Marwadi University
Marwadi Chandarana Group

NAAC A+

28TH ISCB INTERNATIONAL CONFERENCE

ISCBC - 2024

RECENT ADVANCES IN BIOLOGICAL, CHEMICAL, BIOTECHNOLOGICAL AND PHARMACEUTICAL SCIENCES FOR INNOVATION IN HEALTHCARE

JANUARY 8 - 10, 2024
MARWADI UNIVERSITY
RAJKOT, GUJARAT, INDIA

ABSTRACT BOOK

JOINTLY ORGANIZED BY

INDIAN SOCIETY OF CHEMISTS & BIOLOGISTS (ISCB)
FACULTY OF SCIENCE AND FACULTY OF PHARMACY
MARWADI UNIVERSITY, RAJKOT

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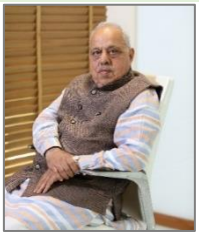

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Dr. Lalji Baldaniya
Principal, Faculty of Pharmacy, Marwadi University

Dr. Vicky Jain
Vice Principal, Faculty of Science, Marwadi University

Shri Ketan Marwadi
President, Marwadi University

Message

We are delighted to commence the 28th ISCB International Conference (ISCBC-2024), a collaborative initiative of the Indian Society of Chemists and Biologists (ISCB) and Marwadi University to be held from 8th to 10th January 2024. The overarching theme, "Recent Advances in Biological, Chemical, Biotechnological, and Pharmaceutical Sciences for Innovation in Healthcare," underscores the focal point of our collective discussions.

We extend a heartfelt welcome and sincere gratitude to our esteemed speakers, researchers, and scientists for gracing us with their invaluable presence and sharing their time and expertise. Your commitment contributes immeasurably to the success and impact of ISCBC-2024.

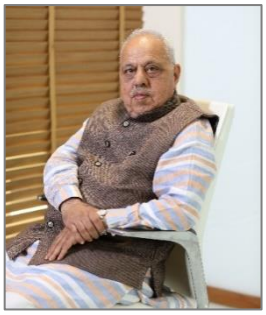
Participation in ISCBC-2024 transcends academic engagement; it's a transformative experience. This event provides a unique opportunity for knowledge exchange, networking, and collaboration, ensuring attendees stay at the forefront of their fields with a diverse program featuring plenary lectures, invited talks, and presentations.

Beyond individual enrichment, the conference fosters a sense of community and collaboration. Connections made here often lead to joint research initiatives and lasting professional relationships, propelling the scientific community forward. May ISCBC-2024 be a catalyst for groundbreaking discoveries, collaborative partnerships, and a lasting impact on the research landscape.

Heartfelt appreciation to the dedicated volunteers and Organizing Committee members for their hard work. Your commitment and passion have been instrumental in making this event a success.

We extend a warm welcome to delegates, dignitaries, and conference attendees. Your presence enriches our event, fostering a collaborative atmosphere for shared knowledge and meaningful interactions.

Thank you all.



Shri Jitubhai Chandarana
Vice President, Marwadi University

Message

It is my distinct pleasure and privilege to announce the 28th ISCB Conference, jointly organized by the Indian Society of Chemists and Biologists (ISCB) and Marwadi University. Scheduled from 8th to 10th January 2024 at our esteemed institution in Rajkot, Gujarat.

Under the theme "Recent Advances in Biological, Chemical, Biotechnological, and Pharmaceutical Sciences for Innovation in Healthcare," this conference promises to be a dynamic convergence of experts, researchers, and professionals in the fields of Biological, Chemical, and Pharmaceutical Sciences.

I take great pride in welcoming you to this intellectual platform, where collaborative discussions and groundbreaking insights will take center stage. Your participation is pivotal to the success of ISCBC-2024, and I anticipate your valuable contributions to the diverse array of plenary lectures, invited talks, and presentations that will characterize our program.

This conference transcends geographical boundaries, offering a unique opportunity for global networking and knowledge exchange. I am confident that your presence will enhance the depth and breadth of our discussions, fostering an environment conducive to the advancement of research and innovation.

Organizing an event of this magnitude requires a tremendous amount of behind-the-scenes effort, and the organizing team has demonstrated an unwavering commitment to excellence. Their attention to detail, thoughtful coordination, and passion for advancing the scientific community are truly commendable.

I extend heartfelt gratitude to our esteemed dignitaries, national and international speakers, and active participants for choosing to be part of this academic gathering. Your presence elevates the significance of our conference, creating an enriching environment for knowledge exchange and collaborative learning.

Best wishes.

Prof. (Dr.) R. B. Jadeja
Pro Vice-Chancellor, Marwadi University

Message

It is with great joy and anticipation that we extend our warmest welcome to all participants of the 28th ISCB International Conference (ISCBC-2024), jointly organized by the Indian Society of Chemists and Biologists (ISCB) and Marwadi University on "Recent Advances in Biological, Chemical, Biotechnological, and Pharmaceutical Sciences for Innovation in Healthcare," to be held during 8th-10th January 2024.

This scientific gathering is expected to provide a conducive platform where global experts will share their cutting-edge insights, exchange research findings, and collaboratively address evolving challenges in these vital fields. The anticipated knowledge-sharing sessions are envisioned to encompass a diverse range of perspectives, methodologies, and discoveries, fostering a dynamic exchange that enriches the collective understanding of participants. The conference is anticipated to serve as a fertile ground for experts to disseminate their expertise, share the latest research outcomes, and engage in meaningful discussions, contributing to the overall advancement of these scientific disciplines. As participants look forward to the knowledge-sharing opportunities, it is expected that the insights gained from these interactions will not only broaden their perspectives but also stimulate collaborative efforts, leading to innovative solutions in the realms of Biological, Chemical, and Pharmaceutical Sciences for the improvement of global healthcare.

Our heartfelt thanks go out to the members of the organizing committee for their tireless efforts in making this event possible. Their dedication ensures the success and seamless execution of ISCBC-2024.

We are looking forward to welcoming distinguished speakers, scholars, and researchers from around the world, making this conference a platform for sharing ideas and contributing to progress in healthcare innovation.

Thank you.

Shri Naresh Jadeja
Registrar, Marwadi University

Message

Dear esteemed participants,

As we eagerly anticipate the 28th ISCB International Conference (ISCBC-2024) hosted by Marwadi University in Rajkot, Gujarat, I extend my heartfelt congratulations to the dedicated staff of the Faculty of Science and Faculty of Pharmacy for their exceptional efforts in organizing this prestigious event.

Marwadi University, Rajkot, Gujarat, has emerged as a beacon of high-quality education, celebrated for its entrepreneurial spirit. In just 14 years, the university has reached an impressive milestone, expanding its educational influence across 51 nations. The commitment to integrating research-based learning into the curriculum and fostering a culture of advancement aligns seamlessly with the vision of university.

The upcoming conference, in collaboration with the Indian Society of Chemists and Biologists, promises to be a convergence of minds, ideas, and innovations. The themes of medicinal chemistry, natural products, pharmaceutical science, and drug discovery underscore the conference's significance in pushing the boundaries of scientific knowledge.

To the researchers, academicians, and industry participants, I extend my best wishes for a rewarding and intellectually enriching experience. May the exchange of ideas, discussions, and collaborations during the conference pave the way for groundbreaking advancements in the realms of science and technology.

May the 28th ISCB International Conference at Marwadi University be a resounding success, contributing to the global pursuit of knowledge and fostering a spirit of innovation.

Best Regards.

Prof. (Dr.) Kantha Deivi Arunachalam
Dean, Faculty of Science

Message

It is my pleasure to announce the upcoming 28th ISCB Conference, a collaborative effort of the Indian Society of Chemists and Biologists (ISCB) and Marwadi University on "Recent Advances in Biological, Chemical, Biotechnological, and Pharmaceutical Sciences for Innovation in Healthcare," taking place from 8th to 10th January 2024.

This conference is anticipated to be a constructive catalyst in fostering collaborative research endeavors within the realms of Biological, Chemical, and Pharmaceutical Sciences. Unlike historical research scenarios marked by individual pursuits, this conference embraces a collective and interdisciplinary approach.

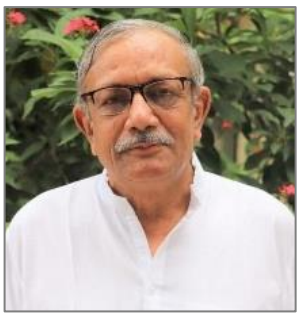
This collaborative shift promises a multitude of benefits. By providing a platform for researchers to share their insights, methodologies, and discoveries, the conference encourages a fruitful exchange of knowledge. This collaborative environment not only deepens our understanding of the interconnected facets of these scientific disciplines but also opens avenues for innovative solutions to intricate research challenges.

Participating in this conference is expected to yield direct benefits for researchers, offering exposure to diverse perspectives and methodologies. These cross-disciplinary interactions are poised not only to enhance individual research pursuits but also to contribute collectively to the advancement of sciences. Ultimately, the conference is poised to be a driving force for transformative progress, fostering collaborative research efforts that hold immense promise for addressing the complexities inherent in global healthcare challenges.

We are honored to host esteemed scientists and keynote/invited speakers from around the world. Their insights and contributions will undoubtedly enrich the discourse on pharmaceutical research and innovation.

I am fortunate to host the 28th ISCB conference and wholeheartedly welcome all the dignitaries, delegates, and conference attendees at Marwadi University, Rajkot. I wish the conference a grand success in terms of generation and fostering knowledge.

Thank you.



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, Lucknow, in collaboration with Marwadi University is organizing the 28th ISCB International Conference (ISCBC-2024). The conference is scheduled to take place at Marwadi University, Rajkot, India, from 8th to 10th January 2024.

The focal theme of the 28th International Conference of ISCB is "Recent Advances in Biological, Chemical, Biotechnological, and Pharmaceutical Sciences for Innovation in Healthcare." Researchers at the conference will engage in discussions on the latest advancements in these fields, with a primary focus on fostering innovation to improve healthcare practices and outcomes.

Distinguished scientists and researchers from around the world, will participate as keynote and invited speakers. The conference will feature over 85 senior scientists and professors addressing the latest advancements and innovations in healthcare.

The scientific committee will compile an abstract book encompassing the presentations to be delivered during ISCBC-2024. Our heartfelt gratitude goes to the members of the organizing committee for their contributions. The conference will facilitate discussions on the trends, prospects, and future directions of research, providing a platform for fruitful deliberations in various scientific research areas.

The comprehensive scientific program includes plenary lectures, invited lectures, and short-gun lectures by eminent scientists from India and abroad. Additionally, oral presentations by young researchers are scheduled, and presentations will be arranged in poster sessions, highlighting the active participation of young scientists and Ph.D. students.

We extend a warm welcome to all national and international delegates from pharmaceutical companies, research organizations, universities, and academic institutes. We hope they have a delightful stay in Rajkot. In conclusion, we express our sincere thanks and gratitude to the members and office bearers of the organizing committee of the 28th ISCB International Conference (ISCBC-2024) at Marwadi University.

Dr. Vicky Jain
Principal, Faculty of Science

Prof. (Dr.) Lalji Baldaniya
Principal, Faculty of Pharmacy

Message

It is with great enthusiasm and honor that we extend a warm invitation to all the resource persons, delegates, research scholars, and esteemed guests for the 28th ISCB Conference, jointly organized by the Indian Society of Chemists and Biologists (ISCB) and Marwadi University. This distinguished event, scheduled to unfold from 8th to 10th January 2024 at our esteemed institution in Rajkot, promises to be an enriching platform for the exchange of knowledge and collaboration in the fields of Biological, Chemical, Biotechnological, and Pharmaceutical Sciences.

The collaborative synergy among Biology, Chemical, and Pharmaceutical Sciences amplifies the potential for groundbreaking discoveries and innovative solutions. As we confront multifaceted challenges in healthcare, environmental sustainability, and technology, the integration of these sciences becomes increasingly pivotal for holistic scientific progress. The upcoming conference stands as a dynamic forum to explore the convergence of these disciplines, fostering dialogue and collaboration that holds the potential for transformative breakthroughs with far-reaching societal impacts.

We extend sincere appreciation to all the upcoming national and international speakers, scholars, and researchers from various corners of the globe, who will grace the 28th ISCB Conference at Marwadi University. Your expected efforts and esteemed presence will play a crucial role in shaping the success of this event. We highly value the wealth of knowledge, diverse perspectives, and innovative insights each of you is set to bring. Your active participation is expected to elevate the quality of discussions and inspire the entire research community present. We express our gratitude in advance for your commitment to fostering collaboration and pushing the boundaries of scientific inquiry. Your contributions are instrumental in making this conference a truly enlightening and impactful event.

A sincere expression of gratitude goes out to the dedicated volunteers, advisors, and esteemed members for their unwavering support, commitment, and collaborative efforts that have contributed significantly to the smooth organization and execution of this event. It is your collective dedication that has enhanced the overall experience for participants, ensuring a fruitful exchange of knowledge and ideas.

Thank you.

डॉ. शैलेंद्र सराफ
निदेशक
Dr. Shailendra Saraf
Director

अहमदाबाद
AHMEDABAD

सत्यमेव जयते

राष्ट्रीय औषधीय शिक्षा एवं अनुसंधान संस्थान (नाईपर), अहमदाबाद
(औषध विभाग, रसायन एवं उर्वरक मंत्रालय, भारत सरकार)
NATIONAL INSTITUTE OF PHARMACEUTICAL EDUCATION AND RESEARCH (NIPER) - AHMEDABAD
(DEPT. OF PHARMACEUTICALS, MINISTRY OF CHEMICALS AND FERTILIZERS, GOI)
Palaj, Opp. Air Force Station Head Quarter,
Gandhinagar-382355, Gujarat, India
December 27, 2023

Message

It gives me immense pleasure to know that the **Indian Society of Chemists and Biologists (ISCB)** and **Marwadi University** are jointly organizing **28th ISCB International Conference (ISCBC-2024)** with the theme "**Recent Advances in Biological, Chemical, and Pharmaceutical Sciences for Innovation in Healthcare**" from **January 8-10, 2024**.

The **ISCB** is always providing leadership in organizing the professional activities on contemporary topics. This International conference will bring all the stakeholders- Academia, Research and Industry on one platform. This conference will provide an excellent opportunity to the participants for the churning on the issues for the translational research.

The **Marwadi University** is known to host such scientific meetings and this conference will witness the presence luminaries from Chemical, Biological, and Pharmaceutical Sciences. The theme is contemporary and needs attention of all the professionals working in different facets of the Biological and Chemical Sciences. The Administration, Staff and students of Marwadi University deserves compliments for the this unique initiative.

I am sure, this conference jointly organized by ISCB and Marwadi University will be remembered for long.I would like to congratulate the organizing committee of **ISCBC-2024** for this pious initiative and wishing a grand success of the Conference.

With Best Wishes

(Dr. Shailendra Saraf)
Director,
National Institute of Pharmaceutical Education and Research (NIPER)- Ahmedabad
Gandhinagar, Gujarat

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- **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**

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Dr. Meghna Seta

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Dr. Ashish Kyada

Scientific Session:
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Dr. Nasir Vadia

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Dr. Malay Udeshi

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Dr. G. Santhanakumar

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Dr. Niralee Patel
Ms. Rinku Manvani

Valedictory function:
Dr. Ashish Kyada
Dr. Dharmesh sur

Exhibitions/ stall:
Dr. Ramesh Parmar

Designing:
Dr. Prakash Kanjariya
Dr. Gaurav Sanghvi

Sponsorship:
Dr. Vicky Jain
Dr. Lalji Baldaniya

SCIENTIFIC PROGRAMME

Monday, January 8, 2024

9.00 AM - 10.00 AM	**Registration**
10.00 AM - 12.00 PM	**Inaugural Session**
12.00 PM - 12.30 PM	**High Tea**

Session – I

Chairpersons: Prof. Anamik Shah and Dr. PMS Chauhan

PL-1 12.30 PM - 1.00 PM	**Nigel G. J. Richards** Department of Chemistry, Cardiff University, Cardiff, UK **Cryo-EM and Molecular Dynamics Simulations Reveal Hidden Conformational Dynamics Controlling Ammonia Transport in Human Asparagine Synthetase**
PL-2 1.00 PM - 1.30 PM	**Michele Vittadello** Professor of Chemistry and Nanoscience, Medgar Evers College of the City University of New York, Energy Nanotechnology and Materials Chemistry Team, Brooklyn, NY, USA **Peristaltic Ion-Conduction Mechanism in Sodium Polymer Electrolytes Based on Perfluoropolyethers, DMSO, and NaTFSI**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session – II A

Chairpersons: Dr. Rakesh Shukla

PL-3 2.30 PM - 3.00 PM	**Anoja Attanayake** Professor in Biochemistry, Department of Biochemistry, Faculty of Medicine, University of Ruhuna, Sri Lanka **Mystery in the development of plant-based nephroprotective agents from Sri Lankan flora**
IL-1 3.00 PM - 3.20 PM	**Dalip Kumar** Senior Professor, Department of Chemistry, Associate Dean, International Programmes and Collaboration Division (IPCD), Birla Institute of Technology & Science, Pilani, Pilani Campus, India **Chlorophyll-a Derived Photosensitizers for Improved Photodynamic Therapy**

IL-2 3.20 PM - 3.40 PM	**Bapurao B. Shingate** Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad, Maharashtra, India **Explorations of Click Chemistry**
IL-3 3.40 PM - 4.00 PM	**Rakesh Kumar Parashar** Bio-Organic Lab, Department of Chemistry, University of Delhi, Delhi, India **Synthesis and Bio-evaluation of Newer benzothiazole appended bis triazoles as antifungal and Tetrahydropyridines based Glycomimetics Azasugars as Anti-Diabetic agents**
IL-4 4.00 PM - 4.20 PM	**Bichismita Sahu** Associate Professor and HOD, Department of Medicinal Chemistry, NIPER-Ahmedabad, Gandhinagar, Gujarat, India **DECIPHERING ROLE OF MINIMALISTIC PEPTIDES AND PEPTIDOMIMETICS TOWARDS BIOMEDICAL APPLICATIONS**
4.20 PM - 4.30 PM	**Tea**

Parallel Session – II B

Chairpersons: Dr M S Shingare and Dr D V Mane

PL-4 2.30 PM - 3.00 PM	**Barbara Zajc** Department of Chemistry and Biochemistry, The City College of New York, USA **Adenosine- and 2'-Deoxyadenosine-8-Carbaldehydes as New Tools for Diverse Purinyl C-8 Modifications**
IL-5 3.00 PM - 3.20 PM	**Mahesh Sharma** Director, Plants Med Laboratories Pvt Ltd, Jaipur, India **Biosap's Rapid-Healing Synergistic Formulas: Debunking Myths in Traditional Medicines**
IL-6 3.20 PM - 3.40 PM	**Evans Coutinho** Bombay College of Pharmacy, Kalina, Santacruz (E), Mumbai, India **Recent Advances in Biological, Chemical and Pharmaceutical Sciences for Innovation in Healthcare**
IL-7 3.40 PM - 4.00 PM	**Deepti Goyal** Assistant Professor, Department of Chemistry, DAV College, Chandigarh, India **Rational design of triazole–peptide conjugates as modulator of Aβ–aggregation, metal–mediated Aβ–aggregation and cytotoxicity**
IL-8 4.00 PM - 4.20 PM	**Hemant Joshi** Department of Chemistry, Central University of Rajasthan, Bandarsindri, Rajasthan, India **Sterically Bulky Ligands Controlled Palladium-Catalyzed Regioselective Organic Transformations**

4.20 PM - 4.30 PM	**Tea**

Parallel Session – II C

Chairpersons: Dr Sanjeev Kumar Shukla and Dr Mahesh Sharma

PL-5 2.30 PM - 3.00 PM	**Dipak P. Ramji** Deputy Head, Cardiff School of Biosciences, Professor of Cardiovascular Science, Cardiff University, Cardiff, UK **Probing the molecular mechanisms underlying the beneficial actions of nutraceuticals in atherosclerotic cardiovascular disease and other inflammatory disorders**
IL-9 3.00 PM - 3.20 PM	**Farukh Arjmand** Department of Chemistry, Aligarh Muslim University, Aligarh, India **RNA-targeted copper-based chemotherapeutic drug candidate derived from bioactive ligand scaffold. that induce ROS -mediated cell death in resistant cancer cells**
IL-10 3.20 PM - 3.40 PM	**Priyankar Paira** Sr. Assistant Professor, Vellore Institute of Technology, Department of Chemistry, School of Advanced Science, Vellore, Tamilnadu, India **Mitochondria targeting Ru(II)/Ir(III)/Re(I) based mono and bimetallic complexes for cancer therapy**
IL-11 3.40 PM - 4.00 PM	**Siddharth Sharma** Assistant Professor, Department of Chemistry, Mohanlal Sukhadia University, Udaipur, India **Transitioning Beyond Flasks: Exploring the Organic Chemistry of Isocyanides through Electrochemical Cells**
IL-12 4.00 PM - 4.20 PM	**Hitendra M. Patel** Professor, Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Synthesis of small Organic Molecules and their Pharmaceutical Applications**
4.20 PM - 4.30 PM	**Tea**

Parallel Session – III A

Chairpersons: Dr Jigna Shah and Dr Alok Jain

PL-6 4.30 PM - 5.00 PM	**Ramaiah Muthyala** Centre for orphan drug development, University of Minneapolis, MN, USA **Development of a broad-spectrum combination antibacterial therapy with metallo beta-lactamase inhibitor against the ESKAPE pathogens for wound healing**

IL-13 5.00 PM - 5.20 PM	**Hitesh D. Patel** Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India **Therapeutic & Diagnostic agents development for Microorganism to AMR through computational chemistry**
IL-14 5.20 PM - 5.40 PM	**Virendra Vikram SIngh** Scientist E, Defence Research & Development Establishment (DRDE), Ministry of Defence, DRDO Gwalior, India **Advanced Materials for Defense: Designing for Performance**

Parallel Session – III B

Chairpersons: Dr N C Desai and Dr Anil Mishra

PL-7 4.30 PM - 5.00 PM	**Harsha Rajapakse** Department of Chemistry and Environmental Science, Medgar Evers College, The City University of New York, Brooklyn, New York, NY 11225, USA **Unveiling Tight Junction Dynamics with Lanthanides**
IL-15 5.00 PM - 5.20 PM	**Ashoke Sharon** Professor & Head, Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Molecular Docking, Dynamics and Chemistry for Hsp90-Cdc37-Cdk4 Protein Complex: A Protein-Protein Modulation Exploration for Drug Discovery**
IL-16 5.20 PM - 5.40 PM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, Rajasthan, India **Metal-Catalyzed Strategies for the Regioselective Functionalization of Amino Acids**

Parallel Session – III C

Chairpersons: Dr Nigel G. J. Richards and Dr Sanjib Bhattacharyya

PL-8 4.30 PM - 5.00 PM	**Erik V. Van der Eycken** Full Professor, University of Leuven (KU Leuven), Department of Chemistry, Division Head of Molecular Design & Synthesis, Head of the Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Celestijnenlaan 200F/box 2404, B-3001 Leuven, Belgium **Synthesis of small complex heterocycles**
IL-17 5.00 PM - 5.20 PM	**Priti Mehta** Dept. of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad, India **Space Pharmaceutical Manufacturing: Beginning of new era of Indian pharmaceutical industry**

IL-18 5.20 PM - 5.40 PM	**Bhupendra Goswami** Assistant Professor, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, Ajmer, Rajasthan, India **Synthesis of Iminophosphonamide Metal Complexes and Their Photoluminescence**

Poster Session -I

Chairpersons: Dr Hardik G. Bhatt and Dr Namrata Rastogi

5.45 PM – 7.00 PM	**Poster Session -I (Poster Number 1 to 50)**

7.00 PM – 8.30 PM	**Cultural Programme**
8.30 PM	**Dinner**

Tuesday, January 9, 2024

Parallel Session – IVA

Chairpersons: Dr Keshav Deo and Prof Diwan Singh Rawat

PL-9 9.00 AM - 9.30 AM	**Marco L. Lolli** Assistant Professor in Medicinal Chemistry, Dept. Science and Drug Technology - University of Turin (UniTO), Italy **Human dihydroorotate dehydrogenase (hDHODH) as drug target: who is going to win the hDHODH golden rush?**
IL-19 9.30 AM - 9.50 AM	**Hardik G. Bhatt** Associate Professor & Head, Dept. of Pharmaceutical Chemistry, Institute of Pharmacy, NIRMA University, Ahmedabad, India **Development of Novel Substituted 1,2,4-Triazole Derivatives Targeting Tankyrase as Anti-Cancer Agents**
IL-20 9.50 AM - 10.10 AM	**Ram Sagar Misra** Professor, School of Physical Sciences, Jawaharlal Nehru University (JNU), New Delhi, India **Efficient Synthesis of Perlin's aldehyde and Electro-Organic Synthesis Isatin derivatives**
IL-21 10.10 AM - 10.30 AM	**Vikas Tyagi** Assistant Professor, School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Promiscuity of enzymes in organic synthesis**
IL -22 10.30 AM - 10.50 AM	**Ved Prakash Singh** Associate Professor & Head, Department of Industrial Chemistry, Mizoram University, Aizawl, Mizoram, India **Pharmacophore-based Drug Design, Synthesis, Structural exploration and study of 2-pyridone-based pharmaceutical precursor**
IL -23 10.50 AM - 11.10 AM	**Yogesh Chandra Sharma** Department of Chemistry, Indian Institute of Technology BHU Varanasi, Varanasi, India **Nanoadsorbents for drinking water remediation**
11.10 AM - 11.30 AM	High Tea

Parallel Session – IVB

Chairpersons: Dr Dalip Kumar and Prof Krishna Nand Singh

PL-10 9.00 AM - 9.30 AM	**Edmond Differding** Managing Director, Differding Consulting, Luxembourg **Drug Discovery and Development in India – An Analysis of BIRAC-Funded Projects**
IL-24 9.30 AM - 9.50 AM	**Sanjeev Kumar Shukla** Senior Principal Scientist (CSIR) and Professor (AcSIR), NMR Lab., SAIF&R Division, CSIR-Central Drug Research Institute, Lucknow, India **Applications of NMR based Metabolomics**
IL -25 9.50 AM - 10.10 AM	**Nabin Sarkar** Customer Success Specialist, ACSI India Pvt. Ltd., India **CAS SciFinder Discovery Platform: Research and Development Trends for Drug Discovery**
IL -26 10.10 AM - 10.30 AM	**Alok Jain** Assistant Professor and Ramalingaswami Fellow, Department of Bioengineering and Biotechnology, Birla Institute of Technology (BIT), Mesra, Ranchi, India **Can Short ECM Hotspot-motifs engineered into Scaffolds for Tissue Engineering Applications?**
IL -27 10.30 AM -10.50 AM	**Satpal Singh Badsara** Assistant Professor, MFOS Laboratory, Department of Chemistry (Centre of Advanced Study), University of Rajasthan, JLN Marg, Jaipur, Rajasthan, India **Electro-Organic Synthesis: Green and Sustainable Approach for Forging New Bonds**
IL -28 10.50 AM -11.10 AM	**Atul Kumar** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Pyrazole-based organic-amine and silver-carbene-based metal-organic cages as artificial Light Harvesting Systems**
11.10 AM - 11.30 PM	High Tea

Parallel Session – IVC

Chairpersons: Dr Donatella Boschi and Dr Tejal Mehta

PL-11 9.00 AM - 9.30 AM	**Mahesh K. Lakshman** Department of Chemistry and Biochemistry, The City College of New York, Convent Avenue, New York, USA **A Unified Route to Carbazolones and Indolones, and a Reactivity Divergence in the Synthesis of 7-Membered Analogues**
IL-29 9.30 AM - 9.50 AM	**Sumit Kumar Pramanik** Senior Scientist, CSIR-CSMCRI, Bhavnagar, India **Stimuli-responsive nanocarriers for bioimaging, targeted drug delivery and**

	therapeutics
IL-30 9.50 AM - 10.10 AM	**Indra Bahadur** Professor in Physical Chemistry, Faculty of Natural and Agricultural Sciences, North-West University, South Africa **Separation of Azeotrope using Green Solvents "Deep Eutectic Solvents and Ionic Liquids"**
IL -31 10.10 AM - 10.30 AM	**Swagat Mohapatra** UGC - Asst. Professor, Institute of Chemical Technology Mumbai (Indian Oil Campus Odisha Bhubaneswar), IIT Kharagpur Extension Center, Bhubaneswar, Odisha, India **A NEW ROUTE TO THE SYNTHESIS OF THE BENZOTHIAZINO-BENZOTHIAZINES**
IL -32 10.30 AM -10.50 AM	**Fateh Veer Singh** Assistant Professor, Chemistry, VIT Chennai, India **Metal Free Oxidative Cyclizations Involving Iodine(III) Reagents**
IL -33 10.50 AM -11.10 AM	**Banibrata Maity** Assistant Professor, School of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed University), Patiala, Punjab, India **Biomass Derived Sustainable Development of Carbon Quantum Dots as Potential Nanosensor**
11.10 AM - 11.30 PM	High Tea

Parallel Session-VA

Chairpersons: Prof Dr Rodney A. Fernandes and Dr Ashoke Sharon

IL-34 11.30 AM - 11.50 AM	**Stefano Sainas** Department of Science and Drug Technology, University of Turin, via Giuria 9, 10125- Turin, Italy **Exploring fluorescent properties of pyrazolo[1,5-a]pyridine to design new fluorosteric compounds as hDHODH inhibitors**
IL35 11.50 AM - 12.10 PM	**Raksh Vir Jasra** R&D Centre, Reliance Industries Limited, Vadodara Manufacturing Division, Vadodara, Gujarat, India **Zeolite Catalytic Technologies for Green Chemical Production**
IL-36 12.10 PM - 12.30 PM	**Dina Nath Singh** Professor, K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Ayodhya, India **Recent Pharmacological Approach toward the Search of Novel Bioactive Leads from Medicinal Plants**

IL-37 12.30 PM - 12.50 PM	**Sunil K. Sharma** Department of Chemistry, University of Delhi, Delhi-110007, India **Design and Development of Non-ionic Amphiphilic Architectures for Transdermal Drug Delivery Applications**
IL-38 12.50 PM - 1.10 PM	**Prakash C Jha** Prof & Dean, SAMS, Central University of Gujarat, Gandhinagar, India **Experimental and Computational Characterization of p-Sulfocalix[4]arene Mediated Delivery System**
IL-39 1.10 PM - 1.30 PM	**Bhupesh Goyal** School of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed to be University), Patiala, Punjab, India **Unravelling the destabilization mechanism of small-molecule inhibitors against α–Syn oligomers using molecular simulations**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session - VB

Chairpersons: Dr Dipak P. Ramji and Dr Hitendra M. Patel

IL-40 11.30 AM - 11.50 AM	**M.V. Raghavendra Rao** Scientist-Emeritus and Director of Research, Apollo Institute of Medical Sciences and Research, Hyderabad, TS, India **Research on Animal, and human clinical trials for Potential High-Risk Therapeutic Products**
IL-41 11.50 AM - 12.10 PM	**Jigna Shah** Professor & Head, Department of Pharmacology, Institute of Pharmacy, Nirma University, Ahmedabad, India **Molecular Signalling Pathways and therapeutic approaches for the treatment of breast cancer**
IL-42 12.10 PM - 12.30 PM	**Amit Shard** Assistant Professor, Department of Pharmaceutics, NIPER, Ahmedabad, Gujarat, India **Unveiling the Mechanism of Tumor Regression in Triple- Negative Breast Cancer with a Thiazole-Based Pyruvate Kinase M2 Inhibitor**
IL-43 12.30 PM - 12.50 PM	**Bhumika Patel** Assistant Professor, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **DESIGN AND SYNTHESIS OF NOVEL NON-NAD+ ANALOGUES AS POLY(ADP-RIBOSE) POLYMERASE1 (PARP1) INHIBITORS**
IL-44	**Pratibha Kumari** Associate Professor, Department of Chemistry, Deshbandhu College, Kalkaji,

12.50 PM - 1.10 PM	University of Delhi, New Delhi, India **Development of nanocellulose-based materials for food safety applications**
IL-45 1.10 PM - 1.30 PM	**Ratnesh Das** Professor of Chemistry, Dr. Harisingh Gour University, Sagar (M.P.), India **Application of TiO 2 Catalyzed Reactions to the Synthesis of Privileged Indole Derivatives for Medicinal Interest**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session - VC

Chairpersons: Prof Anoja Attanayake and Dr Evans Coutinho

IL-46 11.30 AM - 11.50 AM	**N C Desai** Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar, India **Abstract Awaited**
IL-47 11.50 AM - 12.10 PM	**Sanjib Bhattacharyya** Nirma University, Ahmedabad, India **Nano Gold Regulate the Undruggable Pathogenic Tau to Prevent AD**
IL-48 12.10 PM - 12.30 PM	**Sartaj Tabassum** Cancer and Bioinorganic Research Lab, Department of Chemistry Aligarh Muslim University, Aligarh, India **Progress in Metal-based Anticancer Agent Macro to Nano Structure: In vitro and in Vivo Investigations**
IL-49 12.30 PM - 12.50 PM	**Akhilesh Kumar Verma** Department of Chemistry, University of Delhi, Delhi, India ***o*-Alkynyl/alkenyl Arylnitrile: A New Building Block for Construction of Small Organic Molecules of Pharmaceutical Interest**
IL-50 12.50 PM - 1.10 PM	**Vijay M. Khedkar** School of Pharmacy, Vishwakarma University, Pune, India **Abstract Awaited**
IL-51 1.10 PM - 1.30 PM	**C. N. Ramchand** Theragen Biologics Pvt Ltd, Chennai, India **Discovery and Development of Synthetic anti-VEGF FAB for Treating wet- Macular Degeneration and Diabetic Retinopathy**
1.30 PM - 2.30 PM	**Lunch**

Parallel Session – VIA

Chairpersons: Prof Marco L. Lolli and Dr Rakesh Kumar Parashar

IL-52 2.30 PM - 2.50 PM	**Ravindra Kumar** Senior Scientist, Medicinal and Process Chemistry Division, CSIR-CDRI, Lucknow, India **Stereoselective Construction of Alkaloid-Mimicking Polycyclic Scaffolds Through Unified Desymmetrization Strategy**
IL-53 2.50 PM - 3.10 PM	**Niyati Acharya** Dept. of Pharmacognosy, Institute of Pharmacy, Nirma University, Ahmedabad, India **Sialic acid conjugation for target delivery of natural neuroprotective: A case study**
IL-54 3.10 PM - 3.30 PM	**Devesh M Sawant** Asst Professor, Pharmacy, Central University of Rajasthan, NH8, Bandarsindri, Ajmer, Rajasthan, India **Pd-Catalyzed Azide-Isocyanide Cross Coupling Reaction: Concept to application in Medicinal Chemistry and Bioimaging**
IL-55 3.30 PM - 3.50 PM	**Saravanan S** Scientist, Central Salt and Marine Chemicals Research Institute, Bhavnagar, Gujarat, India **Organocatalytic approaches toward the synthesis of important heterocycles**
O-1 3.50 PM - 4.00 PM	**Ankita Doshi** Division of Biomedical and Life Sciences, School of Science, Navrachana University, Vadodara, India **Elucidating synergistic effect of silver nanoparticles of *Butea monosperma* extract and melatonin as anticancer agents against breast cancer cell line**
O-2 4.00 PM - 4.10 PM	**Arnisha Shaileshbhai Italiya** Department of Life Sciences, MKBU, Bhavnagar, India **Isolation, production and comparison of different pigments from Ray fungus**
O-3 4.10 PM - 4.20 PM	**Ashok Garai** Department of Physics, The LNM Institute of Information Technology, PO Sumel, via Jamdoli, Jaipur 302031, Rajasthan, India **Unravelling the Elastic Properties of DNA: Insights from All-Atomistic Molecular Dynamics Study**
O-4 4.20 PM - 4.30 PM	**Asmita Mondal** Department of Chemistry, Durgapur Government College, J. N. Avenue, Durgapur, Paschim Bardhaman, West Bengal, India **Understanding indolizine synthesis from [3+2] cycloaddition reactions of substituted pyridinium methylides with molecular electron density theory perspective**
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VIB

Chairpersons: Prof Barbara Zajc and Dr Bhumika Patel

IL-56 2.30 PM - 2.50 PM	**Tejal Mehta** Professor & Head, Department of Pharmaceutics, Institute of Pharmacy, Nirma University, Ahmedabad, India **Lipid Nanocarriers as Emerging Platform for Targeting in Cancer Therapy**
IL-57 2.50 PM -3.10 PM	**Subhash C. Mandal** Professor, Pharmacognosy & Phytotherapy Research Laboratory, Division of Pharmacognosy, Department of Pharmaceutical Technology, Faculty of Engineering & Technology, Jadavpur University, Kolkata, India **Research and Development of Figs.: My Expertise of the last three Decades**
IL-58 3.10 PM - 3.30 PM	**Manas K Ghorai** Professor, Department of Chemistry, Indian Institute of Technology Kanpur, India **Abstract Awaited**
IL-59 3.30 PM - 3.50 PM	**Sanjay Kumar Patel** Founder & Principal IP Attorney at EXCELON IP, Ahmedabad, Gujarat, India **Role of intellectual property in fostering chemistry and biologics industry**
O-5 3.50 PM - 4.00 PM	**Bhagawati Saxena** Department of Pharmacology, Institute of Pharmacy, Nirma University, S.G. Highway, Ahmedabad, India **PHARMACOLOGICAL EVALUATION OF NEUROPROTECTIVE EFFECT OF ETHANOLIC EXTRACT OF *NARDOSTACHYS JATAMANSI* IN EXPERIMENTAL ANIMAL MODEL OF TRAUMATIC BRAIN INJURY**
O-6 4.00 PM - 4.10 PM	**BRIJESH PATEL** Inorganic Materials and Catalysis Discipline, CSIR- Central salt and Marine Chemical Research institute, Bhavnagar – 364002 Gujarat, India **Unlocking Enhanced Reactivity in julolidine construction: Electrostatic Stabilization of Phenol's Conjugate Bases Through Anion Selection**
O-7 4.10 PM - 4.20 PM	**Charmy S. Kothari** Department of Pharmaceutical Analysis, Institute of Pharmacy, Nirma University, Ahmedabad, Gujarat, India **Development And Validation of Stability Indicating Mass Compatible HPLC Method for Estimation of Deferasirox**
O-8 4.20 PM - 4.30 PM	**CHETAN KISHORBHAI DHOKAI** Research scholar, Marwadi University, Rajkot, Gujarat, India **Watersaving in thermal power plant by use of membrane filter in Cooling tower treatment**
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VIC

Chairpersons: Prof M.V. Raghavendra Rao and Dr Rajeev Sakhuja

IL-60 2.30 PM - 2.50 PM	**Donatella Boschi** Department of Drug Science and Technology, Università degli Studi di Torino, Via Pietro Giuria 9, 10125-Torino, Italy **Structure-guided optimization of new AKR1C3 inhibitors designed by 3-hydroxyazole bioisosteric approach to target prostate cancer**
O-9 2.50 PM - 3.00 PM	**Prakash Pandurang Taur** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333031, India **Design and Synthesis of Pyropheophorbide Derived Photosensitizers and Their Pharmacokinetic, Tumor Uptake and Anti-Cancer Activity Studies**
O-10 3.00 PM - 3.10 PM	**JIGARKUMAR KIRITBHAI VANKAR** School of Chemical Sciences, Central University of Gujarat, Gandhinagar, India **Ester synthesis via cascade alkylation and activation of thioamides**
O-11 3.00 PM - 3.20 PM	**KESUR RAJADE RAM** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar-388 120, Gujarat, India **Synthesis of Pyrazolo[5,1-*b*]quinazoline-3-carboxylates via Three Component DES as a Green Media and their Applicability as Chemosensor**
O-12 3.20 PM - 3.30 PM	**Manas Barik** Central Salt and Marine Chemicals Research Institute, Bhavnagar Gujarat, 364002, India **Revisiting the old material: The impact of boehmite-derived catalytic material on the formation of dihydropyran compounds and its application to access fragrant derivatives**
O-13 3.30 PM - 3.40 PM	**Monika Malik** Department of Chemistry, Birla Institute of Technology and Science, Pilani 333 031, India **A facile and efficient synthesis of *N*-aryl indolylsulfoximines as potent and selective anticancer agents**
O-14 3.40 PM - 3.50 PM	**DEVENDRA PRATAP SINGH** Division of Endocrinology, Council of Scientific and Industrial Research-Central Drug Research Institute, Lucknow, India **MiR-539-3p negatively regulates osteogenesis by suppression of Wnt/Beta catenin pathway and subsequent inhibition of Akap-3 signalling**

O-15 3.50 PM - 4.00 PM	**Nikili K Zhimo** Department of Chemistry, Kohima Science College (Autonomous) Jotsoma, Nagaland India **Potential of Chayote as a precursor for Activated Carbon prepared by chemical activation for the removal of heavy metals**
O-16 4.00 PM - 4.10 PM	**PAYAL BHANUBHAI CHAUHAN** Research Scholar, School of Chemical Sciences, Central University of Gujarat, Gandhinagar, India **Amphipathic Hybrid Foldamers as Antimicrobial Agents**
O-17 4.10 PM - 4.20 PM	**Piyush Bhalla** Chemistry and Bioprospecting Division, Forest Research Institute, Dehradun-248006, Uttarakhand, India **Chemical and *in vitro* biological investigation of *Cupressus torulosa* needles essential oil**
O-18 4.20 PM - 4.30 PM	**Devangi Sojitra** Department of Mathematics, Marwadi University, Rajkot-360003, Gujarat, India **Compactness in unequal crossover model**
4.30 PM - 4.40 PM	**Tea**

Parallel Session – VII A

Chairpersons: Dr Edmond Differding and Prof Sartaj Tabassum

IL-61 4.40 PM - 5.00 PM	**Rodney A. Fernandes** Professor, Chemistry Department, IIT Bombay, Powai Mumbai, India **"SERENDIPITY" in Organic Synthesis: Development of New Synthetic Reactions**
O-19 5.00 PM - 5.10 PM	**Muskanbanu Baloch** Department of Chemistry, Marwaadi University, Rajkot, Gujarat, India **Polymerization of "(E)-4-(4-hydroxy-3-methoxyphenyl)but-3-en-2-one"with chloro acetophenone and formaldehyde solution: Synthesis of □□□unsaturated polymer**
O-20 5.10 PM - 5.20 PM	**Kavan Mehta** Faculty of Pharmacy, Marwadi University, Rajkot – morbi road, Rajkot 360003, Gujarat, India **Advancement in research with the help of AI**
O-21 5.20 PM - 5.30 PM	**Abhay Lodariya** Faculty of Pharmacy, Marwadi University, Rajkot-360003, Gujarat, India **Assessment of *In Vitro* Anti-Glycation Efficacy of Dapagliflozin andRosuvastatin on Human Serum LDL**

O-22 5.30 PM - 5.40 PM	**Rahil Mathakia** Department of Microbiology, Marwadi University, Gujarat, India **Optimizing Patent Processing Time in the Indian Biotechnology Sector: A Comprehensive Analysis of Disposal Types and Their Temporal Impact**

Parallel Session – VII B

Chairpersons: Dr Stefano Sainas and Dr Neelima Gupta

IL-62 4.40 PM - 5.00 PM	**Anirban Pradhan** Assistant Professor, Department of Chemistry, Birla Institute of Technology (BIT) Mesra, Ranchi, India **Green and Renewable Hydrogen Fuel Production based on Porous Carbon Materials**
O-23 5.00 PM - 5.10 PM	**Gaddam Mareechika** Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research, Raebareli, Transit Campus Lucknow, UP, India **Carbon quantum dots, preparation, photophysical properties and application thereof**
O-24 5.10 PM - 5.20 PM	**Priyanka Choudhary** Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076, Maharashtra, India **Chiral Pool Meets Chiral Catalysis: Eight-Step Convergent Total Synthesis of Anticancer Natural Lipid Mycalol**
O-25 5.20 PM - 5.30 PM	**Mital K. Aadesariya** Department of chemistry, Marwadi University, Rajkot- 360003, Gujarat, India **Quantitative, quantitative Analysis as well as bioactivity activity of methanolic and petroleum extract of *Abutilon pannosum* leaves**
O-26 5.30 PM - 5.40 PM	**Neilanuo Huozha** Department of Chemistry, Kohima Science College (Autonomous), Jotsoma, Nagaland, India **Production of activated carbon from *Sechium edule* plant for removal of dyes and fluoride pollutants; Equilibrium, kinetic and thermodynamic studies**

Parallel Session – VII C

Chairpersons: Dr Harsha Rajapakse and Dr Pratibha Kumari

IL-63 4.40 PM - 5.00 PM	**Abu Salim Mustafa** Department of Microbiology, College of Medicine, Kuwait University, Kuwait **Whole Genome Sequencing of Pathogenic Bacterial Genomes: Applications in Clinical Microbiology**

O-27 5.00 PM - 5.10 PM	**Kiran Chauhan** Chemistry and Bio-prospecting Division, Forest Research Institute, Dehradun, India ***Prinsepia utilis* Royle seed oil: A comprehensive study on its fatty acid composition and anti-inflammatory property**
O-28 5.10 PM - 5.20 PM	**Vivek Yadav** Department of Microbiology, Marwadi University, Gujarat, India **Process Development and bio similarity of mAb molecule: a case study**
O-29 5.20 PM - 5.30 PM	**Ravi Shantilal Parmar** Department of Chemistry, Saurashtra University, Rajkot-360005, Gujarat, India **1,2,3-triazoles derivatives via 'click chemistry' approach**
O-30 5.30 PM - 5.40 PM	**Harsh Vithlani** Faculty of Pharmacy, Marwadi University, Rajkot-360003, Gujarat, India **Formulation Characterisation and Optimization of Quick-Dissolving Sublingual Film of Venlafaxine Hydrochloride by Using Design of Experiment**

Poster Session -II

Chairpersons:

5.45 PM –7.30 PM	**Poster Session -II (Poster Number 51 onwards)**
7.30 PM	**Dinner**

Wednesday, January 10, 2024

Parallel Session –VIIIA

Chairpersons: Dr Bapurao B. Shingate

IL-64 9.00 AM – 9.20 AM	**Ramesh Kothari** Professor and Head, Department of Biosciences, Saurashtra University, Rajkot, India **Probiotics and Prebiotics: An Innovative Approach for Improvement of Gut Microbiome**
IL-65 9.20 AM - 9.40 AM	**Brajendra K. Singh** Associate Professor, Department of Chemistry, University of Delhi, Delhi, India **Metal-Catalysed Chalcogenation of Quinoxolinones and Benzoxazines via C-H activation**
IL-66 9.40 AM - 10.00 AM	**Asha Patel** Associate Professor, Parul Institute of Pharmacy, Vadodara, Gujarat, India **DEVELOPMENT OF SURFACE FUNCTIONTIONALISED BIOTHERAPEUTICS FOR THE TREATMENT OF CANCER**
O-31 10.00 AM -10.10 AM	**Ranjan Chhaganlal Khunt** Department of Chemistry, Saurashtra University, Rajkot-360005, India **UGI-mediated an efficient and concise synthesis of anticancer agents**
O-32 10.10 AM -10.20 AM	**Riddhi Naresh Dholakiya** Department of Life Sciences, MKBU, Bhavnagar, India **Xylanase production by marine Actinobacteria**
O-33 10.20 AM -10.30 AM	**Sachinkumar Gunvantrai Modha** Tarsadia Institute of Chemical Science, Maliba Campus, Tarsadi 394350, Uka Tarsadia University, Bardoli, India **Study of photophysical properties of *N*-aryl enaminones and their application in the synthesis of hexahydrocarbazolones via [6π] Photocyclization ‡**
O-34 10.30 AM -10.40 AM	**Santosh Kumar** Division of Medicinal and Process Chemistry, CSIR-Central Drug Research Institute, Lucknow-226031, India **Targeting Methicillin-Resistant Staphylococcus aureus (MRSA) for Antimicrobial Activity Through Hemiaminal 3- Sulfenylated Indoles: Structure-Activity Relationship (SAR), in vitro and in vivo Studies**
O-35 10.40 AM -10.50 AM	**SAURABH KUMAR KAUSHAL** Division of Endocrinology, Council of Scientific and Industrial Research-Central Drug Research Institute, Lucknow, India **Immunomodulating Osteoprotective Effect of IL-33 in D-galactose Accelerated Aging Bone Loss Condition**

O-36 10.50 AM -11.00 AM	**Saurajit Ghosh** Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan 333031, India **Journey of an AIEgen: From mechanochromism to amyloid fibril detection**
11.00 AM - 11.20 AM	**High Tea**

Parallel Session –VIII B

Chairpersons: Dr Nighat Fahmi and Dr Fateh Veer Singh

IL-67 9.00 AM – 9.20 AM	**Saravanan Matheshwaran** Department of Biological Sciences and Bioengineering, Indian Institute of Technology - Kanpur, Kanpur, India **Potential inhibitors of mycobacterial "SOS" response- as an adjuvant therapy**
IL-68 9.20 AM - 9.40 AM	**Ramendra Pratap Singh** Department of Chemistry, University of Delhi, Delhi, India **Synthesis of various functionalized Aza heterocycles from aryl methyl ketones of biological importance**
IL-69 9.40 AM - 10.00 AM	**Navneet Kumar Gupta** Assistant Professor, Center for Sustainable Technologies, Indian Institute of Science, Bangalore, Karnataka, India **Strategies for Producing Renewable Chemicals from Biomass: Advancing the Circular Bioeconomy**
O-37 10.00 AM -10.10 AM	**Shivangi Ambrishkumar Mehta** Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara, 390002, India **Engineering of hybrid SBA-15 for assessment of invitro release of alendronate**
O-38 10.10 AM -10.20 AM	**SOMNATH ARJUN BORADE** Department of Chemistry, Birla Institute of Technology & Science, Pilani, Rajasthan 333031, India **Synthesis of Modified Bile Acids *via* Palladium-Catalyzed C(sp^3)-H (Hetero)arylation**
O-39 10.20 AM -10.30 AM	**Sonu Khanka** Division of Endocrinology, CSIR-Central Drug Research Institute, Lucknow-226031, India **Identification of Novel Pyrimidine derivative as Bone anabolic and fracture healing agent promoting osteogenesis via BMP2/SMAD1 signaling**

O-40 10.30 AM -10.40 AM	**SUNDARAM SINGH** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi – 221 005, U.P., India **A Photo-Catalyst-Free Approach for the Visible-Light Induced N-Arylation of Sulfonamides via Electron-Donor-Acceptor Complex**
O-41 10.40 AM -10.50 AM	**Viralkumar Arvindbhai Doshi** Department of Chemistry, Government Science college, Limkhedda. Gujarat University, Ahmedabad, India **Synthesis and biological evolution 5-chloro thiophene containing novel Hydrazide-hydrazone derivatives**
O-42 10.50 AM -11.00 AM	**Vivek Kumar Vyas** Department of Pharmaceutical Chemistry, Institute of Pharmacy, Nirma University, Ahmedabad 382481, Gujarat, India **INTEGRATED STRUCTURE- AND LIGAND-BASED COMPUTATIONAL MODELLING METHOD FOR THE SUCCESSFUL DESIGN OF DRUG CANDIDATES**
11.00 AM - 11.20 AM	**High Tea**

Parallel Session –VIII C

Chairpersons:

IL-70 9.00 AM – 9.20 AM	**Anil Mishra** Department of Chemistry, University of Lucknow, Lucknow, India **Chemistry of Overcoming the NMR - Stress Connection and Managing Health Made Easy**
IL-71 9.20 AM - 9.40 AM	**Surendra Singh** Professor, Dept. of Chemistry, University of Delhi, Delhi, India **Development of Recoverable Chiral Organocatalysts for Asymmetric Friedel-Crafts Reactions**
IL-72 9.40 AM - 10.00 AM	**Neelima Gupta** Department of Chemistry, University of Rajasthan, Jaipur, India **Computational and Experimental Tools to Recognize Multi-target Binding Profiles of Therapeutic Agents**
O-43 10.00 AM -10.10 AM	**Anjali V. Chhablani** Department of Chemistry, Marwadi University, Rajkot-Morbi Road, P.O. Gauridad, Rajkot 360003, Gujarat, India **Design, Synthesis and Biological Screening of Nitrogen Containing Heterocycles and its Sulphonamide Derivatives**

O-44 10.10 AM -10.20 AM	**Gadavala Sarah** Assistant Professor, Marwadi University1 Rajkot-Morbi Road, Rajkot 360003, Gujarat, India **Evaluation Of Effect Of Ethanolic Extract Of Cassia Tora Seeds On Permeability Of Etoposide Using Everted Chicken Small Intestine**
O-45 10.20 AM -10.30 AM	**Krishna Raval** Faculty of Pharmacy, Marwadi University, Rajkot, Gujarat, 360003, India **AQbD-based optimization and validation of RP-HPLC method for the estimation of Chlorthalidone and Azelnidipine in pharmaceutical dosage form**
O-46 10.30 AM -10.40 AM	**Devanshi Dhinoja** Marwadi University, Rajkot **Formulation and Evaluation of Paracetamol Suspension Prepared by Using Flaxseed Mucilage and Comparative Study Between Different Marketed and In-house Developed Formulation**
O-47 10.40 AM -10.50 AM	**Shreyansh Vagadia** Faculty of Pharmacy, Marwadi University, Rajkot-360003, Gujarat, India **Green Synthesis and Characterization of Silver Nanoparticles from *Cinchona Ledgeriana* Bark Extract**
O-48 10.50 AM -11.00 AM	**Hiral Ranchhod Topiya** Assistant Professor, Faculty of Pharmacy, Marwadi University, Rajkot, Gujarat, India **Karnasphota from Ayurveda as a source of Novel Acetylcholinesterase Inhibitor: a natural scaffold targeting the treatment of Alzheimer's disease**
11.00 AM - 11.20 AM	**High Tea**

11.30 PM - 1.00 PM	**Valedictory Session**
1.00 PM –2.00 PM	**Lunch**

- End of Programme -

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INAUGURAL CEREMONY

Cordially inviting you for the inauguration of

28TH ISCB INTERNATIONAL CONFERENCE

ISCBC-2024

Jointly organized by

Indian Society of Chemists & Biologists (ISCB)

CHIEF GUEST

HON'BLE PROF. (DR) G D YADAV
Padma Shri, Former Vice-Chancellor, ICT, Mumbai

GUEST OF HONOR

DR ANIL GUPTA
Padma Shri, Founder,
The Honey Bee Network, NIF, SRISTI,

DR MUKUL PATEL
Vice Chancellor,
Gujarat Ayurved University, Jamnagar

DR A RAMKISHAN
Deputy Drugs Controller (India),
CDSCO, Hyderabad

DR EDMUND DIFFERDING
Managing Director,
Differding Consulting, Luxembourg

PRESIDED BY

SHRI KETAN MARWADI
President,
Marwadi University

SHRI JITUBHAI CHANDARANA
Vice-President,
Marwadi University

PROF. (DR) R B JADEJA
Pro Vice-Chancellor,
Marwadi University

SHRI NARESH JADEJA
Registrar,
Marwadi University

08 JANUARY, 2024 | 10:00 AM ONWARDS

Venue: Auditorium, Tagore Building, Marwadi University

INVITEES

PROF. PMS CHAUHAN
General Secretary, ISCB

PROF. ANAMIK SHAH
President, ISCB

DR KANTHA D ARUNACHALAM
Dean, Faculty of Science

DR LALJI BALDANIYA
Principal, Faculty of Pharmacy

DR VICKY JAIN
Principal, Faculty of Science

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28TH ISCB
INTERNATIONAL CONFERENCE
ISCBC-2024

Inaugural Ceremony

HON'BLE PROF. (DR) G D YADAV
Padma Shri, Former Vice-Chancellor,
ICT, Mumbai
Has kindly consented to be the Chief Guest

DR ANIL GUPTA
Founder, The Honey Bee Network,
National Innovation Foundation, SRISTI,
will grace the occasion as Guest of Honor

DR MUKUL PATEL
Vice Chancellor, Gujarat
Ayurved University, Jamnagar
will grace the occasion as Guest of Honor

DR EDMOND DIFFERDING
Managing Director,
Differding Consulting, Luxembourg
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CDSCO, Hyderabad
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FACULTY OF SCIENCE | FACULTY OF PHARMACY

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VALEDICTORY CEREMONY

Cordially inviting you for the valediction of

28TH ISCB INTERNATIONAL CONFERENCE

ISCBC-2024

Jointly organized by

Indian Society of Chemists & Biologists (ISCB)

CHIEF GUEST

HON'BLE PROF. (DR) M M SHARMA
Padma Vibhushan, Former Director, UDCT, Mumbai

GUEST OF HONOR

DR UNNAT PANDIT
Controller General of Patents, Design, and Trademarks, Government of India

PROF. (DR) J S YADAV
Former Director, CSIR-IICT, Hyderabad; Director, Research, Indrashil University

DR KESHAV DEO
Executive Director, Almelo Pvt. Ltd., CEO, Lifeactivus Pvt. Ltd.

PROF. (DR) NISHEETH DESAI
Chief Editor, Analytical Chemistry Letters, Taylor & Francis

PRESIDED BY

SHRI KETAN MARWADI
President, Marwadi University

SHRI JITUBHAI CHANDARANA
Vice-President, Marwadi University

PROF. (DR) R B JADEJA
Pro Vice-Chancellor, Marwadi University

SHRI NARESH JADEJA
Registrar, Marwadi University

10 JANUARY, 2024 | 12:30 PM ONWARDS

Venue: Auditorium, Tagore Building, Marwadi University

INVITEES

PROF. PMS CHAUHAN
General Secretary, ISCB

PROF. ANAMIK SHAH
President, ISCB

DR KANTHA D ARUNACHALAM
Dean, Faculty of Science

DR LALJI BALDANIYA
Principal, Faculty of Pharmacy

DR VICKY JAIN
Principal, Faculty of Science

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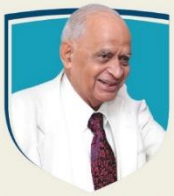
Valedictory Ceremony



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Padma Vibhushan, Padma Bhushan,
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PLENARY

PL-1

Cryo-EM and Molecular Dynamics Simulations Reveal Hidden Conformational Dynamics Controlling Ammonia Transport in Human Asparagine Synthetase

Nigel G. J. Richards

Department of Chemistry, Cardiff University, Cardiff, UK
Email: RichardsN14@cardiff.ac.uk

How dynamical motions in enzymes might be linked to catalytic function is of significant general interest. Recent advances in X-ray crystallography and cryogenic electron microscopy (cryo-EM) offer the promise of elucidating dynamical motions for proteins that are not easily amenable to study using NMR methods. In this lecture, I will describe how 3D variability analysis (3DVA) of an EM structure for human asparagine synthetase (ASNS) has been used to detail how the motions of a single side chain mediates interconversion of the open and closed forms of a catalytically relevant intramolecular tunnel. Our 3DVA results are consistent with those obtained independently from atomistic molecular dynamics (MD) simulations. These MD trajectories further suggest that formation of a key reaction intermediate acts to stabilize the open form of the tunnel in ASNS, thereby permitting ammonia translocation and asparagine formation. This conformational selection mechanism for regulating ammonia transfer in human ASNS contrasts sharply with those employed in other glutamine-dependent amidotransferases that possess a homologous glutaminase domain. This study illustrates the power of cryo-EM to identify localized conformational changes and hence dissect the conformational landscape of large proteins. When combined with MD simulations, 3DVA is a powerful approach to understanding how conformational dynamics regulates function in metabolic enzymes with multiple active sites.

PL-2

Peristaltic Ion-Conduction Mechanism in Sodium Polymer Electrolytes Based on Perfluoropolyethers, DMSO, and NaTFSI

Sumit Kumar[a,b], Rajesh Raghupathy[a,c], Michele Vittadello[a,d,*]

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[b] *Bioorganic Research Laboratory, Department of Chemistry, University of Delhi, University Enclave, Delhi-110007, India.*
[c] *Nano and Bioelectrochemistry Research Laboratory and Carbon Dioxide Research and Green Technology Centre, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Turuvalam Road, Vellore-632014, India.*
[d] *Ph.D. Program in Chemistry and M.S. Program in Nanoscience, The Graduate Center of CUNY, 365 5th Avenue, New York, New York 10016, USA*
E-mail: mvittadello@mec.cuny.edu

The promise of sodium-ion conducting polymer electrolytes in rechargeable power sources is yet to be fulfilled. The possibility to combine the very attractive physical-chemical properties of perfluorinated polyethers (PFPE) with sodium salts has not thus far been considered. Here we investigate a series of eight plasticized polymer electrolytes based on an α,ω-OH-terminated poly[PFPE-block-PEO] (hereafter called PEG-PFPE-PEG), NaTFSI, and dimethylsulfoxide (DMSO) as plasticizer, having general formula PEG-PFPE-PEG/$(NaTFSI)_x(DMSO)_y$ ($0.004 \leq x \leq 0.610$, $3.205 \leq y \leq 3.794$). The thermal analysis results, carried out by means of DSC, indicate that the plasticizer remains intimately integrated in the polymer electrolytes up to the decomposition temperature of PEG-PFPE-PEG (180 ºC ca.) and is not significantly released out of the polymer hosts in closed-cells. The vibrational investigation, carried out by FT-IR spectroscopy in the medium IR region, shed light on NaTFSI-PEG-PFPE-PEG-DMSO interactions. In particular, the role of the OH functional groups in facilitating salt dissolution was elucidated, along with that of the CO and CF moieties. The ionic conductivity was investigated by impedance spectroscopy, in the frequency interval 100 mHz – 1 MHz. The conductivity at 25 ºC is as high as $8.0 \cdot 10^{-4}\ S \cdot cm^{-1}$. Three of at least five polarization events (one electrode and four interdomain polarizations in total) were fully resolved and were associated to different interfacing domains in the polymer electrolytes with increasing DMSO content. The behaviour of the corresponding conductivities and frequencies were fitted with VTF and Arrhenius equations, respectively, highlighting the concomitant roles of segmental motion and ionic hopping in these hybrid systems. Furthermore, it was shown that the presence of DMSO, a well-known cryodepressant, significantly decreases the glass transition temperature of the electrolytes. Reversible Na deposition and stripping was confirmed by cyclic voltammetry.

PL-3

Mystery in the development of plant-based nephroprotective agents from Sri Lankan flora

Anoja P. Attanayake (PhD, FIChem C**)**

Professor in Biochemistry, Department of Biochemistry, Faculty of Medicine, University ofRuhuna, Sri Lanka

Chronic kidney disease has been an emerging global health problem because of its increasing prevalence, associated adverse clinical outcomes, marked reduction in the quality of life of patients, and high healthcare costs. Most of the South Asian countries have witnessed an alarmingly high prevalence of chronic kidney disease during the past ten years. A variety of etiologies contribute to the diverse primary outcomes, but all can eventually lead to the same endpoint which is the chronic kidney disease. With several drawbacks of modern pharmaceuticalagents, the high healthcare cost of renal replacement therapy in the management of end-stage renal disease and the global trend for natural therapeutics among the general public has led to the development of nephroprotective agents from herbal sources that with fewer side effects, less of toxic effects, targeting kidney functions for the management of different pathological conditions of the kidney disease.

Healing with medicinal plants is as old as mankind itself. It is appreciated that traditional systemsof medicine offer some effective medicinal plant preparations from their treatise to be useful indiverse pathological conditions of the kidney. However, many of them have not been subjected to analyze the pharmacological profile and scientific scrutinization through *in vivo* studies. Duringmy talk, I will be discussing a success story of screening selected medicinal plants for nephroprotective activity, phytochemical profiling, and investigation of possible nephroprotective mechanisms in an animal model nephrotoxicity, issues, and challenges in developing commercially viable herbal nephroprotective agents. Scientific findings of the success story would open new vistas for developing potential therapeutic agents/dietary supplements with proven nephroprotective mechanisms for the prevention and/or management of chronic kidney disease. Positive results would complement the efforts in reaching the global health needs of the general public and enhance the quality of life of patients with chronic kidney disease.

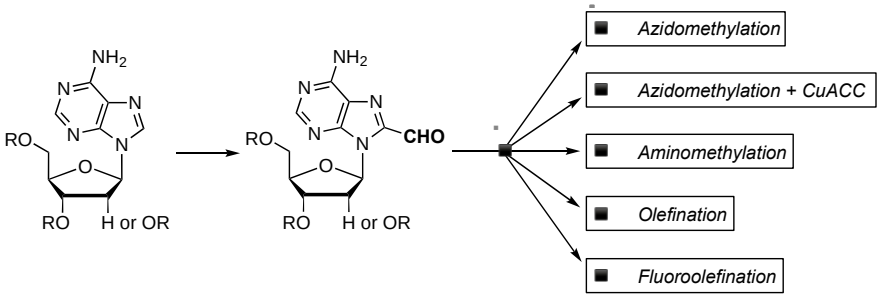
PL-4

Adenosine- and 2'-Deoxyadenosine-8-Carbaldehydes as New Tools for Diverse Purinyl C-8 Modifications

Barbara Zajc

Department of Chemistry and Biochemistry
The City College of New York 160 Convent Avenue, New York, NY 10031
The Ph.D. Program in Chemistry
The Graduate Center of the City University of New York, New York, NY 10016

Nucleosides are a highly important class of biomolecules. Modifications of these has been a focus of research for decades, driven by multitude of applications of their analogs, ranging from therapeutics to biological probes. Commonly, modifications at C8-position of adenine nucleosides involved the 8-bromo or iodo derivatives, *via* various types of metal catalyzed reactions, or reactions of C8 lithiated adenosine derivatives with an electrophile. On the other hand, syntheses, isolation, and reactivity of adenosine and 2'-deoxyadenosine 8-carbaldehyde derivatives have not been explored. A straightforward, scalable syntheses of these two versatile formyl adenine nucleoside derivatives will be presented, along with diverse synthetic applications, ranging from azidation and amination, to reductive amination, olefination as well as fluoroolefination. The ensuing products were deprotected and evaluated for their antiproliferative activities.



PL-5

Probing the molecular mechanisms underlying the beneficial actions of nutraceuticals in atherosclerotic cardiovascular disease and other inflammatory disorders

Professor Dipak P. Ramji, PhD, FLSW

Professor of Cardiovascular Science & Deputy Head of School of Biosciences at Cardiff University
Affiliation: Cardiff School of Biosciences, Cardiff University, Sir Martin Evans Building, Museum Avenue, Cardiff CF10 3AX, UK
Telephone: 0044 (0)2920876753; 0044 (0) 7832380752 (on WhatsApp)

Abstract:

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

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

PL-6

Development of a broad-spectrum combination antibacterial therapy with metallobeta-lactamase inhibitor against the ESKAPE pathogens for wound healing

Ramaiah Muthyala[1]*, Yuk Y Sham[2]

[1]*Experimental Clinical Pharmacology*

[2]*Integrative Biology and Physiology, Medical SchoolUniversity of Minnesota*

The antibiotic revolution began in 1942 with the discovery of penicillin in 1928. The human life expectancy at the beginning of the 20th century jumped from 47 years to 79years by the 1970s in the USA. However, since then, the continuing emergence of antibiotic resistance has become a public health threat and a global burden to our health care. The World Health Organization declared November 18-24, 2022, “World Antimicrobial Awareness Week.”

β-Lactamases function by drug inactivation mechanism. They catalyze the hydrolysis of the amide bond of the β-lactam ring. Unlike serine β lactamases, the metallo-β- lactamases require one or two zinc ions for catalytic activity and are not inhibited by currently approved therapeutics. The metallo-β-lactamase, NDM-1 (subclass B1), was first identified in a patient in New Delhi, India, in 2009. Strikingly, the enzyme was shown to hydrolyze all known β-lactam antibiotics. At the time, it was deemed in the mainstream media as “superbugs.” Due to lack of inhibitors and their ability to hydrolyze a broad spectrum of β-lactam-based drugs, the MBL enzymes are of utmost concern to public health globally.

We have discovered 1-hydroxy pyridine-2 (1H)-thione-6-carboxylic acid (1) (patent 11491146, 2022) as a first-in-class metallo β-lactamase inhibitor (MBLi) with a potentinhibition Ki of 13 nM against VIM-2 that corresponds to a remarkable 0.99 ligand efficiency and possesses low cytotoxicity (CC50) of 97mM with a corresponding therapeutic index of 880, making it a promising candidate for optimization in combination antibacterial therapy.

We will present the mechanism of action of compound (1) and its application in the combination therapy with Augmentin in drug-resistant wound infections.

PL-7

Unveiling Tight Junction Dynamics with Lanthanides

Harsha Rajapakse

Medgar Evers College, City University of New York, NY, USA

Tight junctions (TJs) play an important role in regulating paracellular transport across biological barriers. This abstract explores the impactful application of lanthanides, specifically lanthanum ions (La3+), in the investigation of tight junctions. The combination of low molecular weight, appropriate size and charge, stability, fluorescent properties, selective permeation, biocompatibility, and chelation capabilities makes lanthanides well-suited tracers/ probes for studying tight junction permeation and structural changes. Researchers can leverage these properties to gain insights into paracellular transport dynamics and assess the integrity of biological barriers.

In an experimental brain tumor model, La3+ served as a low-molecular-weight electron microscopic probe to meticulously evaluate microvessel permeability. Complementing in vivo studies, in vitro investigations utilized lanthanides, particularly europium complexes, as permeation tracers for detailed tight junction studies. Time-resolved fluorescence assays confirmed the efficacy of these complexes as practical and novel paracellular indicators. Moreover, a double fluorescence probe strategy, integrating these tracers with a proven paracellular indicator (europium complex), demonstrated effectiveness in calculating changes in structural parameters of tight junctions.

In summary, the utilization of lanthanides, exemplified by La3+ and europium complexes, presents a versatile and potent approach to decipher the intricate dynamics of tight junctions. The adaptability of lanthanides spans from in vivo tumor models to in vitro monolayer assessments, emerging as invaluable tools for investigating paracellular transport. These insights not only deepen our understanding of the complex regulation of biological barriers but also hold implications for drug development.

PL-8

Synthesis of small complex heterocycles

Erik V. Van der Eycken

Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Department of Chemistry, KU Leuven Celestijnenlaan 200F, 3001, Leuven, Belgium.
and
Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya street, Moscow, 117198, Russia,
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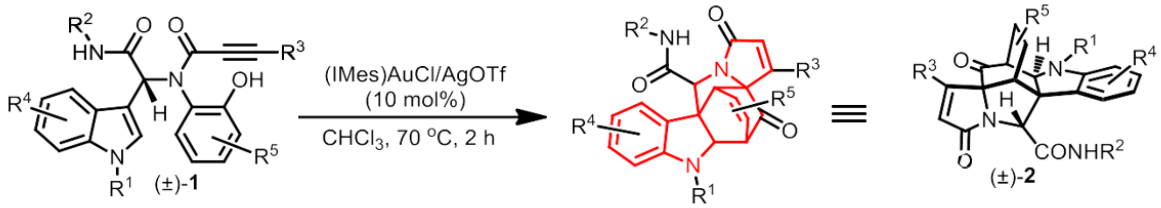
The recent upsurge in the development of mild reaction methodologies for the synthesis of small heterocycles has generated a lot of interest among synthetic organic chemist. To expand this area in organic synthesis, the challenge is to identify novel strategies for the formation of biologically or pharmaceutically important heterocycles under mild conditions as well as continuous flow chemistry to meet up the growing demand for pharmaceuticals as well as agrochemicals. Therefore, in this lecture, an overview will be given about recent synthetic work done in our laboratories regarding this topic. 1) This will include the synthesis of spiroindolines and spiroindoles, which are an important class of spirocyclic compounds present in a wide range of pharmaceuticals and biologically important natural alkaloids. New procedures will be described, including the use of nanoparticles as heterogeneous catalysts. 2) The Ugi-4CR is by far one of the most successful multicomponent reactions leading to high structural diversity and molecular complexity. As the reaction mostly affords a linear peptide backbone, post-Ugi transformations are an elegant solution to rigidify the Ugi-adduct into more drug like species. Not surprisingly, the development of these transformations, leading to new structural frameworks, has expanded rapidly over the last few years. We will comment on the use of homogeneous gold catalysis for performing post Ugi-4CR modifications (Scheme).



3) C-H bond activation/functionalization has demonstrated unprecedented avenues for the streamlined synthesis of pharmaceutically and industrially valuable molecules in a benign manner. This enables the formal functionalization of a C-H bond, which is arguably the most prevalent “functional group” in organic chemistry. We will comment on our recent research regarding this topic. 4) Finally an introduction to our recently started up photo-redox chemistry will be given.

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

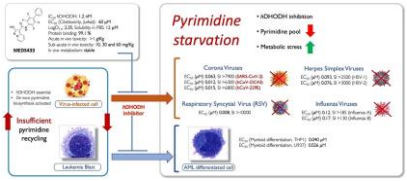
PL-9

Human dihydroorotate dehydrogenase (hDHODH) as drug target: who is going to win the hDHODH golden rush?

Lolli, M. L.;*[a], Sainas, S.;[a] Giorgis, M.;[a] Circosta, P.;[b] Vitale, N.;[b] Pippione, A. C.;[a] Vigato, C.;[a] Martino, E.[a], Mannella, I.;[a] Villella, N.;[a] Poli, G.;[c] Tuccinardi, T.;[c] De Nicolò, A;[d] D'Avolio, A.;[d] B. Bonaldo[e], Gotti, S.;[e] Miggiano, R.;[f] Ferraris, D.;[f] Alberti, M.;[f] Saglio, G.;[g] A. Luganini[f], G. Sibille[f], Gribaudo[f] and Boschi, D.[a]

[a] Dep. Science and Drug Technology, Univ. of Turin (IT); [b] Molecular Biotechnology Center, Univ. of Turin (IT), [c] Dep. of Pharmacy, Univ. of Pisa (IT); [d] Dep. of Medical Sciences, Univ of Turin (IT); [e] Neuroscience Institute Cavalieri Ottolenghi (NICO), Univ of Turin (IT); [f] UPO, Novara (IT); [g] Dept of Clinical and Biological Sciences, Univ of Turin (IT), [f] Dept of Clinical and Biological Sciences, University of Turin, Turin (IT);
Email: marco.lolli@unito.it

At the end of 2016, the connection between Acute Myelogenous Leukemia (AML) and *dihydroorotate dehydrogenase* (*h*DHODH), a key enzyme in *de novo* pyrimidine biosynthesis, generated considerable interest from the pharmaceutical industry as a possible new therapeutic opportunity for this *unmet clinical need*. Since the COVID-19 outbreak, the use of *h*DHODH inhibitors as *Host Targeting Antivirals* (HTA) became one of the most promising therapeutic options for COVID-19 treatment as well as other pandemic outbreaks. In 2023, the discovery of the *h*DHODH role in blocking *ferroptosis* in solid tumors cells open other scenarios also in these fields.
In this occasion, the program active since 2010 at the University of Turin dedicated to design innovative *h*DHODH inhibitors will be fully presented. By using an innovative bioisosteric approach supported by structure-based techniques, **MEDS433**, a potent *h*DHODH inhibitor (IC_{50} = 1.2 nM) was discovered. **MEDS433** is able to induce myeloid differentiation in AML cell lines (THP1 and U937) in the low nM range (EC_{50} = 40 and 26 nM), superior to the AML phase I/II *lead brequinar* (EC_{50} = 249 nM (THP1) and 189 nM (U937)). By leading the cell into *pyrimidine starvation*, **MEDS433** inhibits the *in vitro* replication of a large panel of viruses, with EC_{50} always in the low nM range. On SARS- CoV-2, the replication is inhibited at EC_{50} = 63 nM, being **MEDS433** five folds superior of the antiviral *Molnupiravir* (EC_{50} = 300 nM), recently approved for COVID-19. Beside detailing the **MEDS433** design & SAR, PK, ADME, toxicity (acute/subacute on different species) as well as the *in vivo* efficacy in different AML models (leukemic xenograft and IV (mouse, IP, PO)), its synthetic technological transfer (8 g batches, purity > 98.5 %) is also presented. To reinforce the scenario, the pathway that allowed the discovery of the *backup compound* **MEDS700** (EC_{50} = 17 nM, THP1), is also presented. All these studies, most of them still unpublished, are directed to open the incoming **MEDS433** certified preclinical studies necessary for prepare its Phase I clinical trial for AML.
Moving to the conclusion the lecture, the clinical scenario that involve *h*DHODH inhibitors will be detailed. In particular, the most recent strategies investigated for overcame possible *h*DHODH resistance at clinical level will be presented. This final step will try to answer the title question: *who is going to win the hDHODH golden rush?*



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6. A. Luganini, Lolli M.L. *et al Antiviral Res.* **2021**, *189*, 105057.

PL-10

Drug Discovery and Development in India – An Analysis of BIRAC-Funded Projects

Edmond Differding

Ph.D., Differding Consulting, Contern, Luxembourg

Abstract:

Our comprehensive analysis of over 2000 projects funded up to 2022 by India's Department of Biotechnology since 2005 through private-public partnerships, and as of 2012 through 'Biotechnology Industry Research Assistance Council' (BIRAC) reveals the overwhelming share of human healthcare projects. Of these, therapeutic molecules are one of the main drivers, second only to medical technology, and ahead of vaccines, regenerative medicine, and others. The talk will focus on projects that are aiming at the discovery and development of new chemical entities (NCEs) and new biological entities (NBEs) as novel treatments for diseases.

PL-11

A Unified Route to Carbazolones and Indolones, and a Reactivity Divergence in the Synthesis of 7-Membered Analogues

Mahesh Lakshman

Professor
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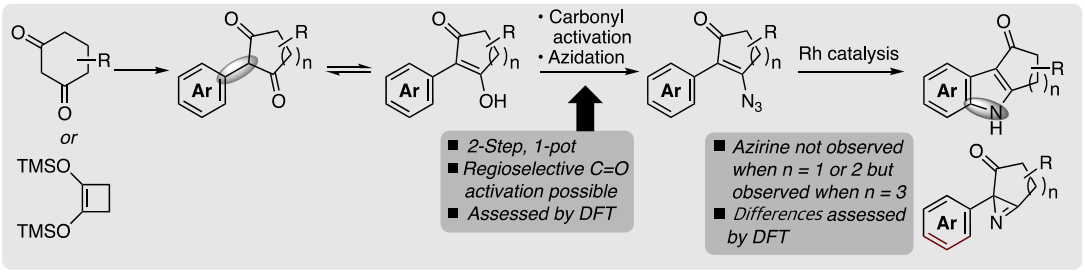
The indole scaffold is ubiquitous, present in a multitude of natural products and synthetic molecules of physiological interest. The famed Fischer indole reaction, discovered in 1883, that relies on aryl hydrazines and a key [3,3] sigmatropic rearrangement is perhaps among the highly important synthetic methods. In the context of the present work, the Fischer chemistry leads to indoles containing fused cycloalkanes and cycloalkanones. Whereas these approaches have become a “go to method”, several other creative approaches have evolved that do or do not involve metal catalysts. We have developed a novel approach to carbazolones and indolones *via* 2-aryl-1,3-cycloalkanediones. These precursors can be obtained either through a Cu-catalyzed arylation of the dione (6-membered) or through a ring expansion of aryl succinoin derivatives (5-membered). Next, a two-step, one-pot activation of the carbonyl group followed by azidation yields 3-azido-2-aryl-cycloalken-2-ones. This particular step is subject to high regiocontrol, a critical aspect for the synthesis of substituted carbazolones. Exposure of these b-azido enones to a Rh-catalyst results in the formation of a nitrene/nitrenoid and insertion in the proximal aryl C–H bond, resulting in the carbazolones and indolones. While this chemistry works very well for 6- and 5-membered rings, comparable reactions on 2-phenyl-1,3-cycloheptanedione do not yield the indole as a major product but leads to an azirine. Product structures are supported by NMR analysis and crystal structures, and various aspects of the chemistry have been assessed by DFT analysis.



Scheme. Synthesis of carbazolones and indolones from 2-aryl-1,3-cycloalkanediones.

INVITED

IL-1

Chlorophyll-a Derived Photosensitizers for Improved Photodynamic Therapy

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Photodynamic therapy (PDT) for being a safe and noninvasive modality has shown great potential for cancer treatment.[1] The efficiency of a photosensitizer is one of the major reasons for the successful implementation of PDT, therefore, continued efforts have been directed towards the development of water soluble and NIR absorbing photosensitizers. To date, pyrrole-based photosensitizers such as porphyrins, chlorins, bacteriochlorins, expanded porphyrins and phthalocyanines have created enormous interest due to their ability to localize in a variety of tumors.[2] In particular, chlorophyll-a derived products such as pyropheophorbide-a and its analogues with unique long-wavelength absorption in the range of 650-700 nm and favourable photophysical properties have been widely used as phototoxic agents in photodynamic therapy.[2] In search of increase in selectivity and accumulation in cancer tissues, recently, we reported the tryptamine pheophorbide conjugates endowed with significant photocytotoxicity against lung cancer cell lines.[3] The pheophorbides have unique characteristics in developing multifunctional agents with a choice for cancer therapy by introducing an iodobenzyl group into the macrocycle. In continuation of our efforts to identify a potent and selective chlorophyll-a derived photosensitizer, we successfully prepared different fluorobenzyl ethers of pyropheophorbide involving the reaction of an appropriate benzyl alcohol with *in situ* Markownikoff's intermediate generated by treatment of pyropheophorbide with HBr in acetic acid.[4] Design, synthesis and photocytotoxicity studies of newly prepared chlorin analogues will be presented during the conference.

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IL-2

Explorations of Click Chemistry

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In recent years, click chemistry has emerged as a fast and powerful approach to the synthesis of novel compounds with desired properties. The concept of “click chemistry” was coined by Sharpless to describe a set of “near perfect” bond-forming reactions which were very selective, high yielding, and wide in scope and describes chemistry tailored to generate substances quickly and reliably by joining small units together. In 2022, the Nobel Prize in Chemistry was jointly awarded to Carolyn R. Bertozzi, Morten P. Meldal and K. Barry Sharpless, "for the development of click chemistry and bioorthogonal chemistry". 1,2,3-Triazoles are important class of target molecules due to their interesting biological properties such as anti-allergic, anti-bacterial, and anti-HIV activity. We were encouraged to combine 1,2,3-triazole moieties with phenol, coumarins, isatin, benzothiazinone, acetophenone, quinoline, 2,4-thiazolidinedione and acid hydrazide in a single molecular framework. All the diversely functionalized molecules were synthesized from commercially available starting materials in minimum steps with high overall yield and screened for antitubercular, antioxidant, antimicrobial, anti-inflammatory and cytotoxic activities and will be discussed.

IL-3

Synthesis and Bio-evaluation of Newer benzothiazole appended bis triazoles as antifungal and Tetrahydropyridines based Glycomimetics Azasugars as Anti-Diabetic agents

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The scientific community has paid close attention to the design and synthesis of new N-containing heterocycles because of their extraordinary biological and pharmacological capabilities. There are numerous medical and biological uses of 2-amino-benzothiazole motifs, including anti-bacterial, anti-fungal, anti-HIV, anti-inflammatory, anti-cancer, and anti-convulsant properties. In this regard, we have synthesized two novel series (**5a-f, 6** and **7a-f, 8**) of benzothiazole appended bis-triazole derivatives-based fungicides that are structural isomer to each other and evaluated for their antifungal activity against Plant pathogen Rhizoctonia solani. All the synthesized compounds have shown excellent antifungal activity in their minimum concentration. Among all synthetics, compounds **5b**, **5f** and **7f** found to be more potent than commercially available fungicide, Hexaconazole. Further, **5f**, **7f**, **6**, and **8** active hybrids have been docked within the active site of sterol 14α-demethylase enzyme to explore their binding interaction energy and possible interactions with receptor.

The work on azasugar glycomimetics includes synthesis and bio-evaluation of new triazolylated dihydropyridine and tetrahydropyridine azasugar scaffolds (**F1-14**) will also be discussed in this lecture. Azasugar glycomimetics are the synthetic substances that mimic the structural and functional characteristics of natural carbohydrates showcasing promising potential as therapeutic agents for diabetes. The α-glucosidase inhibitory activity of synthesized final compounds (**F1-F14**) were evaluated against the commercially available α-glucosidase enzyme. Majority of the screened compounds displayed excellent inhibition with IC_{50} values ranging from 2.12-75.11 μM, when compared to the standard drug Acarbose. Compound **F6** with IC_{50} value of 2.12 μM having a chlorine group and pyrrole ring, was found to be the most active compound among the series. Further molecular docking studies of selected ligands were performed to investigate the binding interactions of compounds with enzyme active sites. Their specific binding patterns have been analysed with amino acids present in the binding sites of *Saccharomyces cerevisiae* α-glucosidase. These findings suggest these candidates as the potential leads for the anti-diabetic activity.

IL-4

DECIPHERING ROLE OF MINIMALISTIC PEPTIDES AND PEPTIDOMIMETICS TOWARDS BIOMEDICAL APPLICATIONS

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Abstract:

Peptides are ubiquitously present in biological system as the key component of various biological signalling in cell as well as extracellular matrix. Peptides have placed themselves in an unique position between small molecules and macromolecules. They possess amalgamation of unique properties offered by both class of molecules (specificity and minimal toxicity). In recent years, role of peptides have been explored beyond drug discovery. Peptides with shorter sequences that provides aforesaid properties are always economical and easy to finetune. Aided with biorecognition/signalling, horizon of peptides have been expanded to the development of soft materials for biomedical applications such as drug delivery and tissue engineering.
Aided with *in-silico tools*, we have deconvoluted antibody-antigen interactions in to short peptides that recognize the antigen (e.g EpCAM, an important biomarker for circulating tumours, CTC) similar to antibody. They offers a cost-effective method for CTC detection and targeted cancer therapy. In parallel we have developed shortest sequence of peptides (dipeptides), which have been structurally modified to gain enzymatic stability. These peptides formed hydrogels through molecular self-assembly with potential applications in tissue engineering and drug delivery.

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IL-5

Biosap's Rapid-Healing Synergistic Formulas: Debunking Myths in Traditional Medicines

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In exploring the depths of Ayurvedic, Unani, Siddha, and TCM traditions, we delve into a legacy enriched by over 1,500 natural ingredients, as detailed in seminal texts like the Charak Samhita, Sushruta Samhita, Ashtanga Hridaya, and others. At the heart of these practices lies the concept of pharmacodynamic and pharmacokinetic synergy in polyherbal preparations, ensuring enhanced therapeutic outcomes through collective herbal action. Biosap's innovative approach, inspired by these ancient principles and bolstered by contemporary scientific insights, has culminated in the development of 30 unique, rapid-healing formulations. These formulations, including Urotone, Medisept, Mediflam, and Hear and Learn, specifically target common health issues across various systems such as musculoskeletal, urinary, digestive, cardiovascular, respiratory, and psychosomatic domains. Our discussion will spotlight these formulations, emphasizing how synergistic herbal interactions mirror an orchestra's harmony, leading to increased bioavailability, minimized side effects, and a multifaceted attack on diseases. This blend of tradition and science not only debunks long-held myths in Ayurvedic medicine but also opens new avenues for holistic and rapid healing.

IL-6

Recent Advances in Biological, Chemical and Pharmaceutical Sciences for Innovation in Healthcare

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Abstract

There are various tools to assess the pharmacodynamics and pharmacokinetics of lead candidates. However, the disparate nature of these tools makes them discomforting to use. To address this issue, we have developed a novel universal methodology termed **E**igen **V**alue **An**alysis (EVANS) that can easily be used to gage the PD, PK and toxicity issues of leads. The approach is centered on the **Q**uantitative **S**tructure **P**roperty **R**elationship (QSPR) formalism. The method has been bench-marked against several PD, PK datasets as well as on datasets that measure Blood Brain Barrier (BBB) permeability, placental permeability, and human skin permeability.The performance of EVANS on these datasets has been compared with standard 2D QSAR methodologies and state-of-the-art ML models, and it is seen that models built using EVANS methodology are comparable or superior to models reported in the literature. Most importantly, the methodology is easy to implement with freely available tools and software.

IL-7

Rational design of triazole–peptide conjugates as modulator of Aβ–aggregation, metal–mediated Aβ–aggregation and cytotoxicity

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Alzheimer's disease (AD) is a complex neurodegenerative condition characterized by misfolding of amyloid–β (Aβ) peptide that hinders the normal functioning of the brain [i]. Histopathologically, AD comprises Aβ deposits, neurofibrillary tangles (τ aggregation), loss of cholinergic transmission, metal ion dyshomeostasis, an imbalance between the generation and removal of reactive oxygen species (ROS), and oxidative stress [ii]. By taking into account the multifaceted nature of AD, we have reported the design and evaluation of mono-triazole and di-triazole derivatives as multi-target-directed ligands against various pathological factors of AD [iii]. In this work, a rational design of triazole–peptide conjugates was followed to combat various pathological hallmarks of AD [iv]. In particular, peptidomimetic DS2 (MLV, Fig.1) showed the best inhibitory activity against Aβ aggregation with an IC_{50} value of 2.43 ± 0.05 µM. In addition, DS2 disaggregates preformed Aβ fibrils, chelate metal ions, inhibit metal–mediated Aβ aggregation, significantly controls reactive oxygen species (ROS) production, and reduces oxidative stress. DS2 exhibited very low cytotoxicity and significantly ameliorate the Aβ–induced toxicity in differentiated neuroblastoma cells, SH–SY5Y. In addition, alteration in the fibrillary architecture of Aβ_{42} in the absence and presence of DS2 was validated by transmission electron microscopy (TEM) images. The molecular dynamics simulations depicted that DS2 suppressed Aβ_{42} monomer aggregation by preserving helical conformations and was able to reduce the production of aggregation–prone β–sheet structures. Moreover, DS2 destabilized Aβ_{42} protofibril structure by significantly reducing the binding affinity between chains D–E of protofibril. The triazole–peptide conjugates can be easily functionalized with functional groups of varying electronic demands and provide a structural framework for designing other triazole–peptide conjugates as MTDLs against AD.

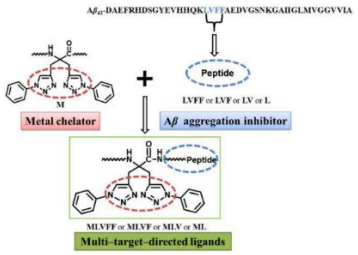

Fig. 1: Rational design of multi–target–directed triazole–peptide conjugates against pathological hallmarks of AD.

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IL-8

Sterically Bulky Ligands Controlled Palladium-Catalyzed Regioselective Organic Transformations

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Controlling reactivity and selectivity of an organic transformation is a long-standing challenge for chemists.[1] Modulating ligand design is one such way for controlling the reactivity and selectivity of organic reactions. Among various ligand designs, synthesizing sterically bulky ligands and their metal complexes is a key strategy for achieving high degree of selectivity.[2] The metal complexes with sterically bulky ligands are known to show excellent catalytic activity and selectivity during catalysis reactions. Our research group is actively working towards the development of new synthetic strategies for synthesizing sterically bulky ligand systems and their *trans*-palladium dichloride complexes. Herein, we are presenting design, synthesis, characterization, and catalytic activities of two new *trans*-palladium dichloride complexes of sterically bulky organoselenium ligands. In these complexes the catalytically active palladium dichloride unit is available in sterically confined space and incoming reactants need to approach the metal center through specific directions, it was envisioned that these complexes could be used for regioselective organic transformations. The proof of concept was tested for two reactions. One of the reaction was between 2-arylimidazo[1,2-*a*]pyridines and diphenylacetylene derivatives, which resulted in an annulated product with reverse regioselectivity. The second reaction was dehydroxymethylation of dihydroxy compounds which generally needs two separate catalysts. Overall, these palladium complexes showed a promising outlook for use in catalysis to enable unique selectivity paradigms.

IL-9

RNA-targeted copper-based chemotherapeutic drug candidate derived from bioactive ligand scaffold that induce ROS -mediated cell death in resistant cancer cells

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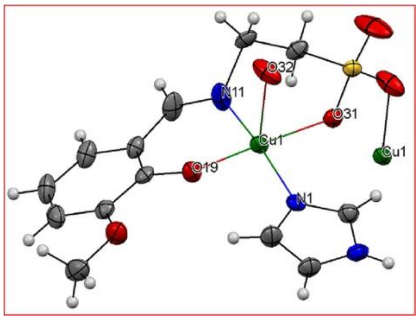
Abstract

RNA-targeted chemotherapeutic drugs are considered as safe treatment option for the cure of many chronic diseases preventing off- targeted delivery and acute toxic manifestations. FDA has approved many such RNA therapies in different phases of clinical trials, validating their use for the treatment of various chronic diseases. Our research group has recently synthesised new water- soluble (μ–oxo) bridged polymeric Cu(II) complexes of taurine (2–aminoethane sulfonic acid) complexes. The therapeutic potency of Cu(II)taurine complexes was ascertained by studying biophysical interactions with tRNA/ct-DNA. The experimental results demonstrated that the complexes interacted avidly to nucleic acids through intercalation mode depicting a specific preference for tRNA as compared to ct–DNA The electrophoretic behaviour of the complexes with plasmid pBR322 DNA and tRNA were examined by gel mobility assay that revealed a concentration-dependent activity with complex 2 performing more efficient cleavage as compared to complex 1. The cytotoxicity of both the complexes was assessed using MTT assay against three cancer cell lines viz., MDA-MB-231 (triple negative breast cancer cell line), HCT 116 (human colon cancer cell line) and A549 (lung cancer cell) The synthesized copper(II) taurine complexes have met the basic criteria of anticancer drug design as they are structurally well-characterized, exhibiting good solubility in water, lipophilic in nature with superior intercalating propensity towards tRNA and cytotoxic in nature



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IL-10

Mitochondria targeting Ru(II)/Ir(III)/Re(I) based mono and bimetallic complexes for cancer therapy

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Chemotherapy is the most prevalent traditional cancer therapy but it lacks tumor specificity and thus it renders normal cells at risk. Therefore, considerable attention should be given on the design and synthesis of new metal complexes by following approaches including (i) selectivity in cancer cell by non-covalent modes of DNA interaction (ii) mitochondria specificity (iii) development of various photo-toxic agents as these produce reactive oxygen species (ROS) at the photo-exposed cancer cells leaving the unexposed healthy cells minimally affected. (iv) "Theranostic", which includes simultaneous diagnostic and therapeutic functions in a single system improving the outcome of a disease state. With respect to therapeutic regimes, improved treatment effect is achieved by effective localization at the tumor specific sites of the therapeutic agents whereas from diagnostic aspect imaging agents along with therapeutic agents combined with biomarkers (tumor specific markers) are carried from one system to another enabling them to differentiate the tumor cells from normal cells. In continuation of our present work on anticancer organoruthenium, organoiridium and organorhenium complexes, we have introduced the convenient and effective synthetic approaches for designing the monometallic and bimetallic Ru(II)/Ir(III)/Re(I) complexes which can address all three approaches. The operational simplicity, good yield, ease of isolation of the products and high chemoselectivity will be the main advantages of these methods (**Fig. 1**).[1, 2]

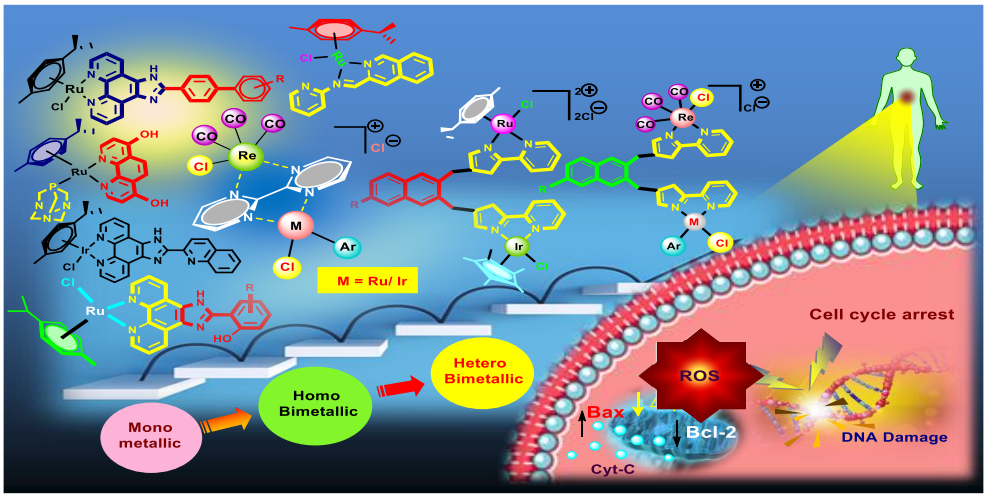

Fig. 1 Schematic diagram of metal complexes in cancer therapy

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IL-11

Transitioning Beyond Flasks: Exploring the Organic Chemistry of Isocyanides through Electrochemical Cells.

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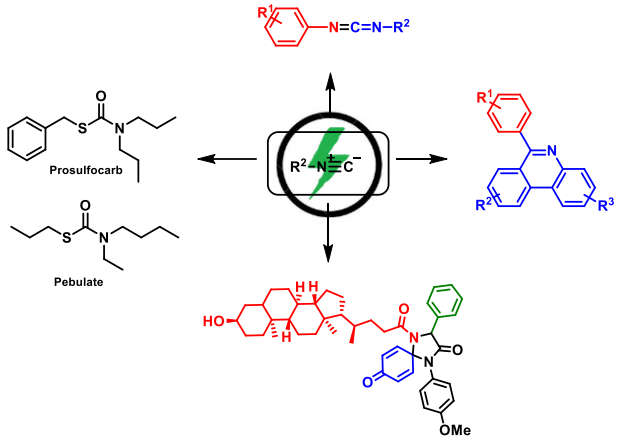

Isocyanides, renowned for their historical significance in organic chemistry, have found utility across academic and industrial realms. Among the pantheon of stable divalent carbon nucleophiles, isocyanides stand out for their remarkable ability to forge multiple bonds on the terminal carbon atom. The allure of isocyanides persists due to their ubiquitous role in organometallics, where they serve as extensively studied ligands, as well as in combinatorial syntheses, offering avenues for novel product discovery through isocyanide-based multi-component processes like the Passirini and Ugi reactions. However, the amalgamation of isocyanides with diverse domains within organic chemistry presents an exciting prospect to populate uncharted 'chemical space' and facilitate the discovery of unprecedented lead compounds. Yet, this endeavor remains a formidable challenge. In this talk, I will delve into our recent strides in the integration of isocyanide chemistry with organic electrosynthesis, culminating in the synthesis of a plethora of medicinally vital scaffolds (refer to the scheme). [1-10]

Keywords: Isocyanides, MCRs, Electrochemical, organic synthesis.

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IL-12

Synthesis of small Organic Molecules and their Pharmaceutical Applications

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Abstract:

At the present time, a synthesis of small organic molecules is a key precursor for the medicinal and pharmaceutical applications. We explore a broader synthetic approach using green and sustainable routes for highly functionalized diastereoselective spiro- and other small heterocyclic scaffolds *via* selective multiple C–C and C-N bond formation under identical reaction conditions. The mentioned protocol works efficiently, tolerates different substituents present in reactants, has a simple equipped procedure, provides excellent reaction yield in a short time, uses a recyclable catalyst, and results in up to 99.7% purity (HPLC) for the synthesized molecules, with high diastereoselectivity, excellent atom economy, reaction mass efficiency, and effective mass yield. The synthesized small library of molecules will be the attractive features for the pharmaceutical applications such as different six solid tumor cell lines including gliomas cell line targets.

IL-13

Therapeutic & Diagnostic agents development for Microorganism to AMR through computational chemistry

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ABSTRACT: AMR is a global health and development threat. It requires urgent multisectoral action to achieve the SDGs. Currently, there are seven common antibiotics used against MRSA, which are: vancomycin, daptomycin, linezolid, Sulfamethoxazole and trimethoprim (TMP-SMZ), quinupristin-dalfopristin, clindamycin and tigecycline. But the microorganisms are very smart and try to get survive in the presence of drugs. So, scientists should be smarter than microorganisms to control them. Computational chemistry is the smartest tool for new drug development. Computational study of existing drugs and other potent molecules from the literature. Based on our previous study we had lead molecule. We have optimized the lead molecule and found better results during the computational study. Now synthesis of the newly designed molecules and their characterization.All newly synthesised molecules will be screened against the MRSA and other AMR strains. The cell line toxicity study of the active compounds will be performed. Then after the study will be carried out in the animal for the potency of the compounds, toxicityand pK-pD. We will complete the phase – 0 (Preclinical). This work will give the best molecules for the Clinical phase which will work as the AMR agents. With the therapeutic development the diagnosis of the microorganismsis equally important. Because early diagnosis can save life better than later treatment.

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IL-14

Advanced Materials for Defense: Designing for Performance

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Materials for defence research aims to develop advanced materials and technologies for military and civil applications, with a goals to improve the equipment performance, weight and size reduction, enhanced durability and reliability in harsh environments, and protecting first responders from chemical and biological threats. Technology is the key to combating terrorism and protecting our citizens, first responders, and soldiers from the threat of chemical warfare agents (CWAs). Our research intends to develop an advanced material having an engineered pore size and high surface area which are capable of providing effective protection against the NBC gases by utilizing the unique features of nanomaterials such as graphene, carbon nanotubes, metal organic framework etc. Different loading of MOF/graphene/CNT over activated carbon was carried out to achieve hybrid carbon system for the efficient adsorption and neutralisation of chemical threats. The hybridization of these carbon structures is meticulously adjusted to provide a synergistic effect that improves the material's overall capabilities in NBC defence applications. Various tests are carried out in order to ensure the performance of the developed materials. Surface area, tuneable pore size, flexibility, and breathability of the material are also assessed to guarantee practical use in a variety of operating situations. Furthermore, the study looks at the possibility of surface functionalization, which involves changes the surface properties of materials by utilizing target chemical moieties to enhance the material's adaptive defence capabilities. The outcomes of this hybrid material research contribute to the advancement of NBC defense technologies by introducing a versatile and efficient hybrid carbon-based material. These advanced carbons based material holds considerable promise for integration into personal protective equipment, air filtration systems, and infrastructure protection, addressing the critical need for advanced defense solutions in the face of evolving and complex NBC threats.

IL-15

Molecular Docking, Dynamics and Chemistry for Hsp90-Cdc37-Cdk4 Protein Complex: A Protein-Protein Modulation Exploration for Drug Discovery

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Abstract

Hsp90 works through its structural flexibility to bind with co-chaperones and client proteins to mediate biological function. The co-chaperone, Cdc37, binds to the Cdk4 client protein and stabilizes the Hsp90-Cdc37-Cdk4 protein complex. Further, the destabilizing protein-protein complex may prevent the requisite folding of the misfolded conformation of Cdk4. Studying the protein-protein interface, followed by designing a suitable ligand or drug, is challenging. However, it may give a direction to discover a therapeutic molecule to alter protein-protein interaction. Overall, the literature suggests targeting HSP90 modulation to yield effective cancer therapy.

Manipulating the interfacial contacts within the heteroprotein complex (Hsp90-Cdc37-Cdk4 protein complex) using drug-like molecules induces conformational changes that affect the maturation of kinase client proteins. We explored the potential of known natural product in modulating Hsp90-Cdc37 interfacial interactions. These modulations could cause instability in the Hsp90-Cdc37-Cdk4 complex, inhibiting the maturation of mutated Cdk4. The findings shed light on the prospective role of drug binding. MD studies validated covalent docking, and the conformational changes were investigated by analyzing the interfacial interactions between Hsp90 and Cdc37 using the Bioluminate, Schrödinger Suite 2022.

Authors acknowledge the High-End Computation Facility and Schrodinger2022/Gaussian 16 Software support from BIT Mesra.

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IL-16

Metal-Catalyzed Strategies for the Regioselective Functionalization of Amino Acids

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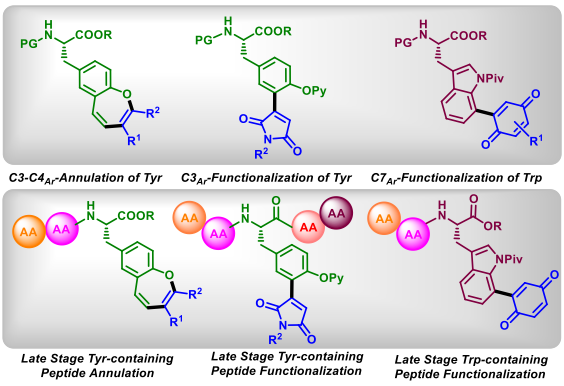
Proteins perform differentiated functions such as metabolic reactions catalysis, DNA replication, stimuli response and transportation of molecules in living organisms [1]. Though, genetic code expansion of natural amino acids results in the synthesis of most proteins, yet, co-translationally amalgamation of a few unnatural amino acids (UAAs) into proteins offers unprecedented capability for site-specific protein manipulation in living systems. The incorporation of UAAs into protein of interest (POI) thus provides an access to synthetically modified natural biologics that could be used in applied areas such as proteomics, diagnostics, asymmetric syntheses and drug delivery. In addition, unnatural amino acids and their resulting peptides are found to be stable towards proteolytic enzymes, populating exclusive conformational space with distinct bioactivities. Accordingly, focused efforts have been devoted in recent past toward synthesizing designer UAAs *via* α-C(sp^3)-H, β-C(sp^3)-H, γ-C(sp^3)-H, δ-C(sp^3)-H and C(sp^2)-H bond functionalization under metal-catalyzed conditions, overcoming the limitations existed with asymmetric synthesis and cross-coupling strategies conventionally utilized for furnishing UAAs [2]. Interestingly, the crucial importance of tyrosine and tryptophan in peptide and protein sequences, and the presence of a phenolic/amidic functionalities in them have provided appealing tunable sites for selective functionalization and assembling heterocyclic architectures over them with the aid of appropriate coupling partners. Under this domain, a few C(sp^2)-H bond functionalization strategies at $C2_{Ar}$ position(s) on aryl/indolyl moieties in tyrosine and tryptophan have been successfully achieved *via* C-H activation notion, respectively. However, efficient strategies involving functionalization at $C3_{Ar}$-position in tyrosine, $C7_{Ar}$-position in tryptophan, or mounting a pharmacologically active heterocyclic moiety on the aryl moiety of tyrosine are limited.

In the backdrop of the above discussion, we have successfully developed [3-5] eye-catching transition metal-catalyzed strategies for the synthesis of synthesis of $C3_{Ar}$-maleimide appended tyrosine, oxepine-mounted tyrosine and $C7_{Ar}$-quinone appended tryptophan and the peptides containing them, which shall be discussed.



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IL-17

Space Pharmaceutical Manufacturing: Beginning of new era of Indian pharmaceutical industry

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Abstract

The rapidly evolving opportunities offered through the new economy of space exploration have opened up numerous exciting areas of research. One of them is In-space pharmaceutical manufacturing and development.

The absence of gravity in space unlocks unique opportunities for drug discovery and development. In microgravity, crystals can grow larger and, in the process, creates better samples than can be grown on Earth. Aging and pathological processes may be accelerated under conditions of microgravity. In addition, bacterial virulence, pathogenicity and resistance to antibiotics have been shown to increase in space. Hence, the knowledge expanded through space research can enable drug screening, improve drug design and delivery and thereby contributing to the development of new technologies and therapeutic products. These include the use of space environment for biological research, including investigation of bacterial virulence, accelerated models for aging, enhanced stem cells proliferation and differentiation; chemical applications like drug polymorphism, protein crystallization, self-assembly of biomolecules etc. and pharmaceutical studies like antibiotic drug resistance, drug delivery systems, microencapsulation, stability of colloidal formulations etc.

In this talk, I will discuss about case studies of drug development using low earth orbit platforms like ISS and will also discuss about future prospectus of research in this emerging field.

IL-18

Synthesis of Iminophosphonamide Metal Complexes and Their Photoluminescence

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Design and synthesis of new ligands and finding the application of corresponding metal complexes is a long-standing interest for chemists. In this regard, the achiral version of the iminophosphonamide (NPN) ligand is well explored in contrast to the corresponding chiral analogue.[1] Therefore, in this work the design of new chiral iminophosphonamide ligands and their various metal complexes is presented.[2] Upon investigating the photophysical properties of the metal complexes it was observed that these complexes showed interesting photoluminescence with thermally activated delayed fluorescence (TADF).[1,2,3] In particular, the alkali metal complexes which exist in the dimeric forms showed the TADF above 150 K. In order to understand the effect of the substituents on the photoluminescence variety of iminophosphonamide ligands were designed. The case study was further extended to calcium and d^{10} configured metal centers (*i.e.*, Cu, Zn) and lanthanide metals coordinated with variety of the iminophosphonamide ligands.[4] In general, the study showed that the photoluminescence and TADF of these metal complexes depends on the metal centers, the ligand orientation around the metal centers and the observation temperature.

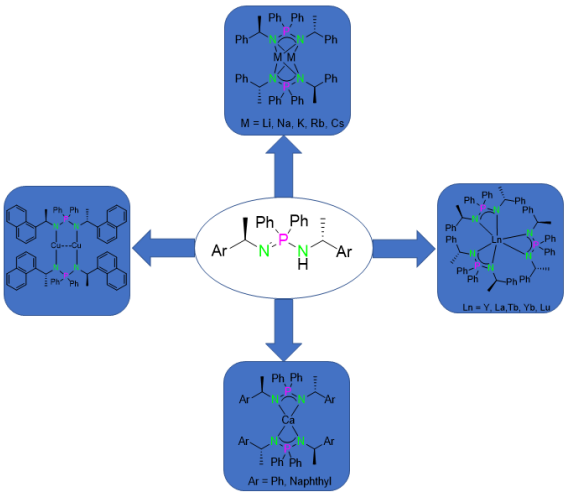

Figure 1. Chiral Iminophosphonamide metal complexes and corresponding photoluminescence.

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IL-19

Development of Novel Substituted 1,2,4-Triazole Derivatives Targeting Tankyrase as Anti-Cancer Agents

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Abstract

Colorectal carcinoma (CRC) is considered the third most deadly cancer with increasingly high rates of prevalence, incidences of mortality, and morbidity as per the WHO reports. The tumor cells involve the aberrant Wnt-signalling pathway in more than 90% of CRC cases which involves tankyrase. Detailed computational studies were carried out to design potent tankyrase inhibitors. The combination of pharmacophore modeling-based virtual screening, 3D-QSAR, molecular docking, and MD simulation studies was carried out using TNKS enzymes as a target. Different software was employed to carry out these extensive computational studies. The designed 1,2,4-triazole derivatives were synthesized and structurally confirmed by various characterization using FTIR, Mass, and NMR spectroscopy (^{1}H and ^{13}C-NMR), and purity was assessed using HPLC analysis. All synthesized molecules were utilized to assess their potential as anticancer agents by *in-vitro* biological evaluation. The cytotoxicity and antiproliferative actions of each synthesized compound at three different concentrations (i.e., 30 µM, 3 µM and 0.3 µM) were evaluated using normal cell line i.e. Vero E6 cell lines, and other cancer cell lines like colorectal cancer cell lines (HT29 & SW480), lung cancer cell line (A549) and breast cancer cell line (MDA-MB231). Doxorubicin and XAV939 were used as reference standards to evaluate the comparative biological activity of these molecules. The best compounds found from this screening were subjected to apoptosis analysis using the flow cytometry-based annexin-V-FITC/PI method at two different concentrations (i.e., 5 µM & 10 µM) to understand the nature of inhibition by the synthesized compounds against the internal standard XAV939. The overall conclusion from these extensive studies is that the currently designed compounds could be considered as the potential hits for the discovery of targeted therapy of CRC through inhibition of TNKS enzymes and Wnt-signalling cascade.

IL-20

Efficient Synthesis of Perlin's aldehyde and Electro-Organic Synthesis Isatin derivatives

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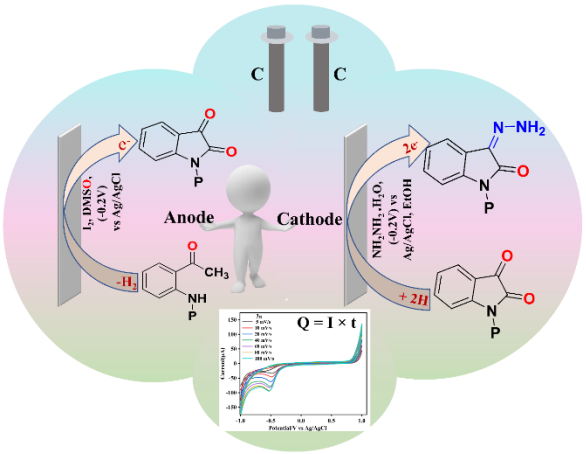

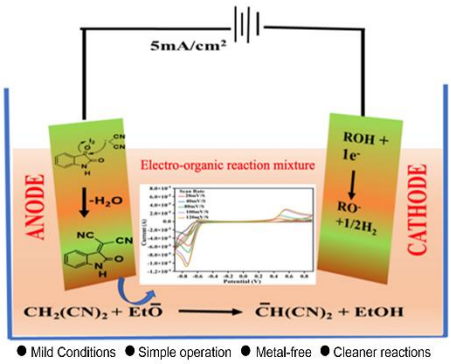

Abstract

Construction of drug like molecules is a challenging task in drug discovery process. These drug like molecules get constructed by using suitable chiral synthons and functionalized precursors. Perlin's aldehyde (2,3-dideoxy-α, β-unsaturated carbohydrate enals) have been demonstrated to be a key precursor as chiral synthons for the synthesis of a wide range of natural products and physiologically active molecules in recent decades due to the existence of structural, functional, and stereochemical properties. Its metal free synthesis will be discussed therein.[1] An efficient and unique approach to synthesize isatin (indole-2,3-dione) from 2-aminoacetophenone under electrochemical conditions supported by I_2-DMSO through C-N Cross-coupling and C(sp^2)-H/C(sp^3)-H functionalization will be presented. This synthetic method spans a wide range of substituted 2-aminoacetophenone substrates.[2] The first electrochemically molecular iodine promoted, domino reactions for the green synthesis of biologically relevant dicyano 2-(2-oxoindolin-3-ylidene) malononitriles from readily available or prepared isatin derivatives, malononitrile, and iodine at room temperature will also be presented. This synthesis method showed tolerance towards various EDG and EWG and getting completed in a short reaction time.[3]

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IL-21

Promiscuity of enzymes in organic synthesis

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Keywords: Biocatalyst, non-natural reactions, α-amylase, lipase, myoglobin, immobilization of enzymes.

Abstract

Biocatalysis is surging interest in chemical, pharmaceutical, and food industries due to its green and efficient synthetic approach.[1] The enigmatic control of enzymes on reactions makes it extremely useful in numerous potential applications e.g., to synthesize chiral drugs or any enantio-, chemo- and region-selective compounds. The enzymatic transformations also happens at physiological temperature with negligible waste production.[2] Therefore, this is not an ambitious claim that biocatalysts have the promising capability to replace traditional catalysts in the near future. Considering the advantages of biocatalysts in synthetic organic chemistry, we have developed the first biocatalysts for several non-natural organic reactions, such as aza-Michael addition of aromatic amines with enone, GBB-multicomponent reaction, cascade reaction consisting aza-Michael addition and Aldol condensation.[1-4] Further, we have also developed the biocatalytic synthesis of N-heterocycles such as bis-indoles, quinolones, piperidines etc.[1-4]

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IL-22

Pharmacophore-based Drug Design, Synthesis, Structural exploration and study of 2-pyridone-based pharmaceutical precursor

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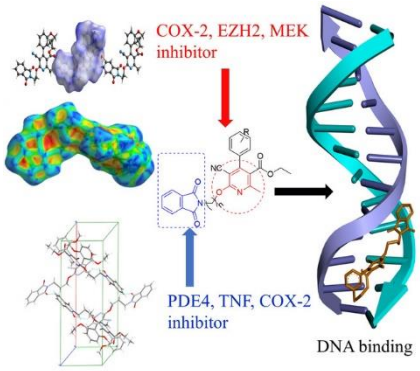
Abstract:

Pyridones/pyridines are structurally similar to thymine and uracil bases, and 2-pyridone exhibits lactam-lactim tautomerization like thymine and uracil bases. Their synthetic derivatives have shown different bio-activities and binding affinities with various receptors like CDK4, FGFR, p38, etc. [1]. The pyridone ring represents the main skeleton of numerous bioactive molecules. Four pyridone-based fleximers were synthesized and characterized using SCXRD, 1 HNMR, 13 CNMR, and IR spectroscopy. Phthalimide is linked to different pyridines/pyridone through a methylene bridge.



The self-assembling of the supramolecular network was studied with SCXRD and Hirshfeld analysis. Vibrational Spectroscopy was used to gain more insight into the non-covalent interactions in solid and liquid phases. More importantly, phthalimide and pyridine of all fleximers can bind with different receptors and are accessed with DNA binding interactions using ct-DNA. Compounds [2-4] exhibited interesting absorption shifts in the titration study with ct-DNA. *In silico* molecular docking of compounds [2-4] was evaluated using Autodock Vina software with B-DNA dodecamer (PDB ID: 1BNA). A docking score ranging from -7.7 Kcal/Mol to -8.9 Kcal/Mol was observed from the docking results. Both results are promising for all compounds to go for in *vivo/vitro* study to develop a new drug.

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IL-23

Nanoadsorbents for drinking water remediation

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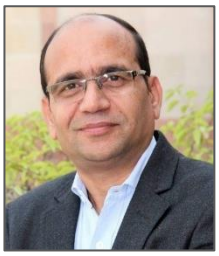
Abstract

Water pollution has been an important topic and ever since industrial revolution started, scarcity of fresh water became concern of the global scientists. Pulp and paper, textile, drugs and pharmaceutics, and steel manufacture are water intensive industries but fresh water is used invariably in all industries, including agriculture practices. More of the global economies are water deficient and are struggling for fresh water. After global industrialisation, there was stress on all natural resources but water resources are worst affected. Drinking water has become scarce in most of the countries. Looking into importance and complexity of the situation, treatment of water became concern of global scientists. There have been several traditional methods for water remediation, especially remediation of metal rich waters. Extraction, osmosis, and oxidation are few important methods but one of the most common methods is application of activated carbons for metal removal from waters. A latest development in this line is application of nanoadsobents for remediation of metal rich waters. Application of nanoadsorbents seems to be more efficient and economically viable and efforts are being made to use these wonderful newer materials at large scale treatment of metal bearing drinking waters.

Keywords: Drinking water; treatment; adsorption; nanoadsorbents; economic viability.

IL-24

Applications of NMR based Metabolomics



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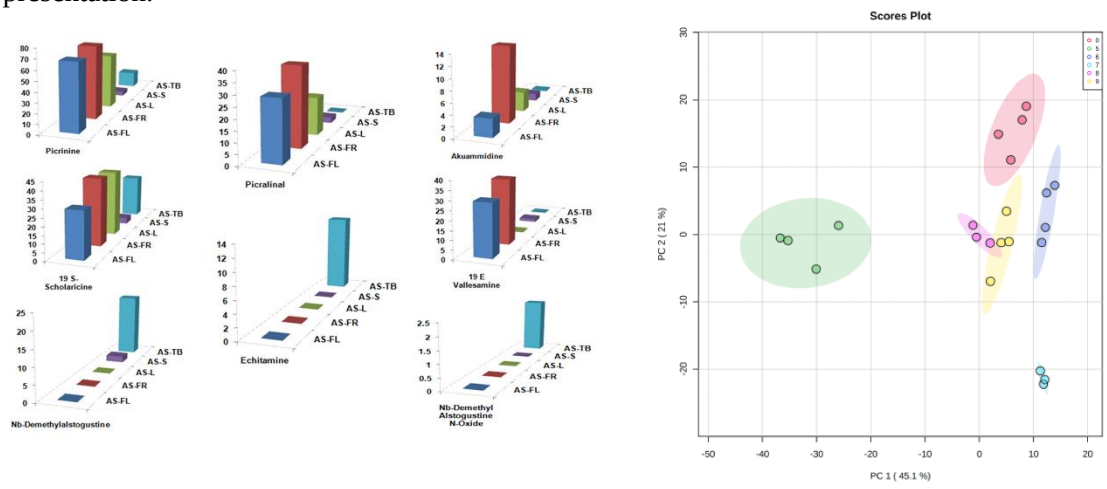
Metabolomics is the youngest member in OMICS family. It is rapidly evolving field in which study of metabolome present in a specific cell, tissue or organism performed. This 'Omics' science has various health applications which includes pharmacology, new born screening, toxicology and clinical chemistry. NMR based Metabolomics has unique and proven advantages in systems biology and biomarker discovery. Biomarkers could detect the biochemical changes, associated with disease processes. Discovering biomarkers for a given disease have become crucial and these studies may help for improving the diagnosis, prognosis and therapy of diseases.

The application of metabolomics is not limited to medical science only; it is widely employed in plant sciences. Metabolomics is being used extensively in plant research because of the benefits created on human health by various plant-derived products such as food, medications and industrial raw materials as well as its usage in plant breeding and nutrition assessment. Furthermore, the huge chemical diversity of plants in comparison to mammals and microorganisms contributes to the importance of metabolomics in plant studies. Metabolic profiling of the medicinally important plants may provide information regarding when and which part of plant should be collected to obtain substantial bioactive ingredients for desirable pharmacological activity. These studies may also provide a complementary tool for quality control of herbal medicinal products when these plants are used. Metabolomics in general and few applications of NMR based Metabolomics will be discussed in this presentation.



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IL-25

CAS SciFinder Discovery Platform: Research and Development Trends for Drug Discovery

Dr. Nabin Sarkar

Customer Success Specialist
ACSI India Pvt. Ltd., India

Abstract: Over the last few years, there have been a rapid advancement in chemical and biological Alternatively, this has a significant implications for the healthcare sector in terms of improving human health through the development of new technologies and more precise treatment of rare diseases.research leading to a better understanding of the chemical process occurring in cells and development of new effective drug molecules.

With advanced analytical tools, SciFinder-n is a robust database curated by expert scientists from CAS that facilitates reference, substance, and reaction searching. The comprehensive content and search capabilities in CAS SciFinder^{n} that will make it your go-to solution for retrieving sustainable approaches related to your research topic in multiple scientific research functions and requirements such as, a) synthesis strategies of drug molecules and optimization of Al-driven synthesis methods, b) searching the present challenges for researchers towards new technologies for undruggable targets, c) staying upto date with evolving research trends for drug designs for sustainable cure.

IL-26

Can Short ECM Hotspot-motifs engineered into Scaffolds for Tissue Engineering Applications?

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Background: Wound healing and selective tissue regeneration have been in scientific investigation for decades, with various strategies involved. One of the key lines of work has been Scaffold designing. These scaffolds are popularly scavenged from natural sources like Extra Cellular Matrix (ECM) proteins or synthetically designed using polymers or both as Composite type. The advantage of hotspot-motifs derived from ECM proteins is they have desirable characteristics of signalling and supporting cell attachment, adhesion, proliferation, and angiogenesis vital for tissue regrowth. The problem with these motifs is that they have poor mechanical properties pertaining to self-assembling, which warrants them for designingscaffolds.

Objective: Here, we aim to use computational tools to scout different combinations of aminoacids to be added to engineer hotspot motifs of ECM proteins that could self-aggregate, be shorter in length, and are suitable for tissue engineering applications.

Methods: A virtual library of peptide sequence were constructed using four different modules of amino acid combinations. Short 8 and 11 residues self-aggregating peptides were designed. A total of 22 multi-peptide systems were investigated using all-atom simulations for their aggregation tendency, aggregate stability, and accessibility of the native motifs.

Results and Implications: Out of 22 models explored, the three best combinations were short-listed based on self-assembling behavior. These top 3 designs had significantly preserved accessibility to native motifs in their aggregates and while maintaining aggregate stability. It was observed that charges on the residues, hydrophobicity, arrangement, and location in the sequence influenced the suitability of these peptides for tissue engineering applications.

Conclusion: This study showed evidence that naturally sourced ECM hotspot motifs can be modified into self-assembling peptides. Currently, we are investigating the influence of other environmental factors such as pH, ionic concentration, temperature, and forcefields on these top three peptide designs for their suitability in tissue engineering applications.

Keywords: Tissue Engineering, Scaffolds Designing, Self-Assembly, MD Simulations

IL-27

Electro-Organic Synthesis: Green and Sustainable Approach for Forging New Bonds

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Abstract:

Due to environmental concerns and cost issues, the development of green and sustainable procedures for the construction of carbon-carbon and carbon-heteroatom bond has attracted much attention in recent years. Electro-organic synthesis has emerged as an environmentally benign technique for the development of novel organic methods due to its benefits such as high atom economy, mild synthetic route, avoiding redox reagents, ligands, or catalyst-free synthetic procedures over traditional reagents-based methodologies. This talk will cover the recent contributions from our group towards the development of electrochemical protocols for carbon-carbon and carbon-heteroatom bond formations.

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IL-28

Pyrazole-based organic-amine and silver-carbene-based metal-organic cages as artificial Light Harvesting Systems.

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Abstract:

The design and implementation of supramolecular emissive materials are one of the important aspects of cutting-edge chemical research that have drawn considerable attention in recent years. Fine-tuning of electronic properties of molecules/materials by modulating parent structure via various external stimuli like non-covalent interactions, light, pH, redox potential, etc., has an important aspect in increasing its efficiencies and functions for practical applications. Switching of emission behaviors in light and dark of stimuli-responsive chromophores was well explored to design optoelectronic materials for bio/chemical sensing as well as artificial light-harvesting materials.[1] Self-assembled discrete organic cages in this regard have attracted wide interest for their remarkable stability. They possess high surface area and have profound applications in host-guest chemistry, catalysis, sensors, and gas storage systems. Dynamic covalent chemistry (DCC) that utilizes reversible imine bond formation between aldehyde and amine functional groups, emerges as one of the smart and efficient approaches toward the design and synthesis of functional organic cages via single pot synthesis in high yield. Organic cages possessing high emission in aggregate/solid-state could be an ideal applicant to construct energy donors in light-harvesting function in the aqueous medium.[2] Supramolecular organic cages based on aggregation-induced emissive cores have bright prospects as in designing artificial light-harvesting systems.[3] In this talk, I will talk about the design and synthesis of an artificial light-harvesting system based on photo-responsive pyrazole-based organic and silver-carbene-based metal-organic cages. The designed cage exhibits multi-step energy transfer which will acts as photocatalyst for clean and sustainable energy.

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IL-29

Stimuli-responsive nanocarriers for bioimaging, targeted drug delivery and therapeutics

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Abstract:

Site-specific delivery of the therapeutic agents to the target site is the most challenging and most important goal from the clinical point of view. Recently, much effort has been indulged in developing targeted drug delivery systems, especially for tumor, instead of introducing new drugs. Stimuli-nanocarriers are the significant results of these efforts. In this regard, internal stimuli such as temperature, pH, hypoxia, redox potential as well as some external stimuli like ultrasound, light, and magnetic field were exploited. The stimuli-responsive nanocarriers can respond to these internal and external stimuli by release of the encapsulated drug. Among the various nanocarriers, nanocapsules have emerged as promising drug cargo that has been well investigated. We have developed such stimuli-responsive nanocarriers that can overcome these drawbacks and provides efficient drug delivery to the desired site of action.

IL-30

Separation of Azeotrope using Green Solvents "Deep Eutectic Solvents and Ionic Liquids"

Indra Bahadur

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Deep eutectic solvents (DESs) are ionic liquids (ILs) analogues that consist of Lewis or Brønsted acids and bases[1]. These systems are characterized by a substantial decrease in melting points as compared to those of neat constituents. DESs have been identified as potentially cost-effective and environmentally friendly replacements for traditional volatile organic solvents. In designing separation techniques, the activity coefficients at infinite dilution of solutes in the DESs and ILs are crucial. The gas-liquid chromatography technique (GLC) was used to determine activity coefficients at infinite dilution of polar and non-polar solutes: alkanes, alkenes, alcohols, ketones, thiophene, heterocyclics, cycloalkanes, acetonitrile, tetrahydrofuran, cycloalkenes, aromatic hydrocarbon and water in DESs and ILs at higher temperatures. Partial molar excess enthalpies at infinite dilution were calculated from the temperature dependence of activity coefficients at infinite dilution. The selectivity and capacity values for separation of azeotrope were calculated and compared to literature values of volatile organic solvents to assess the suitability of the DESs and ILs for possible use as an entrainers. The potential of DESs and ILs to replace traditional solvents were discuss based on (capacity and selectivity) for all chosen systems involving close boiling point mixtures.

Keywords: Azeotrope; Deep eutectic solvents, Ionic liquids, activity coefficients at infinite dilution.

IL-31

A NEW ROUTE TO THE SYNTHESIS OF THE BENZOTHIAZINO-BENZOTHIAZINES

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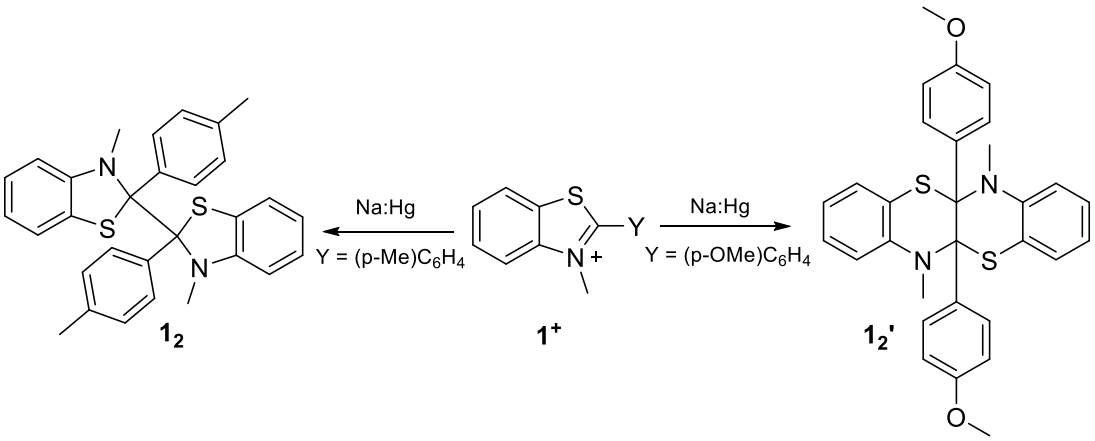
Abstract:

N,*S*-based 5 and 6-membered heterocyclic compounds, such as benzothiazoles and benzothiazines, respectively, have gathered enormous interest in the past few decades. Notably, several reactions have been studied related to benzothiazoles and benzothiazines and their derivatives due to their wide range of pharmacological interest, and in many as synthetic intermediates [1,2]. However, the most exciting part of benzothiazoles is that the 3-alkylbenzothiazolium salts $\mathbf{1}^+$ undergo a myriad of chemical transformations due to their C-2 acidic protons from both chemical and biochemical points of view. Depending on the substituents at C-2 and/or N-atom of the 1,3-thiazole ring and the reaction condition, the chemical reduction of benzothiazolium salts obtain a variety of products. Herein, we report the synthesis of two new fused 5- and 6-membered heterocyclic compounds, bibenzothiazoles $\mathbf{1}_2$ and benzothiazino-benzothiazines $\mathbf{1}_2'$ from the Na:Hg reduction of benzothiazolium salts $\mathbf{1}^+$. Similar bi-benzoimidazoles have already been reported as good electron donors and can be used as n-type dopants in organic electronics [3,4], while the 1,4-benzothiazines and related derivatives stimulate much pharmacological interest [1].



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IL-32

Metal Free Oxidative Cyclizations Involving Iodine(III) Reagents

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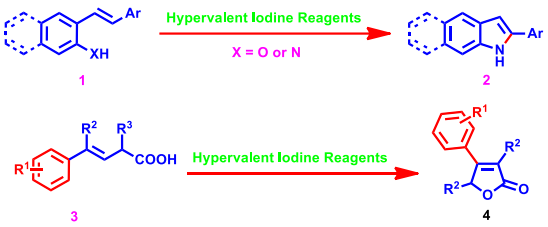
Abstract

In past few decades, hypervalent iodine reagents have been developed as highly valuable reagents in synthetic organic chemistry. Because of mild reaction conditions and environmentally friendly behaviors, these reagents are the key replacements of toxic heavy metals. Various hypervalent reagents have been developed as oxidants but their applications are not limited to oxidative functionalization and several iodine(III) reagents have been known for their electrophilic nature. Various synthetic transformations such as cyclization reactions, α-functionalizations of carbonyl compounds, atom-transfer reactions and oxidative rearrangements have been also achieved successfully. Recently, these reagents have been received a particular attention due to their applications in catalysis. Various synthetic transformations have been successfully achieved using both iodine(III) or iodine(V) reagents as catalyst.



Scheme 1.

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IL-33

Biomass Derived Sustainable Development of Carbon Quantum Dots as Potential Nanosensor

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Abstract

Carbon quantum dots (CQDs) are regarded as a novel fluorescent carbon nanomaterial due to their remarkable properties like high water solubility, low toxicity, tunable photoluminescence, chemical inertness and stability. Scientists have employed various precursors and methodologies to synthesise CQDs. Among them the conversion of biomass-waste into value-added CQDs has been regarded as a green synthesis route for the fabrication of these zero-dimensional nanomaterials. The primary objective of this talk will be utilisation of biomass waste to develop highly fluorescent nanosensor with high quantum yield. Moreover, sustainable synthesis of CQDs from abundance source of biomass-derived precursors have numerous advantages, such as reduced chemical exposure, minimized waste generation, cost-effectiveness, eco-friendliness. As biomass is a plentiful and non-toxic feedstock with a significant carbon and oxygen content. Transforming biomass into high-value products assists efficiently management of solid waste removal and improving the rising resource, environmental, and energy concerns. Moreover, CDs synthesized from biomass have ability to tailor their surface states and size in order to obtain high quantum yield.

IL-34

Exploring fluorescent properties of pyrazolo[1,5-a] pyridine to design new fluorosteric compounds as hDHODH inhibitors

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Receptor target fluorescent probe is an imaging technique used to studying and understanding biological processes in live organisms. Typically, the core structure of these probes involves three key elements: the biological ligand, the linker, and a fluorophore[1]. The alteration of the pharmacological and physiochemical characteristics of the biological ligand, however, is a significant drawback of this method. To avoid these issues, one potential strategy involves merging the concepts of biological target and fluorescent probe, resulting in the design of a *biologically active fluorescent ligand.*
Pyrazolo[1,5-a]pyridin-2-ol is a small molecule characterized by a strong emission in the blue field. Its physicochemical features as carboxylic acid isostere have been widely investigated [2]. The effectiveness of this moiety as carboxylic acid bioisostere is highlighted in MEDS433, a potent *h*DHODH inhibitor [3]. With the purpose of moving the emission profile from blue to red while keeping the scaffold's modest size, two series of compounds were design. In the first series, a yellow-red bathochromic shift was achieved by increasing the π-conjugated network of the scaffold, that was, however, accompanied by a low quantum yield. In the second series, a scaffold rigidification was used to achieve a yellow-red bathochromic shift and an adequate quantum yield.
Here, the comprehensive analysis of the fluorescence properties of this probe, as well as the first biological application achieved by design a new *h*DHODH inhibitor and evaluation of fluorescent propriety in Acute Myeloid Leukemia cell will be discussed.

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IL-35

Recent Pharmacological Approach toward the Search of Novel Bioactive Leads from Medicinal Plants

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Medicinal plants play a vital role in drug discovery for life-threatening ailments like cancer, malaria, diabetes cardiovascular, viral and mycotic problems. Recently, drug discovery from plants for the treatment of cancer gets more focused and leads to the discovery of various novel anticancer drugs such as paclitaxel, docetaxel, topotecan, irinotecan, vincristine and vinblastine. Drugs derived from plants are generally considered safe compared to synthetic drugs. Bioactive constituents obtained from plants have structural diversity and considered as a reference drugs for the discovery of new future semi-synthetic/ synthetic drug candidates. Medicinal plants continue to be an important source of new therapeutic aid for alleviating ailments of humankind. Keeping in view the importance of medicinal plants in the discovery of new or novel drugs and our continuous work [1-3] 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. During the presentation, recent pharmacological approach toward the search of novel bioactive leads from medicinal plants will be discussed in detailed.

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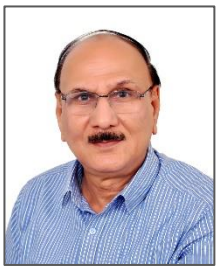
IL-36

Zeolite Catalytic Technologies for Green Chemical Production



Raksh Vir Jasra

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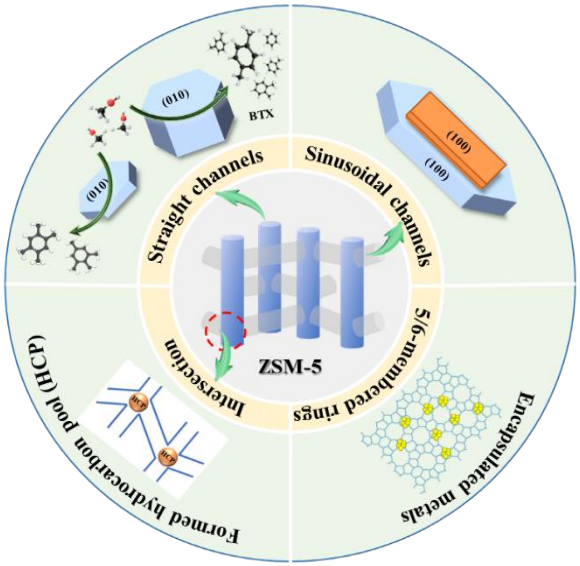
Abstract:

Zeolites due to their high crystallinity, varied surface functionalities, molecular sized pore dimensions and high thermal and hydrothermal stability provide a strong portfolio of heterogenous industrial catalysts for chemical industry. The unique features that zeolites attractive catalytic include:

- Micro-porous crystalline solids (Specific pore opening & channel width)
- Wide variety of pore architecture and shape selectivity that can be tuned in great detail by modern synthetic methods;
- High thermal / hydrothermal stability (> 600 °C); High Surface area (>300 m^2 /gm)



- Tunable Acidity (nature, concentration, strength) as number of acid sites can be controlled by Al content in zeolite; Metal impregnation and exchange to have muti-functional catalytic activity
- Space confinement imposing a unique influence on reaction pathways
- Scalability to tons synthesis.

Zeolites have been conventionally been used as catalysts in a wide variety of industrial processes, especially in oil refining and petrochemistry. Its application has extended to fine chemicals and even in biomass conversion to value added products in recent times.

Present talk will discuss industrial catalytic application of zeolites especially in making chemical processes greener and cleaner. Talk will also discuss in detail about novel zeolite based REL-ORCAT technology developed and commercialized at Aromatic plant of Reliance Industries Limited.

IL-37

Design and Development of Non-ionic Amphiphilic Architectures for Transdermal Drug Delivery Applications

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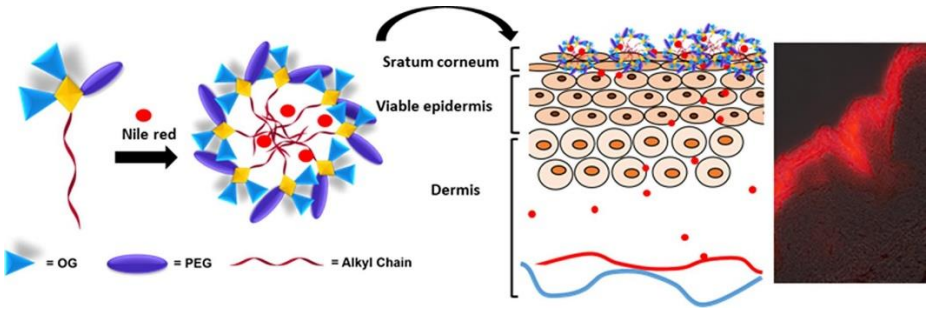
The delivery of many bioactive molecules to their target sites can be improved by utilizing different classes of nanocarriers. Amphiphilic nanocarrier systems are known to have enhanced permeability and retention effect and thus can circulate themselves in the blood for longer duration and are reported to be effective for drug delivery. In response to the increasing need for easy-to-prepare and versatile nano-transport systems for biomedical applications, the importance of polymers and dendrimers has been well recognized. A new class of non-ionic amphiphiles have been synthesised following chemo-enzymatic methodology and using glycerol, polyglycerol, polyethylene glycol (PEG), and alkyl/perfluoro-alkyl moieties as the building blocks. The amphiphiles synthesized were observed to aggregate in aqueous medium. Their aggregation behaviour was studied using Dynamic light scattering (DLS), fluorescence spectroscopy, and cryogenic electron microscopy (*cryo*-TEM). The inner hydrophobic core of these aggregates in aqueous medium is capable of encapsulating lipophilic guest. The biomedical application of synthesized amphiphiles was further investigated for trans-dermal drug delivery on excised human skin using Nile red encapsulated in the nanocarrier. The release profile of drug/dye encapsulated amphiphiles was studied under physiochemical conditions in the presence of immobilized lipase Novozym 435.
An overview of this research area will be given during the conference.



Keywords: Amphiphiles, nanoaggregate, drug/dye, encapsulation, transdermal delivery

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IL-38

Experimental and Computational Characterization of p-Sulfocalix[4]arene Mediated Delivery System

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In past few years, calixarenes are being investigated to improve the physicochemical properties of therapeutic compounds. Calix[n]arene are a macrocyclic compound with different number of phenolic units linked by methylene bridges on ortho positions and possess a 3D cavity that can encapsulate biologically important molecules through host-guest complexation. In this work, we have prepared an inclusion nanocomplex (MH-SC[4]A) between morin hydrate (MH) and p-sulfonatedcalix[4]arene by solvent evaporation method and was evaluated for its anticancer efficacy. With a nanoscale size (23 nm) and negative zeta potential value of -10.5 mV, the prepared complex increased the aqueous solubility of MH by 22 folds, enhanced dissolution in both simulated gastric and intestinal fluids, and provided better stability to MH. The improved solubility of MH was due to strong hydrogen bonding and π- π interactions between MH and SC[4]A. The inclusion complex formation mechanism was determined by FTIR, NMR and Molecular Modelling. Consequentially, the nanocomplex showed substantial antiproliferation activity, apoptosis-mediated cytotoxicity, and inhibition of colony formation activity of A549 human lung cancer cells. Finally, the cellular uptake studies revealed that the increased anticancer activity of MHSC[4]A was led by its higher cellular uptake than the free drug. Thus, these obtained results suggested that the developed nanocomplex could be a promising and therapeutically effective way to use MH.

IL-39

Unravelling the destabilization mechanism of small-molecule inhibitors against α–Syn oligomers using molecular simulations

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The intracellular neuronal aggregates comprising α–Synuclein (α–Syn) protein known as Lewy bodies and Lewy neurites are the key hallmarks of Parkinson's disease (PD)[1]. The destabilization of pre-existing disease-relevant α–Syn fibrils is considered a potential therapeutic strategy against PD (Fig. 1) [2]. Ellagic acid (EA), a natural polyphenolic compound, is experimentally proven as a potential candidate that reverses the α–Syn fibrillization [3]. Hydroxytyrosol (HT), 3,4-dihydroxyphenylethanol, is a naturally occurring polyphenol that lessens the severity of PD by reducing α–Syn aggregation and destabilizing the pre-formed toxic α–Syn oligomers [4]. Continuing with our investigations on elucidating the inhibitory mechanism of various inhibitors against Aβ aggregation and protofibril destabilization [5], molecular dynamics (MD) simulations have been performed in this work to illuminate the destabilization mechanism of EA and HT on α–Syn oligomers[6]. EA interacted primarily with the non-amyloid-β component (NAC) of α–Syn oligomer, disrupting its β-sheet content with a concomitant increase in the coil content. The E46–K80 salt bridge, critical for the stability of Greek-key-like α–Syn fibril, was disrupted by EA. HT binds favorably to α–Syn trimer ($\Delta G_{binding}$= –23.25 ± 7.86 kcal/mol) and a notable reduction in the interchain binding affinity of α–Syn trimer on the addition of HT depicts its potential to disrupt α–Syn oligomers. The computational studies investigating the effect of small molecules on the destabilization of oligomers of varying sizes are worthy for gaining insights into the discovery of new inhibitors of α–Syn aggregation and protofibril destabilization in PD.

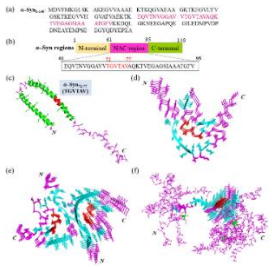

Fig. 1: Amino acid sequence of α–Syn with NAC region (residues 61–95) in pink (panel a). The different regions of α–Syn are shown in panel b. The α–Syn monomer (PDB ID: 1XQ8), α–Syn trimer (residues 37–99) obtained from the cryo-EM derived α–Syn hexamer structure (PDB ID: 6A6B), α–Syn fibril structure (PDB ID: 6CU7), and solid-state NMR structure of a pathogenic fibril of full-length α–Syn (PDB ID: 2N0A) are shown in panels c, d, e, and f, respectively.

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IL-40

Research on Animal, and human clinical trials for Potential High-Risk Therapeutic Products.

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Abstract

There is an old saying- “public health is public wealth”. In the last few decades biomedical research grown tremendously and use of animals was also increased as research model for clinical trials. Over 115 million animals are utilized annually for experiments or to supply the biomedical sector worldwide. The evolution of drug discovery traverses a long and fascinating journey. The security of drugs is pivotal because no drug is absolutely safe for all people, in all places, at all times. Management of Drug Disasters among the human population remains a major therapeutic challenge throughout the world. Drugs showing safety and efficacy in Bio-clinical animal models may show very different pharmacological properties when administered to humans. Clinical trials are crucial for identifying novel disease treatments as well as innovative methods of disease detection, diagnosis, and risk reduction. Researchers can learn things about what works and doesn't work in humans through clinical trials that cannot be discovered through laboratory or animal testing.

Clinical research has undergone a lengthy and fascinating history. Humans are used as test subjects in human clinical trials research, which is a form of scientific investigation. Human clinical trials are used to test new procedures and medications and determine how they affect patient outcomes. Clinical research informs clinical practice and evidence-based medicine. When novel drugs are tested on humans, there are various potential ethical problems. In highly developed countries like the USA and UK, clinical trials are subject to strict regulations, extensive safety measures, and compensation responsibilities. Finding volunteers is a time-consuming and expensive process in western countries. Clinical investigations are currently expanding, particularly in China, India, and other nations. Due to its strong regulatory environment, illiteracy, poverty, lack of awareness about clinical trials, and broken healthcare system, India was a suitable destination to outsource human clinical studies. India has been deemed one of the most promising centers of activity for clinical trials due to the large number of available patients who are treatment-naive, the low cost, and the large number of qualified professionals. Clinical trials are reliable, practical, and available in India.

IL-41

Molecular Signalling Pathways and therapeutic approaches for the treatment of breastcancer

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Abstract:

Breast cancer is the world's second utmost common cancer and the fifth principal source of cancer-related mortalities. It is a heterogeneous disease which is characterized by local or advanced tumors expressing specified hormone receptors such as estrogen (ER), progesterone (PR) and human epidermal growth factor (HER2). Progression of breast cancer depends on various genetic factors such as mutation in ongoing molecular mechanisms involving various pathways such as ER, PR and HER2 signalling as well as Notch signalling, Wnt/βcatenin signalling, SHH signalling, TGF-β signalling and PI3k/Akt/mTOR signalling. Despite of advancements in developing chemotherapeutic agents, therapeutic effect of these drugs lack in ER positive, HER2 positive, ER positive HER2 negative metastatic breast cancer expressing oncogenes. Many targeted therapies such as PI3k inhibitors, mTOR inhibitors, Akt inhibitors CDK4/6 inhibitors, PTEN stimulators, PARP inhibitors and AMPK stimulators have been developed and are currently in clinical use. The talk will cover recent studies in the area of breast cancer and also dwell upon protective action of natural molecules in combination with synthetic molecule for the treatment of breast cancer.

IL-42

Unveiling the Mechanism of Tumor Regression in Triple- Negative Breast Cancer with a Thiazole-Based Pyruvate Kinase M2 Inhibitor

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Triple-negative breast cancer (TNBC) represents a highly aggressive subtype of breast cancer characterized by a dismal prognosis. One of its distinguishing metabolic features is its intensified glucose consumption, a pivotal factor in its initiation and progression. In this regard, pyruvate kinase M2 (PKM2), a critical enzyme governing glycolysis, is notably overexpressed in TNBC. This elevated PKM2 expression intensifies glucose uptake, fosters lactate production, and curbs autophagy, thereby expediting the oncogenic process. Unfortunately, despite advanced platinum-based chemotherapy, around 30% of TNBC patients succumb within five years, underscoring the urgency of innovative therapeuticapproaches. In our research, we present a rational strategy for the development of an anti-cancer compound targeting PKM2, utilizing an imidazopyridine-based thiazole derivative **7d**. Our enzyme assays confirm that these molecules serve as potent PKM2 inhibitors, operating in the nanomolar range, and exhibit favorable drug-like properties. Furthermore, *in vivo* experiments demonstrate that **7d** surpasses the clinical gold standard, lapatinib, in terms of inducing tumor regression by inhibiting PKM2 and multiple metastatic markers. This study introduces a lead-based approach characterized by its simplicity in chemical synthesis and robust efficacy in developing an exceptionally potent PKM2 inhibitor for combating breast cancer. The details will be discussed in the talk.

IL-43

DESIGN AND SYNTHESIS OF NOVEL NON-NAD$^+$ ANALOGUES AS POLY(ADP-RIBOSE) POLYMERASE1 (PARP1) INHIBITORS

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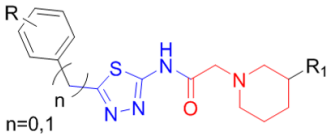
Abstract

Poly (ADP-Ribose) Polymerase1 (PARP1) is a ubiquitous nuclear enzyme which uses NAD$^+$ as a substrate, cleaves it and transfers the ADP-ribose moiety to the proteins and thereby does the parylation of the target proteins. All marketed PARP1 inhibitors; Olaparib, Rucaparib, Niraparib, Talazoparib etc. are NAD$^+$ competitors due to the presence of nicotinamide pharmacophore and are mainly approved for the treatment of BRCAm Ovarian cancer and metastatic breast cancer. They mediate their antitumor effect through catalytic inhibition of PARP1/2. But, as NAD$^+$ is utilized by many enzymes other than PARP1, these conventional NAD$^+$ analogues are nonselective and have many hematological side effects. To circumvent this problem, there is a need to develop next generation selective PARP1 inhibitors. PARP1 activation through its interaction with histone H4 is unique for PARP1 only. We designed series of novel N-(5-substituted-1,3,4-thiadiazol-2-yl)-2-substituted-acetamide derivatives as non-NAD$^+$ PARP1 inhibitors by hybridizing one of reported Non-NAD$^+$ thiadiazole derivative hit molecule with another reported potent non NAD$^+$ lead molecule, 5F02 as shown in Fig. 1 which were subjected to series of *in-silico* studies to check whether they could inhibit the protein-protein interaction between PARP1 (PDB ID 4GV7: A chain) and H4 (PDB ID 5TEG: D chain) in ClusPro 2.0. Promising 11 novel molecules were synthesized, characterized and subjected to *in-vitro* cell viability testing against MDA-MB-231 cell line in MTT assay. The most potent compound, KSBP04 showed 19.34 nM IC_{50} which was found more potent than Olaparib (IC_{50}=11.5 µM). During *in-vitro* PARP1 enzyme inhibition assay, compound KSBP04 IC_{50} was found to be 23.41 nM. Overall, KSBP04 was identified as novel lead under the class of non-NAD$^+$ PARP1 inhibitor and its further development is ongoing.



R= H, 2-CH_3, 3-CH_3, 4-F
R_1= CH_3, NH_2

Fig. 1. Designed Series of N-(5-substituted-1,3,4-thiadiazol-2-yl)-2-substituted-acetamide derivatives

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Acknowledgement:

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IL-44

Development of nanocellulose-based materials for food safety applications

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Nanocellulose is a versatile and sustainable nanomaterial derived from cellulose, which is found in plant cell walls. It has gained significant attention for various applications, including those related to food safety. Nanocellulose-based sensors can be developed to detect contaminants or spoilage in food products [1]. Nanocellulose can be incorporated into food packing materials to improve their barrier properties and it can be combined with antimicrobial agents to create films that inhibits the growth of bacteria and pathogens on the surface of food packaging materials [2]. Herein, we report the synthesis and application a nanocellulose-based composite as an immobilization platform to develop a specialized nano-enabled sensing system for the detection of organophosphate pesticides (OPs) in food samples. The biosensor leverages the colorimetric response generated by an immobilized enzyme during OP hydrolysis, enabling straightforward visual detection. These sensors can provide real-time information about the quality and safety of food items. Further, we developed a novel antioxidant film for food packaging application by incorporating a gallic-based framework into nanocellulose film. These nanocellulose-based materials exhibited prolonged antioxidant activity and durability, offering a promising approach for environmentally friendly food packaging.

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IL-45

Application of TiO 2 Catalyzed Reactions to the Synthesis of Privileged Indole Derivatives for Medicinal Interest

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Abstract:

The present studies include the catalytic synthesis, characterization, and various applications of highly interesting and significantly useful compounds containing nitrogen in the core structure. Manufacture of nitrogen containing biologically active compounds in the interest of pharmaceutical drug design, agrochemical industries, and other synthetic modifications. As nanomaterials have more surface area so they act as a good catalyst for the synthesis of heterocyclic compounds. The work Exclusively devoted to the study of the synthesis of heterocyclic compounds via nanocatalyst. This research containing multicomponent synthesis of novel 2((1H-Indole-3yl) (Phenyl) Methyl) Malononitrile derivative by utilizing Recoverable and efficient TiO 2 nanocatalyst in which we synthesized TiO 2 Nanocatalyst and after that using this nanoparticle as catalyst to synthesized heterocyclic compound and also checked the reusability of TiO 2 Nanocatalyst. Finally, the antioxidant activity, antibacterial activity of synthesized heterocyclic compounds and their electrochemical study was carried out, some of the compounds have shown significant antioxidant and antibacterial properties.
After that synthesized, heterocyclic compound examines the electrochemical study and these compounds show very good electrochemical behaviour.

IL-46

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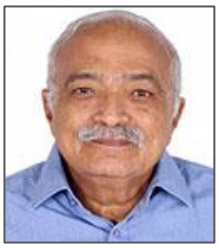

Abstract Awaited

IL-47

Nano Gold Regulate the Undruggable Pathogenic Tau to Prevent AD

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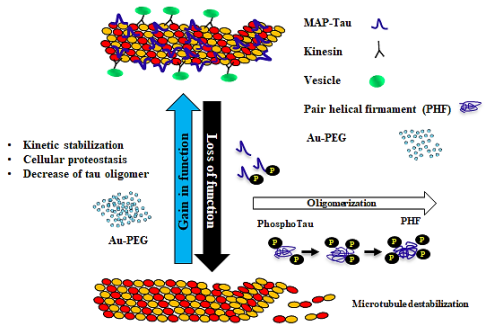
Alzheimer's disease (AD) is a progressive neurodegeneration of CNS with impaired cognition that affects the physical health of patients and social lives. Neuronal fibrillary tangles (NFTs) are proteinous structures found in the autopsy brain section of AD patients and individuals with other neurological disorders. These tangles mainly consist of hyperphosphorylated Tau protein (p-tau) that undergoes aggregation. Tau protein stabilize microtubule-related protein. Hyperphosphorylated tau could disintegrate microtubules, in turn destroy the neuronal cell structure by causing the nerve damage. Growing evidence suggest that insulin resistance or type 2 diabetes could drive the AD progression whereas the underlying mechanism is unclear. In addition, Tau protein forms neuro fibrillary tangle in AD whereas ratio of p-tau to tau in CSF act as an index for the disease state. Therefore, regulating tau protein could be beneficial to alter the disease state of AD. We have observed that the Pegylated self-therapeutic nano gold ameliorates the Tauopathy symptoms and diminish the content of circulating pathogenic Tau. We have prepared both non-targeted and targeted gold conjugates to evaluate the study. Given the small size of the gold nanoparticle, it was observed targeted conjugate localize more inside the brain hippocampal region than the nontargeted control. We have synthesized an AuNPs-Pegylated nanoconjugate and characterized by using TEM, UV-vis, MS and Zetasizer analysis. We further used it to demonstrate whether it can pharmacologically regulate pathological p-tau. Using transferrin as active targeting agent in AuNPs-PEG nano-drug decreases p-tau and subsequently the surface presentation of insulin receptor (IR). AuNPs-PEG conjugate further reduce the PHF tau burden. Further, in okadaic acid chemical induced animal model of AD, AuNPs-PEG transferrin construct boost the cognitive function and enhance of the learning ability of AD mice. Given the insulin resistance and p-tau level holds a connection, further studies are required to understand the gold nanoparticles dependent modulation of insulin signaling during AD.



Scheme 1: Proposed mechanism of nano gold mediated alteration of misfolded mutant tau P301L alone and in hyper phosphorylation state. Loss of Tau function to bind and stabilize microtubule and enters in fatal cascade of protein PHF tau. This destabilizes microtubule and vesicle movement. Au-PEG retain tau function acting as a kinetic stabilizer. Sunil et al; *Small* **2020**, 1906861. DOI: 10.1002/smll.201906861

IL-48

Progress in Metal-based Anticancer Agent Macro to Nano Structure: In vitro and in Vivo Investigations

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Macro and nano metallic cancer drug development is a thrust area of pharmaceutical research [1-3]; developing new nano-drug, delivery, and therapeutic strategies that could target specific receptors on cancer cells is in progress. New potential metallic-drug macro molecules were designed, synthesized, and characterized by various spectroscopic methods and further confirmed by X-ray crystallography. Further, the nano metallic drugs were prepared and characterized by SEM, TEM, XRD, and EDX studies. In vitro DNA binding studies of the compounds, docking studies, and Gel electrophoretic assay demonstrate the ability of the compounds to bind with DNA through the hydrolytic/oxidative process. To understand the macro and nano drug-protein interaction, the affinity of the molecules toward proteins was investigated. The nanoformulations showed high inhibitory activity against enzymes, and IC50, suggesting that nano complexes were efficient DNA-cleaving agents. In vitro, results of anticancer activity against the carcinoma cell lines revealed that complexes can kill the chosen cancer cells. The mode of cell death induced by complexes was apoptosis, as revealed by EB and Hoechst 33258 staining. The drug delivery via graphene oxide loaded nano metallic drugs conjugate was investigated and revealed that the nano conjugate drug has a high potential to inhibit the cancer-promoting enzyme and kill the cancer cells via an apoptotic pathway at low concentration.

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IL-49

o-Alkynyl/alkenyl Arylnitrile: A New Building Block for Construction of Small Organic Molecules of Pharmaceutical Interest

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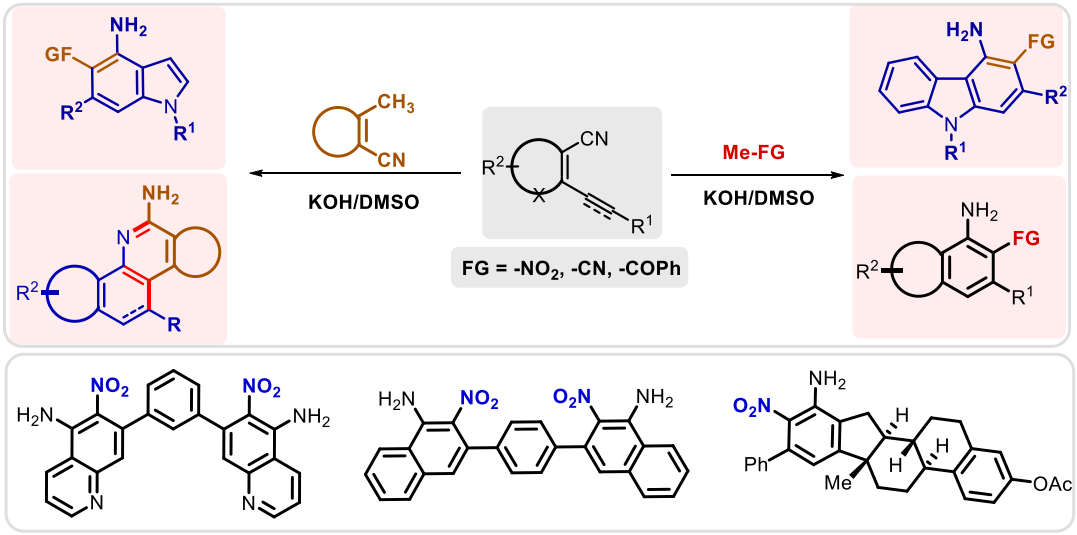
The simplicity, efficiency, and generality of reactions using alkynes have led to its applications in the synthesis of a wide variety of small organic molecules and natural products. Developing synthetic strategies for the direct synthesis of amino-substituted small molecules in terms of selectivity, operational simplicity, functional group tolerance, and environmental sustainability is in constant demand as the majority of drugs; drug-like compounds contain hetero atoms at their core. In continuation of our interest in the synthesis of small organic molecules using alkynes and super-base chemistry, we have successfully engineered the synthesis of a variety of biologically important scaffolds using *ortho*-alkynyl/alkenyl aryl nitriles. In this presentation, I would like to discuss some recent results in this chemistry.



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IL-50

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Abstract Awaited

IL-51

Discovery and Development of Synthetic anti-VEGF FAB for Treating wet-Macular Degeneration and Diabetic Retinopathy

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Abstract: Wet age-related macular degeneration (wet-AMD) is a progressive neurodegenerative disease of the retina, affecting the central vision. Wet-AMD and Diabetic Retinopathy (DR) is a leading cause of irreversible vision loss, worldwide affecting the population older than 50 years. Products that significantly addresses market access representing a global ocular market of >$25B and >200M patients globally. The vision behind FAB201 development is to provide an efficacious and cost- effective treatment for wet-AMD patients. Currently approved anti-VEGF drugs like Lucentis and Eylea in the market are expensive and not widely accessible in developing countries. Keeping this in mind to meet the unmet medical needs and to provide affordable treatment to developing countries.

We have developed an anti-VEGF Fab molecule (FAB201 and FAB293) for wet-AMD and DR, filed US patent, successfully finished the discovery, proof of concept, development, pre-clinical toxicity studies and cGMP manufacturing for our proprietary molecule. FAB201, that is close to going to Phase-1 trails in US and Australia for wet AMD and DR. FAB201 and FAB293 are 48kDa synthetic human anti-VEGF Fab (Fragment Antigen Binding). It is a novel biologic (has unique CDRs in light chain & heavy chain) expressed in microbial system (E. coli BL21). FAB201and FAB293 has been developed using Phage display library with several rounds of affinity maturation for selection of clones with highest binding affinity, followed by site directed mutagenesis in CDRs for improved antigen binding towards hVEGF (Vascular Endothelial Growth Factor).

Both the molecules were engineered to express at a higher level and the downstream processing was optimised to minimise losses during purification. Developmental process of molecular biology where, gene coding for FAB201 and FAB293 was inserted in a modified pBR322 vector and has phoA promoter sequence. E. coli BL21 Pho based expression system offers an efficient and economic system to produce recombinant proteins. Bioreactor and scale-up cultivation was done up to 200L fermentation for the large-scale production of FAB201. The anti-VEGF FAB201 purifications and orthogonal analytical tests were performed. The recombinant protein was extracted from the cell before subjecting for purification, for which a series of steps are performed in sequence so as to efficiently extract the expressed protein from the cell and also maintaining the stability of the protein molecule at the same time inactivating or denaturing any unwanted process related impurities.

The Downstream Process for purification was optimised and was performed by a series of three chromatography steps to reduce impurities. Lysate was homogenized and clarified followed by purification by series of column chromatography. The quality of the product from all three purification steps were assessed by various analytical techniques. The purified drug substance was formulated by buffer exchange & concentration of the drug substance with the formulation buffer. The accelerated stability and stress stability studies are confined to temperature stability studies at ambient temperature and 37°C. Bioanalytical studies included several assays like Quantitation, In-process impurities analysis, Product related impurities and Sterility were performed. Biochemical & Biophysical characterization, analysis of batch consistency. In-vitro binding affinity, In-vitro efficacystudy for batch release assay and In-vivo efficacy studies were performed.

MTD and preclinical studies were done as per the regulatory guidelines. cGMP material was generated for the clinical studies. US FDA IND filing was done, and the molecule is ready for Phase-1 clinical trial.

IL-52

Stereoselective Construction of Alkaloid-Mimicking Polycyclic Scaffolds Through Unified Desymmetrization Strategy

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Stereoselective synthesis of nitrogen-containing complex scaffolds from simple building blocks has significant importance in modern synthetic organic chemistry. Nitrogen-containing bridged ring systems in natural products and pharmaceutically important molecules illustrates the need for the development of efficient synthetic strategies. Unified desymmetrization strategies have been developed to access structurally diverse polycyclic viz linear-, spiro- and bridged- rings systems with endogenous nitrogen.[1-3] Developed reactions demonstrates step-economical, complete control of regioselectivity and stereoselectivity and easily achieved from cheaply available feedstock starting materials.

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IL-53

Sialic acid conjugation for target delivery of natural neuroprotective: A case study.

Dr. Niyati Acharya

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The present talk focuses on the use of sialic acid to design and develop cationic conjugated nanostructured lipid carriers of natural bioactives like Myricetin and Asiatic acid forenhancement of the bioavailability in the brain and cognitive impairment in Alzheimer's disease. MY-NLCs and AA-NLCs were prepared and optimized using central composite design (CCD). *In-vitro* MTT assay and cellular accumulation were evaluated in SH-SY5Y neuroblastoma cells. Further, the pharmacodynamics studies were evaluated in the (Aβ1-42) induced Alzheimer's rat model and cognitive performance was assessed using Morris water maze (MWM) test followed by histological and neurotransmitters analyses in rats' brain.

Based on preliminary successful findings of preparing NLCs we have used sialic acid (SA) grafting and conjugated NLCs were prepared and evaluated for particle size, zeta potential, and entrapment efficiency. SA-grafting was confirmed X-ray photoelectron spectroscopy analysis. *In-vitro* cytotoxicity, cellular uptake, Aβ aggregation inhibition and mitochondrial membrane potential of prepared NLCs were observed in SH-SY5Y cells. The trans endothelial electrical resistance (TEER) was measured through HCMEC/D3 cells. Finally, the pharmacokinetic study was conducted in Sprague Dawley rats to evaluate bioavailability and neuropharmacokinetic parameters after the intraperitoneal administration of optimized NLCs (40mg/kg). Pharmacodynamic findings were also in agreement to show better neuroprotective potential of prepared SA conjugated NLCs. This work has developed a platform technology using sialic acid surface modification for enhanced bioavailability and pharmacological effects for two important neuroprotective bioactives myricetin and Asiatic acid. Prepared NLCs have shown better pharmacokinetic and pharmacodynamic behaviour than the free bioactives.

IL-54

Pd-Catalyzed Azide-Isocyanide Cross Coupling Reaction: Concept to application in Medicinal Chemistry and Bioimaging

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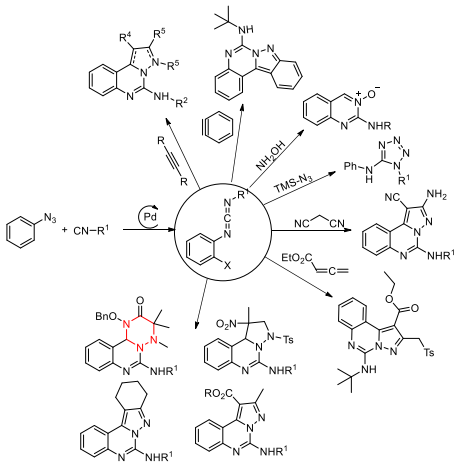
Abstract:

We recently studied transition metal-catalyzed azide-isocyanide cross-coupling reaction in detail.[1] The study revealed that the transfer of nitrene, generated in situ from azide, on isocyanide is a concerted process rather than a two-step process involving a metallaaziridine intermediate as proposed in the literature. The study helped us to fine-tune an elegant method for the synthesis of carbodiimide, a versatile intermediate, in quantitative yield. Encouraged by the result, we devised a four-component reaction promoted by bimetallic relay catalysis for the synthesis of pyrazolo[1,5-*c*]quinozolines.[2] The tricyclic relay cascade involves the formation of five new chemical bonds and concatenation of six discrete chemical steps. Interestingly, pyrazolo[1,5-*c*]quinozolines selectively inhibit EGFR, exhibit apoptosis through the ROS-induced mitochondrial-mediated pathway, and arrest the cell cycle at the G1 phase. The relay catalysis based on nitrene-transfer on isocyanide also provided rapid access to a variety of heterocycles that have application in medicinal chemistry and live-cell imaging.[3]



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IL-55

Organocatalytic approaches toward the synthesis of important heterocycles

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Nature has evolved with a rich diversity of organic molecules, and the creation of similar molecular architectures has been a longstanding fascination of chemists. For instance, Nature enables enzymes as versatile catalysts and provides a practical understanding, that superior performance is achieved by suitably positioning the substrate in close vicinity by collecting non-covalent interactions. In this context, the field of organocatalysis has become a focus of extensive research and brought the prospect of a complementary mode of catalysis with the potential for broader applications. Despite the tremendous achievements in this area, the scope of chemical functionalities and scale-up opportunities remained relatively narrow. We have been working in the design and development of organocatalysis with requisite chemical functionalities for chemical transformations involving oxidation, hydrogenation and CO_2 utilization reactions. In this talk, I would like to share some of our recent developments in the field of organocatalysis with an emphasis on scale-up opportunities. Our organocatalytic approach offers straightforward access to synthetically and biologically important heterocycles such as *N*-alkylated tetrahydroquinolines, spiro cyclic carbonates and benzoquinolizine structures.

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IL-56

Lipid Nanocarriers as Emerging Platform for Targeting in Cancer Therapy

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Abstract:

As cancer is continuously evolving and shows an heterogenous nature, novel therapeutics are required for treating the same. Majority of the cancer therapeutics being poorly soluble and lipophilic in nature ultimately have poor bioavailability and decreased efficacy. It has been reported that a number of methods can improve the solubility and bioavailability of lipophilic medicines. Such lipophilic drugs can be delivered efficiently using nanocarriers composed of vesicular drug delivery systems, emulsion-based systems, solid lipid nanoparticulate systems, etc.
Recent therapies for cancer range from gene therapies to tumor microenvironment targeting therapies. These lipidic nanocarriers can be easily engineered via surface modification strategies to target cancer cells. Though gene therapies have been developed and delivered using lipidic nanocarriers, they are more effective in specific mutations only and hence fall under personalized medication strategies which is not cost effective and scalable. However, lipidic nanosystems have also been surface modified as stimuli responsive systems that are triggered to function and release drug at specific tumor microenvironment (TME). Delivering drugs to TME is more feasible as it is more penetrable and accessible to tumor area. It has broader scope of application with a wide range of application irrespective of tumor heterogeneity. The targeting can be better enhanced by delivering drugs loco-regionally at the site of disease. Potential benefits include better targeting and decreased off-target effects. Such an approach was used in our lab to deliver targeted small molecule using lipidic carrier to oral cancer cells. Lipidic nanocarriers containing anti-cancer drug was incorporated in suitable semi-solid dosage form and applied directly at the site of oral cancer on rat tongue. It has not only shown effect, in-vitro on cancer cells, but also in in-vivo animal models. Thus, the presentation highlights the opportunities and challenges in targeting of lipidic nanocarriers along with its applications in locoregional therapy of oral cancer with suitable case study.

IL-57

Research and Development of Figs.: My Expertise of the last three Decades

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Abstract

Ficus, commonly known as figs, is a genus of around 900 species of woody trees, shrubs, vines and vines of the Moraceae family. It is estimated to be one of the oldest existing plants species, dating back to almost 60 million years. Native to the tropical region, figs are often considered to be source of edible fruits in forests. Distinctive pollination process of figs is carried out by fig wasps of Agaonidae family. The fruits from different species of *Ficus* are consumed for their nutritional value while some species also play important roles in major religions. Apart from its prevalent socio-economic context the species has been widely used for its diverse phytochemical composition. The genus has been reported to be rich source of secondary metabolites including phenolics, flavonoids, terpenoids, sugars, glycosides, and phytosterols among others. Figs are often associated with treatment and management of different human ailments, while some traditional systems of medicine like Ayurveda or the Chinese system of medicine have explicitly explored its biological potential. *Ficus*, often used in the management of certain metabolic, cardiovascular, oxidative stress, inflammation, and infectious diseases, have extensively explored for its cytotoxic and antiviral potential by the researchers through the world. Exploration of the genus has brought light onto the effective nature of the phytoconstituents in management of diabetes mellitus, hepatotoxicity, inflammatory diseases, different types of cancer, and other pathological conditions. Recent studies have followed the trend of isolating phytochemicals from the different species of *Ficus* in the quest for finding lead molecules with multiple mechanistic targets and preparing formulations from them. This plenary session will aim to provide an insight on the historical value, economic importance, ethnopharmacological findings, current scenario and future scope for the species along with my own association with the genus for almost last three decades.

Keywords: Figs, *Ficus*, ethnopharmacology, drug discovery, phytochemistry.

IL-58

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Abstract Awaited

IL-59

Role of intellectual property in fostering chemistry and biologics industry

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The dynamic interplay between intellectual property (IP) and the chemistry and biologics industry is a driving force behind innovation, growth, and sustainable development. In an era marked by rapid scientific advancements and global competitiveness, the role of IP has become paramount in shaping the landscape of this critical sector.

This presentation explores the multifaceted relationship between intellectual property and the chemistry and biologics industry. It delves into how IP frameworks, including patents, trademarks, and trade secrets, function as pillars of protection and incentivization, fostering a conducive environment for research, development, and commercialization of novel chemical and biologic entities.

Through insightful case studies, will examine how IP mechanisms have propelled advancements in drug discovery, formulation, and process optimization. From small molecule therapeutics to biopharmaceuticals, will navigate the nuanced strategies that industry players employ to safeguard their innovations, while also facilitating collaboration and technology transfer.

Furthermore, this presentation will unravel the complex ethical and regulatory considerations that arise in the wake of IP's influence on chemistry and biologics. Balancing exclusivity with access to essential medicines and scientific information poses intricate challenges, demanding a thoughtful exploration of IP's role in addressing global health needs.

IL-60

Structure-guided optimization of new AKR1C3 inhibitors designed by 3-hydroxyazole bioisosteric approach to target prostate cancer

Chiara Vigato,[a] Agnese Chiara Pippione,[a] Iole Mannella,[a] Osman Asghar Mirza,[c] Karla Frydenvang,[c] Francesca Spyrakis,[a] Simonetta Oliaro-Bosso,[a] Marco Lucio Lolli,[a] and Donatella Boschi[a]

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Aldo-Keto Reductase 1C3 (AKR1C3) has a key role in androgen biosynthesis, thus an increasing number of studies have focused on AKR1C3 inhibitors for their potential application in treating *Castration-Resistant Prostate Cancer* and preventing drug resistance [1]. Since *flufenamic acid* (FLU, Figure 1) is known to inhibit AKR1C3 in weak and non-selective mode, we employed in recent years a conformational restriction strategy on FLU anthranilic core to afford a bioisosteric 3-hydroxybenzoisoxazole-scaffold based series of compounds [2].
Thanks to the binding pose of the *lead* compound **1** inside AKR1C3 enzyme,determined through X-ray crystallography [2], we designed the next optimized round of *hydroxybenzazole* derivatives, where the B-ring is modulated by further substituents with the purpose of increasing potency and retaining selectivity through a deeper exploration of AKR1C3 binding pocket (Figure 1). *In silico* design, synthesis, *in vitro* biological evaluation (enzymatic and cellular assays) and X-ray structures of the new AKR1C3 inhibitors are here described and discussed.

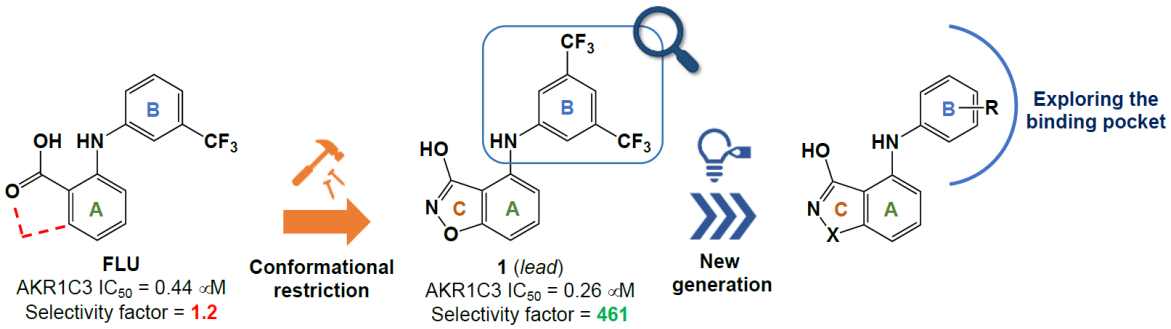

Figure 1: The employed bioisosteric strategy and the suggested modulations of **1**.

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IL-61

"SERENDIPITY" in Organic Synthesis: Development of New Synthetic Reactions

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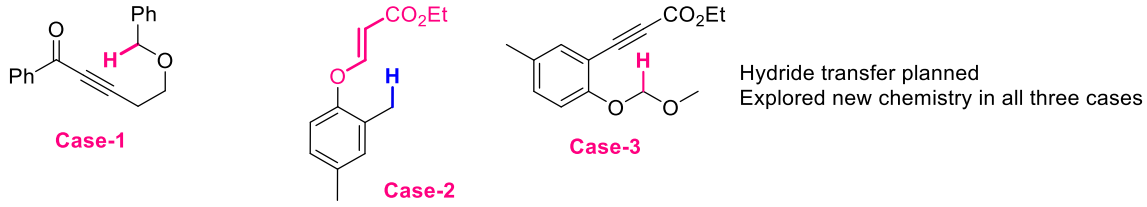
Abstract:

"Luck Favors the prepared mind" as the saying goes, many reactions in a synthetic laboratory are serendipitously found. We plan sometimes based on several parameters, particular reaction or an extension of known reaction. However, the reaction may take a different course and give entirely different products. The analysis of such reaction and the mechanistic steps involved help in understanding the new course of reaction leading to unusual chemistry and new reaction profiles, where serendipity favours the prepared mind. We in our laboratory, have extensively been benefitted with new reactions being discovered serendipitously while attempting hydride transfer chemistry.[1] Some of the new reactions developed paved excellent paths toward total synthesis of natural products. Many such reactions developed in our laboratory will be discussed in this lecture.[2-5]



Keywords: Hydride transfer, Lewis-acid catalysis, Rearrangements, Total synthesis, New Reactions, Serendipity

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IL-62

Green and Renewable Hydrogen Fuel Production based on Porous Carbon Materials

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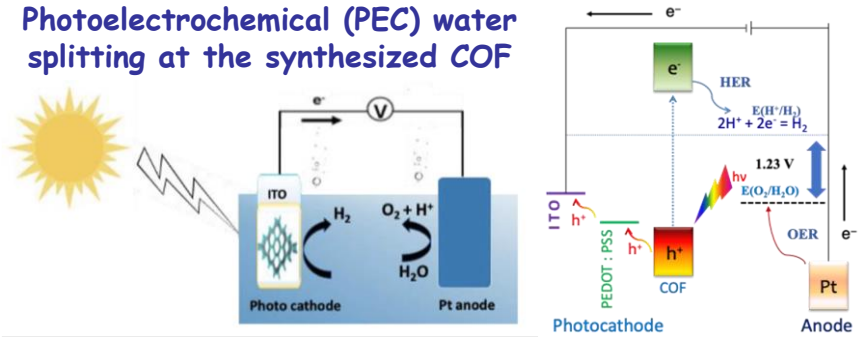
Rapid global warming has forced people to replace conventional energy sources with green renewable solar and wind energies. Hydrogen, as a renewable and clean energy resource, is a promising future fuel. Hydrogen production through metal-free electro-catalyst water splitting is crucial for obtaining sustainable and clean fuel. Due to its high efficacy along with zero pollution and zero greenhouse gas emission, intensive research effort is ongoing for the development of the HER technology.[1-4]
Herein, we devoted to developing, greener energy through integration of Chemistry and Materials, Optimal utilization of carbon resources Chemical energy storage and conversion, commercially viable low-cost carbon materials preparation for energy production and storage applications.



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.

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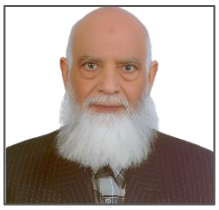
IL-63

Whole Genome Sequencing of Pathogenic Bacterial Genomes: Applications in Clinical Microbiology



Abu Salim Mustafa

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Abstract

The success in determining the nucleotide sequence of a pathogenic bacterial genome was first achieved in 1995 by sequencing the complete genome of *Haemophilus influenzae* strain Rd (genome size = 1.83 Mb) by Fleischmann et. al. The methodology used in these experiments was the first-generation DNA sequencing technology using chain-terminating dideoxy nucleotide analogs, which was established by Sanger et al. in 1977. However, the first-generation DNA sequencing technology is laborious, costly and time consuming. After 2000, next generation sequencing (NGS) technologies have been developed for whole genome sequencing (WGS) to provide efficient and cost-effective results. WGS provides the details of an organism's genetic makeup and includes all the coding and non-coding sequences and regulatory regions present in the genome. In the recent years, WGS coupled with the bioinformatics analysis of the sequenced genomes have been projected to revolutionize clinical microbiology practices. The applications of WGS technologies can be used in identification of bacterial species from cultured specimens and directly from clinical specimens. Furthermore, strains and genotypes of pathogenic bacteria can be determined. It can also help in detection of antimicrobial resistance mechanisms, identification of virulence factors, and epidemiologic tracking of organisms in a hospital setting as well as in communities. This talk will focus on the above-mentioned applications of WGS in clinical microbiology settings.

IL-64

Probiotics and Prebiotics: An Innovative Approach for Improvement of Gut Microbiome

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ABSTRACT

The human body lives in close harmony with a complex ecosystem; diverse microbiota inhabit different areas of the human body, collectively known as microbiota, especially gut microbiota, which lives with us in a mutually beneficial life-long relationship. The human body's gut microbiota, a vital part of the complex ecosystem, plays a vital role in maintaining and improving health through various metabolic activities. These benefits are enhanced by consuming probiotics and prebiotics or combining both (synbiotics). The interest in these particular research areas increased after COVID-19 due to interesting scientific evidence of benefits on human gut health, eventually influencing overall health. Recent studies have pointed out the association between the gut microbiota and the nervous system, including the brain, which can support treating mental health issues such as anxiety, depression, and neurological conditions. These findings led to a new concept: '*Psychobiotics*'.
The ongoing research in our lab on probiotics focuses on the characterization of probiotic bacteria, their synergistic synbiotic properties, prebiotic utilization ability, and their significance on important probiotic properties such as antimicrobial activity and galactosidase activity. Optimization of nutritional components and prebiotics had been carried out for antimicrobial activity against pathogens such as *E. coli*, and *S. typhi.* Further, whole genome sequencing (WGS) and analysis have been conducted on *Lactobacillus* spp. with synergistic symbiotic properties.

Keywords: Gut microbiome, Probiotics, Prebiotics, Synbiotics, Psychobiotics

IL-65

Metal-Catalysed Chalcogenation of Quinoxolinones and Benzoxazines *via* C-H activation.

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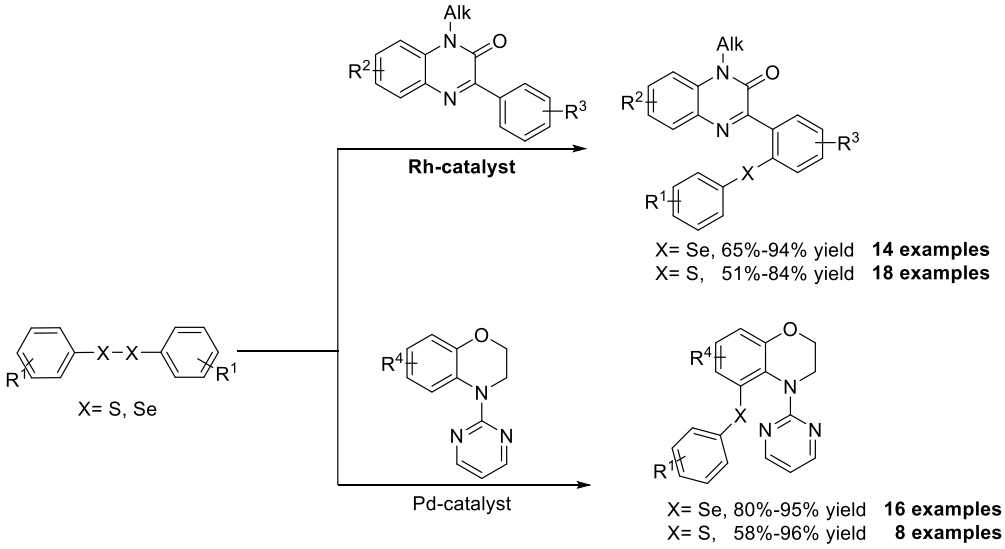
In continuous pursuit to develop newer methodology for synthesis of bioactive molecules, we have developed green and sustainable methodologies for the regioselective direct C-H chalcogenation of quinoxolinones and benzoxazines using Rhodium and Palladium as catalyst. Metal-directing property of the nitrogen atom has been exploited for the synthesis of bioactive compounds. Several control experiments and Kinetic studies have also been performed in order to establish the mechanism. A wide variety of diphenyl disulphiles, diphenyl diselenides were exposed to these newly developed methodologies and all of them have delivered the chalcogenated products in excellent yields. Detail of this chemistry would be discussed during the talk.



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IL-66

DEVELOPMENT OF SURFACE FUNCTIONTIONALISED BIOTHERAPEUTICS FOR THE TREATMENT OF CANCER.

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Introduction and Objective: Increasing multi drug resistance and immune escape surveillance with resurgence have risen the need for development of strategy that can maximize the treatment and minimize the off-target delivery, natural building blocks of proteins can be utilized by exploring their structural properties for ligand conjugation. As protein like lactoferrin offers numerous assets with anti-inflammatory responses, iron scavenging as well as host defense mechanism can be an attractive tool. The study rationalized to develop and characterize lyophilized Lactoferrin Nanoparticles containing targeting drug and conjugated with known biomarkers like folate, Biotin-streptavidin and Her2 antibody, in order to design the way to target, prolong action with less chances of frequent dosing as well as provide immune-targeted therapy.

Methods: Fabrication of protein nanoparticles by Desolvation technique [(1)], that is based on nanoprecipitation principle and further functionalized with ligands by EDC-NHS Carbodiimide chemistry. The Optimization by AQbD based risk assessment studies using Design Expert was employed.

Results: The Protein Nanoparticles were found to be uniformly distributed. The drug loading and entrapment was found to be 14% and 76±2.14% with 6 days of prolong release at physiological pH, that delineates the successful attempt to reduce frequent dose. Confirmation of folate conjugation NMR shows successful conjugation with superimposed aromatic protons at down field as well as for biotin-streptavidin by DLS with uniform size distribution.

Conclusions: The study is currently on level 4 in technology readiness and aims to reach at TLR 7 for ecstatic demonstration of nano-cargo based formulation.

Acknowledgments: The author would like to acknowledge the financial assistance from GsBTM, Gandhinagar, GsBTM/JM (R&D 610).

IL-67

Potential inhibitors of mycobacterial "SOS" response- as an adjuvant therapy

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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 in mycobacteria.

IL-68

Synthesis of various functionalized Aza heterocycles from aryl methyl ketones of biological importance

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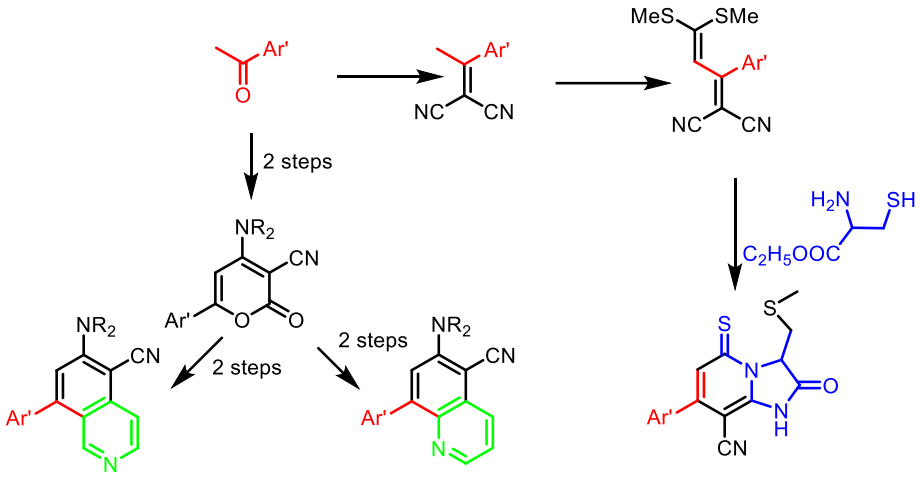
ABSTRACT



Aryl methyl ketones are very well-known primary precursor for the synthesis of a large class of molecules. Our group is involved in using ketone for the synthesis of various ketene dithioacetals and pyran and to explore further chemistry.[1] Imidazopyridines are interesting heterocyclic compounds containing two fused heterocyclic motifs, i.e., pyridine and imidazole, in one molecule. we have developed a cascade one-pot methodology to synthesize Imidazopyridines using 1,6-Michael acceptor ketene dithioacetals under mild conditions. we also reported iodine and DMSO-promoted synthesis of multifunctional quinolines and isoquinolines using 6-aryl-4-*sec*. amino-2-oxo-2*H*-pyran-3-carbonitriles and 1-Boc-4-piperidone/1-Boc-3-piperidone as precursors. Synthesis of N-Boc-1,2,3,4-tetrahydroisoquinoline was carried out by ring transformation of suitably functionalized 2-pyranones with 1-Boc-4-piperidone in DMSO under basic conditions. The N-Boc-1,2,3,4-tetrahydroisoquinoline crude was obtained and treated with iodine and DMSO to afford the desired isoquinoline. Using iodine and DMSO, consecutive two-step Boc deprotection and aromatization of isoquinolines occur. The reaction proceeded efficiently, and the desired isoquinolines were achieved in good yields. The generality of the protocol was tested by using various functionalized 2-pyranones with 1-Boc-4-piperidone. Earlier we have achieved a one-pot approach for the synthesis of benzo[h]quimolines[2] and now new azaheterocycles were established ketene dithioacetals.[3]

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IL-69

Strategies for Producing Renewable Chemicals from Biomass: Advancing the Circular Bioeconomy

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Abstract

The evolving societal changes necessitate the adoption of novel sustainable technologies and methodologies to address the depletion of fossil resources and reduce CO_2 emissions. Therefore, the establishment of a circular economy in the chemical industry requires not only the safer design of new processes using renewable feedstocks but also the utilization of existing processes with drop-in chemicals. Catalysts play a crucial role in promoting sustainability in the chemical industry, serving as the backbone of numerous industrial processes that convert raw materials into valuable products. Even a small quantity of catalyst can significantly enhance reaction rates and achieve high product selectivity, while its cost remains negligible compared to the overall processing expenses. Consequently, the development of nanostructured catalysts is vital for the chemical industry.

In his presentation, the speaker will discuss strategies for designing new catalysts that exhibit enhanced activity, selectivity, and durability in the production of various furanic compounds (such as FDCA and furoic acid, etc.) derived from biomass sugars (*ACS Catal*., 2017, 7, 2430; *ACS Catal*., 2018, 8, 283; *ACS Sustain. Chem. Eng*., 2018, 6, 3434) as a new class of important chemicals. Furthermore, the speaker will explore the development of renewable pathways for the production of amines (*ACS Catal*., 2022, 12, 10400; *ACS Sustain. Chem. Eng*., 2022, 10, (44) 14560) and aromatics (*Green Chem.*, 2023,25, 1588; *Catal. Commun*., 2022, 163, 106402) in the context of drop-in production.

IL-70

Chemistry of Overcoming the NMR - Stress Connection and Managing HealthMade Easy

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Nuclear Magnetic Resonance Spectroscopy (NMR) is a physical tool to study the magnetic properties of nucleus under the influence of a strong magnetic field andradio-frequency. Initially the basic details of NMR spectroscopy would be explained. Starting from the importance of free spin in the nucleus up to the theory of multi- dimensional NMR and MRI.

Studying about NMR and interpreting the spectra could be stressful. Stress is responsible for causing several diseases from common cold to cancer and COVID infections. There may be multiple reasons to be stressed and it is necessary for a person to evaluate and find out the reason. It is therefore important to first understandwhat is stress and then find out ways of how it can be controlled. Stress does this by weakening our immune system and making our body prone to them. Stress starts from worry which is caused if we are unable to solve the problems. This leads to anxiety and then to stress. Stress is just an accumulation of worry. If we could stop it at the worry level stress can be controlled. There are several ways to control worry. In the Practical Approach emphasis is on how easily a person can manage his/her own life by following some basic principles which we usually tend to forget. These areAcceptance and Gratitude. Usually we do not remember these when it comes to our own problems. Here methods and examples will be given as to how these principles can be easily applied for one's own betterment. People apply acceptance unknowinglyplenty of times but the important thing is to apply it knowingly and this will help in having a life with lesser stress. Meditation also plays an important role in controlling our thoughts. Conscious Breathing, the simplest form of meditation also plays an important role in reducing stress. Overall these simple methods can be used to manage stress in our life and make it more peaceful.

IL-71

Development of Recoverable Chiral Organocatalysts for Asymmetric Friedel-Crafts Reactions

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Abstract:

The enantioenriched compounds have various applications including pharmaceuticals, agricultural chemicals, flavours, fragrances and material.[1,2] Asymmetric catalysis is defined as an enantioselective transformation controlled by a chiral catalyst. We are working on the development of recoverable organocatalysts for asymmetric organic transformations. Imidazolium ionic liquids containing MacMillan second generation catalysts (**2-4**) were synthesized and evaluated as organocatalyst (10 mol%) for enantioselective Friedel-Crafts reaction between *N*-benzylindole and crotonaldehyde using trifluoroacetic acid as co-catalyst (10 mol%) at -60°C, the corresponding product was obtained in 87% yield and 89% *ee*.[3] Imidazolium-based chiral ionic liquid **5** containing *α,α*-diaryl-(*S*)-prolinol trimethylsilyl ether as an efficient and reusable organocatalyst was used for the first time in the enantioselective Friedel-Crafts reaction between indoles and *α, β*-unsaturated aldehydes.[4]

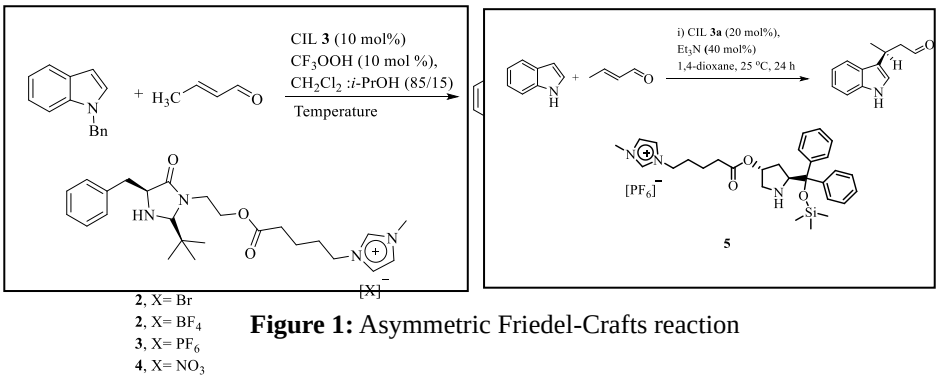

Figure 1: Asymmetric Friedel-Crafts reaction

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IL-72

Computational and Experimental Tools to Recognize Multi-target Binding Profiles of Therapeutic Agents

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Abstract

During recent times, analysis of the drug-biomolecule interactions has occupied an important domain in modern drug discovery process. Drugs interact with biological molecules via a variety of mechanisms, which is the basis for particular therapeutic effect of a drug candidate. Lately, the focus is shifting single target drug to polypharmacology or drug repurposing as an effective means to find new therapeutic applications of known drug candidates due to their multi-target affinities. Among analytical strategies available to understand such interactions between therapeutic agent and biological receptor, spectroscopic techniques such as UV, Fluorescence and CD are advantageous to estimate the strength of important interactions. Some of these methods have been utilized to provide an estimate of the overall binding along with stoichiometric assessment of drug-receptor complex. Besides, computational approaches such as Docking, MD and QM-MM calculations have also been applied to study effectively the structural aspects of these complexes. Computational tools have provided structural information in terms of position and orientation of in the receptor pockets along with their binding free energy values. Results from our recent investigations of the multi-target binding profile of few anticancer agents with DNA and HSA in a dynamic physiological environment using spectroscopic, molecular dynamics simulations, and quantum mechanical calculations to evaluate the structural features, mode, ligand, and receptor flexibility and energetics of complexation will be discussed.

ORAL

O-1

Elucidating synergistic effect of silver nanoparticles of *Butea monosperma* extract and melatonin as anticancer agents against breast cancer cell line

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The utilization of green synthesis has garnered considerable interest as an environmentally conscious, economically viable, energy-efficient, and safe approach for fabricating silver nanoparticles (AgNPs) aimed at cancer therapy. In this study, silver nanoparticles (AgNPs) were synthesized using aqueous and methanolic extracts of *Butea monosperma* leaf and gum extracts. The prepared AgNPs (BM-AgNPs) were examined by ultraviolet-visible spectroscopy, DLS, Zeta sizer, Fourier transform infrared (FTIR) spectroscopy and scanning electron microscopy (SEM). The anticancer potential of synthesized silver nanoparticles with and without melatonin was investigated against MDA-MB-231 and MCF-7 (human breast cancer cells) and HEK 293 (Human embryonic kidney). The primary responses i.e. cytotoxic response was assessed by 3-(4, 5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide (MTT), viability assay and clonogenic assay were studied. The result obtained suggests significant ameliorative effect of the prepared nano-formulations. However, synergistic action of melatonin and plant extracts were found to be more effective. We have also tried to study the mechanism of the interaction of melatonin and plant extracts using spectroscopy.

O-2

Isolation, production and comparison of different pigments from Ray fungus

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ABSTRACT

Actinomycetes are heterogeneous group of bacteria that are gram positive, filamentous with mycelial growth pattern. The present study was conducted with an objective to isolate and physiological characterized using different biochemical tests and different pigment producing Actinomycetes were screened and compared based on different pigments. The samples were collected from different places of Kumbharwada wetland, Bhavnagar. Nowadays, natural pigments are in great demand, have been replacing its place instead of artificial pigments. In correlation, biological pigments have been variety of applications in various fields of day-to-day concepts. These pigments are produced by living organisms. The more potent one is Actinomycetes. The producing pigments from Ray fungus can be assessed for different applications in textile as well as in food industries.

Keywords: Ray fungus, Natural pigments, Textile industry, Food industry

O-3

Unravelling the Elastic Properties of DNA: Insights from All-Atomistic Molecular Dynamics Study

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ABSTRACT:

Biological processes such as transcription, replication, recombination, DNA repair, and DNA packaging engage with bent DNA structures at the nanometer scale [1]. Investigating DNA elasticity and conformational changes at this scale is crucial. Molecular dynamics simulations, meticulously analyzing atomic-level fluctuations, offer a precise approach to extracting structural information and biomolecular properties of DNA [1,2]. Atomistic molecular dynamics simulations play a pivotal role in calculating elastic properties across diverse DNA scenarios, considering varying salt concentrations, and hydrated ionic liquid (IL) environments [3,4]. Notably, macroscopic elastic theory proves inadequate for calculating the elastic properties of short DNAs in monovalent salt, contrasting with the behavior observed in dsDNA within IL concentrations [3]. Moreover, our study highlights that ionic liquids confer rigidity to DNA. This work contributes to a profound understanding of DNA nanomechanics, offering broadly applicable methodologies for studying other DNA-protein complexes [1,2,3,4]. The findings shed light on the impact of ionic liquids, revealing their role in modulating DNA flexibility [3].

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O-4

Understanding indolizine synthesis from [3+2] cycloaddition reactions of substituted pyridinium methylides with molecular electron density theory perspective

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Indolizines display a wide spectrum of biological and pharmaceutical activities. The [3+2] cycloaddition (32CA) reactions of methylides serve as one of the powerful synthetic strategies for the stereo- and regioselective construction of indolizines. The molecular electron density theory (MEDT) proposed by Domingo in 2016, [1] identifies the decisive role of electron density changes on the molecular reactivity [2-6]. The main purpose of this study is to understand how substitution on cyclic azomethine ylides changes the reactivity relative to the simplest azomethine ylide (Figure 1). Herein, electron localization function, reactivity indices, and AIM parameters (Figure 2) have been applied [7].

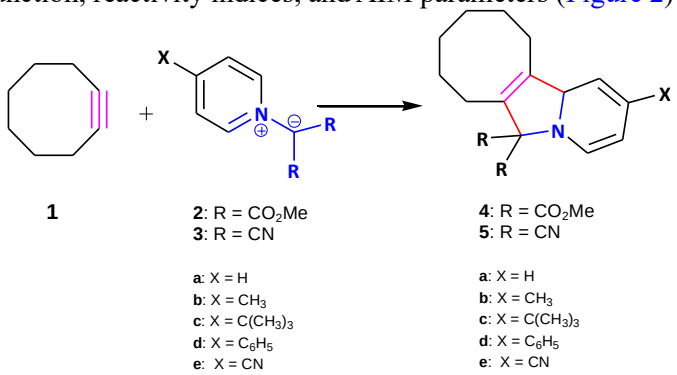

Figure 1. 32CA reactions of substituted pyridinium methylides for indolizine synthesis

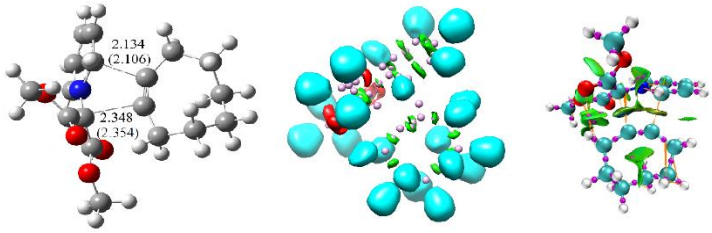

Figure 2. MPWB1K/6-311G(d,p) optimized geometry, ELF domain, and NCI isosurface of transition state

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O-5

PHARMACOLOGICAL EVALUATION OF NEUROPROTECTIVE EFFECT OF ETHANOLIC EXTRACT OF *NARDOSTACHYS JATAMANSI* IN EXPERIMENTAL ANIMAL MODEL OF TRAUMATIC BRAIN INJURY

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Abstract:

Traumatic brain injury (TBI) is a multiphased neurological disorder caused by mechanical impact on the head that impairs the brain function, resulting in cognitive, behavioural, and physical defects [1]. TBI causes blood brain barrier disruption, neuronal inflammation, axonal degeneration, and reactive oxygen species [2, 3]. *Nardostachys Jatamansi* is having anti-oxidative and anti-inflammatory activities. The present research examines the effect of ethanolic extract of *Nardostachys Jatamansi* impact on Marmarou's weight drop-induced TBI in rats. In study, female Wistar rats were grouped in five groups with six animals in each. Groups assigned were normal control group, TBI group, and three treatment groups with different doses of *Nardostachys Jatamansi* (100 mg/kg, 200 mg/kg and 400 mg/kg). *Nardostachys Jatamansi* was pre-treated orally once a day for seven days. The behaviour studies were done using actophotometer, rearing test, beam walk test, rotarod, novel arm discrimination test (NADT) and wire hang test, 24 hr after TBI induction. Lastly animals are sacrificed and brain were isolated. Half of the brain's hemisphere was utilized for histopathological studies and estimation of biochemical parameters that include levels of MDA, nitrite and reduced glutathione. The other half was used to measure % water content in brain (brain oedema). Results of the study showed the neuroprotective effect of ethanolic extract of *Nardostachys Jatamansi* in TBI exposed animals. *Nardostachys Jatamansi* ameliorated the deficits in locomotor and neuro motor co-ordination induced by trauma. *Nardostachys Jatamansi* was also found to effective in improving the TBI induced memory impairment. *Nardostachys Jatamansi* mitigated oxidative stress (lowered level of lipid peroxidation and nitric oxide), while improved antioxidative mechanisms (reduced glutathione). The histopathology shows decrease in vasogenic oedema and lesion in treated group in contrast of disease manifested group. The results signify the *Nardostachys Jatamansi* is a potential therapeutic agent for neuroprotection in condition like TBI. *Nardostachys Jatamansi* by acting on secondary cascade of TBI pathogenesis reduces reactive oxidants levels, reduces neuroinflammation, neurodegeneration and oedema, can be a potential alternative therapy for the management of TBI.

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O-6

Unlocking Enhanced Reactivity in julolidine construction: Electrostatic Stabilization of Phenol's Conjugate Bases Through Anion Selection

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Abstract:

In the domain of catalysis research, a pivotal quest revolves around uncovering the factors that confer superior catalytic capabilities upon specific molecular structures when compared to their counterparts. Consider, for instance, the extraordinary efficiency exhibited by enzymes in the natural world as versatile catalysts. Nature appears to have provided us with a practical blueprint for this achievement, elucidating that superior catalytic performance frequently arises from the meticulous coordination of non-covalent interactions, facilitating the close proximity of substrates. Nonetheless, translating this knowledge to non-biological catalysts presents a formidable challenge. In this study, we present our synthesis of the julolidine ring using our previously designed, straightforward, and scalable electrostatically tuned phenol (ETP) as an organocatalyst. The catalyst's ability to engage in hydrogen bonding facilitates the reaction, resulting in high conversions and excellent selectivity. Furthermore, we conducted a kinetic analysis of the reaction and quantified the catalyst's hydrogen-bonding capacity using ^{31}P NMR, establishing a clear correlation between the catalyst's acidity due to electrostatic stabilisation of conjugate base and the rate of the reaction.

O-7

Development And Validation of Stability Indicating Mass Compatible HPLC Method for Estimation of Deferasirox

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Deferasirox (DFR) is a new drug treatment for Beta-thalassemia. A simple, specific, linear, accurate, robust, sensitive and precise high-performance liquid chromatography method was developed for Deferasirox. The column used was Phenomenex C18 Column (250 x 4.6mm, 5µm), mobile phase was a ACN:Buffer (60:40 v/v) Buffer consists of 10 mM ammonium acetate, pH of mobile phase was adjusted to 3.5 with 0.1 % formic acid. The flow rate was 1.0 mL/min. Detector wavelength was monitored at 250 nm, and the injection volume was 20 µL and run time was 10 min. The developed method was validated in terms of linearity, range, accuracy, precision, repeatability and specificity, robustness, LOD and LOQ as per ICHQ2(R1). The method as found to be linear in the concentration ranges of (1-25 µg/mL) having LOD 30.01 ng/mL and LOQ 90.96 ng/mL with regression coefficient (R2) of 0.9991. The recovery ratio was in the range of 98-102 %. The precision was evaluated by studying intermediate precision and repeatability. The %RSD values for repeatability were 1.8 % and intermediate precision were 0.8 % respectively. Deferasirox (DFR) was subjected to the forced degradation studies showed degradation in acidic condition (15.92 %), alkaline condition (4.8 %), oxidative condition (68.7 %), photolytic condition (1.03 %) while stable in thermal condition. The developed stability indicating mass compatible HPLC method can be used to monitor the quality control of the drug and it can be applied to stability study.

O-8

Watersaving in thermal power plant by use of membrane filter in Cooling tower treatment

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Abstract

A study was carried to investigate by placing a side stream filter in a cooling tower to observe the water conservation in the system. For any coal based power plant cycles of concentration plays important role for water conservation. The cycles of concentration in cooling tower was increased by installation of membrane system .The drain of the side stream filter was disposed to effluent treatment plant(ETP), while the filtered water will be recycled to the cooling tower inlet. The water parameter was measured by using various flow rates, pressure, and other factors. Significant water savings were demonstrated in the pilot. Maximum make-up water and outflow were both reduced by 14 and 48 percent, respectively. To save the most water, permeate recovery must be as high as possible. Water savings were minimal due to silica scaling on the membranes. Selected membranes are capable of lower total dissolved system (TDS) rejection than the 88% of total required membranes in the primary study, which might help to save water. The increased energy consumed by membrane treatment was compensated for by lower water outlays. To prevent scaling antiscalent chemical with chemical dosing system was installed along with membrane system.

O-9

Design and Synthesis of Pyropheophorbide Derived Photosensitizers and Their Pharmacokinetic, Tumor Uptake and Anti-Cancer Activity Studies

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Cancer ranks as one of the leading causes of death globally that poses a major health problem, not only due to cancer-related deaths but also because of treatment toxicities[1]. Therefore, to facilitate recovery and prevent deaths, early diagnosis and image-guided therapies are of utmost importance. Among heterocyclic systems, pyrrole-based compounds[2] including porphyrins, chlorins, bacteriochlorins, expanded porphyrins, phthalocyanines, porphycenes, corroles have gained considerable interest due to their ability to localize in a variety of tumors, and they have shown great potential in fluorescence-imaging and photodynamic therapy (PDT)[3]. Some of the tetrapyrrolic systems, after appropriate modifications, have also been used for cancer imaging and PDT[4]. Among the chlorophyll-a-based analogs, the pyropheophorbides are of particular interest due to their localization and retention in tumors for a long period of time. Very recently we reported the tryptamine pheophorbide conjugates endowed with IC_{50} of 695 nM against lung cancer cell lines[5]. These compound have unique characteristics in developing multifunctional agents (PET/fluorescence) with an choice for cancer therapy by introducing an iodobenzyl group into the macrocycle[6]. In continuation of our efforts herein we synthesized fluoro-benzyl ethers of pyropheophorbide having fluorine at ortho, meta and para-positions (methy ester and carboxylic acid) by the reaction of benzyl alcohol with *in situ* Markownikoff's intermediate of pyropheophorbide generated by treatment of pyropheophorbide with HBr in acetic acid[7]. The prepared fluoro-benzyl ethers of pyropheophorbides were well characterized using NMR and Mass spectrometry and purity was confirmed by HPLC. The photoxicity study of prepared photosensitisers has been carried out and compared with iodinated photosensitizer. Replacing fluorine did not cause significant difference in photophysical properties as well as singlet oxygen production. However, nature of delivery vehicle and tumor type shows significant difference not only on pharmacokinetic profile but also in uptake. Fluorinated photosensitizers showed a high tumor uptake at 2 h post injection. All isomers were screened against mice bearing U87 (brain) or bladder (UMUC3) tumors, among them m-fluoro substituted photosensitizer showed excellent PDT efficacy. The long-term tumor response (cure) results are interesting and useful in developing tumor specific agents for PET imaging and fluorescence-guided photodynamic therapy. Detailed synthesis and comparative pharmacokinetic study of the prepared arylethers of pyropheophorbide will be presented during the conference.

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O-10

Ester synthesis via cascade alkylation and activation of thioamides

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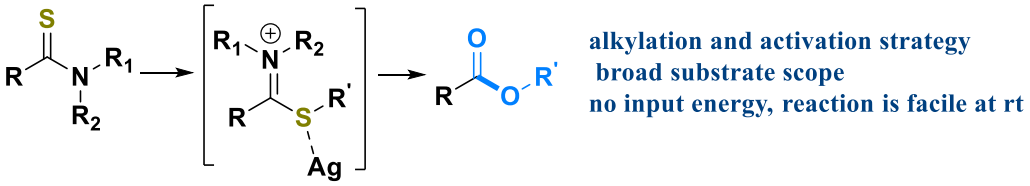

ABSTRACT:

The synthesis of esters from thioamide precursor is successfully accomplished in one pot under mild reaction conditions. The cascade alkylation and activation of stable thioamides results in the cleavage of stable C-N and C-S bonds to valuable ester. Readily available substrates, reactants, and activating agents enable facile transformation at room temperature with a broad substrate scope. Besides esters are crucial components of natural flowers and fruits due to their innate perfume, and they are used in the fragrance industry [1]. Ester is a crucial component of many different products, including food, drinks, medicines, and personal care items like soap, shampoo, and cosmetics [2]. As intermediates, solvents, and protective groups in synthesis, esters are fascinating substances for organic chemists. By creating crucial for industry scent esters, the presented technique was put to the test.

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O-11

Synthesis of Pyrazolo[5,1-*b*]quinazoline-3-carboxylates via Three Component DES as a Green Media and their Applicability as Chemosensor

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In recent time, the use of green solvents has got great attention in organic synthesis. Tremendous efforts are made worldwide by researchers to replace toxic and volatile solvents by sustainable solvents form renewable sources. The Deep Eutectic Solvents (DESs) are green and sustainable replacements for volatile organic compounds (VOCs). DESs are one of widely used sustainable solvents as possess various advantages like preparation from easily available chemicals, low vapour pressure, non-toxic nature, can solubilize wide range of reactants and are reusable.[1-3] The pyrazolo[5,1-*b*]quinazoline scaffold is of great biological significance as they exhibits wide range of biological activities.[4-5] We are recently involved in exploring application meglumine based catalytical systems for synthesis of biologically important organic molecules.[6]

Here in efforts were made for preparation of three component-DES (3c-DES) based on meglumine. The 3c-DES was synthesized using meglumine, PTSA, and acetic acid. The formation of 3c-DES was confirmed by ^{1}H NMR and is thermal stability was studied using TGA and DTA analysis. We employed the developed 3c-DES in the synthesis of novel pyrazolo[5,1-*b*]quinazoline-3-carboxylate derivatives via three-component one pot reaction between 3-amino-1*H*-pyrazole-4-carboxylate, aldehydes and 1,3-dicarbonyls. Our 3c-DES has dual role as solvent and catalyst. Key features of the present catalyst free-protocol are good functional group tolerance, short reaction time, good to excellent yields, reusability of reaction media, scalability, and easy isolation of products. Further, we checked chemosensor properties of newly synthesized pyrazolo[5,1-*b*]quinazoline-3-carboxylate derivatives against various metal ions. One of the synthesized pyrazolo[5,1-*b*]quinazoline-3-carboxylate displayed great potential as chemosenser for Cu^{2+} ions with the lower limit of detection (LOD) of 52.26 x 10^{-5} M, which is also supported by ^{1}H NMR titrations. DFT study was also carried out to get more insights into the electrostatic interactions between the metal and ligand.

Keywords: Pyrazolo[5,1-b]quinazoline-3-carboxylates, Three Component DES (3c-DES), Cu^{2+} chemosensor, DFT study

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O-12

Revisiting the old material: The impact of boehmite-derived catalytic material on the formation of dihydropyran compounds and its application to access fragrant derivatives

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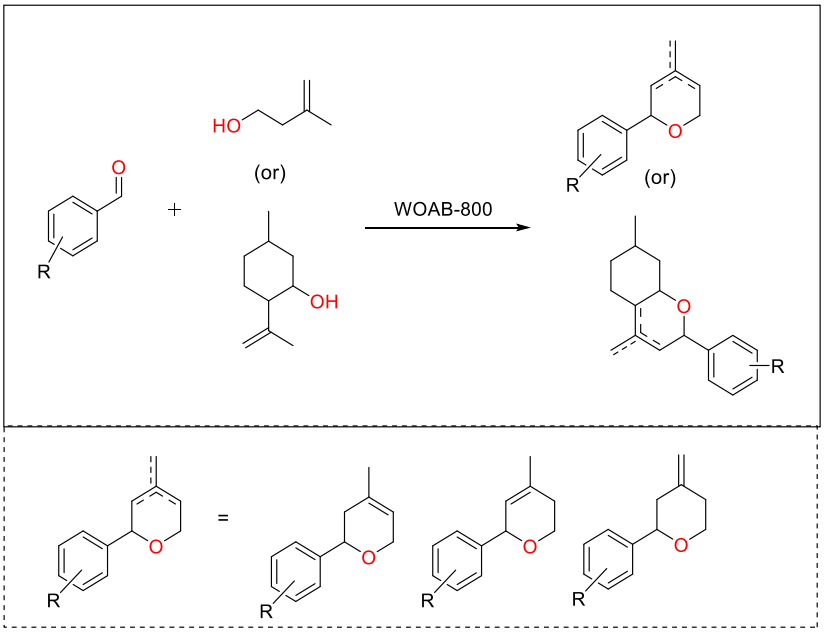
Bulk materials are the oldest in heterogeneous catalysis, but with the resurgence of recent interest, it has emerged as one of the best catalytic tools to unlock their full potential. Boehmite-derived alumina materials are widely studied for catalytic organic transformations. Despite the progress, understanding the mechanistic insights of its catalytic behaviour has remained obscure. Here, we demonstrate the catalytic performance of a boehmite-derived alumina material to a highly selective catalytic process for the preparation of dihydropyran compounds. The catalytic material displayed excellent activity in terms of conversion (up to 99%) and selectivity (up to 99%). The material was characterized using different techniques and observed that the □-alumina phase with inherent mild acidic character are key feature for the catalytic activity. Based on NMR and *in situ* FT-IR spectroscopic investigations a probable mechanism is proposed. This study expands the application of robust material for the preparation of industrially important fragrance compounds. The scope of the catalytic study encompasses a range of substrates and scale-up activities.



Scheme 1: Synthesis of dihydropyran compounds [R is selected from -H, -CH_2CH_3, -OCH_3, -NO_2, -CN, -CF_3, -F, Cl, Br.]

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O-13

A facile and efficient synthesis of *N*-aryl indolylsulfoximines as potent and selective anticancer agents

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Indole core has been continuously attracting the attention of researchers owing to its outstanding pharmacological properties [1]. Indole derived natural and synthetic compounds are reported to display a range of biological activities including antiviral, anti-inflammatory, anticancer, anti-HIV, antioxidant, antitubercular, antidiabetic and antimalarial [2]. Similar to indole containing compounds, sulfoximine derivatives have recently been emerged as interesting compounds for medicinal and synthetic chemists [3, 4]. The combination of these two important chemical moieties, indoles and sulfoximines, offers an unique opportunity to develop novel compounds with potentially enhanced biological activities and therapeutic applications. As part of our efforts to develop novel anticancer agents, in the present work we have successfully synthesized and conducted cytotoxicity studies on a series of indolylsulfoximines. A facile and efficient approach utilizing copper-mediated cross-coupling reaction of *N*-boc-3-indolylsulfoximines with aryl iodides was developed to synthesize a diverse range of *N*-arylated indolylsulfoximines in excellent yields (up to 91%). Indolylsulfoximines were readily prepared by the treatment of *N*-boc-3-methylthioindoles with a combination of IBD and ammonium carbamate. The reaction is highly chemoselective and tolerant of a wide range of functional groups. The prepared indolylsulfoximines are well characterized using NMR and Mass spectrometry. Some of th *N*-arylated indolylsulfoximines displayed a broad spectrum of cytotoxicity (1.2-8.2 μM) against the tested prostate and breast cancer cell lines. These compounds were found to be non-cytotoxic to normal HEK293 cells, indicating their potential selectivity for cancer cells. In cellular assay, the indolylsulfoximines were found to increase the endogenous level of ROS, leading to the increased level of p-53 and c-jun inducing apoptosis. *N*-arylated indolylsulfoximines also induced mitochondrial dysfunction, further promoting apoptotic pathways [5,6]. Our data shows that *N*-aryl indolylsulfoximines could serve as potent and selective anti-cancer agents. Synthesis and biological results of the prepared indolylsulfoximines will be shared during the conference.

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O-14

MiR-539-3p negatively regulates osteogenesis by suppression of Wnt/Beta catenin pathway and subsequent inhibition of Akap-3 signalling

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X-linked hypophosphatemia (XLH), is a hereditary form of rickets, which emerges from the mutations within the Phex gene [1]. However, the mechanism by which Phex gene mutation leads to XLH is relatively unknown. In the past decade a class of non-coding RNA molecules i.e. miRNAs have emerged significantly as post transcriptional gene regulators and have been linked to various disease's aetiology [2]. Hence, in this study, the role of signature microRNAs in osteoblast cells transfected with Phex siRNA and their effects in the process of osteogenesis was investigated. Differential expression of numerous miRNA candidates was discovered during miRNA profiling of Phex-silenced osteoblast cells. We chose miR-539-3p as it was more than eight-fold upregulated. Overexpressing miR-539-3p lowered the osteoblast differentiation. Through predictive algorithms and subsequent experimental validation via Dual Luciferase Reporter Assay, LRP6 emerged as one of the direct targets of miR-539-3p. Overexpression of miR-539-3p suppressed the Wnt/beta catenin signalling components and led to deterioration of skeletal parameters in ovariectomized mice. Moreover, serum samples from mice treated with miR-539-3p mimic exhibit heightened levels of bone resorption markers like CTX and Trap-5b and lesser levels of bone formation marker, P1NP. All these parameters were reversed by anti-miR-539-3p treatment. Furthermore, transcriptome analysis of osteoblast cells overexpressing miR-539-3p has unveiled the presence of an unexplored and uncharacterized Akap-3 gene in osteoblasts. Akap-3 silencing downregulates osteoblast differentiation markers at both transcriptional and translational levels. In summary, we present first report of a novel miRNA, miR-539-3p and its downstream target, Akap-3 in regulation of osteoblastogenesis.

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O-15

Potential of Chayote as a precursor for Activated Carbon prepared by chemical activation for the removal of heavy metals

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Heavy metal disposal into the environment and even more so the aquatic environment has increased significantly in the last few decades due to rapid industrialization. These metals not only severely harm human life and the environment but also are difficult to decompose biologically as they resist the environment's natural process of self-purification. In addition to that, the conventional wastewater treatment plants add pressure to the already existing problem of availability of clean water. All these factors bring about the main objective of this paper i.e. the removal of heavy metals from contaminated water. With the constant development of methods to purify contaminated water, recent researches have been focused on converting agricultural wastes into Activated Carbon solving not only the problem of waste disposal but also the conversion of a potential waste into Activated Carbon which can be used as an efficient adsorbent for the treatment of waste water. The Activated Carbon which is not only cost effective but environmentally friendly will be prepared from the agriculture waste i.e. leaves and stems of the “Chayote/ Squash/Eskos” plant, undergoing chemical activation and will be used in the heavy metal removal via the Adsorption process which has not only shown promising results in the removal process but also because of its simple preparation process, cost effectiveness and wide range of application. The prepared Activated Carbon will further undergo characterization and adsorption studies which will give us a more detailed knowledge on the prepared Activated Carbon.

Keywords: contaminated water, heavy metal, Activated Carbon, Chayote, Cost Effective, Adsoprtion

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O-16

Amphipathic Hybrid Foldamers as Antimicrobial Agents

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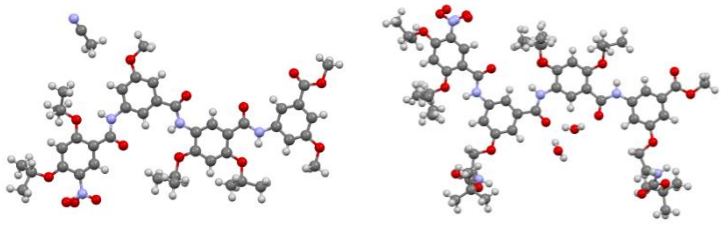
ABSTRACT:

Bacterial infections that are resistant to antibiotics are beginning to threaten public health globally. This spotlight on application provides a summary of our research investigation, with a particular emphasis on the investigation of small compounds that imitate host-defence peptides (HDPs) and have membrane-active antibacterial activity[1]. Recently, membrane-active foldamers have been identified as promising antimicrobial peptide (AMP) mimics. Small molecules are selected for development because of their potential for more beneficial applications and low production costs. Innate defence peptide development and use are hampered by issues with absorption, off-target toxicity, and pharmacokinetics. They have broad-spectrum activity against both Gram-positive and Gram-negative bacteria, including two strains that were multidrug resistant, according to in vitro studies.[2]
In this work, we illustrate the synthesis of short hybrid foldamers, characterization, conformational analysis, and antibacterial studies are included.



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O-17

Chemical and *in vitro* biological investigation of *Cupressus torulosa* needles essential oil

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Abstract:

The current investigation was undertaken in response to the growing interest in natural alternatives within the realm of medicine. Specifically, this study sought to explore the chemical composition and biological potential of the essential oil extracted from the needles of *Cupressus torulosa* (CTEO), an evergreen tree abundant in the western Himalayan region of India, yet lacking in comprehensive studies. The hydro-distillation process of *C. torulosa* needles produced a greenish-yellow oil, with a moisture-free yield of 0.60 ± 0.07%. The chemical composition of the essential oil was analyzed using GC-MS, leading to the identification of 29 compounds. Additionally, GC-FID was employed for the quantification of these compounds. The major constituents included terpinen-4-ol (393.8 µg/mg), totarol (55.0 µg/mg), sabinene (43.7 µg/mg), and sempervirol (40.8 µg/mg). Biological evaluation of CTEO revealed promising *in vitro* anti-inflammatory activity (IC_{50} 27.32 µg/mL) that was comparable to standard sodium diclofenac (IC_{50} 15.03 µg/mL) in the egg albumin denaturation assay. Additionally, CTEO demonstrated notable α-amylase inhibitory activity, with an IC_{50} value of 31.54 µg/mL, comparable to the standard acarbose (IC_{50} 32.87 µg/mL). In terms of skin whitening effects, CTEO exhibited modest activity in the tyrosinase inhibitory assay, with an IC_{50} value of 2038 µg/mL, in contrast to the standard kojic acid (IC_{50} 203.3 µg/mL). The observed promising *in vitro* anti-inflammatory and anti-diabetic activities suggest potential avenues for further exploration through *in vivo* assays. This study contributes valuable insights into the pharmacological properties of CTEO, paving the way for future research and development in the field of alternative medicine.

O-18

Compactness in unequal crossover model

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Abstract

Crossover is a genetic operator, that leads to the recombination of chromosomes. Unequal crossover plays a crucial role in genetic evolution. In this paper, we discuss the general topological structures on the set of chromosomes and the property of compactness in unequal crossover model.

Keywords: Recombination, Unequal Crossover, Topology, Pretopology, Compactness

O-19

Polymerization of "(E)-4-(4-hydroxy-3-methoxyphenyl) but-3-en-2-one"with chloro acetophenone and formaldehyde solution: Synthesis of α–β unsaturated polymer.

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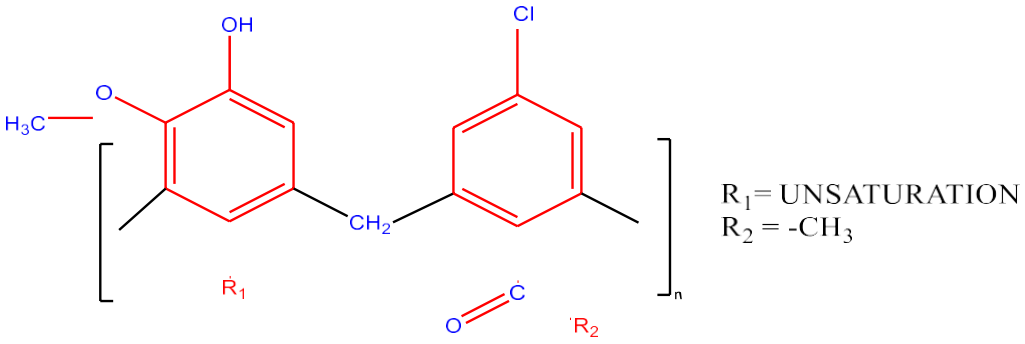
Abstract

vanillin -based polymers are found biologically active against, Bacillus subtitlis, Escherichia coli, Staphylococusaureus, and Pseudomonas aeruginosa. Synthesis of Schiff base polymers has also shown structural importance and biological activity, due to its eco-friendly nature.[1] Due to biodegradability and multiple biological importance including antioxidant properties, and wound healing properties ferulic acid polymers have their own importance in literature. Various applications of FA-polymers are well-known in the literature. Moreover, FA- polymers have no toxic effect, and cyclotoxicity thus useful in drug delivery applications. Ferulic acid derivative-based synthesized using the simple method from vanillin. The condensation reaction of vaniline with acetone converted to α–β ferulic acid ketone, derivatives with unsaturation. Ferulic acid polymers have importance in various healthcare applications. Ferulic acid ketone derivatives were converted to oxime monomers by condensation reaction with hydroxyl amine hydrochloride. The polymerization of oxime ferulic acid ketone with 4-chloro acetophenone gave novel α–β unsaturated polymer with oxime. Polymerization was carried out in the presence of NaOH, and formalin in a short time. We want to present the complete process and characterization of the above polymer in the present study.

Keywords: Co-polymer, Ferulic acid polymers, novel α–β unsaturated polymer

Graphical Abstract



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O-20

Advancement in research with the help of AI

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As the new era of technological advancements begin and with every piece of technology the new AI (Artificial Intelligence) is being added why not the some of the most important researches should be aided with it.

Yes, research in pharmaceutical drug design or discovery should be aided with AI. There are several reason for why it should be and mainly is that its way more efficient than the traditional method. I am not stating the traditional method is wrong but slow just like Ayurveda is the traditional old fashion way of treating the disease and eradicating it from the roots but we also know that it also takes sometimes years to do it. That's why we have to rely on modern drug packed medicines and liquids but with the help of AI. From recent discoveries one of the most fascinating one was "An Antibiotic identified by AI" by Angela Cesaro & Cesar de la Fuente-Nunez where they found out that when they did it traditionally the success rate of finding out with human labor was only 6% but with the help of AI the chances went upto 16%, i.e, up to 2.5 times higher.

So to conclude it I would say with the help of AI we can speed the manual process we can't completely rely on it but we can take aid of it so to increase the efficiency of the process

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O-21

Assessment of *In Vitro* Anti-Glycation Efficacy of Dapagliflozin andRosuvastatin on Human Serum LDL

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Introduction: Glycation of LDL is regarded as one of the atherogenic modifiers of LDL and glycated LDL is more prone to oxidation than native LDL. A majority of Type-2 diabetic patients have comorbid hyperlipidemia. Therefore, the treatment of diabetic patients with hyperlipidemia demands the use of agentswith pleiotropic effects to reduce the risk of diabetic complications such as atherosclerosis.

Objectives: The primary objective is to study the protective effect of dapagliflozin and rosuvastatin against LDL glycation.

Methodology: *In vitro* non-enzymatic glycation of human serum LDL was carried out in triplicates in the absence and presence of dapagliflozin, and rosuvastatin. The reaction mixture containing LDL was incubatedfor 7 days at 37 ^{o}C and % inhibition of fructosamine adduct formation was measured. The level of thiobarbituric acid reactive substances (TBARS) was also estimated after CuSO4-induced oxidation of glycated LDL.

Results: Dapagliflozin and rosuvastatin showed a significant reduction in fructosamine monoformazan in the LDL glycation system, the highest at 5 mM concentrations (P<0.0001). Dapagliflozin produced statistically significant inhibition of TBARS formation at 0.5 mM, 1 mM and 5 mM concentrations (P<0.01 for all concentrations) which was comparable to that of reference standard aminoguanidine (P<0.01 for 0.5 mM, 1 mM and 5mM). In the case of rosuvastatin-treated LDL, reduced TBARS was observed at 1 mM (P<0.05) and 5 mM (P<0.05) concentrations.

Conclusion: In the present investigation, we found that dapagliflozin and rosuvastatin are effective in inhibiting glycation-induced LDL modification. Therefore, both drugs may be recommended for diabetic patients with hyperlipidemia. However, further investigations are required to ascertain the mechanism of action and *in vivo* efficacy.

Keywords: Diabetes mellitus, Advanced glycation end-products, Anti-glycation, Diabetic complications, Low-density lipoproteins (LDL).

O-22

Optimizing Patent Processing Time in the Indian Biotechnology Sector: Comprehensive Analysis of Disposal Types and Their Temporal Impact

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Abstract:

In the rapidly evolving landscape of biotechnology, a key facet lies in ensuring efficient and timely processing of patent applications. This study focuses on the Indian biotechnology sector, a burgeoning domain of innovation and intellectual property. Spanning the years 2017 to 2021, we delve into the intricate relationship between disposal types—specifically 'Abandoned U/S 21(1),' 'Granted,' and 'Refused'—and the temporal dynamics of patent processing. Through an extensive analysis employing descriptive statistics, ANOVA, and meticulous multiple comparisons, this research uncovers profound disparities in processing durations across these disposal types. 'Abandoned U/S 21(1)' patents showcase a relatively shorter processing time, contrasting the extended duration associated with 'Refused' patents. 'Granted' patents occupy an intermediate position, indicating a streamlined processing approach. These findings elucidate the pivotal influence of disposal types on the timelines of patent processing, holding profound implications for stakeholders, patent applicants, and policy architects.

Keywords: Patent Processing, Disposal Types, Biotechnology Sector, Statistical Analysis

O-23

Carbon quantum dots, preparation, photophysical properties and application thereof

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Abstract

Eco friendly, water soluble and blue fluorescent quantum dots with an average size of 7nm were synthesized from natural carbon source by using microwave assisted bottom-up approach[1] and they are labelled as GFQDs, the characterisation and surface functionalities of the GFQDs were done by using FTIR, XRD, SEM and HR-TEM. The synthesized GFQDs has exhibited pH and excitation dependent emission spectra. GFQDs exhibited emission spectra at two different wavelengths with 24% QY. The as synthesized GFQDs are crystalline in nature which is confirmed by powder XRD analysis. GFQDs are used for the detection of two different class of antibiotics i.e., fluoroquinolones and tetracyclines of which it selectively detects tetracycline antibiotic in water, food samples and bacterial cell lines[2].

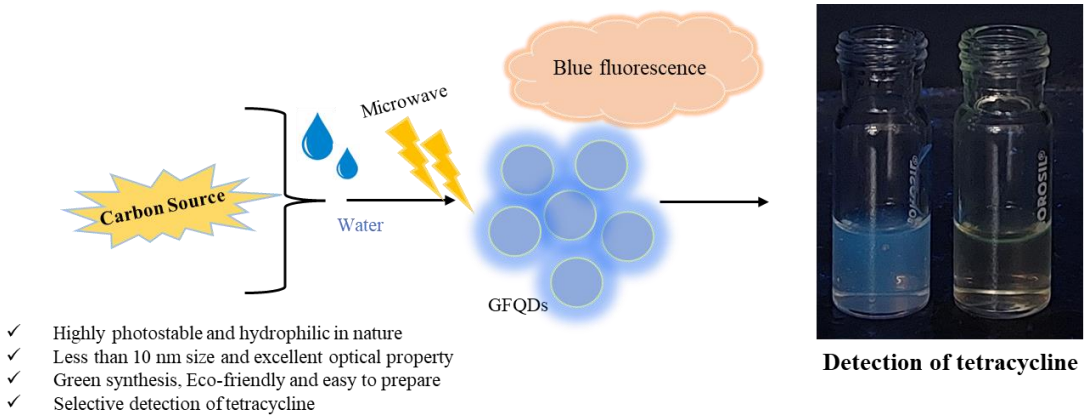

Figure 1. Schematic representation of GFQDs synthesis and application.

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O-24

Chiral Pool Meets Chiral Catalysis: Eight-Step Convergent Total Synthesis of Anticancer Natural Lipid Mycalol

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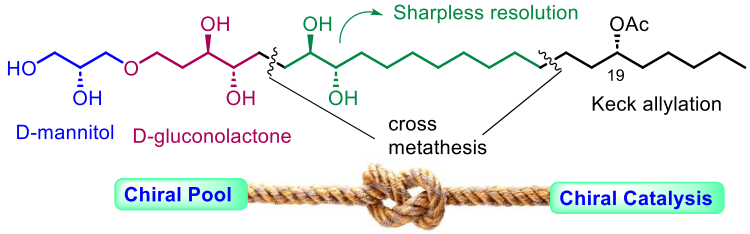
An exemplary blend of chiral pool with chiral catalysis is exhibited in the eight-step (longest) convergent asymmetric total synthesis of mycalol, a promising anticancer natural lipid from the marine source. It displayed potent and selective cytotoxicity against human anaplastic thyroid carcinoma (ATC) as evidenced by its IC_{50} values against different human ATC-derived cell lines: FRO-HMGA1as = 7.3 µM, ACT1 = 4.5 µM, and 8505c = 3.8 µM.[1] The polyhydroxy lipid is constructed by using four blocks, two of which are derived from the chiral pool (D-mannitol and D- gluconolactone) and the other two by chiral catalysis (Sharpless epoxidation and Keck allylation). Alkylation and metathesis were used to knit the blocks in an excellent display of modular convergent eight-step synthesis. Also, a modular approach not only enables the synthesis of target molecules in a convergent design but also assist in rapid building of analogues for bioactivity studies.



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(Oral Presentation)

Priyanka Choudhary
DOB- 4 July, 1998

O-25

Quantitative, quantitative Analysis as well as bioactivity activity of methanolic and petroleum extract of *Abutilon pannosum* leaves

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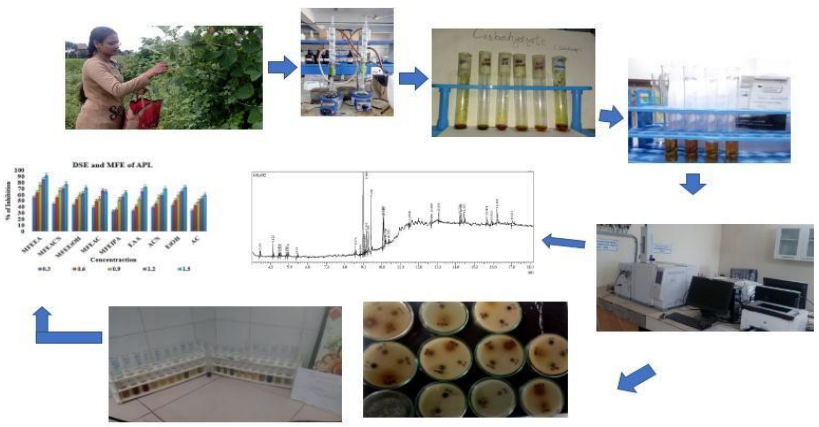
Abstract

The aim of the study is to identify, both qualitatively and quantitatively, the presence of several phytoconstituents in the petroleum ether and methanolic extract of *Abutilon pannosum* leaves. The qualitative and quantitative experiments were performed by its standard method which is reported in higher impact factor journals and separation of extracts has been done using GC-MS techniques. Phytochemical screening of plant extracts revealed the presence of total phenol, flavonoids, alkaloids, total phenol, steroids, terpenoids, and cardiac glycosides, etc. Quantitative determination of total phenolics, total flavonoids, and alkaloids was carried out using UV-vis spectroscopy methods. These phytoconstituent has responsible for the medicinal activity of plant samples like antibacterial, antioxidant, and antifungal wound and urinary tract cleaning, trachoma as well as for treating hemorrhoids, diabetes, and anemia which is reported in higher impact factor journals. Out of these antimicrobial and antioxidant activities has been performed using different techniques. According to the result plant samples have potent antioxidants against ABTS and DPPH scavenging radical and good antibacterial against *E. fecalis*, *S. epidermidis*, *S. typhi*, *S. pneumoniaee* and *P. aeruginosa*. The antioxidant activity of *Abutilon pannosum* leaves has been observed due to phytochemicals which is reported that chemicals are trans-phytol, Hexadecanoic acid, Methyl tetradecanoate ,11-Eicosenoic acid, Tridecanoic acid, palmitic acid, Pentadecanal. The antibacterial activity *Abutilon pannosum* leaves have been observed due to Octadecanoic acid**,** dl-.alpha and beta.-tocopherol , trans-squalene, 1-hexadecanol which is identified by GC-MS.

Keywords: *Abutilon pannosum* leaves, qualitative, quantitative, antimicrobial and antioxidant activities

Graphical Abstract



O-26

Production of activated carbon from *Sechium edule* plant for removal of dyes and fluoride pollutants; Equilibrium, kinetic and thermodynamic studies.

Neilanuo Huozha

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Mode: Podium Presentation.

Abstract:

Today's public awareness is growing and international guidelines are becoming more closely regulated which has made environmental issue related to wastewater more difficult. Worldwide developments, multiple industrial and agricultural practices, all contribute to water contaminations, as such various techniques are being employed for their treatments. However, the techniques are found to be costly, ineffective and produce secondary waste products. Hence it is vital to find a method to cleanse contaminated waters that is both affordable and environmental friendly. The choice of a specific wastewater treatment method should take into account both the environment and the economy rather than solely relying on how effective it is. Through adsorption process, researchers are concentrating on the production of activated carbons from inexpensive sources to replace costly commercial activated carbons as an effective way to reduce the level of water contaminants. Within this context, the goal is to create a chemically activated carbon from the leaves and stems of *Sechium edule* plant commonly known as "Chayote" to purge water of fluoride and dye pollutants. The issue of waste disposal will be resolved as a result, and a potentially wasteful product will be rendered into a useful one that maybe utilized as an adsorbent for wastewater treatments.

Keywords: Activated carbon, Adsorption, Water treatments, Adsorbents, Chemical activation

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O-27

Prinsepia utilis Royle seed oil: A comprehensive study on its fatty acid composition and anti-inflammatory property

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Abstract:

Prinsepia utilis (PU) Royle, known as the Himalayan Cherry, is a deciduous thorny shrub native to the Himalayas, thriving up to 3000 meters. Traditionally used for medicinal purposes, its roots, leaves, and seeds address rheumatic pain, joint pain, arthritis, and inflammation. To meet rising demand for natural healthcare, this pioneering study scientifically validates traditional healing claims. In this study, PU Seeds collected from Kanasar, Uttarakhand (India), were Soxhlet extracted using n-hexane and fatty oil was isolated. Focusing on fatty oil from PU seeds, Gas Chromatography-Flame Ionization Detection (GC-FID) and Gas Chromatography-Mass Spectrometry (GC-MS) determined its composition. *In vitro* assays (trypsin inhibitory, bovine serum albumin denaturation) and *in vivo* models (carrageenan, formalin-induced edema) confirmed anti-inflammatory properties, marking a significant step in systematic assessment. GC-FID and GC-MS analysis of the oil revealed the presence of linoleic acid (59.06±0.00%), oleic acid (28.11±0.01%), palmitic acid (9.51±0.01%) and stearic acid (3.32±0.01%). *In vitro* trypsin inhibitory and bovine serum albumin denaturation assay revealed dose-dependent notable activity of the oil with IC_{50} value of 63.57 µg/mL and 518.14 µg/mL, respectively. The oil exhibited noteworthy anti-inflammatory efficacy, manifesting positive effects persisting up to four hours post-dose administration in carrageenan-induced and formalin-induced rat paw edema at tested doses of 100 and 200 mg/kg body weight. These outcomes, in addition to corroborating traditional assertions, indicate the prospective therapeutic utility of PU seed oil as a natural anti-inflammatory agent. Further investigations are imperative to elucidate its mechanisms of action and ascertain its potential applications within the pharmaceutical and nutraceutical industries.

O-28

Process Development and bio similarity of mAb molecule: a case study

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Abstract

Human epidermal growth factor receptor 2 (HER2) dimerization with other HER receptors is inhibited by the specific monoclonal antibody as biosimilar, preventing them from signalling in ways that encourage cell growth and proliferation. A comparable analytical bio similarity study is performed to evaluate the biosimilar against innovator. This article briefly illustrates the outcomes of the mAb molecule process development approach. Studies such as medium screening, clone screening, cell culture process parameter optimization, aeration, and trace metals, enzymes supplementation for n-Glycosylation optimization have been carried out in the process development. Shake flask and two-Liter bioreactor scales were used for the screening and development research. The parameters like Growth profile, culture length, protein titre, and most importantly the resemblance of the biosimilar mAb product with the innovator were all factors in cell culture performance. It will be scaled up to production scale using the defined process at small scale. Overall, the Upstream process for the mAb molecule described a final output with a sufficient level of productivity and equivalent quality characteristics. The consistency of the outcomes further demonstrates the process's robustness.

Keywords: consistency, bio similarity, lab scale, manufacturing & Biopharma

O-29

1,2,3-triazoles derivatives via 'click chemistry' approach"

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Abstract:

This work summarize the synthesis of imidazo[1,2-a]pyrazine containing 1,2,3-triazole derivatives and the importance of this motif as a lead structure for novel drug molecule discovery. With the help of "click chemistry" 1,2,3-triazoles can be obtained on a multigram scale under comprehensive conditions. The design strategy claimed in this work for the synthesis of imidazo[1,2-a]pyrazin hybrid 1,2,3-triazole derivatives is novel. Novel nine compounds were synthesized and evaluated on eight microbial strains such as E. coli, P. aeruginosa, E. aerogenes, B. megaterium, S. aureus, B. subtilis, A. niger and A. flavus. All the compounds were characterized by various analytical methods such as ^{1}H-NMR, ^{13}C-NMR, IR and MS. The compounds were evaluated with Minimum Inhibitory Concentrations (MICs) and some of them showed excellent results. The synthesized compounds show potential antimicrobial agents against Gram-positive, Gram-negative bacteria and fungi.

Keywords: 1,4-disubstituted 1,2,3-triazoles; CuAAC; Click chemistry

O-30

Formulation Characterisation and Optimization of Quick-Dissolving Sublingual Film of Venlafaxine Hydrochloride by Using Design of Experiment

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The present investigation was focused on developing a quick-dissolving sublingual film of venlafaxine hydrochloride. The sublingual film was prepared by solvent casting method. The combination of drugs with a polymer such as HPMC E5, HPMC-E15, SSG and Pullulan was used to prepare the film. PEG 400 used as a plasticizer The compatibility between Venlafaxine HCl and excipients was confirmed by the FTIR study. A 3^2 full factorial design was used to study the effect of HPMC E5 and SSG on disintegration time and % CDR of the film. The following parameters were assessed for each of these formulations: thickness, drug content, surface pH, folding endurance, disintegration time, weight variation, tensile strength, and percentage elongation. The optimized formulation of the quick-dissolving sublingual film (batch F8) has shown 99.13 per cent drug release within 1 min and disintegration time was found to be 25.20 ± 0.614 second., the drug content was found to be 96.69 ± 0.36 percentage and the pH of the film is near to neutral (6.89 ± 0.05). The dependent variables were analysed using ANOVA and the polynomial equation was developed for the same parameters, it was found that the concentration of HPMC E5 and SSG significantly effects on disintegration time and percentage CDR (at 1 min) for the film. The quick dissolving sublingual film of venlafaxine hydrochloride was successfully developed and hence was concluded that the film would improve patient compliance and efficacy of the drug in cases of depression.

Keywords: Venlafaxine Hydrochloride, HPMC E5, SSG, factorial design, quick-dissolving sublingual film.

O-31

UGI-mediated an efficient and concise synthesis of anticancer agents

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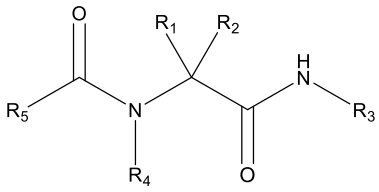
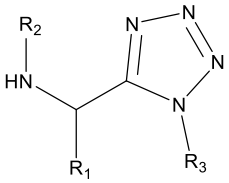
Abstract:

Cancer is becoming a major health issue worldwide and new anticancer agent is one of the need due to adverse side effect of chemotherapy. From the ancient chemistry, Heterocycles have a significant role in medicinal chemistry. One effective way to create novel derivatives of heterocycles is through multicomponent reactions. I have described both conventional and unconventional UGI-4C reactions here, such as those aided by microwaves. By using spectroscopic techniques, all the synthesized compounds have been identified and tested against a panel of nine cancer cell lines.





Keywords: Ugi multicomponent reaction, heterocyclic compounds, anti-cancer activities, Medicinal chemistry

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O-32

Xylanase production by marine Actinobacteria

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Department of Life Sciences, MKBU, Bhavnagar

ABSTRACT

Actinobacteria bacteria exhibited maximum enzyme production with growth where as the fungi require acidic pH. The marine environment contain complex polysaccharides derived from sources like terrestrial and aquatic plants, algae, fungi, bacteria and crustaceans; thus, it is the richest resource for microorganisms equipped with the novel enzymes for complex polysaccharide. Screening of actinomycetes for their xylanolytic property was carried out by growing them on xylan-agar medium with yellow clear zone against red background were identified as xylanase producers. Based on maximum zone of clearance, isolate *Streptomyces labedae* RD 16 was identified as a potential xylanase producer and selected for further studies. Xylanase activity was determined using different buffers having varying pH and Stability of the crude enzyme with respective pH (6.0 to 12.0) by preincubating the enzyme in respective buffer for 30 min and then the residual activity was determined. The optimum temperature required for xylanase activity was determined by incubating the system in the temperature ranging from 20 to 80°C. Also temperature stability of xylanase was determined by preincubating enzyme at respective temperature for 30 min. The kinetic properties of xylanase were determined using varying concentration of the substrate, xylan. Km and Vmax values were calculated by Lineweaver Burk double reciprocal plots. Though several potential strains which produce xylanases with higher yield, improved stability with extreme conditions have been recently identified, there is a need to isolate novel microbe producing robust xylanase for their industrial applications. An appropriate enzyme for commercial pulp bleaching applications must have a high specific activity, a broad pH range and high thermal stability because pulp bleaching is usually done at high temperature and pH.

Keywords: Actinobacteria, Xylanase, Pulp bleaching, Optimum study

O-33

Study of photophysical properties of *N*-aryl enaminones and their application in the synthesis of hexahydrocarbazolones via [6π] Photocyclization ‡

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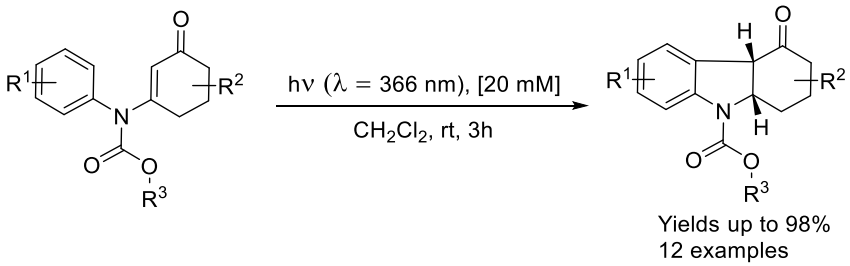
Photochemical organic transformations provide easy access to molecular structures that are difficult, if not impossible, to obtain via conventional reactions. Numerous approaches toward natural product synthesis have been reported where a photochemical transformation represents a key step.[1] Indoline derivatives are a very important class of heterocyclic compounds due to their presence as core structures in many naturally occurring alkaloids and pharmaceutical compounds. We were intrigued by the photocyclization of enaminones to hexahydroindoline derivatives.[2] During our initial attempts, we found out that the reported photoproducts were not stable on silica and the substitution on nitrogen plays an important role in stability of the photoproducts.[3] For this modification UV-Vis absorption was used as a tool to determine the substitution change on nitrogen.



The energy of excited states and intermediates as well as final products were calculated with the help of computational calculations which provide insight into the mechanistic pathway of this interesting reaction.

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O-34

Targeting Methicillin-Resistant Staphylococcus aureus (MRSA) for Antimicrobial Activity Through Hemiaminal 3- Sulfenylated Indoles: Structure-Activity Relationship (SAR), in vitro and in vivo Studies

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The design of small molecules has been used for the treatment of a vast array of diseases including microbial infections. Indole is one of the most valuable privileged heterocyclic compounds[1] in synthetic as well as medicinal chemistry owing to their omnipresence in many drugs and drug-like molecules with a wide range of biological activities such as antibacterials[2] and anti-inflammatory.[3] Particularly, 3-sulfenyl indole derivative has a wide range of pharmaceutical activities such as anticancer[4], antiviral, and antibacterial. We also reported synthesis and discovery of diaryl disulphides as potent inhibitors of drug-resistant *S. aureus*.[4] Reports revealed that hemiaminals of pyrazole and imidazole group showed enhanced antimicrobial activity against *S. aureus* over parent heterocycles.[5] Based on the literature and our own hypothesis, we have developed a new method of synthesis of hemiaminal-3-sulfenyl indole derivatives in good to excellent yield. All the synthesized compounds were investigated for biological activity against anti-microbial activities on gram-negative and gram-positive bacteria strains. Some of the compounds were active selectively against *S. aureus* ATCC 29213 (MIC 2-32 µg/mL). We also established the structure-activity relationship and their study against MDR *S. aureus*. We found the most active compound MIC 2 µg/mL and *SI* = 50. Around SAR in vitro and in vivo study has been done. Time kill kinetics, bio-film inhibition, and drug combination study with different antibiotics were also studied. The details will be presented during the presentation.

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O-35

Immunomodulating Osteoprotective Effect of IL-33 in D-galactose Accelerated Aging Bone Loss Condition

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Recent studies have identified a new TH2 cytokine, IL-33, whose implications in osteoporosis is slowly emerging. It has been shown to inhibit RANKL induced osteoclastogenesis. Another report showed that IL-33 levels in postmenopausal osteoporotic women were significantly lower compared to healthy controls. However, no study has been carried out to assess the role of IL-33 in senile osteoporosis. For inducing senescence, we exploited D-galactose (D-gal)-induced accelerated aging model due to its convenience and least side effects. Treatment of osteoblast cells with D-gal showed typical characteristics of senescence and bone loss. D-gal treated cells exhibited reduced ALP activity and downregulation of osteogenic genes like RUNX-2, osteocalcin and Type 1 Col. It also upregulated senescence-associated markers like p53 and p21. On the contrary, in the cells treated with IL-33 along with D-gal, all the osteogenic parameters were elevated and senescence markers were lessened. These results were also validated in D-galactose induced accelerated aging mice model. In the mice treated with only D-gal, various skeletal parameters were compromised. On the other hand, supplementation of IL-33 restored the skeletal parameters. Additionally, reduction in osteoclastogenic TH17 and elevation in T regulatory cell population was observed. Overall our study demonstrates that IL-33 is an important bone-protecting cytokine which may be a novel therapeutic tool in the prevention and therapy of senile osteoporosis.

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O-36

Journey of an AIEgen: From mechanochromism to amyloid fibril detection

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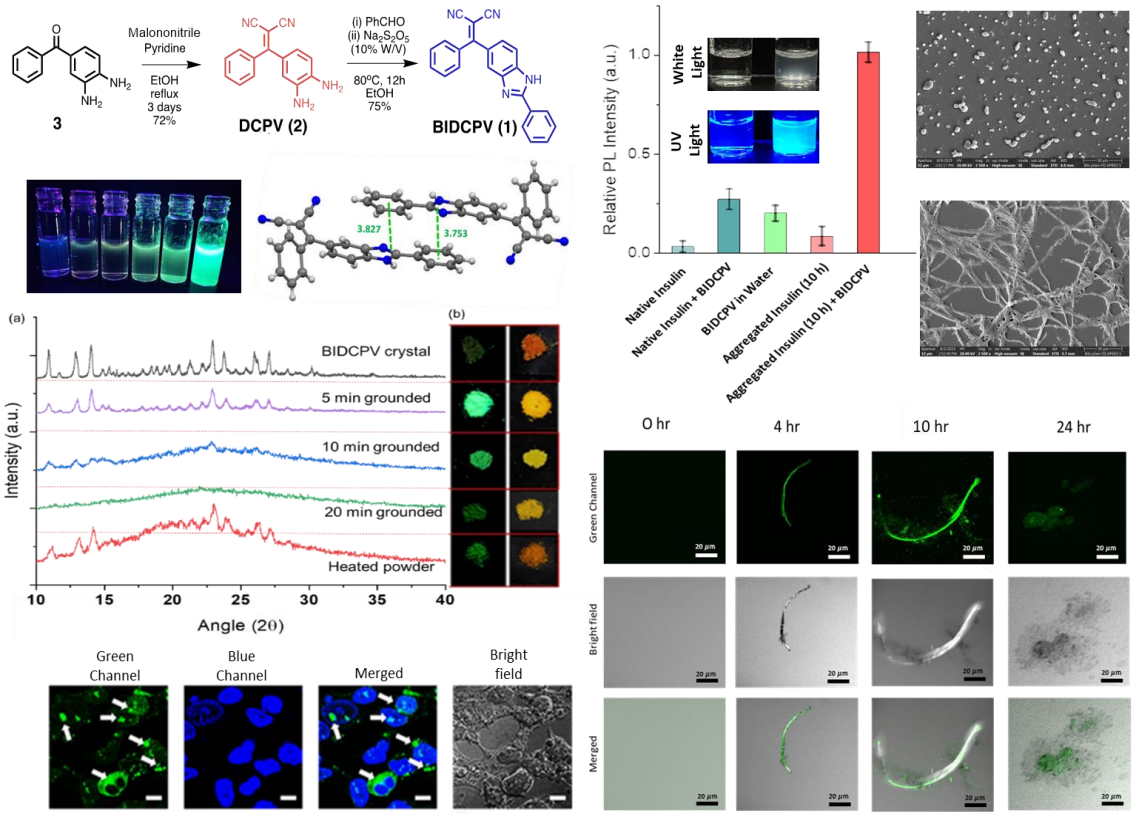
Biocompatible organic fluorescent probes with environment sensitive properties are highly demanding. These molecules are useful to unravel various biological secretes and their potential application for the development of optical materials. Despite such need commercially viable synthesize of such fluorescent molecules is a challenging task. Here we present, a convenient two step synthetic protocol to obtain an aggregation induced emission based luminogen (AIEgen), BIDCPV (benzimidazole dicyano phenyl vinyl) which shows mechanical force responsive solid state optical response. On top of that based on its AIE property we have explored the strength of aggregates to detect aggregates. In this trail we observed BIDCPV can monitor different stages of protein aggregation inside or outside the cells.



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O-37

Engineering of hybrid SBA-15 for assessment of invitro release of alendronate

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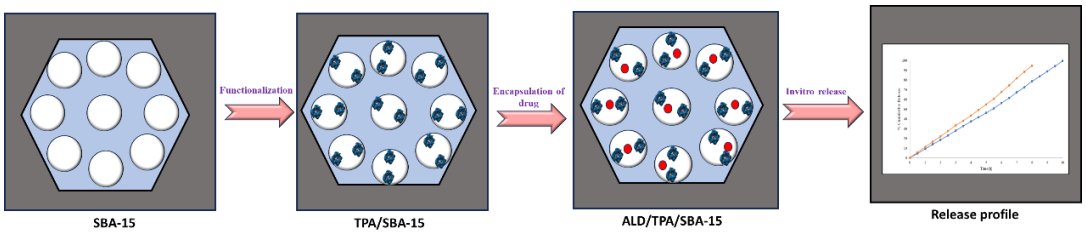
Email- shivangimehta2000@gmail.com
Mode: Podium Presentation

Osteoporosis is skeletal disorder in which microarchitectural deterioration of bony tissue occur. This condition emerges out due to imbalance cause in bone remodeling process. Alendronate (ALD) which is nitrogen containing bisphosphonate has been widely used for healing postmenopausal osteoporosis, Paget disease as well as metastatic bone disease. However, ALD has lower bioavailability that can causes gastrointestinal irritation and oral route causes cardiovascular risk [1]. The above-mentioned limitations can be resolved by using a controlled drug delivery system. Functionalized Mesoporous silica- based carriers having high surface area and pore volume serve as promising material for controlled drug delivery [2]. The present work includes the synthesis of SBA-15, functionalization of SBA-15, encapsulation of ALD, characterization using various physico-chemical techniques, invitro release study of drug in simulated body fluid (SBF). To study the kinetics and mechanism using various models have also been proposed.



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O-38

Synthesis of Modified Bile Acids *via* Palladium-Catalyzed C(sp^3)-H (Hetero)arylation

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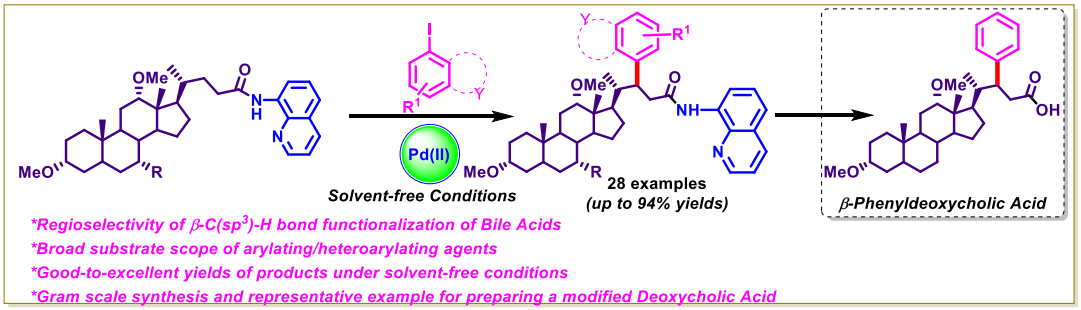
Bile acids are the acidic sterols present in physiological enterohepatic circulation that have proven to be one of the desirable scaffolds for anticancer drug development. In addition to drug delivery applications exhibited by bile acid conjugates with chlorambucil, tamoxifen, floxuridine, foscan, artemisinin, dihydroartemisinin, a few bile acids and their taurine conjugates have been identified as potent inhibitors of apoptosis in different cell types. Numerous bile acid conjugates of amino acids and nucleosides (hetero)arenes have been synthesized over the years and have demonstrated micromolar levels of cytotoxicity against a variety of cancer 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]. Embracing the rich possibility our group designed of arylation at *β*-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 aryl and heteroaryl iodides under solvent-free conditions using 8-aminoquinoline auxiliary as a directing group [4]. Further, the 8-aminoquinoline (AQ) auxiliary was easily removed to obtain a *β*-aryl bile acid derivative. Interestingly, all the (hetero)arylated products were obtained in almost single diasteroisomeric form as evident from the ^{1}H NMR and their respective HPLC profiles (dr ranging from 87:13 to 99:1). Hence, the overall strategy can be considered as an excellent approach for producing *β*-(hetero)aryl bile acids in a regioselective and diastereoselective fashion.



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O-39

Identification of Novel Pyrimidine derivative as Bone anabolic and fracture healing agent promoting osteogenesis via BMP2/SMAD1 signaling

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Abstract

Osteoporosis is a major health problem among the elderly characterized by reduced bone mass and micro-architectural deterioration of bone tissue leading to fragility fractures. Limited efficacy and serious side effects of current therapies led to the need for identifying orally available small-molecule based novel therapeutics. Pyrimidine derivatives possesses broad spectrum of biological activity; however, their potential as bone anabolic agents have never been explored. Therefore, aim of present study is to explore the bone forming potential of pyrimidine derivatives. A series of pyrimidine derivatives was screened primarily using ALP assay and further *in vitro* experiments like cell viability, mineralization, real time PCR and western blotting were carried out to find the potential compound. Results showed that out of 31 compounds, 6 compounds were found active for ALP activity. Moreover, cell viability and mineralization data indicated that **compound B_2P.H** was found most efficacious anabolic agent with activity at 1pM. Further, RT-PCR and immunoblotting exemplified that **B_2P.H** promoted osteogenesis by upregulating the expression of osteogenic genes (RUNX2 and Type 1 col) via activation of BMP2/SMAD1 signaling pathway. The osteogenic efficacy of **B_2P.H** was further evaluated in *in vivo* fracture defect model in ovariectomized Balb/C mice. *In vivo* experiments revealed that **B_2P.H** at 5mg/kg dose promoted bone formation rate, upregulated expression of BMP2, RUNX2, and type 1 col, and increased bone healing at fracture site as confirmed by increased bone volume/trabecular volume, trabecular number and trabecular thickness. Overall, this study confirmed pyrimidine derivatives as therapeutic option for the osteoporosis treatment.

Key words: Pyrimidine derivatives, Osteogenesis, Fracture healing, BMP2/SMAD1signaling

O-40

A Photo-Catalyst-Free Approach for the Visible-Light Induced N-Arylation of Sulfonamides via Electron-Donor-Acceptor Complex

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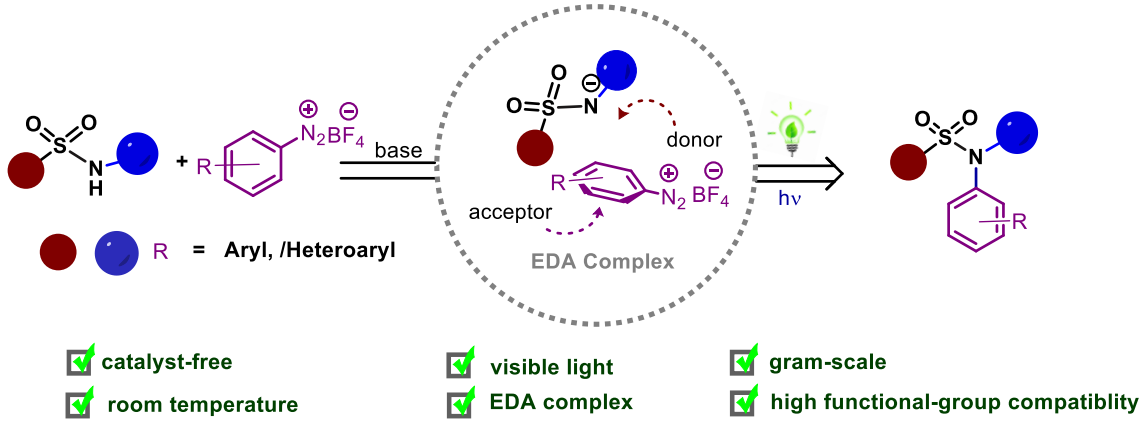
ABSTRACT:

In the pharmaceutical sector, functionalized aryl sulfonamides are fundamental building blocks. Direct N-aryl sulfonamide is more effective because it is free from genotoxic and undesirable potential impurities. Most known previous methods have a limited scope and depend on the catalyst, ligand availability, and high temperature. The photoexcitation of aryl(hetero)diazonium salt and sulfonamide enabled this strategy under visible light irradiation through an EDA complex used to generate a one-step synthesis without a catalyst. The approach tolerated various functional groups of primary sulfonamide and (hetero)aryl diazonium salt frequently found in modern medications and pharmacological intermediates. This method also enabled the direct arylation of secondary sulfonamide. The mechanistic study showed that the formation of electron donor-acceptor EDA complex and sulfonamide radical rapidly interact with aryl radical intermediate through radical coupling to gen-erate the desired product.



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O-41

Synthesis and biological evolution 5-chloro thiophene containing novel Hydrazide-hydrazone derivatives.

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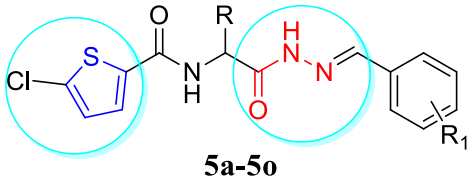
New hydrazide-hydrazone derivatives(5a-5o) were synthesized by reacting 5-chloro thiophene containing hydrazine derivative with aromatic aldehydes. These derivatives underwent analysis using IR, NMR, and Mass spectroscopy. Their antibacterial activity against 4 bacterial stains and antifungal activity against 3 fungal stains were evaluated using Broth Dilution Method. Furthermore, an *in-silico* analysis was performed to predict the pharmacokinetic properties (ADME) of the newly synthesized derivatives. The results are statistically treated as its significance. Further Investigation regarding the mechanistic pathway are still underway.



5a-5o

R = Alkyl

R_1 = Alkyl, heterocycle, halogens

Keywords: Hydrazide-hydrazone, Schiff base, Antibacterial, Antifungal, ADME.

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O-42

INTEGRATED STRUCTURE- AND LIGAND-BASED COMPUTATIONAL MODELLING METHOD FOR THE SUCCESSFUL DESIGN OF DRUG CANDIDATES

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Structure-based drug design (SBDD) strategies are very useful in the beginning of drug discovery and development process. With the availability of co-crystal structures of biological targets, numerous target selective drug candidates can be design using SBDD approaches. Ligand-based drug design (LBDD) strategy is also is very popular and effective if co-crystal structural details of target is not available. Studying this mechanism using SBDD methods such as docking and molecular dynamics simulations is extremely useful in the early stages of drug discovery process and even in the lead to hit optimization process. Structure-based pharmacophore modelling guide toward the selection of a core moiety, and selection of substituents on core moiety per the features. Through docking study, the molecular basis of the binding modes of newly designed compounds can be discovered. MD simulation study was determining the overall stability of the protein-ligand complex. Similarly, LBDD approach 3D-QSAR study help in the selection of substitutions for favourable interactions with the target and also help in the activity prediction of designed compounds prior to their synthesis for selection of better designed compounds for wet-lab experiments. The integration of SBDD and LBDD approaches have been successfully employed in successful design of drug candidates along with investigations of structural, chemical and biological data.

Abstract as podium (oral)
Name: Dr. Vivek K. Vyas
Date of Birth: 02/05/1981

O-43

Design, Synthesis and Biological Screening of Nitrogen Containing Heterocycles and its Sulphonamide Derivatives.

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Abstract:

The preparation of **Heterocycles** and their biological activities are very important in pharmaceutical industries as heterocyclic derivatives shows excellent pharmacophore activity. Furthermore, **Nitrogen-containing heterocycles** are a diverse organic compound class that contains at least one nitrogen atom within a ring structure. These compounds are prevalent in nature and have various biological activities like **antibiotics**, **antivirals**, **antifungals**, **anticancer**, **antimicrobe**, etc. due to their unique chemical properties. Moreover, **Sulfonamide** compounds have been used as biologically active agents, it's worth noting that sulphonamides have played a significant role in the history of antibiotics. sulphinamides remain valuable in certain clinical scenarios and continue to be studied for potential applications in various fields of medicine and biology. Here in this research, we have focused on three various nitrogen-containing heterocycles, namely **Benzimidazole**, **Indole**, and **Pyrazole** having a sulfonamide functional group. Significantly less work has been reported on Benzimidazole, indole, and pyrazole-containing Sulfonamides which might be very potent antimicrobial agents. In conclusion, while benzimidazole, indole, and pyrazole derivatives with sulfonamide functional groups have demonstrated diverse biological activities in research studies, their clinical use as antibiotics or drugs varies. However, the practical application of these compounds in medicine depends on further research, optimization, and evaluation of their safety and efficacy in clinical settings.

Keywords: Heterocycles; Nitrogen-containing heterocycles; Sulfonamide; Benzimidazole; Indole; Pyrazole.

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O-44

Evaluation Of Effect Of Ethanolic Extract Of Cassia Tora Seeds On Permeability OfEtoposide Using Everted Chicken Small Intestine.

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ABSTRACT

Objective: Etoposide, a widely used anticancer drug, exhibits low and variable oral bioavailability mainly because of being substrate for the efflux transporter, P-glycoprotein (P-gp). Therefore, the present study was aimed to investigate the effect of Ethanolic extract of *Cassia tora* seeds (EECTS) as P-gp inhibitors onthe intestinal absorption of etoposide.

Method: Everted sacs of chicken small intestine were incubated in Krebs buffer solution which contained etoposide in the absence or presence of various concentrations of EECTS. The effect of EECTS as a knownP-gp inhibitor on the absorption of drug was studied.

Result: The absorptive transport of etoposide (25µg/ml) was significantly enhanced ($p < 0.001$) in the presence of EECTs (50,200 & 400 µg/ml) suggesting that the inhibition of P-gp located in the intestine maybe involved in the enhancement of etoposide absorption. There was significant increase in permeability values in the presence of the maximum concentration of EECTS as compared to etoposide alone.

Conclusion: The result of the study suggests that by adding EECTS, permeability of etoposide increases and emodin present in EECTS is may be responsible for enhanced permeability of etoposide. Further preclinical and clinical studies are warranted.

Keywords: Etoposide, EECTS, Everted gut sac, Permeability, P-glycoprotein.

O-45

AQbD-based optimization and validation of RP-HPLC method for the estimation of Chlorthalidone and Azelnidipine in pharmaceutical dosage form

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Abstract

Achieving a certain predictable quality with intended and predetermined parameters is known as quality by design (QbD). Due to the emphasis on risk assessment and management compared to a traditional or conventional approach, a quality-by-design approach to method development may result in a more robust or rugged method. Understanding dependent variables, different factors, and their interaction effects by a desired set of experiments on the responses to be studied is a crucial part of the QbD. The development and validation of an AQbD-based HPLC technique for Chlorthalidone (CLT)and Azelnidipine (AZL) in pharmaceutical dosage form are described in the current study. The mobile phase and flow rate, two essential elements of the RP-HPLC process, are crucial to an effective experimental design that is based on a central composite design (CCD). The chromatographic conditions were optimized using the Design Expert tool, i.e., Gemini Phenomenex ODS column C^{18} (250 mm × 4.6 mm, 5.0 µ), mobile phase used acetonitrile and methanol: 0.1 % formic acid (38: 62, v/v), and the flow rate was 0.9 ml/min with retention time 4.15 min for ranges of 6.25 to 125 g/ml for CLT and for ranges of 8 to 160 g/ml for AZL, the devised technique was discovered to be linear with $r^2 = 0.999$. The robustness percentages were under 2%. The assay yielded a result of 99.73 0.61%. According to ICH rules, the technique validation parameters were within the allowed range. The QbD methodology was used to construct analytical methods and improve knowledge of method variables at various stages.

Keywords: Quality by design, HPLC

Reference:

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O-46

Formulation and Evaluation of Paracetamol Suspension Prepared by Using Flaxseed Mucilage and Comparative Study Between Different Marketed and In-house Developed Formulation.

Devanshi Dhinoja*, Meera Maru

Marwadi University, Rajkot

Abstract:

The research aimed to discover substitutes for synthetic suspending agents derived from natural sources, create and assess a unique, efficient, and natural paracetamol suspension, contrast various formulations, establish UV spectrophotometric techniques, and reduce the formulation expenses.

In pediatric patients, fever is a common occurrence, and the administration of antipyretic medications like paracetamol (acetaminophen) is often necessary to alleviate fever. When preparing a paracetamol solution for pediatric use, it is notable that the solubility of paracetamol need to be enhanced through the addition of synthetic suspending agents. However, in this specific formulation, there is no need for the inclusion of any solubilizers or synthetic suspending agents.

This is because the formulation is being prepared using natural components exclusively. The absence of artificial components or synthetic suspending agents is intentional, as it aligns with the principle of utilizing only naturally derived substances in the formulation. This approach is taken to minimize any potential risks associated with synthetic additives, particularly in the context of pediatric patients who may be more sensitive to such additives.

This investigation was carried out at Marwadi University, Rajkot. The wet process was employed to extract flaxseed mucilage from whole flaxseed obtained. Phytochemical assessments revealed that the mucilage exhibited a substantial content of carbohydrates, proteins, sugars, amino acids. Various concentrations of the mucilage were utilized to ascertain the optimal quantity for formulating a paracetamol suspension. The evaluation parameters encompassed sensory observations, pH measurements, viscosity assessments, sedimentation rates, stability assessments, flow properties, re-dispersibility, assay analyses, and dissolution testing.

The findings emanate from a comparative investigation of commercially available paracetamol suspension formulations with Developed paracetamol suspensions. The salient data under scrutiny included pH values, viscosity quantification, stability assessments, re-dispersibility, flow characteristics, assay analyses, and dissolution testing using UV-Spectroscopy. UV-Spectroscopy was employed to perform a comparative analysis between the developed paracetamol suspension and the commercially available counterpart.

O-47

Green Synthesis and Characterization of Silver Nanoparticles from *Cinchona Ledgeriana* Bark Extract

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Introduction: Silver nanoparticles (AgNPs) and their applications have piqued the curiosity of many researchers due to nanoparticles' efficiency in targeting specific tissues and pathogenic microbes. The green synthesis of AgNPs has emerged as an eco-friendly and cost-effective alternative to conventional chemical synthesis methods.

Objective: The present study was undertaken to perform green synthesis of AgNPs using *Cinchona ledgeriana* bark.

Methodology: AgNPs were biosynthesized using the methanolic bark extract of *C. ledgeriana*, which acted as a reducing and capping agent. The synthesized *C. ledgeriana* silver nanoparticles (Cl-AgNPs) were characterized by surface charge, particle size and distribution using zetasizer and UV–visible spectroscopy.

Results: The formation of silver nanoparticles has been confirmed by visual detection in which the color changes from yellow to dark brown as a result of the reduction of silver ions. In addition, UV-Vis spectroscopy revealed a characteristic absorbance peak at 443 nm indicating the formation of Cl-AgNPs. Zetasizer analysis confirmed the size in a range of 200 – 400 nm and zeta potential values of -26.85 mv. The negative zeta potential value of Cl-AgNPs could be due to the capping by the organic components of plant extract. High negative values of zeta potential indicate the electrostatic repulsion between the particles, thereby rendering them highly stable without aggregation.

Conclusion: According to this study, green synthesis is an effective way to produce AgNPs using *C. ledgeriana* and may have promising antibacterial properties due to the plant's antibacterial phytochemicals such as flavonoids and essential oils.

Keywords: Green synthesis, Silver nanoparticles, Cinchona ledgeriana, Zeta potential

O-48

Karnasphota from Ayurveda as a source of Novel Acetylcholinesterase Inhibitor: anatural scaffold targeting the treatment of Alzheimer's disease

Hiral Ranchhod Topiya

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Abstract:

Alzheimer's disease (AD), a neurological ailment that affects older people and progresses overtime, is characterized by increasing memory loss and declines in intellectual capacity, impacting daily activities. The major treatment for Alzheimer's disease involves acetylcholinesterase (AChE) inhibitors, which prevent acetylcholine from being broken down.Important triterpenoids and sterols found in Karnasphota (*Cardiospermum halicacabum Linn.)* roots by GCMS analysis interacted strongly with the AChE's binding site. The Ayurvedic assertion that plant roots are potent memory boosters (Medhya) is supported by these studies and may aid in the development of novel treatments. In this research, our approach is to analyzethe effect of phytochemicals from roots of Karnasphota on multiple culprit enzymes inAlzheimer's disease, such as AChE (Acetylcholinesterase), BChE (Butyrylcholinesterase). Additionally, in-silico ADME prediction using the ADMET lab revealed that these compoundssatisfied all the requirements for CNS-acting medications. Butyrylcholinesterase (BuChE) is significantly inhibited by phytochemicals found in the roots of Karnasphota, including Ergosterol (BA = 9.2 kcal/mol), β-Amyrin acetate (BA = 8.4 kcal/mol), Lupen-3-one (BA = 7.5 kcal/mol), and Lupeol acetate (BA = 7.3 kcal/mol). This research work provides fresh information and opens up new perspectives on how the bioactive compounds present in Karnasphota can be used to treat Alzheimer's disease.

POSTER

P-1

Insights into Synergistic Effects of 1, 5- disubstituted Tetrazole Derivatives via a TMS-N_3 Based Ugi Reaction and their Anti-cancer Activity

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Abstract

In the current study situation, an efficient synthesis for new tetrazole scaffolds via single-step multicomponent reaction has been established. The Ugi multi-component technique for connecting four separate components in a single reaction step and isolating lead compounds, which may offer a better living in society, is one of the most promising approaches. The syntheses of tetrazoles were undertaken by the Ugi-Multi Component approach with the condensation of aromatic aldehyde containing active pharmacophore, various aryl amines, isocyanide (cyclohexyl isocyanide) and TMS-N_3 under catalyst-free reaction condition at room temperature. The structural conformation was carried out by the most acceptable spectroscopic technique *i.e*. MS, IR, NMR, and single crystal study (XRD), and the potency of compounds **(4a to 4h)** was checked at NIH (National Institute of Health) use 60 different cell-lines with respect to nine cancer panels among which compounds **4a** and **4b** have been found to be more potent against different cell lines.

Keywords: U-4CC condensation, Anticancer, NCI-60 cell line, UGI-TMS N_3 reaction.

P-2

Coumarin-Benzopyran Fused Bioheterocycles via Intramolecular Cross Dehydrogenative Coupling (CDC) Strategy: A Potential Scaffold against Monoamine Oxidase A and B

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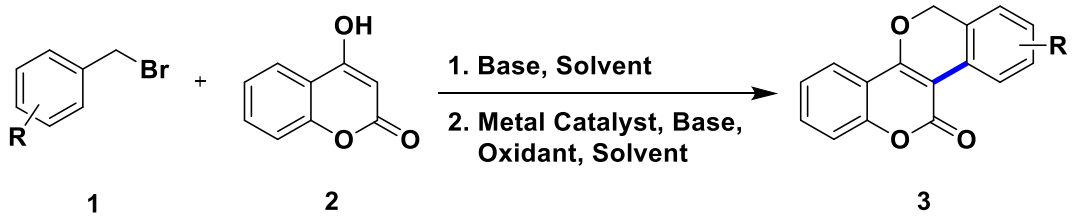
Abstract:
The cross-dehydrogenative coupling (CDC) is used for the most sustainable and efficient synthesis strategies for constructing C–C bonds. Monoamine oxidase (MAO) is a flavoenzyme bound to the mitochondrial outer membranes of the cells, which is responsible for the oxidative deamination of neurotransmitters and dietary amines. It has two distinct isozymic forms, MAO-A and MAO-B (Tripathi et al. 2019).



In our endeavor to develop MAO-A and B inhibitors from natural-product-inspired bioactive heterocycle 6*H*,11*H*-isochromeno[4,3-*c*]chromen-11-one **3.** The development of a new methodology for their synthesis, involving intramolecular palladium-catalyzed cross-dehydrogenative coupling reaction. *In silico* studies revealed that there is a strong interaction between the active sites of MAO-A and B enzymes and compound **3**, could be utilized as MAO-A and B inhibitors. The details of the study will be presented.

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P-3

Synthesis of Bis(oxazolenes): A ligand system having antimicrobial activity

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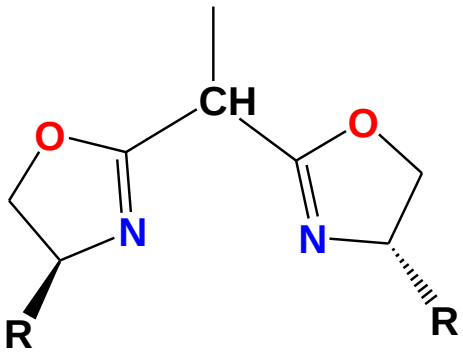
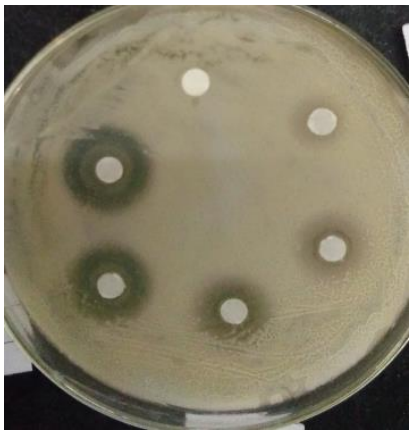
Heterocyclic compound plays important role in biological science with varieties of applications. An oxazole is an oxygen and nitrogen containing unsaturated 5-membered heterocyclic ring, which exhibits anticancer, antitubular, antimicrobial, antidiabetic, antioxidant etc. properties. Bis-Oxazolenes (BOX) ligands are known for their catalytic activity but their biological activities are least explored. 2,2'-(ethane-1,1-diyl) bis (4-methyl-4,5-dihydrooxazole) (L1) & 2,2'-(ethane-1,1-diyl) bis(4-ethyl-4,5-dihydrooxazole) (L2) were successfully synthesized by employing cyclisation of substituted 2-amino alcohol with methyl malonyl chloride. L1 & L2 are being applied as antimicrobial agents against S. aureus NCTC 10788, B. subtilis NCTC 10400, E. coli NCTC 12923, P. aeruginosa NCTC 12924; and antifungal activity against at least the C. albicans.



R = CH_3.....L1
R = C_2H_5.....L2



P-4

The synthesis, biological evaluation and structure–activity relationship of 2-phenylaminomethylene-cyclohexane-1,3-diones as specific anti-tuberculosis agents

Ali Mohd Lone,‡[c] Muzafar Ahmad Rather,‡[ab] Bisma Teli,[cd] Zubair Shanib Bhat,[ad] Paramjeet Singh,[e] Mubashir Maqbool,[a] Bashir Ahmad Shairgojray,[c] Mohd Jamal Dar,[de] Shajrul Amin,[b] Syed Khalid Yousuf,*[cd] Bilal A. Bhat*[cd] and Zahoor Ahmad

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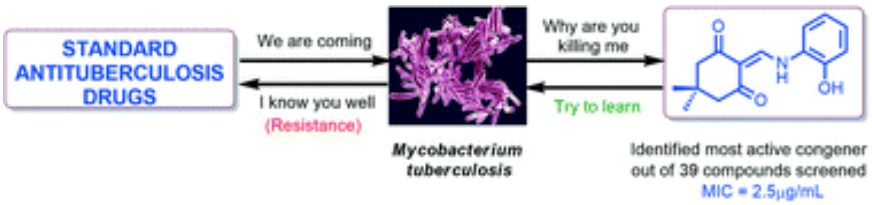
Abstract

The present study utilized whole cell based phenotypic screening of thousands of diverse small molecules against *Mycobacterium tuberculosis* H37Rv (*M. tuberculosis*) and identified the cyclohexane-1,3-dione-based structures **5** and **6** as hits. The selected hit molecules were used for further synthesis and a library of 37 compounds under four families was synthesized for lead generation. Evaluation of the library against *M. tuberculosis* lead to the identification of three lead antituberculosis agents (**37**, **39** and **41**). The most potential compound, 2-(((2-hydroxyphenyl) amino) methylene)-5,5-dimethylcyclohexane-1,3-dione (**39**) showed an MIC of 2.5 μg mL^{-1}, which falls in the range of MICs values found for the known antituberculosis drugs ethambutol, streptomycin and levofloxacin. Additionally, this compound proved to be non-toxic (<20% inhibition at 50 μM concentration) against four human cell lines. Like first line antituberculosis drugs (isoniazid, rifampicin and pyrazinamide) this compound lacks activity against general Gram positive and Gram negative bacteria and even against *M. smegmatis*; thereby reflecting its highly specific antituberculosis activity.



P-5

Is CiNA a potential candidate for TNF-alpha induced atrophy as well?

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Abstract

Inflammation and oxidative stress are major contributors to skeletal muscle loss, which can lead to increased mortality rates under various physiological and pathological conditions. The regulation of both factors can efficiently prevent atrophy and thus increase the survival rate. We hypothesize that pre-incubation with the bioactive compound of cinnamon (CiNA), known for its anti-oxidative and anti-inflammatory properties can mitigate skeletal muscle loss. Recently, our lab explored the anti-atrophic potential of CiNA in oxidative stress-induced myotube atrophy. To examine the protective impact of CiNA under inflammation-induced atrophic conditions as well, C2C12 post-differentiated myotubes were treated with TNFα (25 ng/ml, a pro-inflammatory cytokine) in the presence or absence of CiNA (50µM). Our data show that TNFα treatment induced atrophic effect (i.e. thinning of myotubes and a decrease in the fusion index), which were prevented by 4h pre-administration of CiNA. Furthermore, the decreased level of ROS, achieved by modulating the altered antioxidant defense system, also underscores the protective effect of CiNA even in the presence of inflammation in cultured C2C12 myotubes. Altogether, our initial study provides insights into the multi-targeted approach of CiNA in mitigating skeletal muscle loss.

Keywords: C2C12 myotubes, Cinnamon, TNFα, CiNA

P-6

"Green Synthesis of Dihydropyranopyrazole Derivatives at Elevated Temperatures"

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Abstract:

In this study, we have reported here the synthesis of dihydropyranopyrazole by the condensation of suitable aldehyde, phenyl hydrazine, malononitrile and ethyl acetoacetate in the presence of sodium ascorbate as catalyst and Polyethylene glycol(PEG) as solvent under reflux conditions at 80-85 ℃. This reaction leads to the formation of dihydropyranopyrazole derivatives, which have significant interest due to their potential biological activities. The study include comprehensive Mass and Infrared Spectroscopy data providing valuable insights of molecular structure of the synthesized compounds. This aspect of the study aims to assess of the potential pharmacological properties of the synthesized compounds, which could have applications in drug discovery and medicinal chemistry.

Keywords: Dihydropyranopyrazole derivatives, sodium ascorbate, PEG, Mass Spectrometry, IR Spectroscopy, drug discovery, Medicinal chemistry.

P-7

In vitro Assessment of Antioxidant and Anticancer Potential of *Tinospora cordifolia* Leaf Extract

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Since time immemorial, herbal medicines have been used for combatting various diseases and are now seen as a safer alternative against currently used drugs that come with a myriad of adverse effects, or protect against those adverse effects when co-administered, as clearly seen in the case of cancer. *Tinospora cordifolia* is an ayurvedic medicinal plant with manifold pharmacological properties, which makes it useful for treating an array of diseases.

The leaves of *Tinospora cordifolia* were dried, pulverized into fine powder and subsequently, the hydro-methanolic extract was prepared using Soxhlet extraction method. The phytochemical screening and qualitative analysis was done using preliminary biochemical tests, FTIR, and thin-layer chromatography which confirmed the presence of its bioactive phytocomponent Tinosporin in the extract. The quantitative estimation of phenols, flavonoids and tannins in the extract showed its abundance. The excellent antioxidant activity of the extract was proved by various assays like DPPH, ABTS, Nitric oxide and Superoxide anion scavenging assays. The toxicity of the extract was investigated, and confirmed non-toxic by Brine shrimp lethality assay whereas the anticancer activity of the extract was determined through MTT assay using MCF-7 and HCT-116 cell lines. The extract exhibited inhibition of proliferation of both cancer cells.

The results of this study prove that *Tinospora cordifolia* has a diverse range of phytochemicals with vital medicinal properties and can be used as a potential therapeutic drug for the treatment of cancer.

P-8

Organocatalytic Photoinduced Carboamination of Dienes

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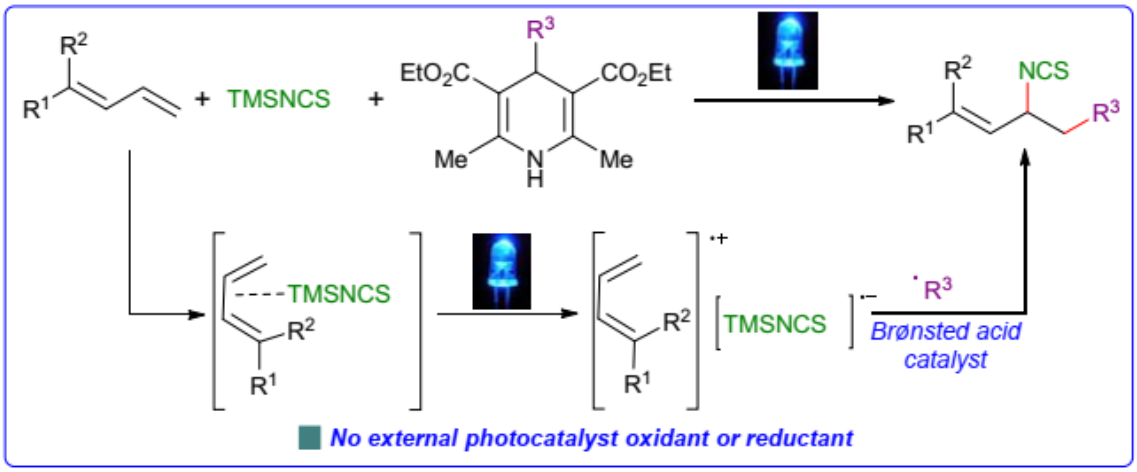
Email: arunyadav092@gmail.com

Abstract:

An organocatalytic photoinduced 1, 2-carbofunctionalization strategy for conjugated dienes has been developed. No exogenous photocatalyst or additive are required in this mild protocol and it allows for highly regioselective and efficient 1, 2-carboisothiocyanation through coupling of diene, alkyl radical and TMSNCS.The reaction is proposed to proceed through EDA complexation between diene and TMSNCS.



Keywords: reaction through EDA complex, no external photocatalyst, oxidant or reductant

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P-9

"Green Synthesis and Biological Studies of 5-(Trifluoromethyl)-4,7-Dihydro [1,2,4] triazolo[1,5-a]Pyrimidine-6-Carboxamide Based Hybrid Molecules as *Plasmodium Falciparum* DHFR Inhibitors"

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[1]Ashok & Rita Patel Institute of Integrated Studies and Research in Biotechnology and Allied Sciences, Affiliated to CVM University, Vallabh Vidyanagar-388120, Gujarat, India.

ABSTRACT:

New 5-(trifluoromethyl)-4,7-dihydro [1,2,4] triazolo[1,5-a] pyrimidine-6-carboxamide derivatives have been synthesized by the combination of 3-amino-1,2,4-triazole, aldehyde and N-substituted acetoacetanilide in the presence of thiamine hydrochloride (VB_1) catalyst. The antimalarial activity of obtained products were evaluated against P. *falciparum.* In this study, thirty 5-(trifluoromethyl)-4,7-dihydro[1,2,4]triazolo[1,5-a]pyrimidine-6-carboxamide derivatives were prepared and subjected to an anti-malarial study using molecular docking study, out of which five compounds AMP-19, AMP-24, AMP-27, AMP-28, and AMP-29 showed good activity against P. *falciparum* and their IC_{50} values range from 0.068 to 0.092 µg/mL, nearly equal to those of the antimalarial drugs pyrimethamine and chloroquine (IC_{50}=0.25, 0.02µg/mL). Further, molecular docking and 3D-QSAR investigation using CoMSIA/CoMFA contour map suggested that P*f*-DHFR enzyme binds efficiently with AMP-24 and AMP-27 structures with the lowest binding energy and high score value.

P-10

Ethanol Gas Sensing Properties of La doped α-Fe_2O_3 nanoparticles

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[2]*Department of chemistry, Mahatma Jyotiba Fule Arts, Commerce and Science College, Bhatkuli, Dist. Amravati (M.S) India*
[3]*Department of Physics, R.D.I.K.N.K.D. Badnera-Amravati (M.S) India*

Abstract:

In the present work, thick film of nanostructured La doped (5 wt%, 7 wt% and 10 wt%) α-Fe_2O_3 were synthesized by sol-gel citrate method. The structural properties of La doped α-Fe2O3 nanoparticles were analysed using x-ray diffractometer (XRD) and scanning electron microscope (SEM). The minimum crystallite size of 7 % La doped α-Fe_2O_3 calculated from Scherrer's formula is found to be around 40 nm. The sensitivity of 7% La doped α-Fe_2O_3 to reducing gases like acetone, ethanol, H_2S and LPG was been compared. 7% La doped α-Fe_2O_3 is adopted to improve the gas sensitivity of pure α-Fe_2O_3, especially to enhance the response to ethanol gas. The maximum values of sensitivity and percentage sensor response were found at an operating temperature 180^0C of ethanol gas. The quick response and fast recovery are the main features of this sensor. The effects of microstructure and additive concentration on the gas response, selectivity, response time and recovery time of the sensor in the presence of ethanol gas were studied and discussed.

Keywords: Sensitivity; Gas Sensor; Sol-gel method; Nanomaterials

P-11

Bioactive compound of cinnamon and garlic guard chemotherapy-induced cachexia

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Abstract

Chemotherapeutic agents, a common approach used for their anti-cancer effects, can also lead to a variety of complications, including cachexia characterized by loss of muscle mass and strength due to alteration in protein metabolism. Till date, there is no approved treatment available against chemotheraphy-induced cachexia. In the present study, we explored the anti-chemotheraphy-induced cachectic effect of bioactive compounds of cinnamon (CiNA) and garlic (S-ACys) on cisplatin/doxorubicin-induced myogenesis in skeletal muscle specific cells i.e.C2C12. Myoblast (C2C12 undifferentiated cells) were treated with cisplatin/doxorubicin in the presence or absence of CiNA/ S-ACys. Initial morphological data show that during myogenesis (muscle formation process, 0-72h), 8h pre-administration of CiNA (100□M)/ S-ACys (200□M) prevents the negative effect of cisplatin (50□M)/doxorubicin (0.1□M & 0.15□M) and helps in the formation of healthy myotubes (C2C12 differentiated cells) after 72h incubation in cultured differentiation media compared to cislatin/ doxorubicin-treated C2C12 cells. Our initial data suggests that CiNA and S-ACys may represent possible potential compounds against cisplatin/doxorubicin-induced cachexia.

Keywords: Chemotheraputic agent, C2C12 myotubes, myogenesis, Cinnamon, Garlic

P-12

"Synthesis and Characterization of chalconyl ester homologous series with different lateral and terminal group"

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Abstract:

A chalconyl ester homologous series α-4-(4'-n-alkoxy-3'-methoxy benzoyloxy) benzoyl-β-3",4"-dimethoxy phenyl ethylene is synthesized and studied with a view to understand and establish the relation between molecular structure and mesomorphism. The new homologous series consists of twelve homologous (C_1 to C_8, C_{10}, C_{12}, C_{14} & C_{16}) and show mesomorphic in nature. The members of the series were characterized by IR, NMR, Mass, and Optical polarizing microscopy with a heating stage. The mesomorphic properties of the present series are compared with other structurally related series.

Keywords: Chalconyl ester, Mesomorphism, Homologous, Mesomorphic, Homologues

P-13

Paclitaxel-BODIPY Carrier Free Heterodimeric Nano-Prodrug as versatile Nanoplatform for Cancer Chemotherapy and Bioimaging.

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[b]Department of Chemical Sciences and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research, Kolkata, West Bengal, India.
[c]Academy of Scientific and Innovative Research (AcSIR), CSIR-Human Resource Development Centre, Ghaziabad, Uttar Pradesh 201 002, India
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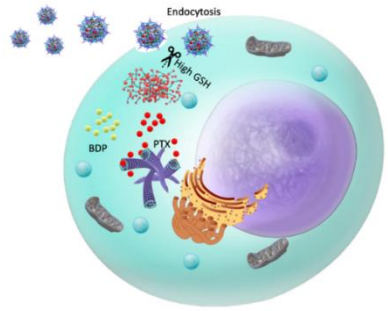

ABSTRACT

All Anticancer drugs as they have a very narrow therapeutic window, show many side effects and toxicity to healthy tissue[1]. Most anticancer drugs are hydrophobic, low bioavailable and nonspecific in their actions, which reduces their use in cancer management[2]. Target-specific drug delivery with improved bioavailability, low side effects as well as real-time imaging and monitoring drug release in biological systems, is still a huge challenge in cancer management. Recently emerging dimeric prodrug-based strategy can overcome these issues especially when coupled with nanotechnology[3]. With the advantages of passive tumour targeting by the EPR Effect, high drug loading capacity and spatiotemporal drug release, such prodrugs can greatly enhance the benefits of chemotherapy[4]. Here, we develop an activable fluorescent dimeric nano-prodrug (PTX-SS-BDP NPs) by taking advantage of tumorous heterogeneity. Paclitaxel (PTX) and BODIPY (BDP) are covalently conjugated through the disulphide bond which acts as a glutathione-responsive linker, for fluorescence imaging-guided chemotherapy. The drug conjugate, PTX-SS-BDP was converted into a stable nanoparticle by co-assembling it with DSPE-PEG_{2K} using a simple nanoprecipitation method. The emerging nano platform will contribute to the visual chemotherapy tool, by virtue of refined cellular imaging and real-time action of chemotherapeutics through fluorescence.

KEYWORDS: Heterodimeric Prodrug, bio-Imaging, Theragnostic, Chemotherapy.

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P-14

"An unconventional synthesis and characterization of nitrogen and oxygen infused heterocyclic compounds with anticancer activity"

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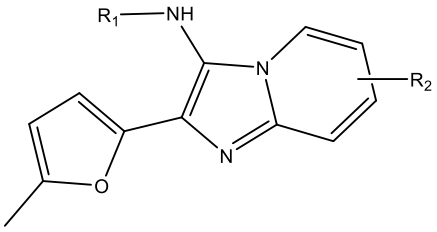
Abstract:

Heterocyclic compounds have emerged as promising agents in the realm of medicinal chemistry for their potential as anticancer agents. These compounds exert their anticancer properties by modulating various cellular processes and interacting with crucial biological molecules, such as DNA and proteins. Among these, nitrogen and oxygen containing heterocyclic compounds have garnered significant attention for their versatile applications in cancer therapy. In this study, we have reported here the synthesis of imidazo[1,2-a]pyridine-furan hybrids via the Groebke-Blackburn-Bienayme multicomponent reaction method, employing PEG 400 and microwave irradiation. We further investigate the anticancer efficacy of these compounds against NCI-60 Cell lines. Harnessing the potential of imidazo[1,2-a]pyridine-furan hybrids may have the way for more precise and efficacious cancer treatments in the future.



Keywords: Heterocyclic compound, Imidazo[1,2-a]pyridine-furan, Groebke-Blackburn-Bienayme Reaction, PEG 400, Microwave irradiation, Anticancer agent

P-15

ARGYROPHILIC NUCLEOLAR ORGANIZER REGIONS STAINING BY SILVER NITRATE FOR HPV DETECTION

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[2] *Multi-Disciplinary Research Unit, Shri M. P. Shah Government Medical College, Jamnagar.*
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Introduction:

Cervical cancer is one of the most common disease and it accounts for 16 to 29% in India of total cervical cancer cases occurring globally. There are various screening techniques available such as visual inspection, colposcopy testing, and cervical cytology screening has been found effective in reducing incidence of the disease. Objective: Feasibility of different screening method has been assessed to find out the most suitable mode applicable and also to assess Argyrophilic nucleolar organizer regions (AgNOR) counts to discriminate high-risk and low-risk dysplasia cases. Materials and methods: The cervical smears for the study were collected from the Gynecology department of Shri M. P. Shah Government Medical College, Jamnagar. The cervical smears were collected in pairs, one for the specialized AgNOR staining and one for the PAP test. HPV by PCR was performed from smear sample. PAP test was performed by pathology department and results were collected. Result and discussion: 498 patients were screened for cervical lesions using Pap smear and AgNOR staining. 4 cases were confirmed using HPV by PCR. It was observed that the AgNOR dots were single larger and compact in the normal cervix. They appeared small and loosely arranged in the dysplastic and malignant lesions of the cervix. Sensitivity and specificity of AgNOR stain we found was 93.20% (95%CI: 86.50-97.22%) and 100% (95%CI: 99.06-100%) respectively. Conclusion: Alternative screening test of AgNOR is simple and cost-effective method and AgNOR can be used as proliferative marker. It is rapid, precise, and impartial compare to conventional techniques.

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P-16

Catalytic Enantioselective Synthesis of Aryl–Methyl Organophosphorus Compounds

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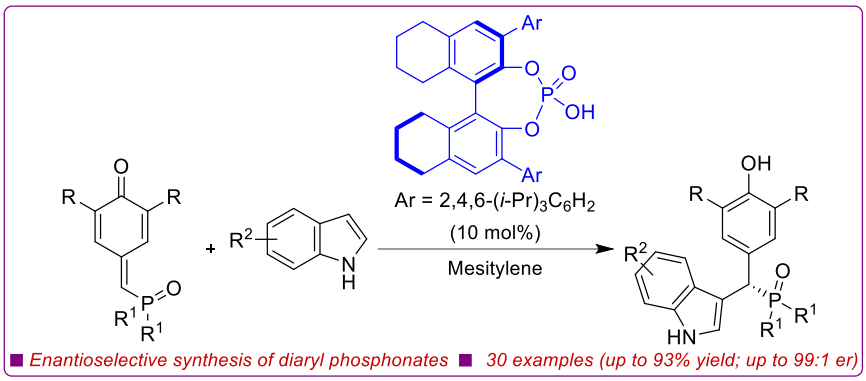
Abstract:

A catalytic enantioselective protocol for the synthesis of aryl–methyl organophosphorus compounds is reported. Uti-lizing a chiral phosphoric acid as a catalyst, a wide range of indole derivatives reacted with phosphorylated quino-methanes in high yield with excellent enantioselectivity. This is the first report on application of phosphorylated quinomethanes in asymmetric synthesis.



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P-17

Rhodium-Catalyzed Regioselective C7$_{Ar}$-Functionalization of Tryptophan with Quinones and its Late-Stage Peptide Exemplification

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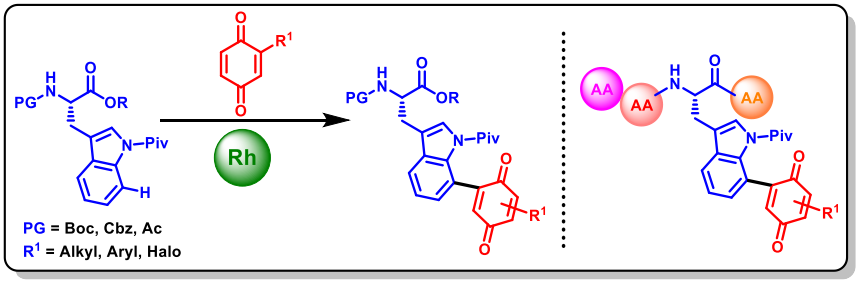
Site-selective modification of peptides and proteins has now become an established practice for modulating their metabolic stability towards proteolytic enzymes, and eventually improving their pharmacological properties [1]. Such reformed biologics have been successfully employed in cellular tracking, diagnostics, imaging and drug therapeutics [2]. However, the transformation of native proteins into engineered proteins that requires selective functionalization at the amino acid side chain(s) while conserving the structural integrity of remaining peptide fragment, exemplifies a formidable mission. Consequently, chemical manipulation of lesser-abundant proteinogenic tryptophan (Trp) residue, which constitute an integral part of numerous natural-products and native proteins has been specifically targeted in recent past [3]. These strategies have manifested designer Trp-containing peptides and proteins with minimum undesired isoforms. In this expedition, Trp-based unnatural amino acids/peptides have been successfully prepared *via* arylation, sulfenylation, alkylation, allylation, alkynylation, difluoralkylation, trifluoromethylation and macrocyclization at C2$_{Ar}$-H position of indole moiety *via* transition metal-catalyzed or metal-free thermal/photocatalytic approaches [4]. While, the C7$_{Ar}$-H functionalization in tryptophan and tryptophan-containing peptides are limited to boronation by Movassaghi's group, amidation by Ackermann's group, alkylation by Shi & Wang's group and maleimidation by Zhu, and recently by Wang and Liu's group [5]. In pursuit of novel C-H functionalization strategies on amino acids and peptides, we successfully developed a Rh^{III}-catalyzed strategy for the pivolyl-directed C(sp^2)-H alkenylation of protected tryptophans with alkyl and aryl decorated benzoquinones to afford a series of benzoquinone-appended tryptophan based unnatural amino acids and peptides in good yields.



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P-18

The Effect of Laterally Substituted Methoxy -OCH_3 Group on Mesomorphicity

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Abstract:

To understand structure-activity relationship, comparative A study of newly synthesised homologous series with structurally similar known homologous series is carried out. Newly synthesised homologous series 1 to 7[6-12] and selected other series-X and -Y for comparative study, resemble to each other in all respect i.e., two phenyl rings, central bridge -COO-, right-handed tail -CH=CH-COOR, left n-alkoxy end-group for the same homologue, but differs with respect to laterally substituted -OCH3 group. Especially this study is focused to understand the effect of laterally substituted methoxy group on mesomorphicity. Different liquid crystalline properties (viz. type of mesophase, mesophase length, and relative thermal stabilities, upper transition temperatures etc are mutually compared. 1) Presence and/or absence, 2) Size 3) Position and 4) Polarity of laterally substitution of methoxy group affect the mesomorphic characteristics of similar type compounds. A phenomenon of mesomorphism is very sensitive and susceptible to molecular structure of a substance. Present comparative study supports the views and conclusions drawn earlier.

Keywords: Smectiogenic, nematogenic, mesophaselength, polarity, steric effect, structure-activity relationship

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P-19

New Directions in Diene Functionalization: Regioselective Hydroalkoxylation and Hydroxyperoxidation of 1-Aryl/Alkyl-1,3-dienes

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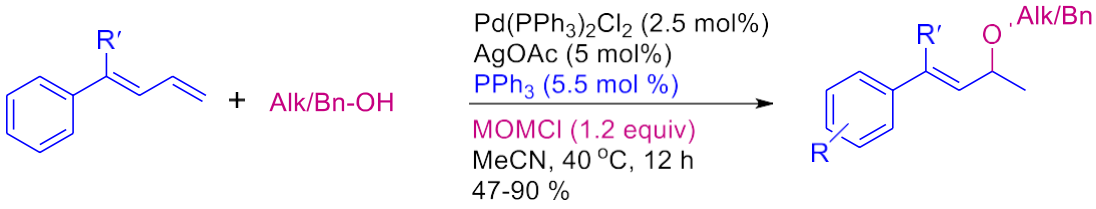
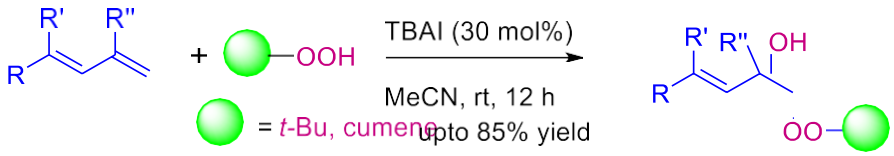
Abstract:

We have developed efficient and regioselective methods for hydroalkoxylation and hydroxyperoxidation of 1-aryl/alkyl-1,3-butadienes. In the first case the reaction was catalysed by Pd-catalyst and additive chloromethyl methyl ether (MOMCl) to deliver allylic alkoxylated products (Scheme 1).[1] Secondly, a new method has been developed for the selective production of 4-aryl/alkyl-1-peroxy-but-3-en-2-ols from 1- substituted-1,3-butadienes (Scheme 2).[2] This process uses hydroperoxides with TBAI as the catalyst. It is distinguished by its simplicity because it doesn't require dry conditions and can work with a variety of substrates to produce hydroxyperoxidates in good yields. Both the methods developed illustrate excellent regioselective hydroalkoxylation and dioxygenation in a diene system.



Scheme 1. Hydroalkoxylation of dienes.



Scheme 2. Hydroxyperoxidation of 1-aryl/alkyl-1,3-dienes.

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P-20

Synthesis of thiazolidin-4-one bearing pyrimidine analogues by Microwave irradiation and their *in vitro* antimicrobial, antituberculosis, antimalarial and anti protozoal studies

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Abstract:

Synthesis of biologically active thiazolidin-4-one by microwave irradiation method and evaluate against different species of bacteria, fungi and protozoa is aim of this study. Microwave irradiation method is serviceable for rapid and sustainable synthesis. Thiazolidin-4-one is a valuable motif because of its broad-spectrum biological evaluation. It is famous for many types of biological profiles, mainly antimicrobial, anti-tuberculosis, antihypertensive, hypoglycemic agent and antimalarial [1-4]. This biological response leads our attention towards the change of Thiazolidin-4-one skeleton to enhance potential. Present study aims to carry out a rapid synthesis of Thiazolidin-4-one derivative of pyrimidine by microwave-assisted heating. All newly synthesized motifs were characterized by spectral analysis (IR, ^{1}H NMR, ^{13}C NMR) and screened for different biological profile. The excellent biological response of the compounds was observed.

Keywords: Pyrimidine, Thiazolidin-4-one, Antituberculosis, Antimicrobial, Anti protozoal

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P-21

Synthesis of novel Diclofenac N-Derivatives as Therapeutic Agents

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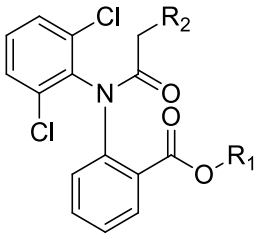
ABSTRACT:

Diclofenac sodium is well known for their therapeutic use as a nonsteroidal anti-inflammatory drug. However, it is associated with some adverse effects like gastrointestinal toxicity and severe liver injury. Numbers of diclofenac analogues were synthesized involving functionalization of the acid group of drug moiety, but modification on the secondary amine of diclofenac is much more limited. In order to develop new N-substituted Diclofenac analogues, herewith we are reporting a series of diclofenac N-substituted derivatives. The structure of the synthesized derivatives was confirmed by various analytic techniques like Mass, IR and NMRs. The detailed report will be presented in a poster.



R1 = H, Me, Et etc
R2 = Various secondary amines

P-22

Exploring the Antimicrobial Potential of *Cynodon dactylon*: Phytochemical Profiling and Efficacy Against Pathogenic Organisms

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Cynodon dactylon is rich in diverse phytochemical compounds, showcasing antimicrobial properties against pathogenic organisms. The pharmaceutical industry increasingly relies on medicinal plants to develop alternative drugs combating drug-resistant pathogens. This study focused on exploring the antimicrobial potential of *C. dactylon*, a perennial plant. To assess bioactive compounds' antimicrobial efficacy, three solvents (methanol, acetone and water) were employed. Qualitative and quantitative phytochemical tests revealed over 10 secondary metabolites, including alkaloids, glycosides, flavonoids, saponins, tannins, phytosterols, terpenoids, carbohydrates, and reducing sugars. Antimicrobial assays against pathogenic organisms such as *E. coli, Streptococcus aureus, Klebsiella pneumoniae, Bacillus,* and *Aspergillus niger*, using the well diffusion method, demonstrated significant antimicrobial activity in all extracts. Particularly noteworthy was the broad-spectrum antimicrobial efficacy observed in the methanolic extraction, suggesting potential effectiveness against diverse pathogenic microbes. Further research is essential to isolate and identify specific bioactive compounds responsible for these antimicrobial effects. In conclusion, *C. dactylon* extract emerges as a promising antimicrobial agent, holding potential for the development of substances to treat microbial infections.

Keywords: Antimicrobial compounds, Extraction, Phytochemical tests, Antimicrobial activity, Pathogens.

P-23

Rapid analytical technique for determining pendimethalin and metribuzin in suspoemulsion formulation

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Pendimethalin and metribuzin are combined to generate a suspoemulsion (SE) herbicide that is used as a preemergence and early postemergence herbicide. For the simultaneous measurement of metribuzin and pendimethalin in suspoemulsion formulation, a reverse phase high performance liquid chromatography technique was validated and used. The method used an acetonitrile:water (65:35v/v) mobile phase with a flow rate of 1.0 mL/min and quantitation at 237 nm. The approach was developed and validated using a Hypersil ODS column. The RTs of metribuzin and pendimethalin were determined to be 3.6 and 11.9 minutes, respectively. Metribuzin and Pendimethalin had detection limits of 0.03 mg/l and 0.04 mg/l, respectively. Metribuzin and pendimethalin have quantitative limits of 0.09 mg/l. The suggested method's linearity was evaluated in the ranges of 2.51 to 100.54 mg/l and 0.25 to 9.80 mg/l for pendimethalin and metribuzin respectively. For pendimethalin and metribuzin, the percentage recovery ranged from 99.8 to 100.1% and 99.8 to 100.3, respectively. According to the modified Horwitz equation, the % RSD values for intraday precision study and interday precision study for metribuzin and pendimethalin were <2.22 and <1.57, respectively, as required by SANCO. According to SANCO criteria, the method's performance was verified in terms of selectivity, specificity, precision, linearity, accuracy, LOD, LOQ, and robustness. For the first time, a simple and quick reverse phase high performance liquid chromatography method for the simultaneous measurement of pendimethalin and metribuzin in SE formulation is described in this work.

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P-24

Synthesis of Pyrimido[4',5':3,4] pyrazolo[1,2-b]phthalazine-4,7,12-triones and their *In silico* Docking Studies

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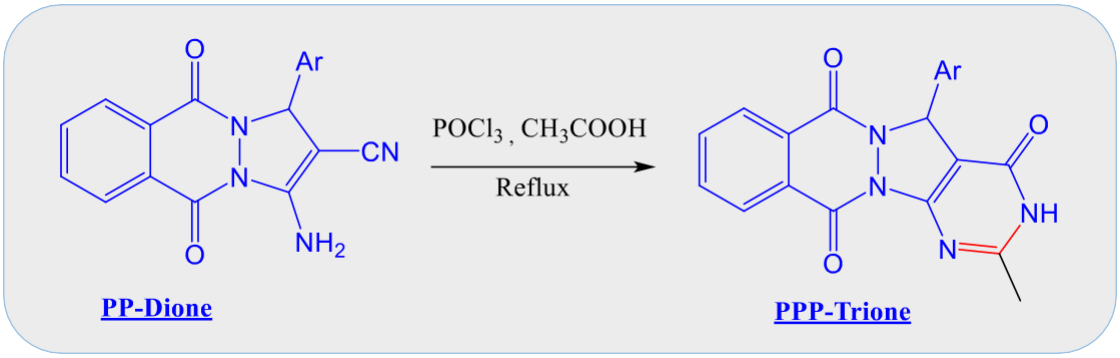
Abstract:

Pyrazole and 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, antifungal, anti-inflammatory, antibacterial, and antipyretic properties. Due to these significant characteristics, our research group has been interested in creating such heterocycles and investigating their synthetic methodologies. Thus, this new pyrimido- pyrazolo-phthalazine-trione (PPP-Trione) derivatives were synthesized by reacting pyrazolo- phthalazine-dione (PP-Dione) with acetic acid in the presence of well-known chlorinating agent POCl3 under the reflux condition. Previously limited derivatives were synthesized by Hosseininasab et al.[1]. Herein, we report additional derivatives of PPP-Trione. The starting materials PP-Dione were 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]. Here, we also investigated the in-silico docking study of the PPP-Trione derivatives. The scheme of the reaction is given below:



PP-Dione PPP-Trione

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P-25

Evaluation of JAK Inhibitor in Modulation of Astrocyte Expression in Scopolamine-induced Cognitive Impairment Model in Rats

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Alzheimer's disease (AD) is a neurodegenerative disorder that impairs memory and cognitive function. The pathology includes loss of cortical and subcortical neurons, and cerebral atrophy caused by the proliferation of neurofibrillary tangles of tau and amyloid-beta plaques. Scopolamine antagonizes muscarinic acetylcholine receptors and causes neuroinflammation and neurodegeneration. JAK inhibitors prevent the phosphorylation of key proteins involved in the signal transduction that leads to immune activation and inflammation. This study was undertaken to evaluate the neuroprotective potential of JAK inhibitors through modulation of astrocyte expression and neuroinflammation. Scopolamine (2 mg/kg, IP for 6 weeks) was utilized to induce cognitive impairment in rats. 3 doses of JAK inhibitor were administered orally for 4 weeks. Donepezil served as the reference standard. The percentage time spent in the closed arm of the modified Y Maze and discrimination index in the novel object recognition test was found to be significantly reduced ($p<0.05$) in the DC group as compared to the treatment animals. Scopolamine administration significantly increased ($p<0.05$) the levels of interleukin-6 and GFAP immunoreactivity which revealed astrogliosis and neuroinflammation which was found to be decreased in the investigational drug group. The histopathological evaluation showed that the DC group showed marked morphological changes which were found to be improved in the treatment groups. It can be concluded from the results that the JAK inhibitor ameliorated memory and cognitive impairments by reducing astrogliosis and neuroinflammation and thus possesses neuroprotective potential. Further studies are warranted for the elucidation of mechanistic pathways.

P-26

Role of Probiotics and Pharmabiotics in Clinical Diseases

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Abstract

Probiotics are live microorganisms such as bacteria & yeast, which play a significant role in exerting a beneficial impact on human health when administered in enough amounts. Intestinal microflora composition plays a vital role in various pathological conditions by altering gut microflora. Probiotic products with pharmacological action in health and diseases are known as pharmabiotics, mainly developed for therapeutic purposes. Pharmabiotics are still under development, but they have shown promise in treating various diseases. Probiotics and pharmabiotics are effective in the treatment and prevention of a wide range of clinical diseases, including Diarrhea, Inflammatory bowel disease (IBD), irritable bowel syndrome(IBS), Eczema, Allergies, Cardiovascular disease, Cancer, Obesity, Diabetes, Mental health condition, Gastrointestinal disorders, Infectious diseases, Metabolic disorders, and Neurological disorders.

A variety of pharmabiotic strategies, such as the use of specific members of the microbiota, their surface components, or metabolites, as well as genetically modified commensal bacteria, are being investigated for their ability to enhance the beneficial components of the microbiota. Probiotics and pharmabiotics are generally safe and well tolerated for most people. Nowadays, the widespread high throughput technology helps us assess microorganism communities that inhibit the gut microbiota. In recent years, increasing evidence has shown the modification of gut microbiota by using probiotic products as current treatments for various diseases. Clinical trials and *in vivo*, experiments give ideas about probiotics and pharmabiotic role in shaping the balance in intestinal microbiota & improve overall wellness.

In the present study, we have isolated potential probiotic bacteria from fruit sources and evaluated their probiotic properties to identify potential probiotic candidates that may be further helpful in several clinical diseases.

Keywords: Gut microflora, Pathological condition, Clinical trial, Pharmabiotics, Probiotics

P-27

3D-QSAR Studies, Molecular Docking, Molecular Dynamic Simulation, and ADMET Proprieties of Novel *Pf*DHODH Enzyme as *Pf*DHODH Inhibitors for the Treatment of Malaria

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Abstract:

This research explores new possibilities for antimalarial drugs by focusing on the *Plasmodium falciparum* Dihydroorotate Dehydrogenase (*Pf*DHODH) enzyme, a critical enzyme in the parasite's pyrimidine biosynthesis pathway. Unlike humans, the malaria parasite cannot salvage pyrimidines, making *Pf*DHODH an ideal target [1–3]. The study combines various techniques, including 3D-QSAR, molecular docking, molecular dynamics (MD) simulations. A dataset of 99 triazolopyrimidine derivatives was examined using CoMFA and CoMSIA models. PLS analysis provided statistically validated results for CoMFA (r^2_{ncv} = 0.952, q^2 = 0.634, r^2_{cv} = 0.652) and CoMSIA (r^2_{ncv} = 0.942, q^2 = 0.761, r^2_{cv} = 0.673) models. The two models that were established suggested R^2_{pred} = 0.683, and R^2_{pred} = 0.767, respectively. The relations between the different features and activities were well demonstrated by the contour maps of the CoMFA and CoMSIA models. Molecular docking identifies key binding sites in the *Pf*DHODH protein (PDB code: 6I55) and highlights specific residues, such as Arg265, His185, Tyr528, Phe188, Phe227, and Ile263, as crucial for inhibitor binding. The results from MD simulations confirm the stability of these inhibitors within *Pf*DHODH's active sites over a 100 ns duration, reinforcing their potential as effective inhibitors. Additionally, when we checked the compounds for their ADMET properties we found that 25 our designed triazolopyrimidine derivatives showed promising results that make them potential candidates for antimalarial drugs. In summary, this research provides a robust approach for the design and of *Pf*DHODH inhibitors as novel leads for the treatment of malaria, offering hope in the fight against this deadly disease.

Keywords: 3D-QSAR; *Pf*DHODH inhibitors; molecular docking; dynamic simulation; antimalarial

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P-28

Antimycotic sensitivity evaluation and synthesis of 1,2,4-triazole containing pyrimidine analogous

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Abstract:

A large number of 1,2,4-triazole, a heterocyclic derivative exhibits important therapeutic activities such as antifungal, anticonvulsant, anti-tubercular, antioxidant, anti-inflammatory, anticancer and antimicrobial activity[1-5]. Furthermore, 1,2,4-triazole ring system has been incorporated into a wide variety of therapeutically interesting drug candidates like ribavirin (antiviral agent), rizatriptan (antimigraine agent) and fluconazole, itraconazole (an antifungal agent)[6]. Thus, there is a need to explore these pharmacophores for the development of novel molecules with different activities. Present work deals with the synthesis of 1,2,4-triazole clubbed pyrimidine analogous derived from 1,2,4-triazole . Newly synthesized compounds were characterized by spectral studies (IR, ^{1}H-NMR and ^{13}C-NMR). They were screened for their antimycotic activity and compared with standard drugs.

Key words: 1,2,4-triazole, Pyrimidine, Antimycotic study

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P-29

Phytochemical Characterization of Two Marketed Anti-urolithiatic Herbal Formulations

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Urolithiasis is the formation of stone in the human urinary system and it is a very common and painful disease. Recently there is an increased interest in the alternative and traditional system of medicine for the management of urolithiasis using herbal drugs and Ayurvedic formulations.
Many medicinal plants are used to treat kidney stones and the most commonly used plants are *Bergenia ligulata*, *Boerhavia diffusa*, *Crataeva nurvala*, and *Tribulus terrestris.*
Two marketed formulations which are containing some of these plants and are commonly used for kidney stone treatment were selected for phytochemical characterization and estimation of bioactive constituents. The reported plants contain significant amount of phenolics, flavonoids and triterpenoids which are responsible for the activity so it was thought worthwhile to estimate these constituents in the selected marketed formulations. Phytoconstituents like Quercetin, Lupeol, Rutin, and Gallic acid were mainly estimated in the selected formulations.[1]
The two market products were analysed for Ash value, extractive value, LOD, total phenolic estimation and total flavonoid content. The extracts of the marketed formulations were estimated by HPTLC densitometric scanning method for estimation of active phytoconstituents. After several TLC trials, Toluene, ethyl acetate, methanol, and formic acid in the ratio of (6.6: 6.6:5.3:1.3) were selected as mobile phase for Quercetin and Gallic acid in formulation II, Toluene:Ethyl Acetate:Formic Acid (5:4:1) for Gallic acid in Formulation I, Butanol:Acetic Acid :Water (7:7:7) for Rutin in both formulations, and Toluene:Ethyl Aetate:Formic Acid:Methanol (7:6:1:2) for lupeol in Formulation II. Thus, the major phytoconstituents which are responsible for the activity in both the marketed formulations were estimated by HPTLC.[2]

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P-30

Synthesis and Characterization of Schiff Bases Containing Quinazolinones as Potent Biological Scaffolds

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ABSTRACT

Similar to aliphatic or aromatic compounds, heterocyclic molecules have a chemistry that makes sense. It is believed that heterocyclic molecules and their derivatives, which have become important drug moieties, are the basis of medicinal chemistry research. A number of unique (E)-3-(substituted benzylideneamino)-8-methyl-2-(p-tolyl) quinazolin-4(3H)-one molecules were synthesized in the proposed investigation using benzoxazinone. In order to avoid the issue of ring opening, which is frequently experienced when synthesizing quinazolines from benzoxazinone, we changed the method for the synthesis of 3-amino-8-methyl-2-(p-tolyl) quinazolin-4(3H)-one to a fusion reaction at 100° to 140° C with hydrazine hydrate solution and separated by water. These newly synthesized Schiff bases were characterized using IR, 1H NMR, 13C NMR, MASS spectrum data, and elemental analyses. A wide variety of antimicrobial potential is introduced by the synthesis of quinozolinone derivatives employing amine group substituted benzoic acid derivatives as starting materials.

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P-31

Synthesis, antimalarial and antiprotozoal evaluation of 1, 2, 4-triazole containing pyrimidine analogous

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Abstract:

To synthesize more biologically active motif of triazole is our ongoing effort. N-[4-(substituted phenyl)-6-(substituted aryl) pyrimidine-2-yl]-2-[(4H-1,2,4-triazol-4-yl)amino]acetamide (3A-J) were carried out by chemical processes like cyclization, condensation, purification and crystallization. Characterization of the entire newly synthesized compound were done by IR, 1H NMR, 13C NMR and mass spectral analysis and screened for antiprotozoal and antimalarial activities. Antiprotozoal activity performed on *L. mexicana* and *T. cruzi.* Antimalarial activity done on Plasmodium falciparum. Significant co-relation of these compounds were observed on the basis of statistical analysis was good. Newly synthesized compounds showed potent as antimalarial and antiprotoaoal Thus, there is a need to explore these pharmacophores for the development of novel molecules with different activities. Present work deals with the synthesis of 1,2,4-triazole clubbed pyrimidine analogous derived from 1,2,4-triazole. Newly synthesized compounds were characterized by spectral studies (IR, ^{1}H-NMR and ^{13}C-NMR).

Key words: 1,2,4-triazole, Pyrimidine, Antimalarial, antiprotozoal

P-32

Imidazolium-based Chemosensor for dual Detection of Al^{3+} and As^{3+}

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Aluminium in its ionic form (Al^{3+}) is found in abundance inside several biological tissues and natural water sources. Uncontrolled concentration of Al^{3+} has a detrimental impact on plant physiology and can result in the mortality of several aquatic organisms, including fish, bacteria, algae and other species inhabiting aquatic environments [1]. Human exposure to aluminium occurs as a result of its widespread utilization in food preservatives, storage and cooking utensils, as well as pharmaceutical products containing aluminium compounds [2]. Overconsumption of Al^{3+} has been found to result in disruptions of enzymatic, neurotransmitter and neurofibrillary processes within the central nervous system of organisms and the development of several diseases, including Parkinson's disease, Alzheimer's disease, microcytic hypochromic anaemia and dementia. Arsenic is the 20th most abundant element in earth's crust. The main source of arsenic exposure in the environment is ground water or drinking water [3][4]. The continuous exposure to arsenic is known to have harmful effect on human health, including the development of skin cancer, neurotoxicity, cardiovascular disorders and diabetes. Ion-tagged compounds are a fascinating class of organic materials because they have unique, tuneable features that come from a balanced ratio of cations and anions. Nevertheless, the limited solubility of chemosensors in aqueous solution poses a challenge to their utilization in biological and environmental sample analysis. Herein, a water-soluble imidazolium-tagged probe has been designed, synthesized and characterized. The probe displayed a turn-on fluorescence response on the addition of Al^{3+} and As^{3+} ions in aqueous medium.

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P-33

HIGH PERFORMANCE OF PALLADIUM DOPED MoO_3 FOR ADVANCE APPLICATION TOWARDS AMMONIA GAS SENSING

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Abstract:

The purpose of this study is to determine the effect of temperature on the microstructure of MoO_3 nanoparticles. The synthesis was carried out by using sol - gel citrate method followed by calcinations. The nanocomposite was characterized by means of x-ray powder diffraction to study the properties of pure and different wt % Pd. The structural XRD revealed monoclinic crystal structure of the MoO_3 thick films with high purity and highest crystal size of 54 nm. Additionally, sensor performance of undoped and surface modified by different wt % Pd over MoO_3 were studied under different operating temperature and different reducing gases such as NH_3, H_2S, CO and ethanol. The result reveals that material exhibit excellent sensitivity and selectivity toward ammonia gas at 180^0C proving their applicability in gas sensors.

Keywords: MoO_3, Pd, XRD, Sensitivity, Selectivity.

P-34

Design, Synthesis and Characterizations of Some New Series of Fused Pyrimidines for their Pharmacological Activity

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Fused pyrimidine derivatives have attracted significant interest in pharmaceutical industries as they were found to be effective for the treatment of many diseases such as antineoplastic, antiviral, antibacterial, expectorant, urinary tract infection, parkinsonism, anthelmintic, vasodilator, liver disorder, infections of the respiratory tract and ear, treatment of gastrointestinal roundworms, peripheral neuropathies and disorders associated with hyperuricaemia [1,2]. Keeping in view the above importance of pyrimidine heterocycles in various therapeutic areas and our continuous work [3] to design and synthesis of the novel pyrimidines based new chemical entities for biological significance; recently, we have designed, synthesized and characterized a series of some new fused pyrimidine derivatives. In this presentation, the detailed synthetic procedure and characterizations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

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P-35

Stability Indicating RP-HPLC Method for Assay of Flucloxacillin From Tablet Dosage Form

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Flucloxacillin is a semi-synthetic isoxazolyl penicillin class of antimicrobial drug. It can be used to treat bacterial infections caused by microorganisms. A simple and accurate stability indicating RP-HPLC method was developed to determine flucloxacillin sodium by using Inertsil ODS C_{18} column (150 X 4.6mm, 5µ). The mobile phase was phosphate buffer (pH 5.0) : acetonitrile (70:30 v/v) and the flow rate was 1mL/min. The column temperature was set at 25 °C and column eluent was monitored at 225 nm using PDA detector. The retention time of flucloxacillin was found to be 9.99 min. The method was validated as per ICH guidelines for various validation parameters. The method was found to be linear in the concentration range 10-150 µg/mL and the value of correlation coefficient was found to be 0.9999. The method was specific for flucloxacillin as there is no interference of impurity/degradant peak on flucloxacillin main peak. The method demonstrated good accuracy as the mean recovery value was found to be 97.56%. The method was robust and %assay was found to be with in the limit mentioned in the ICH guidelines. Degradation study of flucloxacillin was also performed under various stress degradation conditions i.e. acidic, alkaline, thermal, and oxidative stress degradation. The flucloxacillin found susceptible in all degradation conditions and showed degradation between 12.2 to 18.0 % in various degradation conditions.

P-36

Revolutionizing Agriculture with Nanotechnology: Rice-Based Silica Nanoparticles for the Remediation and Quantification of Toxic Heavy Metals in Potatoes

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Abstract

Today, metal pollution in agricultural soils poses a growing concern due to its potential health risks through the consumption of contaminated plants like potatoes. Heavy metal concentrations in the environment can exceed safe levels due to various human activities, including industrialization, mining, and agricultural practices. Consequently, potatoes and other vegetables may contain toxic heavy metals like Co, Ni, Pb, Cd, and Cr. Effective removal techniques are needed to mitigate these risks to food safety and human health. In this study, a simple and inexpensive green synthesis method is described to extract mesoporous silica nanoparticles taken from Navsari region "GNR-3 (Gujarat Navsari Rice – 3)" rice using the bottom-up approach for removal of toxic heavy metals contamination present in North Gujarat region Banaskantha district's special variety potatoes named "KUFRI BADASHAH". Rice husk (RH) calcinated to obtain rice husk ash (RHA) with high silica purity (>98% wt), as determined by the EDX analysis. Calcination at 650°C for four hours in a box furnace yielded RHA that was devoid of metal impurities and organic matter. The present study defines successfully minimization of toxic heavy metal contamination present in potatoes by employing silica nanoparticles (SNPs) as a biomass adsorbent and also includes all basic characterization of SNPs. The X-ray diffraction pattern showed a broad peak at 2θ≈22.1°C and was free from any other sharp peaks, indicating the amorphous property of the GNR-3 variety rice SNPs. Scanning electron micrographs (SEM) showed clusters of spherically shaped uniform aggregates of SNPs while transmission electron microscopy analysis indicated an average particle size of < 50 nm. Peaks in the Fourier transform infrared spectra were found at 1083.29 cm^{-1} and 795.48 cm^{-1}, corresponding to O-Si-O symmetric stretching vibration and O-Si-O asymmetric stretching, respectively. The Brunauer-Emmet-Teller, obtained value of 11.1984 m^2/g reflects the extent of surface available for adsorption. Concurrently, the pore size, a crucial factor influencing the accessibility of adsorption sites, was measured at 196.202 Å. The specific surface area of 11.1984 m^2/g suggests a considerable active surface for potential interactions, respectively. In conclusion, Agriculture waste-derived SNPs (Silica Nanoparticles) offer a compelling solution for the removal of toxic heavy metals from potatoes. This technique is characterized by its simplicity, as it leverages readily available agricultural waste materials, requiring minimal processing.

Keywords: Toxic heavy metals, potatoes, silica nanoparticles, rice husk ash, food product remediation.

P-37

Biological and catalytic applications of the newly synthesised and characterized benzothiazole-based Pd (II) metal complex in the Suzuki reaction

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Abstract:

N, N, O-donating ligand was prepared from the condensation of 2-amino benzothiazole with various aromatic aldehyde. Metal complex of this ligand is neither air nor moisture sensitive. The effects of varying solvents, bases and ligand/copper ratio on the performance of the coupling reaction were investigated. This method is a very simple, efficient and mild protocol for the cross-coupling of aryl bromides with arylboronic acids and the reactions proceeded effortlessly in excellent yields within short reaction times. All reaction were carried out in anhydrous condition. Antibacterial activity of synthesized compounds were tested against Gram-positive and Gram-negative strain.

Keywords: N, O, O donating ligand, Schiff Base, Antimicrobial activity, Suzuki reaction.

P-38

Sonochemical synthesis and characterization of rod-like nano-sized Cobalt (III) complexes and their application as textile dyeing agents

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Nanotechnology has gained interest in recent years due to its vast variety of applications and lucrative potential. So now a days, the synthesis of nanomaterials is a crucial field of study. These inorganic nanomaterials' morphologies have a significant impact on their characteristics. Out of numerous synthetic methods, the ultrasonic approach is particularly intriguing among them since sonochemistry itself is a sonoluminescence application, and it still has a variety of uses, including wastewater treatment, synthesis, and degradation. In this work, two nano-sized cobalt complexes, $[Co(NH_3)_5N_3](4\text{-np})_2.H_2O$ (1 N) and $[Co(NH_3)_5N_3](3\text{-np})$ (2 N) {np= nitrophenolate} were synthesized via sonochemical synthesis method and compared to their bulk counterparts, which were made under the same circumstances without ultrasounds. All the complexes were characterized by elemental analysis and spectroscopic techniques (UV–visible and IR). Morphology and particle size of nano-sized complexes was determined by SEM and Zeta-sizer respectively. The ions $[Co(NH_3)_5N_3]^{2+}$ and (4-np) create alternate organic-inorganic layers in the crystals that are stabilized by the O-H...O and N-H...O hydrogen bonds, according to the single-crystal X-ray diffraction of complex-1. Additionally, studies of the coloring abilities of nano-sized cobalt (III) complexes on silk and wool fibers revealed effective dyeing behavior.

Keywords: Sonochemical process, band gap energy, semiconductor, cobalt complexes

P-39

Marble Slurry Waste Material as Solid Support for Palladium-Catalysed Heck and Suzuki Reactions

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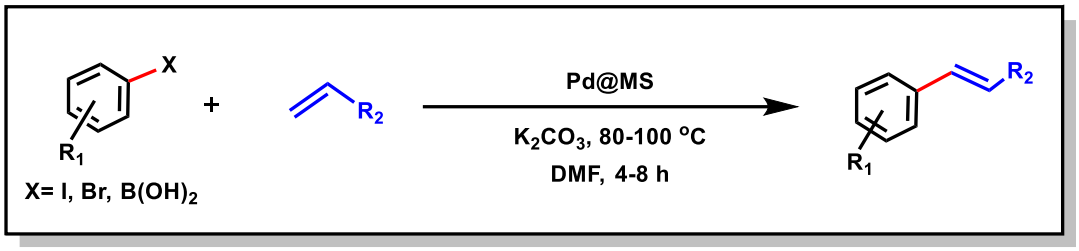
Abstract:

Solid supported catalysis is an excellent substitute to homogenous catalysis which offers many advantages mainly, recovery and recycling of the metal catalyst.[1,2] As far as sustainability is concerned, solid-supported catalysts are highly recommendable for the demand of modern chemical industry. Marble slurry (MS) waste material from marble processing industries can facilitate cost-effective and environmentally sustainable catalyst support for metal catalyzed organic transformations.[3] It is envisioned to use MS as catalyst support for palladium nanoparticles owing to its excellent adsorption capacity, large surface area and resistant to reaction conditions that can offer a waste-to-wealth concept. Mizoroki-Heck and Suzuki-Miyaura C–C coupling reactions are being very important in organic synthesis due to impressive outcome with high chemoselectivity under mild reaction conditions.[4,5] Herein, Pd@MS catalyst was prepared by modest wet impregnation method and used for ligand-free palladium nanoparticles catalyzed Mizoroki-Heck and Suzuki-Miyaura coupling reactions. The prepared catalyst is found to be very efficient and facile with maximum TON 4.13×10^2 and TOF 102 h^{-1} with good to excellent yields in aerobic conditions.[3] The catalyst was recuperated after each reaction and reused upto five catalytic cycles affording quite satisfactory stability.



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P-40

"Synthesis and characterization of thiazole compounds as biologically active agent"

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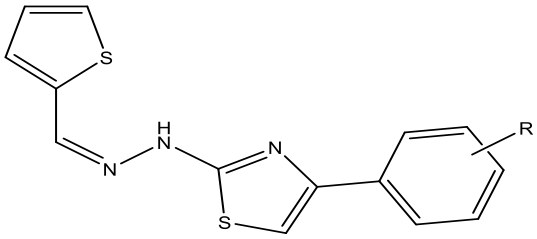
Abstract:

Thiazole derivatives have attached a great deal of interest due to their association with various kinds of biological properties found in many potent biologically active molecules such as ritonavir(an antiretroviral drug), sulfathiazole(antimicrobial drug), etc. due to its wide range of applications, consist of a core structure for the synthesis of a chemical library. We reported here the synthesis of thiazole derivatives(PMS-1 to PMS-10) by using a novel aldehyde, a scaffold from which a diverse range of other biologically active crucial new chemical entities could be generated. This aspect of the study aims to assess the potential pharmacological properties of the synthesized compounds, which could be applied in drug development and medicinal chemistry.



Keywords: Heterocyclic compounds, Thiazole derivatives, Pharmacological properties, Drug development, Medicinal chemistry

P-41

Multivariate Application of Post Synthetically Modified Co-Coordination Polymer Based on bis-pyridyldiamide.

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The reaction of Co(II) with N1 ,N3 - di(pyridine-4-yl)isophthalamide gave one-dimensional looped chain coordination polymer (CP1). Transmetalation reaction of CP1 with Cu(II) showed the formation of CP2 which is again a one-dimensional coordination polymer. Tauc plot calculations revealed that CP1 and CP2 have bandgaps of 2.41 eV and 1.30 eV, respectively. Photocatalytic dye degradation experiments reflected the change in optical bandgap reported between CP1 and CP2. It was observed that CP1 has much greater efficiency in degrading the dyes (Methylene blue, Methyl orange and Rhodamine B) as compared to that of CP1.Adsorption and desorption studies of Iodine was done by CP1 and CP2.In both the CP's the rate of reaction is found to be first order. Benzotriazole was incorporated as guest in CP1 and then impedance study was done.

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P-42

AGGREGATION INDUCED EMISSION-BASED PRODRUG FOR TARGETED DRUG DELIVERY

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Abstract:

In order to overcome the drawbacks and maximize the drug therapeutic potential, drug molecules are strategically modified to create prodrugs. Prodrugs are designed to undergo enzymatic or chemical changes after administration. The active medication is released as a result of these transformations at the intended site of action. Prodrugs have found use in a variety of therapeutic fields, such as the treatment of cancer, the control of pain, and the disorders of the central nervous system. Here, we have synthesized an AIE-based prodrug with real-time imaging and target selectivity[1]. Aggregation-Induced Emission (AIE) is a phenomenon that occurs in some molecules when they aggregate in a particular environment, dramatically increasing their fluorescence. An intriguing area of research uses this phenomenon to transport and activate medications using AIE-based prodrugs[2]. An AIE-based prodrug is one in which the AIE property is used to create a prodrug molecule that, when delivered, displays modest fluorescence but undergoes a certain biological transition to become highly fluorescent. This led to a significant increase in fluorescence, which can be visualized and monitored using imaging techniques. This fluorescence signal provides information about the prodrug's location and activation, allowing researchers and clinicians to track its distribution and therapeutic effects. The advantages of AIE-based prodrugs include enhanced drug delivery, targeted activation, and the potential for real-time monitoring through fluorescence imaging[3]. This concept is still an area of ongoing research and innovation, and its successful implementation requires a deep understanding of both AIE properties and the specific biological processes that can trigger prodrug activation[4].

Keywords: AIE, Prodrug, Targeted delivery, Real time imaging.

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P-43

ARGYROPHILIC NUCLEOLAR ORGANIZER REGIONS STAINING BY SILVER NITRATE FOR HPV DETECTION

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Introduction:

Cervical cancer is one of the most common disease and it accounts for 16 to 29% in India of total cervical cancer cases occurring globally. There are various screening techniques available such as visual inspection, colposcopy testing, and cervical cytology screening has been found effective in reducing incidence of the disease. Objective: Feasibility of different screening method has been assessed to find out the most suitable mode applicable and also to assess Argyrophilic nucleolar organizer regions (AgNOR) counts to discriminate high-risk and low-risk dysplasia cases. Materials and methods: The cervical smears for the study were collected from the Gynecology department of Shri M. P. Shah Government Medical College, Jamnagar. The cervical smears were collected in pairs, one for the specialized AgNOR staining and one for the PAP test. HPV by PCR was performed from smear sample. PAP test was performed by pathology department and results were collected. Result and discussion: 498 patients were screened for cervical lesions using Pap smear and AgNOR staining. 4 cases were confirmed using HPV by PCR. It was observed that the AgNOR dots were single larger and compact in the normal cervix. They appeared small and loosely arranged in the dysplastic and malignant lesions of the cervix. Sensitivity and specificity of AgNOR stain we found was 93.20% (95%CI: 86.50-97.22%) and 100% (95%CI: 99.06-100%) respectively. Conclusion: Alternative screening test of AgNOR is simple and cost-effective method and AgNOR can be used as proliferative marker. It is rapid, precise, and impartial compare to conventional techniques.

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P-44

"Synthesis and Characterization of Bromo-Terminated Azoester Derivatives: Mesophase Behavior and Comparative Study for Liquid Crystal Materials Design"

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Abstract:

In this research, we have synthesized and characterized a novel series of azoester derivatives featuring a bromo terminal group, comprising a total of 12 variants. These compounds displayed a unique combination of primarily nematogenic and partially smectogenic behaviors, with mesophase initiation observed from the first homologue and mesophase temperature ranges spanning from 4.9 to 30.9 °C. Notably, the isotropic temperature of the liquid crystal (LC) compounds decreased with increasing carbon chain length, indicating the influence of the flexible chain on mesophase properties. Employing various characterization techniques, including FT-IR, mass spectroscopy, ^{1}H-NMR, Gauss view, and elemental analysis, We gained comprehensive insights into the compound properties. Polarized optical microscopy confirmed the presence of mesogenic phases, while DSC revealed thermal behavior. Furthermore, a comparative analysis with structurally similar series shed light on the distinct properties and potential applications of these compounds, contributing valuable insights to the design of advanced liquid crystal materials.

Keywords: Azo Ester derivatives, Bromo terminal group, Mesophase behavior, Polarized optical microscopy, DSC, Liquid crystal materials design, Advanced liquid crystal materials

P-45

Biogenic synthesis of Surface Engineered copper oxide nanoparticles using *Tridex procumbens* leaf extract and their biological activities

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Abstract

Growing interest has recently been shown in plant-based nanoparticle synthesis, mainly when using plant parts, including leaves, stems, and flowers. A new technology that has recently gained increasing attention due to various advantages over traditional chemical methods is the creation of nanoparticles through a green path. Different plant parts are used in the manufacture of metallic nanoparticles because they include metabolites that act as reducing agents to create nanoparticles, such as alkaloids, flavonoids, phenols, terpenoids, alcohols, sugars, and proteins. They also serve as a stabilizer and capping agent for them. A new technology that has recently gained increasing attention due to various advantages over traditional chemical methods is the creation of nanoparticles through a green path. The current study presents the fabrication of copper oxide nanoparticles(CuO) using dried *Tridex procumbens* leaf extract in an aqueous media. The synthesized CuO nanoparticles were characterized by ultraviolet-visible spectroscopy, field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray analysis, transmission electron microscopy (TEM), and Fourier transform infrared spectroscopy (FTIR) analysis techniques. The nanoparticles were screened for antibacterial activity, antifungal, antidiabetic, antioxidant and anti-inflammatory activities.

Keywords: Biogenic synthesis; copper oxide nanoparticles; *Tridex procumbens*; biological activities.

P-46

Syntheses and biological evolution of some novel pyrrolo [2, 3-d]pyrimidine urea derivatives

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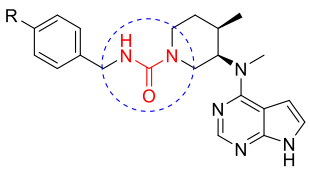
Abstract

Our area of interest is allied to study targeted antimicrobial agents. We focused on pyrrole fused pyrimidines. This ring system is tied up with carbamate in order to form corresponding urea derivative. The present study compiled syntheses, antibacterial and antifungal activity of some novel Pyrrolo [2, 3-d] pyrimidines urea derivatives. The targeted compounds have been synthesized by condensation reaction between (3R, 4R) -(4-Methylpiperidin-3-yl) methyl-(7Hpyrrolo [2, 3-d] pyrimidin-4-yl)amine[1] and 4-nitrophenyl (4-substitutedbenzyl)carbamate. The structures of synthesized compounds have been confirmed by various spectroscopic techniques like ^{13}CNMR, ^{1}H NMR, mass spectrometry (MS) and Infrared spectroscopy (IR). All the synthesised compounds have been screened *in-vitro* antimicrobial activities. Four different bacterial strains like Escherichia coli, P.aeruginosa, S.aureus, S.pyogenus and also two different fungal strains like Calbicans, A.niger and A.clavatus have been used. The standard drugs like Gentamycine, Ampicillin, Chloramphenicol, Ciprofloxacin and Norfloxacin have been used to compare antibacterial activities while two standard drugs Nystatin and Greseofulvin have been used to compare antifungal activities. The tabulated results are promising and encourage us for further expansion in our study.

Graphical abstract



Pyrrolo pyrimidine urea derivative
R= alkoxy group and halide group

Keywords: Pyrrolo[2,3-d]pyrimidine, Urea, antifungal, antibacterial.

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P-47

Effect of diverse chemically modified bis(pyrenyl) spacer group-di-imines on the photophysical properties.

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1-pyrene substituted bis(pyrenyl)-di-imine Schiff bases were synthesized using **(SB1**)=phenylene ,**(SB2)**= absence of any alkyl/aryl spacer , **(SB3)**= ethylene ,**(SB4)**= butylene ,**(SB5)**= hexylene ., the photophysical characteristics of bis(pyrenyl)-di-imines were studied in solution and solid form. It was found that the type of spacer group affects the light-emitting characteristics. The structural characteristics of a molecule determine molecular aggregation, which in turn determines aggregation-caused quenching (ACQ) and aggregation-induced emission (AIE). Bis(pyrenyl)-di-imines showed AIE at higher concentrations and in the solid state when an alkylene spacer [ethylene (SB3), butylene (SB4), and hexylene (SB5)] was present. In contrast, a phenylene (SB1) spacer and the absence of an alkyl/aryl spacer (SB2) in the compound led to ACQ in the solid state. Its crystal structure explained SB1's non-emissive solid-state properties. In contrast, the AIE in the compounds SB3-SB5, which contain flexible alkylene spacers, was given insight into the arrangement of the molecules in solid form.

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P-48

ARGYROPHILIC NUCLEOLAR ORGANIZER REGIONS STAINING BY SILVER NITRATE FOR HPV DETECTION

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Introduction: Cervical cancer is one of the most common disease and it accounts for 16 to 29% in India of total cervical cancer cases occurring globally. There are various screening techniques available such as visual inspection, colposcopy testing, and cervical cytology screening has been found effective in reducing incidence of the disease. Objective: Feasibility of different screening method has been assessed to find out the most suitable mode applicable and also to assess Argyrophilic nucleolar organizer regions (AgNOR) counts to discriminate high-risk and low-risk dysplasia cases. Materials and methods: The cervical smears for the study were collected from the Gynecology department of Shri M. P. Shah Government Medical College, Jamnagar. The cervical smears were collected in pairs, one for the specialized AgNOR staining and one for the PAP test. HPV by PCR was performed from smear sample. PAP test was performed by pathology department and results were collected. Result and discussion: 498 patients were screened for cervical lesions using Pap smear and AgNOR staining. 4 cases were confirmed using HPV by PCR. It was observed that the AgNOR dots were single larger and compact in the normal cervix. They appeared small and loosely arranged in the dysplastic and malignant lesions of the cervix. Sensitivity and specificity of AgNOR stain we found was 93.20% (95%CI: 86.50-97.22%) and 100% (95%CI: 99.06-100%) respectively. Conclusion: Alternative screening test of AgNOR is simple and cost-effective method and AgNOR can be used as proliferative marker. It is rapid, precise, and impartial compare to conventional techniques.

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P-49

Efficient Synthesis and Comprehensive Characterization of Oxomorpholine-Imidazole Derivatives: Investigating Remarkable Antimicrobial Efficacy

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Abstract:

This research is dedicated to the synthesis of aromatic or heteroaromatic compounds with profound potential in pharmaceutical and medicinal domains. Imidazole derivatives have emerged as focal points of interest due to their versatile therapeutic applications, spanning a broad spectrum of diseases encompassing cancer, bacterial infections, fungal infections, and malaria. In pursuit of these objectives, we have devised an efficient synthetic route to explore a diverse array of 2-((1,4-diphenyl-1H-imidazol-2-yl)thio)-N-(4-(3-oxomorpholino)phenyl)acetamide derivatives. The structural elucidation of the synthesized compounds is conducted with precision, employing advanced techniques including 1H and 13C NMR, FT-IR spectroscopy, mass spectroscopy, and elemental analysis. This exhaustive characterization ensures a comprehensive understanding of the molecular composition and configuration of the compounds, laying a solid foundation for subsequent investigations. Moreover, the oxomorpholino-imidazole derivatives derived from this synthesis are further utilized in the creation of a diverse range of chemotherapeutic agents, showcasing significant potential for clinical applications. This study contributes not only to the enrichment of our knowledge regarding imidazole derivatives but also to the development of novel compounds poised to make substantial contributions in the realm of medical science, promising advancements in the ongoing pursuit of effective therapeutic interventions.

Mode of Presentation: Poster

Keywords: Heteroaryl compounds, oxomorpholine, 1,4-Diaryl imidazoles, biological implications

P-50

mIBG-Doxurubicin conjugate for neuroblastoma targeted chemotherapy:synthesis and in-vitro evaluation

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Neuroblastoma is the most common extracranial solid tumor in children, accounting for approximately 8% of all childhood cancers and 15% of childhood cancer mortality [1]. meta-Iodobenzylguanidine (mIBG) has been utilized as a radiopharmaceutical ligand for targeting therapies to bind to the norepinephrine transporter (NET) expressed on 90% of neuroblastoma cells. On the other hand, standard chemotherapeutics viz. Doxoribicin (Dox) is clinically used as a non-targeting anticancer therapeutic, with serious life-threatening side effects. A combination of mIBG with Doxmay lead to a neuroblastoma targeted chemotherapeutic and circumvent these side effects. This would improve the therapeutic efficacy, diminish the undesired side effects and reduce the cost of treatment. Towards this, we have chosen m-Iodobenzylguanidine (mIBG) as the targeting ligand, which is an analog of the catecholamine norepinephrine and is known to bind with the norepinephrine transporter (NET) receptors resulting in accumulation in neuroblastoma [2]. mIBG was successfully synthesized from p-xylene via a multistep synthetic route, and was conjugated to the well-known chemotherapeutic Doxorubicin via an acid-cleavable imine linkage, resulting in a novel mIBG-Dox (**Figure 1**) conjugate. The conjugate was obtained in an overall yield of 4.5%, purified by preparative RP-HPLC, and was characterized using FT-IR, NMR, elemental analysis and UV-VIS absorption spectroscopy. Further, the efficacy of mIBG-Dox was investigated in-vitro in neuroblastoma vs other cancers. Our results revealed that both Dox and mIBG-Dox are highly effective against neuroblstoma cancer (IMR32) with slightly lower efficacy was observed for mIBG-Dox. Interestingly, Dox was also quite effective in reducing clonogenic growth of battery of different other cancers and normal cells (with no NET expression), while efficacy of mIBG-Dox was drastically reduced in these cells, suggesting the specificity of mIBG-Dox towards neuroblastoma only. Overall, we could successfully synthesize a chemotherapeutic, mIBG-Dox, for effectively targeting neuroblastoma.

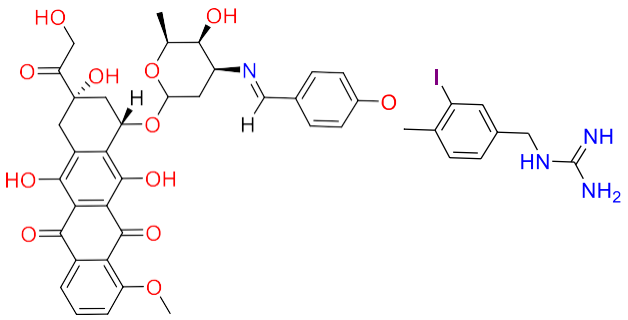

Fig.1. Structure of the mIBG-Doxorubicin conjugate.

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P-51

Cinnamaldehyde and its derivatives: Potential protective agents against oxidative-stress induced myotube atrophy using chemical, biological and computational analysis

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Abstract

Skeletal muscle atrophy, associated with increased morbidity, mortality and poor quality of life, is a metabolic disorder with no FDA approved drug. Oxidative stress is one of the key mediators of atrophy by influencing various cell signaling molecules. The goal of this study is to identify potential antioxidant agents that could be used to treat atrophy. In this study *invitro* and *insitu* screening of different cinnamaldehyde (CNA) derivatives for their antioxidant effects was done along with computational analysis to understand the relationship between their chemical structure and biological activity. Data show that 2-hydroxycinnamaldehyde (2HCNA) worked better than other CNA analogues at physiological pH, while 4-Fluoro-2-methoxycinnamaldehyde (4FoCNA) showed the maximum antioxidant activity under acidic conditions. However, these derivatives (2HCNA and 4FoCNA) were found to be toxic to the cultured myotubes (mature myofiber) under both physiological and pathophysiological conditions. Immunofluorescence, bright-field microscopic and biochemical studies conducted using live C2C12 cells showed that pre-incubation with other CNA analogues *i.e.* 2-methoxycinnamaldehyde (2MeCNA) and 2-benzyloxycinnamaldehyde (2BzCNA) not only maintained the normal morphology of myotubes but also protected them from H2O2-induced atrophy. These compounds (2MeCNA and 2BzCNA) showed higher stability and antioxidant potential, as indicated by computer simulation data analyzed by Density Functional Theory (DFT) based molecular modeling. Overall, the chemical, biological, and computational studies reveal the therapeutic potential of CNA analogues (BzCNA and MeCNA) against oxidative-stress induced muscle atrophy in C2C12 cells.

Keywords: CNA-derivatives, C2C12 skeletal muscle cells, Oxidative stress, Atrophy

P-52

"Design, Synthesis, and Molecular Docking Analysis of Novel Benzo[4,5]imidazo[1,2-*a*]pyrimidine Hybrids Targeting Plasmodium falciparum DHFR: A Comprehensive *In Silico* and Biological Study"

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Synthesis of Benzo[4,5]imidazo[1,2-*a*]pyrimidine derivatives using an environmentally friendly Biginelli-type reaction in ionic liquid DIPEAc. Remarkably, this ionic liquid exhibits efficient recyclability over five cycles. Synthesized compounds underwent rigorous *In vitro* antimalarial efficacy screening, complemented by computational and *In vitro* studies, assessing their potential as Plasmodium falciparum dihydrofolate reductase (*Pf*-DHFR) inhibitors. A robust 3D-QSAR model was established and validated, elucidating structure-activity relationships. Estimated ADMET descriptors highlighted favorable pharmacokinetics, suggesting their role in new antimalarial drug development. This study exemplifies the synergy of sustainable synthesis, enzyme inhibition, and pharmacokinetic profiling, promising a transformative outlook for antimalarial innovation.

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Computational Designing of Novel Inhibitors Targeting Dengue Virus RdRp: A Promising Avenue for Antiviral Drug Development

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Dengue fever arises from viral infection caused by Dengue Virus (DENV) transmitted by mosquitoes, particularly in warm, tropical areas. In the recent past, the World Health Organization (WHO) has pinpointed dengue as a potential threat among ten diseases, a concern validated by ongoing outbreaks in numerous countries.[1] Infection is primarily caused by any one of four closely related DENV serotypes with manifestations ranging from mild symptoms to those that may require medical intervention and hospitalization and in some extreme cases, can also lead to fatalities.[2]

Evidence indicates that among all the serotypes, two virus-encoded nonstructural (NS) proteins, namely NS3 and NS5, play a crucial role in regulating the essential enzymatic processes for RNA replication. DENV NS5 protein is bifunctional and has the RNA-dependent RNA polymerase (RdRP) catalytic domain.
RdRPs are involved in genome replication, mRNA synthesis, RNA recombination, etc. and are essential for the survival of viruses. Viral polymerases are clinically proven therapeutic targets.[3]

In the present study, inhibitors of DENV RdRP were identified using docking-based Virtual screening of small-molecule databases. An exhaustive computational assessment, which included the evaluation of binding interactions and an assessment of the pharmacokinetics and toxicity profiles, was carried out to filter five molecules targeting DENV 2 and six molecules targeting DENV 3 serotypes. The protein-ligand interactions were further studied using a 50 ns molecular dynamics (MD) simulation to establish dynamic stability.

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P-54

Ultrasonic-Assisted 1, 3-Dipolar Cycloaddition Reaction for the Synthesis of Novel Spirooxindole Derivatives as Anti-cancer Agents

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ABSTRACT:

Spirooxindoles has been recognized as a promising bioactive heterocyclic scaffold and are associated with a broad array of biological activities such as anticancer, antimicrobial, antifungal, antitumour, antiproliferative, anti-inflammatory, antimycobacterial, acetylcholinesterase inhibitory activity etc. In our endeavour to search for potent anticancer compounds; a series of novel spirooxindole-pyrrolizidines **4a-r** were synthesized *via* 1,3-dipolar cycloaddition reaction under ultrasonic irradiation conditions by the one-pot reaction of various substituted isatins **1a-j**, L-proline **2** and substituted chalcones **3a-d** as the starting precursors (Figure 1). The reaction provides spirooxindole-pyrrolizidine derivatives with high regio and stereo-selectivity under mild reaction conditions. The structures of the synthesized **4a-r** were confirmed by FT-IR, ^{1}H and ^{13}C NMR, HR-MS and X-ray single crystal studies. All the synthesized spirooxindoles **4a-r** showed potential anticancer activity *in vitro* using MTT assay. *In Silico* studies validated the wet results and predicted expected drug-receptor interaction against cancer protein targets.

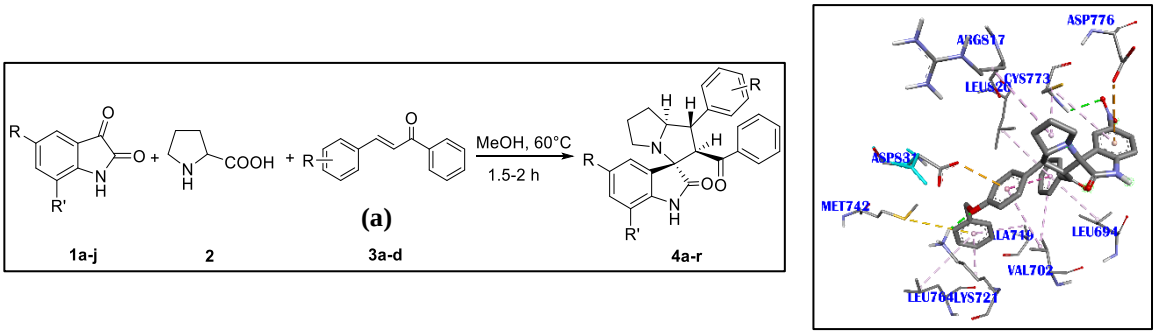

Figure 1. (a) Synthesis of novel spirooxindole-pyrrolizidines **4a-p**. (b) Binding energy of compound **4d** inside EGFR (PDB ID: 1M17): 10.3 Kcal/mol.

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P-55

In vitro Antioxidant and Anticancer Activity of Hydro-methanolic and n-Hexane Extract of Ocimum basilicum L. Leaves: A Comparative Analysis

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According to the World Health Organization's 2022 report, cancer is the leading cause of death worldwide, accounting for about 10 million fatalities in 2020, or nearly one in every six deaths. Herbal medicines are currently gaining attention as a potential source of anticancer agents and are widely used due to the availability and affordability with few or no side effects. *Ocimum basilicum* L. is a medicinal herb of the family Lamiaceae which has been used traditionally in the treatment of various diseases.

Hydro-methanolic extract (HME) and n-hexane extract (HE) of *Ocimum basilicum* L. leaves was prepared by Soxhlet extraction method. The extracts were subjected to physical analysis and phytochemical screening. Antioxidant properties of both extracts were determined by DPPH, ABTS, NO and SO anion scavenging assays. Brine shrimp lethality assay was performed to investigate toxicity of both the extracts. HCT-116 and MCF-7 cell lines representative of colorectal and breast cancer respectively, were used to determine anticancer potential of both the extracts using MTT assay. Phytochemical screening of both extracts revealed that *Ocimum basilicum* L. is rich in major phytochemicals such as phenols, flavonoids, tannins, terpenoids, etc. TLC and HPTLC confirmed the presence of bioactive compound Alpha-Terpineol in HME and HE. HME was found to be good source of natural antioxidants and was nontoxic with potential anticancer activity as compared to HE. These findings suggest that both extracts could have great importance as therapeutic agents but HME is more potent to fight against cancer.

P-56

Novel Pyrazole-Oxindole Conjugates with Cytotoxicity in Human Cancer Cells *via* Apoptosis.

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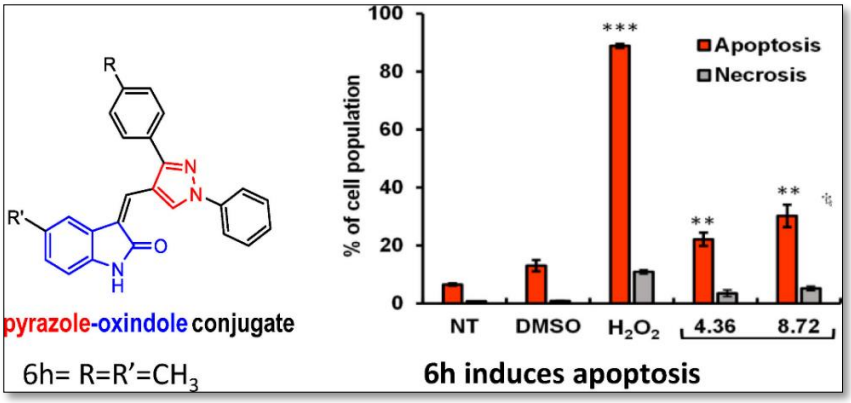
Novel pyrazole-oxindole conjugates were prepared and tested as potential cytotoxic agents in the Jurkat acute T cell leukemia, CEM acute lymphoblastic leukemia, MCF10 A mammary epithelial, and MDA-MB 231 triple negative breast cancer cell lines. Among the tested conjugates, the 5-methyl-3-((3-(1-phenyl)-3-(*p*-tolyl)-1*H*-pyrazol-4-yl) methylene) indolin-2-one **(6h)** emerged most cytotoxic (CC_{50} of 4.36+/−0.2 µM) against Jurkat cells. The mechanism of cell death was investigated through the Annexin V-FITC assay *via* flow cytometry. Reactive oxygen species (ROS) accumulation, mitochondrial health, and the cell cycle progression were also evaluated. Results demonstrated that **6h** induces apoptosis in a dose-dependent manner, without generating ROS and/or altering mitochondrial health. In addition, **6h** disrupted the cell cycle distribution causing an increase in DNA fragmentation and an arrest in the G0-G1 phase. Taken together, the **6h** compound revealed a strong potential as an antineoplastic agent evidenced by its cytotoxicity in leukemia cells, the activation of apoptosis, and restriction of the cell cycle progression, Jain et al. [1]



Keywords: Pyrazole, Oxindole, Human cancer cells, Apoptosis.

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P-57

Trans-Palladium Dichloride Complex of Macrocyclic Organoselenium Ligand as Catalyst for Dehydroxymethylation of Dihydroxy Compounds

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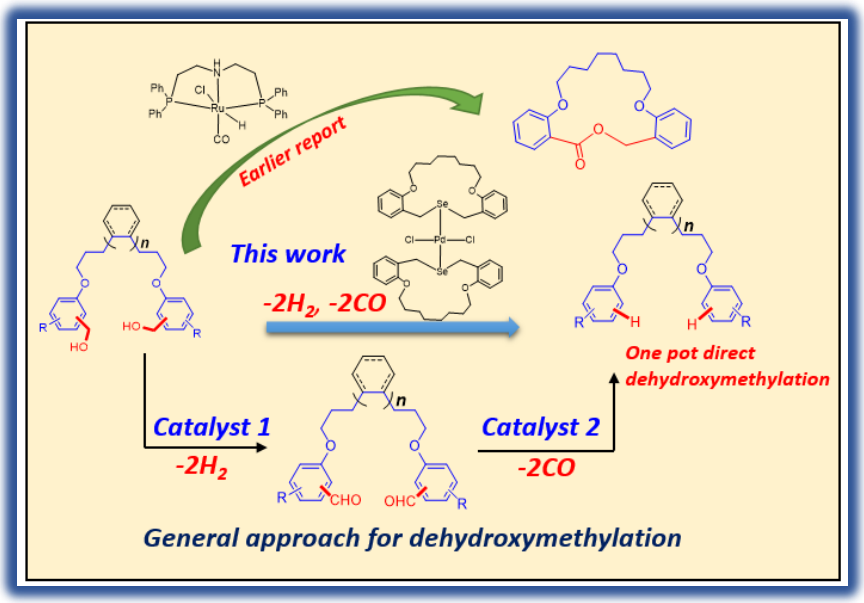
Abstract:

To achieve specific reactivity and selectivity during catalysis reaction we have planned the design, and synthesis, of novel metal complexes where central metal is present in sterically confined spheres that showed excellent potential for catalysis leading to better activities and selectivities. Here we have reported easily synthesized and characterized novel seventeen-membered macrocyclic ring containing selenium ligand and its *trans*-palladium dichloride complex.[1] The ligand and complex are air and moisture-insensitive. The ligand and complex were fully characterized by various spectroscopy techniques such as ^{1}H and $^{13}C\{^{1}H\}$ NMR, HRMS, FTIR, UV-visible, and elemental analysis. The single crystal XRD studies showed that the complex possesses a distorted square planar geometry around the palladium center. The variable temperature NMR data and computational studies suggest selenium inversion in the complex with an inversion barrier of ~22.6 kcal/mol. This palladium complex was efficiently utilized as a catalyst for the dehydroxymethylation of long alkyl chains containing dihydroxy compounds. This catalytic route is beneficial because generally, two separate catalysts are used for dehydroxymethylation (one for oxidation of alcohol and another for decarbonylation of aldehyde). Here, a single catalyst shows dual action of dehydroxymethylation up to 91% yield with 5.0 mol% catalyst loading.



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P-58

2-Phenylbenzo[*d*]imidazo[2,1-*b*] thiazoles as Potential Anticancer Agents: Design, Synthesis, Bioevaluation and *in-silico* studies

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ABSTRACT:

Imidazo[2,1-*b*] thiazoles have been recognized as a promising bioactive scaffold for wide array of biological activities including anti-proliferative, anti-tumor, anti-bacterial, analgesic, anti-allergic, anti-inflammatory, antioxidant, antifungal, antipsychotic, antiviral etc. Based on the reported literature of anti-carcinogenic efficacy of thiazole and imidazothiazole derivatives, we have synthesized a new series of various substituted 2-phenylbenzo[*d*]imidazo[2,1-*b*] thiazoles derivatives **3a-r** by the reaction of 2-amino benzothiazole **1** with substituted phenacyl bromide **2a-i** in ethanol under microwave (MW) irradiation conditions at 100 °C for 15 min [Figure 1(a)]. The structures of the synthesized molecules were confirmed by FT-IR, ^{1}H and ^{13}C NMR, HR-MS spectroscopic techniques. Compound **3a-r** shows promising anticancer activity *in vitro* against various cancer cell lines. The wet results were validated by *in silico* studies [Figure 1(b)]. The details of the study will be presented.

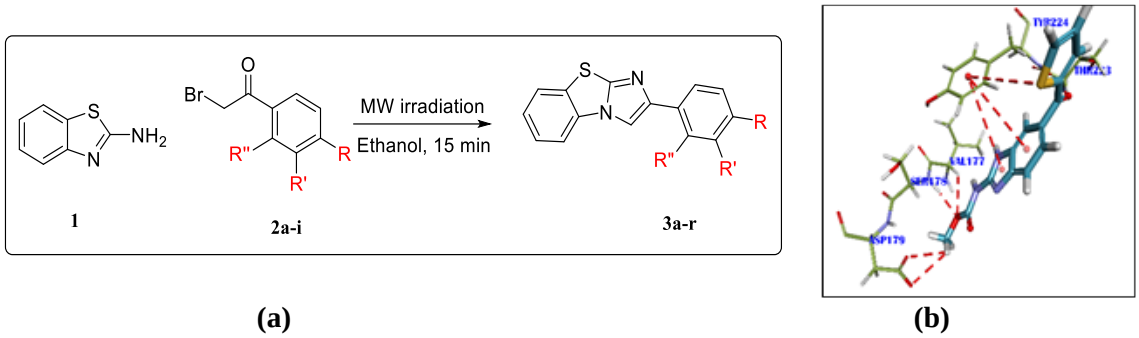

Figure 1. **(a)** Synthesis of various 2-phenylbenzo[*d*]imidazo[2,1-*b*] thiazoles **3a-r (b)** Binding interaction of potent molecule **3e** (CDOCKER Interaction Energy 12.7 Kcal/mol compare with 7.7 Kcal/mol energy of Nocodazole) with 3E22 protein.

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P-59

Synthesis of Quinoline Derivatives Using Acceptorless (de)hydrogenation Strategy

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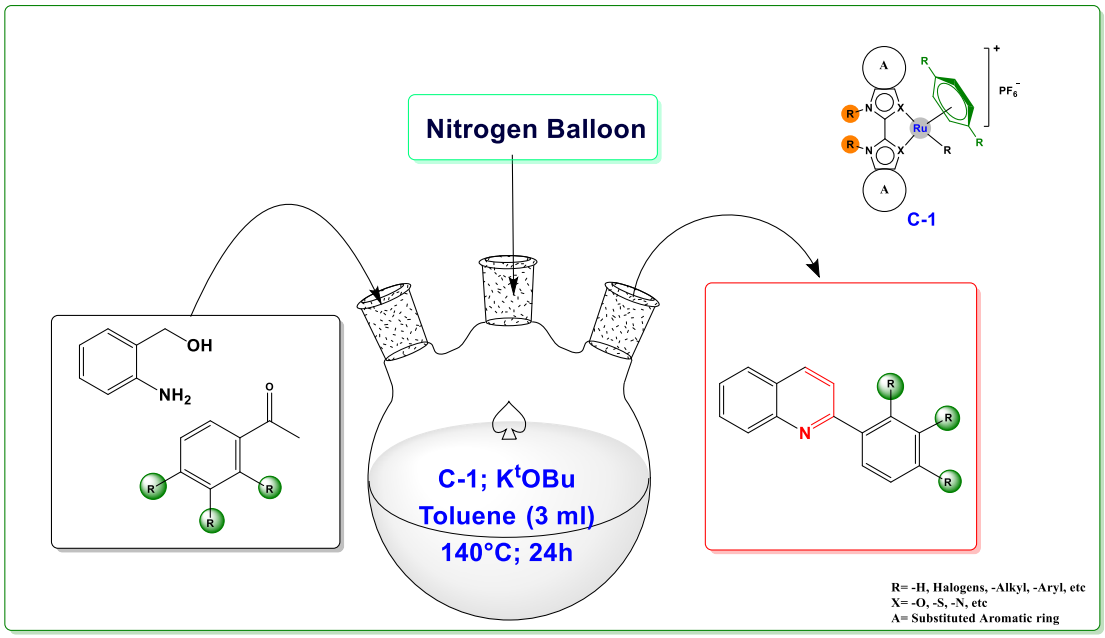
Abstract:

In the past few decades, attention has been paid to the catalytic methodologies of quinolone as it represents an important synthon for many pharmaceutically important drug molecules.[1] Although there are verities of synthetic routes available for quinoline but transition metal based modified Friedlander synthesis has been emphasized recently.[2] In particular, transition metal based catalytic routes involving tandem de(hydrogenation) reaction between 2-amino benzyl alcohol and acetophenone/2-phenyl ethanol is one of the simplest routes for said molecule.[3] [4] Herein, we developed a ruthenium metal based robust, bifunctional, metal-ligand cooperative, air and moisture stable catalyst (**C-1**) for synthesis of quinoline from reaction between 2-aminobenzyl alcohol and acetophenone via tan dem de(hydrogenation) reaction. The products were isolated in good to excellent yield and methodology provides a broad substrate scope.



Keywords: Bifunctional catalyst, Metal-ligand cooperativity, Modified Friedlander quinoline synthesis, robust catalyst, high TOF etc.

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P-60

Rapid synthesis of highly functionalized novel asymmetric 1,4 dihyropyrimidines using glacial acetic acid as solvent

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Abstract

A new series of 1,4-dihydropyridines bearing a coumarin moiety in the 3-position were synthesized by a variation of the classical Hantzsch synthesis. The reaction of derivatives of coumarin-3-aldehyde with 3-amino crotononitrile and different β-keto-ester active methylene in the presence of glacial acetic acid afforded novel 1,4-dihydropyridines. The procedure has short reaction time (15–20 min), easy workup, and good yield of product. The structures of all synthesized compounds were well characterized by mass, infrared, ^{1}H NMR.

Keywords: 1,4-Dihydro pyridines; glacial acetic acid; coumarino aldehyde

P-61

Synthesis and antimicrobial evaluation pyrrole and coumarin fused derivatives.

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Abstract:

This study reports the successful synthesis of a novel series of pyrrole derivatives featuring a coumarin moiety at the 4-position. The synthetic process involved the reaction of 4-amino coumarin derivatives, aromatic aldehydes, and α-diketo compounds using anhydrous ZnCl2 as a catalyst in nitromethane. Characterization via mass spectrometry, infrared spectroscopy, and 1H NMR confirmed the structures of the synthesized compounds. Additionally, their antimicrobial activity was evaluated. This research contributes to the expanding field of antimicrobial agents through the development of these specialized pyrrole-coumarin derivatives.

Keywords: coumarino, nitro methan, diketones

P-62

Synthesis, characterizations, biological activity of Pd(II), Ni(II), Zn(II), Cu(II) metal complexes of quinazolinone Schiff-bases

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Abstract

Schiff base was obtained from the reaction between 2-amino benzohydrazide and 2-Hydroxy-4-methoxy benzaldehyde using the reflux method in HPLC grade methanol for 2 hours producing 71% yield. 2-amino benzohydrazide 2-Hydroxy-4-methoxy benzaldehyde schiff base was slight yellow color. The structures characterized by ESI-mass, Mass, 1H NMR, IR, 13C NMR, the metal complex of quinazolinone schiff base derivative were tested for antibiotics such as Streptomycin, Ampicillin and Nystatin. Metal complexes of Ni, Zn, Cu, and Pd were prepared in which Ni metal complex and Pd metal complex are highly potent drug that inhibit only gram-negative bacteria. All the metal complexes are able to inhibit gram negative bacteria. Zn and Cu metal complexes are effective broad-spectrum drug which can inhibit the growth of both gram-positive and gram-negative bacteria. All the metal complexes exhibited antifungal activity. Among them, Pd metal complex is most potent antifungal drug.

Keywords: Schiff base, Metal complex, Antimicrobial, Quinazoline

P-63

Distractive Impact of Lepidopteran Larvae Infestation on Kesar Mango (*Mangifera indica L.*): An Anatomical and Physiological Analysis

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The infestation of leaf webbers on *Mangifera indica L.* (Kesar mango) represents a significant pest issue, particularly in densely cultivated regions of Gir. Over a two-year observation period (2022-23), more than three species of lepidopteran larvae were identified on Kesar mango. The leaf webber, from egg to larva, develops within the leaf buds, causing substantial damage to the leaves during their feeding phase. The physiological structure of the mango is adversely affected by larval infestation, with observable anatomical changes in young shoots, characterized by irregular cell growth in the epidermal region, cortex, and extensive damage to the xylem and phloem tissues. This larval activity leads to the desiccation of buds, contributing to morphological and physiological damage. Consequently, the mango leaf bud experiences a significant reduction in flower and fruit production, leading to an overall decline in the growth of the entire Kesar mango plant.

Keywords: Lepidopteran Larvae, Physiological Impact, Pathogenic Damage, Xylem and Phloem Tissues, Morphological Damage, Agricultural Impact.

P-64

Phytochemical Analysis and Medicinal Potential of *Punica granatum L.* Leaves: A Gas Chromatography-Mass Spectrometry Study

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Abstract:

Punica granatum L., commonly known as Pomegranate, is a commercially significant fruit plant belonging to the Punicaceae family. In addition to being a nutritious fruit, Pomegranate is also recognized for its rich phytochemical content, which exhibits remarkable medicinal properties. This study aimed to identify the phytochemical constituents present in Pomegranate leaves utilizing Gas Chromatography-Mass Spectrometry (GC-MS) technique, and to assess their medicinal potential using the PASS online software. The results of the analysis revealed the presence of several important phytochemicals, including Lupeol, Phytol, Maltol, D-glucopyranose, and Pyragallol, known for their medicinal properties such as anti-inflammatory effects, membrane integrity agonism, and Nicotinamide adenine dinucleotide phosphate (NADPH) peroxidase inhibition. Notably, Lupeol demonstrated significant anticancer activity, suggesting its potential as an in vivo anticancer drug candidate. Further evaluation of Lupeol's therapeutic properties is necessary for potential clinical applications. This study contributes to the understanding of the phytochemical composition and medicinal potential of Pomegranate leaves, highlighting its significance as a valuable natural resource for pharmaceutical research and development.

Keywords: *Punica granatum L.,* Pomegranate, phytochemicals, Gas Chromatography- Mass Spectrometry (GC-MS), medicinal properties, Lupeol, Phyton, Maltol, D- glucopyranose, Pyragallol, anti-inflammatory, membrane integrity agonist, NAPDH peroxidase inhibitor, anticancer activity, in vivo drug evaluation.

P-65

Design, synthesis and biological evaluation of Thieno[2,3-*d*] pyrimidine derivatives

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Abstract:

There are ten thieno[2,3-*d*]pyrimidine 200erivatives have been synthesized from ethyl 2-amino-4,5-dimethylthiophene-3-carboxylate. All the synthesized compounds are characterized by elementary analysis, spectral studies, such as Mass, FTIR, ^{1}H NMR, ^{13}C NMR. The synthesized compounds are screened for their antibacterial, antifungal and antimalarial activities.

Keywords: Thieno[2,3-*d*]pyrimidine, Antibacterial, Antifungal.

P-66

SYNTHESIS, CHARACTERIZATION, BIOLOGICAL ACTIVITIES, AND MOLECULAR DOCKING STUDIES OF NOVEL BIS-SCHIFF BASES

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In this study, A series of novel bis-benzaldehyde-imines ligands were made and their properties were studied using different spectroscopic methods. The antimicrobial activity of the compounds have been investigated for their minimum inhibitory concentration (MIC) to gram-negative and gram-positive bacteria and yeast cultures. Both gram-negative and gram-positive bacteria were used to test the antibacterial qualities of the compounds. The results showed that, at different concentrations, the compounds have antibacterial action, especially against S. aureus, E. coli, B. subtilis, and K. pneumoniae. The study also looked at how the nitro-containing substituent group affects the benzaldehyde part of the ligands. This suggests that this chemical change affects the ability of the compounds to stop the growth of certain types of bacteria. This study shows that synthesized benzaldehyde-imine ligands could be used as antibacterial agents. It also shows how important chemical substitutions are for fine-tuning the biological activity of these ligands. Furthermore, Molecular docking is also performed by Authors for some Proteins with using of these novel Schiff bases.

Keywords: Schiff bases, MIC, Benzaldehyde, Biological activity, Molecular Docking

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P-67

Stability Indicating UPLC method for Quantification of Famotidine from its pharmaceutical Dosage: Green Analytical Approach and Stress Study

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Abstract

Famotidine is a histamine H_2-receptor antagonist that inhibits stomach acid production, and it is commonly used in the treatment of peptic ulcer disease and gastroesophageal reflux disease. The aim of the present study was to develop a green UPLC method for quantitative estimation of Famotidine. An isocratic mobile phase (Buffer: Acetonitrile (80:20), %v/v) was used in this study. The method development was performed on ACQUITY UPLC HSS T_3 C18 (100*2.1) mm ,1.8 µ particle size column, and the detection was achieved at 266 nm on diode array detector. The temperature of the column oven was set at 30 °C. The developed flow rate and injection volume were optimized and set at 0.3 mL/min and 1 µL with retention time of 1.5 minutes. The stability indicating green analytical method was validated as accordance with ICH guidelines. The correlation coefficient value (R^2) was 0.9991 with 0.2 µg/ml and 0.5 µg/ml, limit of detection and limit of quantification, respectively. The method precision was determined by calculating intraday (%RSD = 0.18) and interday precision (%RSD = 0.25). The mean recovery of the accuracy study was between 99.00-101.00%. The stress degradation studies of Iron sucrose were performed in acidic, thermal, oxidative and photolytic condition. The greenness of the method was calculated by using Analytical Greenness calculator[1], Green Analytical Procedure Index (GAPI)[2] and Analytical Eco scale. Moreover, the method has proven to be reliable when applied to quantitative determination of commercial products.

Keywords: UPLC, Method Greenness, Famotidine, Validation, Force degradation study

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P-68

A Quality By Design Approach For Bacoside Nanosuspension For Improved Solubility And Herbal Drug Registration: An Indian, US And EU Perspective

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Solubility is an important physiochemical factor affecting absorption of drug and its therapeutic effectiveness. Consequences of poor aqueous solubility would lead to failure in formulation development. One of the main problems responsible for the low turnout in the development of herbal constituents as herbal formulations is poor solubility and poor permeability of the lead herbal compounds. The present research work was aimed at preparing nanosuspensions of a poorly soluble mode herbal entity, *Bacopa monnieri* (Linn.) [1] for enhancing its solubility and bioavailability using novel QbD approach with the help of high-pressure homogenization. The Response Surface Methodology was applied for the production of optimized nanosuspensions. Box-Behnken design was applied for optimization of formulation [2]. The effect of poly dispersibility index, type of stabilizer, and its concentrations were studied with regards to the particle size and drug release. The prepared nanosuspensions were evaluated for its particle size, zeta potential, redispersibility index, solubility, and dissolution studies. The developed formulation was characterized by instrumental techniques like XRD, DSC, FTIR analysis. The data of in-vitro study revealed that nanosuspension showed better dissolution; nearly 2-3-fold increase in the dissolution for the nanoparticles in comparison with the raw extract. The developed herbal formulation was reviewed as per the current regulatory guidelines provided especially US, UK [3] and India [4]. It has been found that regulations for herbal drug products in Europe and United States are more stringent than in India which has been reflected by some reports of safety issues of Indian herbal drug [4].

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P-69

Neuroprotective Role of Apremilast In Scopolamine & Lipopolysaccharide Induced Experimental Model Of Alzheimer's Disease

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Abstract

Apremilast is a PDE4 inhibitor which is used to treat moderate to severe plaque psoriasis. In vitro studies have reported Apremilast can reduce the synthesis of cytokines such as TNF-α, IL-12 and IL-23 and chemokines such as CXCL10, CCL2, and CCL3 associated with causing inflammation. Neuroinflammation plays an important role in the pathogenesis of AD(. The overstimulated microglia releases cytokines such as TNF- α, IL-6 etc. The elevated levels of cytokines for prolonged period of time leads to neuronal damage and neuronal death. So, this study was aimed to evaluate the anti-neuroinflammatory effect of Apremilast in scopolamine and LPS induced AD in rats and mice (Li, Heng, et al. [1]) (Schafer et al. [2]). Upon treatment with scopolamine (1 mg/kg/day) and LPS (0.5 mg/kg) intraperitoneally (i.p.) injections for 10 and 7 days respectively, there was a significant increase ($p \leq 0.05$) in acetylcholinesterase enzyme (AchE) activity, lipid peroxidation (LPO) activity and TNF- α levels whereas significant decrease in superoxide dismutase, reduced glutathione, catalase activity. In the Morris water test and probe trial tests, scopolamine and LPS treated rats and mice showed longer escape latencies and reduced time spent in target quadrant than the normal group. Whereas the apremilast groups had shorter escape latencies and spent more time in the target quadrant as compared to the scopolamine and LPS groups. With daily treatment of apremilast (2.5, 5, and 10 mg/kg. p.o. in rats and 5,10, and 20 mg/kg p.o. in mice) for 21 days attenuated the effect of scopolamine in rats and LPS in mice by significantly reducing the AchE activity ($p < 0.05$), MDA ,GSH activity ($p < 0.001$) and TNF- α levels ($p < 0.001$) whereas increase in SOD ($p < 0.001$) than alone Scopolamine and LPS treated group. The present study confers that Apremilast possess neuroprotective effect in scopolamine and LPS induced AD in rats and mice. Apremilast improves the cognitive deficit possibly by reducing the neuroinflammation via CAMP/CREB pathway and could be an alternative therapeutic approach for the treatment of Alzheimer's disease (Zou et al.[3]).

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P-70

Ameliorative effect of Curcumin in combination with probiotic (L.rhamnosus) in rotenone induced Parkinson's disease in Sprague Dawley rats.

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ABSTRACT

Curcumin, a natural polyphenolic compound obtained from rhizomes of Curcuma Longa have potential neuroprotective effect on Parkinson's disease. Though, oral use is highly restricted due to its poor aqueous solubility, rapid metabolism and clearance from the body. Till date, numerous novel approaches have been made in order to increase its systematic bioavailability. Amongst them, an effective natural way is to target its metabolic pathway by the use of curcumin adjuvant. β glucuronidase activity in Lactobacillus rhamnosus(LR) by invitro assay and also studied the increase in bioavailability of curcumin by the use of probiotic. Further, Curcumin and LR were administered together to evaluate the neurobiochemical and histopathological change in PD rats. The result demonstrated that Curcumin and LR combination depicted lass neuronal damage to the midbrain, restoration of dopamine levels, maintaining the AChE levels, improvement in the motor and behave behavioral characteristics, and increment in antioxidant levels. The present investigation focuses on the role of probiotic *Lactobacillus rhamnosus* as a curcumin-adjuvant (to potentiate its effect) in retenon induced Parkinson's disease in SD rats.

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P-71

Formulation Optimization and Charactrization of Compression CoatedTablet of Budesonide for Colon Specific Drug Delivery

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Abstract:

Solvent free compression coating was one of the approaches for carrying drugs to the colon. The investigation was focused to develop compression coated Budesonide tablet using mixture of pH responsive soluble polymer Cellulose Acetate Phthalate (CAP) and Eudragit S-100 (ED) in different ratios along with hydrated polymer Xanthan gum. The effect of proportion of CAP and Eudragit S-100 in the coat on premature release and the drug release in colon target area was determined. It was found that core tablets compression-coated with CAP and Eudragit S-100 fails to prevent drug release in upper part of gastrointestinal tract. The formulations were released 1.02% to 5.29% of drug in physiological environment of stomach and small intestine respectively depending upon proportion of CAP and ED in the coat. The core tablets compression-coated with CAP and ED mixture in the ratio 70:30 (CTF7) along with Xanthan gum was found to be suitable for targeting Budesonide to the colon owing to its minimal drug release in physiological environment of stomach and small intestine and shown drug release 99.27% in the colon area. The presence of ED in hydrophilic compression coat retarded the initial swelling of the coat in acidic to weakly acidic pH, but in alkaline pH, enhance the drug release in faster and controlled manner.

Key Words: Compression Coating, Budesonide, Eudragit S-100, CAP.

P-72

Identification of Biomarkers for the sex determination in Date Palm (*Phoenix dactylifera L.*) Cultivars using ISSR Markers

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Abstract

Date palms (*Phoenix dactylifera L.*) hold immense global economic and nutritional significance, serving as a vital food source in numerous regions. Their cultivation sustains livelihoods and plays a pivotal role in conserving arid land ecosystems, contributing significantly to sustainable agriculture and food security. In India, date palm cultivation thrives in arid regions like Gujarat, Rajasthan, Tamil Nadu, and Kerala, employing various propagation methods, including seeds, offshoots, and tissue culture techniques. While offshoots and tissue culture plants are costlier, seed-raised plants offer a cost-effective alternative through simple germination. Seed-raised plants revealed 50% of each male and female plant. Gender of the date palm can be identified only at the flowering stage i.e., after 3-5 years of planting. Female date palms are valued commercially for their fruit production, while males are crucial for pollination, with an ideal ratio of 2 to 5% for optimal farming. However, a major challenge arises from the absence of available kits for date palm sex determination. Early sex identification at the seedling stage holds immense potential for efficient farm management, enhancing productivity and socioeconomic development. This research aims to fill this critical gap by developing a sex-identification molecular marker tailored to Indian (particularly Gujarat) date palm cultivars using Inter Simple Sequence Repeat (ISSR) markers. In this investigation, 79 different ISSR primers were initially screened for the identification of gender-specific molecular markers that were analyzed on 100 samples of each male and female date palms. Among these, the primer ISSR-49 successfully identified a female-specific DNA band measuring 400bp, which is absent in male date palm samples. This marker can be converted into more reliable Sequence Characterized Amplified Region (SCAR) markers for the sex determination of date palms in the seedling stage. This will help Gujarat farmers with efficient strategy and management of date palm cultivation.

Keywords: Date palm, molecular marker, gender discrimination, ISSR primer

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Development of Green novel Nano catalyst for Catalytic degradation of dye in Water

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Abstract

For graphene-based applications in electronic, optical, chemistry, energy storage, and biology, graphene oxide (GO) is a useful and promising material. Our research has resulted in the production of strontium ferrite graphene composite (SF-GOC), which has undergone thorough physico-chemical characterization employing methods including TGA, TEM, SEM-EDX, FTIR, AFM, XRD, and nitrogen adsorption desorption analysis. Only a small number of catalysts have been created that can degrade Orange (II) and Eosin-Y dyes in water using a heterogeneous catalytic approach. The current work provides a comprehensive description of the biodegradable nanocomposite SF-GOC that was used under mild reaction conditions to break down the potentially harmful water pollutant dyes Orange (II) (98.7 %) and Eosin-Y (96.2 %). It can also be employed for new multifunctional processes in the fields of biological applications, solar energy, heterogeneous catalysis, composite materials, and others.

Keywords: Graphene oxide, Strontium Ferrite Graphene Composite, Dye degradation

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P-74

Synthesis and Application of Sustainable Strontium Ferrite Nanocomposite for fluoride removal in water

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Abstract

It is now important to remove fluoride from contaminated water sources using easily controllable and ecologically friendly adsorbents and catalysts. Because prolonged exposure to fluoride above the allowed limit causes both dental and skeletal fluorosis, this is a serious problem. The current study has produced strontium ferrite graphene composite (SF@GOC), which has been fully analysed by physico-chemical techniques as XRD, FTIR, SEM-EDX, TEM, AFM, TGA, and nitrogen adsorption desorption analyses. Using a UV-Visible spectrophotometer, the maximum amount of fluoride that could be eliminated under ideal conditions was found to be 97.5%, demonstrating that SF-GOC can be used as an effective, thermally stable, recyclable, and environmentally acceptable nano catalyst for the simple removal process of fluoride from contaminated water.

Keywords: Adsorption, Langmuir isotherm, Strontium Ferrite Graphene Composite, Graphene Oxide

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P-75

Screening and isolation of novel nattokinase-producing microorganisms from marine sources

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Abstract:

Cardiovascular diseases (CVDs) are one of the most life-threatening diseases reported throughout the globe and the mortality rate has increased by 111% in the last three decades. Since the COVID-19 pandemic, 20-30% of COVID-19 patients admitted to hospitals have shown increased troponin levels in the blood which is an indicator of cardiac arrest. Research data shows that 1% of people out of the total population in the world, who have experienced COVID-19 have a higher risk of CVDs. For the treatment of CVDs, several natural and synthetic medicines are available in the market where synthetic medicines have major side effects *i.e.,* kidney failure, heart attack, paralysis, etc. Whereas, the natural medicine, nattokinase (NK) is used for the treatment of various CVDs without any side effects. The majority of the nattokinase has been produced by *Bacillus* species which were isolated from fermented soybeans, soil and water sources. However, there are limited reports on the screening and isolation of NK producers from marine resources. Hence the present investigation has been aimed to isolate NK-producing microorganisms from marine environments. Marine water, soil and coral samples were collected from the coastal regions of Kutch, Somnath, Dwarka, Surat, Narara and Pirotan, Gujarat. These samples were serially diluted and screened on 4 different media namely Sea-water agar, Zobell-marine agar, Nutrient agar and Luria-Bertani agar with a pH range of 5-10. Various fibrinolytic, thrombolytic and nattokinase assay was performed to find the NK producers. A total of 512 microorganisms were initially isolated from which 48 strains were primarily selected as NK producers. From these strains, 26 potential nattokinase producers were selected where 18 non-Bacilli and 6 Bacilli strains were recorded. These novel marine non-bacilli isolates can be used for NK production as an alternative nattokinase source towards fulfill the social demand for the treatment of CDVs at a lower cost.

Key words: Cardiovascular diseases, Corona, Nattokinase, Marine resources, non-Bacilli strain

P-76

Authentication of Medicinal Plants and Detection of Adulterants: A Molecular Approach Using ISSR Markers

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Abstract

Herbal products play a pivotal role in addressing a diverse spectrum of diseases, including life-threatening conditions. The global acknowledgment and surging demand for these products emphasize the imperative need for rigorous quality control measures. Regrettably, the escalating demand has given rise to pervasive adulteration and substitution of medicinal plant materials, thereby posing substantial threats to consumer health. In response to this challenge, diverse techniques have been deployed worldwide, among which chemical and molecular methodologies have emerged as indispensable tools for the precise quantification of adulteration levels. This study focuses on the application of Inter Simple Sequence Repeat (ISSR) markers to authenticate and distinguish between two important herbal species, *Asparagus racemosus* and *Saraca asoca* and their adulterants *Asparagus sermentosus* and *Polyalthia longifolia,* respectively. In this investigation, 79 different ISSR primers were initially screened for species-specific molecular marker identification. The ISSR analysis unveiled distinctive genetic markers, notably in primer ISSR-73, which yielded a 600bp band specific to *Saraca asoca*, and 800bp and 900bp bands for *Polyalthia longifolia*. Moreover, primer ISSR-47 revealed species-specific bands of 500bp and 600bp for *Asparagus racemosus* and a 700bp band for *Asparagus sermentosus*. These markers could be used to develop Sequence characterized amplified region (SCAR) markers that will serve as reliable methods for authenticating herbal products derived from these medicinal plants. This discriminative approach, harnessing ISSR molecular markers, holds significant potential for ensuring the quality and safety of herbal products, while concurrently addressing the challenges posed by resource limitations and escalating global demand. Furthermore, it contributes to the preservation of traditional medicinal practices and upholds the integrity of herbal medicine within the contemporary healthcare paradigm.

Keywords: ISSR, herbal drug authentication, molecular markers, SCAR development

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Sustainable Copper and Zinc Bimetal-Immobilized SBA-15 Composite for Improved Wet Catalytic Oxidation of Dye Capacity

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Wet catalytic decomposition of Yosin Y dye was carried out with copper and zinc bimetal incorporated mesoporous SBA-15 (Cu-Zn@SBA-15) under visible light. The synthesized hybrid composite material was characterized by physicochemical methods, powder X-ray diffraction (PXRD) spectroscopy, scanning electron microscopy combined with energy-dispersive X-ray (SEM−EDX) spectroscopy studies, Fourier transform infrared (FT-IR) spectroscopy, transmission electron microscopy (TEM), atomic force microscopy (AFM), thermogravimetric analysis (TGA), and surface property studies to understand the nature of the dye degradation process and for catalytic studies. The maximum degradation of Eosin Y dye measured by a UV−visible spectrophotometer was 99 % at a contaminant volume of 2.7×10^{-4} mol/L and a catalyst quantity of 2 g/ L in 180 min reaction time. Using gas chromatography−mass spectrometry (GC−MS), the final products were chemically identified. The mechanistic steps of the process were carried out through a series of experiments. The recyclability of the catalyst added a novel feature for such a heterogeneous catalysis that can reduce secondary pollutants in water with no leaching effect observed.

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Next Generation Diagnosis Techniques for the Accurate Diagnosis of Urinary Tract Infections

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Abstract:

Urinary Tract Infection (UTI) is the second most common problem worldwide with around 150 to 250 million cases reported annually. Approximately 40% of women experience at least one symptomatic episode during their lifetime, compared to 12% of men. Poor hygiene, anatomical abnormalities, and catheterization are the major reasons for UTIs. The majority of these infections are caused by *Escherichia coli* and others including *Klebsiella pneumoniae*, *Proteus spp*., *Enterobacter* spp., etc. The burden of UTIs leads to increased antibiotic usage, including both self-administration and inappropriate prescribing. Inappropriate empirical therapies are associated with prolonged treatments and increased antimicrobial resistance (AMR) in uropathogens. Uropathogens are currently detected by various diagnostic approaches such as urine culture, ELISA, multiplex PCR, MALDI -TOF, PNA-FISH, Dipstick, etc. Urine culture is a gold-standard technique for culturable uropathogen detection however, non-culturable uropathogens cannot be detected with this method as well as it takes much time. Therefore, over the past two decades, solutions that have been pursued to shorten the time-consuming methods include developing advanced molecular-level assays and nanotechnologies. It can reduce the analysis time and also provide detailed information about the microenvironment of a patient's urinary tract. However, these techniques are costly and time-consuming. Therefore, further research is required to develop an advanced UTI diagnosis kit using new high-throughput genomic technologies that provide rapid and accurate results by detecting all the uropathogens along with antimicrobial susceptibility. This will help effective infectious disease management and enable healthcare personnel to use 'precision medicine' for the genuine treatment of UTIs.

Keywords: Urinary Tract Infection (UTI), Uropathogens, Antimicrobial Resistance (AMR), UTI Diagnosis.

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Synthesis and Biological evaluation of 1,2,3-triazole derivatives of Ranolazine

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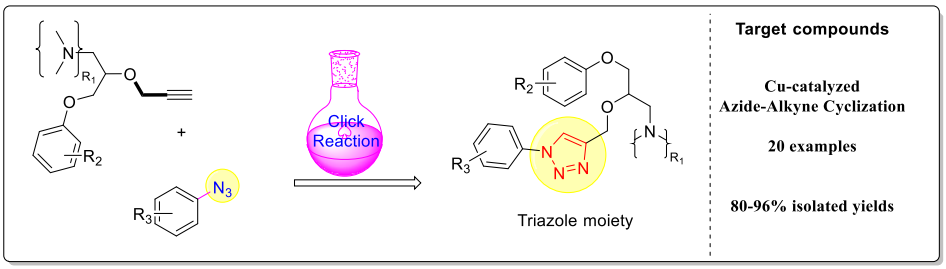
Ranolazine is a novel antianginal agent developed by Syntex with the brand name Ranexa. Ranolazine is a new cardio selective and metabolism regulating antianginal drug. The scope and limitations of method development and biological screening of the derivatives of Ranolazine is the main objective of the presented work. In the present work, a series of new 1,2,3-triazole derivatives have been synthesized by the click chemistry approach. The phenyl azide derivatives with various acetylene derivatives {1-(2-phenoxy-1-(prop-2-yn-1-yloxy)ethyl)derivatives} undergoes 1,3-dipolar cycloaddition reaction to afford 1,2,3-triazole in presence of the $CuSO_4$ and Na-ascorbate. Efforts has been made to synthesize the triazole based derivatives of the drug which on further analysis and biological screening, their potency will be compared. The newly synthesized compounds were characterized by the 1H NMR, 13C NMR and mass spectral data.



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P-80

A Series of Dipeptide Derivatives Containing (S)-5-Oxopyrrolidine-2-carboxylic acid Conjugates: Design, Solid Phase Peptide Synthesis, in vitro Biological Evaluation, and Molecular Docking Studies

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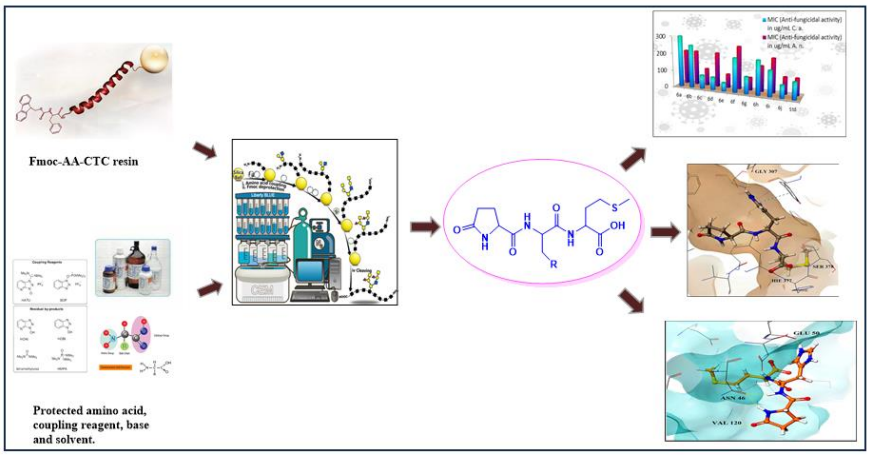
Abstract

Utilizing the solid phase peptide synthesis protocol, we have designed and prepared a novel dipeptide library containing (S)- 5-oxopyrrolidine-2-carboxylic acid moiety. All the newly synthesized dipeptides were characterized by spectroscopic techniques as well as elemental analysis. Furthermore, the in vitro antimicrobial activities of the synthesized dipeptide conjugates were evaluated. Two Gram-positive (Streptococcus pyogenes and Staphylococcus aureus) and two Gram-negative bacteria (Escherichia coli and Pseudomonas aeruginosa) were utilized to evaluate the antibacterial activity of the screened derivatives. In contrast to the standard drug Ampicillin, the targeted derivatives exhibited good antibacterial activity. Additionally, two fungi (Candida albicans and Aspergillus Niger) were used to evaluate the antifungal activity of the target dipeptides. The targeted derivatives also exhibited good antifungal activity compared to the standard drug Nystatin. In continuous, the molecular docking study of the targeted derivatives was also carried out, which revealed that the dipeptide analogs showed encouraging binding interaction networks with Escherichia coli DNA gyrase B and lanosterol-14 alpha demethylase resulting in antibacterial and antifungal activities, respectively. Such synthesis, biological evolution, and molecular docking study of peptide derivatives with oxo pyrrolidine conjugates open the door for the future development of new therapeutics containing heterocycle and peptide hybrids with potency as antimicrobial agents.



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P-81

Document Requirement for Marketing Authorization Application of Generic Parenteral Products – A Comparison

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Abstract

Marketing authorization application preparation and its submission is a crucial task, especially in terms of non-regulated market. This non-regulated market is sometimes also referred as Rest of the World (ROW) market. Non-regulated market regions are highly in demand and trending for manufacturing and selling the pharmaceutical products. Due to its less documentation requirements (legal as well as technical), less competition and low cost application requirements non-regulated market has drawn attention of numerous pharmaceutical industries.[1] Furthermore, global expansion of generic products, especially life-saving low cost general and parenteral products has increased generic market tremendously. Almost 70% of drugs provided for the treatment to the patients are generic medicines and from that most of the medicines given to the in-house patients of the hospitals are in a form of injections; therefore, generic product requirements become important.[2,3] Moreover, parenteral products control in pharmaceutical companies are crucial and extensively regulated than other dosage forms that increase the demand of understanding the regulatory requirement for these dosage forms.[4] As the pharmaceutical market expanding globally, it is required by the pharmaceutical companies to keep updated with latest regulatory requirements to ensure their place in not only to regulated market but also to non-regulated market. Current research approaches the marketing authorization requirements, especially the legal and technical documents required in a dossier of generic parenteral products, that help pharmaceutical companies to prepare for multi-country registration in rest of the world market.

Keywords: Non-regulated Market, Rest of the World, Documents, Generic, Parenteral, Marketing Authorization, Registration

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P-82

1,4-Dihydropyridines-Based Triazole Derivatives: InSilico and In Vitro Study on Green Synthesis and Anticancer Potential

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Abstract

Cancer is a disease in which cells divide in ungovernable manner and spread in tissue which further leads to death of healthy cells. Yearly approximate 41 million people are diagnosed with life threatening non- contagious disease named cancer; out of which 10 million people losses their clover life and their family lost elixir of their life. The cytotoxic potential of a library of 1,4-dihydropyridine-based 1,2,3-triazol derivatives on colorectal adenocarcinoma (Caco-2) cell lines has been assessed. Based on the 1H and 13C NMR spectroscopic data of each chemical, it was possible to characterize and identify each one. Furthermore, the mechanism of action of the two most active compounds, 13ab0 and 13ad0, revealed that they enhance cell cycle arrest during the G2/M phase and induce cell death through apoptosis in the late apoptotic phase as well as dead phase.

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Identification of Bio-Markers for Dengue Serotype Discrimination

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Abstract

Dengue is a mosquito-borne arboviral disease that majorly spreads to tropical and subtropical regions worldwide. The incidence of dengue has grown dramatically around the world in recent decades, with cases reported to increase from 0.5 million in 2000 to 5.2 million in 2019 according to WHO reports. The Americas, Southeast Asia, and western Pacific regions are the most seriously affected with Asia representing around 70% of the global disease burden. The clinical manifestations of dengue infection include fever, joint pains, arthralgia, rashes, and haemorrhagic shock which can lead to morbidity and mortality. From the available diagnostic methods in the market, the serological test also known as antibody–antigen test is widely performed to detect the presence of a virus with poor sensitivity. No efficient kit is available for the detection of specific dengue serotypes by qRT-PCR. Hence, the present investigation is aimed at identifying serotype-specific bio-markers. The whole genome of each serotype has been retrieved from public domains (NCBI). The sequence has been analysed using MSA, Codon Code Aligner to identify the unique signature of each serotype. By using Primer 3, at present, 5-6 biomarkers for serotype 1, 2, 3, and 4 has been identified. Further, these identified bio-markers primers will be validated on control and test samples for the development of the kit prototype. This bio-marker-based detection of the dengue virus and its serotypes will help in early detection of the infection effectively.

Keywords: Dengue, biomarker, serotype, epidemiology.

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Assessment of Genetic Diversity in Date Palm Cultivars collected from different locations of Gujarat using SCoT marker

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Abstract

Date palm (*Phoenix dactylifera* L.) is a perennial monocotyledonous fruiting crop belonging to the family Arecaceae. It has been cultivated since 6,000 years ago and there are existence of almost 3,000 varieties in the world. Despite of huge genetic structure and base, the genetic diversity of Indian date palm cultivars is not yet deciphered. Hence the present investigation has been aimed at analyzing the genetic diversity of date palm cultivars using Start Codon Targeted (SCoT) polymorphism markers. In this study, 30 male and 30 female date palm cultivars were collected from five different farming lands in Gujarat and were analyzed using SCoT markers. A total of 36 SCoT primers were initially screened from which eleven SCoT primers were selected for further analysis. Eleven SCoT primers successfully amplified a total of 149 reproducible DNA fragments, out of which 120 polymorphic bands, 15 monomorphic and 14 unique bands. Fragment sizes range from 100 to 10500 bp and the ratio of amplified fragments per primer is 13.5. The highest polymorphism of 100% is recorded in primer SCoT 15 and the lowest 54% in SCoT 35 with the average polymorphism is 79%. Maximum Polymorphic Information Content (0.5) was observed in primer SCoT 21 whereas SCoT 1 exhibits the lowest PIC value of 0.27. Jaccard's coefficient of similarity and SHAN clustering showed that pairwise genetic similarity coefficients ranged between 37 to 95%. The highest similarity is 95% between the genotypes F1 & F6 and F3 & F4 whereas the highest diversity (63%) was observed between F25 & M6 and F5 & M30. In conclusion, the genetic diversity of the genotypes are directly correlated with geographical distance as well as gender of the crop. The information generated from the study will help in the crop breeding program for the development of new promising date palm cultivars.

Keywords: Breeding program, Genetic diversity, Polymorphism, SCoT marker

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Triethyl amine catalyzed, thermal oxidopyrylium ion and [3+2] cycloadditionreaction for Synthesis of Oxa-bridged cyclic ethers

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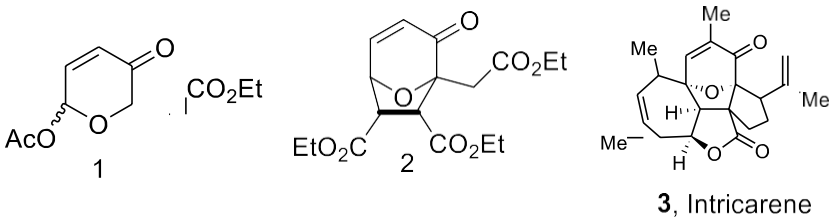
Abstract

Bioactive natural products can be synthesized by Multicomponent reactions, cascade reactions, and cycloaddition reactions. Cycloaddition reactions are one most important tools to achieve a synthesis of complex molecular structures with hetrocyclics. Molecular complexity from simple molecules becomes a challenge to build up complex bioactive natural products. In view of that and to develop oxygen-containing polycyclics from simple aromatic compounds, we with present synthesis of bicyclic ether synthesis from simple furfural. Stereoselectivity [3+2] cycloaddition of oxidopyrylium species and generation oxo pyridinium ion in from the pyronone acetate is the key step in our method. Furfural was converted to b-keto ester via reformatsky rearrangement, which upon MCPBA rearrangement gave alchol which is the source of acetate 1. Dipolar 3+2 cycloaddition is used to achieve oxo-bridged bicyclic ethers 2. Thus, in-situ generation of oxidopyrylium ion prepared in the presence of Et3N, and 3pi+2p intermolecular cycloaddition reaction studied. The adducts were obtained was characterized using spectroscopic data. The structure was confirmed by ^{1}H NMR, ^{13}C NMR, and Infrared spectroscopy.

Keywords: Cycloaddition; oxidopyrylium ion, intermolecular cycloaddition; oxo-bridged.

Graphical Abstract



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HPLC profile of Organic acid secreted by various Phosphate solubilizingGroundnut nodule endophytes

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Abstract

Arachis hypogyeae also known as groundnut or peanut is one of the leading oilseed and protein dietary cash crop. India ranks 2nd after China in World groundnut production with (66 LMT; 13%). Gujarat produces 42% of India's and 5.46% of World's total groundnut production. Saurashtra region in Gujarat is leading and renowned for its groundnut production,with Junagadh, Amreli, and Rajkot as some of the top groundnut-producing districts.

Sustainable groundnut production in Saurashtra faces major challenges of abiotic and biotic stress like Nitrogen-availability, Phosphate-deficiency, salinity, drought, fungal infestation, chemical-toxicity etc. Plant growth promoting rhizobacteria (PGPR) are solution to these challenges owing to their properties like Nitrogen-fixation, Phosphate-solubilization, antagonistic, phytohormone production, etc. Groundnut nodule serve as a unique niche for the colonization of endophytic bacteria with the potential to fix nitrogen and solubilize phosphate.

We isolated various groundnut nodule-entophytes from the organic farming fields of Rajkot region and evaluated their PGP potentials. 19 bacterial isolates showed nitrogen fixation and phosphate solubilization phenotypes. 16s rDNA sequencing revealed that isolates belong to *Rhizobium and Pseudomonas* species. Cell free supernatant of Pikovskaya broth were subjected to HPLC analysis to detect organic acids responsible for pH drop and P- solubilization. Organic acid profile was checked for presence of acids like Gluconic, Citric, Malic, Succinic, Glucoronic, Oxalic, Fumaric, Ascorbic, etc. Isolates with N2-fixation and strong P-solubilization phenotypes may prove to be strong candidates for Biofertilizer development with their multiple PGP traits for sustainable groundnut production.

Keywords: Groundnut, Nodule-Endophytes, *Rhizobium*, Phosphate solubilization, Organic acids, HPLC.

P-87

Design, Synthesis, Characterization and Biological Evaluation Study of Tetrazole Containing or N-Containing Heterocyclic Compounds

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Abstract

Most of the active pharmaceutical ingredient (API) contain the tetrazole ring. The tetrazole ring provides them a vast significance for the designing of new drug descriptors. It is known that tetrazole family is a well-known class of nitrogen containing compounds that recently attracted much attention due to its potential applications in various field such as powerful explosives, solid rocket propellant fuels as well as novel biologically active substances. Tetrazoles are not found in nature. So the synthesis of tetrazole ring containing drug molecules is a challenging job. Synthesis of tetrazole using different reaction conditions such as a N-alkylation, sodium azide, TMS azide etc via traditional method (reflux) and microwave technology have been reported. The synthesized compounds are well characterized by physical properties, UV-Vis, LC-MS, ^{1}H and ^{13}C NMR analysis. The newly synthesized tetrazole and its derivatives exhibit a large range of biological properties towards antifungal, antibacterial, anticancer, analgesic, antidiabetic, ant tubercular and anti-hyperlipidemic activity.

Keywords: Tetrazole, active pharmaceutical ingredient (API), biological study etc.

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P-88

Synthesis and Characterization of Pyrrolopyridone Derivatives: Potential Drug Candidates

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ABSTRACT

BET (Bromodomain and Extra-Terminal Domain family of proteins) inhibitors are considered to have potential therapeutic benefits for various diseases like cancers, infections, metabolic diseases, CNS disorders etc. It is critical to identify potent inhibitors suitable for phenotypic profiling that are highly selective over other bromodomain family members. Pyrrolopyridone derivatives have demonstrated significant therapeutic potential as enzyme inhibitors in various disease as it serves as the acetyl lysine mimetic with the pyridone carbonyl and pyrrole nitrogen forming a 2-point interaction[1]. In addition, Pyrrolopyridone is a fragment derived molecule with strong binding across bromodomain family members, with ligand efficiencies (LE)> 0.54 for all eight bromodomains screened [1], which proves its high selective ligand efficiency. Pyrrolopyridone derivatives have also been recognized as an important core to inhibit the activity of BRD^9 through small molecules [2], which has been a novel and reliable pathway for tumor treatment. Moreover, the mechanism responsible for DUX4 expression are poorly understood for the treatment of FSHD disease[3] and also limited drug targets have been identified based on Pyrrolopyridone derivative. In summary, Pyrrolopyridone derivatives represent a versatile and powerful enzyme inhibitor with diverse pharmacological applications. Their thoughtful design and synthesis make them an exciting area of exploration in modern drug development. This work provides an overview of synthesis and characterization of Pyrrolopyridone derivatives and showcasing their potential as enzyme inhibitors in various biological applications like antibacterial, antifungal, anticancer, and anti-tubercular treatments.

Keywords: Pyrrolopyridone derivatives; antibacterial and antifungal, anticancer, anti-tubercular; heterocyclic compounds.

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P-89

Molybdovanadophosphoric acid supported kaolin hybrid catalyst for dye degradation inwater: A review

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Recyclable molybdovanadophosphoric acid immobilized on kaolin (MVPA/Kaolin) is a hybrid substance that can be used to catalyze the degradation of the dye Chromotrope 2R in water undermild reaction conditions. The current study offers a comprehensive perspective on this subject. Novel MVPA/Kaolin was produced using an advanced impregnation method. The substance was characterized using PXRD, FTIR, ICP-OES, SEM-EDX, TEM, TGA, surface area, porosity, and ^{31}P NMR studies. The oxidation of aromatic azo (-N=N-) dyes with -OH and -SO_3H functional groups in hydrogen peroxide might be accomplished using the Keggin type of catalyst. The deterioration showed outstanding conversion of 99.1% under optimum conditions of normal pressure and 60 °C temperature. By using GC-MS analysis, the end products have been identified as chemicals like malonic acid and oxalic acid. In the current work, it was demonstrated how to degrade azo dyes with a simple and effective catalyst and that the catalyst could be recycled up tosix times without losing its potency.

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P-90

Cur-cumin a therapy for covid -19

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ABSTRACT

Coronavirus disease 2019 outbreak is an ongoing pandemic caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) with considerable mortality worldwide. The main clinical manifestation of COVID-19 is the presence of respiratory symptoms, but some patients develop severe cardiovascular and renal complications. There is an urgency to understand the mechanism by which this virus causes complications so as to develop treatment options. Cur-cumin, known for its pharmacological abilities especially as an anti-inflammatory agent, can be hypothesized as a potential candidate in the therapeutic regimen. COVID- 19 has an assorted range of pathophysiological consequences, including pulmonary damage, elevated inflammatory response, coagulopathy, and multi-organ damage. This review summarises the several evidences for the pharmacological benefits of cur-cumin in COVID-19-associated clinical manifestations. Cur-cumin can be appraised to hinder cellular entry, replication of SARS-CoV-2, and to prevent and repair COVID-19-associated damage of pneumocytes, renal cells, cardiomyocytes, hematopoietic stem cells, etc. The modulation and protective effect of cur-cumin on cytokine storm-related disorders are also discussed.

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P-91

HPTLC method for rapid chemical screening and simultaneous determination of major bioactive constituents of Butterfly pea

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ABSTRACT

Butterfly pea (*Clitoria ternatea*) is herbaceous climbing plant, belonging to the family Fabaceae and originated from tropical Asia then now distributed in various parts of the world. Different phytocompounds like triterpenoids, flavonol glycosides, proteins, tannins and carbohydrates are reported from the plant and also it showed vast pharmacological activities.[1,2] The bioactive constituents such as β-sitosterol and taraxerol are reported with higher content in the herb. In the present study is therefore, an effort to develop a simple, and accurate high-performance thin layer chromatography (HPTLC) method for rapid chemical fingerprinting and simultaneous estimation of β-sitosterol and taraxerol in the Butterfly pea. The developed HPTLC method was validated as per ICH guidelines. [3] Solvent selection for enriched extraction with the aforementioned bioactive constituents was also evaluated using the developed method.

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P-92

Rapid, diversity-focused method for producing 3-tetrahydropyrimidinyl coumarins using MCRA gentle, efficient, and practical synthetic method for producing unknown tetrahydropyrimidinyl substituted 3-coumarins.

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Abstract: The synthesis of unknown tetrahydropyrimidinyl substituted 3-coumarins as hybrid scaffolds, possibly beneficial novel chemical entities (NCEs), by metal- and catalyst-free multicomponent cyclization is reported as a helpful, moderate, and high-yielding synthetic method. The difference in the 13C NMR values (Δδ) of vinylic carbons explains why 3-amino coumarins are more nucleophilic than 4-amino coumarins. A representative set of examples' structure is described through X-ray crystallography.

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One-pot synthesis and structural elucidation of barbiturate analogues

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ABSTRACT

Pyrimidine is a prominent heterocyclic constituent presents in the biologically active compounds, which reported as chemicals, flavors, and stains but they mainly used as drugs because of their derivatives play a significant role in the field of medicine.[1] Numerous natural substances, including coenzymes, uric acid, purines, and some marine microbes, have the pyrimidine ring structure. Barbituric acid is a chemical compound with pyrimidine heterocyclic skeletons, their derivatives are sedative medicines that suppress the central nervous system.[2] Certain substituted thiobarbituric acids have a long history of use as intravenous anaesthetics and as intermediates in the manufacture of dyes.[3] Parent barbiturates and thiobarbiturates are convenient starting materials for the creation of distinct fused heterocycles because of their accessibility and range of functional possibilities.[4] Structure activity relationship shows heterocyclic substituted aryl moieties at the 5-position of barbiturates nucleus increase biological activities. In pharmaceutical chemistry and drug development, the significance of barbiturates is widely known,[5] because they are good target molecules for organic and medicinal chemists due to their diversified biological actions and covering of a wide chemical spaces. In continuation of our efforts, we synthesized the barbituric acid derivatives using a multi-component, environmentally friendly process and one-pot synthesis. The structural elucidation was carried out using various spectroscopic techniques.

Keywords: One-pot synthesis, barbiturate analogues, biological activities

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P-94

Development of assay method and forced degradation study of Multaq by RP-HPLC in Pharmaceutical Dosage Form

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Abstract:

Multaq in pharmaceutical dosage form has been estimated using a reverse phase UPLC approach that is simple, reliable, fast reproducible, selective, and stability suggesting [1-2]. On an Acquity BEH C18 (100 mm∗2.1 mm) 1.7 μm μm column, multaq was estimated using a buffer consisting of 20 mM KH2PO4 + 1 mL Triethylamine (pH = 2.5 by orthophosphoric acid) and methanol in a ratio of 40: 60 as the mobile phase at 30∘C. The effluents were seen at 290 nm, at a flow rate of 0.4 mL/min. In terms of linearity, accuracy, precision, LOD, LOQ, and robustness, the procedure was validated. The linearity of the technique was observed over the concentration range of 0.38–90 μg/mL ($r2$ = 0.999), with 0.1 and 0.38 μg/mL for the detection and quantification limits, respectively [3]. Acid and alkali hydrolysis, chemical oxidation, thermal degradation, and photo (sunlight) degradation were all performed on multaq. The degradation product peaks were well separated from the drug peak, and their retention time values differed significantly [4-7].

Keywords: HPLC, Analytical method validation, Pharmaceutical analysis, Specificity, Precision, Accuracy.

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Development of the Bio Active Pyridine Based Hetero Cyclic Compounds for Medicinal Application.

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Abstract:

Pyridine is a heterocyclic aromatic compound with a six-membered ring containing five carbon atoms and one nitrogen atom. It is a basic structure found in many biologically active molecules. Pyridine and its derivatives are widely used in medicinal chemistry due to their diverse biological activities. Pyridine and its derivatives have been studied for their microbial activity (1), both as antimicrobial agents and as compounds that can influence microbial metabolism (2). Indeed, pyridine derivatives have been extensively studied in medicinal chemistry, and they play a crucial role in the development of various pharmaceutical agents. The development of bioactive pyridine-based heterocyclic compounds for medicinal applications involves a systematic process that combines synthetic chemistry, computational modeling biological testing. Some pyridine derivatives have been found to exhibit antibacterial properties. For example, 2,6-dimethylpyridine has been studied for its antibacterial activity against certain strains of bacteria (3). Certain pyridine derivatives have also demonstrated antifungal properties (4). Researchers have explored the potential of pyridine compounds in the development of antifungal agents (5). In this current research the following steps will be covered Target Identification and Validation, Lead Compound Identification, Synthetic Chemistry Medicinal Chemistry Optimization and Biological Assays (6). Research in this field continues to explore the potential applications of pyridine and its derivatives in medicine, as well as to understand the microbial interactions with these compounds.

Keywords: pyridine hybrids, antimicrobial activity & antifungal, nitrogen containing Heterocycle antioxidant agent.

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In-Silico molecular docking studies on drug molecules to treat the breast cancer

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Among various diseases, cancer has become a big threat to human beings globally including Indian population. All types of cancers have been reported in the Indian population, including the skin, lungs, breast, rectum, stomach, prostate, liver, cervix, esophagus, bladder, blood, mouth, etc. Amongst all of these, breast cancer is expected to rise to 2.3 million new cases. The present *in-silico* work incorporates the basic techniques for docking the chemical molecules related to breast cancer to find their chemical potential. The parameters related to structures and energy status of those chemical drug molecules treating the cancer are clearly presented.

Argus lab was used to investigate the docking proportion for the treatment of breast cancer with the help of three drugs Tamoxifen, Decitabine, and Capecitabine. It was found the least energy (Max Stability) was observed as (-15.1394 Kcal/mol) for Tamoxifen, (-10.9912 Kcal/mol) for Decitabine, and (-9.68165 Kcal/mol) for Capecitabine.

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Biomass Derived Green Solvents – A Review

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With ever growing impact of climate change, environment sustainability has become one of the most critical concerns. Synthesis and separation of various chemicals and pharmaceutical intermediates involves solvents. Selecting solvent for these processes having least harmful effect on environment and most economically viable is crucial for sustainability. Green solvents can help in achieving these goals. They can be synthesised via traditional chemicals where green solvent itself might not be harmful to environment but base or raw material used for its synthesis might be having adverse effect on environment. A recent approach to mitigate this is to explore various biomass to derive or obtain said green solvent. In this work, various biomass green solvents are identified. Also, their synthesis and application are reviewed comprehensively.

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P-98

Mesomorphic Study of some chiral derivatives involving of 6-*n*-alkoxy-2-naphthoic acid

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Abstract:

In this contribution, we are presenting synthesis and mesomorphic properties of two homologues series by judicious choice of optically active S(+)-2-methyl butyric acid. We compare various homologues and look for tendencies in behavior of physical properties, when changing the length of the non-chiral chain. Thus, the aim of our research is to develop a wide range of materials and have origins in basic structure–property relationships and in the development of ferroelectric materials. Hence, this area research is completely different to that of non-chiral liquid crystals, which generate mesophases that are of a different category to those reported here. In this work, we focus our studies on the SmC* phase stability of these materials in relation to their molecular structure and structures of these two new series of chiral compounds are shown in Series **I** and **II**.

Keywords: Liquid crystal, mesophase, nematic, smectic

P-99

Removal of Lead Ions from aqueous solutions using Bimetallic Oxide Impregnated Silicate Composites

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Abstract

Despite the implementation of various mitigation strategies to combat lead ion toxicity in water bodies, lead can still enter these ecosystems through a range of anthropogenic activities. These activities include industrial processes, mining, smelting, manufacturing, and improper disposal of products containing lead. Managing agricultural fly ash is crucial due to environmental concerns. Using it for wastewater treatment holds promise in addressing waste management and improving water quality. Despite challenges, this approach aligns with sustainability and pollution reduction goals. The present work executes the fabrication of a low cost silica supported bimetallic oxide impregnated silicate sorbents, namely (FeZn)Ox/Silicates, (FeMn)Ox/Silicates, and (FeCu)Ox/Silicates, using the Incipient Wetness Impregnation (IWI) method. The Bagasse fly ash (BFA), a low cost raw material as an agricultural waste utilized for the silica source. Scanning Electron Microscopy (SEM) images and Energy Dispersive X-ray Spectroscopy (EDX) images of the bimetallic oxide impregnated silicate sorbents provides support to the successful grafting. The batch sorption studies conducted, with parameters such as pH, contact time, sorbent dosage, initial sorbate concentration, and temperature being optimized. The sorption capacity in terms of q_e was found maximum in case of (FeMn)Ox/Silicates at pH 5.0 for the removal of Lead in aqueous media. The Langmuir and Freundlich sorption isotherm models found in support of the sorption capacities.

Keywords: Lead removal, Fly ash utilization, Environmental remediation, Agricultural waste, Waste Utilization, Waste minimization.

P-100

Novel Dihydropyrimidinone Derivatives as Potent Drugs that inhibit of P-Glycoprotein

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Abstract: Cancer multidrug resistance is brought about by the ATP-dependent efflux pump p-glycoprotein (Pgp), an ATP binding cassette (ABC) transporter. We applied a synthetic method that is well studied for producing compound libraries to build a series of novel triazole-conjugated dihydropyrimidinones as part of our attempts to locate human Pgp (hPgp) inhibitors. With low micromolar EC_{50} values, some of these dihydropyrimidinone derivatives modify the activity of human P-glycoprotein (hPgp). Based on molecular docking studies, these substances link to the transporter's M-site.

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Design, Synthesis and Biological Evaluation of Piperazine-arylamide Derivatives as Antitubercular Agents.

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Abstract:

Tuberculosis (TB), an ancient, highly contagious and chronic infectious diseases caused by Mycobacterium tuberculosis has affected millions of peoples and has been the cause of death of more than 60 million people since 2000. The estimated number of deaths officially classified as caused by TB (1.3 million) in **2020.**The currently used DOTS therapy have failed to cure TB completely, due to poor or inadequate treatment against the emergence of MDR-TB and XDR-TB. The failure of current drug-regimen and worsening situation of TB have sensitized the urge for discovery of new anti-TB agents. In search of the panacea for TB, several research groups have designed, synthesized new anti-TB hits. Moreover, the recent trend has been shifted to adopt the design and synthesis of entirely new chemical scaffold acting on the new targets with least scope of resistance.

In search of InhA inhibitors (PDB-ID: 4TZK), For virtual screening Enamine Hit locator library (Library code: HILL-200, compound: 2,00,000) was selected. The designed compounds have been docked against this protein using FlexX and compared with reported inhibitor of InhA. After virtual screening, we found piperazine-arylamide scaffold in common. Further, we analysed the 3D interaction along with their ADMET properties through *in silico* tools. These studies have provided an important start-point in the field of anti-mycobacterial agents through virtual screening in search InhA inhibitors.

Keywords: Piperazine-arylamide derivatives, Inha inhibitors, Antitubercular agents.

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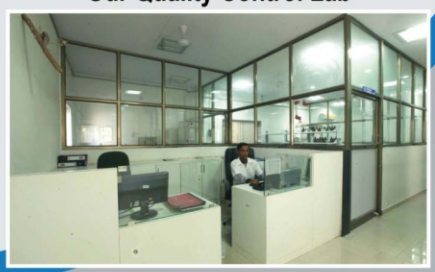

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