact on biodiversity preservation. Sustainable agriculture development through organic farming not only provides food requirements for the current creation in an environmentally friendly way manner also provides food for prospective generations and controls our surroundings. Modern agriculture, which involves the use of pesticides and fertilizers, harms the environment by affecting soil fertility, water hardness, the development of insect resistance, and an increase in toxic residue through the food chain and animal feed, resulting in increased health problems, and many other serious health concerns and environmental degradation. Organic farming is one of the most widely used methods, and is regarded as the best alternative to avoiding the negative effects of chemical farming. It also has far more benefits than conventional and other modern agricultural practices. In conclusion, organic farming emerges as an environmentally friendly and economically viable alternative to conventional agriculture. By promoting soil health, reducing chemical residues in food, and meeting consumer demand for nutritious products, organic farming offers a pathway towards sustainable agricultural practices. The objective of this review paper is to identify synthetic fertilizers and pesticides that can be replaced with natural alternatives as well as to examine how organic farming might promote sustainability in agriculture.

Keywords: Conventional farming, soil health, food safety, organic farming, sustainable agriculture

O-15

Targeted Phytochemical Investigation of *Calamus leptospadix* Griff.

Dwipen Kakati,* Utpal Dutta

Department of Chemistry, Rajiv Gandhi University, Rono Hills, Doimukh, Arunachal Pradesh-791112, INDIA
E-mail: dwipen.kakati@rgu.ac.in

Plant-derived natural products have long been recognised as a rich source of bioactive molecules for drug discovery. Arunachal Pradesh, the largest state in Northeast India, is situated in the Eastern Himalayas, a biodiversity hotspot harbouring approximately 5,800 plant species, of which nearly 2,000 are endemic.[1] *Calamus leptospadix* Griff., a member of the genus *Calamus*- the largest genus of rattans with around 370 species in the family Arecaceae and subfamily Calamoideae- is native to India (Assam and the Indian Eastern Himalayas), Bangladesh, Myanmar and Nepal. Locally, *C. leptospadix* is known as "lejaibet" in Assam and "jeying" in East Siang, Arunachal Pradesh, where its tender shoots are consumed as vegetables. Previous studies have reported that extracts from the shoots of *C. leptospadix* possess antimicrobial, antioxidant, anthelmintic and antidiabetic activities.[2]

In this study, tender shoots of *C. leptospadix* were extracted using methanol, water and ethanol to investigate the effects of solvent type and extraction temperature on antioxidant, antidiabetic, and antibacterial activities, as well as total phenolic and flavonoid contents. A flavan-type compound was subsequently isolated from the most bioactive cold methanolic extract and fully characterised.

REFERENCES

1. P S Roy and M D Behera, Current Science 88, 2005, 250.
2. B Borah, P Phukon, M P Hazarika, R Ahmed, D K Sarmah, S B Wann, A Das and B S Bhau, Industrial Crops and Products 82, 2016,127.

O-16

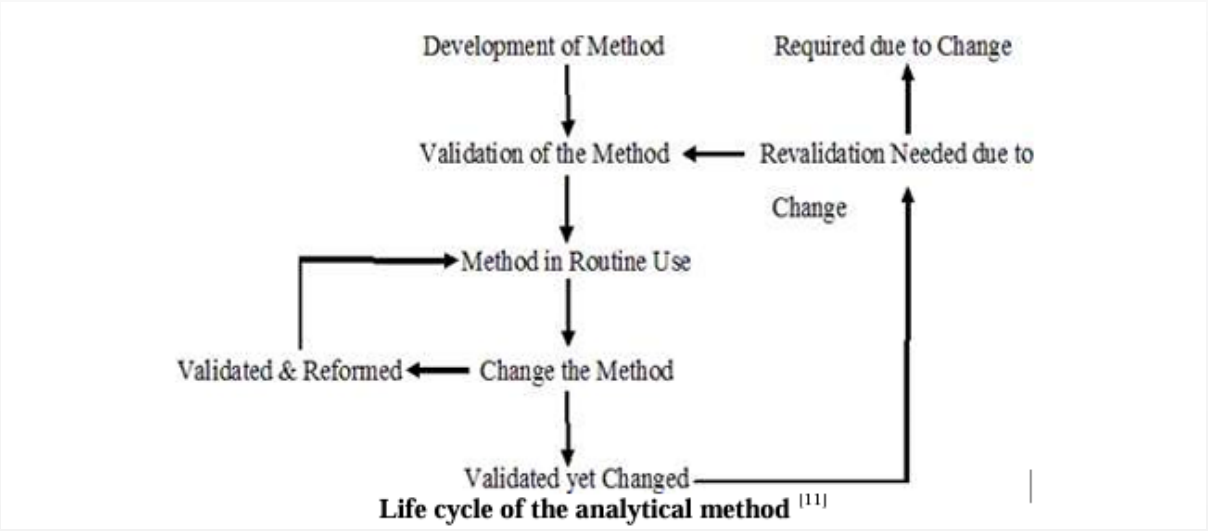
Chromatographic Method Development, Validation and Analytical Studies of Ceftazidime and Avibactam in its Bulk and Pharmaceutical Formulation.

Hitesh Tank*[1], Dr. Mayank Pandya[1]

[1] *Department of Chemistry, School of Science, Dr. Subhash University, Junagadh (362001), Gujarat, India.*
Email: hiteshtank091@gmail.com

Abstract

A simple, precise, accurate and robust method of Ceftazidime and Avibactam was developed and validated, including the separation, identification and quantification of said analytes from its bulk and pharmaceutical formulation. The method was developed and validated as per ICH guidelines. The method employed a Shim-pack GIST C18 (250 × 4.6 mm, 5.0 µm) column as a stationary phase, and the mobile phase consisted ratio of buffer: Acetonitrile (90:10) v/v buffer solution prepared of 2.75 gm potassium dihydrogen orthophosphate, adjusted pH 4.0 with diluted o-phosphoric acid . The flow rate of mobile phase was set at 1.0 mL/minute, chromatographic analysis of drug and degradation products were carried out through PDA detector in the absorbance mode at 230 nm, respectively. The Avibactam drug was found at retention time at 4.0 minutes and the Ceftazidime drug was found at retention time 7.8 minute on the chromatogram with the working concentration range of 250-500 µg/mL. The linear regression analysis data for the calibration plot showed a good linear relationship with R^2- 0.9982. The method was validated for its linearity, accuracy, precision, robustness, limit of detection, and limit of quantification. At last, the method was employed to analyse pharmaceutical formulations of the said APIs and found successful in the detection for the same.



Life cycle of the analytical method [11]

Keywords: Development, Validation, Ceftazidime, Avibactam, chromatography

O-17

Valorization of Food Bioprocess Waste for Production of Prebiotic Oligosaccharides

Rohit Maurya, Koushik Mazumder*

Department Food and nutrition Biotechnology, BRIC-National Agri-Food Biomanufacturing Institute Mohali sector, Institute

The valorization of food bioprocess waste offers a ssustainable opportunity to generate high-value functional ingredients while reducing environmental burden. This study focuses on converting diverse agro-industrial residues including amla waste, Aloevera peel, Tomato waste, and potato peel into prebiotic oligosaccharides through integrated bioprocessing. Pectin extracted from fruit wastes was subjected to chemo-enzymatic hydrolysis using magnetic nanoparticle-immobilized pectinase, optimized via Response Surface Methodology (RSM) to produce pectic oligosaccharides (POS). Structural characterization by GC–MS, MALDI-TOF, NMR, and HPAEC-PAD confirmed the formation of bioactive low-molecular-weight POS with strong prebiotic potential. Simultaneously, potato peel starch was valorized for isomaltooligosaccharides (IMOs) production through liquefaction, saccharification, and transglucosylation. The α-transglucosidase gene from *Aspergillus niger* (GH31) was cloned into *E. coli* BL21 (DE3), overexpressed, purified, and immobilized on magnetic nanoparticles, enhancing its operational stability and enabling reuse for up to five cycles while retaining >60% activity. Enzyme immobilization was confirmed through FTIR, TEM, FE-SEM, EDX, XRD, TGA, and DLS analyses. RSM-optimized reaction conditions (enzyme–substrate ratio 6.9 U g^{-1}, pH 5.5, 45 °C, 9 h) yielded 70 g L^{-1} IMO, with MALDI-TOF–MS confirming DP 2–10 and GC–MS/NMR indicating α-(1→4), α-(1→6), and minor α-(1→2)/(1→3) linkages. Both POS and IMOs significantly enhanced the growth of *Lactobacillus* and *Bifidobacterium* spp., demonstrating strong prebiotic functionality. This work establishes a scalable waste-to-wealth bioprocess for producing prebiotic oligosaccharides, supporting circular bioeconomy principles and enabling future applications in functional foods and nutraceuticals.

Keywords:- Pectic oligosaccharides (POS), Bioprocess waste, Isomaltooligosaccharides (IMOs), Magnetic nanoparticles

O-18

Caffeic acid O-methyltransferases (COMTs) from *Eleusine coracana*: A key melatonin biosynthetic enzyme confers salinity and drought stress tolerance

Vikash Kumar[1], Mohini Yadav[1], Prafull Salvi[#] and Saurabh C. Saxena[1*]

[1]Department of Biochemistry, Central University of Haryana, Mahendergarh, Haryana-123031, India
[2]BRIC-National Agri-Food and Biomanufacturing Institute, Sector 81, Sahibzada Ajit Singh Nagar, Punjab 140308
**Email: saurabhcs@cuh.ac.in (Presenter)*

ABSTRACT

Abiotic stresses, such as salinity, drought, and extreme temperatures, impose significant constraints on crop productivity. These stresses initiate a series of physiological, biochemical, and molecular reactions in plants, resulting in poor yields and diminished crop quality. Caffeic acid O-methyltransferase (COMT) plays an important role in plants by methylating caffeic acid, which is crucial for lignin biosynthesis. Additionally, COMT contributes to melatonin biosynthesis by methylating N-acetylserotonin. In turn, melatonin enhances antioxidants in plants, thereby enhancing abiotic stress tolerance in plants. In this study, we investigated the function and regulation of COMT genes in the C4 plant *Eleusine coracana* under abiotic stress conditions. We performed a genome-wide analysis of the COMT gene family in *E. coracana*, focusing on genetic diversity, structural variation, expression patterns, and gene function under salinity and drought stress. Our results show that the expression levels of two COMT genes, *EcCOMT7* and *EcCOMT49*, are significantly increased under salinity and drought stress. Ectopic overexpression of *EcCOMT7* and *EcCOMT49* in yeast leads to improved stress endurance, as demonstrated by growth analysis and spot assay. Similarly, under stress conditions, transgenic Arabidopsis plants overexpressing EcCOMT7 and EcCOMT49 exhibited better growth than wild-type plants. Overall, these findings highlight the potential role of COMT in improving the stress response and mitigating stress-induced ROS, making it an important target for crop improvement.

O-19

Comparative Study Of Endo-β-1,4-Mannanases From Novel Bacterial Strains For The Production Of Galactomannooligosaccharides

Shruti Saini[1,2], Dr. Koushik Mazumder[1]*

[1] *BRIC-National Agri-food and Bio-manufacturing Institute, SAS Nagar, Punjab, India*
[2] *Regional Centre of Biotechnology, Faridabad- 121001, Faridabad, Haryana*
shruti.saini@nabi.res.in

Prebiotics are compounds including sugar polyols, polysaccharides, oligosaccharides, resistant starches, and fibers which are non-digestible and not absorbed by gastro-intestinal tract. Galactomannan is a polysaccharide which is made of linear mannose chain and galactose is present as the side branch group. It has prebiotic potential, but its usage is limited because of its highly viscous nature. Galactomannan oligosaccharides are the emerging prebiotic which can be used to develop the functional foods for the benefit of human. In the presented work we performed a comparative analysis of endo-1,4- β-mannanase which was produced from novel bacterial strains. The bacterial strains were isolated form the guar fields of Rajasthan and Haryana. The recombinant construct made by inserting gene into pET vectors using rDNA technology. The comparative analysis of the purified enzyme showed that all were highly active in the pH 6, showed more than 50% activity in the low and high temperature (30-90˚C). The RJ 32 showed the optimum activity with 0.1U of enzyme/mg dosage in pH 6 at 55˚C temperature, RJ 35 optimal activity was found at pH 6 and 50 ˚C with 0.09U of enzyme/mg and HR 10 showed the optimal activity at pH 6 and 65 ˚C with 0.08U of enzyme/mg. The endomannanase of the RJ 32 and RJ 35 showed thermal stability with 50% of enzymatic activity upto 7 days. The enzymes were active at high temperatures even though they are not thermophilic strains; highly stable for longer duration at their optimal temperature which increase their industrial application.

Keywords: Endo-1,4- β-mannanase, Galactomannan oligosaccharides, Prebiotics, Thermal stable

O-20

Development and Validation of Analytical Device for rapid Iron determination

Charmy Kothari, Raveena Udhani

Department of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad-382481, Gujarat, India

Iron is one of the most essential trace elements in the human body. It is a vital component of haemoglobin & myoglobin, responsible for oxygen transport, DNA synthesis and electron transport. Despite its importance, both iron deficiency and overload are major clinical concerns worldwide. Accurate determination of iron concentration in biological samples is therefore crucial for clinical diagnosis and disease monitoring. Conventional methods such as CLIA, AAS, ICP and colorimetric assays provide high accuracy but require more time, expensive instrumentation and trained personnel. These limitations restrict their use in clinical settings. Hence, there is a growing need for simple, rapid, and cost-effective analytical platforms for iron determination that can be adapted for field use or self-monitoring applications. In this study, we report a thin-film-based colorimetric device for iron determination using the colorimetric dye assay. Analytical signal acquisition was achieved with a smartphone and free software (imageJ, RGB detector), making the method low-cost and user-friendly. The device was optimized to allow rapid iron estimation within approx. 120 seconds, requiring only 10 µL of biological specimen. Under optimized conditions, the limit of detection found was 5.9 µg/dL, and all quality controls (low, mid and high) demonstrated precision with %CV < 15. The method exhibited acceptable selectivity in various other minerals like, magnesium, potassium, calcium and sodium. Samples from healthy volunteers were successfully analysed, concentrations determined in the range of 25–800 µg/dL. This is the first report of a thin-film-based analytical platform for iron determination in human biological specimen, offering a rapid, reliable and POC alternative to conventional methods.

Keywords: Iron, POC, ImageJ, Colorimetric assay, RGB detection

O-21

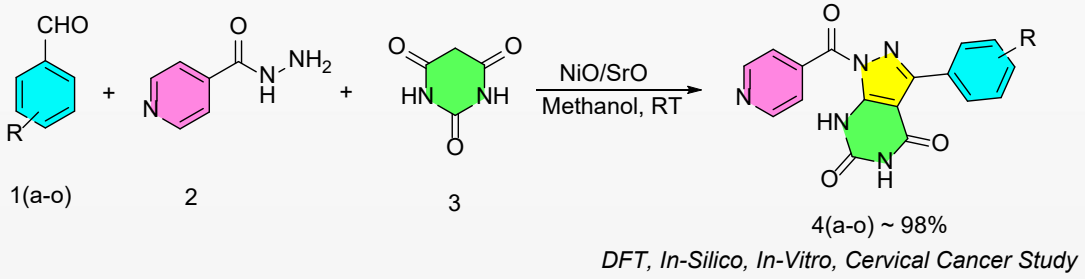
MOF-Derived NiO/SrO Nanocatalyst Enabled Multicomponent Synthesis of Novel AIPDs with Promising Anticancer Potential

Mueataz G. Thabet, Ashlesha Jadhav, Giribala M. Bondle*

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University Chhatrapati Sambhaji Nagar-Maharashtra, 431004, India.
Email: gmbondle@gmail.com

Abstract

A sustainable nanocatalyst approach was developed for the efficient synthesis of aryl-isonicotinoyl-pyrazolopyrimidine-dione (AIPD) derivatives using a MOF-derived NiO/SrO (75:25 wt%) nanocomposite. The catalyst achieved up to 98% yield within 60 minutes under mild conditions and was recyclable for multiple cycles without loss of activity. Structural characterization confirmed its crystalline and hierarchical morphology, enhancing catalytic performance. Density Functional Theory (DFT) and molecular docking studies revealed compound 4i as a potent binder to the cancer target 5IVE (−10.4 kcal/mol) and compound 4m as highly reactive (ΔE = 0.104 Hartree). ADMET analysis indicated favorable pharmacokinetics, and in vitro studies against HeLa cells showed significant cytotoxicity (IC50 = 94.5 µg/mL). This work demonstrates how integrating nanocatalysis, synthetic methodology, computational modeling, and biological screening can accelerate the development of new anticancer scaffolds.



Keywords: NiO/SrO Nanocomposite, Molecular Docking, DFT, ADMET Profiling, HeLa Cell Line

References

1. A.V. Sadybekov, V. Katritch, Computational approaches streamlining drug discovery, Nature 2023, 616 .
2. D.C. Onwudiwe, N.H. Seheri, L. Hlungwani, H. Ferjani, R. Rikhotso-Mbungela, NiO nanoparticles by thermal decomposition of complex and evaluation of the structural, morphological, and optical properties, J. Mol. Struct.,2024.
3. A.K. Shimi, C. Parvathiraj, S. Kumari, J. Dalal, V. Kumar, S.M. Wabaidur, Z. Alothman, Green synthesis of SrO nanoparticles using leaf extract of Albizia julibrissin and its recyclable photocatalytic activity: an eco-friendly approach for treatment of industrial wastewater, Environ. Sci.*: Adv.* 1, 2022.
4. Z. Yang, Z.Y. Liu, M. Ablise, A. Maimaiti, Z. Mutalipu, Y. Alimujiang, A. Aihaiti, Design, synthesis, and anti-cervical cancer and reversal of tumor multidrug resistance activity of novel nitrogen-containing heterocyclic chalcone derivatives, Molecule*s* 28, 2023.

O-22

Design and Development of a Thermo-Mechanical Leaf Processing System for Sustainable Biodegradable Material Production

Shikha Singh; Anish Pandey; Ruby Mishra; Rajiva Lochan Mohanthy

shikha11129@gmail.com

Abstract

This study presents a novel approach to sustainable material production through the design and development of a thermo-mechanical leaf processing system. The developed machine integrates three key processes—shredding, hot compression rolling, and pulping—to convert raw plant leaves into durable sheets and fibrous substrates suitable for biodegradable applications. Structural components, including the conveyor system, shredder mechanism, compactor, and control units, were optimized using Computer-Aided Design (CAD) modeling and Finite Element Analysis (FEA) to enhance operational efficiency and reduce energy consumption. Experimental investigations revealed that appropriate roller dimensions and controlled pressure-temperature parameters achieved up to 90% uniform compression under optimal load conditions. The processed leaf pulp exhibited enhanced microbial accessibility, accelerating biodegradation and contributing to improved nutrient recycling within soil ecosystems. By mitigating greenhouse gas emissions, reducing thermal losses, and minimizing landfill waste, the system demonstrates a sustainable and energy-efficient pathway for transforming agricultural leaf waste into eco-friendly products. The research further underscores the environmental potential of replacing single-use plastics with biodegradable, leaf-derived materials, thereby supporting global initiatives toward a circular bioeconomy and ecological sustainability.

Keywords: Thermo-mechanical processing, Leaf-based materials, Biodegradable composites, Sustainable design, Finite Element Analysis (FEA), Circular bioeconomy, Environmental sustainability

O-23

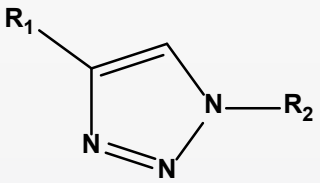
Triazole-Linked Heterocyclic Hybrids via Click Chemistry: Structure–Activity Insights Toward Potent Anticancer Agents

Dr. Ranjan C. Khunt

Department of Chemistry, Saurashtra University, Rajkot-360005, India
Email id: rckhunt@sauuni.ac.in

Abstract

The triazole moiety has attracted significant attention in medicinal chemistry owing to its stability, bioisosteric properties, and ability to interact with diverse biological targets. In this study, a series of triazole-linked heterocyclic hybrids such as purine–triazoles**[1]**, benzoxazole–triazoles**[2]**, phthalimide–triazoles**[3]**, and indole–triazoles**[4]** were synthesized using Cu(I)-catalyzed azide–alkyne cycloaddition (click chemistry) under optimized reaction conditions. The intermediates and final compounds were characterized by ^{1}H NMR, ^{13}C NMR, IR, and mass spectrometry, ensuring structural integrity and purity. The synthesized compounds were screened for anticancer activity against a panel of human cancer cell lines, including leukemia (CCRF-CEM, K562), non-small cell lung cancer (A549), renal cancer (UO-31), and melanoma (SK-MEL-5). Among them, benzoxazole–triazole derivatives (7b, 7c, 7d, 7g, and 7i) and phthalimide–triazole derivatives (6a, 6b, 6e, 6g, and 6j) exhibited notable cytotoxicity with GI_{50} values between 5.6 and 20.8 µM, indicating promising potency. Molecular docking studies further confirmed strong binding interactions with the EGFR tyrosine kinase receptor, suggesting a potential mechanism of action through inhibition of cancer cell proliferation. The incorporation of the triazole pharmacophore into heterocyclic frameworks significantly enhanced anticancer activity, particularly against leukemia and non-small cell lung cancer cell lines. These results demonstrate that triazole-linked hybrids represent a valuable scaffold for further optimization toward potent anticancer therapeutics.



Keywords: Triazole, Click chemistry, Anticancer activity, EGFR inhibition, Leukemia, Lung cancer

References:

1. Kapadiya, K., Jadeja, Y., & Khunt, R. C. (2018). *Journal of Heterocyclic Chemistry*, *55*(1), 199-208.
2. Jivani, A. J., Lunagariya, K. S., Kapadiya, K. M., Dholaria, P. V., Khedkar, V. M., & Khunt, R. C. (2022). *Analytical Chemistry Letters*, *12*(1), 44-57.
3. Mori, N. P., Parmar, P. K., Khedkar, V. M., & Khunt, R. C. (2023). *Polycyclic Aromatic Compounds*, *43*(6), 5354-5374.
4. Manvar, P., Katariya, D., Vyas, A., Bhanderi, P., & Khunt, R. C. (2025). *Reviews and Advances in Chemistry*,

POSTER

Design, Synthesis, and Anticancer Evaluation of Triazolyl-Pyrimidine-2,4-Diones

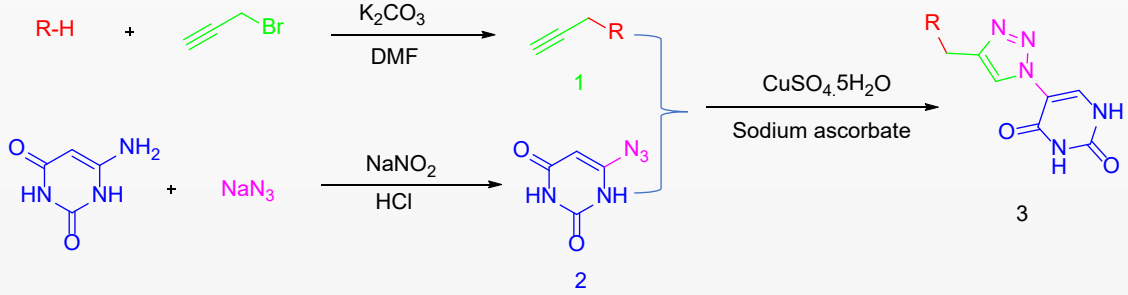
Ms. Ashvini A. Jadhav (DOB:15/03/2001), Dr. Anusaya S. Chavan*

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati sambhajinagar, Maharashtra, India
*Email: *aschavan.chemistry@bamu.ac, aj7338264@gmail.com*

Abstract:

A novel series of substituted 1-(1,2,3-triazol-1-yl)pyrimidine-2,4(1H,3H)-dione derivatives were efficiently synthesized from appropriately functionalized precursors [1,2,3]. The structural identity and purity of all the synthesized compounds were thoroughly characterized. The synthesized hybrids will be evaluated as potent anticancer agents and tested against different human cancer cell lines, including A549 (lung), MCF-7 (breast), HeLa (cervical), and HepG2 (liver) [4,5]. This approach aims to assess their broad-spectrum anticancer potential and ability to affect multiple cancer-related pathways, providing insights into their suitability as promising anticancer candidates [5]. The details and other aspects will be debited.

Scheme:-



References:

1. P. Sivaguru; Y. Ning; X. Bi. Chemical Reviews 2021, 121, 4253–4307.
2. T. Deshmukh; A. Sarkate; D. Lokwani; S. Tiwari; R. Azad; B. Shingate. Bioorg. Med. Chem. Lett. 2019, 29, 126618.
3. D. Veeranna; L. Ramdas; G. Ravi; S. Bujji; V. Thumma; J. Ramchander. ChemistrySelect 2022, 7, 202201758.
4. K. Shaik; K. Pandurangan; T. Allaka; S. Nalla; S. Ganta; M. Ahmed; S. Venkatesan; P. NandaKishore. Scientific Reports 2025, 15, 95669.
5. N. Reddy; S Hung; M. Swamy; A. Sanjeev; V. Rao; R. Rohini; A. Raju; K. Bhaskar; A. Hu; P. Reddy. Molecules 2021, 26, 1952.

P-2

Microenvironment-Regulated Ultraslow Microstructural Dynamics of Phenoxazine Dyes

Ritu Kumari, Vineeta Chaturvedi, Mudit Pithi, and Avik K. Pati*

Department of Chemistry, Birla Institute of Technology and Science Pilani, Pilani, Rajasthan 333031, India
Email ID: p20220016@pilani.bits-pilani.ac.in

Phenoxazine class of dyes, including nile red, cresyl violet, and nile blue, have been extensively used in chemical and biological studies, particularly for probing lipid membranes.[1–3] In this presentation, we will share our recent findings on a general phenomenon of hours-long spectral dynamics in the phenoxazine dyes, evidenced by systematic changes in their electronic spectra over an hour. Detailed mechanistic investigations reveal that such spectral dynamics of the dyes can be reduced by tuning microenvironments, where microsolvation (interactions of the dyes with their immediate solvent microenvironment) plays a key underlying role. These microsolvation-induced microstructural changes in a single dye species tend to follow zeroth-order kinetics. The half-life values of such processes systematically vary with solvent hydrogen bonding strength and ionic radius of the dyes' counter anions. Using lipid membrane model systems, this work showcases the importance of longer dye incubation time inside the bilayers for studying membrane properties. We believe that the observed phenomenon holds significance for the practical use of phenoxazine dyes in understanding chemical and biological systems. This work also advances the fundamental understanding of dye-solvent interactions and provides key guidelines for the optimized use of phenoxazine-based fluorescent probes in biophysical and analytical studies.[4]

References:

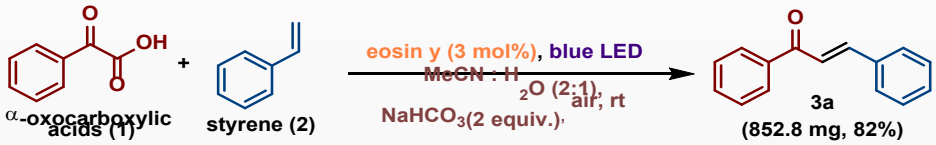
1. Sadhu, C.; Mitra, A. K., Synthetic, biological and optoelectronic properties of phenoxazine and its derivatives: a state of the art review. *Molecular diversity* **2024,** *28* (2), 965-1007.
2. Klymchenko, A. S., Fluorescent Probes for Lipid Membranes: From the Cell Surface to Organelles. *Accounts of Chemical Research* **2023,** *56* (1), 1-12.
3. Kumari, R.; Sharma, P.; Chaturvedi, V.; Pati, A. K., Organic Fluorophores for Studying Lipid Membrane Structures and Dynamics. *Chemistry – An Asian Journal* **2025**, e00328.
4. Kumari, R.; Chaturvedi, V.; Pithi, M.; Pati, A. K., Microsolvation-Driven Hours-Long Spectral Dynamics in Phenoxazine Dyes. *The Journal of Physical Chemistry A* **2025,** *129* (1), 82-93.

Photoredox catalysed decarboxylative acylation of unsaturated hydrocarbon *via* Csp^2-Csp^2 cross-coupling: α-keto acids as acyl radical precursor

Aman Singh and Sundaram Singh*.

Department of Chemistry, Indian Institute of Technology (BHU), Varanasi– 221005, U.P., India,
Amansingh.rs.chy23@itbhu.ac.in

We describe a streamlined and efficient strategy for synthesizing chalcones *via* photocatalytic decarboxylative cross-acyl coupling of α-oxocarboxylic acid with styrenes, employing an organic photoredox catalyst under visible light irradiation as a sustainable energy input. Detailed mechanistic studies demonstrate that the transformation proceeds through a radical mechanism. Furthermore, the broad functional group tolerance, compatibility with structurally complex and biorelevant substrates, and facile scalability collectively underscore the robustness and synthetic utility of the developed methodology. This methodology holds significant promise for the late-stage modification of bioactive molecules and natural products.



References

1. Kushwaha, Ambuj Kumar, Arsala Kamal, Pooja Kumari, et al. "Metal-Free Photoredox Catalyzed Sulfonylation of Phenylhydrazines with Thiols." *Organic Letters*, vol. 26, no. 18, May 2024, pp. 3796–800. *ACS Publications*, https://doi.org/10.1021/acs.orglett.4c00849.
2. Beil, Sebastian B., et al. "Carboxylic Acids as Adaptive Functional Groups in Metallaphotoredox Catalysis." *Accounts of Chemical Research*, vol. 55, no. 23, Dec. 2022, pp. 3481–94. *ACS Publications*, https://doi.org/10.1021/acs.accounts.2c00607.
3. Elkanzi, Nadia A. A., et al. "Synthesis of Chalcones Derivatives and Their Biological Activities: A Review." *ACS Omega*, vol. 7, no. 32, Aug. 2022, pp. 27769–86. *ACS Publications*, https://doi.org/10.1021/acsomega.2c01779.

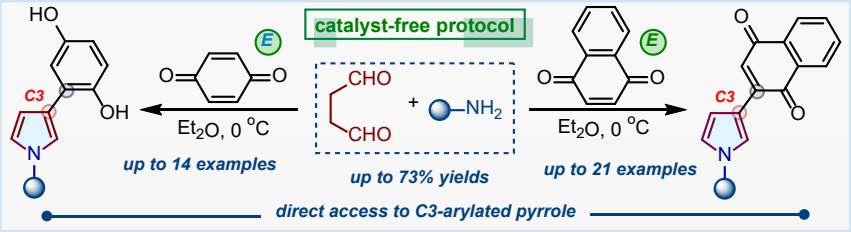
P-4

Direct Multicomponent Synthesis of C3-Arylated Pyrroles Under Catalyst-Free Conditions

Reena Jangir, Amol Prakash Pawar, Atul Jankiram Dolas, Yadav Kacharu Nagare and Indresh Kumar*

Department of Chemistry, Birla Institute of Technology & Science, Pilani, Pilani campus, Rajasthan, 333031
Email: *jangirr2031995@gmail.com*

Pyrroles are valuable scaffolds in pharmaceuticals, natural products, and functional materials (Young et al. [1]), yet selective C3-functionalization remains a challenge due to the electron-rich heteroaromatic core (Hunjan et al. [2]). An operationally simple, catalyst-free multicomponent protocol has been developed for the direct synthesis of C3-arylated and alkenylated pyrroles under open-flask, one-pot conditions. Readily available succinaldehyde (Pawar et al. [3]), primary amines, and activated carbonyl electrophiles (Son et al. [4]) generate an enamine intermediate in situ, which is intercepted before Paal–Knorr cyclization. This "just-mix" strategy affords diverse C3-substituted N-alkyl pyrroles in good yields while avoiding metal catalysts and protection–deprotection steps. The method demonstrates improved atom- and step-economy consistent with sustainable synthesis principles (Pawar et al. [5]) and enables access to fused heterocyclic scaffolds via quinone electrophiles, offering a practical route to medicinally relevant pyrrole derivatives. The details of the concept and outcome in this direction will be discussed.



REFERENCES

1. I. S. Young, P. D. Thornton and A. Thompson, Natural Product Reports 27, 2010, 1801.
2. M. K. Hunjan, S. Panday, A. Gupta, J. Bhaumik, P. Das and J. K. Laha, The Chemical Record 21, 2021, 715.
3. A. P. Pawar, J. Yadav, N. A. Mir, E. Iype, K. Rangan, S. Anthal, R. Kant and I. Kumar, Chemical Communications 57, 2021, 251.
4. E. J. Son, J. H. Kim, K. Kim and C. B. Park, Journal of Materials Chemistry A 4, 2016, 11179.
5. A. P. Pawar, R. Jangir, A. J. Dolas, Y. K. Nagare, K. Rangan, E. Iype and I. Kumar, Synthesis 57, 2025, 380.

P-5

Switchable and Stereoselective Synthesis of Tetrasubstituted Azines and Olefins via Electricity-Mediated Homo-Coupling of Diazo Compounds

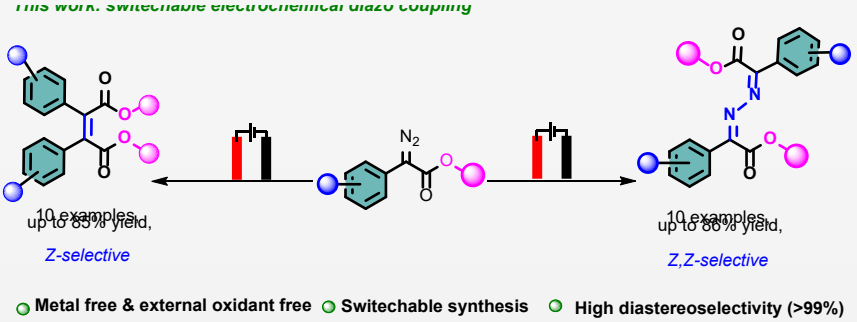
Abinash Mohapatra, Vaneet Saini, and Vikas Tyagi*

Department of Chemistry and Biochemistry, Department of Chemistry, Panjab University, Chandigarh 160014, Thapar Institute of Engineering and Technology, Patiala-147004, Punjab, India
Email: vikas.tyagi@thapar.edu

Keywords: Electrosynthesis, transition metal-free coupling, stereoselective synthesis, tetrasubstituted azine & olefin synthesis, machine learning.

Abstract:

Diazo compounds are widely recognized as versatile intermediates in organic synthesis, enabling diverse transformations such as X–H carbene insertions, C–C coupling, and cyclopropanation[1]. They serve as key precursors for constructing azines and tetrasubstituted olefins, both of which are valuable synthetic motifs in bioactive and functional molecule synthesis. However, achieving switchable selectivity and stereocontrol between azine and olefin formation within a single catalytic system remains a major challenge. Conventional transition-metal-catalyzed or photocatalytic strategies have advanced this chemistry but often suffer from narrow substrate scope, harsh conditions, and metal contamination issues[2,3]. In this work, we report a transition-metal-free, electricity-mediated homo-coupling of aryl diazoesters that enables highly stereoselective and switchable synthesis of tetrasubstituted azines and olefins. The electrochemical approach eliminates the need for external oxidants or catalysts, providing a sustainable and tunable platform for diazo transformations. Systematic screening of solvents, electrolytes, and electrode materials revealed that product selectivity between azines and olefins can be finely controlled by reaction conditions. This method demonstrates broad substrate tolerance for both electron-donating and electron-withdrawing substituents, affording excellent yields (up to 95%) and stereoselectivities (up to 99%). Overall, this electricity-driven, metal-free protocol introduces an environmentally benign and stereoselective route to diazo-derived azines and olefins, merging synthetic innovation with machine learning-guided electrochemical design. It offers a powerful platform for the development of sustainable methodologies in modern organic and materials synthesis.



References:

1. Durka, J.; Turkowska, J.; Gryko, D. Lightening Diazo Compounds? *ACS Sustainable Chem. Eng.* **2021**, *9*, 8895–8918.
2. Dong, Y.; Lipschutz, M. I.; Witzke, R. J.; Panetier, J. A.; Tilley, T. D. Switchable Product Selectivity in Diazoalkane Coupling Catalyzed by a Two-Coordinate Cobalt Complex. *ACS Catal.* **2021**, *11*, 11160–11170.
3. Kuzhalmozhi Madarasi, P.; Sivasankar, C. Grignard Reagent Dictated Copper(I) Phosphines Catalyzed Reductive Coupling of Diazo Compounds: The Chemistry beyond Carbene Generation. *Appl. Organomet. Chem.* **2022**, *36*, e6522.

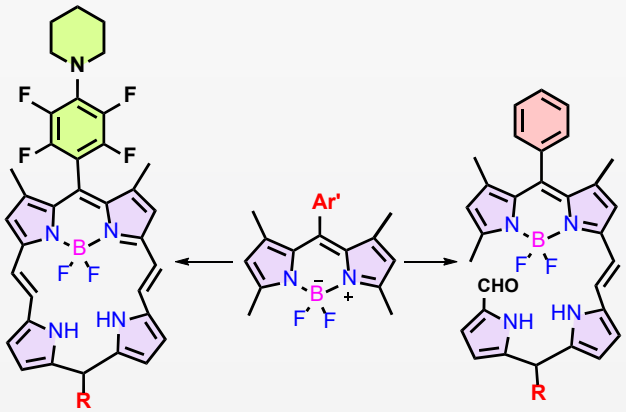
P-6

Synthesis and Photophysical Analysis of BODIPY-DPM Conjugates

Sonia Swami, Harshita Saroj and Nitika Grover*

Department of Chemistry, BITS Pilani Pilani Campus, Rajasthan -333031, India
Email: nitika.grover@pilani.bits-pilani.ac.in

Organic dyes with tunable electronic and optical properties are becoming an important tool in modern biomedicine, imaging, and phototherapies. Among these, boron dipyrromethenes (BODIPYs) gained special attention due to their modular design, strong absorption, and low toxicity, making them excellent photosensitizers (PSs) for photodynamic therapy (PDT). [1] Traditional triplet harvesting via heavy atoms enhances intersystem crossing (ISC) but compromises biocompatibility and stability. Consequently, recent efforts emphasize heavy-atom-free molecular designs that achieve efficient ISC through structural engineering, such as BODIPY–anthracene and benzothiophene-fused systems with enhanced spin–orbit coupling and strong ROS generation. [2,3] Parallel studies on dipyrrin and dipyrromethane (DPM) derivatives, including prodigiosin analogues, reveal potent anticancer and antimicrobial properties, underscoring the biomedical potential of pyrrole-based scaffolds. Inspired by these advances, we envisioned merging BODIPY with dipyrrin/DPM frameworks to create multifunctional, heavy-atom-free systems integrating imaging, anticancer, and antimicrobial capabilities. We selected 5-tolyl-1,3,7,9-tetramethyl BODIPY as a model substrate. Reaction with pyrrole-2-carboxaldehyde under microwave irradiation yielded the mono- and di-substituted derivatives depending on aldehyde stoichiometry. Extending this, condensation of BODIPY with various DPMs furnished mono- and cyclic BODIPY–DPM conjugates in good yields. Further, we tested the 1O2 generation capabilities of synthesized compounds. These results demonstrate a versatile strategy for constructing BODIPY–DPM hybrids, uniting efficient triplet harvesting with potential biomedical functionality in next-generation photosensitizers.



References

1. I S Yadav and R. Misra J. Mater. Chem. C, 2023,11, 8688.
2. W Bu, C Yu, Y Man, J Li, Q Wu, S Gui, Y Wei, L Jiao and E. Hao Chem. Commun., 2024,60, 9809.
3. M A Filatov, S Karuthedath, P M Polestshuk, H Savoie, K J Flanagan, C Sy, E Sitte, M Telitchko, F Laquai, R W Boyle, M O Senge J. Am. Chem. Soc 2017, 139, 6282.

Urea-Appended Push-Pull Chromophores as Efficient Colorimetric Sensors for Fluoride Ions: Design and Mechanistic Insights

Kritika Nag, Pooja Das, Arun Kumar Solanki, Md. Ehesan Ali and Govindasamy Jayamurugan*

Institute of Nanoscience and Technology (INST), Mohali, Punjab, 140306, India.
E-mail: *jayamurugan@inst.ac.in*

Abstract:

Fluoride ions are widespread in the environment, and while trace levels are beneficial, excessive exposure poses serious health risks. Rapid, selective, and sensitive detection is therefore crucial. In this study, we present two urea-based tetracyanobutadiene (TCBD) chromophores designed as colorimetric fluoride sensors with distinct substitution patterns. **Urea-TCBD-Si**, containing a silyl-protected benzyl urea–TCBD unit, and **NP-Urea-TCBD**, featuring a 4-nitrophenyl urea–TCBD framework, both exhibit remarkable fluoride responsiveness. Upon interaction with F^-, each sensor undergoes a visible color transition from yellow to pink, coupled with characteristic UV/vis spectral changes. These responses stem from fluoride-induced deprotonation of urea –NH groups, which enhances intramolecular charge transfer within the push–pull TCBD core. The detection limits were determined to be **3.6 µM** for **Urea-TCBD-Si** and **68 nM** for **NP-Urea-TCBD**, highlighting the superior sensitivity of the latter. Binding studies indicate 2:1 and 1:1 probe-fluoride stoichiometries, respectively. ^{1}H NMR mechanistic analysis confirms silyl deprotection followed by di-deprotonation for **Urea-TCBD-Si**, and direct di-deprotonation for **NP-Urea-TCBD**. These findings establish urea–TCBD systems as efficient, low-cost platforms for naked-eye fluoride sensing.

References

1. V Gowri, S Jalwal, A H Dar, A Gopal, A Muthukrishnan, A Bajaj, Md E Ali, and G Jayamurugan, *J. Photochem. Photobiol. A.* 410, 2021, 113163.
2. A Sharma, S Dhiman, S Sartaliya, K M Neethu, K Nag, and G Jayamurugan, *ACS Appl. Polym. Mater.* 7, 2025, 1271-1278.

P-8

Structure–Activity Relationship of Extended TCBD Derivatives for Nitric Oxide Radical Scavenging and Sensing

Sarita Kumari, Malika Arora, Arun Kumar Solanki, Deepa Ghosh, and Govindasamy Jayamurugan

Institute of Nanoscience and Technology (INST), Mohali, Punjab, 140306, India
E-mail: jayamurugan@inst.ac.in

Abstract:

Excessive nitric oxide (NO) production triggered by bacterial or inflammatory stimuli is implicated in multiple pathological conditions. Traditional strategies targeting nitric oxide synthase (NOS) or downstream pathways often face limited clinical success. To address this, we developed urea- and amine-functionalized push–pull chromophores incorporating expanded 1,1,4,4-tetracyanobuta-1,3-diene (eTCBD) cores as efficient NO radical scavengers. Two derivative classes were synthesized: (i) urea–eTCBD hybrids bearing primary, secondary, or tertiary amines and (ii) amine–eTCBD systems. Griess assay evaluations demonstrated strong scavenging efficiency (≥85%) at 200 µg/mL. Urea-eTCBD1 and Urea-eTCBD3 (3° and 1° amines) achieved ~90% activity, while Urea-eTCBD2 (2° amine) showed 85%. Among amine derivatives, Amine-eTCBD1 and Amine-eTCBD3 exhibited >98% efficiency, highlighting the superior reactivity of primary amines. Fluorescence studies revealed PET-based emissive quenching upon NO exposure in urea-functionalized systems, while amine derivatives remained non-emissive. ^{1}H NMR spectra showed downfield proton shifts confirming diazeniumdiolate (NONOate) adduct formation, with Job's plot analysis indicating a 2:1 NO-to-probe stoichiometry. These results establish eTCBD scaffolds as promising candidates for NO scavenging and sensing applications.

References

1. H S Roy, K M Neethu, S Rajput, S Sadhukhan, V Gowri, A H Dar, M Monga, N Salaria, R Guha, N Chattopadhyay, G Jayamurugan and D Ghosh, *Chem. Euro. J.* 29, 2023, p.e202301748.
2. J Yeo, Y M Lee, J Lee, D Park, K Kim, J Kim, J Park and W J Kim, *Nano Lett.* 19, 2019, 6716-6724.
3. Z Huang, Y Zhang, L Fang, Z Zhang, Y Lai, Y Ding, F Cao, J Zhang and S Peng, *Chem. Commun.* 13, 2009, 1763-1765.

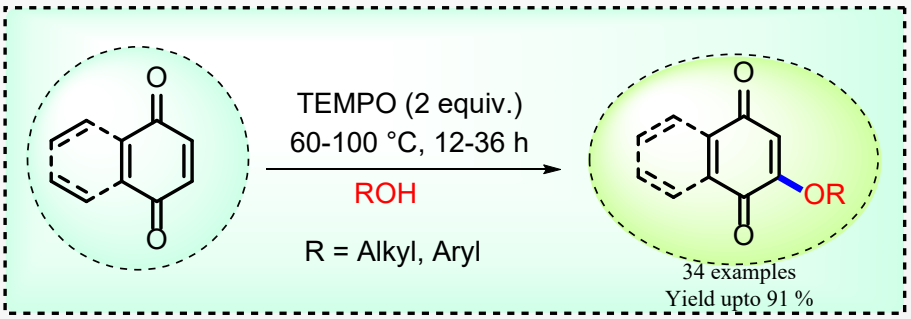
P-9

TEMPO-Mediated Direct C(sp^2)-H Alkoxylation/Aryloxylation of 1,4-Quinones

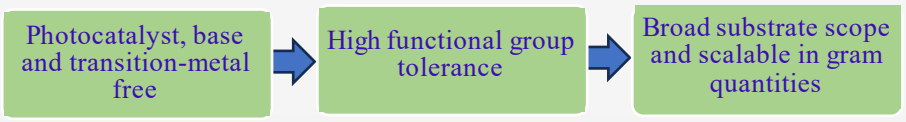
Amol B. Gadekar, Dhananjay S. Nipate, Krishnan Rangan, and Anil Kumar*

Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India
E-mail: anilkumar@pilani.bits-pilani.ac.in

1,4-Quinones are vital molecular frameworks found in nature, particularly in plants, bacteria, fungi, and several natural products and pharmaceuticals, showing a wide range of biological activities.[1-2] It shows unique redox properties through 1 or 2-electron transfer processes.[3] Introducing a heteroatom onto the quinone ring increases their stability and makes them more prevalent in bioactive natural products.[4] A key strategy to modify their properties is through the introduction of alkoxy or aryloxy groups. However, traditional methods for creating these C-O bonds often rely on pre-functionalized starting materials and hazardous metal catalysts, which can be inefficient and environmentally unfriendly. On the other hand, the stable nitroxyl radical TEMPO is commonly used in organic synthesis, serving as a catalyst, reagent, hydrogen acceptor and radical generator.[5] In this work, we have developed a straightforward and efficient metal-free method for the direct alkoxylation and aryloxylation of 1,4-quinones by direct cross-dehydrogenative coupling of readily available alcohols and phenols in the presence of TEMPO as radical initiator. The mechanistic study, including all control experiments, strongly supports the radical-based pathway (Scheme 1).[6] Details of the protocol will be presented in the poster.



Scheme 1. Alkoxylation or Aryloxylation of 1,4-quinones.



Scheme 1. Alkoxylation or aryloxylation of 1,4-quinones.

Reference:

1. K. W. Wellington, *RSC Adv*. **2015**, *5*, 20309-20338.
2. D. Aminin, S. J. C. Polonik, P. *Chem. Pharm. Bull.* **2020**, *68*, 46-57.
3. E. A. Hillard, F. C. de Abreu, D. C. M. Ferreira, G. Jaouen, M. O. F. Goulart, C. Amatore, *Chem. Commun*. **2008**, 2612-2628.
4. E. O. M. Orlemans, W. Verboom, M. W. Scheltinga, D. N. Reinhoudt, P. Lelieveld, H. H. Fiebig, B. R. Winterhalter, J. A. Double, M. C. Bibby, *J. Med. Chem.* **1989**, *32*, 1612-1620.
5. H. A. Beejapur, Q. Zhang, K. Hu, L. Zhu, J. Wang, Z. Ye, *ACS Catal.* **2019**, *9*, 2777-2830.
6. A. B. Gadekar, D. S. Nipate, K. Rangan, A. Kumar, *J. Org. Chem.* **2025**, *90*, 1044-1053.

P-10

Advances in Phytomedicine: A Promising Future for Neurodegenerative Disease Treatment

Banaja Panigrahi[1], Satyabrata Nanda[1*]

[1]School of Biotechnology, Centurion University of Technology and Management (CUTM), Bhubaneswar, Odisha 752050, India
Presenting author email: banajapanigrahi1@gmail.com

Abstract

Neurodegenerative disease (ND) is next leading cause of death, disease burden and disability in the world after cardiovascular disorders; they undergo progressive degeneration of neurons in CNS that control memory, cognition as well as motor structuralfunctions. AD, PD, HD and ALS are among the commonest NDs. Current treatment modalities are primarily symptomatic, and numerous ones are limited by corticosteroid resistance, drug-related toxic effects, nonsufficient blood–brain barrier penetration or bioavailability. Natural products from plants are increasingly recognized for their neuroprotective and therapeutic effects. Phytochemicals (e.g., quercetin, curcumin, EGCG, apigenin and cannabinoids) are shown to modulate the common pathways of NDs in disease pathogenesis. Herein, we critically analyze their pharmacological characteristics, therapeutic potential and inherent limitations as well emphasizes the urgent necessity of thorough preclinical/clinical researches for advancement of second-generation phytomedicines against NDs.

Keywords: Neurodegenerative disorders, Phytomedicine, Molecular docking, MD Simulation.

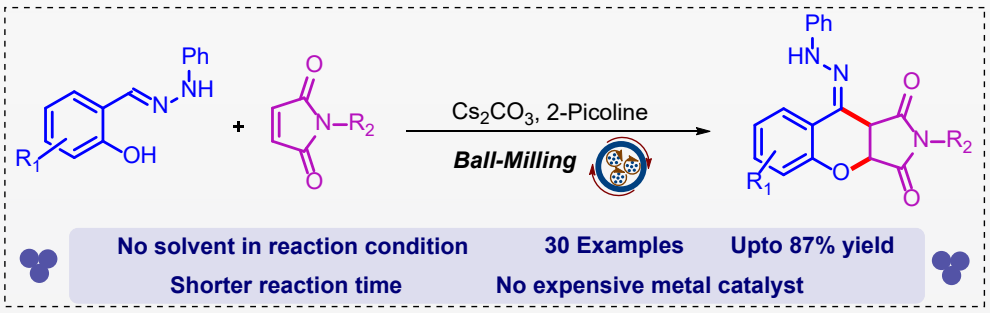
P-11

Base-Catalysed Synthesis of 4-Chromenones by [4+2] Annulation of *β*-Hydroxyhydrazones with Maleimides using Ball-Milling

Pratiksha Jangir, Bhawani, Prakash N. Swami, Anil Kumar*

Department of Chemistry, Birla Institute of Technology & Science, Pilani 333031, India
**Email: anilkumar@pilani.bits-pilani.ac.in*

Chromones are structural isomers of coumarins and are often regarded as highly valuable scaffolds due to their pharmacological and biological properties, along with the relatively low toxicity associated with these derivatives.[1] Their derivatives have been recognized as potent inhibitors of enzymes responsible for serious diseases such as Alzheimer's and Parkinson's.[2] Several metal-catalysed chelation-assisted C–H activation reactions of aldehydes with unsaturated hydrocarbons have been reported for the synthesis of chromone derivatives.[3] Among aldehydes, salicylaldehyde (SA) stands out as one of the best chelating partners, owing to its bifunctional nature (presence of both *ortho*-hydroxy and formyl groups).[4] Numerous strategies have been developed involving the reaction of SA with alkynes,[5] alkenes,[6] and allenes,[7] most extensively using transition-metal catalysts, to access 4-chromenone derivatives. Interestingly, masking of the –CHO functional group in salicylaldehyde can enhance reactivity *via* the hydroxyl handle, thereby opening the door to greater structural diversity.[8] With this idea and motivated by our ongoing interest in mechanochemical synthesis of organic compounds, we propose a base-catalysed, mechanochemically driven [4+2] annulation of *β*-hydroxyhydrazones with maleimides, leading to synthesis of 4-chromenone derivatives under ball-milling conditions. The key advantages of this method include shorter reaction times, solvent-free reaction conditions, and the absence of expensive metal catalysts. Details of the reaction conditions, mechanism, and substrate scope will be presented.



Scheme 1. [4+2] Annulation of *β*-hydroxyhydrazones with maleimides under ball-milling conditions

References:

1. Matos, M. A. R.; Sousa, C. C. S.; Miranda, M. S.; Morais, V. M. F.; Liebman, J. F., *J. Phy. Chem. B* **2009,** *113*, 11216-11221; (b) Khadem, S.; Marles, R. J. *Molecules*, **2012**, *17*, 191-206.
2. (a) Sharma, K., *ChemistrySelect* **2022,** *7*, e202200540; (b) Li, F.; Wu, J.-J.; Wang, J.; Yang, X.-L.; Cai, P.; Liu, Q.-H.; Kong, L.-Y.; Wang, X.-B., *Bioorg. Med. Chem.* **2017,** *25*, 3815-3826.
3. Benny, A. T.; Arikkatt, S. D.; Vazhappilly, C. G.; Kannadasan, S.; Thomas, R.; Leelabaiamma, M. S. N.; Radhakrishnan, E. K.; Shanmugam, P., Chromone, *Mini Rev. Med. Chem.* **2022,** *22*, 1030-1063.
4. Yang, J.; Yoshikai, N., *Angew. Chem., Int. Ed.* **2016,** *55*, 2870-2874.
5. Du, X.-W.; Stanley, L. M., *Org. Lett.* **2015,** *17*, 3276-3279.
6. Shi, Z.; Schröder, N.; Glorius, F., *Angew. Chem., Int. Ed.* **2012,** *51*, 8092-8096.
7. Kumar, N. N. B.; Reddy, M. N.; Swamy, K. C. K., *J. Org. Chem.* **2009,** *74*, 5395-5404.
8. Diana, E. J.; Kanchana, U. S.; Mathew, T. V., *Org. Biomol. Chem.* **2021,** *19*, 7995-8008.

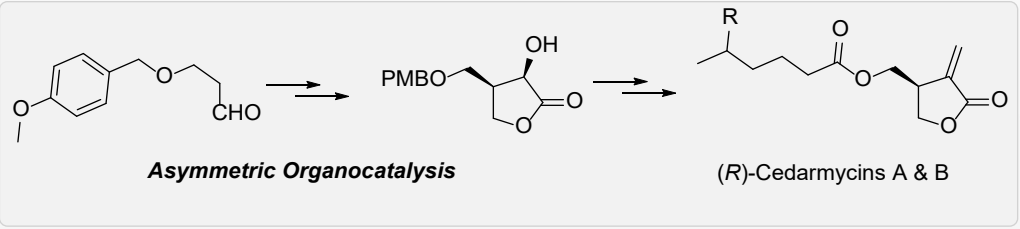
P-12

An approach towards (*R*)-cedarmycins via organocatalytic direct cross-aldol reaction

Dr. Shashank N. Mhaldar*, Prof. S. G. Tilve

Department of Chemistry, DCT'S Dhempe College of Arts & Science Miramar Goa (Affiliated to Goa University), Miramar Goa, 403001
Email ID: shashank@dhempecollege.edu.in

Chiral γ-butyrolactones represent one of the most common structural motifs in bioactive natural products and pharmaceuticals.[1] In enantiomerically pure form, γ-butyrolactones and their derivatives display a remarkable range of biological activities, including pesticidal, ratogenic, embryotoxic, and cytotoxic effects against human tumor cell lines, thereby underscoring their potential as novel physiological and therapeutic agents.[2] Among these, chiral γ-butyrolactones such as cedarmycins are particularly significant, as they exhibit potent antibiotic activity against *Candida glabrata* IFO 0622, comparable to amphotericin B.[3] The asymmetric cross-aldol reaction between two different aldehydes has long been established as one of the most powerful carbon–carbon bond-forming strategies for the generation of highly enantiopure chiral compounds.[4] However, despite extensive advances in this area, its application to the synthesis of γ-butyrolactones bearing stereogenic centers at both the α- and β-positions remains relatively rare. Motivated by this challenge, and building on our earlier work[5] in hydroxy lactams and (+)-allokainic acid, we sought to develop novel γ-butyrolactones through enantioselective cross-aldol reactions, followed by further synthetic modifications to access the desired natural products.



References:

1. R. R. A. Kitson, A. Millemaggi and R. J. K. Taylor, Angew. Chem. Int. Ed., 48, 2009, 9426.
2. M. A. Blázquez, A. Bermejo, M. C. Zafra-Polo and D. Cortes, Phytochem. Anal., 10, 1999, 161.
3. Ismiyarto, N. Kishi, Y. Adachi, R. Jiang, T. Doi, D. Zhou, K. Asano, Y. Obora, T. Suzuki, H. Sasai and T. Suzuki, RSC Adv., 11, 2021, 11606.
4. B. Alcaide and P. Almendros, Angew. Chem., 42, 2003, 858.
5. S. N. Mhaldar and S. G. Tilve, Org. Biomol. Chem., 21, 2023, 5469.

P-13

Exploring Benzotriazole–Oxadiazole Hybrids as Promising Scaffolds in Medicinal Chemistry

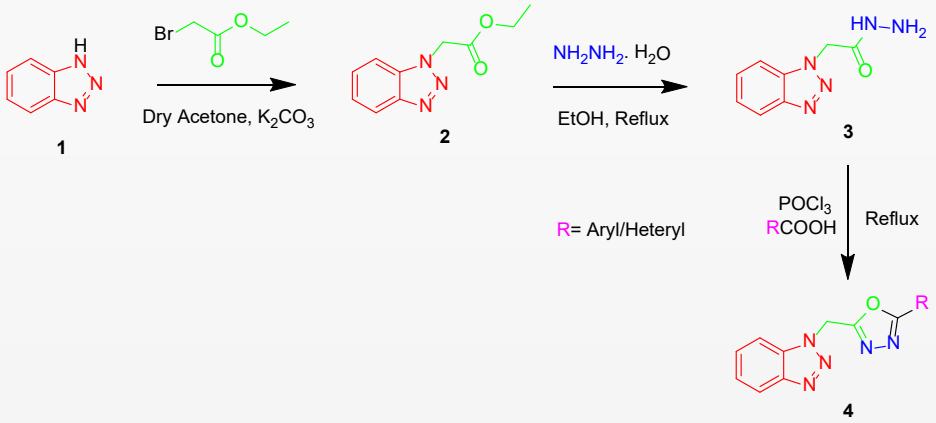
Ms. Nupur M. Jalewar (DOB: 29/04/1998), Dr. Anusaya S. Chavan*

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar, Maharashtra, India
*Email: *aschavan.chemistry@bamu.ac, nupur.jalewar@gmail*

Abstract:

Molecular hybridization is an effective strategy in medicinal chemistry for generating scaffolds with improved pharmacological potential. Benzotriazoles are well-known for their wide spectrum of biological activities, including antibacterial [1], anticancer [2], and anti-viral [3] effects, while 1,3,4-oxadiazoles are recognized as versatile pharmacophores with antimicrobial [4], anticancer [5], and anti-tubercular [6] properties. In this study, a new series of 1H-benzo[*d*][1,2,3] triazole–substituted 1,3,4-oxadiazole hybrids was designed and synthesized via a multistep synthetic route [7], yielding good yields and characterized by spectroscopic techniques, confirming the successful construction of the target framework. The biological evaluation of these compounds is planned to explore their potential as novel pharmacological agents. Other details will be debated during the presentation.

Scheme:



References:

1. A Gujar, K Danao and U Mahajan, Int. J. Pharm. Chem. 10, 2020, 5474.
2. A Dwivedi, S Rawat, V Kumar, N Kumar, V Kumar, R Yadav, S Baranwal, A Prasad and V Kumar, Curr. Cancer Drug Target 23, 2023, 278-292.
3. P Corona, S Piras, R Ibba, F Riu, G Murineddu, G Sanna, S Madeddu, I Delogu, R Loddo, and A Carta, Open Med. Chem. J. 14, 2020, 83-98.
4. T Glomb and P Swiatek, Int. J. Mol. Sci. 22, 2021, 6979.
5. M Salem, K El-Adl, A El-morsy and H Abulkhair, RSC Adv. 15, 2025, 32778.
6. T Chaudhary, P Upadhyay, Neuro Quantology 20, 2020, 2917-2931.
7. A Mermer, M Bulbul, S Kalender, I Keskin, B Tuzun, O Eyupoglu, J. Mol. Liq. 359, 2022, 119264.

P-14

A Facile Synthesis of Azepino-Fused Porphyrins with Enhanced Absorption as Singlet Oxygen Generators

Ankit Yadav, Narshimha Verma, Dalip Kumar

Department of Chemistry, BITS Pilani, Pilani Campus, Rajasthan-333031, India
E-mail: p20240421@pilani.bits-pilani.ac.in

Extending the π-system of porphyrinoids unlocks unique electronic and optical properties. Such designer molecules are emerging as key materials for next-generation technologies, including NIR displays, solar energy harvesting, advanced optical devices, targeted photodynamic therapy, and molecular electronics.[1] The fusion of a hetero-aromatic segment directly to the porphyrin macrocycle is one of the promising methods to expand electronic conjugated systems.[2] Therefore, several research groups have focused on the synthesis and chemical transformation of porphyrins into new derivatives with improved features that may turn them into possible candidates for different applications.[3] Our group has recently developed efficient protocol for the fusion of pyrrolo- and indolo[1,2-a]quinoxalino-appended porphyrins via I(III) mediated oxidative cyclization.[4] In continuation of our efforts herein,[5] we developed a high yielding protocol for synthesis of imidazo-azepine-fused porphyrins *via* Iodine(III)-promoted oxidative intramolecular cyclization of readily accessible *β*-imidazole/benzimidazole substituted porphyrins. Iodine(III) reagents have emerged as highly attractive tools in organic synthesis, offering a combination of remarkable stability, ready availability, and environmentally benign character.[6] The prepared *N*-heterocycle annulated porphyrinoids with structural rigidity and extended conjugation are of potential interests in photodynamic therapy (PDT) and optoelectronic applications.[7] The electronic absorption spectra of the fused porphyrins displayed a sharp and intense Soret band between 440–460 nm, while prominent Q-bands appeared in 550-750 nm region, consistent with π-π^* transitions.[8] Interestingly, zinc(II)-metalated imidazoazepine-fused porphyrin exhibited a significantly enhanced singlet oxygen quantum yield ($\Phi_\Delta \approx 0.78$ in DMF), which is much higher than that of the standard zinc tetraphenylporphyrin (ZnTPP, $\Phi_\Delta \approx 0.53$).[9] This study thus establishes azepine-fused porphyrins as promising next-generation functional chromophores with potential biomedical and materials relevance.[10] The detailed synthesis, characterization and photophysical studies of azepine-fused porphyrins will be discussed in the conference presentation.

References:

1. Tian, J.; Huang, B.; Nawaz, M. H.; Zhang, W., *Coord. Chem. Rev.* **2020,** *420*, 213410.
2. Tanaka, T.; Osuka, A., *Chem. Soc. Rev.* **2015,** *44* (4), 943-969.
3. Berthelot, M.; Hoffmann, G.; Bousfiha, A.; Echaubard, J.; Roger, J.; Cattey, H.; Romieu, A.; Lucas, D.; Fleurat-Lessard, P.; Devillers, C. H., *Chem. Comm.* **2018,** *54* (43), 5414-5417.
4. Kumar, B.; Khandagale, S. B.; Verma, N.; Pandurang, T. P.; Iype, E.; Kumar, D., *Org. Biomol. Chem.* **2022,** *20* (35), 7040-7046.
5. Taur, P. P.; Verma, N.; Sharma, D.; Kumar, D., *J. Org. Chem.* **2025,** *90* (10), 3570-3579.
6. Yoshimura, A.; Zhdankin, V. V., Chem. Rev. *Chemical Reviews* **2024,** *124* (19), 11108-11186.
7. Lan, M.; Zhao, S.; Liu, W.; Lee, C. S.; Zhang, W.; Wang, P., *Adv. Healthc. Mater.* **2019,** *8* (13), 1900132.
8. Brahmi, J.; Nasri, S.; Saidi, H.; Nasri, H.; Aouadi, K., *ChemistrySelect* **2019,** *4* (4), 1350-1359.
9. Fan, Y.; Zeng, Z.; Shu, H.; Zhou, M.; Xu, L.; Rao, Y.; Gu, T.; Liang, X.; Zhu, W.; Song, J., Org. Chem. Front. *Organic Chemistry Frontiers* **2021,** *8* (21), 6080-6088.
10. Thanjavur, N.; Bugude, L.; Kim, Y.-J., *Biosensors* **2025,** *15* (1), 38.

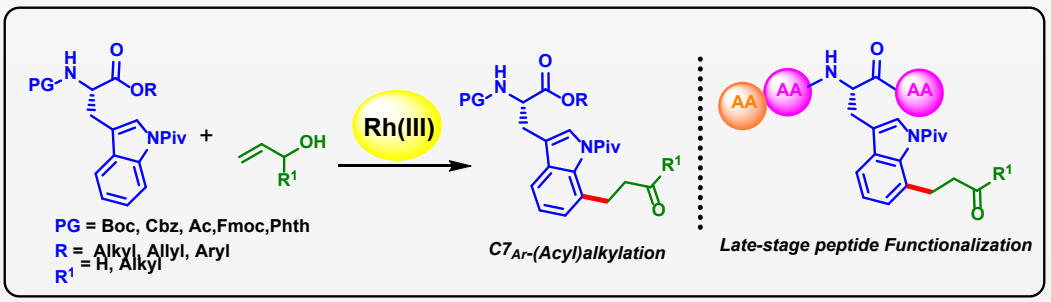
P-15

Rhodium-Catalyzed Regioselective $C7_{Ar}$-(Acyl)alkylation of Tryptophan with Allyl Alcohols and its Late Stage Peptide Exemplification

Disha Harsukhbhai Tank,[a] **Rajeev Sakhuja***[a]

[a]*Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan 333031, India*
Email: p20210409@pilani.bits-pilani.ac.in

Strategic synthesis of unnatural amino acids (UAAs) by functionalization at specified locations of natural amino acids is a key strategy for preparing designer peptides that have showcased profound applications as diagnostics and drug therapeutics in chemical biology [1]. Among the various proteinogenic amino acids, tryptophan (Trp) holds a special stature in cell biology due to its active participation in human body growth, in addition to acting as a chief precursor for the biosynthesis of melatonin, serotonin, vitamin B_6, kynurenine, 3-hydroxykynurenine, tryptamine, and quinolinic and xanthurenic acids [2]. Transition metal-catalyzed late-stage functionalization (LSF) of complex molecules has good site specificity, high tolerance of functional groups, and therefore, providing a straightforward method for an efficient C-H functionalization/macrocyclization of peptides. This strategy provides new distinct peptide scaffolds that are not easily achievable with traditional methods, which has been explored by Shi, Ackermann, Wang, and others. Our group has also disclosed a Rh(III)-catalyzed strategy for the regioselective $C7_{Ar}$-H alkenylation of N-pivaloyl tryptophan with variedly substituted 1,4-benzoquinones and its late stage peptide exemplification [3]. In sharp contrast, the regioselective functionalization of tryptophan with inexpensive allyl alcohols that are often used for alkylation, alkenylation and annulation of (hetero)arenes, remains unexplored. Herein, we report an efficient and Pivolyl-directed Rh(II)-catalyzed $C7_{Ar}$-(acyl)alkylation of tryptophan was achieved with allyl alcohol derivatives, furnishing tryptophan-based unnatural amino acids in good yields. Notably, this catalytical system has excellent regioselectivity and high tolerance of functional groups which enable late-stage exemplification. The strategy was successfully accomplished in tryptophan-containing dipeptides, tripeptides in moderate yields. This methodology is distinguished by scalability, and retention of the chiral configuration for tryptophans motifs.



References:

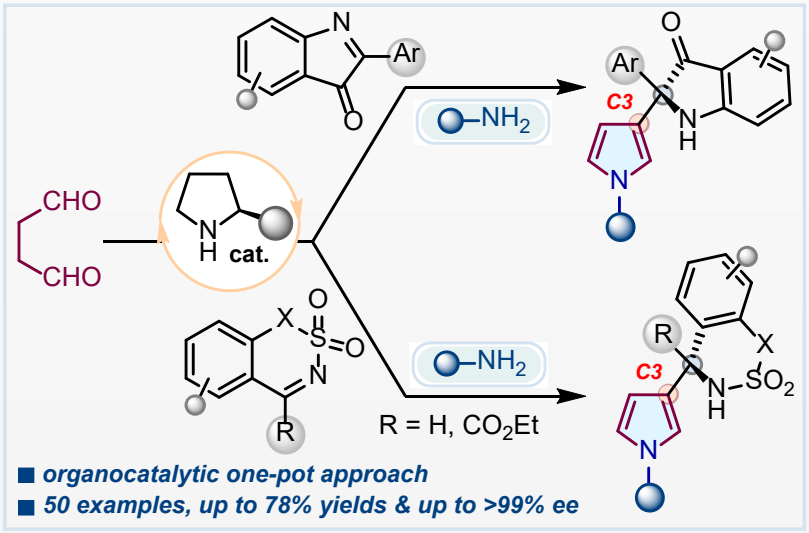
1. D. J. Drucker, Nat. Rev. Drug Discov., 2020, 19, 277.
2. a) E. M. Phizicky and S. Fields, Microbiol. Rev., 1995, 59, 94.
   b) L. G. Milroy, T. N. Grossmann, S. Hennig, L. Brunsveld and C. Ottmann, Chem. Rev., 2014, 114, 4695.
3. a) W. Wang, J. Wu, R. Kuniyil, A. Kopp, R. N. Lima and L. Ackermann, Chem., 2020, 6, 3428.
   b) L. Liu, X. Fan, B. Wang, H. Deng, T. Wang, J. Zheng, J. Chen, Z. Shi and H. Wang, Angew. Chem. Int. Ed., 2022, 61,e20220 6177.
   c) D. H. Tank, N. D. Kharat, K. Bajaj, S. S. Panda and R. Sakhuja, Asian J. Org. Chem., 2023, 12, e202300503.

Organocatalyzed Asymmetric Synthesis of 3-Pyrrolyl Methanamines *via* Direct Mannich/Paal-Knorr Reaction Sequence

Atul Jankiram Dolas, Jyothi Yadav, Yadav Kacharu Nagare and Indresh Kumar*

Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031.
E-mail: dolasatul@gmail.com

The inherent complexity of the pyrrole structure, coupled with the need for precise stereo-chemical control presents a formidable challenge to synthetic chemists (Borah et al. [1] and Philkana et al. [2]). Since the C2-substitution of pyrroles typically occurs in good yields, (Hunjan et al. [3]) recent research studies in this area have focused on promoting electrophilic attack at the C3-position by using bulky substituents on the nitrogen atom (Johannsen [4] and Borah et al. [5]). Herein, we reveal an organocatalytic one-pot synthesis of 3-pyrrolyl methanamine in an asymmetric fashion. This study introduces an approach wherein an amine-catalyzed direct Mannich reaction between aqueous succinaldehyde and cyclic imines, followed by a Paal-Knorr reaction with primary amines, connect to furnish regiospecific β-substituted chiral pyrroles. A range of 3-pyrrolyl methanamine scaffolds possessing chiral center were generated in 59-78% isolated yields with excellent enantioselectivity (≥99:1).



REFERENCES

1. B. Borah, K. D. Dwivedi and L. R. Chowhan, RSC advances 11, 2021, 13585.
2. S. C. Philkhana, F. O. Badmus, I. C. Dos Reis and R. Kartika, Synthesis 53, 2021, 1531.
3. M. K. Hunjan, S. Panday, A. Gupta, J. Bhaumik, P. Das and J. K. Laha, The Chemical Records 21, 2021, 715.
4. M. Johannsen, Chemical Communication, 1999, 2233.
5. B. Borah, K. D. Dwivedi and L. R. Chowhan Asian Journal of Organic Chemistry 10, 2021, 2709.
6. A. J. Dolas, J. Yadav, Y. K. Nagare, K. Rangan, E. Iype and I. Kumar, Organic & Biomolecular Chemistry 23, 2025, 98.

P-17

Targeting Ferroptosis Defenses with Phytochemicals: *In Silico* Insights into xCT, GPX4, & FSP1 inhibition

Akash Rao G[1,2], Advait P Dubey[1,2], Vikram Gota[1,2*]

[1]Clinical Pharmacology, Tata Memorial Center, Advanced Center for Treatment, Research and Education in Cancer (TMC-ACTREC), Navi Mumbai, Maharashtra 410210.
[2]Homi Bhabha National Institute, Mumbai, 400094, India.

Ferroptosis, a non-apoptotic, iron-dependent form of regulated cell death characterized by lipid peroxidation has gained attention as a novel strategy for overcoming therapy-resistance in cancer especially in the apoptosis resistant tumors (Zhang et al., [1]). Targeting the major regulators of this pathway including glutathione peroxidase (GPX4), ferroptosis suppressor protein (FSP1), and cystine/glutamate antiporter system xc- (xCT) has shown to be a promising approach to induce ferroptosis (Nakamura et al., [2]). However, clinically viable inhibitors remain limited. In this context, phytochemicals offer a promising resource with vast chemical diversity and inherent biological activities.

In the present study, a large-scale computational screening of phytochemicals was carried out to identify novel compounds that have strong affinity for major ferroptosis regulators. The binding affinities of thousands of phytochemicals against xCT, GPX4 and FSP1 was evaluated through Molecular docking and the potential hit compounds were subsequently assessed using Molecular dynamics (MD) simulations to examine the persistence of binding and affinity in a dynamic environment. Binding free energies were calculated using MM-GBSA prioritizing lead compounds with favorable thermodynamics. Insights into key molecular features contributing to affinity and selectivity were assessed through Structure-activity relationship (SAR) and off-target docking against related proteins was also carried out to evaluate compound specificity. Additionally, drug-likeness and pharmacokinetic profiles of lead compounds were analyzed ensuring their potential translational relevance.

The study is one of the most extensive in silico screenings of natural compound-based inhibitors of ferroptosis providing a rational foundation for experimental validation of top-hit compounds as potential ferroptosis inducers.

References:

1. Liu, X., Zhang, Y., Wu, X., Xu, F., Ma, H., Wu, M., & Xia, Y. (2022). Targeting Ferroptosis Pathway to Combat Therapy Resistance and Metastasis of Cancer. *Frontiers in pharmacology*, *13*, 909821. https://doi.org/10.3389/fphar.2022.909821
2. Nakamura, T., & Conrad, M. (2024). Exploiting ferroptosis vulnerabilities in cancer. *Nature cell biology*, *26*(9), 1407–1419. https://doi.org/10.1038/s41556-024-01425-8

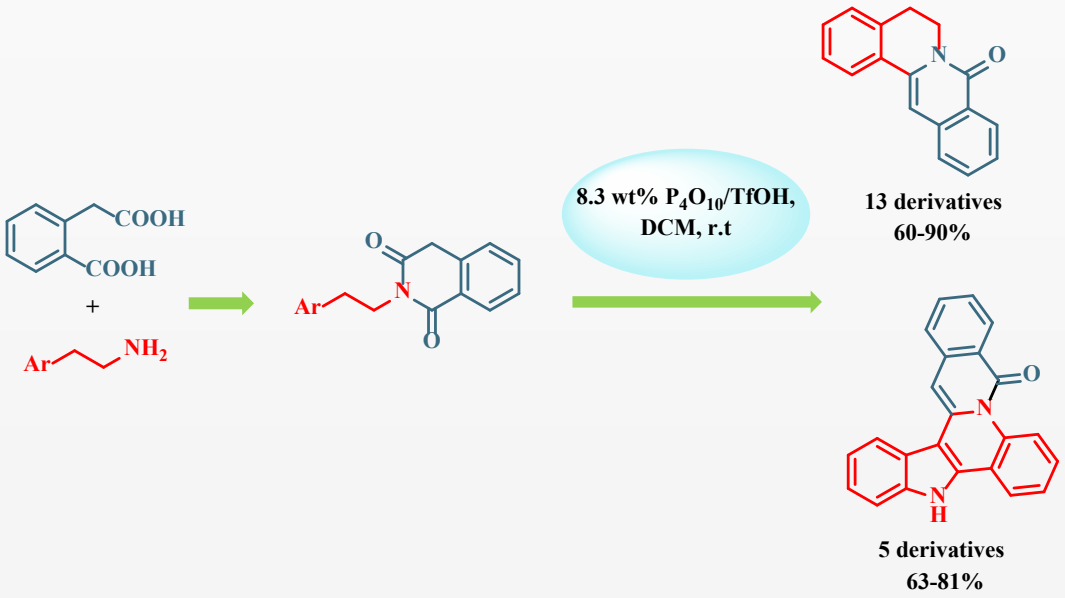
P-18

Triflic Acid Mediated Cascades Towards Indoloquinolines and Protoberberine Alkaloids

Madhuri Gaikwad and S.G. Tilve*

School of Chemical Sciences, Goa University, Taleigao Plateau, 403206, India
**Email: stilve@unigoa.ac.in*

One-pot cascade reactions have become a powerful and sustainable strategy in modern organic synthesis, especially for constructing **complex natural products such as alkaloids**. Alkaloids often possess intricate polycyclic frameworks, making their synthesis both challenging and time-consuming. Cascade reactions provide an efficient way to achieve these complex architectures in a single operational step. In this work, we report the one-pot synthesis of synthetic analogues of naturally occurring indoloquinoline alkaloids and 8-oxoprotoberberine alkaloids *via* domino condensation-cyclization method which can afford the target molecules in moderate to excellent yields. The amide activation of homopthalimides proceeded smoothly in presence of 8.3 wt% of P_4O_{10}/TfOH reagent. This protocol avoids multiple steps of the reaction and offers an efficient and convenient route to complex heterocyclic alkaloids without using either a metal catalyst or solvent.



References

1. S. C. Lu, F. Q. Wen, X. D. Guan, ***Green Chem.***, *23*, **2021**, 8964.
2. M. Lamba, P. R. Singh, S. Bhatt, A. Goswami, ***Green Chem.,*** *26*, **2024**, 448.
3. K. S. Mandrekar, S. G. Tilve, *RSC Adv.*, *12*, **2022**, 17701.

P-19

Selective and Sensitive Detection of 2,4,6 trinitrophenol (TNP) by Imidazolium Salt in Aqueous Medium

Nidhi, Bharti Khungar*

Department of Chemistry, Birla Institute of Technology and Science Pilani, Pilani Campus, Pilani, Rajasthan, 333031, India
***Corresponding Author:** bkhungar@pilani.bits-pilani.ac.in*

Research on nitro explosive detection has significantly increased in relation to environmental protection and national security.[1] Picric acid (PA), or 2,4,6-trinitrophenol (TNP), is categorized as a strong nitro explosive material.[2] TNP is a more powerful explosive than TNT, even though RDX and 2,4,6-trinitrotoluene (TNT) are the most often used nitro-explosives due to their low safety coefficient and rapid detonation velocity. TNP is used as an important component in the dye industries, military, pharmaceutical industries, chemical laboratories, manufacture of rocket fuel as well as in the fireworks industries and forensic investigations.[3] It possesses high water solubility and violent explosive nature that easily contaminates air, soil and water leading to severe health effects on living beings.[4] Many chronic disorders, including gastritis, anemia, liver/kidney malfunction, sycosis, asphyxiation, eye or skin irritation, haemorrhage, nephritis, hepatitis, cancer, and cyanosis, are brought on by direct exposure to TNP.[5] Therefore, it is essential to monitor and detect traces of TNP effectively to protect homeland security, public safety, and human health. Imidazolium salts are a fascinating class of organic materials because they have unique, tuneable features that come from a balanced ratio of cations and anions.[6] Additionally, the imidazole nucleus provides room for one of the N atoms to be quaternized, increasing the hydrophilicity and providing the ability to sense in aqueous media. Herein, we report a highly selective turn-off fluorescent chemosensor, **AQIm** for the detection of TNP. Detection of TNP is also demonstrated in simulated water and soil samples assessing the sensor efficacy.

Keywords: Imidazolium; Aqueous medium; TNP

References:

1. A. S. Tanwar, S. Patidar, S. Ahirwar, S. Dehingia and P. K. Iyer, *Analyst,* 144**,** 2019, 669-676.
2. H. Li, R. Jia and Y. Wang, *Spectrochim. Acta A Mol. Biomol. Spectrosc. ,* 228, 2020, 117793.
3. B. Naskar, A. Bauzá, A. Frontera, D. K. Maiti, C. D. Mukhopadhyay and S. Goswami, *Dalton Trans. ,* 47, 2018, 15907-15916.
4. G. Chakraborty and S. K. Mandal, *ACS omega,* 3, 2018, 3248-3256.
5. B. K. Kundu, S. M. Mobin and S. Mukhopadhyay, *New J. Chem. ,* 43, 2019, 11483-11492.
6. V. Saini, R. Krishnan and B. Khungar, *Photochem. Photobiol. Sci,* 19, 2020, 931-942.

P-20

Synthesis and Photophysical Investigation of Mono-Annulated Indigo Derivatives

Huma and Nitika Grover*

Department of Chemistry BITS Pilani, Pilani Campus, Rajasthan 333031 India
Email: nitika.grover@pilani.bits-pilani.ac.in

Mono-annulated indigo (MAI) derivatives have recently gained attention as potential candidates for singlet-fission materials.[1] Structural modification at the indigo framework via one-sided π-annulation improves molecular planarity, extends π-conjugation, and introduces distinct photophysical properties along with thermal and photostability. [2.3] Despite these interesting features, MAI derivatives remain overlooked and unexplored in the literature. To this end, a series of MAI derivatives was synthesized and investigated to understand the effect of structural modifications on their photophysical behavior. The reaction of aryl acetyl chlorides with indigo in refluxing xylene yielded a mixture of mono- and di-annulated products, whereas selective formation of MAIs was achieved via stoichiometric control of the corresponding acetyl chlorides. Various electron-donating and electron-withdrawing substituents were introduced at the 5- or 6-position of the indigo unit to understand their effect on optical and electronic properties.

The synthesized compounds were characterized using NMR, HRMS, UV-vis spectroscopy, fluorescence spectroscopy, and transient absorption spectroscopy. UV-vis and fluorescence spectra revealed that the aryl ring at the annulation site significantly modulates absorption and emission properties. For example, the thiophene-annulated derivative (**A**) exhibited a 20 nm red shift compared to the corresponding phenyl-annulated compound (**B**). Solvent polarity further affected the HOMO–LUMO gap, as observed from UV–vis spectra.

Density functional theory (DFT) calculations supported the experimental findings, showing reduced HOMO–LUMO gap and enhanced charge delocalization upon annulation. Overall, MAI derivatives integrate classical dye chemistry with new photoactive materials, providing tunable platforms for organic photovoltaics and optoelectronic devices.[4]

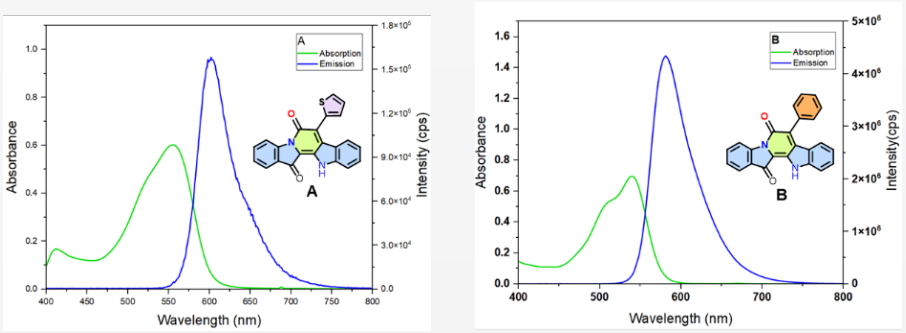


Figure 1. Comparative UV-Vis and Emission spectra for compounds **A** and **B**.

References

1. B Das, S Bora, S Bishen, H Mishra, D Kalita, and A Wahab, J. Phys. Chem. A. 128, 2024, 2565.
2. T Furuyama, M Uchiyama, D Tamura, H Maeda, M Segi, Dyes and Pigments. 193, 2021, 109535.
3. B He, A Pun, D Zherebetskyy, Y Liu, F Liu, L Klivansky, A McGough, B Zhang, K Lo, T Russell, L Wang, Y Liu, J. Am. Chem. Soc. 2014, 136, 42, 15093.
4. M Purdy, J Walton, K Fallon, D Toolan, P Budden, W Zeng, M Corpinot, D Bucar, L Turnhout, R Friend, A Rao, H Bronstein, J. Am. Chem. Soc. 145, 2023, 10712.

Potential α-Amylase Inhibitors from Plants for the Treatment of Type 2 Diabetes: An In silico Evaluation

Charmy Kothari[1]*, Manoj Godhaniya[1] and Dhyey Kothari[2]

[1]*Department of Biotechnology, Christ Campus, Rajkot, Gujarat*
[2]*Government Medical College, Bhavnagar, Gujarat*
E-mail: *dr.charmykothari@gmail.com*

.

This research examines the efficacy of phytochemical substances as natural inhibitors of human α-amylase (PDB ID: 1B2Y) for the treatment of type 2 diabetic mellitus (T2DM). Molecular docking was conducted on a collection of 3,320 phytochemicals sourced from 20 medicinal plants and synthetic anti-diabetic agents. The highest-ranked compounds demonstrated enhanced binding affinities (-11.7 to -18.6 kcal/mol) in comparison to the control medication Acarbose (-8.7 kcal/mol). Goyaglycoside-g, Goyaglycoside-e, and Momordicoside R were identified as the most effective inhibitors, with Momordicoside R preferentially interacting with the catalytic residue TYR151. Compounds derived from *Momordica charantia* (Kuguacin M, β-Amyrin, α-Amyrin) and *Azadirachta indica* (Melianoninol, Odoratone) shown significant inhibitory effects. Analysis of contacts revealed many binding mechanisms, including van der Waals forces, hydrogen bonding, and hydrophobic interactions with critical residues like TYR151 and TRP58. ADME investigation revealed the difficulties associated with the low bioavailability of some glycosides, however toxicity projections indicated Melianoninol as a viable option with a favorable efficacy-safety profile. This research corroborates the ethnopharmacological use of *Momordica charantia* and *Azadirachta indica* in the treatment of T2DM and underscores the potential of phytochemicals as safer alternatives to pharmaceutical medications. Subsequent investigations should concentrate on structural modification and sophisticated formulations to improve the bioavailability of these substances. This analysis illustrates the enhanced efficacy of phytochemicals as natural α-amylase inhibitors compared to synthetic drugs, with compounds from *Momordica charantia* and *Azadirachta indica* exhibiting a 2.14-fold superior binding affinity relative to Acarbose. This establishes a basis for the development of safer, bioavailable anti-diabetic therapeutics via computationally guided structural optimization and advanced formulation strategies for clinical application in type 2 diabetes management.

Keywords: Phytochemicals, Type 2 Diabetes, Molecular Docking, *Momordica Charantia, Azadirachta Indica*

P-22

In Silco Simulations: Unveiling The Interactions Of Jev Ns3 Helicase Through Dft, Molecular Docking And Molecular Dynamic Simulations.

Krupali Patil, Vrushali Patil, Ashish Asrondkar.

[a] *Haffkine Institute for Training, Research and Testing, Aacharya Donde Marg, Parel, Mumbai, Maharashtra, India-400012, chemotherapy@haffkineinstitute.org.*

Abstract

Japanese encephalitis is a viral infection that primarily affects the central nervous system.It is transmitted to humans through the bite of infected mosquitoes, especially those found in rural and agricultural areas of Asia. The disease has a significant impact on public health, causing inflammation in the brain and often leading to severe neurological complications or even death. In this paper we report the spectroscopic characterization and reactivity studies on potential ligands using computational techniques such as Molecular Dynamic (MD) simulations and Density Functional Theory (DFT). Comparing the three derivatives computed findings with the conventional drug's yields more insights. Molecular docking study is also performed to scrutinized ligand which having high binding affinity towards desired protein of JEV. After evaluation, the desired ligand has highest binding energy of -9.597 kJ/mole, the graph of RMSD, RMSF, Radius of gyration, SASA indicates stability of protein-ligand in the equilibrated system as compared to standard drug.

Keywords: Encephalitis, Molecular Dynamic (MD) simulations and Density Functional Theory (DFT), JEV.

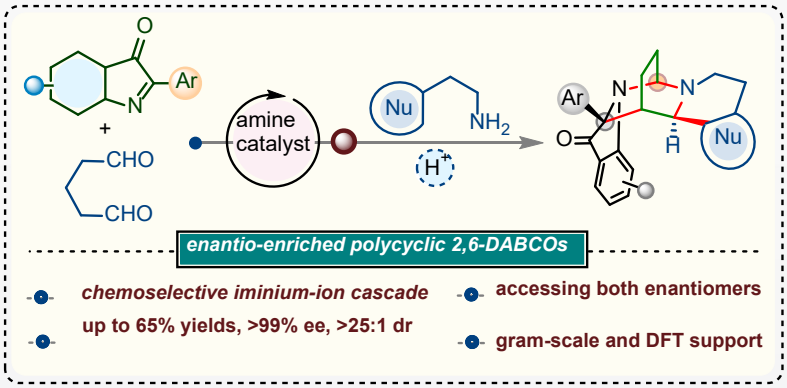
P-23

Organocatalytic Asymmetric Construction of 2,6-Diazabicyclo-[2.2.2]octanes by Harnessing the Potential of 3-Oxindolium Ion Intermediates

Jyothi Yadav, Arun Patel, and Indresh Kumar*

Department of Chemistry, Birla Institute of Technology & Science, Pilani 333031 (Rajasthan)
E-mail: p20220411@pilani.bits-pilani.ac.in

Diazabicyclo[2.2.2]octanes (DABCOs) are a special class of conformationally locked bridging diamines widely sought as catalysts and an integral part of many natural and medicinally important scaffolds.[1-2] Due to its structural complexity and sensitivity of the bridged aminal junction, the asymmetric access of 2,6-diazabicyclo[2.2.2]octane (2,6-DABCO) is still not explored.[3-4] Due to the scarcity of methods in this direction, developing 2,6-DABCOs by overcoming the existing limitations of finding substrates with suitable functionalities to engage in double aza-cyclization through sequential iminium ion trapping is highly valuable. Our novel metal-free approach delivers polycyclic chiral 2,6-DABCOs *via* stereoselective amine catalyzed [4+2] annulation and acid-mediated Pictet-Spengler/intramolecular aza-cyclization. This one-pot domino process, leveraging in situ 3-oxindolium ion intermediates for the first time, constructs five new bonds and four stereocenters, yielding fused 2,6-DABCOs in high yield and enantioselectivity.[5]



Scheme 1: One-Pot Sequential Aza-Cyclization to Access Polycyclic Chiral 2,6-DABCOs

Reference:

1. Z. Halimehjani, and E. Badali, RSC Adv. 9, 2019, 36386.
2. X. Zhang, Nat. Prod. Rep. *41*, 2024, 784.
3. J. A. Leitch, T. Rogova, F. Duarte, and D. J. Dixon, Angew. Chem. Int. Ed. *59*, 2020, 4121.
4. Q. Cai, C. Zheng, and S.-L. You, Angew. Chem. Int. Ed. *49*, 2010, 8666.
5. J. Yadav, A. Patel, A.J. Dolas, E. Iype, K. Rangan, and I. Kumar, Angew Chem Int. Ed. 64, 2025, e202416042.

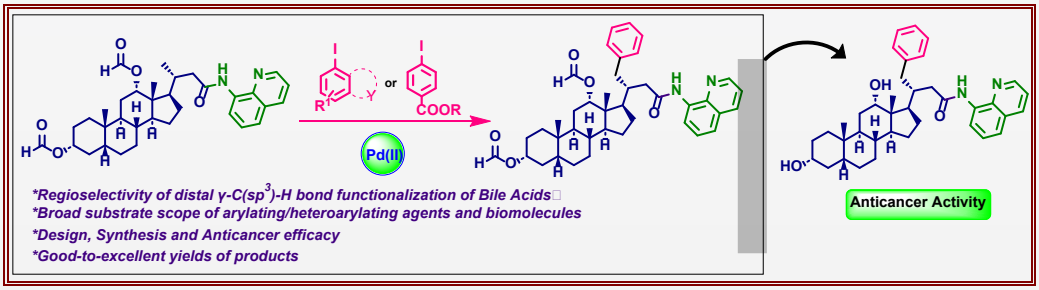
P-24

Synthesis of novel bile acid scaffolds via Pd-catalyzed Sp^3C-H distal arylation : Design, Synthesis and Anticancer efficacy

Somnath Arjun Borade,[a] **Deepak Chitkara**,[d] **Rajeev Sakhuja***[a]

[a]*Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan 333031, India*
[c]*Department of Pharmacy, Birla Institute of Technology & Science, Pilani, Rajasthan 333031, India*
Email: p20210411@pilani.bits-pilani.ac.in

Bile acids are the acidic sterols present in physiological enterohepatic circulation that have proven to be one of the desirable scaffolds for anticancer drug development. In addition to drug delivery applications exhibited by bile acid conjugates with chlorambucil, tamoxifen, floxuridine, foscan, artemisinin, dihydroartemisinin, a few bile acids and their taurine conjugates have been identified as potent inhibitors of apoptosis in different cell types [1]. Interestingly, the previous synthetic wisdom collated for the construction of modified bile acids mainly focused on commencement of functional group inter-conversion(s) either at/nearer to the hydroxyl groups in ring A/C or application of conventional strategies to undergo A/C-ring expansion, [2] while the alteration in bile acid scaffold *via* directing group-assisted site-selective C(sp^3)-H functionalization, such as *β*-alkynylation, *β*-hydroxylation and *α*-oxidation have been reported only to a limited extent [3]. Our group recently did *β*-arylation of bile acids [4]. Embracing the rich possibility our group designed of distal arylation at C(sp^3)-H bond with aryl iodides in bile acids, we successfully developed a Pd(II)-catalyzed strategy for the (hetero)arylation of unactivated C(sp^3)–H bonds in bile acids with (hetero)aryl iodides. Parallel to this, different natural products like menthol and geraniol, amino acids (tyrosine and phenylalanine), drug like paracetamol and steroids (cholesterol) have great importance in biological activity. After Further, the 8-aminoquinoline (AQ) auxiliary was easily removed to obtain a distal arylation of bile acid derivatives. All the synthesized γ-arylated compounds and hydroxyl free compounds were studied for their anticancer activity against MCF-7 (human breast adenocarcinoma cell line) respectively. Furthermore, these compounds were tested on a normal human embryonic kidney cell line (HEK 293), indicating cell viability above 75%, thus confirming they are non-toxic to normal cells and it is cancer specific. Then also extend this work upto apoptic study. Interestingly, all the products were as evident from the ^{1}H NMR. Hence, the overall strategy can be considered as an excellent approach for producing distal aryl bile acids in a regioselective fashion.



REFERENCES

1. (a) M. L. Navacchia, E. Marchesi and D. Perrone, Molecules 25, 2020. (b) C. Faustino, C. Serafim, P. Rijo and C. P. Reis, Expert Opin Drug Deliv. 13, 2016, 1133.
2. (a) J.-Y. Lee, S.-J. Chung, H.J. Cho and D.D. Kim, Eur. J. Pharm. Biopharm. 94, 2015, 532. (b) D. S. Agarwal, H. S. Anantaraju, D. Sriram, P. Yogeeswari, S. H. Nanjegowda, P. Mallu and R; Sakhuja, Steroids 107, 2016, 87.
3. Y. Ano, M. Tobisu and N. Chatani, J. Am. Chem. Soc. 133, 2011, 12984.
4. S. A. Borade, S. Naharwal, H. Bhambri, S. Mandal, K. Bajaj, D. Chitkara, and R. Sakhuja. Organic & Biomolecular Chemistry. 2023.

P-25

Virtual Screening Using ML Model To Find Novel KDM4C Inhibitors For The Treatment Of Cancer

Timir Naskar, Debashis Mandal*

Department of Chemistry and Biochemistry, Thapar Institute of Engineering & Technology, Patiala-147004, Punjab, India
Email: debasish.mandal@thapar.edu

Abstract:

Histone H3 lysine residues (H3K9me3/2 and H3K36me3/2) are demethylated by the lysine demethylase enzyme KDM4C. Its overexpression has been linked to tumour proliferation in several malignancies, including colorectal, breast, and prostate cancer. The majority of current inhibitors exhibit poor selectivity, low permeability, and adverse pharmacokinetics. Using an integrated virtual screening strategy that combines pharmacophore modelling, machine learning (ML)-based categorisation, and molecular docking techniques, this study aims to identify new KDM4C inhibitors.

Using Pharmit, ligand-based pharmacophore modelling was done to find inhibitors. KDM4C (ChEMBL6175) bioactivity data were curated (n = 874), and substances were categorised as either inert (IC_{50} > 1000 nM) or active (IC_{50} ≤ 1000 nM). RDKit and Mordred were used to calculate a total of 2D molecular descriptors, which were then reduced using feature reduction (low variance < 0.2, correlation > 0.8). Several machine learning algorithms (RF, KNN, GB) were subjected to forward feature selection and GridSearchCV-based hyperparameter optimisation. Y-randomisation, 5-/10-fold cross-validation, and external test sets were used to evaluate the model's performance. Accuracy, sensitivity, specificity, ROC-AUC, and Cohen's kappa were among the evaluation criteria. Chemical space analysis based on Euclidean distance was used to identify the applicability domain. Drug-likeness and toxicity filters (Lipinski RO5, PAINS, Brenk, QED, SA score) were used to filter predicted active compounds. Molecular dynamics (MD) simulation using AMBER 2013 was used to evaluate stability and binding free energy after top-ranked hits were docked with KDM4C (PDB ID: 4XDO) using AutoDock Vina. The optimised machine learning model successfully distinguished between active and inactive substances with high balanced accuracy and ROC-AUC values. During MD simulations, a number of new scaffolds showed stable protein–ligand interactions, excellent pharmacokinetic characteristics, and significant binding affinity toward KDM4C.These results show that ML-driven virtual screening, when combined with molecular docking and pharmacophore modelling, offers a reliable and economical method for finding specific KDM4C inhibitors for the development of anticancer drugs.

Reference:

1. Ghosh, D.; Lo, J.; Morton, D.; Valette, D.; Xi, J.; Griswold, J.; Hubbell, S.; Egbuta, C.; Jiang, W.; An, J.; Davies, H. M. L. Novel Aromatase Inhibitors by Structure-Guided Design. *J Med Chem* **2012**, *55* (19), 8464–8476. https://doi.org/10.1021/jm300930n.
2. Thinnes, C. C.; England, K. S.; Kawamura, A.; Chowdhury, R.; Schofield, C. J.; Hopkinson, R. J. Targeting Histone Lysine Demethylases — Progress, Challenges, and the Future. *Biochimica et Biophysica Acta (BBA) - Gene Regulatory Mechanisms* **2014**, *1839* (12), 1416–1432. https://doi.org/10.1016/j.bbagrm.2014.05.009.
3. Nielsen, A. L.; Kristensen, L. H.; Stephansen, K. B.; Kristensen, J. B. L.; Helgstrand, C.; Lees, M.; Cloos, P.; Helin, K.; Gajhede, M.; Olsen, L. Identification of Catechols as Histone–Lysine Demethylase Inhibitors. *FEBS Lett* **2012**, *586* (8), 1190–1194. https://doi.org/10.1016/j.febslet.2012.03.001.

P-26

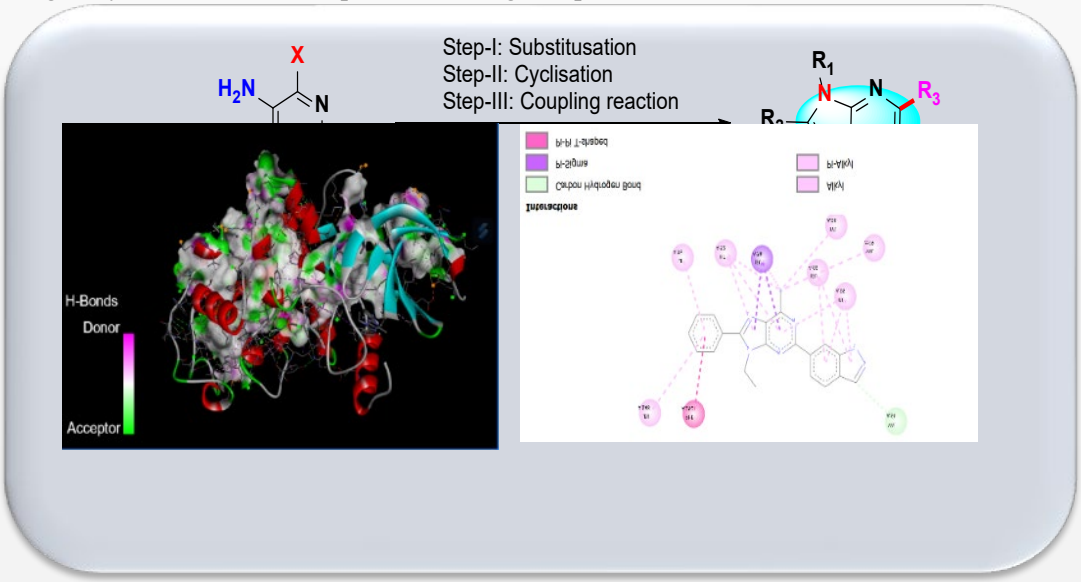
Purine Derivatives: Structural Diversity, Synthesis, and Biological Applications

Vishal Pathak [a], Mayank K. Pandya [*a]

Dr. Subhash University, Junagadh -362001, Gujarat, India
Email: vishalpathak263@gmail.com, mayank.pandiya@dsuni.ac.in

ABSTRACT

Purine derivatives have emerged as a cornerstone of modern drug discovery due to their structural similarity to naturally occurring nucleobases and their ability to interact with a wide range of biological targets. The purine ring system composed of a fused imidazole and pyrimidine ring is a privileged scaffold in medicinal chemistry, found in many FDA-approved drugs used to treat cancer, viral infections, autoimmune diseases, and parasitic infections. This poster highlights recent advances in the design, chemical synthesis, and pharmacological evaluation of purine-based therapeutics. Emphasis is placed on structure–activity relationship (SAR) studies that guide the rational modification of the purine nucleus at key positions (C2, C6, C8, and N9), optimizing their potency, selectivity, and pharmacokinetic profiles. Examples include 6-mercaptopurine and azathioprine (anticancer/immunosuppressive agents), acyclovir and tenofovir (antiviral agents), and emerging kinase inhibitors targeting oncogenic signalling pathways. Innovative synthetic methodologies such as metal-catalysed cross-coupling, microwave-assisted synthesis, and click chemistry have expanded the chemical space around purines, enabling the rapid generation of analogues with diverse biological activities. In parallel, advances in computational drug design and molecular docking have facilitated the identification of novel purine-based ligands with high affinity and selectivity for nucleic acid-processing enzymes, kinases, and purine-binding receptors.



Keywords: Purine derivatives, Medicinal chemistry, Antiviral agents, Anticancer drugs, Molecular docking.

References

1. ones, G. (2009). Pyrimidines and purines in medicinal chemistry. *Medicinal Research Reviews*, 29(3),581–609. https://doi.org/10.1002/med.2014.
2. De Clercq, E. (2004). Antiviral drugs in current clinical use. *Journal of Clinical Virology*, 30(2), 115– 133. https://doi.org/10.1016/j.jcv.2004.01.00.
3. Robak, T., & Lech-Maranda, E. (2004). Purine analogs as immunosuppressive and anticancer age, current medicinal chemistry, 11(16), 1973–1989. https://doi.org/10.2174/0929867043364827.

P-27

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

Dishant Pahelajani Jeet Bhatt *Dr. Mayank Pandya[1]

Centre for Research and Development, Dr. Subhash University, Junagadh (362001), Gujarat, India.
Email – mayank.pandya@dsuni.ac.in

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

References

1. Hong, D.; Hai-Bo, Y.; Yong, Q. L,; Xin, Z.; Zhen-Fang, Q.; Ting, W.; Jian, X. F.; Synthesis and bioactivity of novel trifluromethylated pyarzole oxime ether derivative containing pyridyl moiety.ARKIVOC 2009, 12,126-142
2. Patel, N.B.; Agravat, S.N.; Shaikh, F.M. Synthesis and antimicrobial activity of new pyridine derivatives-I. Med. Chem. Res. 2011, 20, 1033–1041.
3. Srivastava, A.; Pandeya, S.N.; "Indole" a versatile nucleuse in pharmaceutical field. Int. J. Curr.Pharm. Rev. Res. 2011, 4, 5–8.
4. Paronikyan, E.G.; Noravyan, A.S.; Dzhagatspany, I.A.; Nazaryan, I.M.; Paronikyan, R.G. Synthesis and anticovulsant activity of isothiazolo-[5,4-b]-pyrano (thiopyrano)-[4,3-d]-pyridine and isothiazolo [4,5-b]-2,7-naphthyridine derivatives. Pharm. Chem. J. 2002, 36, 465–467.
5. Bernardino,A.M.R.;DeAzevedo,A.R.; Pinheiro,L.C.D.;Borges,J.C.;Carvalho,V.L.; Miranda,M.D.; DeMeneses,M.D.F.; Nascimento, M.; Ferreira, D.; Rebello, M.A.; et al. Syntehsis and antiviral activity of new 4-(phenylamino)/4- [(methylpidin2-yl) amino]-1- phenyl-1H-pyrazolo- [3,4-b]-pyridine-4-carboxylic acid derivatives. Med. Chem. Res. 2007, 16, 352–369.
6. Tucker, T.J.; Sisko, J.T.; Tynebor, R.M.; Williams, T.M.; Felock, P.J.; Flynn, J.A.; Lai, M.;Liang, Y.; McGaughey, G.; Liu, M.; et al. Discovery of 3-{5[(6-Amino-1H-pyrazolo-[3,4-b]-pyridine-3-yl)methoxy]-2- chlorphenoxy}-5-chlorobenzonitrile (MK-4965): A potent, orallybioavailable HIV-1 non-nucleoside reverse transcriptase inhibitor with improved potency against key mutant viruses. J. Med. Chem. 2008, 51, 6503–6511.
7. Mamolo, M.G.; Zampieri, D.; Falagiani, V.; Vio, L., Fermeglia, M.; Ferrone, M.; Pricl, S.; Banfi, E.; Scialino, G. Antifungal and antimycobacterial activity of new N1-[1-aryl-2-(1Himidazol-1-yl and 1H- 1,2,4-triazol-1-yl)-ethylidene]-pyridine-2- carboxamidrazone derivatives:A combined experimental and computational approach. ARKIVOC 2004, 5, 231–250.
8. M.S. Karthikeyan,; B.S. Holla,; N.S. Kumari, Synthesis and antimicrobial studies on novel chloro-fluorine containing hydroxy pyrazolines, Eur. J. Med. Chem.42 (2007) 30e36.
9. M.E. Shoman,; M.A. Aziz,; O.M. Aly,; H.H. Farag,; M.A. Morsy, Synthesis and investigation of anti-inflammatory activity and gastric ulcerogenicity of novel nitric oxide-donating pyrazoline derivatives, Eur. J. Med. Chem. 44 (2009) 3068e3076
10. K.S. Girisha,; B. Kalluraya,; V. Narayana,; Padmashree, Synthesis and pharmacological study of 1-acetyl/propyl-3-aryl- 5- (5- chloro-3-methyl-1-phenyl-1Hpyrazol-4-yl)-2-pyrazoline, Eur. J. Med. Chem. 45 (2010) 4640e4644.
11. G.T. Zitouni,; P. Chevallet,; F.S. Kiliç,; K. Erol, Synthesis of some thiazolylpyrazoline derivatives and preliminary investigation of their hypotensive activity, Eur. J. Med. Chem. 35 (2000) 635e641.
12. T.S. Jeong,; K.S. Kim,; J.R. Kim,; K.H. Cho,; S. Lee,; W.S. Lee, Novel 3,5-diaryl pyrazolines and pyrazole as low-density lipoprotein (LDL) oxidation inhibitor, Bioorg. Med. Chem. Lett. 14 (2004) 2719e2723.

P-28

Indole-3-Carbinol Inhibits Angiogenesis in the Chick Chorioallantoic Membrane Model

Subhalaxmi Pattanayak and Priya Ranjan Debata

Department of Zoology, Maharaja Sriram Chandra Bhanja Deo University, Takatpur, Baripada-757003, Mayurbhanj, Odisha
Email: pbs.laxmi97@gmail.com, prdebata@gmail.com

Angiogenesis, the process of forming new blood vessels, is vital for normal growth and tissue repair but also contributes to disease progression in cancer, chronic inflammation, and diabetic complications. Natural plant-derived compounds are increasingly recognized as potential anti-angiogenic agents because of their ability to act on multiple molecular targets while maintaining low toxicity (Aggarwal et al., 2006). Indole-3-carbinol (I3C), a phytochemical found in cruciferous vegetables, is well known for its anticancer and antiproliferative effects, but its direct influence on angiogenesis has not been fully elucidated (Bradlow et al., 1991; Sarkar & Li, 2004). In this study, the chick chorioallantoic membrane (CAM) assay was employed to evaluate the anti-angiogenic activity of I3C (Ribatti, 2016). Fertilized chicken eggs were incubated and exposed to different concentrations of I3C, followed by microscopic examination of vascular development. Treatment with I3C resulted in a marked reduction in blood vessel branching and overall vascular density in a concentration-dependent manner. These results suggest that I3C effectively suppresses neovascularization and may serve as a promising candidate for the development of novel therapies targeting pathological angiogenesis.

Keywords: Indole-3-carbinol, angiogenesis, chick CAM model, phytochemicals, cancer therapeutics

References

1. Aggarwal, B. B., Ichikawa, H., Garodia, P., Weerasinghe, P., Sethi, G., Bhatt, I. D., Pandey, M. K., Shishodia, S., & Nair, M. G. (2006). From traditional Ayurvedic medicine to modern medicine: identification of therapeutic targets for suppression of inflammation and cancer. *Expert Opinion on Therapeutic Targets*, *10*(1), 87–118.
2. Bradlow, H. L., Michnovicz, J. J., Telang, N. T., & Osborne, M. P. (1991). Effects of dietary indole-3-carbinol on estradiol metabolism and spontaneous mammary tumors in mice. *Carcinogenesis*, *12*(9), 1571–1574.
3. Ribatti, D. (2016). The chick embryo chorioallantoic membrane (CAM). A multifaceted experimental model. *Mechanisms of Development*, *141*, 70–77.
4. Sarkar, F. H., & Li, Y. (2004). Indole-3-carbinol and prostate cancer. *The Journal of Nutrition*, *134*(12), 3493S-3498S.

P-29

Peptide-Based Antiviral Design: Computational Repurposing of α-Bungarotoxin Against Rabies

Vrushali Patil, Harshada Sawant, Ashish Asrondkar.

[a] *Haffkine Institute for Training, Research and Testing, Aacharya Donde Marg, Parel, Mumbai, Maharashtra, India-400012, chemotherapy@haffkineinstitute.org.*

This study explores a computational approach to the design and optimization of alpha-bungarotoxin (α-BGT) peptide analogues aimed at inhibiting the rabies virus (RabV). Alpha-bungarotoxin, a neurotoxin known for its strong interaction with nicotinic acetylcholine receptors, serves as the structural basis for developing novel peptide variants with potential antiviral activity. By employing molecular docking and molecular dynamics simulations, the research predicts and evaluates the interactions between the designed peptides and key RabV proteins, particularly the glycoprotein responsible for viral attachment and entry into host cells.

Through structure-based drug design, the α-BGT analogues were computationally engineered to improve binding affinity, stability, and selectivity. The simulation outcomes revealed that several designed peptides exhibited strong and stable interactions with the RabV glycoprotein and phosphoprotein, suggesting their potential to interfere with viral entry and replication mechanisms. These findings highlight the promise of the designed peptides as lead candidates for further in vitro and in vivo investigations.

Overall, this research underscores the effectiveness of in silico methodologies in accelerating antiviral drug discovery and provides a foundation for the development of targeted therapeutics against the rabies virus.

Keywords: Rabies, Peptide, Alpha-Bungarotoxin, Glycoprotein, MDS, HADDOCK

P-30

Integrating Molecular Docking, DFT, and ADME–Tox Predictions to Identify Imidazole–Benzothiazole Hybrids as Selective Estrogen Receptor (ERα) Inhibitors

Ashish Asrondkar, Vrushali Patil

Haffkine Institute for Training, Research and Testing, Aacharya Donde Marg, Parel, Mumbai, Maharashtra, India-400012, chemotherapy@haffkineinstitute.org.

Abstract:

Breast cancer continues to be a leading cause of cancer-related death for women worldwide, highlighting the urgent need for effective and targeted therapeutic agents. The diverse biological actions of imidazole and benzothiazole scaffolds make them well-known favored structures in medicinal chemistry. A distinguishing series of imidazole–benzothiazole hybrids was rationally synthesized and developed in this study. The synthesized compounds' structures were verified by mass spectrometry, NMR, and infrared spectroscopy. An extensive investigation of these compounds was conducted, which included in vitro cytotoxicity screening against MCF-7 breast cancer cells, molecular docking, DFT-based quantum chemistry investigations, and ADME predictions. Among the tested compounds, S1.4 demonstrated notable biological potential, exhibiting a strong binding affinity (–6.677 kcal/mol) toward the estrogen receptor alpha (ERα, PDB ID: 2RD0) through interactions with key residues GLU-172, LYS-271, and ARG-818. DFT calculations revealed a narrow HOMO–LUMO energy gap (ΔE = 0.17794 eV), indicating favorable electronic characteristics for biological reactivity. In vitro cytotoxic assays showed that S1.4 displayed potent anticancer activity (IC_{50} = 26.7 µg/mL), surpassing the standard drug doxorubicin (IC_{50} = 74.2 µg/mL). Additionally, antioxidant activity of S1.4 (IC_{50} = 7.94 µg/mL) exceeded that of ascorbic acid. ADME profiling revealed no carcinogenic or mutagenic risks, high gastrointestinal absorption, and ideal drug-likeness. According to these results, S1.4 is a potential imidazole–benzothiazole-based scaffold for the treatment of breast cancer and needs more in vivo testing and structural improvement.

Keywords: Imidazole-Benzothaizole, Breast cancer, ERα, Molecular docking, DFT,

P-31

Synthesis, X-ray Structural Studies with DFT calculation of carboximidamide-substituted pyridone scaffold

Kumari Suprita, Ashoke Sharon*

Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, 835215
Email: asharon@bitmesra.ac.in

Abstract

This study reports the synthesis and structural characterisation of a novel heterocyclic compound featuring a carboximidamide-substituted pyridone scaffold. The synthesis was achieved via a two-step process: initially, a condensation reaction under basic conditions produced a cyano intermediate with a pyridone core. Subsequently, this intermediate was converted into an amidoxime derivative using hydroxylamine hydrochloride and triethylamine, maintaining the basic environment. Structural analysis using single-crystal X-ray diffraction revealed a pyridone ring system bearing amino, hydroxyl, and methylthio functionalities, which may suggest potential biological activity. The molecular geometry was confirmed, and a network of stabilising non-covalent interactions was identified, including intramolecular hydrogen bonds and π-π stacking interactions. Hirshfeld surface analysis, performed with Crystal Explorer, indicated that H…H contacts (43.5%) predominantly contribute to crystal packing, followed by O…H (9.3%), C…H π (8.5%), and N…H (6%) interactions. Density Functional Theory (DFT) calculations using B3LYP/6-311++G(d,p) indicated a moderate HOMO-LUMO gap, implying balanced reactivity and stability. Preliminary ADME predictions suggest favourable pharmacokinetic properties, positioning this scaffold as a promising candidate for further biological activity studies.

Keywords: Amidoxime, Structural studies, Single Crystal X-ray studies

P-32

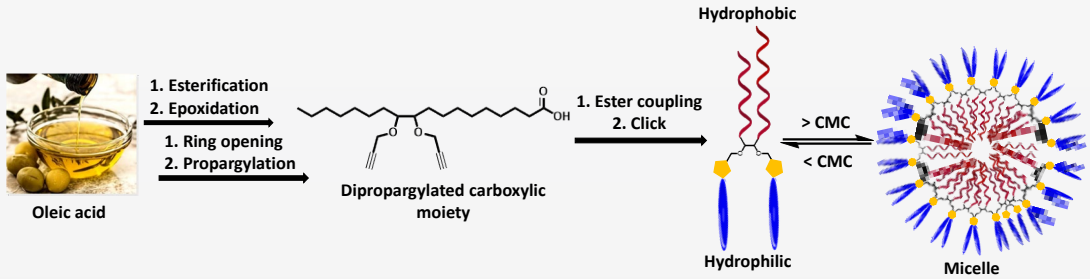
Development of Oleic Acid-Based Gemini Amphiphilic Architectures for Efficient Drug Transport

Sudhanshu Vats, Saumya Shukla, S. K. Sharma*

Department of Chemistry, University of Delhi, Delhi-110007, India
sksharma@chemistry.du.ac.in

Abstract

The major obstacles in the area of drug delivery are the low aqueous solubility of drug, non- targeted delivery, and less duration of circulation in the blood. In the past few decades the contribution of nano-transporters have been recognized worldwide for addressing these challenges and improving the overall drug efficacy. As a part of our ongoing research program to design and develop efficient drug delivery agents,[1] herein we report the synthesis of a newer type of non-ionic Gemini amphiphilic architectures. These amphiphiles possess desirable physicochemical properties to enable them to form nano-sized aggregates in aqueous medium allowing them to act as promising drug transporters.[2] For this study we have used commercially available and biocompatible oleic acid as a starting material which is suitably modified at its olefinic bond using epoxidation followed by the opening of the epoxide ring to yield a diol. The diol was propargylated and the carboxylic acid group esterified with hydroxy alkyl/perfluoro chain to develop a hydrophobic core. Further, the hydrophobic core was clicked coupled with hydrophilic monomethoxy polyethylene glycol (mPEG) azide (M_n: 550/750) and lactose azide. The decision to incorporate polyethylene glycol and lactose was made on the basis that its derivatives are highly biocompatible and are frequently used in drug delivery systems to improve the solubility, immunogenicity, toxicity, and regulated drug release of therapeutic agents.[3] The physicochemical characterization of the synthesized amphiphiles was carried using dynamic light scattering and spectroscopic tools. The encapsulation and nano-transport potential studies were carried using fluorescence spectroscopy. The preliminary results will be discussed during the poster presentation.



References:

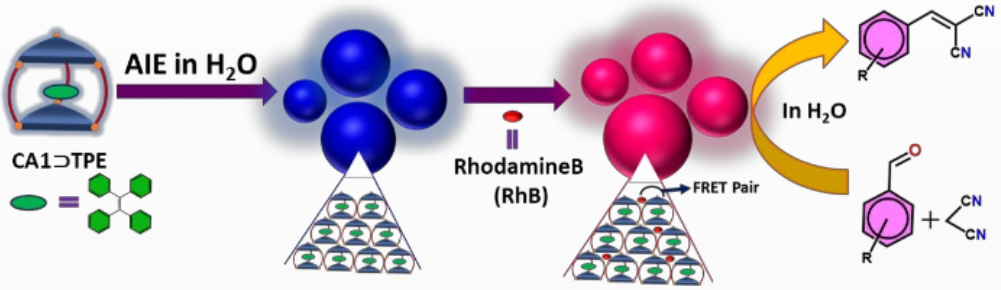
1. Gupta, S.; Tyagi, R.; Parmar, V. S.; Sharma, S. K.; Haag, R. Polymer, 2012, 53, 3053-3078.
2. Rashmi; Singh, A. K.; Achazi, K.; Ehrmann, S.; Böttcher,C.; Haag,R.; Sharma,S.K. Polymer Chemistry, 2022, 11, 6772-6782.
3. Verma, D.; Rashmi; Rathore, D.; Achazi, K.; Schade,B.; Haag, R.;Sharma, S. K. ACS Applied Polymer Materials, 2022, 4, 8269-8276.

P-33

Design and Synthesis of Organic–Imine Cage-Based Artificial Light-Harvesting System for Photocatalytic Applications

Chanchala Kumari, Dr. Atul Kumar*

Chemistry, Birla institute of technology Mesra, Ranchi Jharkhand
Email id: chanchalakumari8986@gmail.com



Recent advancements in supramolecular chemistry have emphasized the potential of dynamic covalent chemistry (DCC) in constructing complex three-dimensional organic cage structures with high efficiency and precision Wang et al. [1]. Traditional synthetic methods often faced challenges such as low yields and poor structural control. By utilizing DCC, particularly with multifunctional amine and aldehyde components, robust and self-correcting organic amine cages can now be reliably synthesized. Here, we report the design and synthesis of a supramolecular [2 + 3] triazine-based organic-imine cage (**CA1**) via dynamic covalent amine condensation featuring tunable cavity sizes and diverse functional groups, confirmed by NMR spectroscopy and mass spectrometry (MS) Kumari et al. [2]. Encapsulation of an aggregation-induced emissive fluorophore, tetraphenylethylene (TPE), forming a 1:1 host–guest complex (CA1⊃TPE). The rigid cage framework effectively restricts the intramolecular motion of TPE, suppressing non-radiative decay and producing bright blue emission. In the aggregated state, CA1⊃TPE acts as an efficient energy donor to Rhodamine B (RhB) through Förster resonance energy transfer (FRET). The resulting artificial LHS (CA1⊃TPE@RhB) demonstrates remarkable photocatalytic performance in the visible-light-induced Knoevenagel condensation between substituted benzaldehydes and malononitrile in green aqueous media, yielding significantly enhanced conversions compared to individual catalysts. This study provides a rational supramolecular design strategy that integrates AIE-active chromophores within organic cages to construct efficient, photostable, and environmentally benign artificial photosynthetic systems for visible-light photocatalysis. Beyond fundamental interest, these cages can be a promising material in biomedical applications Sezgin et al. [3]. Their ability to encapsulate guest molecules within well-defined cavities enables their usage toward targeted drug delivery vehicles, offering controlled release and improved bioavailability. Our work paves the way for future research in engineering smart supramolecular systems precision medicine.

Keywords: Dynamic Covalent Chemistry, Organic Imine Cages, Supramolecular Chemistry, FRET, aggregation-induced emission.

REFERENCES:

1. Q Wang, C Yu, C Zhang, H Long, S Azarnoush, Y Jin and W Zhang, Chemical Science 7, 2016, 3370.
2. C Kumari and A Kumar, RSC Advances 15, 2025, 43366.
3. P Sezgin, E Gulcay-Ozcan, M Vučkovski, A M Bondžić, I Erucar and S Keskin, Industrial and Engineering Chemistry Research 64, 2025, 1907.

P-34

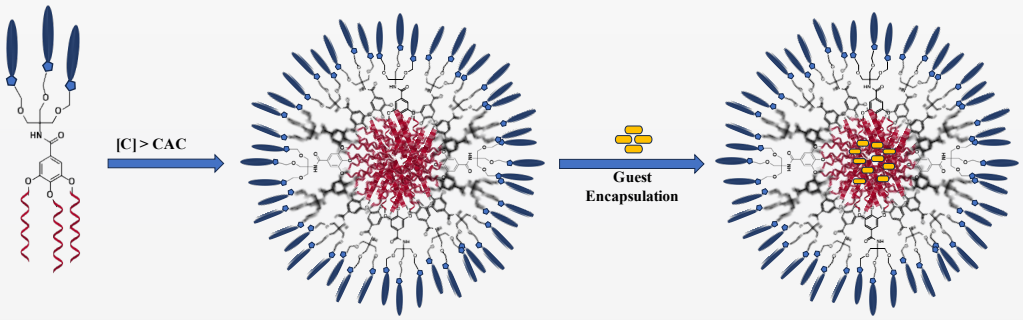
Synthesis of Gallic Acid Derived Non-ionic Janus Amphiphiles as Nanotransporters

Bajrang Sharma, Shakira, S.K. Sharma*

Department of Chemistry, University of Delhi, Delhi-110007, India
Email: sk.sharma90@gmail.com

Abstract

Stimuli-responsive polymer assemblies have garnered significant attention over the past two decades owing to their potential in biomedical and nanotechnological applications. Among them, non-ionic amphiphilic systems capable of spontaneous self-assembly into nanocarriers in aqueous environment are particularly attractive.[1] Herein, we report the rational, design and synthesis of novel non-ionic Janus amphiphiles derived from gallic acid as a tri-functional central core. Gallic acid was initially esterified and subsequently functionalized with long alkyl chains (C_{12} and C_{16}) via ester coupling to form the hydrophobic segment. The resulting intermediate on controlled hydrolysis and subsequent amide coupling, followed by propargylation, afforded a clickable hydrophobic scaffold. The hydrophilic units - second-generation polyglycerol dendron (PG_2), lactose azide, and $mPEG_{750}$ azide were then conjugated through click chemistry approach to yield the final amphiphilic architectures.[2] The self-assembly and aggregation behaviour of the synthesized amphiphiles were systematically investigated using dynamic light scattering (DLS) and fluorescence spectroscopy, revealing the formation of stable nanostructures. Furthermore, their encapsulation efficiency towards hydrophobic guest molecules was examined to assess their drug-loading potential.[3] Overall, these newly developed non-ionic Janus amphiphiles present a versatile platform for constructing biocompatible nanocarriers with potential applications in targeted drug delivery and controlled release systems. The research data will be shared during the poster presentation.



References:

1. Phan, V. G.; Trang Duong, H. T.; Tran, P. T.; Thambi, T.; Ho, D. K.; Murgia, X. *Biomacromolecules*, 2020, *22*, 572-585.
2. Kumar, A.; Krishna; Sharma, A.; Dhankhar, J.; Syeda, S.; Shrivastava, A.; Sharma, S. K. *ChemistrySelect*, 2022, *7*, e202203274.
3. Singh, A. K.; Achazi, K.; Ehrmann, S.; Böttcher, C.; Haag, R.; Sharma, S. K. *Polymer Chemistry*, 2020, *11*, 6772-6782.

P-35

Changes in Phytochemicals from Leaves of *Rauvolfia tetraphylla* with seasonal variation

Sneha Mundary, Saswat Nayak and Subhendu Biswal

Department of Forest Products &Utilisation, College of Forestry, Odisha University of Agriculture and Technology, Bhubaneswar

The present study entitled "Changes in Phytochemicals from Leaves of *Rauvolfia tetraphylla* with seasonal variation" was carried out under department of Forest Products and Utilisation, College of Forestry, OUAT, Bhubaneswar during 2025.

Rauvolfia tetraphylla L. belonging to family Apocynaceae is an evergreen, pubescent shrub with a woody plant that grows to a height of 4-6 feet with pubescent leaves are typically seen in whorls of four. It has emerged as a vital alternative source of reserpine and other essential alkaloids [1]. Phytochemicals in plants changes in their content with seasonal variation. In the case of *Rauvolfia* it was observed that Reserpine content also varies with different harvesting time coinciding with different seasons [2]. During this study an attempt was made for estimating the Changes in major active principle content from Leaves of *Rauvolfia tetraphylla* with seasonal variation.

The plants were selected from a natural population based on basis of plant height and categorized into two classes (I &II) based on plant height i.e. Class- I (50-75 cm) and Class- II (75-100 cm) . Under each category 3 plants were selected and leaves were harvested during different seasons. The harvested leaves were then subjected to methanolic extraction from which the major active principles were separated by using a Thin Layer Chromatography and identified spot corresponding to the Standard Reserpine. The total active principle content was estimated by UV-VIS Spectrophotometer method as reserpine equivalent. The Active Principle content was found maximum in the month of winter both the classes i.e. in class –I (2.268%) and Class-II (1.270%), whereas, the minimum content was found in the rainy month for Class-I (0.650%) and Summer month for class-II (0.881%).

Table-1: Changes in Active Principle content in leaves of *Rauvolfia tetraphylla* L.

Season	Class-Active Principles content (%) in leaves of class-I	Class-Active Principles content (%) in leaves of class-II
Winter	2.268	1.270
Spring	0.940	1.071
Summer	0.655	0.881
Rainy	0.650	0.927
MEAN	**1.128**	**1.037**
f-value	**22.3216**	**1.0076**
p-value	**0.0003052 (S)**	**0.4381 (NS)**

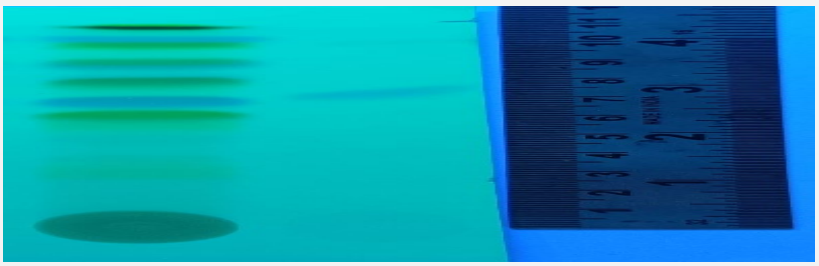


Figure-1: Separation of Active Principle from methanolic leaves extract by TLC

References:

1. Kar MK and Panda T. *JMPS,* **11**(5), 2023, 137-145.
2. Irshad S and Khatoon S. *Journal of Botany*, **142,** 2021. 193-200.

P-36

Assessment of Essential oil and Camphor content in the leaves of *Ocimum kilimandscharicum* Gürke

Subhendu Biswal, Saswat Nayak and Sneha Mundary

Department of Forest Products &Utilisation, College of Forestry, Odisha University of Agriculture and Technology, Bhubaneswar

The present study entitled "Assessment of Essential oil and Camphor content in the leaves of *Ocimum kilimandscharicum* Gürke" was carried out under Department of Forest Products and Utilisation, College of Forestry, OUAT, Bhubaneswar during 2024-25.

O. kilimandscharicum is a herb grows to height of 0.5-1 meter forming a bushy structure with multiple stems originating from the base. Its leaves are 4–8 cm in length with width of 2–5 cm which are ovate to elliptical shaped and arranged oppositely on the stem. The essential oil of *O. kilimandscharicum* is characterized by high camphor content, along with other aromatic compounds like 1,8-cineole, eugenol, limonene, and β-caryophyllene [1]. These bioactive compounds contribute to a range of pharmacological effects, including antimicrobial, antifungal, anti-inflammatory, and antioxidant activities [2]. The phytochemicals and their content percentage in oil found to vary when grown in different climatic and edaphic conditions. The present study was to assess the oil content, yield and phytochemical presences in oil extracted from the plant grown in this local condition.

The planting materials were raised from apical cuttings of the available plant source in the Ekamravana, Bhubaneswar which were planted in the Instructional unit of college of Forestry, OUAT. The transplanting was done in the month of December 2024 at a spacing of 45cm x45cm and leaves were harvested after 6 months of planting in the month of June1st week of 2025. The harvested leaves were weighed and then subjected to hydro distillation by Clevenger's apparatus for oil extraction. The camphor deposited around the condenser was recovered by dissolving it in Ethanol, evaporating it and finally weighing the Camphor devoid of ethanol. The Oil content (%), Oil yield/ha, Camphor recovered (%) and Camphor recovered yield /ha were estimated. The extracted Oil was subjected to GCMS for determination of major compounds in the essential Oil.

Table 1: Evaluation of Essential Oil and recovered Camphor from Ocimum *kilimandscharicum*

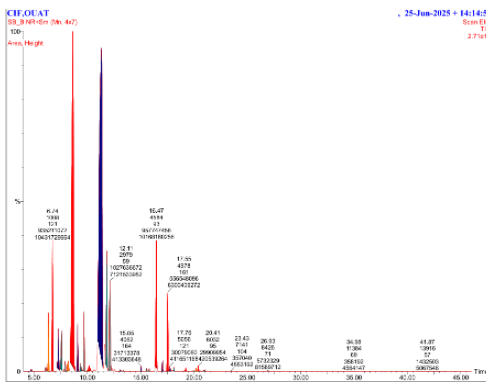
Total fresh Leaf Yield /Plant	Oil Content(%)	Recoverd Camphor(%)	Oil Yield/Plant (mL)	Recovered Camphor Yield/plant (g)	Oil Yield/ha (L)	Recovered Camphor Yield/ha (kg)
142.84	1.048	0.41	1.496	0.585	73.875	28.888

GCMS analysis of essential oil carried out by dissolving the oil in n-Hexane and found to have nearly 30 compounds in it of which 5 major compunds isolated were given in the below table.

Table 2: Major compounds identified from GCMS of Essential oil of *Ocimum kilimandscharicum*

Compound	RT	REV	Area (%)
Camphene	6.77	983	4.44
Eucalyptol	8.65	938	24.18
Camphor	11.27	972	29.72
(+)-2-Bornanone	11..37	971	12.83
Caryophyllene	16.50	982	5.05
Germacrene D	17.57	960	2.65

Figure-1: Peaks of GCMS of *Ocimum kilimandscharicum*



References:

1. Sakuntala, P., Ch. Pradyutha, A. and Selvaraju, R. *Natural Product Research*,2024, 1-7.
2. Sharma, S. and Dubey, R. C. *South Eastern European Journal of Public Health*, 2025,139–149

P-37

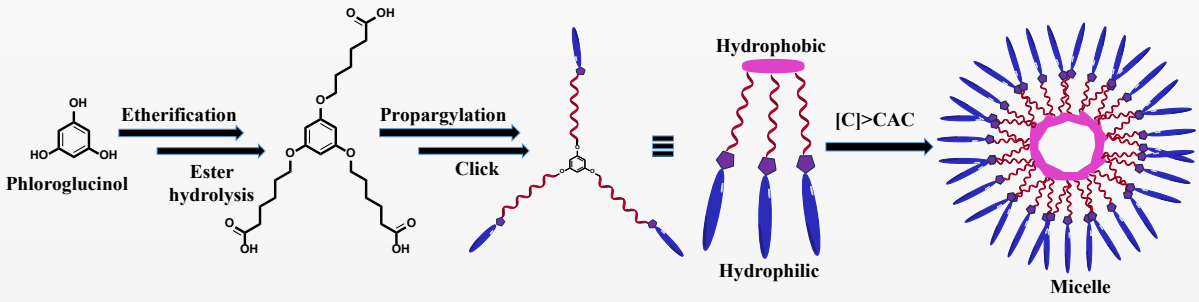
Synthesis of Phloroglucinol Based Stimuli-Responsive Non-ionic Amphiphiles for Drug Delivery

Kamal Kaushik, S. K. Sharma*

Department of Chemistry, University of Delhi, Delhi-110007, India
Email: sksharma@chemistry.du.ac.in

Abstract

Amphiphiles are a versatile class of molecules capable of self-assembling into diverse nanostructures. Their utility is drug encapsulation and delivery has been extensively explored.[1-2] In the present work, we report the synthesis of a newer series of non-ionic amphiphiles by incorporating a phloroglucinol moiety as the central core.[3] Phloroglucinol was first reacted with ethyl 6-bromohexanoate to afford the corresponding triester, which was subjected to ester hydrolysis. The resulting triacid which was then reacted with propargyl bromide to yield tri-propargylated ester, marked as the lipophilic moiety. The hydrophilicity was conferred by introducing monomethoxy poly(ethylene glycol) azide (mPEG- azide, M_n: 350/550), lactose azide, and polyglycerol G_1-azide *via click chemistry approach*. The self-assembly behavior of the resulting amphiphiles was examined through dynamic light scattering (DLS) and fluorescence spectroscopy. Their encapsulation efficiency and controlled guest-release characteristics were systematically evaluated.[4] Since our amphiphiles contain ester functionality they exhibit sensitivity towards enzymes for the release of encapsulated guest in a controlled manner. The preliminary results from this study will be shared during the poster presentation.



References

1. Parshad, B.; Prasad, S.; Bhatia, S.; Mittal, A.; Pan, Y.; Mishra, P. K.; Sharma, S. K.; Fruk, L. *RSC advances*, 2020, *10*, 42098-42115.
2. Mittal, A.; Prasad, S.; Mishra, P.K.; Sharma, S. K.; Parshad, B. *Materials Advances*, 2021, *2*, 3459-3473.
3. Parshad, B.; Yadav, P.; Kerkhoff, Y.; Mittal, A.; Achazi, K.; Haag, R.; Sharma, S. K. *New Journal of Chemistry*, 2019, *43*, 11984-11993.
4. Fleige, E.; Ziem, B.; Grabolle, M.; Haag, R.; Resch-Genger, U. *Macromolecules*, 2012, *45*, 9452-9459.

P-38

Design, Synthesis and Characterisation of Some New Series of Substituted Pyrimidines for their Biological Potential

N. Verma# and D. N. Singh*

Department of Chemistry, K. S. Saket PG College, Dr. R.M.L. Avadh University Ayodhya-224001, India.
**E-mail:dnsinghsaket@yahoo.com; #Ex-Research Scholar*

Pyrimidine derivatives having diverse biological functions and their many therapeutic uses have attracted a lot of research in the field of medicinal chemistry. Due to its synthetic accessibility and structural diversity, the pyrimidine scaffold has found widespread therapeutic applications, including antimicrobial, antimalarial, antiviral, anticancer, antileishmanial, anti-inflammatory, analgesic, anticonvulsant, antihypertensive, antioxidant, central nervous system (CNS)-active agents, calcium channel blockers and antidepressants. Keeping in view the above facts and importance of pyrimidine nucleus in various therapeutic targets and continuous of our work, recently, we have synthesized and characterised some new series of substituted pyrimidine derivatives for their biological potential. 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.

REFERENCES

1. DN Singh, N Verma, Bentham Science, Frontiers in Medicinal Chemistry, 10, **2023**,81.
2. DN Singh, N Verma, LP Pathak, PK.Shukla, Indian J. Heterocyclic Chemistr, 19,**2010**,229.

Recent developments in the synthesis, biological assessment, and therapeutic uses of pyrimidine derivatives

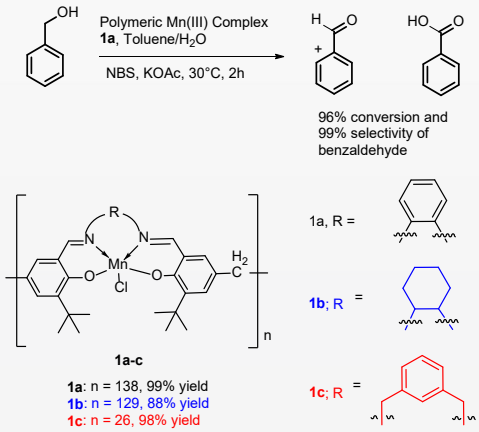
Polymeric Mn(III) Salen complexes as efficient catalysts for the selective oxidation of primary and secondary alcohols

Rashmi Meena [1], Dhan Raj Meena [1,2] Surendra Singh[1,*]

[1] *Department of Chemistry, University of Delhi, India -110007*
[2] *Department of Chemistry, Rajdhani College, University of Delhi, Delhi, India 110015*
Email: ssingh1@chemistry.du.ac.in

Abstract

The transition metal complexes of the salen ligands are widely used as catalysts in different organic transformation.[1] Synthesis and evaluation of polymeric Mn (III) Salen complexes as oxidation catalysts for primary and secondary alcohols are carried out at room temperature. The monomers used for the synthesis of the polymeric Schiff base ligands were disalicylaldehyde and ortho-phenylenediamines/ 1,2-diaminocyclohexane/ 1,3-phenylenedimethanamine, which were reacted under microwave irradiation. The resulting polymeric ligands were then treated with $Mn(OAc)_2.4H_2O$ to obtain polymeric Mn(III) Salen complexes **1a-c**. These complexes were characterized using CHN analysis, FT-IR, UV-Vis spectroscopy.[2] The polymeric Mn(III) Salen complexes showed efficient and selective oxidation catalytic activity towards primary and secondary alcohols with N-bromo succinimide (NBS) used as the oxidant at room temperature in a mixture of Toluene and H_2O (1:1). The catalyst **1a**, which was discovered to be the most effective catalyst for the oxidation of various primary and secondary alcohols demonstrated the ability to produce aldehydes and ketones with isolated yields ranging from 64-99%.



Scheme: Oxidation of benzyl alcohol to benzaldehyde

References

1. (a) W. Zhang, J. L. Leobach, R. S. Wilson, E. N. Jacobson, *J. Am. Chem. Soc.* **1990**, *112*, 2801; (b) N. H. Lee, J. S. Baik, S. B. Han, *Bull Korean Chem. Soc.* **1998**, *19*, 726-728. (c) T. Katsuki, *J. Synth. Org. Chem. Jpn.*, **1995**, *53*, 940-951.
2. (a) P. Chaudhary, Geeta D. Yadav, K. K. Damodaran, S. Singh, *New J. Chem.*, **2022**, *46*, 1308; (b) P. Chaudhary, D. R. Naikwadi, A. V. Biradar, S. Singh*, *Langmuir* 2023, 39, 31, 10925–10934

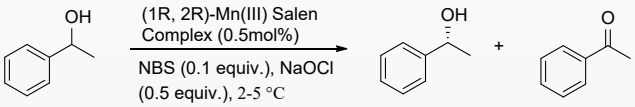
Oxidative Kinetic Resolution of Secondary Alcohols Catalysed by Recoverable Mn (III) Salen Complexes

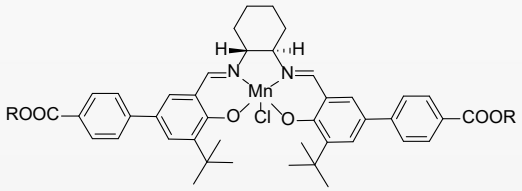
Geeta[1], Surendra Singh*

Department of chemistry, University of Delhi, Delhi-110007

Abstract

The asymmetric catalysis is one of the efficient methods for the synthesis of asymmetric compounds by using organocatalyst, enzyme as a biocatalyst and chiral metal complexes. The chiral secondary alcohols are valuable intermediates for pharmaceutical, flavour and fragrance and agrochemical industries.[1] Oxidative kinetic resolution of secondary alcohols catalysed by Mn(III) Salen complexes is and efficient method to enantioselective resolve the one enantiomer.[2] We have synthesised a variety of Mn(III) Salen complexes having different alkyl chain on ester moiety. The reaction conditions for Oxidative kinetic resolution using NBS and NaOCl as oxidant were optimised. Oxidative kinetic resolution of 1-phenylethanol shows 65% conversion of acetophenone with 98% *ee* of (R)-1-pehylethanol. The catalyst was recovered and reused for oxidative kinetic resolution of secondary alcohols.





1a: R = Et; **1b**: R = ^{i}Pr; **1c**: R = C_5H_{11},
1d: R = $C_{12}H_{25}$

Keywords: Mn (III) Salen Complexes, OKR, 1-Phenylethanol, NBS, NaOCl

References

1. K. Laumen, D. Breitgoff, M.P. Schneider J. Chem. Soc., Chem. Commun., **1988**, 1459-1461
2. P. Chaudhary, G. D. Yadav, K. K. Damodaran, S. Singh, *New J Chem*, **2022**, 1308-1318.
3. I. Ahmad, Shagufta, A. R. AlMallah, *Chirality*, **2017**, 798-810.

P-41

Mosquito diversity studies of University Campus of Khallikote Unitary University

Santhosh Goud

Department of Zoology, Khallikote Unitary University, Berhampur, Ganjam, Odisha, India, 760001

Abstract

Mosquitoes (Diptera: Culicidae) are of immense medical importance as vectors of significant diseases, including malaria, dengue, chikungunya, and filariasis. University campuses provide diverse ecological niches that favor mosquito breeding and survival. The present investigation was conducted to document the diversity, abundance, and seasonal distribution of mosquitoes within the University Campus of Khallikote Unitary University, Odisha, India. Field surveys were conducted during the pre-monsoon, monsoon, and post-monsoon seasons, covering hostels, academic blocks, gardens, stagnant water bodies, and waste-dumping sites. Adult mosquitoes were collected using light traps and aspirators, while larvae were sampled from breeding habitats and reared to confirm the species. Identification was performed using standard morphological taxonomic keys. A total of 18 species belonging to 5 genera were recorded, with *Anopheles, Culex,* and *Aedes* being the dominant genera. The Shannon–Wiener diversity index (H′) ranged from 1.89 to 2.47, with the highest diversity observed during the monsoon season. Species richness and evenness also peaked during this period due to the increased availability of breeding habitats. The predominance of vector-competent species indicates a potential public-health risk within the campus. The study provides essential baseline data for continuous vector surveillance and the development of effective integrated mosquito management strategies.

Keywords: Mosquito diversity; Culicidae; University campus; Vector-borne diseases; Seasonal variation; Shannon–Wiener index; Odisha.

P-42

PREDICTORS OF QUALITY OF LIFE IN CHRONIC KIDNEY DISEASE PATIENTS UNDERGOING HEMODIALYSIS: A CROSS-SECTIONAL STUDY

Dr Soumya Mishra, Dr Ayush Arora, Dr Pratyush Kanungo, Dr Magna Manjareeka

Department of Physiology, Kalinga Institute of Medical Sciences, KIIT University, Bhubaneswar, Odisha

Abstract

Background: Hemodialysis (HD) prolongs survival in chronic kidney disease (CKD) but imposes substantial physical, psychological, and socioeconomic burden, negatively affecting quality of life (QoL). Identifying modifiable predictors of QoL is important for patient-centered care.

Objective: To assess QoL in CKD patients undergoing HD and determine demographic and clinical predictors associated with QoL.

Methods: A hospital-based cross-sectional study was conducted among adult CKD patients receiving HD at a tertiary-care center in Bhubaneswar, India. Demographic characteristics, lifestyle factors, comorbidities, and treatment-related variables were recorded. QoL was assessed using the WHOQOL-BREF questionnaire across four domains, and Total QoL score was calculated as the mean of domain scores. Group differences were analyzed using the Mann–Whitney U test and odds ratios; predictors of QoL were examined using multivariable linear regression.

Results: A total of 120 HD patients were included. The mean age was 51.52 ± 15.10 years and 71% were male. Higher QoL was significantly associated with use of dietary supplements ($p = 0.001$), employment ($p = 0.015$), and absence of comorbidities ($p = 0.048$). HD duration < 5 years was linked to lower QoL ($p < 0.0001$). In multivariable regression, use of dietary supplements remained an independent positive predictor of QoL ($\beta = -7.073$; $p = 0.017$). Age, sex, smoking, alcohol intake, diet pattern, exercise, and dialysis frequency were not significantly associated with QoL.

Conclusion: QoL in HD patients is influenced by nutritional supplementation, comorbidity burden, occupational status, and dialysis duration. Integrating targeted nutritional support, comorbidity management, and socioeconomic assistance may improve QoL in CKD.

Keywords - Chronic kidney disease; Hemodialysis; Quality of life; WHOQOL-BREF; Predictors

$BaWO_4:Eu^{3+}$, Ag^+ nanocatalyst for efficient reduction of 4-nitrophenol in aqueous solution

Dasrathi Murmu[1], Rajkumari Bindiya Devi[2], Ningombam Yaiphaba*[3], Bibhuti Bhusan Parida[1], Ganngam Phaomei[1,4*]

Presenting Author: Dasrathi Murmu, Department of Chemistry, Berhampur University, Odisha
Email: dasrathim8@gmail.com

Abstract:

$BaWO_4$ nanoparticles doped and co-doped with various metal ions like Eu^{3+}, Ag^+, Li^+, Zn^{2+} and Bi^{3+}, etc., are synthesized using a simple polyol route. The synthesized NPs were characterized by XRD, TEM, XPS, EDX and a UV-VIS spectrometer. From the TEM image, the NPs are spherical in shape with an average particle size of 15 nm. The band gap of the NPs is calculated using Tauc's plot, and it is found to change with the concentration of co-dopant ions and the pH of the synthesis medium. The crystal size, crystallinity %, and lattice strain are calculated from the XRD data and it is found that $BaWO_4:Eu^{3+}$, Ag^+ NPs have a smaller size and larger strain. However, this nanoparticle demonstrated better catalytic activity in reducing the organic pollutant, 4-Nitrophenol (4-NP). The rate constant (k) for the reduction of 4-NP is 6.14×10^{-3} s^{-1}. The catalyst is stable and can be reused for five consecutive cycles.

Keywords: $BaWO_4:Eu^{3+}$, Ag^+, 4-Nitrophenol, Nanocatalyst, Catalytic reduction.

Molecular Regulation of Kidney Development in Zebrafish

Deepak Singh[1,2] and Rajeeb k. Swain[1]

[1]*Institute of Life Sciences, Nalco Square, Chandrasekharpur, Bhubaneswar, Odisha, India*
[2]*Regional centre for biotechnology, Faridabad, India*

Abstract

The cilia-flagella-associated gene *cfap90* remains poorly uncharacterized in vertebrate development. Here, we provide a comprehensive characterization of cfap90 in zebrafish by integrating expression profiling, sequence and domain analysis and morphological characterization after generating the CRISPR/Cas9-mediated knock out. Spatiotemporal whole-mount in situ hybridization of *cfap90* revealed its dynamic expression pattern, at otolith, pronephric region in the early developmental stage and in the anterior and posterior lateral line at later stages. Comparative protein sequence analysis revealed the conserved region and DUF-containing regions across vertebrates, supporting an evolutionary preserved function. Together, these findings establish the first functional framework of *cfap90* as a developmentally regulated gene with potential contribution to both early kidney patterning and lateral line formation, offering a foundation for future mechanistic studies into its ciliary and developmental functions.

Keywords: Zebrafish, *cfap90*, Pronephros, Otolith, Lateral line

P-45

Isolation and characterization of novel mouse pancreatic cancer cell lines from KC ($kras^{G12D}$, pdx1-cre) model of pancreatic adenocarcinoma

Salona Kar[1,2], Amlan Priyadarshee Mohapatra[1,2], Deepti Parida [1,2] , Swayambara Mishra [1,2] , Supriya Halder [1,2] , Ritwik Biswas [1,2] , Prajna Paramita Saran [1,2] Shantibhusan Senapati 1

[1] Institute of Life Sciences, Bhubaneswar, Odisha, India; [2] Regional Center for Biotechnology, Faridabad, Haryana, India

Abstract:

Regardless of substantial advancements in treatment approaches and improved knowledge of pancreatic cancer pathophysiology and molecular mechanisms, the disease remains one of the most fatal human malignancies with a dismal prognosis. Significant progress in cancer research necessitates suitable use of potential pre-clinical models that accurately mimics the complexities of tumor biology. Xenograft models have long been used to unravel the biological intricacies contributing towards the development and progression of cancer. However, the use of immune compromised hosts in these models limits their application in cancer immunotherapy. Conversely, immunocompetent syngeneic mouse models of pancreatic cancer could be of great importance for gaining better insights into the complex interactions between different therapy regimens and the host immune system. Thus there is a demand for the development of a research platform comprising an array of syngeneic cell lines representing multiple heterogeneous characteristics of pancreatic tumors. Pancreatitis has long been reported as a major risk factor for pancreatic cancer. Besides, researchers have successfully used genetically engineered mice models to prove the progression towards an aggressive malignancy with the induction of pancreatitis. In this study we have established a panel of syngeneic cell lines from the KC mice challenged with pancreatitis inducing agent caerulein. The cell lines were characterized based on their morphology, growth kinetics and response towards radiation and chemotherapeutic drug gemcitabine. In addition, the gene expression status of selective genes was examined. Furthermore, the tumorigenicity potential of a few of the clones was validated by heterotopic and orthotopic implantation. The clones had varying metastatic potential and from histopathological examinations the tumors were found to be poorly to moderately differentiated and even showed different degree of fibrosis. In the future we aim to use these cell lines as suitable platforms for addressing different aspects of pancreatic cancer and thereby accelerate the discovery of potential therapy with improved knowledge of disease complexities.

P-46

High-Throughput Screening of FDA-Approved Drugs in TGF-β–Induced Myofibroblast Activation

Ritwik Biswas[1,2], Amlan Priyadarshee Mohapatra[1,2], Shri Krishna Bhagat[1,2], Asutosh Tripathy[1,2] Supriya Halder[1,2], Shantibhusan Senapati[1]

[1] Institute of Life Sciences, Bhubaneswar, Odisha, India; [2] Regional Center for Biotechnology, Faridabad, Haryana, India
ritwikb1020@gmail.com

Introduction:

Transforming growth factor-β (TGF-β) is a central regulator of myofibroblast activation, a key process that drives fibrosis across multiple pathological conditions, including pulmonary fibrosis and cancer-associated fibrosis. Extensive clinical and experimental evidence highlights the pivotal role of TGF-β in promoting fibroblast-to-myofibroblast transition, extracellular matrix accumulation, and tissue remodelling. Consequently, there is considerable interest in identifying novel inhibitors or repurposing existing FDA-approved drugs that can effectively block TGF-β–mediated fibroblast activation.

Objective:

To identify FDA-approved drugs capable of inhibiting TGF-β–induced myofibroblast activation using high-throughput screening, and to validate top candidates in patient-derived cancer-associated fibroblasts through molecular and phenotypic assays.

Materials & Methods:

A high-throughput screening of FDA-approved drugs was performed in TGF-β–induced human lung fibroblast cell lines. Top candidate compounds were subsequently evaluated in cancer-associated fibroblasts isolated from human pancreatic tumor tissue. Multiple molecular assays were conducted to validate their anti-fibrotic effects.

Results and conclusion:

High-throughput screening in TGF-β–induced human lung fibroblasts identified several FDA-approved drugs that significantly reduced myofibroblastic features, including decreased α-SMA expression and altered fibroblast morphology. When tested in patient-derived CAFs, the top candidate compounds similarly suppressed TGF-β–driven activation. Molecular analyses further confirmed downregulation of key fibrotic genes, indicating a consistent anti-myofibrotic effect across both fibroblast models.

Keywords: High-throughput screening; TGF-β; Myofibroblast activation; Cancer-associated fibroblasts (CAFs)

P-47

Altering the Optical and Magnetic Properties of ZnO Nanoparticles by Co Doping

Subhashree Dash [a] M. Bhoi [a], S. Kavita [b], A. Priyam [c] B. Bhushan [a]

[a]*Department of Physics, School of Applied Sciences, KIIT, Deemed to be University, Bhubaneswar 751024, India*
[b] *International Advanced Research Centre for Powder Metallurgy and New Materials(ARCI), Chennai 600113, India*
[c]*Department of Chemistry, Central University of South Bihar, NH-120, Gaya 824236, India*
**E-mail: bbhusanfpy@kiit.ac.in*

A dilute magnetic semiconductor (DMS) is a semiconductor doped with transition metals, which have both magnetic and semiconducting properties. Doped ZnO is considered the most promising dilute magnetic semiconductor material for use in spintronics devices [1] .Because of their flexible semiconducting and magnetic capabilities at ambient temperature, DMSs like Co doped ZnO are attracting attention as possible candidates for information storage and processing systems in the spintronics, opto-electronics, magneto-electronics devices. In this work, co-precipitation method was used to synthesize Co doped ZnO nanocrystals. The substitution of Co atoms causes the crystallites in the nanocrystal to become smaller, even at low concentrations. When the doping concentration increases the average crystallite size decreases from 20 nm to12 nm[2]. From the FESEM analysis, we found that the NPs are homogeneous in particle distribution and uniform. It was found that the excitonic absorption peak expanded with the doping of Co. Through Co doping, ZnO nanocrystals with significant ferromagnetic capability were created [3]. The observed results suggest that ZnO nanoparticles doped with Co may find application in optoelectronic and spintronic systems.

References:

1. S. Singh, M.R. Rao, Optical and electrical resistivity studies of isovalent and aliovalent 3 d transition metal ion doped ZnO, Phys. Rev. B (2019).
2. S. Dash, M. Bhoi, S. Kavita, A. Priyam, and B. Bhushan, "Structural, optical and magnetic properties of $Zn_{0.98}Co_{0.02}O$ dilute magnetic semiconductor nanoparticles," 82, 118–122, (2023)
3. S. Dash, B. K. Dadhich, S. K. Patra, A. Priyam, S. Kavita, and B. Bhushan, "Iron(II)-induced defect luminescence and deconvolution of ferromagnetic and paramagnetic behaviour in Zn(1−x)FexO (x = 0.01, 0.03, 0.05) nanoparticles," 385, 115500, (2024).

P-48

Synergistic MOF-Cerium Oxide Composites: Design, Functionality, and Biomedical Potential

Jyotiranjan Behera[1], Tapas Ranjan Sahoo[1*]

[1]Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India
Email: trsahoofch@kiit.ac.in

ABSTRACT

Metal-organic framework (MOF)/cerium oxide (CeO_2) composites are an important development in hybrid nanomaterials, especially for biomedical applications. These composites exploit the unique redox-switchable Ce^{3+}/Ce^{4+} chemistry and the ROS-scavenging properties of cerium oxide, combined with the porous structure, tunable design, and functional surface chemistry due to its high surface area of various MOFs (e.g., ZIF, UiO- 66, MIL-101, and MOF-74). The MOF@CeO_2 composites are characterized by enhanced catalytic activity, controlled drug loading and release, and improved physicochemical stability. This innovation has spurred interest in applications such as biosensing, photothermal and chemodynamic therapies for cancer, antibacterial effects, antioxidant and anti-inflammatory treatments, and targeted drug delivery. Furthermore, these composites can exhibit responsive therapeutic behavior based on physiological triggers, including pH changes, glutathione levels, or hydrogen peroxide concentrations, owing to the synergy between MOF architecture and the catalytic functions of ceria. The study underscores the potential of MOF@CeO_2 composites as versatile multifunctional nanoplatforms, highlighting their structural diversity, synthesis methods, and expanding roles in various biological fields.

KEYWORDS: Cerium oxide, MOF composites, ROS scavenging, Drug delivery, Cancer therapy, Antibacterial activity, Nanomedicine

REFERENCES:

1. Liu, J., Ye, L. Y., Xiong, W. H., Liu, T., Yang, H., Lei, J. (2021). *Chemical Communications*, 57, 2820
2. Zhou, X., He, Z., Xiao, Y., Liu, Z., Sun, Y., (2024). *Nano-Micro Letters*, 16, 156

P-49

Anticancer, Antibacterial and Antibiofilm Effects of Green Synthesized CeO_2, Mn and Mg-Doped CeO_2 Nanoparticles

Nibedita Nayak[1], Tapas Ranjan Sahoo[1*]

[1]Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India
Email: trsahoofch@kiit.ac.in

ABSTRACT

In this study, pure cerium oxide (CeO_2) nanoparticles along with manganese-doped and magnesium-doped CeO_2 nanoparticles were synthesized using an eco-friendly sol-gel approach. *Acacia concinna* fruit extract and *Actinidia deliciosa* peel extract served as natural reducing, surfactant, and stabilizing agents for Mn-doped and Mg-doped CeO_2 nanoparticles, respectively. Comprehensive characterization using XRD, FESEM, HRTEM, FTIR, Raman, UV–Vis spectroscopy, BET, and PL analyses confirmed the formation of highly crystalline, uniformly dispersed nanoparticles with a cubic fluorite CeO_2 phase. Cytotoxicity assays revealed that Mn-doped CeO_2 nanoparticles exhibited strong anticancer efficacy, inhibiting 50% of MCF-7 breast cancer and HCT 116 colon cancer cells at optimized concentrations, while maintaining biocompatibility toward normal HEK 293 cells, highlighting their potential as redox-active nanotherapeutics. In parallel, Mg-doped CeO_2 nanoparticles demonstrated excellent antibacterial and antibiofilm performance against pathogenic strains including Methicillin-resistant *Staphylococcus aureus* (MRSA), *Escherichia coli*, and *Pseudomonas aeruginosa*. Mg-doped CeO_2 NPs displayed enhanced zones of inhibition and low minimum inhibitory concentration (MIC) values, accompanied by significant biofilm suppression. ROS-mediated bactericidal activity was identified as the underlying mechanism for their antimicrobial potency. Overall, the green- synthesized Mn and Mg-doped CeO_2 nanoparticles exhibit promising multifunctional properties, demonstrating potent anticancer and antibacterial effects. These findings offer a sustainable platform for developing advanced nanomedicine strategies targeting both cancer therapy and antimicrobial resistance.

KEYWORDS: Cerium oxide nanoparticles; Green synthesis; Anticancer; Antibacterial; Antibiofilm

REFERENCES:

1. N. Nayak, U. Suryakanta, D. Mandal, T.R. Sahoo, *ChemistrySelect,* 9 (2024) e202402964
2. S. Sarangi, U. Suryakanta, N. Nayak, D. Mandal, T. R. Sahoo, *Journal of Rare Earths*, (2025)

P-50

Eco-Friendly Synthesis of Gadolinium-Doped Cerium Oxide Nanoparticles as Multifunctional Anticancer Agents Against Colon and Breast Cancer Cell Lines

Sasmita Sarangi[1], Tapas Ranjan Sahoo[1*]

[1]Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India
E-mail: trsahoofch@kiit.ac.in

ABSTRACT

Nanoparticles have emerged as prospective cancer therapeutic agents due to their unique physicochemical features caused by surface functionalization. This work focuses on the green synthesis, characterisation, and anticancer potential of cerium dioxide nanoparticles and gadolinium-doped cerium dioxide nanoparticles in human colon cancer (HCT-116) and breast cancer (MCF-7) cell lines. CeO_2 and Gd-doped CeO_2 NPs were synthesised via sol–gel method using a fruit extract from *Acacia Concinna* as a surfactant. Their structural, morphological, and physico-chemical properties were characterised using different analytical techniques, like X-ray diffraction, Raman spectroscopy, UV–visible spectroscopy, field emission scanning electron microscopy, transmission electron microscopy and Fourier transform infrared spectroscopy. XRD analysis confirms the cubic fluorite-type structure of CeO_2 nanoparticles, with average crystallite size ranging between 7 and 14 nm. Raman spectroscopy validates this structure with F_{2g} band observed at 462.58 cm^{-1}. FE-SEM images reveal irregular spherical morphologies with grain sizes estimated between 40 and 56 nm. The CeO_2 nanoparticles exhibit a prominent absorption peak at 345 nm in the UV–visible spectrum. Increasing the Gd-doping concentration from 2% to 6% results in a rise in the bandgap energy from 2.8 to 3.12 eV. *In vitro* cytotoxicity assays were performed to evaluate the anticancer efficacy of these nanoparticles. The Gd-doped CeO_2 NPs exhibit dose- dependent cytotoxicity, reducing cell viability to 52% and 53% in HCT-116 and MCF-7 cells, respectively, at 200 µg/mL, while sparing the non-cancerous cell line. The experimental results corroborate the emergence of promising CeO_2-based therapeutic molecules, thereby opening new avenues for research in invasive nanomedicine.

Keywords: Gd-doped CeO_2 NPs, Anticancer activity, Colon cancer (HCT-116), Breast cancer (MCF-7), Green synthesis

REFERENCE:

1. **Sarangi, S**., Suryakanta, U., Nayak, N., Mandal, D., Sahoo, T. R. *Journal of Rare Earths*. (2025).
2. Nayak N, Suryakanta U, Mandal D, Sahoo T R. Chemistry Select. 2024 Nov; 9 (41): e202402964.

P-51

The impact of Nd-doping on structural, optical, dielectric and magnetic features of $BiFeO_3$ multiferroic nanoparticles

Subhasmita Jena[1], S. S Parida[2], A. Priyam[3], B. K. Singh[2,*] and B. Bhushan[1,*]

[1]*Department of Physics, KIIT, Deemed to be University, Bhubaneswar 751024, India*
[2]*Department of Physics, Central University of South Bihar, NH-120, Gaya 824236, India*
[3] *Department of Chemistry, Central University of South Bihar, NH-120, Gaya 824236, India*
[*]*Email: bbhusanfpy@kiit.ac.in*

Abstract

Materials with two or more of the primary ferroic characteristics (ferroelectric, ferromagnetic, and ferroelastic) combined in a single phase are called multiferroics. $BiFeO_3$ (BFO) is a promising multiferroic material that has shown potential in the manufacturing of memory devices. The ethylene glycol-based sol-gel technique was used to synthesize multiferroic nanoparticles (NPs) of $BiFeO_3$ (BFO) and Nd-doped BFO, $Bi_{1-x}Nd_xFeO_3$ (x=0.01, 0.03,0.05, and 0.07) Bhushan et. al. [1] The influence of Nd concentration on their structural, optical, magnetic and dielectric properties has been investigated. The phase purity of the materials was validated using X-ray diffraction (XRD). Following Nd doping, the rhombohedral distorted perovskite structure remained unaltered. The crystallite size of Nd-doped BFO samples was determined using Debye-Scherrer's formula, and it decreased from 41 nm to 37nm, respectively. The FESEM image also shows that the average particle size reduces from 46 nm to 38 nm, respectively. In Raman Spectroscopy, both the Bi-site occupation states and the Bi-O covalent bonds have altered when the Nd concentration increases, so the Raman peaks have shifted to higher wave numbers. UV-vis spectroscopy reveals that the absorption edges of BFO and Nd-doped BFO NPs are in the visible range. This shows a 13-nm shift toward a shorter wavelength at increasing doping concentrations. which improves optical absorption power after doping. The PL spectra revealed three bands between 400 and 500 nm. The M-H loops of BFO and Nd doped BFO NPs demonstrated a weak ferromagnetic character. Pure BFO showed the largest saturation and remanent magnetisation values at room temperature, 0.335 emu/g and 0.019 emu/g, respectively. Sinha et al. [2] Nd doped BFO suppresses the real part of the dielectric constant (ε') while effectively mitigating dielectric loss (tan δ) at higher doping concentrations BNFO7. Nd doped BFO NPs promise various technological applications in optoelectronic devices and photocatalytic activity.

REFERENCES

1. B. Bhushan, A. Basumallick, N.Y. Vasanthacharya, S. Kumar, D. Das, *Solid State Sciences*, vol. 12, 1063-1069,2010.
2. A.K. Sinha, B. Bhushan, Jagannath, R.K. Sharma, S. Sen, B.P. Mandal, S.S. Meena, P. Bhatt, C.L. Prajapat, A. Priyam, S.K. Mishra, S.C. Gadkari, *Results in Physics*, vol 13, 2019.

P-52

Nanoceria: A rare-earth nanoparticle as a promising anti-cancer therapeutic agent in colon cancer

Tapas Ranjan Sahoo[1*]

[1]*Department of Chemistry, School of Applied Sciences, KIIT deemed to be University, Bhubaneswar 24, Odisha, India*
Email: trsahoofch@kiit.ac.in

ABSTRACT

The biological performance and physicochemical properties of cerium oxide nanoparticles (CeO_2 NPs) are strongly influenced by their particle size, morphology, and defect structure. In this study, pure CeO_2 nanoparticles were successfully synthesized using a facile, rapid, and cost-effective microwave-assisted combustion (MACS) method. The obtained nanoparticles were comprehensively characterized to correlate their structural features with their anticancer behavior. X-ray diffraction analysis confirmed the formation of a single-phase cubic fluorite CeO_2 structure (Fm-3m), while FESEM images revealed aggregated irregular nanoparticles with a grain size of 20-40 nm. TEM further demonstrated square-shaped particles (50–95 nm), and HRTEM confirmed high crystallinity through distinct lattice fringes in the corresponding FFT patterns. BET analysis indicated a specific surface area of 25 m^2/g, and UV-visible spectroscopy revealed a direct band gap of approximately 2.8 eV, supporting the presence of oxygen vacancy–related defects. The biologically synthesized CeO_2 nanoparticles exhibited remarkable differential cytotoxicity toward normal (BHK121) and human colon cancer (HCT116) cells. Nuclear fragmentation assays revealed pronounced DNA fragmentation in HCT116 cells, whereas normal cells retained intact nuclei, demonstrating nanoceria-induced apoptotic cell death selectively in colon cancer cells. Overall, the MACS-derived CeO_2 nanoparticles show strong potential as a promising and selective anticancer nanotherapeutic, providing a new avenue for colon cancer treatment.

KEYWORDS: Cerium oxide nanoparticles; Microwave-assisted combustion synthesis; Anticancer activity; Human colon cancer

REFERENCES:

1. Sahoo, T. R., Armandi, M., Arletti, R., Piumetti, M., Bensaid, S., Manzoli, M., Panda, S.R., Bonelli, B., (2017) *Applied Catalysis B: Environmental*, *211*, 31-45
2. Sarangi, S., Suryakanta, U., Nayak, N., Mandal, D., Sahoo, T. R., *Journal of Rare Earths*. (2025)

P-53

Cholera Outbreak in Jajpur District, 2025: Clinical, Environmental, and Antibiotic Resistance Findings

Archana Jena, Debasish Samal, Jyotirmayee Turuk*

Microbiology Division, ICMR-Regional Medical Research Centre, Bhubaneswar, Odisha, India
E-mail: officialarchana062@gmail.com

In eastern India, cholera outbreaks continue to be a major public health concern (Samal et al. [1]). An acute watery diarrhea were reported in the Jajpur district, in June 2025. Of the 16 clinical samples analyzed, three were identified as *Escherichia coli*, while thirteen (81.25%) were confirmed *Vibrio cholerae* O1 serotype of both Ogawa and Inaba. High resistance to azithromycin (83%) and ciprofloxacin (75%) was observed, while tetracycline showed moderate resistance. All isolates retained sensitivity to ofloxacin and doxycycline, indicating their suitability for therapeutic management. Previous outbreak data indicate 75% resistance to ciprofloxacin (Samal et al. [2]). Based on sensitivity findings, the ICMR-RMRC, Bhubaneswar, recommended ofloxacin or doxycycline for clinical management.

Environmental assessment revealed the presence of *Shigella flexneri* in contaminated tube-well water. Continuous monitoring of antibiotic resistance and improvement of water sanitation infrastructure are essential to prevent recurring outbreaks in vulnerable populations (Samal et al. [2]).

REFERENCES

1. D Samal, J Turuk*, SR Nayak, S Pany, BB Pal & S Pati, *Genomic insights into the dynamic antibiotic resistance landscape of **Vibrio cholerae** during the Cholera outbreak 2022 in Odisha, India.*
2. D Samal, RR Nayak, UK Rout, S Kerketta, D Bhattacharya, JS Kshatri, AS Kerketta, S Pati & J Turuk, *Unraveling the 2023 cholera outbreak in Rourkela Municipal Corporation of Odisha, India: Antibiotic resistance, virulence factors, and water contamination insights.*

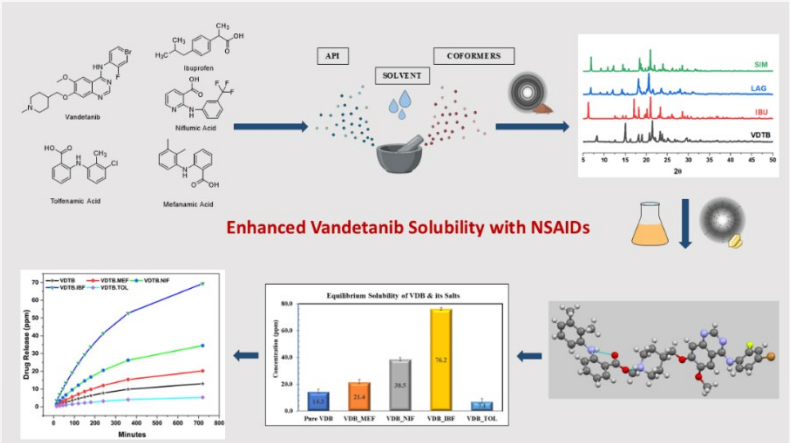
P-54

A current insight into the drug-drug molecular adducts of an anti-cancer drug Vandetanib with various NSAIDs

K. G. Abishek [a], Gowtham Kenguva [a], E. V. V. S. Ramarao [b], Gorja Dhilli Rao [c], Lopamudra Giri [d]*, Rambabu Dandela [a]*

[a] *Department of Industrial and Engineering Chemistry, Institute of Chemical Technology-Indian Oil Bhubaneswar Campus, Bhubaneswar, India.*
Email: kgabishek2001@gmail.com and r.dandela@iocb.ictmumbai.edu.in

Vandetanib (VDTB), a BCS class II anticancer medication, has a low water solubility, requiring large dosages and causing a variety of adverse effects. The current study aims to enhance the solubility of VDTB using a well-known crystal engineering technique, Bolla et al. [1]. A series of NSAIDs: Ibuprofen (IBU), Mefenamic acid (MEF), Niflumic acid (NIF) and Tolfenamic acid (TOL) were screened to prepare novel solid forms using the liquid-aided grinding (LAG) method followed by the slow evaporation crystallization process. Various characterisation techniques such as Single Crystal X-ray Diffraction, Powder X-Ray Diffraction, Thermogravimetric analysis and Differential Scanning Calorimetry were used to screen the newly obtained adducts, Rout et al. [2]. The crystal structure study confirmed salt formation, indicating proton transfer from the carboxylic acid group of NSAIDs to the piperidine nitrogen atom of VDTB. A comprehensive study of the solubility and in-vitro release kinetics of these newly obtained entities showed that, as compared to the parent medication, most of the binary adduct has a much higher solubility rate, especially VDTB.IBU, which shows ~5-fold enhanced solubility compared to the parent drug. Furthermore, a detailed study of the residue recovered following solubility indicated that all the molecular adducts were stable. To the best of our grasp, this is the first study to look at drug-drug interactions of VDTB with improved physicochemical properties. We anticipate that the new discovery will provide some helpful insight prior to the VDTB medication development and that the usage of NSAIDs can avoid side effects, in addition to their anti-cancer attributes, Bandaru et al. [3].



References

1. G. Bolla and A. Nangia, Chem. Commun., 2016, 52, 8342–8360
2. S. R. Rout, G. Kenguva, L. Giri, A. Kar and R. Dandela, Chem. Commun., 2023, **59**, 4640–464.
3. R. K. Bandaru, L. Giri, P. Kesharwani and R. Dandela, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2024, **682**, 132835

P-55

Graphene oxide - Carbon dot fluorescent hybrids for Optical Glucose and H_2O_2 Detection

Akanshya Mishra, Jasaswini Tripathy*

Department of Chemistry, School of Applied Sciences, KIIT deemed to be University
**Corresponding author's email address: jtripathyfch@kiit.ac.in*
Choice of mode: Poster

Abstract

A fluorescence nanosensor has been engineered for the dual detection of glucose and hydrogen peroxide (H_2O_2). The sensing platform is built from a nanocomposite of nitrogen doped carbon dots (N-CDs) and graphene oxide (GO). Strong interactions between N-CDs and GO initially suppress the fluorescence signal [1]. When glucose is introduced, the quenched emission is restored due to the affinity of glucose molecules for the oxygen rich sites on GO [2]. Further, H_2O_2 enhances the electron transfer dynamics within the nanocomposite, leading to a measurable quenching of fluorescence [3]. These features establish the N-CDs/GO hybrid nanocomposite as a versatile, rapid and cost effective platform for monitoring glucose and H_2O_2 in biological samples, offering significant promise for biomedical diagnostics and therapeutic applications.

Keywords: Glucose; H_2O_2; Fluorescence sensing; Carbon dots; Graphene oxide; Nanocomposite

References

1. Y Zhang, L Wang, Y Liu, Y Zhao, X Yang and H Xu, Sens. Actuators B Chem. 228, 2016, 296.
2. S P Rajmane, O S Nille, G B Kolekar and S B Sadale, Sci. Rep. 2025, 88491.
3. C Carrera, A Galán-González, W K Maser and A M Benito, Chem. Sci. 16, 2025, 3662.

P-56

Sol-gel Synthesis and Structural Characterization of Ag-doped $BiFeO_3$ Multiferroic Nanoparticles

Anil Kumar Munda[1], Subhasmita Jena[2], Mrutyunjaya Nayak[1], Bhavya Bhushan[2,*]

[1]Department of Physics, School of Indigenous Knowledge Science and Technology, KISS University, Bhubaneswar
[2]Department of Physics, School of Applied Sciences, KIIT, Deemed to be University, Bhubaneswar
E-mail: bbhusanfpy@kiit.ac.in

ABSTRACT:

Multiferroic materials combine two or more ferroic characteristics in a single phase. $BiFeO_3$ (BFO) is one of the most extensively researched multiferroic materials. The multiferroic nanoparticles (NPs) of BFO and Ag-doped BFO, $Bi_{1-x}Ag_xFeO_3$ (x = 0.01, 0.03, and 0.05), were synthesized using an ethylene-glycol-assisted sol–gel method [1]. The effect of Ag incorporation on the structural and magnetic properties was systematically examined. X-ray diffraction (XRD) confirmed the rhombohedrally distorted perovskite structure of BFO and Ag doped BFO nanoparticles. The crystallite size, calculated using the Debye–Scherrer equation, showed a slight increase from 43 nm to 56 nm with increasing Ag concentration. The FESEM image also shows that the average particle size was enhanced from 63 nm to 75 nm after increasing doping concentration. The M-H loops of BFO and Ag-doped BFO NPs exhibited a modest ferromagnetic property [2]. At room temperature, pure BFO had the highest saturation and remanent magnetization values of 0.294 emu/g and 0.019 emu/g. The bismuth ferrite multiferroic materials have many technological applications in optoelectronics, spintronics, sensors, and memory devices.

REFERENCES:

1. B Bhushan et. al, Enhancing the magnetic characteristics of BiFeO3 nanoparticles by Ca, Ba co-doping, Materials Chemistry and Physics, 135 (1), 144-149, 2012
2. A. K. Sinha et. al, Enhanced dielectric, magnetic and optical properties of Cr-doped BiFeO3 multiferroic nanoparticles synthesized by sol-gel route, Results in Physics, 13, 102299, 2019

P-57

Quorum Sensing: A key driver of cooperative and competitive behaviors in bacteria

Adarsh A Kalua, Om Ashutosh, Isheeta Mohanty, Subhashree Sahu, Rahul Pradhan, Sakti Prasad Ojha, ShilaLipi Samantraya* Chirasmita Mishra* and Arup Sarkar

School of Biotech Sciences, Trident Academy of Creative Technology, F-2/B Chandaka Industrial Estate, Bhubaneswar-751024
**Corresponding Author Email: arup.s2010@gmail.com*

Bacteria exhibit sophisticated collective behaviors regulated by quorum sensing (QS), a communication system that uses chemical signaling molecules to detect population density and coordinate gene expression. One important QS-regulated trait is biofilm formation, where cells attach to surfaces and produce extracellular polymeric substances (EPS). Although EPS is essential for biofilm structure and protection, bacteria differ in how QS controls its production: some increase polymer secretion at high cell density, whereas others reduce it after biofilms mature.

To investigate this variation, a computational QS model based on *Pseudomonas aeruginosa* were developed, an opportunistic pathogen associated with chronic lung infections and medical device-related biofilms. Using individual-based evolutionary simulations, we compared strains with different QS thresholds and EPS regulation patterns. Study showed that early activation of polymer production gives a competitive advantage by promoting rapid biofilm establishment, spatial dominance, and exclusion of non-producing strains. However, the model demonstrates that downregulating polymer secretion at high density can be advantageous under certain ecological conditions. When dispersal opportunities arise, such as through immune stress or physical disruption redirecting resources from EPS production to cell growth enhances transmission and colonization of new environments. In contrast, continuous polymer production is favored in stable, long-lasting biofilms typical of chronic infections, where structural integrity and resistance to antibiotics are essential. Overall, study suggests that variation in quorum-regulated EPS production reflects adaptive responses to ecological context. These findings highlight how infection dynamics shape QS evolution and support the development of anti-QS strategies to manage *P. aeruginosa* biofilm-related disease.

P-58

Development of an IoT-Enabled Smart Agricultural Monitoring System for Optimized Irrigation and Precision Farming

Prabhat Rishi[1], Ashmit Kumar[1], MD Safiullah[1] and Bhavya Bhushan[2]

[1]B.tech 1st year, Department of Computer Engineering, KIIT Deemed to be University, Bhubaneswar
[2]Department of Physics, School of Applied Sciences, KIIT, Deemed to be University, Bhubaneswar
**E-mail: bbhusanfpy@kiit.ac.in*

Precision agriculture has transitioned to an essential sector due to global water shortages and the need to increase crop yields through technology. This research work proceeds to depict the fabrication and deployment of a very affordable Internet of Things (IoT) based environmental measuring system designed for home gardening and smart farming applications. The proposed system's primary control unit is the ESP32 microcontroller (Alternative of Arduino UNO and WIFI Sensor), which is chosen for its dual-core architecture and the fact that the Wi-Fi/Bluetooth capabilities are integrated, which makes the data transmission simple to carry out. The system commits a DHT11 sensor for real-time acquisition of the ambient.

Temperature and humidity, and a resistive soil moisture sensor are used to measure the volumetric water content of the soil. The environmental parameters gathered are handed to and then sent wirelessly to a remote server by the ESP32. Data Recording is achieved through a cloud-based spreadsheet interface (Google Sheets), which facilitates the review of the logged data and has been made accessible from any internet-enabled device. The arrangement here is specifically meant to cope with the problems brought about by over- and under-irrigation, which, in the former case, causes root rot and plant death, and in the latter, it hampers development, respectively. By equipping the user with accurate information, the system allows for the production of microclimates, which provide the necessary temperature and moisture for rare plants. The experimental results demonstrate that the future environmental parameters can be disseminated very quickly from the system, so that it is possible to use same system as a scalable irrigation automation process solution. This system is a great step in the direction of water conservation and a source of empowerment for farmers to embark on data driven decision making for sustainable agriculture.

References:

1. K. Lakshmisudha et al., "Smart Precision Based Agriculture using IoT," Recent Technology and Engineering (IJRTE), Vol. 8, Issue 2, 2019.
2. Espressif Systems, "ESP32 Series Datasheet: 2.4 GHz Wi-Fi + Bluetooth + Bluetooth LE SoC," .
3. D. H. T. Sensor, "DHT11 Humidity & Temperature Sensor Datasheet," AosongElectronicsCo.,Ltd.

P-59

Laser-targeted photothermal therapy with functionalized gold nanoparticles

Jasaswini Tripathy*, Rupayana Panda, Akanshya Mishra

Department of Chemistry, School of Applied Sciences, KIIT Deemed to be University, Bhubaneswar-751024, Odisha, India
Email-jtripathyfch@kiit.ac.in

Recent research has increasingly focused on NIR-based therapeutic methods, including NIR-triggered photothermal therapy (PTT) for cancer treatment. In this study, surface-functionalized plasmonic gold nanoparticles were developed for targeted laser-induced PTT. These nanoparticles showed absorption in the near-infrared (NIR) range and were modified to specifically target tumor cells. Characterization of the nanoparticles was performed using techniques such as UV-Vis spectroscopy, FT-IR, dynamic light scattering (DLS), transmission electron microscopy (TEM), atomic force microscopy (AFM), and energy-dispersive X-ray spectroscopy (EDX). The anticancer effects of these gold nanostructures were evaluated in vitro through cytotoxicity assays, flow cytometry, and DNA damage assessments. The results indicated that NIR irradiation induced apoptosis in cancer cells, enhancing the precision and effectiveness of PTT in destroying tumor cells.

Keywords: PTT, AuNPs, NIR, Cancer

P-60

Study of genetic polymorphism of AGER gene in type 2 diabetes mellitus with and without complications

[*]Sweta Singh, [1]Rajlaxmi Sarangi, [2]Sambit Das, [3]K.P. Tripathy

[*]PhD Scholar in Biochemistry,KIMS,Bhubaneswar
[1]Professor, Biochemistry, KIMS, Bhubaneswar
[2]Professor, Endocrinology,KIMS,Bhubaneswar
[3]Professor, Medicine,KIMS,Bhubaneswar
Kalinga Institute Of Medical Sciences,Bhubaneswar,Odisha,India
Email: swetasingh5040@gmail.com

Abstract:

Diabetes is a complex metabolic disorder caused by insufficient insulin secretion,as in type 1 diabetes mellitus,or insulin resistance,as in type 2 diabetes mellitus. According to the international diabetes federation,537 million adults worldwide had diabetes in 2021,which is projected to increase to 783 million by 2045.Chronic hyperglycemic condition in diabetics promotes the development of several microvascular and macrovascular complications,such as diabetic retinopathy,diabetic nephropathy,diabetic neuropathy,and cardiovascular diseases. The receptor for advanced glycation end products(RAGE) is a transmembrane protein that interacts with its ligands,advanced glycation end products(AGEs).

AGEs are elevated in diabetes and diabetic complications,leading to increased oxidative stress and activation of pro-inflammatory pathways facilitated by AGE-RAGE signaling.Polymorphisms in the RAGE gene can potentially affect AGE-RAGE interaction and its downstream signaling.The receptor for advanced glycation end products(RAGE) is a cell surface transmembrane multiligand receptor,encoded by the AGER gene.RAGE presents many transcripts,is expressed mainly in the lung,and involves multiple pathways(such as NFkB,Akt,P38 and MAP kinases)that initiate and perpetuate an unfavorable proinflammatory state.Due to these numerous functional activities,RAGE is implicated in multiple diseases.AGER is a highly polymorphic gene,with polymorphisms or SNP(single-nucleotide polymorphism)that could be responsible or co-responsible for disease development.Six polymorphisms of AGER are described:rs2070600,rs1800624, rs1800625,rs184003,and rs3134940,rs55640627.The rs2070600 SNP may be associated with the development of human autoimmune disease,diabetes complications,Cancer,and lung diseases such as chronic obstructive pulmonary disease and acute respiratory distress syndrome.The rs1800625 SNP may be associated with the development of diabetic retinopathy,cancer,and lupus but may be protective against cardiovascular risk.The rs184003 SNP seems related to coronary artery disease,breast cancer and diabetes.Here,these potential associations between AGER polymorphisms and the development of diseases are discussed,as there have been conflicting findings on the pathological impact of AGER SNPs in the literature.These contradictory results might be explained by distinct AGER SNP frequencies depending on ethnicity.

Keywords: Type 2 diabetes,Receptor for advanced glycation endproducts, Polymorphism

References:

1. Ahuja P, Waris A, Siddiqui SS, Mukherjee A. Single nucleotide variants of receptor for advanced glycation end-products (AGER) gene: is it a new opening in the risk assessment of diabetic retinopathy?-a review. J Genet Eng Biotechnol. 2022 Jan 31;20(1):17.
2. Chaurasiya AH, Khilari AA, Kazi R, Jaiswal MR, Bhoite GM, Padwal MK, Momin AA, Shanmugam D, Kulkarni MJ. Nanopore Sequencing of *RAGE* Gene Polymorphisms and Their Association with Type 2 Diabetes. ACS Omega. 2023 Jul 10;8(29):25727-25738.
3. Serveaux-Dancer M, Jabaudon M, Creveaux I, Belville C, Blondonnet R, Gross C, Constantin JM, Blanchon L, Sapin V. Pathological Implications of Receptor for Advanced Glycation End-Product (*AGER*) Gene Polymorphism. Dis Markers. 2019 Feb 4;2019:2067353.
4. Tripathi AK, Chawla D, Bansal S, Banerjee BD, Madhu SV, Kalra OP. Association of RAGE gene polymorphism with vascular complications in Indian type 2 diabetes mellitus patients. Diabetes Res Clin Pract. 2014 Mar;103(3):474-81.
5. Cheng H, Zhu W, Zhu M, Sun Y, Sun X, Jia D, Yang C, Yu H, Zhang C. Susceptibility of six polymorphisms in the receptor for advanced glycation end products to type 2 diabetes: a systematic review and meta-analysis. Endocr J. 2021 Aug 28;68(8):993-1010.
6. Bansal S, Chawla D, Banerjee BD, Madhu SV, Tripathi AK. Association of RAGE gene polymorphism with circulating AGEs level and paraoxonase activity in relation to macro-vascular complications in Indian type 2 diabetes mellitus patients. Gene. 2013 Sep 10;526(2):325-30.
7. Chawla D, Bansal S, Banerjee BD, Madhu SV, Kalra OP, Tripathi AK. Role of advanced glycation end product (AGE)-induced receptor (RAGE) expression in diabetic vascular complications. Microvasc Res. 2014 Sep;95:1-6.

P-61

ELUCIDATING THE MOLECULAR, CELLULAR AND FUNCTIONAL HETEROGENEITY IN NORMAL AND MALIGNANT PANCREATIC FIBROBLAST CELLS

Amlan Priyadarshee Mohapatra[1,2], Sudeshna Dutta[1], Aliva Prity Minz[1], Swayambara Mishra[1,2], Deepti Parida[1,2], Salona Kar[u], Sunil K Raghav[3*], Shantibhusan Senapati[1*]

[1]Tumor microenvironment and Animal models lab, Institute of Life Sciences, Bhubaneswar, Odisha, India
[2]Regional center for Biotechnology, Faridabad, Haryana, India
[3]Immuno-genomics and Systems biology lab, Institute of Life Sciences, Bhubaneswar, Odisha, India
e-mail: priyadarshee1998@gmail.com

ABSTRACT

Background: Heterogeneity in Carcinoma associated fibroblasts (CAFs) and their functionality have been identified recently in pancreatic ductal adenocarcinoma (PDAC), yet it warrants further investigations. Normal pancreatic fibroblasts (PFs) could be heterogenous shaping CAF heterogeneity and certain CAF subtypes might significantly confer tumorigenic and/or therapy refractory attributes in the TME.

Objectives: Here, we set two objectives first, to understand PF heterogeneity and their contribution to PDAC development and lastly, to evaluate the role of different CAF-subtypes in PDAC therapy outcomes.

Materials and Methods: Single cell analysis of an enriched fraction of mouse PFs in normal mouse whole pancreas and its different lobes was conducted. Fibroblasts were sorted into two subtypes using the marker LY6C by FACS. *In-vitro* and *in-vivo* models and several molecular techniques were used to check the tumor modulating properties of these subtypes.

Results and conclusions: The fibroblasts in normal mice pancreas and its different lobes exhibited distinct molecular heterogeneity corroborating with already reported populations of pancreatic normal fibroblasts and CAFs of mice. Additionally, we captured some novel molecular subtypes and predicted their functionality. The phenotypic diversity and tumor modulating properties of LY6C positive and negative fibroblasts were characterised and validated with cell-line based *in-vitro* and *in-vivo* mice models. Our study will help understand different novel normal fibroblast subtypes, their contribution to CAF heterogeneity and their function in determining cancer development and therapeutics, which will help in developing targeted therapy in PDAC.

Keywords: PDAC, Fibroblast heterogeneity, Normal pancreatic fibroblasts, Single cell sequencing, LY6C, Tumor modulation

Presenting authors name- Amlan Priyadarshee Mohapatra
Presenting authors mail id: priyadarshee1998@gmail.com
Mentor's affiliation and e-mail: Scientist-F, Tumor microenvironment and animal Model's lab, Institute of Life Sciences, Nalco Square, Bhubaneswar-751023
e-mail: senapati@ils.res.in

P-62

Aristolochia indica-based Synthesis and Characterization of Silver-Manganese Oxide Composite Nanoparticles

Prangya Prajjwalita Gajendra, Archita Lenka

P.G. Department of Zoology, Berhampur University, Berhampur, Odisha-760007, India
E-mail: archita191@gmail.com, prangya.1235@gmail.com

Leaf extract of *Aristolochia indica* is rich in aristolochic acid, which acts as a very good reducing agent to reduce both the KMnO4 and $AgNO_3$ into oxides of manganese and silver, respectively, at 95°C. The L.E. can reduce the mixture of $KMnO_4$ and $AgNO_3$ (in ratios of 1:3, 3:1, and 1:1) into composite nanoparticles. The synthesis of the NP was monitored in real-time using UV/Vis spectrophotometry. The NPs were then recovered and characterized for their optical properties by using UV/Vis spectrophotometry (190-1100 nm) (Dwivedi et al., 2018; Li et al., 2018) and chemical composition by FTIR (500-4000 cm^{-1}) spectroscopy (Iyer and Panda, 2018) and EDAX. The morphology of the NPs was detected through SEM and TEM at 120-300 KeV. Powder XRD study using a diffractometer (40 kV, 15 mA, and Cu-Kα of 1.541 Å) to understand their crystalline nature, grain size, and alignment of the NPs.

Keywords: Biogenic, Charcterization of NPs, Plant-based synthesis of NP

References

Dwivedi, C., Chaudhary, A., Srinivasan, S., Nandi, C.K., 2018. Polymer Stabilized Bimetallic Alloy Nanoparticles: Synthesis and Catalytic Application. Colloid Interface Sci. Commun. 24, 62–67.
Iyer, R.I., Panda, T., 2018. Biosynthesis of Gold and Silver Nanoparticles Using Extracts of Callus Cultures of Pumpkin (Cucurbita maxima). J. Nanosci. Nanotechnol. 18, 5341–5353.
Li, X., Odoom-Wubah, T., Huang, J., 2018. Biosynthesis of Ag–Pd bimetallic alloy nanoparticles through hydrolysis of cellulose triggered by silver sulfate. RSC Adv. 8, 30340–30345. https://doi.org/10.1039/C8RA04301A

Electrostimulation-based induction of defensive skin secretion in *Duttaphrynus melanostictus*

Abhaya Kumar Behera

P.G. Department of Zoology, Berhampur University, Ganjam, Odisha, 760007
E-mail: akbehera.in@gmail.com

ABSTRACT

Amphibians represent one of the most ecologically significant group of vertebrates. Among them frogs (anurans) have gained notable attention in biological science and biomedical research due to their unique skin properties. The skin of frogs is a vital organ that plays a critical role in defense against environmental threats. This defense mechanism is primarily facilitated by secretion of various chemical compounds. In nature environments, frog are constantly exposed to wide array of microbial pathogens including bacteria, fungi, and viruses. They rely heavily on their innate immunity which includes the skin secretion of antimicrobial peptides (AMPs), these secretions are known to contain a complex mixture of biologically active compounds such as peptides, proteins, alkaloids, and steroids that protect them from microbial infection. The project aims to extract crude skin secretions from the species, and evaluate their antimicrobial efficacy against selected bacterial and fungal strains. The present study investigates the electro stimulation based induction of skin secretions in *Duttaphrynus melanostictus* . Collected specimens were maintained in a naturalistic terrarium environment with regulated temperature and humidity, ensuring minimal stress and optimal physiological activity. Morphometric analyses including measurments of body length, breadth, and weight were performed to determine species specific stimulation thresolds. A custom stimulation apparatus was developed using a step down transformer capable of delivering adjustable voltages from 3 – 18 V, with output verified using a multimeter. Experimental stimulation trials indicated that effective secretion induction occurred primarily between 9 – 18 V, applied for 2 – 5 minutes depending on the size of specimen. Crude secretions obtained were subjected to biochemical assesment, where protein estimation using biuret assay and bovine serum albumin used as the standard, confirms the presence of peptide rich components. Preliminary antimicrobial screening using the agar well diffusion and disc diffusion method showed weak inhibition zones against selected bacterial strains, suggesting either need further purification and extraction of anti microbial peptide. The study highlights the potential of *D. melanostictus* as a source of bioactive compound and emphasizes the future directions including isolation and characterization of AMPs, advanced purification techniques, and functional assays to evaluate therapeutic potential.

Keywords: Amphibians, Duttaphrynus melanostictus, Anti microbial Peptide, therapeutic potential

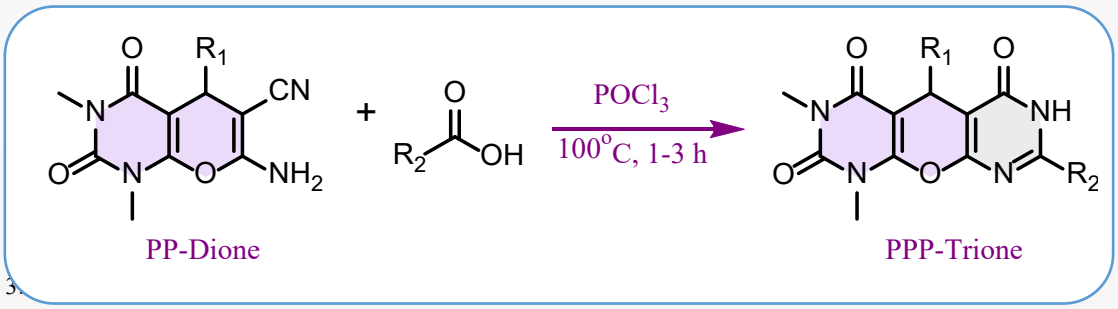
P-64

Synthesis, Molecular Docking and Pharmacokinetics Study of Pyrano-dipyrimidine Derivatives

Jayesh Sarvaiya[a], Paritosh Shukla[a*]

[a] *Department of Chemistry, Birla Institute of Technology and Science, Pilani – 333031 Rajasthan, India*
E-mail: p20210408@pilani.bits-pilani.ac.in , shukla_p@pilani.bits-pilani.ac.in

Pyran, pyrimidine derivatives, either alone or as fused rings, are extremely important in organic chemistry as well as biological science because of their significant biological actions viz., anticancer, antitubercular, anti-HCV, antiviral, anti-inflammatory, antibacterial, antipyretic properties. Due to these significant characteristics, our research group has been interested in creating such heterocycles and investigating their synthetic methodologies. Thus, these new pyrano-dipyrimidine-trione (PPP-Trione) derivatives were synthesized by reacting to pyrano-pyrimidine-dione (PP-Dione) with acid in the presence of well-known chlorinating agent $POCl_3$ under the reflux condition. Previously limited derivatives were synthesized by Asadian et al. [1]. Herein, we report on additional derivatives of PPP-Trione. The starting materials PP-Dione was prepared according to the literature reports [2]. A Tandem intramolecular Pinner-Dimroth rearrangement-based process was also suggested as a plausible mechanism for the synthesis of PPP-Trione derivatives [3]. In addition to that, we also carried out the Pharmacokinetics study and in silico docking analysis of the PPP-Trione derivatives. The scheme of the reaction is given below:



3.

P-65

In vitro Cytotoxicity of Chalk Particles Released in Public Secondary School Classrooms in the Johannesburg Region in South Africa

Setlamorago Mbazima [1,2] and Jitcy Joseph[2, 3]

[1] *School of Geography, Archaeology and Environmental Studies, University of the Witwatersrand, Johannesburg, Republic of South Africa*
[2] *Department of Toxicology and Biochemistry, National Institute for Occupational Health, Division of the National Health Laboratory Service, Johannesburg, Republic of South Africa*
[3]*Department of Life and Consumer Sciences, College of Agriculture and Environmental Sciences, University of South Africa, Johannesburg, Republic of South Africa*

Introduction: Teaching in low- and middle-income countries (LMICs) heavily relies on chalkboards, releasing chalk particles that contribute to poor indoor air quality and pose inhalation risks. Despite traditional views of chalk as inert, its potential health effects, especially on respiratory cells, remain understudied in LMICs. This study aimed to investigate the cytotoxicity of different chalk particle types on human bronchial epithelial (BEAS-2B) cells *in vitro*.

Methods: BEAS-2B cells, a relevant model for respiratory exposure, were cultured and exposed to varying concentrations of pulverized, airborne, and settled chalk particles. Cell viability and proliferation were continuously monitored using the xCELLigence Real-Time Cell Analyzer (RTCA), which measures cell index (CI). Untreated cells served as a negative control, while 10% DMSO was used as a positive control for maximum toxicity. Statistical significance was determined by using GraphPad prism 10.5.

Results and discussion: The study revealed a concentration-dependent toxicity across all chalk particle types. Pulverized chalk showed significant cytotoxicity at 100 µg/ml, while lower concentrations had minimal effects. Airborne chalk exhibited less toxicity from 0.13 mg/ml, with increasing severity at higher doses. Settled chalk caused moderate effects at 100 µg/ml and 1 mg/ml, with high toxicity at 10 mg/ml. Untreated cells showed robust growth, and controls validated the assay. These findings challenge the assumption that chalk dust is harmless, demonstrating its capacity to impair cell viability. The varying toxicity thresholds underscore the need for further research into particle characteristics. The results have significant implications for respiratory health in classroom environments.

Conclusion: The research provides compelling evidence that chalk particles exhibit concentration-dependent toxicity on BEAS-2B cells. This study highlights an under-recognized health hazard, particularly in LMICs. The results underscore the importance of minimizing chalk dust exposure through improved ventilation, frequent cleaning, and considering alternative teaching materials to enhance classroom safety and inform public health policies.

P-66

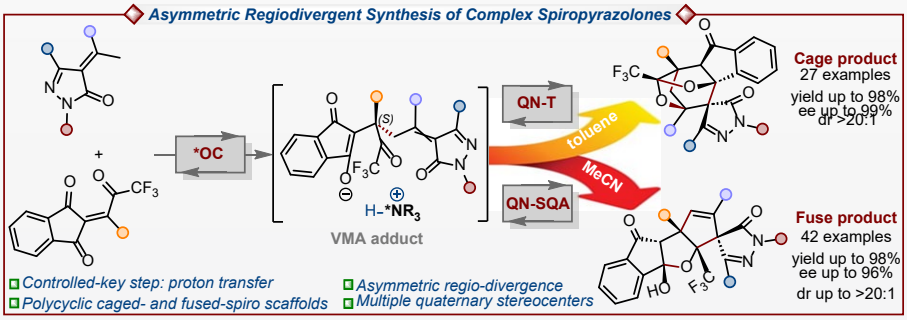
Solvent-Assisted Organocatalyst-Enabled Enantioselective Regiodivergent Cascade Reactions: Overriding Intrinsic Reactivity of Vinylogous Pyrazolones

Ganesh Shantaram Khomane, and Wenwei Lin*

Department of Chemistry, National Taiwan Normal University, 88, Sec. 4, Tingchow Road, Taipei 11677, Taiwan, R.O.C. Fax: (+886)-2-2932-4249
E-mail: ganeshkhomane91@gmail.com

Asymmetric organocatalytic vinylogous Michael addition (VMA) is a powerful platform for constructing chiral building blocks.[1] Previously, we synthesized polycyclic compounds with high stereoselectivity and complexity from sterically biased indandione-derived acceptors and oxindole- or pyrazolone-based vinylogous precursors via VMA in a cascade fashion.[2] However, enantioselective regiodivergent cascades remain challenging, requiring precise control of both regio- and stereoselectivity.

Herein, we present a quinine-derived bifunctional catalyst strategy for the cascade construction of diverse asymmetric polycyclic spiro-pyrazolone scaffolds. The reaction is initiated by the asymmetric VMA of arylidene pyrazolones to indandione-derived acceptors, followed by regioselective transformations that afford structurally diverse products. The divergent outcomes are governed by the interaction between the in situ-generated conjugate acid of the catalyst and the anionic VMA adduct, and can be further modulated by tuning the reaction conditions, particularly the solvent polarity. This strategy establishes a versatile platform for asymmetric regiodivergent cascade reactions.[3]



References:

1. Y. Yin, Z. Jiang, *ChemCatChem*, **2017**, *9*, 4306.
2. (a) S.-M. Yang, P. Karanam, M. Wang, Y.-J. Jang, Y.-S. Yeh, P.-Y. Tseng, M. R. Ganapuram, Y.-C. Liou, W. Lin, *Chem. Commun*., **2019**, *55*, 1398. (b) G. S. Khomane, T. -C. Yen, G. Marri, W. Lin, *Org. Lett.* **2025**, *27*, 9189-9194.
3. Unpublished results.

P-67

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

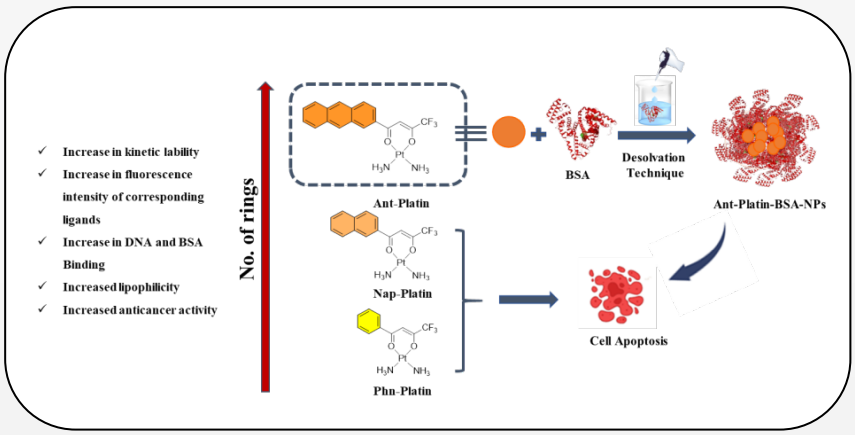
Kanakasree Mohan[1], Megha Biswas[2], Rakesh Kumar Pathak*

Department of Chemical Sciences, IISER Berhampur, India
*E-mail: * rpathak@iiserbpr.ac.in*

Abstract

Platinum-based chemotherapeutics such as cisplatin and carboplatin remain mainstays of cancer treatment, yet their clinical success is limited by dose-limiting toxicity, poor aqueous solubility, and the emergence of resistance. Addressing these challenges requires innovative molecular design coupled with smart delivery platforms that can modulate pharmacokinetics and improve tumor selectivity. Protein-based nanocarriers, particularly bovine serum albumin (BSA) nanoparticles, have gained attention for their biocompatibility, stability, and ability to enhance the solubility and circulation of hydrophobic drugs (Ji Yeon et al. [1]; Khandelia et al. [2]). A series of Pt (II) prodrugs, termed aromaplatins, featuring β-diketonate ligands with progressively extended aromatic ring systems, was synthesized. HPLC-based stability studies revealed that an increase in the ring size enhanced chemical reactivity and biomolecular interactions but reduced aqueous solubility and formulation stability. Among them, Ant-Platin, the most reactive analogue, showed poor stability in biological media, necessitating the use of a nanocarrier. Accordingly, Ant-Platin was encapsulated in biocompatible BSA nanoparticles, achieving high encapsulation efficiency and drug loading capacity. The resulting nanoformulations were monodisperse, colloidally stable under both refrigerated storage and serum incubation, and exhibited a cumulative release profile with an initial burst followed by sustained release exceeding 90% over 72 hours. This encapsulation strategy mitigated the solubility and stability limitations of aromaplatins and provided controlled release, thereby expanding their therapeutic applicability.

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



References

1. Ji Yeon, J.; Hoang Hai, N.; Sae-Yeol-Rim, P.; Hyang Sook, C.; Byeong-Cheol, K.; Sanghoon, K. *Food Chem*, 2011, 127 (4), 1892-1898.
2. Khandelia, R.; Hodgkinson, T.; Crean, D.; Brougham, D. F.; Scholz, D.; Ibrahim, H.; Quinn, S. J.; Rodriguez, B. J.; Kennedy, O. D.; O'Byrne, J. M.; *et al.*, *ACS Appl Mater Interfaces*, 2024, 16 (12), 14633-14644.

P-68

Synthesis, Photophysical Evaluation and Computational Study of 2-Pyrone Carboxylic Acid Analogs

Preeti Christina Beck, Dr. Debdutta Chakraborty, Dr. Ashoke Sharon*

Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India-835215
Email Id: phdac10052.23@bitmesra.ac.in

2-Pyrone, a six membered heterocyclic medicinally important scaffold, possesses a privileged structure having characteristics of lactones, conjugated dienes and arenes. It possesses multiple potential reactive sites for a variety of chemical reactions. The synthesis of 2-pyrone based 4-(methylthio)-2- oxo-6-phenyl-2H-pyran-3-carboxylic acid analogs follows a simple yet efficient one pot bottom-up synthesis protocol.[1] The synthesized compounds are characterized using ^{1}H NMR, ^{13}C NMR, HRMS, UV, and IR spectroscopic methods. The functionalization of 2-pyrone allows vast derivatisation at C3, C4 and C6 positions of the heterocyclic ring. Addition of a carboxylic acid group at C3 position of the scaffold and appropriate substitution at C4 and/or C6 position renders the scaffold emissive with significant quantum yield. In the 4-(methylthio)-2-oxo-6-phenyl-2H-pyran-3-carboxylic acid derivatives reported herein, a donor-acceptor based intramolecular charge transfer in solid state has been demonstrated and justified through photoluminescence analysis. Computational analysis based on the DFT calculations has been performed using hybrid functional B3LYP in order to investigate stability and reactivity through inferred from the HOMO-LUMO energy gaps fundamental reactivity descriptors such as electronegativity, chemical potential, hardness, softness, electrophilicity index and molecular electrostatic potential.[2][3]

Keywords: 2-Pyrone, heterocyclic, photoluminescence analysis, DFT, reactivity descriptors

References:

1. Ananda Kumar Konreddy, Massaki Toyama, Wataru Ito, Chandralata Bal, Masanori Baba, and Ashoke Sharon, ACS Med. Chem.Lett. 2014, 5, 259−263
2. Shetgaonkar, S.E.; Kollur, S.P.; Pillai, R.R.; Thangavel, K.; Armakovi´c, S.J.; Armakovi´c, S.; Shivamallu, C.; Amachawadi, R.G.; Syed, A.; Elgorban, A.M.; et al. Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. Symmetry 2021, 13, 161
3. M. Govindarajan , M. Karabacak, S.Periandy,and D.Tanuja. Spectroscopic (FT-IR,FT-Raman,UV and NMR) investigation and NLO, HOMO–LUMO, NBO analysis of organic 2,4,5-trichloroaniline. Spectrochim. Acta, Part A: Mol. Biomol. Spectrosc., 2012, 97, 231-245.

P-69

Tributyltin Chloride Promotes Obesity Through SIRT1-Mediated Adipogenesis and Inflammation

Shruti Sharan[1,2*], Sthitiprajna Samantaray[1], Prajnya Das[1], Shilalipi Samantaray[1], Partha Roy[2*]

[1]*Trident Academy of Creative Technology, Bhubaneswar, Odisha, India*
[2]*Indian Institute of Technology Roorkee, Uttarakhand, India*

While diet and sedentary lifestyle remain important factors in the development of obesity, recent findings have shown the possible involvement of environmental obesogens, which disrupts homeostatic energy balance and increases adiposity. One of the food contaminants i.e., tributyltin chloride (TBTCl) is an endocrine disrupting compound (EDC) promoting adipogenic differentiation *in vitro* and *in vivo*. Although TBTCl exposure has been shown to induce obesity, the underlying mechanisms are not yet well understood. Here we investigated the effect of TBTCl in promoting adipogenesis and inflammation in adipose tissue, in a manner that promotes obesity and to elucidate the involvement of SIRT1 in this action using both *in vitro* and *in vivo* models. Our result showed that knockdown of SIRT1 enhanced TBTCl induced peroxisome proliferator-activated receptor (PPARγ) expression and adipogenesis while simultaneously causing NFκB activation promoting inflammation. Further, TBTCl enhanced the recruitment of RAW264.7 macrophage to 3T3-L1 adipocytes and also increased the expression of genes associated with adipogenesis (leptin, adipsin, adiponectin) and inflammation (IL-6, TNF-α, COX-2, NFκB). In vivo exposure to TBTCl significantly increased the body weight, perigonadal fat mass and lipid deposition in liver of female Swiss albino mice after 45 days of treatment. In conclusion, the results demonstrate the obesogenic potential of TBTCl both *in vitro* and *in vivo* involving multiple mechanisms including increased adipogenesis and inflammation. Thus, TBTCl may be considered as a potential chemical stressor for obesity and obesity-related disorders.

P-70

"Synthesis of Nitrogen Containing Heterocyclic Entities"

Yash Kholakiya[1], Jeet Bhatt

Centre for Research and Development, Dr. Subhash University, Junagadh (362001), Gujarat, India.
Email – bhattjeet94@gmail.com

Abstract:

The importance of Nitrogen containing Heterocyclic compounds in chemistry, Biology and other Pharma Technology makes them an important class of organic molecules. The imidazole molecules are amphoteric in nature that is they can be acidic as well as basic in nature. The selection of Imidazole and pyridine is due to it holds an immense appeal due to their structural activites and pivotal role in biological and therapeutic activities. Sulfa pyridine was the first antibiotic to treat Winston pneumonia. Activity.The2-phenylimidazo [1,2-*a*] pyridine-3-carbaldehyde derivatives were synthesized using substitute phenacyl bromides with 2-aminopyridines and later Vilsmeier and Albrecht Hack reaction. When a ketone is reacted with aldehyde it forms a β- ketone intermediate followed by dimethylaminomethylation reaction. This intermediate further followed by Hantzsch pyridine synthesis to form a pyridine Moiety which further undergoes nucleophilic aromatic substitution to from an imidiazopydridine moiety. Pyridine is a nitrogen bearing heterocyclic entities showing wide range of biological activites and its therepuactic applications. The Imidazopyridine is synthesized using Hantzsch pyridine synthesis or multicomponent reaction leading to formation of pyridines or pyrimidines. Imidazole which is two nitrogen containing heterocyclic molecule also known as 1,3 diazole which is simultaneous to pyrrole nitrogen heterocyclic molecule shows various biological activites such as Anticancer, antibacterial, anti-inflammatory, antitumor,anti-diabetic,anti-allergic, antifungal etc.

Keywords: Imidazole, Pyridine, 1, 3 Imidazole, 2-Phenylimidiazo, [1,2 –a] pyridine, Hack reaction, Vilsmeier reaction, Albrecht Reaction, Hantzsch synthesis, Anticancer, Antibacterial, Anti- tumor, Anti-inflammatory, Antifungal.

P-71

Green Synthesis and Characterization of Silver Nanoparticles for Transdermal Insulin Patch Applications

Debasis Behera[1], Jagnyaseni Tripathy[1]

[1]Department of Physics, School of Applied Sciences, KIIT deemed to be university BBSR-751024, Odisha, India

Silver nanoparticles (Ag NPs) are extensively explored in biomedical research due to their distinctive physicochemical and biological properties, such as high surface-to-volume ratio, excellent antimicrobial activity, catalytic behaviour, and good biocompatibility. The presented work focuses on, a comprehensive literature review was carried out on green synthesis method of Ag NPs, their properties, and their relevance in biomedical applications with a prominence on their potential application in transdermal insulin patches. Emphasis was placed on the design and structural components of transdermal insulin patches, including polymer matrices, adhesive layers, and drug release mechanisms. To date, silver nanoparticles were synthesized via a green approach using plant-based extracts and characterized using UV–Visible spectroscopy to confirm surface plasmon resonance and X-ray diffraction (XRD) to determine crystalline structure. Future work will focus on the fabrication of Ag NP-loaded insulin patches, evaluation of their mechanical properties, and investigation of insulin release kinetics to assess their suitability for effective diabetic management.

P-72

Impedance Spectroscopy Analysis and polaron transport mechanism in Sol-Gel Synthesised of Gd_2MnFeO_6 Double Perovskite

Siddhartha Swarup Parida[a], Abhijeet Kumar[a], Budhendra Singh[a*]

[a] *Electroceramics and Crystal Laboratory, Department of Physics, Central University of South Bihar, Gaya, Bihar, India-824236*
Email-ID- siddharthaswarupparida@gmail.com , budhendrasingh@cusb.ac.in

Rare-earth double perovskite Gd_2MnFeO_6 (GMFO) was synthesised via a modified low-temperature sol-gel technique. The structural analysis were done using X-ray diffraction and Rietveld refinement which confirmed a an orthorhombic structure with space group ***Pbnm***[1]. Scanning electron microscopy were used to analyse the morphology of the synthesised ceramic. A heterogeneous plate-like morphology with well-defined grain boundaries were observed. X-ray photoelectron spectroscopy were done to verify elemental composition and valance states of the individual elements viz. Gd^{3+}, Mn^{3+}, Fe^{2+}/Fe^{3+} [2]. The electrical conduction mechanism was explored using impedance spectroscopic study. The study suggested a dominant grain boundary contribution with a decreasing value of bulk resistance with increasing temperature. An extensive investigation of Variable Range Hopping (VRH) conduction mechanism was done to understand the polaron-dominated charge transport behaviour. The study suggested a typical hopping length in the order of 11.5–13 Å [3]. A quantitative correlation between synthesis-induced microstructural features and electrical properties through electrical modulus analysis revealed an enhanced short-range carrier mobility at higher frequencies. A fairly low value of activation energy for conduction (0.286 eV), with an excellent dielectric thermal stability ($\varepsilon' \approx 800$) below 100°C was observed. The present report underlines a direct correlation between microstructural parameters of the sample with VRH type polaron transport mechanisms. The study suggested the suitability of the synthesised sample for next-generation electronic and sensor applications. The results are analysed and discussed in details.

REFERENCES

1. M. Rani, P.K. Kamlesh, S. Kumawat, Anuradha, U. Rani, G. Arora, A.S. Verma, Rare earth-based oxides double perovskites A2NiMnO6 (A=La and gd): Applications in magneto-caloric, photo-catalytic and thermoelectric devices, Physica B: Condensed Matter, 680 (2024) 415645, https://doi.org/10.1016/j.physb.2023.415645.
2. J.S. Punitha, A. Nataraj, V. Anbarasu, M. Dhilip, K.S. Kumar, Synthesis and characterization of phase-stabilized Gd2FeMnO6 double-Perovskite compound, Journal of Materials Science: Materials in Electronics, 32 (2021) 10266-10276, https://doi.org/10.1007/s10854-021-05682-3.
3. M.Y. Gneber, I. Elhamdi, J. Messoudi, R. Dhahri, F. Sahnoune, M. Jemmali, M. Hussein, E. Dhahri, B. Faria Oliveira Costa, Investigation of variable range hopping and dielectric relaxation in GdCrO(3) orthochromite perovskites, RSC Adv, 14 (2024) 36161-36172, https://doi.org/10.1039/d4ra06104g.

AUTHOR INDEX

Author Index