योगः कर्मसु कौशलम्

INDRASHIL UNIVERSITY

A LIFE SCIENCES UNIVERSITY

Sustained Excellence with Relevance

An educational initiative by

CADILA PHARMACEUTICALS LIMITED

The Care Continues...

Department of Chemistry, School of Science,
Indrashil University
Organizes

1st International Conference on

SUSTAINABLE INNOVATIONS IN DRUG DEVELOPMENT (SIDD-2025)

Monday 24th to Wednesday 26th March, 2025

Organised by
Department of Chemistry, School of Science,
Indrashil University, Rajpur – Kadi, Mehsana, Gujarat, India-382715

School of Science (SoS)

B. Sc. Chemistry

B. Sc. Biotechnology | Ph.D. in Science

B. Sc. Forensic Science

M. Sc. Chemistry (Organic & Analytical Chemistry) | M. Sc. Microbiology

M. Sc. Zoology | M. Sc. Biotechnology

Nuclear Magnetic Resonance (NMR)

Received Research Grant of 3+ Crore from Govt.Organizations 2021&22

Department of Chemistry, School of Science Received DST-FIST Grant 2022

Received Research Grant of 1.13 Cr Crore from Industries Commissionerate, Department of Industries and Mines, GoG, Gandhinagar

Chemical & Biochemical Eng. Department Recognised as Schedule 1 Environmental Auditor by GPCB

Startup & Incubation Facilities

IU is having a clear focus on supporting startup and entrepreneurship in our institutional & industrial goals. Our university is closely working with both State and Central Government, to give 360 degree support to aspirants in both technical and business domains. IU has received the recognition from state government to support startup & entrepreneurship through Gujarat Knowledge System to support student startups since 2020 and Industry commissionerate to support any novel startups to take the idea from lab to market with incubation support. The central government guided Atal Incubation Centre functioning since 2019. AIC-ISE Foundation is supported by the Atal Innovation Mission, NITI Aayong, Government of India is to promote 'Make in India' & 'Atmanirbar' Bharat' scheme & ideology. It is supporting more than 40 student projects, 20 registered startups with over 10 IPR.

About SIDD-2025

The three-day international conference titled "Sustainable Innovations in Drug Development (SIDD-2025)" is scheduled to be held from March 24th (Monday) to March 26th (Wednesday), 2025 at Indrashil University. The conference will be held at the IU campus and conducted in a Hybrid Mode, enabling speakers to join and deliver their talks online as well.

SIDD-2025 aims to provide a platform for researchers, professionals, and students from academia and industry to discuss cutting-edge sustainable innovations in drug discovery and development. Approximately 200 participants are expected to join this conference, featuring keynote, plenary, and invited lectures by eminent scientists across the globe with interdisciplinary expertise, alongside poster and oral presentations by young researchers. The thematic areas include sustainable innovations in Natural Product Synthesis, Asymmetric Catalysis, Chemical Biology and Bioconjugate Therapeutics, Medicinal Chemistry, Process Development and Computational Drug Development. The whole activity aligns with Government of India initiatives like "Viksit Bharat @2047" and "Make in India". By encouraging sustainable practices, India can achieve a balance between industrial growth and environmental responsibility in the pharmaceutical sector.

CONFERENCE OBJECTIVES:

1. *Foster collaboration between academia and industry in drug discovery and chemical synthesis.*
2. *Provide a platform for students and researchers to showcase their work.*
3. *Highlight innovations which have high impact in life.*
4. *Encourage interdisciplinary dialogue to solve complex challenges in drug research and advanced synthesis.*

About Indrashil University

Indrashil University aims to provide an epitome of excellence in higher education by imparting knowledge and high-quality teaching and learning experiences to students in the field of Chemical Sciences, Biological Sciences, Pharmaceutical Sciences, Engineering, Technology and Management domain. This university was established by its Founding Chancellor, Dr. Rajiv I. Modi in the loving memory of his parents, Shri Indravadan Ambalal Modi and Smt. Shilaben Modi, who laid the foundation stone of Cadila Pharmaceuticals Ltd. in 1951. To honour their legacy of care and compassion, Indrashil University is determined to transform lives of students by providing holistic education and knowledge in cutting-edge research and technology and to develop the university into a hallmark of global academic excellence. All the programs of Indrashil University offer updated course curriculum with choice-based credit system and industry-inculcated syllabus to provide future-ready skilled professionals.

The research and development activities of Indrashil University is largely boost up by its modern laboratory facilities with advanced analytical instruments. Indrashil University has also received prestigious DST-FIST grant and Industries Commissionerate, Govt. of Gujarat fund to procure high-cost instruments and equipment for cutting-edge research and data analysis.

Indrashil University is the only private university in Gujarat which has Atal Incubation Centre (AIC-ISE), a foundation under Section-8, not-for-profit organization, instituted as per the direction of Atal Innovation Mission, NITI Aayog, Government of India to promote Innovation, startups and entrepreneurship. The prime objective of AIC is to provide requisite facility in nurturing the ideas & start-ups for personalized as well as societal growth and development.

The Indrashil University has received several award and accreditations including recently awarded four-star rating by GSIRF (KCG, Govt. of Gujarat) for the quality of teaching and research activities.

About The Department of Chemistry

The Department of Chemistry offers UG, PG, and PhD programs in chemical sciences at Indrashil University. These programs provide ample opportunities for the students to choose courses from a broad spectrum of cutting-edge areas in addition to fundamentals of organic, inorganic, physical, analytical, nano, polymer, and computational chemistry. Sessions on improving technical skills, scientific writing, oral presentations and research expertise have been incorporated in the curriculum. Furthermore, the students will have the scope to pursue their graduation and post-graduation thesis work at various national and international institutions and industries. Overall, by integrating the in-depth core and elective courses, and research work, instructed and guided by highly qualified and well-experienced faculty members, students gain the foundation and skill to advance their careers in higher studies and industry.

Programs offered:

- B.Sc. and M.Sc. Chemistry in collaboration with Cadila Pharmaceuticals Ltd.
- B.Sc. (Specialization in Chemistry)
- M.Sc. Chemistry (Specialization in Organic Chemistry)
- M.Sc. Chemistry (Specialization in Analytical Chemistry)
- Ph. D. Chemistry

Internship, placement and higher studies opportunities for the B.Sc. and M.Sc. students in reputed companies, national and international universities.
100% students from the previous academic years have secured internships and placements in various renowned industrial and academic organizations.

Areas of Innovation and Research in the Department of Chemistry:

- Organic Chemistry
- Catalysis
- Environmental Chemistry
- Inorganic Chemistry
- Physical Chemistry
- Supramolecular Chemistry
- Computational Chemistry
- Medicinal Chemistry
- Molecular self-assembly
- Material Chemistry (Nano materials, porous materials, metal organic gel)
- Lasers and Spectroscopy

Fostering Innovation for a sustainable future

It is with immense pride and deep personal commitment that I welcome you to the **1st International Conference on Sustainable Innovation in Drug Development (SIDD-2025)**. This landmark event, the first of its kind in Gujarat, is a testament to our unwavering commitment to research, innovation, and sustainable advancements in pharmaceutical science.

This institute, named in honour of my beloved parents, stands as a testament to their values of integrity, perseverance, and pursuit of knowledge for the greater good. Their legacy fuels our mission to create a world-class centre of excellence where academia, industry, and research converge to drive meaningful impact in healthcare and beyond.

As someone deeply engaged in the pharmaceutical industry, I have witnessed first-hand the transformative power of research and development. While ground-breaking therapies have revolutionized patient care, it is imperative that we approach innovation with sustainability, ethics, and accessibility at the forefront. The future of our industry will be shaped not just by scientific discoveries but by our collective responsibility to create eco-friendly, affordable, and effective solutions.

SIDD-2025 is more than just a meeting of minds— it is a platform for scientific dialogue, collaboration, and action. With a focus on Natural Products, Stereoselective Synthesis, Chemical Biology, Computational Drug Design, and Sustainable Process Development, this conference brings together global pioneers, leading academicians, and industry experts to shape the next era of pharmaceutical innovation. With the right vision and commitment, we can shape an industry that not only delivers world-class medicines but does so in a way that safeguards our planet and future generations.

This conference is not just about sharing knowledge; it is about shaping the future. Through interdisciplinary collaboration, cutting-edge research, and industry-academia partnerships, we have the opportunity to redefine pharmaceutical sustainability, ethical practices, and regulatory advancements. Let us collectively work toward solutions that balance scientific excellence with environmental and social responsibility.

As we embark on this exciting journey at SIDD-2025, I encourage all participants—scientists, faculty, students, and industry leaders—to actively engage, exchange ideas, and forge collaborations that transcend borders and disciplines. Together, let us inspire new possibilities, drive impactful research, and create a legacy of innovation that serves humanity for generations to come.

Dr. Rajiv I. Modi
President
Indrashil University

Driving Research Excellence & Community Impact Through Innovation

It is with immense pride that I extend my heartfelt welcome to all participants of the Sustainable Innovations in Drug Development Conference (SIDD-2025). This international conference is a reflection of Indrashil University's unwavering commitment to research, innovation, and knowledge-sharing in the field of pharmaceutical sciences and drug development. It provides a unique opportunity for scholars, industry leaders, and young researchers to engage in meaningful discussions, fostering collaborations that can redefine the future of sustainable healthcare solutions.

At Indrashil University, we strongly believe in the transformative power of research. Our state-of-the-art research facilities, industry-driven curriculum, and strategic global partnerships position us as a university that drives innovation with societal impact. We recognize that academic research must not only contribute to scientific advancements but also serve the greater good by addressing global healthcare challenges and sustainability concerns.

In today's rapidly evolving global landscape, drug development and pharmaceutical research are undergoing transformative shifts. The emergence of precision medicine, artificial intelligence-driven drug discovery, and green chemistry has revolutionized how we approach treatments. However, these advancements must align with sustainable and ethical research practices to ensure accessibility, affordability, and minimal environmental impact.

Indrashil University is committed to fostering research that:

- Explores novel drug discovery pathways through computational modelling and AI-driven approaches.
- Develops eco-friendly and sustainable pharmaceutical processes, minimizing waste and optimizing resource utilization.
- Strengthens academia-industry partnerships to accelerate translational research and real-world applications.
- Encourages interdisciplinary collaborations that integrate chemistry, biology, and engineering for holistic healthcare solutions.

Innovation in Drug Development: A Global Necessity -The pharmaceutical industry today faces multifaceted challenges, from antimicrobial resistance to the need for rapid vaccine development. The COVID-19 pandemic demonstrated the urgent need for agility, collaboration, and cutting-edge innovation in the healthcare sector. Sustainable drug development is no longer an option—it is an imperative.

SIDD-2025 serves as a platform where faculty and students can immerse themselves in cutting-edge discussions, interact with distinguished experts, and explore interdisciplinary approaches to problem-solving in drug discovery, green chemistry, and computational advancements. Such conferences play a pivotal role in the academic and professional growth of our university community, ensuring that we remain at the forefront of scientific excellence and industry relevance.

I extend my gratitude to all the eminent speakers, researchers, and participants who have joined us for SIDD-2025. Your presence and contributions make this conference a significant milestone in our journey towards academic distinction and societal progress. Let us utilize this opportunity to build stronger networks, share groundbreaking ideas, and take a step forward in shaping a future where innovation meets responsibility.

Wishing you all an enriching and inspiring experience during SIDD-2025 at our green university.

Prof. (Dr.) Dharmesh J. Shah
Provost
Indrashil University

Prof. (Dr.) J. S. Yadav

FNA, FTWAS

It is an honor to welcome you to the Conference on Sustainable Innovations in Drug Development (SIDD-2025). This event brings together some of the brightest minds in science, including stalwarts of organic chemistry, to discuss cutting-edge advancements that are shaping the future of pharmaceutical research.

As a director of a national laboratory, I have dedicated my career to pioneering innovation while ensuring that sustainability and ethical responsibility remain at the forefront of our work. Today, as we navigate the evolving landscape of drug development, it is imperative that we embrace greener, more efficient technologies to minimize environmental impact and maximize scientific breakthroughs.

This conference is not only a platform for intellectual exchange but also a celebration of excellence. With numerous poster awards and recognitions, we honor the outstanding contributions of researchers who are driving meaningful changes. I encourage you to engage, learn, and collaborate, as these discussions will inspire the next generation of sustainable solutions in our field.

Beyond science, I hold strong personal values that guide my vision. Just as we acknowledge the mentors and pioneers who paved the way, I urge everyone to show the same respect and gratitude to their parents—the foundation of our success and character. Staying humble amidst our achievements reminds us that knowledge is a lifelong journey, and true progress is made when we uplift and learn from one another.

Thank you for being part of this incredible gathering. I look forward to insightful discussions, ground-breaking ideas, and a shared commitment to excellence.

Prof. (Dr.) J. S. Yadav
Research Director
Indrashil University

Message

The First International Conference on Sustainable Innovations in Drug Development (SIDD-2025) is a testament to Indrashil University's unwavering commitment to advancing the frontiers of science in the drug discovery process while addressing the global challenges with sustainable solutions. It gives me immense pleasure to extend a hearty welcome to all the distinguished delegates, dignitaries, and participants on the campus of Indrashil University for this international conference.

Drug development is a multidisciplinary domain that requires a multi-facet approach to balance cost-effectiveness, environmental considerations, and regulatory compliances. With the advent of novel chemical processes like electrochemical synthesis, photo-redox catalysis, and mechanochemical processes, there has been a big paradigm shift in achieving sustainable solutions for existing academic and industrial concerns. This conference aims to bring together a galaxy of intellectuals, eminent researchers, passionate academicians, professional industrial experts, and strategic policymakers across India and around the world to discuss their expertise. This conference will also provide a platform and opportunity for specialists to exchange and share their path-breaking novel ideas and discoveries in chemical and pharmaceutical sciences and forge collaborations amongst participants.

The deliberations and outcomes of this conference will inspire many young and budding researchers to look for transformative and translational solutions to existing societal and environmental concerns in drug research and innovation. The members of the Organizing Committee owe a sincere applause for their remarkable efforts in making this international conference a grand success. We look forward to a memorable and enjoying stay for all the delegates and participants on our campus and to benefit from the enriching discussions and useful interactions that this conference promises to deliver.

Dr. Keshri Nath Tiwari
Dean, School of Science
Indrashil University

Message

It is my pleasure to welcome you to the Conference on Sustainable Innovations in Drug Development (SIDD-2025) on 24th - 26th March 2025 at Indrashil University, Rajpur, Mehsana, Gujarat. This conference serves as a vital platform for students, researchers, industry experts, and academicians to exchange their ground-breaking research, ideas and foster collaborations that drive the future of chemical, biological and pharmaceutical sciences. This conference features an engaging line-up of plenary, keynote addresses, technical sessions, academia-funding-industry panel discussions, and interactive dialogues on the latest advancements in the field of chemistry, drug discovery and development.

In an era where sustainability and innovation are paramount, SIDD-2025 brings together some of the finest minds in organic chemistry, medicinal sciences, nanotechnology, and biotechnology to discuss transformative approaches in drug discovery and development. From green chemistry solutions to cutting-edge biopharmaceuticals.

This conference provides a distinctive platform and a valuable opportunity for scientific networking, contributing to the nation's growth and development in line with the vision of Vikshit Bharat 2047. It serves as a forum to explore emerging technologies and ground-breaking discoveries, inspiring and educating students, scientists, researchers, clinicians, industry professionals, and key stakeholders. Through knowledge exchange and collaborative learning, the conference seeks to reinforce the pillars of science, technology, and innovation, paving the way for a brighter future.

I urge all participants to actively engage in thought-provoking discussions, embrace new perspectives, and cultivate meaningful collaborations that will drive a more sustainable and innovative pharmaceutical industry.

Vijai Singh

Prof. (Dr.) Vijai Singh
Dean (R & I)
Indrashil University

Message

Dear Esteemed Delegates, Participants and Future Innovators,

It is with great enthusiasm that we welcome you to the International Conference on 'Sustainable Innovations in Drug Development (SIDD-2025)', hosted by Indrashil University from March 24–26, 2025.

SIDD-2025, where science meets sustainability and innovation fuels discovery! Over the next three days, we dive into cutting-edge breakthroughs in drug development, exploring Natural Product Synthesis, Asymmetric Catalysis, Medicinal Chemistry, and more—all through the lens of sustainability.

Expect powerful keynotes, dynamic discussions, and game-changing ideas from global experts. Our Students' Special Interactive Session is set to spark fresh perspectives on industry-academia collaboration with a special emphasis on translational research.

Let's take this opportunity to network, learn, and drive innovation towards a sustainable and transformative future in drug development.

Wishing you an intellectually stimulating and successful SIDD-2025!

Vishnumaya

Dr. Vishnumaya Bisai
Convener
Associate Professor
Indrashil University

Message

Dear Esteemed Guests and Participants:

I am pleased to announce that Indrashil University will be hosting its inaugural 1st International Conference on Chemical Sciences for a Sustainable Future: Research, Innovations, and Solutions (SIDD-2025). This landmark event is dedicated to tackling some of the world's most urgent challenges by leveraging advancements in chemical and biological sciences. By integrating cutting-edge research, pioneering technologies, and sustainable solutions. With a strong emphasis on global collaboration, SIDD-2025 will serve as a dynamic platform where scientists, researchers, policymakers, and industry leaders can exchange knowledge, share breakthroughs, and explore innovative solutions for a more sustainable future. Furthermore, this conference presents a valuable opportunity for students, early-career researchers, and stakeholders to engage with renowned experts, fostering an environment of intellectual exchange, innovation, and meaningful dialogue.

As we embark on this exciting journey of scientific discovery and sustainable development, SIDD-2025 marks a significant milestone in promoting research-driven innovation and addressing critical global challenges. I extend my best wishes for the success of this impactful and forward-thinking conference, and I look forward to the collaborative efforts that will emerge from this esteemed gathering.

Dr. Shally Rana
Co-Convener
Assistant Professor
Indrashil University

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Scientific Program Schedule

Day 1 – March 24th, 2025, Monday

Time	Session Speaker(s)
Inaugural Session-Chairs-Prof. Keshri Nath Tiwari & Dr. Vishnumaya Bisai	
9:30 am – 10:30 am	**Welcome Address by Dignitaries & Release of 'Souvenir'**
Session I: Chairs-Prof. J. S. Yadav & Prof. G. Mugesh	
10:30 am – 11:05 am	**Keynote Lecture: Prof. Vinod K. Singh,** IIT Kanpur *Creativity in Organic Synthesis and its Implications on Drug Discovery*
11:10 am – 11:40 am	**Plenary Lecture (PL-1): Dr. T. Rajamannar,** Sun Pharma Advanced Research Company Ltd. *Process Development and Sustainable Chemistry*
11:45 am – 12:05 pm	**Tea Break and Networking***
Session II: Chairs-Prof. Tapas K. Kundu & Prof. Alakesh Bisai	
12:10 pm – 12:40 pm	**Plenary Lecture (PL-2): Prof. G. Mugesh,** IISc Bangalore *Small Molecules as Redox Active Artificial Enzymes for Biomedical Applications*
12:45 pm – 1:15 pm	**Plenary Lecture (PL-3): Dr. D. S. Reddy,** IICT Hyderabad *Efforts in Drug Discovery through Natural Products and Process Development of a Lifitegrast Intermediate with Low Carbon Footprint*
1:20 pm – 2:30 pm	**Lunch Break and Networking***
Session III: Chairs-Prof. Sivapriya Kirubakaran & Dr. Poulomi Sengupta	
2:30 pm – 3:00 pm	**Virtual Plenary Lecture (VPL-1): Prof. Janine Cossy,** ESPCI Paris-France *Powerful Tools for The Synthesis of Bioactive Heterocycles Towards Sustainability*
3:05 pm – 3:35 pm	**Virtual Plenary Lecture (VPL-2): Prof. Lutz Ackermann,** Georg-August-University Göttingen- Germany, TBA
3:40 pm – 4:10 pm	**Virtual Plenary Lecture (VPL-3): Prof. Varinder Aggarwal,** University of Bristol- UK *Synthesis with Boron at the Helm*
4:20 pm – 4:40 pm	**Tea Break and Networking***
Session IV: Chair- Chairs- Dr. Debendra Mohapatra & Dr. Vijai Singh	
4:45 pm – 5:05 pm	**Dr. Bakulesh Khamar:** Cadila Pharmaceuticals Ltd. **CADILA Special Session** on 'CADILA's Innovation'
5:10 pm – 5:30 pm	**Dr. Manjul Joshipura:** Cadila Pharmaceuticals Ltd. **CADILA Special Session** on 'CADILA's Innovation'
Session V: Chairs- Chair-Dr. Sriram K. Gundimeda & Moderator-Prof. Santosh Gharpure	
5:35 pm – 6:45 pm	**Students' Special Academia/Industry Interactive Session** **Prof. J. S. Yadav** (Research Director, Indrashil University) **Prof. V. K. Singh** (Institute Chair Professor, IIT Kanpur) **Dr. T. Rajamannar** (Non-Executive Director, SPARC Ltd.) **Prof. Tapas K. Kundu** (Professor, JNCASR Bangalore) **Prof. G. Mugesh** (Professor & Dean, IISc Bangalore) **Dr. D. S. Reddy** (Professor & Director, IICT Hyderabad) **Dr. Debesh Das** (President, Branded SBU, CADILA) **Dr. Vinay Kr. Srivastava** (Prof. IU & Asst. Vice President, VFS, CADILA)
6:45 pm – 7:30 pm	**Cultural Program**

Time	Session Speaker(s)
Inaugural Session-Chairs-Prof. Keshri Nath Tiwari & Dr. Vishnumaya Bisai	
7:30 pm onwards	**Banquet Dinner and Networking**

Day 2 – March 25th, 2025, Tuesday

Time	Session Speaker(s)
Session VI: Chairs- Dr. Vinay Kumar Srivastava & Prof. Satyendra Pandey	
9:30 am – 10:00 am	**Plenary Lecture (PL-4): Prof. Tapas K. Kundu,** JNCASR Bangalore *Epigenetic Regulation of Neurological Disorders: Role of Lysine Acetyltransferases p300/CBP*
10:05 am – 10:25 am	**Invited Lecture (IL-1): Prof. Santosh J. Gharpure,** IIT Bombay *New Avenues in Radical Based Approaches to Heterocycles*
10:30 am – 10:50 am	**Invited Lecture (IL-2): Prof. Debendra Mohapatra,** IISER Berhampur *Molecular Mysteries - The Art of Structure Elucidation in Drug Research*
10:55 am – 11:15 am	**Invited Lecture (IL-3): Prof. Alakesh Bisai,** IISER Kolkata *Architecturally Complex Natural Products of Biological Relevance: A Platform for the Discovery of New Strategy/Methodology*
11:20 am – 11:35 am	**Tea Break and Networking***
Session VII: Chairs-Prof. Debendra Mohapatra & Prof. Keshri Nath Tiwari	
11:35 am – 11:55 am	**Invited Lecture (IL-4): Prof. Satyendra Pandey,** Banaras Hindu University *Metal-Free Approaches for the Synthesis of Bioactive Molecules*
12:00 Noon – 12:20 pm	**Invited Lecture (IL-5): Prof. Sivapriya Kirubakaran,** IIT Gandhinagar *Achieving new avenues in Prostate Cancer therapy via TLK1 inhibition*
12:25 pm – 12:45 pm	**Invited Lecture (IL-6): Dr. Janakiram Vaitla,** IIT Delhi *Switchable Divergent Benzannulation using Vinyl Sulfoxonium Ylides and Electron-Deficient Alkynes*
12:50 pm – 1:10 pm	**Invited Lecture (IL-7): Dr. Ch. Raji Reddy,** IICT-Hyderabad *Cascade Functionalization/Annulation of Alkenyl Precursors: Construction of Fused- Heterocycles*
1:15 pm – 2:25 pm	**Lunch Break and Parallel Poster Session***
Session VIII: Chairs-Prof. Chandrakumar Appayee & Dr. Ankit Srivastava	
2:30 pm – 3:00 pm	**Virtual Plenary Lecture (VPL-4): Prof. Rene Gree,** Rennes Institute of Chemical Sciences- France *Discovery of new potent and selective inhibitors for CLKs kinases*
3:05 pm – 3:25 pm	**Invited Lecture (IL-8): Dr. Ekambaram Balaraman,** IISER Tirupati *Turning CO_2 into Poly (ether carbonate) diol: A Circular Economy Approach*
3:30 pm – 3:50 pm	**Invited Lecture (IL-9): Dr. Sudipta Basu,** IIT Gandhinagar *Powerhouse targeted small molecule-mediated chemo-photodynamic therapy induces apoptosis in cancer cells*
3:55 pm – 4:15 pm	**Invited Lecture (IL-10): Dr. Ravi Barnwal,** Panjab University *Drug development for RNA target from Neisseria meningitidis*
4:20 pm – 4:35 pm	**Tea Break and Networking***
Session IX: Chairs-Dr. Sudipta Basu and Dr. Ekambaram Balaraman	
4:40 pm – 5:00 pm	**Invited Lecture (IL-11): Prof. Ravi P. Singh,** IIT Delhi *Expanding the Repertaire of Chiral Fulvene-Based Bioactive Scaffolds*
5:05 pm – 5:25 pm	**Invited Lecture (IL-12): Dr. Namrata Rastogi,** CDRI Lucknow *Sustainable Organo photocatalytic Synthesis of Carbo/Heterocycles*
5:30 pm – 5:50 pm	**Invited Lecture (IL-13): Dr. Amrendra Kumar,** IIT Indore *Ruthenium Complexes as Promising Anti-Cancer Agents*
Session X: Chairs- Dr. Namrata Rastogi & Dr. Manas Pal	

Time	Session Speaker(s)
Session VI: Chairs- Dr. Vinay Kumar Srivastava & Prof. Satyendra Pandey	
5:55 pm – 6:15 pm	**Invited Lecture (IL-14): Prof. Hitesh Patel,** Gujarat University *Research Makes Zero to Hero*
6:20 pm – 6:55 pm	**RSC Special Session: Dr. Aayushi Arora & Dr. Rajdip Roy**
7:00 pm – 7:30 pm	**Plenary Session by Cadila** on **'Therapeutic Areas' -TBA-**
7:30 pm onwards	**Dinner and Networking**

Day 3 – March 26, 2025, Wednesday

Time	Session Speaker(s)
Session XI: Chairs-Dr. Janakiram Vaitla & Dr. Ankit Srivastava	
9:30 am – 9:50 am	**Invited Lecture (IL-15): Prof. Chandrakumar Appayee,** IIT Gandhinagar *Development of chiral organo catalysts and their applications*
9:55 am – 10:15 am	**Invited Lecture (IL-16): Dr. Nidhi Gour,** Indrashil University *Investigating the role of metabolite assemblies in the etiology of Inborn Errors of Metabolism*
10:20 am – 10:40 am	**Invited Lecture (IL-17): Dr. Ramendra Pratap,** Delhi University *Cyanomethylarenes: A Source to develop new molecular entity*
10:45 am – 11:05 am	**Invited Lecture (IL-18): Dr. Gourisankar Roymahapatra,** HIT Haldia (IPS Representative) *Chitosan integrated Polysaccharide-Hydrogel; fluorescence responses for bioimaging*
11:10 am – 11:25 am	**Tea Break and Networking**
Session XII: Chairs-Dr. Amrendra Kumar & Dr. Ramendra Pratap	
11:30 am – 11:50 am	**Invited Lecture (IL-19): Dr. Subhash Ghosh,** CSMCRI Bhavnagar *Regioselective C-H Functionalization/Annulation: An Efficient Route to Medicinally n Relevant Heterocycles*
11:55 am – 12:10 pm	**Invited Lecture (IL-20): Dr. Nabanita Sadhukhan,** ICT Mumbai **–TBA-**
12:15 pm – 12:30 pm	**Invited Lecture (IL-21): Dr. Santanu Ghosh,** Shiv Nadar University *Concise Strategy for the Synthesis of Napthylisoquinoline Alkaloids*
Session XIII: Chairs-Dr. Ravi Barnwal & Dr. Manasi Roy	
12:35 pm – 12:50 pm	**Invited Lecture (IL-22): Dr. Joyee Mitra,** CSMCRI Bhavnagar *Exploring amine-rich supramolecular silver(I) metallogels for catalyst and as membrane-targeting broad-spectrum antibacterial agent*
12:55 pm – 1:10 pm	**Invited Lecture (IL-23): Dr. Dinesh Kumar,** NIPER Ahmedabad *A Novel Chemotype for Oral Cancer via Dual (Distal) C–H Bond Activation Relay Protocol*
1:15pm – 1:45 pm	**Session XIV: Chairs-Dr. Vishnumaya Bisai & Dr. Shally Rana**
	Valedictory: Certificate and Prize Distribution
1:45 pm Onwards	**Lunch Break and Departure**
***Lunch Breaks on and 24th & 25th is Parallelled and extended by short oral/Poster Presentations/Exhibit booths Display**	

Abstract Section
Plenary and Invited Lectures

PL-01

Process Development and Sustainable Chemistry

Rajamannar Thennati

Executive Vice President
Head, High Impact Innovations (HISHS) & Advisor to MD
Sun Pharmaceutical Industries Ltd., Vadodara 390 012
E-Mail: *rajamannar.thennati@sunpharma.com*

Abstract:

Making affordable medicines is a success story of Indian Pharma. However, designing a process with predictable quality requires a complete understanding on each element of process chemistry, e.g. reacting components, desired bond making energies, reaction time, temperature, possible side reactions, pH sensitivity, product isolation procedures, etc.

Novel process should aim to maximize the carbon efficiency, selection of raw materials and batch overall energy resulting in a production of high-quality APIs, batch after batch are essential. Leading to sustainable business with cost efficiency and benign to environment.

Feasibility of technology at an industrial scale, with ease of handling, quick turnaround time, maximal product recovery with desired purity and crystal habit / attributes, least solvent inventory for manufacturing and safety aspects needs to be part of process development.

Innovations and measuring the metrics of the process shall be discussed with reference to few pharmaceutical developments.

Reference:

1. Rajamannar T et al., 62/MUM/**2000**; 76/MUM/**2000, WO 03**/057132A2.
2. Zanon J, Klapars A, Buchwald SL, *J. Am. Chem. Soc.,* **2003,** 125(10), 2890 – 91.

PL-02

Small Molecules as Redox Active Artificial Enzymes for Biomedical Applications

Prof. G. Mugesh

Department of Inorganic and Physical Chemistry Indian Institute of Science, Bangalore
E-mail: *mugesh@iisc.ac.in*

Abstract:

Oxidative stress is caused by an imbalance between the production of reactive oxygen species (ROS) and the biological system's ability to detoxify these reactive intermediates. It is well known that oxidative stress is associated with diverse diseases, including cancer, renal disease, and neurodegenerative disorders such as Alzheimer's and Parkinson's disease. Antioxidant treatment has been found to be unsuccessful in many cases as they promote disease and increase mortality in humans. The reason for this unexpected behaviour is that antioxidants with strong reducing ability can act as pro-oxidants and increase the oxidative stress. Therefore, it is important to develop antioxidants without pro-oxidant activity. In this regard, our group is working on the design and synthesis of antioxidant enzyme mimetics such as small molecules and nanomaterials that can combat oxidative stress without affecting the cellular antioxidant systems. In this lecture, I will discuss our recent results on the development of redox active small molecules that can be used for cellular and biomedical applications.

References

1. Singh, N.; Sherin, G. R.; Mugesh, G. *Angew. Chem., Int. Ed.* **2023**, *62*, e202301232.
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PL-03

Efforts in Drug Discovery through Natural Products and Process Development of a Lifitegrast Intermediate with Low Carbon Footprint

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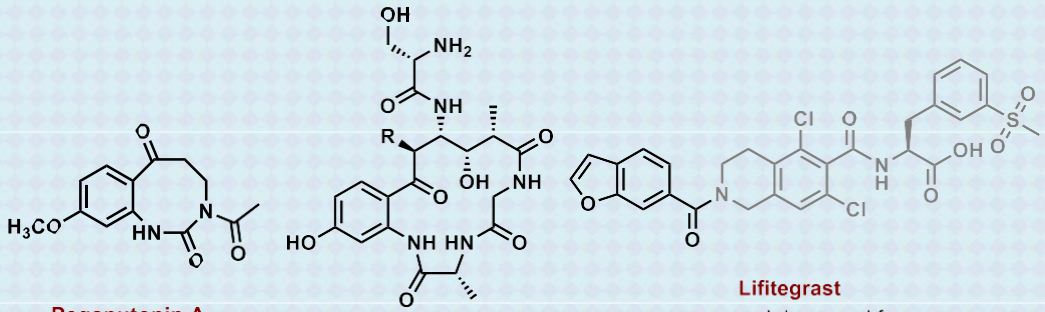
Abstract:

Our research group focuses on total synthesis of biologically active compounds and medicinal chemistry with an ultimate aim of discovering drugs. We have accomplished the synthesis of more than 50 natural products which include cell-adhesion inhibitors, anti-bacterial, anti-inflammatory, anti-cancer agents, and CNS agents sex pheromones and insect repellents. Here, I would like to about a couple of recent projects from my group. In particular, Peganutonin and Solomonamides towards identification of lead compounds towards antiviral and anti-inflammatory agents, respectively. In the later part, Scalable synthesis of benzofuran-6-carboxylic acid, a key fragment of an ophthalmic drug Lifitegrast The life cycle analysis comparison of existing and present routes indicated roughly that the present route leaves less carbon footprint.



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PL-04

Epigenetic Regulation of Neurological Disorders: Role of Lysine Acetyltransferases p300/CBP

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Abstract:

Epigenetics is gene function beyond the DNA sequence, operated by DNA modifications, DNA-associated protein modifications, and noncoding RNA. It is reversible and metabolically regulated, thus directly related to habit and lifestyle. Reversible histone acetylation is one of the most investigated epigenetic modifications shown to be involved in diverse physiological as well as pathological phenomena. However, its role in memory and neurological disorders is not fully understood. Several studies have demonstrated that the master Lysine acetyltransferases CBP/p300 catalytic activity could be critical for long-term memory formation. We have shown that specific activation of p300/CBP KAT activity significantly prolongs the long-term memory in mice. We have discovered a small molecule (TTK21) activator of CBP/p300, which, after conjugating to the glucose-derived carbon nanospheres (CSP), crosses the blood-brain barrier and reaches different parts of the brain without apparent toxicity. It induces adult neurogenesis and long-term memory. By administrating this activator to the tauopathy mouse model of Alzheimer's Disease (AD), we could significantly reverse the memory loss in young and older mice. In the course, we identified that the cholesterol biosynthesis pathway is severely deregulated in older AD mice, which could be correlated with available human patient data. Activating p300/CBP KAT activity could normalize cholesterol biosynthesis, reversing cognitive function. Recently, we have found that in Syngap1+/-, a mouse model on intellectual disability (ID) and autism spectrum disorder (ASD), the p300 KAT activity is dramatically reduced in the CA1 region of the hippocampus. Our results demonstrate that the oral administration of CSP-TTK21 in adult *Syngap1*$^{+/-}$ mice rescued physiological and cognitive/emotional functions, presumably through restoring p300/CBP mediated histone acetylation and adult neurogenesis. The molecular pathways of the amelioration of symptoms are being elucidated.

PL-05

Powerful Tools for The Synthesis of Bioactive Heterocycles Towards Sustainability

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Abstract:

Heterocycles are present in a great diversity of natural products and/or bioactive compounds. They are also present in ligands, dyes, materials, etc. Due to the importance of heterocyclic compounds, the development of chemo-selective, efficient and versatile methods is one of the main areas of research. Itt is worth mentioning that, in the literature, two third of the publications are related to heterocycles.

In this lecture, different methods will be presented to construct small and large heterocycles containing nitrogen and we will show that, if transition metals can be useful tools, they can be replaced easily by heat or enzymes which are more sustainable. The application of the developed methods to the synthesis of an anti-inflammatory compound and bioactive macrocyclic compounds will be presented.

PL-06

Bond Activation for Late-Stage Diversification of Biomolecules

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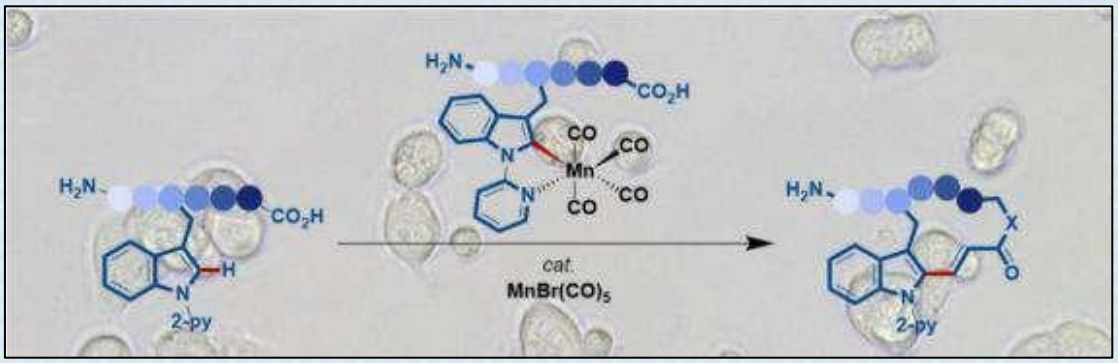
Abstract:

The continuously increasing demand for complex molecular scaffolds in biology and material sciences, as well as agrochemical and pharmaceutical industries translates into a continued strong demand for innovative molecular syntheses. Non-natural peptides have emerged as increasingly potent scaffolds in medicinal chemistry and the pharmaceutical industry. As a consequence, the chemo-selective assembly and modification of structurally complex peptides continues to be of utmost importance. Significant recent momentum was gained through the development of palladium-catalyzed cross-couplings of peptides.



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PL-07

Synthesis with Boron at the Helm

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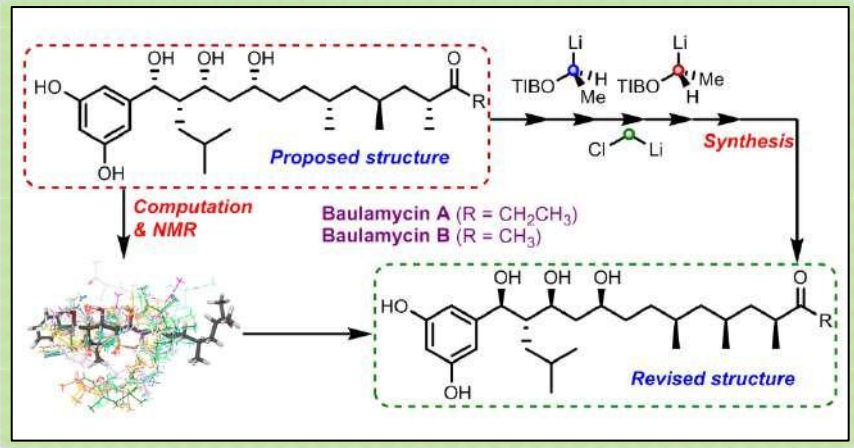
Abstract:

Nature has evolved highly sophisticated machinery for organic synthesis, many of which resemble molecular assembly-line processes. So far chemists have been able to apply this type of approach in the synthesis of peptides, oligonucleotides and polysaccharides but it is much more difficult to apply iterative methodologies to organic synthesis.

Here, we describe the application of iterative homologation of boronic esters using chiral lithiated carbamates and chloromethyl lithium enabling us to grow carbon chains with control over both relative and absolute stereochemistry. Application of this strategy to the synthesis of the proposed structure of baulamycin and the real structure will be presented as well as other complex targets. In addition, the methodology is used to answer fundamental questions about nature and the specific role of methyl substituents in carbon chains. By understanding their role, I will show that molecules can be created with linear or helical conformations and how this can be exploited in the design of protein mimetics.



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PL-08

Discovery of new potent and selective inhibitors for CLKs kinases

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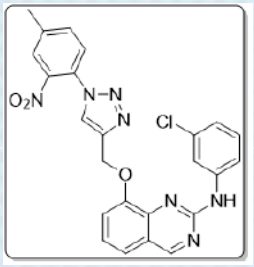
Abstract:

The human kinome comprises 538 kinases playing essential functions, in particular by catalysing protein phosphorylation. Protein kinases (PKs) are involved in the regulation of numerous cellular processes, such as metabolism, cell cycle progression, cell adhesion, vascular function and angiogenesis, often in response to an external stimulus. Aberrant kinase activity plays an important role in the pathogenesis of many diseases including neurodegenerative, cardiovascular, autoimmune and inflammatory diseases as well as in numerous cancers. Over the past three decades, this family of enzymes has emerged as one of the most important suppliers of drug targets and there are already more than 80 kinases inhibitors marketed around the world.



CLKs (Cdc2-like kinases) and DYRKs kinases (Dual specificity tyrosine-phosphorylation regulated kinases) are known for their important biological properties and recently CLKs have been explored as attractive targets for their pharmacological inhibition. Many of the marketed drugs targeting PKs are multi kinase inhibitors and selective inhibition of a kinase remains clearly a challenging problem. Even if a few CLKs selective inhibitors have been reported recently, more selective drugs are awaited, as second-generation molecules. Identification of selective inhibitors targeting CLKs is a non-trivial task since CLKs are in particular structurally very closely related to DYRKs and to homeodomain. Interacting protein kinases (HIPKs) leading to inhibitor cross reactivity. We have discovered a molecule called ***DB18*** which exhibit very attractive properties: it is a potent inhibitor of the human CLK1, CLK2 and CLK4 kinases in the 10-20 nm range. On the other hand, it is not active at 100 µm on the human DYRK1A kinase, thus demonstrating a remarkable selectivity (in the 10^5range) between these kinases which are very close from a structural point of view.

New Avenues in Radical Based Approaches to Heterocycles

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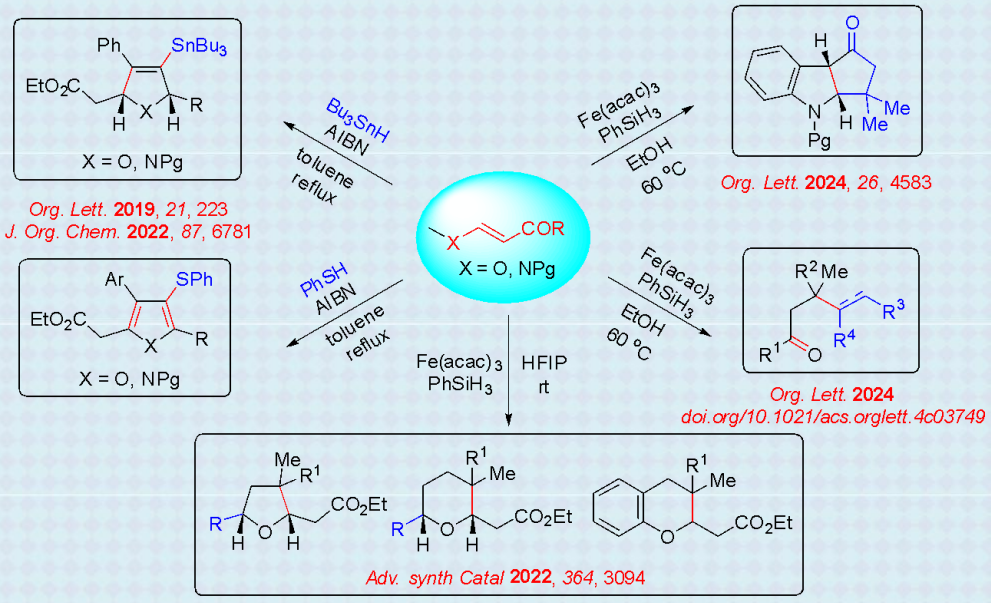
Abstract:

Heterocycles such as substituted tetrahydrofurans (THFs), tetrahydropyrans (THPs), chromans, and pyrroles are important scaffolds in many natural products and biologically active compounds. Although, vinylogous carbonates/carbamates have emerged as excellent radical acceptors for the synthesis of cyclic ethers, their utility for the synthesis of furan/pyrrole derivatives remains underexplored. In this context, we have reported the divergent synthesis of tetrasubstituted furans, dihydrofurans and pyrroles using Bu_3SnH/PhSH mediated cascade radical cyclization on vinylogous carbonates and carbamates. In recent years, metal hydride hydrogen atom transfer (MHAT) radical hydro-functionalization of isolated olefins has emerged as a powerful tool for the construction of carbon–carbon and carbon–heteroatom bonds. We have showcased utility of MHAT for the synthesis of heterocycles such as THFs, THPs, chromans as well as fused indoles/pyrroles. The talk will focus on these studies and interesting new discoveries made along the way.



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Molecular Mysteries - The Art of Structure Elucidation in Drug Research

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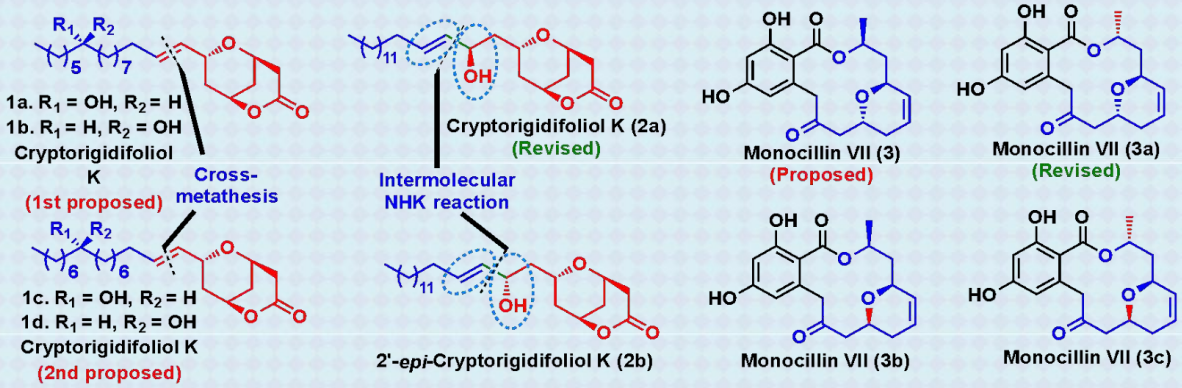
Abstract:

Despite significant advances in NMR spectroscopy and other analytical techniques, structure elucidation of natural products with limited availability, is still a challenging task for chemists. From the year 2000 to 2020, more than 300 natural products have been incorrectly assigned (stereochemical and/or structural). Surprisingly, the examples cover almost all class of compounds, including steroids, terpenes, indole alkaloids, peptides and encompass molecules of all sizes and stereochemical complexity.[1] The first asymmetric convergent total synthesis of four isomers of proposed structures of cryptorigidifoliol K[2] (**1a**, **1b**, **1c**, and **1d**) and discrepancies between the spectroscopic data of synthetic isomers of cryptorigidifoliol K and the data reported for the natural product, suggested that the structure proposed for the natural products needs revision[3].

In this talk, the first asymmetric total synthesis of proposed structures, correct structure and absolute configuration of cryptorigidifoliol K, Monocillin VII, and Diplopyrone will be discussed.[3-6]



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IL-3

Architecturally Complex Natural Products of Biological Relevance: A Platform for the Discovery of New Strategy/Methodology

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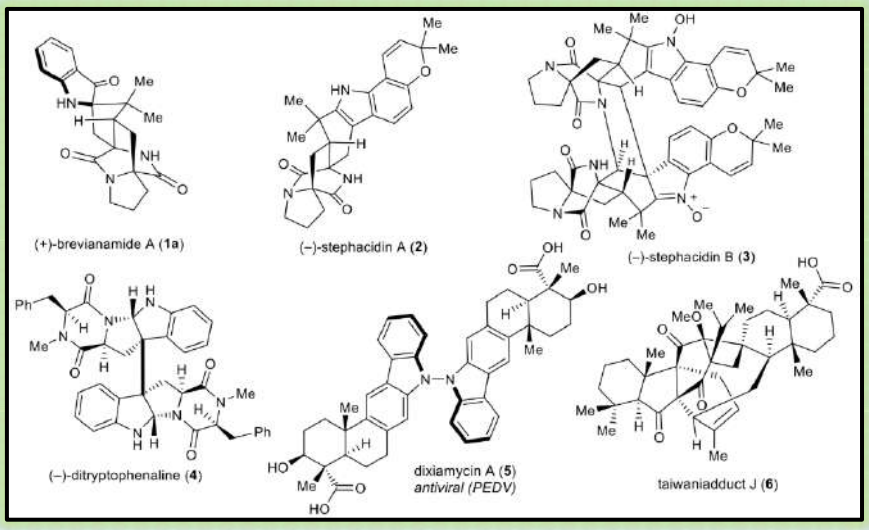
Abstract:

The natural product chemical diversity is more closely aligned with drugs than synthetic libraries, thus making them ideal candidates for drug discovery projects.[1] Marine organisms can be considered the most recent source of bioactive natural products in relation to terrestrial plants and nonmarine microorganisms.[2] The beauty of Nature is that she produces a variety of complex natural products in enantioenriched form (Figure).[3] Since biomimetic processes avoid a protection and deprotection groups, it is an attractive strategy.[4]In the above context, naturally occurring alkaloids with impressive diversity of biological activities drew our interest for the development of bio-inspired strategies.[5]



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IL-4

Metal-Free Approaches for the Synthesis of Bioactive Molecules

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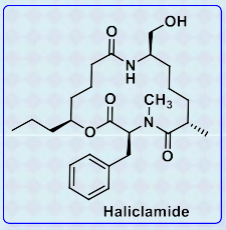
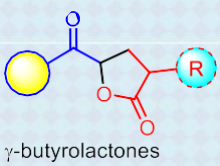
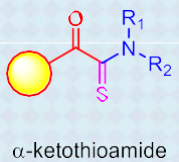
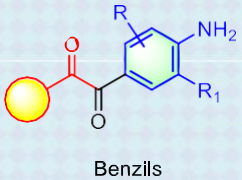
Abstract:

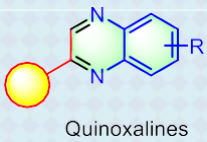
Metal-catalyzed transformations of sulfoxonium ylides have gained prominence for the synthesis of a number of heterocyclic compounds, such as pyrrole, indole, furan, pyrimidine, and quinolone. However, their utility under metal-free conditions is still under-explored. In this context, we have demonstrated that the sulfoxonium ylides can be used as a precursor for the synthesis of various bioactive molecules. These studies were expanded to include the diverse synthesis of several bioactive molecules such as γ-butyrolactones, α-ketothioamides, α-ketoamides, benzils, quinoxalines, quinazolines, quinazolinones, and others under mild and metal-free conditions. The talk will focus on recent advances in the chemistry of sulfoxonium ylides and our laboratory's asymmetric total synthesis of bioactive compounds such as (R)-Lacosamide, Reboxetine, Haliclamide, and others.

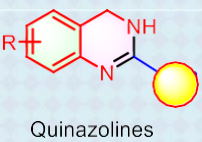


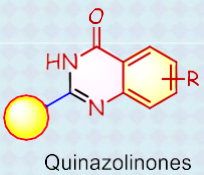

γ-butyrolactones


α-ketothioamide


Benzils


Quinoxalines


Quinazolines


Quinazolinones

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IL-5

Achieving New Avenues in Prostate Cancer Therapy via TLK1 Inhibition

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Abstract:

Tousled-like kinases (TLKs) are associated with chromosomal integrity, DNA replication, and repair. However, the dysregulation of these genes can give rise to different aberrations. The activity of TLK1, a human isoform of TLK, is found to be attenuated in the case of prostate cancer (PCa), especially after the administration of Androgen deprivation therapy using anti-androgens, hence making TLK1 a novel clinical target. Currently, phenothiazines—widely known as antipsychotic drugs—are the only reported inhibitors of TLK1, with none advancing to clinical trials.

Our recent research aims to expand the understanding of TLK1 inhibitors by designing, synthesizing, and validating a diverse series of potent molecules. This effort led to the discovery of J54, a phenothiazine analogue with strong TLK1 inhibitory activity. J54 induces apoptosis in androgen-responsive prostate cancer (PCa) xenografts and shows potential for clinical application in combination with anti-androgens.

Furthermore, using a ligand-based drug design approach, we synthesized novel pyridazine one fused indole derivatives, identifying them as potent TLK1 inhibitors. Among them, SPK DJ115 exhibited enhanced TLK1 inhibition and binding affinity compared to J54. SPK-DJ115 effectively suppresses TLK1 activity in metastatic prostate cancer cells and, when combined with anti-androgens, promotes apoptosis. Overall, our studies highlight phenothiazine and pyridazine one-fused indole derivatives as promising TLK1 inhibitors. We believe our results pave an important milestone for future research in TLK1 drug designing, treating PCa, overcoming resistance mechanisms, and improving patient outcomes.

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Switchable Divergent Benzannulations using Vinyl Sulfoxonium Ylides and Electron-Deficient Alkynes

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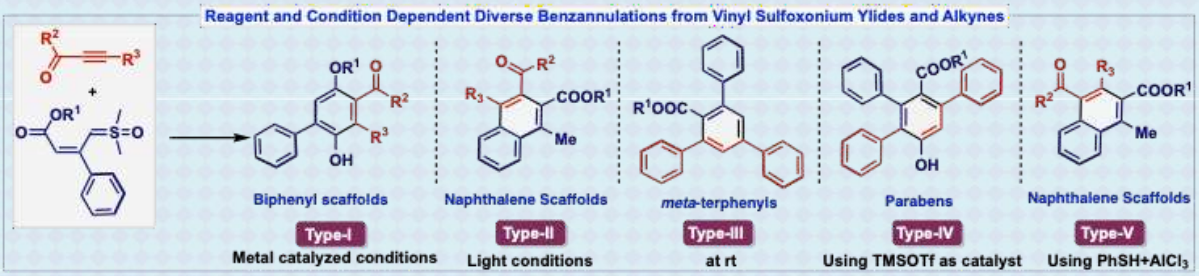
Abstract:

Highly substituted arene is a ubiquitous core motif in various natural products, pharmaceuticals, and polymer materials. Of the top 200 best-selling drugs, nearly 70% of molecules contain at least one arene scaffold. Due to most of the small molecule drugs being constructed around the benzene scaffold, there is a growing impetus within the industry to develop arene libraries. Thus, the synthesis of substituted arenes receives continuous attention from the synthetic community. We developed various highly substituted arenes using vinyl sulfoxonium ylides [1] and electron-deficient alkynes. The reaction of vinyl sulfoxonium ylides with ynoates under ruthenium-catalyzed conditions afforded biphenyl scaffolds.[2] A similar reaction under blue light irradiation provided various naphthalene derivatives.[3] By employing different reaction conditions, it has been possible to access not only naphthalene derivatives but also meta-terphenyls and parabens through a [3+3] benzannulation.[4] This switchable benzannulation from vinyl sulfoxonium ylides enables the selective synthesis of diverse, highly substituted arenes with different scaffolds. A combined theoretical and experimental investigation provided strong evidence for the mechanism of each annulation.



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IL-7

Cascade Functionalization/Annulation of Alkenyl Precursors: Construction of Fused-Heterocycles

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Abstract:

Heterocyclic molecules and their analogues are commonly present in bio-active natural as well as unnatural products exhibiting significant pharmaceutical activities.[1] Motivated by the importance and need to access diverse heterocycles towards drug discovery program, a plethora of methods are being developed involving different approaches. Over the last one decade, the development radical-promoted cascade functionalization/annulation of handy precursors holding alkenyl/alkynyl functionalities has been the attention of research initiatives.[2] In this direction, alkenyl precursors are one of the convenient substrates for the construction of complex molecular scaffolds including spirocyclic or fused-heterocyclic compounds. The present lecture will focus on the recent accomplishments on cascade functionalization/annulation of alkenyl precursors for the assembly of fused-heterocycles (Figure 1).[3-5]

Figure 1:

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IL-8

Turning CO_2 into *Poly (ether carbonate) diol*: A Circular Economy Approach

Ekambaram Balaraman

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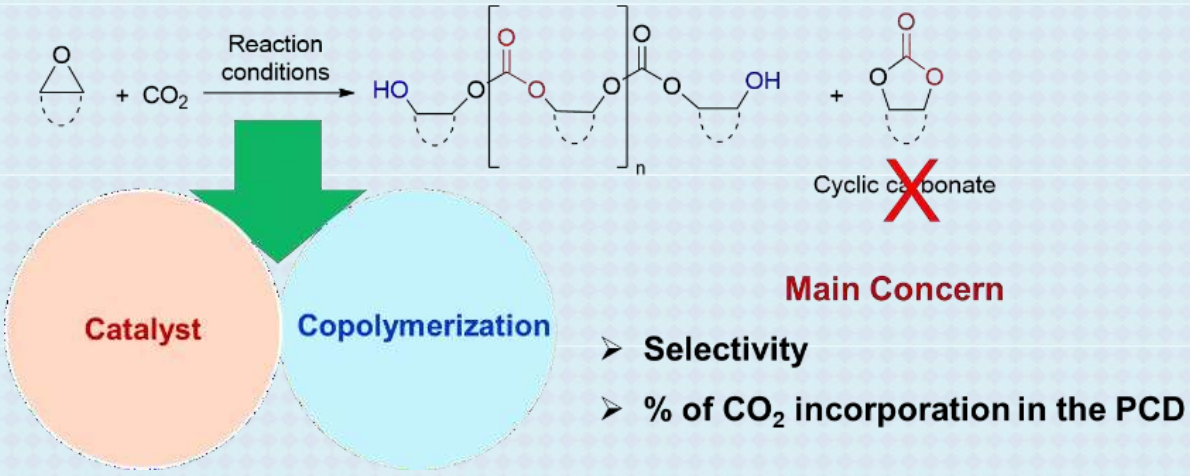
Abstract:

Carbon dioxide (CO_2) as an abundant, non-flammable, economical, and renewable C1 feedstock is of strategic importance for our dependence on depleting non-renewable fossil derivatives. One of the most attractive areas of CO_2 utilization is its direct application as a renewable raw material for polymer synthesis, as large amounts of CO_2 can be utilized to make value-added polymeric products. 1 Polycarbonate has a terminal hydroxyl group (polycarbonate diol/ poly (ether carbonate) diol; PCD) plays a role in its excellent adhesive properties. The primary application of low-molecular-weight polycarbonate diol is widely used as an intermediate in the production of polyurethane (PU) foams. PCD-derived polyurethane has both financial and environmental benefits. The present work mainly involves the development of efficient, scalable catalysts for the production of PCD with excellent selectivity as well as tunable molecular weights and enhanced CO_2 incorporation[2]. The production of polycarbonate diol will be achieved at ambient temperature and low pressure of CO_2. This process may open varied opportunities and emerge as a game-changer technology for engineering polyurethane foams.



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IL-9

Powerhouse Targeted Small Molecule-Mediated Chemo-Photodynamic Therapy Induces Apoptosis in Cancer Cells

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Abstract:

Mitochondria, often referred to as the powerhouse of the cell, play a crucial role in various biological processes, including bioenergetics, biosynthesis, and stress signaling. Given their significant involvement in numerous cancers, targeting mitochondria has emerged as an unconventional yet promising anti-cancer therapeutic strategy. However, achieving precise spatial targeting of mitochondria within the cancer cell environment has remained a major challenge. In recent years, phototherapy has garnered immense attention in cancer treatment due to its non-invasive nature. Despite its tremendous potential, the development of small molecule probes for mitochondria-targeted phototherapy remains in its infancy. To address this gap, we have designed and synthesized a mitochondria-targeted small molecule, Cy-(Indo)2, featuring a penta-methine cyanine-based donor-π-acceptor system for simultaneous fluorescence imaging, phototherapy, and mitochondria homing moiety conjugated with indomethacin V as a drug to inhibit cyclooxygenase-2 (Cox-2) in mitochondria. Notably, Cy-(Indo)2 self-assembled into nanoscale particles in water and successfully localized into the mitochondria of HCT-116 colon cancer cells within 3h. Upon irradiation with a 740 nm LED light (0.9 W/cm2), Cy-(Indo)2 induced mitochondrial outer membrane permeabilization (MOMP), leading to mitochondrial impairment and the generation of reactive oxygen and superoxide species. This light-triggered, mitochondria-targeted chemo-photodynamic effect efficiently inhibited Cox-2 and the anti-apoptotic protein Bcl-2, culminating in remarkable cancer cell death, without exhibiting selective toxicity towards non-cancerous Cos-7 cells. We envision that this novel mitochondria-targeted small molecule-mediated chemo-photodynamic strategy will pave the way for innovative organelle-specific chemical biology approaches, leveraging light-matter interactions for non-invasive cancer therapy.

IL-10

Drug Development for RNA Target from Neisseria Meningitidis

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Abstract:

RNA targeting with small molecules has been a relatively new and rapidly evolving concept with promise to expand its utility in drug discovery field. Until recently, RNAs were mentioned as 'undruggable' however few molecules are reported in last few years for treating few diseases, i.e., Risdiplam. RNAs serve important regulatory functions beyond canonical protein synthesis and their dysregulation has been reported in many diseases. Due to its functional diversity and structural complexity, RNA can be perceived as a prospective target for therapeutic intervention. My lab has been exploring several RNA targets involved in HIV-1, dengue, influenza, *Neisseria meningitidis* and postmenopausal women.

In my presentation, I will brief upon an RNA thermo sensing molecular rheostat from *Neisseria meningitidis* that modulates immune evasion, a leading cause of bacterial meningitis and septicemia. The bacterium evades the host complement system by upregulating expression of three immune evasion factors in response to changes in temperature. RNA thermometers within mRNAs control expression of bacterial immune evasion factors; of which the best studied is CssA, located in the 5′-untranslated region of the operon necessary for capsule biosynthesis. I will discuss how even small changes in stability and the dynamics (as shown by NMR and other biophysical methods) induced by mutations of imperfect base pairs/temperature, as observed in naturally occurring polymorphisms, shift the thermometer response outside of the desired temperature range. This suggests that its activity could be modulated by small molecules based pharmacological intervention, a goal being explored in my lab.

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Expanding the Repertoire of Chiral Fulvene-Based Bioactive Scaffolds

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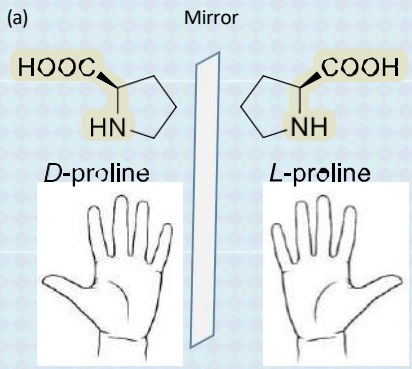
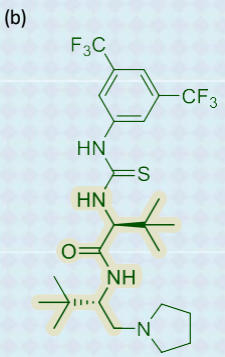
Abstract:

Bioactivity is often associated to the unique structural features of a molecular scaffold and chirality plays an important role in governing it. Unfortunately, due to lack of appropriate synthetic protocols chiral versions of many known scaffolds remain unexplored. While drug molecules are quite common, bioimaging probes rarely get developed. Particularly, chiral fluorescent organic small molecule probes that might have enhanced optical properties are highly valued for their stable luminescence, good biocompatibility, and high signal-to-noise ratio.[1] In this regard chiral conjugated polycyclic cores,[2] axially chiral molecules, chiral planar molecules, and conjugated helices are very important.

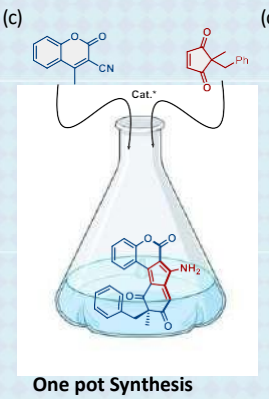
Protocols for the simultaneous installation of multiple stereogenic axes onto different substrate sites have not been widely reported because of the difficulties in managing the sterically impacted multiple stereo-genic axes diastereo and enantioselectively.[3] An efficient cross-dehydrogenative coupling of electronically rich and sterically congested benzofulvene with bi-(hetero)aryl moieties to construct an axially chiral benzofulvene core has been realized.[4]Atropisomeric pyrazoles are widely found in natural products, pharmaceuticals, ligands and catalysts.[5]



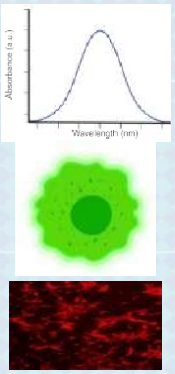
Chirality in natural Amino acids (Non-superimposable on each other)



Amino acid-derived catalyst (cat.)



One pot Synthesis Functionalized Chiral Fulvenes



Np table photophysical Chiral bioimaging

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IL-13

Sustainable Organo photocatalytic Synthesis of Carbo/Heterocycles

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Abstract:

The philosophy behind visible light photo redox catalysis is to develop chemical transformations using clean, green and sustainable source of energy i.e. (sunlight). The use of visible light for carrying out chemical transformations has helped discovering hitherto unexplored activities of several classes of chemicals compounds. Subsequently, the field of visible light photo-redox catalysis has seen unprecedented refinement, innovation, and application in the last decade. However, the use of metal-based photocatalysts i.e. (polypyridyl complexes of iridium and ruthenium) in these reactions is not only against the principles of green chemistry, the high cost of these photocatalysts also render them unsuitable for industrial applications. The continuous exploration of novel metal-free photocatalysts has uncovered several highly oxidizing as well as highly reducing organo-photo-redox catalysts lately. In this context, we explored the reactivity of selected strong photo-reductants (Hantzsch ester and Rh-6G) 1-3 as well as strong photooxidants (acridinium salts and pyrydium salts)[4-5]. In this presentation, our group's results on visible light-mediated synthesis of several valuable heterocycles/carbocycles employing the abovementioned organo-photocatalysts will be discussed.)

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IL-14

Ruthenium Complexes as Promising Anti-Cancer Agents

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Abstract:

The ongoing search for effective and less toxic alternatives to platinum-based chemotherapeutic agents has led to significant interest in ruthenium complexes as promising anti- cancer drugs. Key ruthenium-based drug candidates that have progressed to clinical trials include NAMI-A, KP1019 (and its sodium derivative NKP1339), RM175, RAPTA-C, and TLD1433. During our investigations of ruthenium complexes for catalytic transformations towards sustainable development, we have developed a rich library of Ru-NHC complexes including Ru (III)-NHC complexes 1a and 1a' (Figure 1). 1,2 These Ru (III)-NHC complexes, analogous to RuCl3·H2O, serve as excellent metal precursors for the preparation of new Ru (II) complexes. Complexes 1a, 1a', and related complexes are being also investigated as anticancer agents. Complex 1a was found potent in inducing the apoptosis by elevating the levels of p53 and pRb tumor suppressors in all the cell lines tested except MDA-MB-231. Both 1a and 1a' show significant apoptosis inducing potential in colon cells (HT-29). This shows the anticancer potential of these Ru (III)-NHC complex against colorectal cancer that is one of the highest drug-resistant carcinomas.

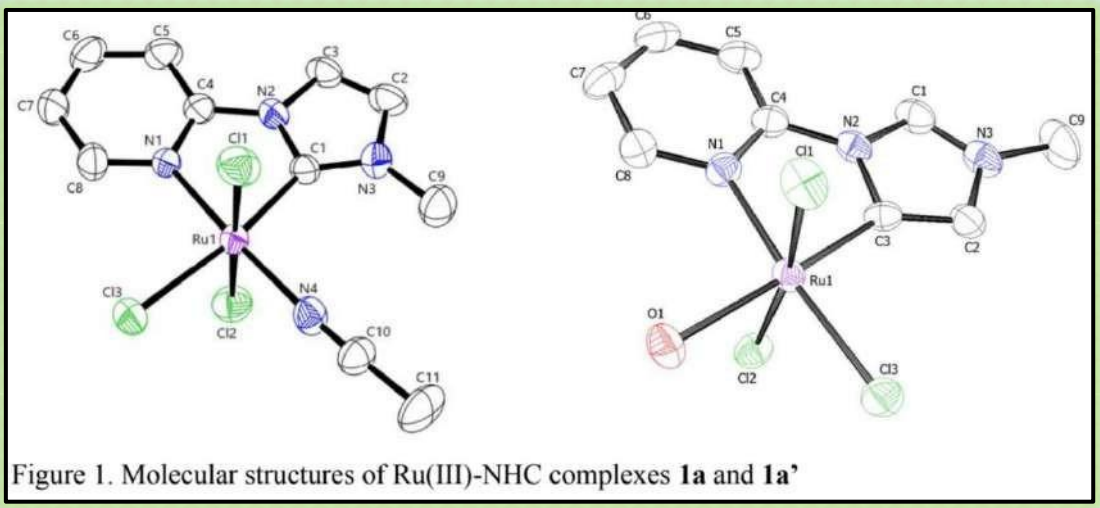

Figure 1. Molecular structures of Ru(III)-NHC complexes **1a** and **1a'**

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IL-15

Research Makes Zero to Hero

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Abstract:

Research creates you if you believe in innovation with a multidimensional approach. As mentioned about the conference's aim, we are working on various areas. Natural Product Synthesis – we are working on seaweeds, collection, identification, extraction, isolation of products, structure identification, biological screening, total synthesis and lead optimization. Asymmetric Catalysis – we have used a selective catalyst for asymmetric synthesis and confirmed the structure geometry by Single Crystal - XRD, the synthesized compounds were used for anticancer activity. Medicinal Chemistry – is the field where we are working for therapeutic and diagnostic reagents development. Process Development—Our focus is on synthesizing products via green routes, and for that, we have designed synthesis and used solid acid catalysts. Computational Drug Development – we are working in in-silico designing using Schrodinger's software. This topic/talk is for the motivation of all young beginner researchers.

IL-16

Development of Chiral Organo-catalysts and their Applications

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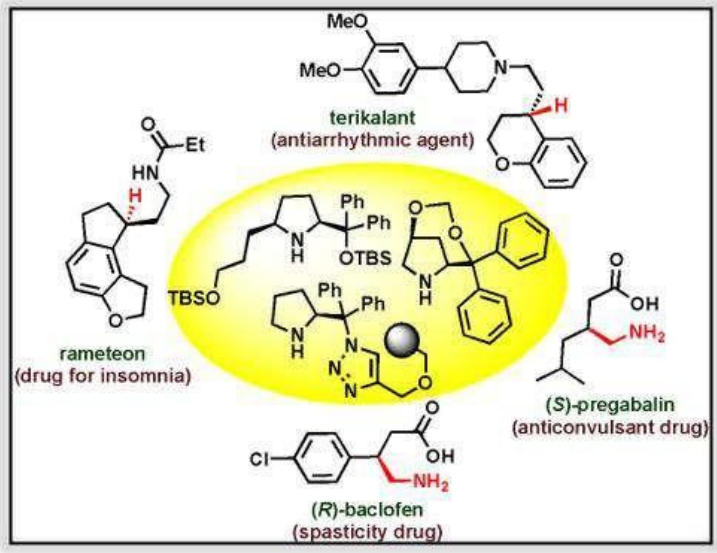
Abstract:

Single enantiomer drugs are preferred over the racemic mixtures.[1] Asymmetric catalysis is the most attractive method to access single enantiomer drugs. Recently, asymmetric organo-catalysis has emerged as an important tool for the synthesis of several bioactive chiral molecules as they are usually inexpensive, non-toxic, insensitive to moisture and air, and environment friendly. Asymmetric secondary amine organo-catalysis has been extensively used for multicomponent, tandem, or domino-type multistep reactionsdue to the generation of multiple reactive intermediates during the reaction.[2]



L-Proline and their derivatives such as silyl protected diaryl prolinols (Hayashi–Jørgensen catalysts) are considered as the privileged catalysts due to their outstanding levels of enantio discrimination in a wide range of organic transformations. However, the catalyst decomposition, higher catalytic loading (usually 20 mol %), and poor regioselectivity are the major challenges associated with the secondary amine organo-catalysis. To address these limitations, novel chiral secondary amine organo-catalysts were developed in our laboratory.[3,4,5] The application of these catalysts to the key organic transformations, and the concise asymmetric synthesis of pharmaceutical drugs were also demonstrated. In this talk, I would like to discuss the challenges associated with the development of chiral secondary amine organo-catalysts and their application to the asymmetric synthesis of bioactive molecules.

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IL-17

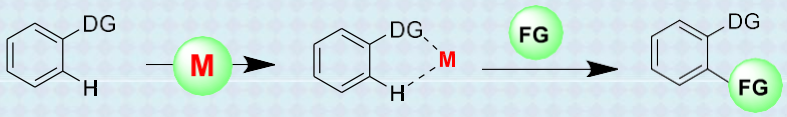
Transition Metal-Catalyzed C–H Functionalization of Bioactive Heterocycles: A Directing Group Approach

Kamaldeep Paul

Abstract:

Nitrogen-containing heterocyclic scaffolds hold a pivotal position in organic chemistry due to their immense significance in both photophysical properties and pharmaceutical applications. Their widespread occurrence in natural products, drugs, and functional materials has driven extensive research into their synthesis and modification. Despite numerous studies focusing on the development of nitrogen-containing heterocycles and the design of novel skeletons, there remains a continuous demand for innovative synthetic methodologies and structurally diverse scaffolds. This is primarily due to the ever-growing importance of these compounds in various fields, including drug discovery, material science, and fluorescent probe development.

One particularly powerful and sustainable approach is transition metal-catalyzed C–H functionalization using directing groups, which enables the regioselective transformation of inert C–H bonds into functional groups, thereby facilitating the efficient construction of nitrogen-containing heterocycles. This strategy not only expands the range of functionalized heterocyclic compounds but also unlocks new opportunities for the discovery of novel molecules with enhanced biological and material properties. Late-stage functionalization through C–H activation has proven particularly useful for the substitution of key heterocyclic frameworks, including coumarins, benzimidazoles, naphthalimides, and 1H-phenanthro[9,10-d] imidazoles. These scaffolds have demonstrated remarkable applications in medicinal chemistry, optoelectronic materials, and fluorescence-based sensors, further emphasizing the importance of innovative synthetic strategies in expanding the heterocyclic library for diverse applications.



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IL-18

Patenting Chemical Innovations– Science Vs Scientific Art: The Synergy

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Abstract:

Innovation and Technology is widely recognised as an essential feature of strategic thinking and management efforts in contributing for economic growth. The innovative technological development depends increasingly on collaborations between different stakeholders.

Exploring the role of IPR (Patents) in technology and innovation processes on a strategic level and utilization of IPR (Patents) aspects for decision making may find huge and unexploited potential for an effective outcome in any kind of organization. It is intended to enable any organization to assess the value of road-mapping in its own particular context by means of a rapid first application. This session/lecture gives an overview on integrating IPR (Patents) aspects for strategic planning and technology road-mapping of the research activities and throws a light on how IPR (Patents) plays a crucial role in design and planning for conducting an effective R&D works focusing to chemical and allied areas of research.

Key words: Innovation, Intellectual Property Rights (IPR), Patents, Technology Development, Chemical and allied areas of research

IL-19

Investigating the Role of Metabolite Assemblies in the Etiology of Inborn Errors of Metabolism

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Abstract:

Metabolite assemblies are structures formed by metabolites that spontaneously self-assemble into amyloid- like aggregates. Proteins and peptides are known to form assemblies which cause amyloid-associated diseases. However, recent studies suggest metabolites such as single amino acids, nucleobases, and glucosylceramides can also aggregate to form amyloid-like toxic structures and have possible implications in the etiology of rare inborn errors of metabolism (IEM).[1] Our group is interested in studying the self-assembly of molecules to assess its implications in healthcare and material science. In this context, we started studying the self-assembly of single amino acids to decipher its role in the pathogenesis of in-born errors of metabolisms (IEM's).[2a] Hence, for the very first time we reported the self-assembly of non-aromatic amino acids like cysteine and methionine to amyloid-like cytotoxic structures.[2b] We also reported unusual aggregates formed by other amino acids proline, hydroxyproline and lysine.[2c] Furthermore, we reported a chemical perspective on the anti- amyloid of compound using diphenylalanine self-assembly as a reductionist model.[2d] We have also investigated the controlled aggregation properties of single amino acids modified with protecting groups and, to our surprise, could decipher distinct well-defined unique morphologies.[2e-g] We investigated the self- assemblies formed by metabolites of the urea cycle and uric acid pathway, as well as other metabolites such as homogentisic acid, isovaleric acid, and N-acetyl aspartic acid. Additionally, we studied amyloid-mimicking assemblies formed by single amino acid, including branched-chain amino acids (BCAAs) and other polar non- aromatic amino acids such as glutamine, glutamic acid, and aspartic acid. We envisage that the outcomes has potential of unravelling the relevance of amyloidogenic pathways in the etiology of multiple orphan diseases like Lesch-Nyhan Syndrome, Xanthinuria, Alkaptonuria, Canavan and Maple Syrup Urine Disease (MSUD) to name a few and possible identification of new therapeutic targets for treatment of these diseases. [2h-k] We have also studied the antimicrobial activity of the self-assembled structures formed by protected single amino acids (SAAs)[2l] and amyloid-like aggregation propensities in nucleobases.[2m]

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IL-20

Cyano-methylarenes: A Source to Develop New Molecular Entity

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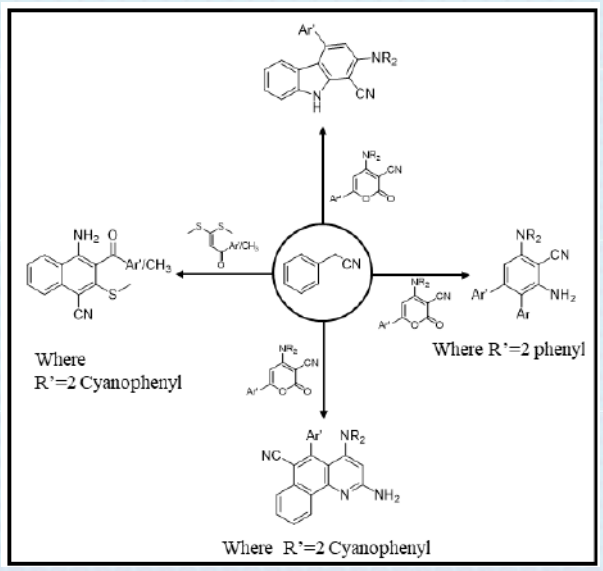
Abstract:

Our research group recently explored the functionalized cyano-methylarenes as a carbanion source for various reactions. Various functionalized naphthalene's was afforded in good to excellent yield by reactions of ketene dithioacetals with 2-cyanomethylbenzonitrile.1,2 We studied 2-cyanomethylbenzonitrile, benzyl cyanide and o- and p-substituted benzyl cyanide and used them as a carbanion source to explore their chemistry. Furthermore, 2-cyanomethylbenzonitrile provides highly functionalized beno[h]quinolines by ring transformation with 2-pyranone.3 5,6-Dihydro-2H-benzo[h] chromenes react with cyano-methyl benzonitrile to afford 4,5-dihydro-1H-benz[e]indenes.4 1H-Naphtho[1,2-d] imidazole was also synthesized in three steps involving 2-(1-cyno-2,2-bis methyl sulfanyl vinyl)-benzonitrile1,5 as an intermediate obtained from 2-cyanomethylbenzonitrile. We have also used functionalized benzyl cyanide as a carbanion source to carry out the ring transformation of 2-pyranone and various tert-aryls and enones achieved under different reaction conditions.



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IL-21

Chitosan integrated Polysaccharide-Hydrogel; fluorescence responses for bioimaging

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Abstract:

Functionalized hydrogels, known for their versatile and adaptable structures, have garnered significant interest in materials and biomaterials research. Among them, fluorescent hydrogels stand out due to their exceptional sensing capabilities and their ability to replicate cellular environments, aiding in cell infiltration and drug delivery tracking. Understanding the structural composition of hydrogels is essential for assessing their reactions to various stimuli, such as pH, temperature, and solvents. Here we have developed a fluorescent hydrogel by modifying chitosan with p-cresol-based quinazolinone aldehyde. Confocal microscopy highlighted the hydrogel's remarkable fluorogenic properties. The hydrogel displayed enhanced fluorescence and a tuneable network morphology, which was influenced by the THF-water ratio. The study also explored how gel network reformation could be controlled in different media while examining fluorescence responses and structural changes in the sugar backbone and fluorophore. Selecting the appropriate combination of solvents is crucial for optimizing the hydrogel as a fluorescence probe for bioimaging applications. Additionally, the hydrogel exhibited superior swelling properties, making it highly suitable for drug delivery purposes.

IL-22

Regioselective C-H Functionalization/Annulation: An Efficient Route to Medicinally Relevant Heterocycles

Subhash Chandra Ghosh

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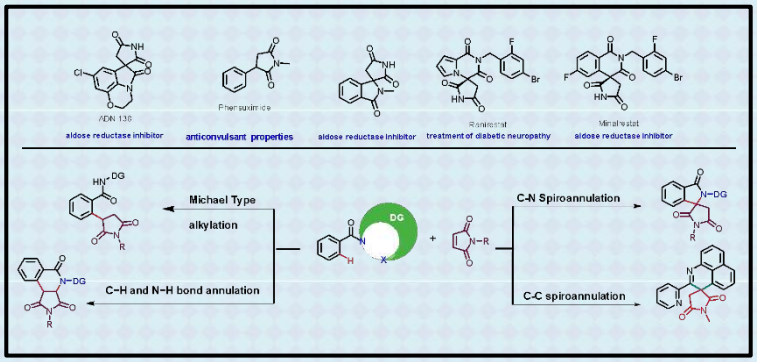
Abstract:

Direct C-H bond functionalization offers a step and atom-economical and sustainable alternative, for the traditional C-C and C-N bond formation through functional group interconversions or transition metal-catalyzed cross-coupling reactions. However, achieving selective C-H bond functionalization within complex molecules remains a significant challenge. Directed C-H activation strategies address this challenge by employing directing groups to guide the catalyst towards the desired C-H bond, enabling site-selective bond formation. N-containing heterocyclic compounds are a very important class of organic molecules in medicinal chemistry; around 59% of commercial drugs contain a nitrogen heterocycle. Among them, iso indolone and succinimide moieties are present in several natural products and biologically active molecules. Spiro succinimides derivatives like ranirestat and minalrestat are used as aldose reductase inhibitors. Synthesis of a spirocyclic succinimide compound is always a challenging task for the synthetic organic chemist starting with a maleimide as it prefers a Michael-type conjugate addition products. Our research group has developed a diverse array of catalytic systems for the C-H functionalization for accessing medicinally relevant heterocycles fused with spiro succinimides.[1]



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IL-23

TEGylation To Achieve Known Molecules with Unique Theragnostic: Benzothiazole for Protein Responsive Drug Delivery and Copper Phthalocyanine for Anticancer Applications

Nabanita Sadhukhan

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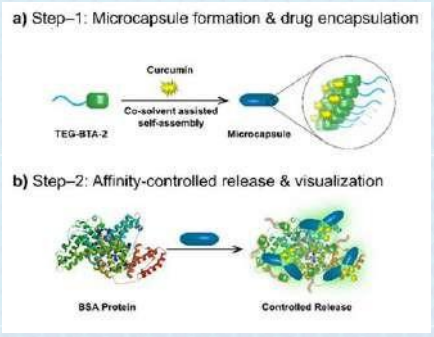
Abstract:

Tetraethylene glycol is a non-toxic, non-ionic, commercially abundant, short, monodisperse PEG (<500 D). Herein, we focus on a meticulously designed amphiphilic small molecule by TEGylation to achieve unique molecular structure and properties for biomimicking applications. In the first example, we have designed a tetraethylene glycol and benzothiazole dye conjugate (**TEG-BTA-2**). TEGylated benzothiazole **TEG-BTA-2** can act as an amphiphilic molecular rotor that can self-assemble to form a microsphere in aqueous medium at room temperature. Interestingly, **TEG-BTA-2** microsphere transforms into microcapsule to encapsulate drug molecules that undergo controlled drug delivery in the presence of protein-based external stimuli. In the second example, we have synthesized TEGylated copper phthalocyanine **CuPc(TEG)$_4$** substituted with four tetraethylene glycol for anti-cancer applications. Ideally, the desirable active anticancer agent would be only effective in an oncological condition, such as a higher concentration of GSH and H_2O_2, a low pH, hypoxic tumour microenvironments. Remarkably, the **CuPc(TEG)$_4$** - catalysed GSH oxidation reaction to make GSSG, and subsequently produced hydroxyl radical (•OH) following the Fenton-like process. The MTT assay suggested **CuPc(TEG)$_4$** effectively destroys cancer cell (**A549, MCF-7**) with cell viability 30%, and it showed minimal effect on normal cells (**3T3**) with cell viability (85%). Detailed investigation on (**i**) bullet-shaped molecular capsule formation of **TEG-BTA-2** for protein-responsive controlled drug delivery inspired by the rabies virus in nature, (**ii**) chemo-, photo-dynamic effect (CDT and PDT) of the **CuPc(TEG)$_4$** revealing selective cancer cell death will be discussed in the presentation.



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Concise Strategy for the Synthesis of *Naphthylisoquinoline* Alkaloids

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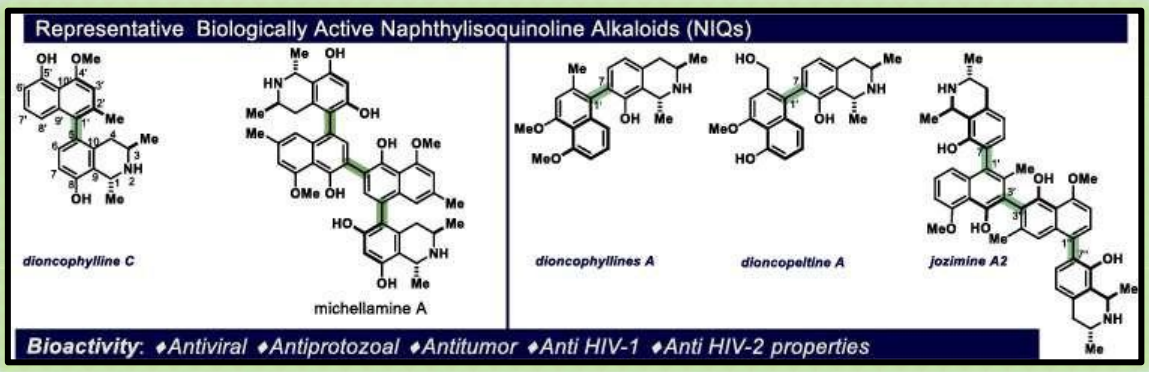
Abstract:

Malaria is a life-threatening infectious disease caused by protozoan parasites belonging to the Plasmodium genus, with Plasmodium falciparum (P. falciparum) being the most virulent species. The disease is primarily transmitted through the bites of infected mosquitoes.[1] In 2015, malaria affected approximately 212 million individuals worldwide, leading to an estimated 429,000 fatalities.[2] Although antimalarial drug treatments have been effective, the emergence of drug-resistant P. falciparum strains poses a significant challenge to disease control efforts. This highlights the urgent need for novel therapeutic agents. Naphthylisoquinoline (NIQ) alkaloids have garnered significant interest due to their strong antimalarial properties, promising pharmacological characteristics, and minimal cytotoxicity.[3] We put forward our effort for the synthesis of various NIQ natural products. Our strategy employs metal-mediated asymmetric desymmetrization reactions, followed by a Pictet Spengler cyclization, to achieve the desired synthesis with high efficiency and selectivity.[4]



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IL-25

Exploring Amine-Rich Supramolecular Silver(I) Metallogels for Catalysis and as Membrane-Targeting Broad-Spectrum Antibacterial Agent

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CSIR-Central Salt & Marine Chemicals Research Institute Bhavnagar

Abstract:

The design of supramolecular gels can be tuned on-demand, catering to desired applications, including catalytic transformations and facile bacterial membrane perturbation. A series of Ag(I) supramolecular organo-aqueous gels have been synthesized in the presence of an amine-rich triazole ligand, DATr (3,5-diamino-1,2,4-triazole) as a gelator. Judicious choice of the triazole derivative and counter anion allows a desired spatial orientation of the pendant amine functionality to accentuate the gelation ability and autonomous self-healability via hydrogen bonding. In addition, the hydrogen bond donors, i.e. pendant –NH2 groups, offer a critical proximity of counter anions to the Lewis acidic Ag(I) and the reactants for promoting a three component coupling reaction of an aldehyde, a terminal alkyne and an amine, giving expedient access to propargyl amines, with remarkable functional group tolerance for both aromatic and aliphatic aldehydes, and aryl acetylenes.

Considering the strong biocidal properties of Ag-based systems and the bacterial membrane-targeting potential of appended primary amine groups, we designed self-assembled multicomponent supramolecular Ag(I)-hydrogels with urea and DATr as ligands, which are predisposed for hydrogen bonding and interacting with negatively charged bacterial membranes at physiological pH. Ag(I)-hydrogels facilitated the disruption of the negatively charged bacterial membrane of both gram positive (Staphylococcus aureus; S. aureus) and gram-negative bacteria (Campylobacter jejuni; C. jejuni) due to electrostatic interaction and complementary hydrogen bonding facilitated by DATr and urea. Sustained intracellular ROS generation in the presence of Ag(I)- hydrogel further expedited cell lysis. The multicomponent supramolecular Ag(I)- hydrogels studied herein can be employed in designing effective antibacterial coatings on a range of medical devices, including surgical instruments in the future.

IL-26

A Novel Chemotype for Oral Cancer *via* Dual (Distal) C–H Bond Activation Relay Protocol

Dinesh Kumar

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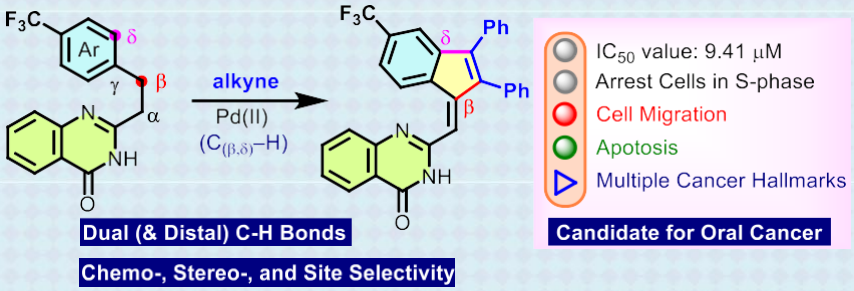
Abstract:

In contrast to proximal C–H bond activations, distal C–H bond activation is fundamentally more challenging and requires distinctly specialized directing partners or techniques. In this context, we develop a dual (distal) β-C(benzylic)–H and δ-C(aryl)–H bond activation relay protocol for the chemo-, regio-, and stereoselective construction of heterocycle-tethered benzofulvenes via [3 + 2] CH/CH-alkyne annulation under palladium catalysis. The synthesized new chemical entities (NCEs) constitute a novel scaffold with favorable anticancer activity against oral squamous cell carcinoma (OSCC). Detailed biomolecular studies, including RNA-sequencing and analysis, indicate that these compounds arrest the cell cycle at the S-phase and target multiple cancer hallmarks, suggesting their chemotherapeutic potential for oral cancer by addressing the complexity and adaptability of



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Abstract Section
Oral and Poster Presentations

OP-01

Computational Insights into Momordin II from Bougainvillea Extract: Molecular Docking, ADMET Profiling, and Molecular Dynamics Simulation Against MHC Class I and II

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*[a]*Department of Horticulture, School of Agriculture, Lovely Professional University, Phagwara, Panjab.*
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Dr Homraj Anandrao Sahare

Abstract:

Natural phytochemicals are gaining attention as potential immunotherapeutic agents due to their ability to interact with key immune system components. In this study, GC-MS analysis of *Bougainvillea* leaf extract identified several bioactive compounds, among which Momordin II exhibited the highest binding affinity to major histocompatibility complex (MHC) class I and II molecules. Molecular docking results showed strong interactions, with binding energies of -11.0 kcal/mol for MHC I and -8.9 kcal/mol for MHC II. ADMET profiling indicated poor absorption but favourable safety and metabolism characteristics, with no significant hepatotoxicity or cardiotoxicity. Molecular dynamics (MD) simulations performed using GROMACS at 100 ns confirmed the stability of the Momordin II-MHC complexes. These findings suggest that Momordin II holds promise as an immunomodulatory agent and warrants further experimental validation.

OP-02

Microwave-Assisted Catalyst-Free Conjugate Addition of Amines to Maleimide

Akshay Bharodiya[a], Bhargav Desai[a], Bhavyesh Desai[a], Areti Sivaih[a], Eeshwaraiah Begari*[b], Togati Naveen*[a]

Catalysis Research Laboratory, Department of Chemistry, SVNIT, Surat, Gujarat, India-395007
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Abstract:

A catalyst-free approach has been introduced for the conjugate addition of aromatic amine nucleophiles to *α, β*-unsaturated *N*-methyl maleimide under microwave irradiation by utilizing water as a promoter. Catalyst-free, environmentally friendly, short-reaction time, green solvent, and mild reaction conditions are the advantages of this protocol. This reaction provided good to excellent yields with aromatic anilines as nucleophiles. The benefits of this reaction align with the principles of green and sustainable synthetic chemistry, making it widely applicable in organic synthesis and pharmaceutical chemistry.

OP-03

A study of Mesomorphism in laterally substituted homologous series of Sulfamethoxazole with azomethine, Sulphonamide linkages

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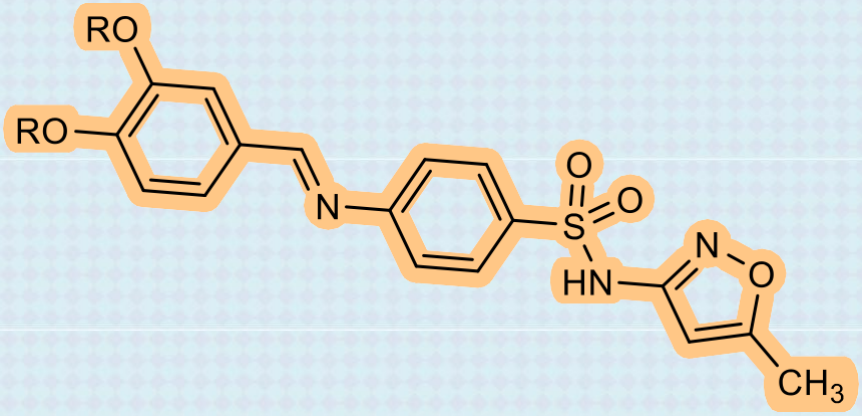
Abstract:

The Fourteen compounds i.e. 4-((4-Alkyloxy benzylidene derivative) amino)-N-(5-methylisoxazol-3-yl) benzene sulfonamide and 4-((4-Alkyloxy-3mrthoxy benzylidene derivative) amino)-N-(5-methylisoxazol-3-yl) benzene sulfonamide having an -SO_2NH- and -CH=N- linkages were synthesized and studied for their mesogenic behavior. The nematic phase of liquid crystals, although observed in sulfamethoxazole 's Schiff base, All the synthesized compounds are enantiotropic Nematic and behaving in a normal manner on transition curve. Thermal phase transitions were recorded on polarizing optical microscope equipped with heating stage. Structures of the synthesized compounds were established on the basis of ^1H NMR, C^{13} NMR and IR Spectral analysis. A methoxy (-OCH_3) substitution at meta position in phenyl ring with a terminal alkyl chain depressing the transition temperatures for phase Nematic transition than unsubstituted molecules. The average thermal stability for unsubstituted homologous series is 152.2 °C and that of for methoxy substituted homologous is 135.2 ˚C



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OP-04

Design and Synthesis of Stable GBF- Inhibitors to Investigate Clathrin and Dynamin-Independent Endocytic Pathways

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[b]Academy of Scientific and Innovative Research, (AcSIR), Ghaziabad 201002, India.
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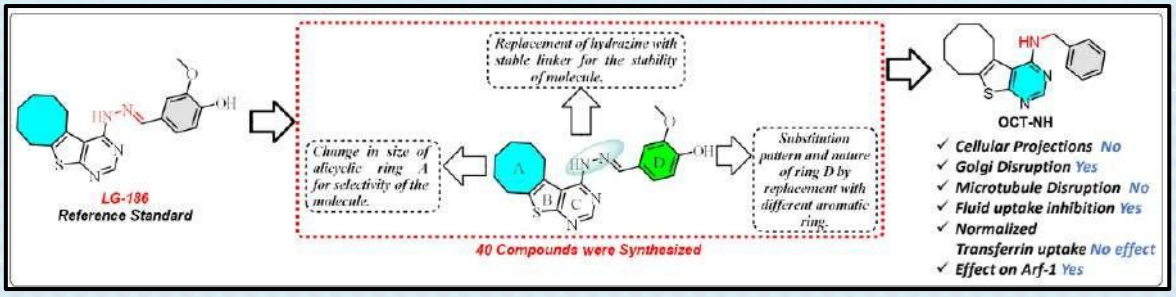
Abstract:

The development of GBF (Golgi Brefeldin A-Resistant Factor) inhibitors plays a vital role in studying Clathrin- and Dynamin- independent endocytic pathways, particularly the CLIC/GEEC (CG) pathway. These inhibitors are designed to selectively interfere with
GBF proteins, which regulate key processes, nutrient uptake, maintaining membrane tension, and cell adhesion, and are also implicated in disease processes such as cancer metastasis and viral infections. A deeper understanding of these mechanisms through GBF inhibitors could pave the way for new therapeutic strategies. In the literature, LG-186 is reported as a selective and reversible inhibitor of GBF, however, its limited long-term stability requires further intervention. In this direction, we have started an extensive medicinal chemistry program on LG-186 and developed a novel, specific, selective, and stable GBF inhibitor, which selectively disrupts the Golgi apparatus and



OP-05

The Power of NMR in Molecule-Based Drug Development

Ms. Anjali Luhana, Ms. Riddhi Prajapati, Ms. Namrata Vyas, Dr. Nidhi Solanki, Mr. Mahesh Patel

Shree Swaminarayan science college and Shree Swaminarayan college of pharmacy, Swaminarayan University, kalol
Shree Swaminarayan college of pharmacy, Swaminarayan University, kalol
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Abstract:

In the evolution of NMR in the pharmaceutical business, NMR's unique ability to offer dynamic and atomic level information has been used to find and design new medications. NMR has a long and proven track record as a potent analytical technique in the search of more effective pharmaceuticals. It has evolved to play an important part in fragment screening procedures that have effectively transformed molecular substrates into actual medicines. Several nuclear magnetic resonance (NMR) applications have been developed for structure-based drug discovery (SBD). NMR has several benefits over other technologies, including the capacity to directly view chemical compounds and target bio-molecules, as well as to be employed for ligand - and protein-based approaches. In just three decades, NMR has become the "gold standard" platform technology in medical and pharmacological studies. In the early phases of drug development, two major techniques are utilized to uncover drug-like candidates: high throughput screening (HTS) and fragment-based drug design (FBDD). Immobilising the target protein is frequently required in drug discovery campaigns that use biophysical techniques to characterise protein-small molecule interactions. Immobilized protein is necessary for both of our primary technologies, one of which is NMR-based and the other is surface plasmon resonance (SPR).In this review, we present the major applications of NMR spectroscopy in medical drug discovery and development The fundamental ideas, hypotheses, and uses of the most widely utilized NMR methods are discussed. Additionally, we provide an overview of the benefits and drawbacks of the main NMR techniques used in drug development.

OP-06

Design and synthesis of coumarin-heterocycle hybrid compounds, *pyrano[3,4-c]pyran-1,8-diones* and as an Anticancer Agents

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University of Delhi, Delhi-110021
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Abstract:

Cancer, a leading cause of death, is influenced by genetics and has been treated with various medications, but often leads to severe side effects, necessitating efficient treatment. Over the years, cancer medications have been discovered, ranging from organometallic to purely organic compounds. Unfortunately, these drugs often come with severe side effects because they target rapidly dividing cells. Consequently, there is an urgent need for an efficient cancer treatment that minimizes adverse reactions. We are actively participating on developing an anticancer agent and exploring a novel approach to synthesize functionalized heterocyclic hybrids. Pyrazole-based compounds exhibit diverse chemotherapeutic properties, including scavenging free radicals, analgesic and antipyretic effects, antiviral, anti-inflammatory, and antimicrobial properties, attracting interest in developing heterocyclic fused hybrid compounds.

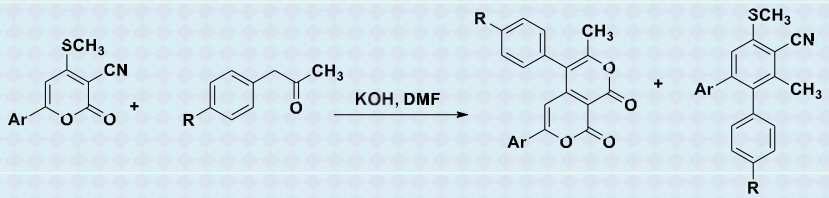

Figure: Synthetic Scheme for the pyrano-pyran

Our research involves synthesizing precursors for design pyrano-pyran molecules and further synthesizing different pyrano-pyran derivatives by optimizing reaction conditions using various base, solvents for desired derivatives, and using them for functionalized heterocyclic hybrids. Characterization has been done using various spectroscopic techniques such as ^{1}HNMR, ^{13}CNMR and mass spectroscopy. Synthesized pyrano-pyran derivative were submitted for their anticancer activities. A molecular docking simulation was conducted using Schrodinger and Auto Dock to assess drug binding with breast cancer target receptor aromatase.

OP-07

Modular Synthesis of Unsymmetrical Indolyl Diketones from Ynediones via Sequential Aza-Michael Addition/C–H Functionalization

Naveed Abdul [a,b] Bag Debojyoti [a,b] Sawant D. Sanghapal [a,b,*]

[a]*Natural Product & Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Jammu 180001, India;*
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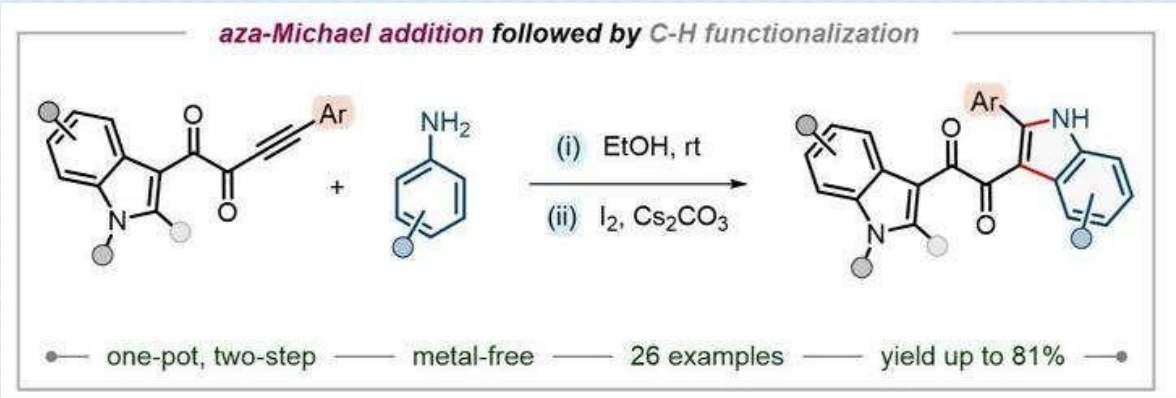
Abstract:

A modular synthesis of unsymmetrical indolyl diketones from ynediones is presented, employing a sequential aza-Michael addition and C–H functionalization strategy. This approach leverages the reactivity of ynediones, which are functionalized via a nucleophilic aza-Michael addition, introducing an amine component to the system. The resulting intermediate undergoes selective C–H functionalization to afford a diverse array of indolyl diketones. This synthetic methodology offers a highly efficient and versatile pathway for constructing unsymmetrical indolyl derivatives with potential applications in medicinal chemistry, particularly in the design of bioactive molecules. The modular nature of the synthesis provides flexibility in selecting diverse starting materials and functional groups, allowing access to a broad spectrum of indole-based diketones, which are of significant interest for their pharmacological properties.



OP-08

A Facile Ultrasonic Promoted Green Synthesis of Modified *2-Oxochromane* Derivatives and their Antimicrobial Profile

Priti Patel, Sarika Patel

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Abstract:

The preparation of 2-oxochromane containing derivatives is achieved through divergence assembly known as ultrasound irradiation. The principle for the operation of the ultrasonic irradiation approach is green synthesis. 2-oxochromane derivatives are synthesized via a onepot multicomponent reaction. In this study, water is employed as a green solvent. A bicyclic heterocycle that has a benzene ring fused to a dihydro-pyran ring that serves as the building block for tocopherols. All newly synthesized compounds are characterized by Mass, IR, 1H and 13C NMR spectra and Elemental analysis. The molecules described are tested for antimicrobial activity. Many substances' biological activity has been demonstrated in various studies.

OP-09

Statistical Analysis of Magnesium and Aluminum Ion Concentrations in Antacid Samples from Rural Areas of Rajkot, Gujarat.

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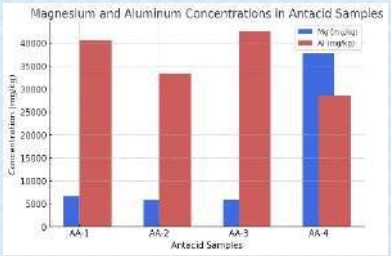
Abstract:

Over-the-counter (OTC) antacids are commonly used for self-medication in rural areas of Rajkot to manage acidity and indigestion. However, the composition of these antacids, particularly their Magnesium (Mg^{2+}) and Aluminum (Al^{3+}) ion concentrations, plays a crucial role in their effectiveness and potential health implications. This study aims to analyze the elemental composition of selected antacid samples using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) to quantify Mg^{2+} and Al^{3+} concentrations in mg/kg.

A descriptive statistical analysis was performed to assess the variation in Mg and Al content across different samples, including measures such as mean, standard deviation, range, and median. Additionally, a correlation analysis was conducted to examine the relationship between Mg and Al concentrations, providing insights into possible formulation trends in commercially available antacids. The study also presents graphical representations of the obtained data to enhance understanding of the elemental composition of antacids used in rural self-medication.

The findings from this study are valuable in evaluating the quality and consistency of OTC antacids and their potential effects on consumer health. Understanding the balance between Mg and Al in antacid formulations is essential, as excessive consumption of either component can lead to side effects such as diarrhea (Mg-based) or constipation (Al-based). This research contributes to the growing body of knowledge on self-medication practices and highlights the importance of monitoring elemental composition in OTC pharmaceutical products to ensure safe and effective use.



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OP-10

Sustainable Approach for Synthesis of Novel *Isoindolinone* Based Small-Molecule Inhibitors Against Enzyme Sortase

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Abstract:

In this present world of globalization with increase in Antimicrobial Resistance (AMR) there is an urgent need for discovery of new targets and Sortase family proteins are attractive target for treating microbial infections by playing an essential role in biofilm formation. It is mostly found in Gram-positive bacterium, which is present amongst the most prevalent multidrug resistant hospital pathogens. According to the findings, this surface protein can attach to and colonize abiotic surfaces, where it plays a key role in the development of biofilms. A membrane anchored transpeptidase enzyme Sortase A (Srt A) plays a major role in the formation of biofilms. Therefore, Srt A has been recognized as an ideal drug target. In this regard we have synthesized in house a library of 40 novel Isoindolin one derivative bearing lactam group to inhibit Srt A. All these compounds were synthesized via one pot synthesis from 2-aminobenzyl alcohols & phthaladi-aldehyde with sustainable approach. Further in accordance to which we performed several In-silico approach such as Docking, Density Function Theory (DFT), Molecular Dynamics studies for synthesized compounds. It showed Binding Energy between -8.8 to -7.5 Kcal/mol. Six derivatives are strongly binding to active site with the orientation similar to which substrate (LPXTG) binds. Through DFT studies it was observed that these compounds exhibit stable interactions and high reactivity. In-vitro studies are under process. A further effort for crystallization and determining 3D structure of protein is going on.

OP-11

Synthesis, Characterization, and Molecular Docking Study of *2-(4-((4-(6-nitroH-imidazo[1,2-a] pyridin-2-yl) phenoxy) methyl)-1H-1,2,3-triazole-1-yl)*-N-Substituted Phenyl Acetamide as in Antimicrobial Screening

Shital Y. Patel[1], Jigar S. Patel[2]

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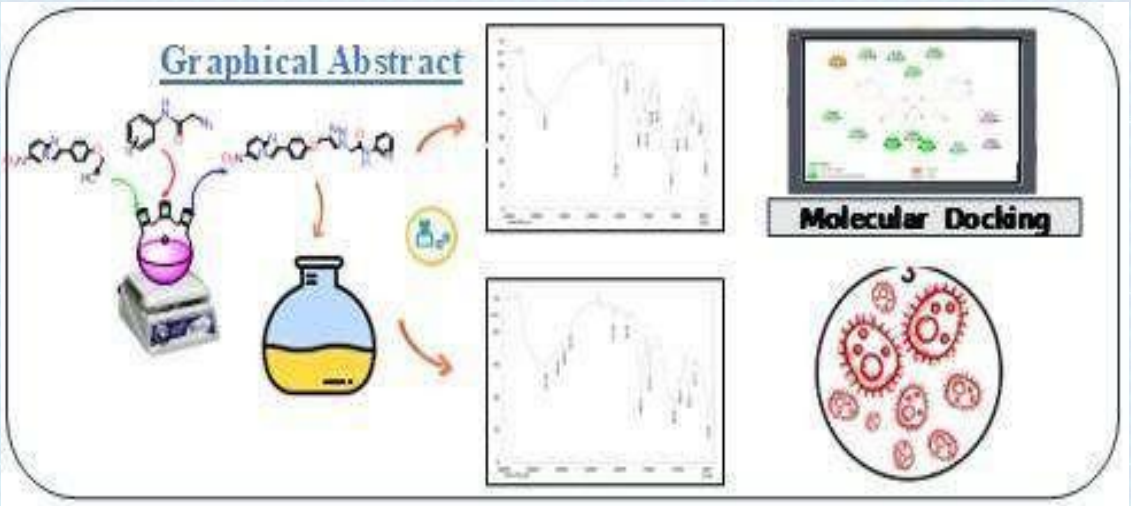
Abstract:

Reactions of 6-nitro-2-(4-(prop-2-ynyloxy) phenyl) H-imidazole[1,2-a] pyridine with substituted-2-azido-N-substituted phenyl-acetamide gave 2-(4-((4-(6-nitroH-imidazo[1,2-a] pyridin-2-yl) phenoxy) methyl)-1H-1,2,3-triazol-1-yl)-N-substituted phenyl acetamide. The compounds were analysed and characterized using elemental analysis, mass spectrometry, 1H NMR, 13C NMR, and infrared spectroscopy. These new compounds were evaluated for their in vitro antibacterial and anti-fungal activity. Compound 7b exhibited significant efficacy against S. aureus, S. epidermidis, E. coli, and P. aeruginosa, with MIC values of 5, 2.5, 5, and 8, respectively. Molecular docking analysis demonstrated that compound 7b exhibited a notable glide score of -10.0kcal/mol, reflecting strong binding interactions with the VEGFR2 tyrosine kinase domain of homo sapiens protein (PDB ID: 2OH4).



Flag

OP-12

Exploring Anti-Quorum Sensing Strategies: Staphylococcus-Derived Compound as a Potential Inhibitor of Pseudomonas Aeruginosa PAO1 QS System

Saklain Mustak Saiyad, Shreya Kansara, Nisha Daxini

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Abstract:

Quorum sensing (QS) is a key regulatory system in Pseudomonas aeruginosa PAO1, controlling virulence, biofilm formation, and multidrug resistance (MDR). Targeting QS with anti-quorum sensing (anti-QS) compounds presents a novel approach to mitigating bacterial pathogenicity without exerting selective pressure for resistance development. In this study, we evaluated an anti-QS compound isolated from Staphylococcus spp. and compared its QS inhibitory potential with cinnamaldehyde, a well-established QS inhibitor, through molecular docking analysis.

Docking results demonstrated that the Staphylococcus-derived anti-QS compound exhibited strong binding to LasR (7.2 kcal/mol), RhlR (-5.0 kcal/mol), and PqsR (-5.9 kcal/mol), suggesting its ability to interfere with multiple QS pathways in P. aeruginosa PAO1. Cinnamaldehyde, used as a standard, showed the highest affinity for LasR (-8.2 kcal/mol), further validating its QS inhibitory potential. In silico pharmacokinetic analysis of the Staphylococcus-derived compound indicated favorable absorption, distribution, metabolism, and excretion (ADME) properties with minimal toxicity concerns, supporting its potential as a safe therapeutic candidate.

These findings highlight the Staphylococcus-derived anti-QS compound as a promising candidate for QS disruption in P. aeruginosa PAO1. Further in vitro and in vivo studies are needed to confirm its role in attenuating QS-regulated virulence and biofilm formation, offering a potential alternative for combating MDR infections.

OP-13

A Study on the Antimicrobial Potential of Substituted (Z)-5-Benzylidene Thiazolidine-2,4-diones with 1,3,4-Oxadiazole Functionalities

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Abstract:

A variety of antimicrobials with distinct modes of action is vital for tackling the challenges associated with multidrug resistance. Herein, we have designed and synthesized novel thiazolidine-2,4-dione derivatives (1–10). These scaffolds analyzed for their potent antibacterial and antifungal activities. Among all, (10) exhibited excellent antibacterial activity at minimum zone of concentration values ranging between 1.9 to 2.4 mg/mL against pathogenic strains Staphylococcus aureus, Streptococcus pyogenes, Escherichia coli, and Pseudomonas aeruginosa. The synthesized compounds (1) and (7) was exhibited moderate antifungal activity with zone of concentration 2.4 and 2.3 mg/mL respectively against Aspergillus niger compared to standard drug Nystatin. Furthermore, the molecular binding affinity of the synthesized thiazolidine-2,4-dione derivatives with proteins of various bacteria fungi was ascertained using a molecular docking studied.

OP-14

A Review of PNPLA3 I148M and TM6SF2 E167K Polymorphism in NAFLD: Pathophysiological Mechanisms.

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Abstract:

Non-alcoholic fatty liver disease (NAFLD) is a complex metabolic disorder linked to obesity and metabolic syndrome, affecting 25% of the global population. Among the main genetic determinants, the PNPLA3 I148M and TM6SF2 E167K polymorphisms have emerged as significant contributors to disease susceptibility and progression. The PNPLA3 I148M variant is associated with impaired triglyceride hydrolysis, leading to hepatic fat accumulation and increased fibrosis risk. The Patatin-like Phospholipase Domain Containing 3 (PNPLA3) gene, particularly the I148M variant (rs738409), plays a key role in the development and progression of NAFLD, influencing lipid metabolism and increasing susceptibility to more severe liver conditions, such as Non-Alcoholic Steatohepatitis (NASH), fibrosis, and hepatocellular carcinoma (HCC). Similarly, the Transmembrane 6 Superfamily Member 2 (TM6SF2) E167K variant (rs58542926) mutation disrupts lipid metabolism, reducing very-low-density lipoprotein (VLDL) secretion and promoting liver steatosis. These polymorphisms influence multiple pathophysiological pathways, including lipid droplet remodelling, inflammation, and fibrogenesis, exacerbating NAFLD severity and its progression to non-alcoholic steatohepatitis (NASH) and finally to hepatocellular carcinoma (HCC) especially PNPLA3 gene. This review explores the mechanistic roles of PNPLA3 and TM6SF2 variants in NAFLD, highlighting their potential as biomarkers for risk stratification and therapeutic targets. Understanding these genetic factors provides deeper insights into NAFLD pathogenesis, paving the way for precision medicine approaches in liver disease management.

OP-15

Elemental Sulfur-Catalyzed Synthesis of Quinoxalines from Sulfoxonium Ylides and O-Phenylenediamines

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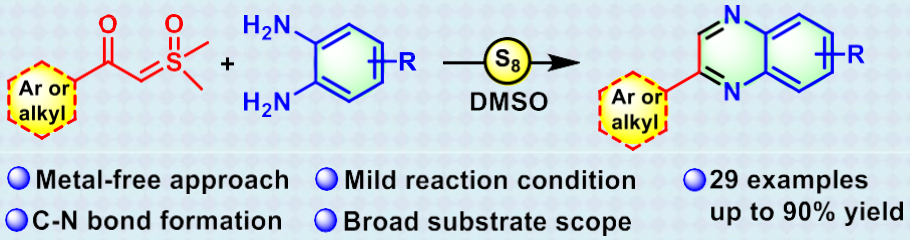
Abstract:

A novel and efficient synthetic protocol has been developed for the synthesis of quinoxaline derivatives. This methodology involves the ambient-temperature reaction of β-ketosulfoxonium ylides with o-phenylenediamines, exhibiting excellent compatibility with various substituted sulfoxonium ylides and o-phenylenediamines. Notably, this approach yields moderate to high yields of the desired products. Furthermore, the synthesized quinoxaline derivatives have been utilized to prepare biologically active compounds, highlighting the potential applicability of this methodology. Additionally, the developed strategy has been successfully extended to the synthesis of certain pyrazine derivatives.[1]



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Mn(I)-Catalyzed Site-Selective C–H Activation of 2-Aryl Pyridines and Maleimides: A Convenient Route to 3-Arylated Succinimides

Ajay Kant Gola and Satyendra Kumar Pandey*

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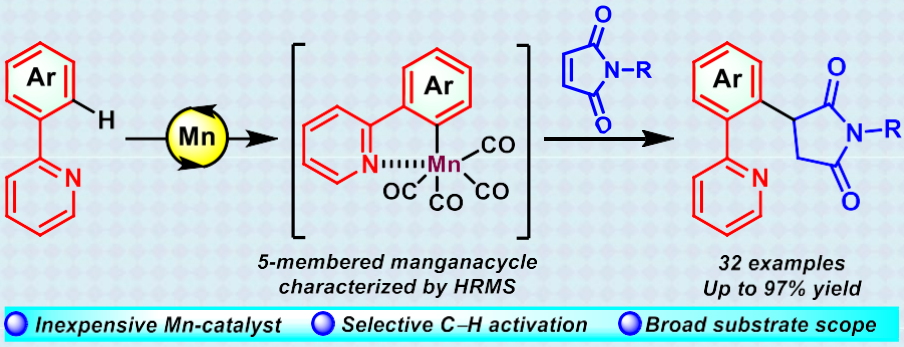
Abstract:

We report a Mn(I)-catalyzed, site-selective C–H activation of 2-aryl pyridines with maleimides that furnishes 3-arylated succinimides in a straightforward manner. This protocol proceeds under mild conditions, tolerating a wide range of functional groups and offering a highly efficient synthesis of valuable succinimide derivatives. The reaction works well with a variety of substrates while maintaining excellent chemoselectivity. Furthermore, the practicality of this approach is highlighted by its successful application in large-scale reactions and the facile transformation of the synthesized succinimide derivatives into other valuable compounds, underscoring its synthetic utility.[1]



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PP-17

Possible Role of Proinflammatory Biomarkers Interleukins Among the Prostate Cancer Patients.

Abbas abdulhasab jebur

Gujarat University

Abstract:

Prostate Cancer is a non-cutaneous cancer that primarily affects men over 50. It affects over 1.6 million people and causes over 3,000 fatalities globally. According to reports, it is the fifth leading cause of cancer-related mortality and the second most frequent kind of cancer among men. Furthermore, a thorough assessment and consistent viewpoints about the role of interleukins in prostate cancer are still lacking. Here, in the current study, we planned to investigate the role of possible correlation between the incidence of PCa vs age patterns along with PCa vs cytokines levels.

The study was a prospective longitudinal observational study, which was performed between January 2019 and March 2020. Seventy patients (n=70) (healthy individuals as control =20) at the Urology Service of the Gujarat medical college diagnosed with prostate cancer and treated with standard chemotherapy were recruited in the study. Interleukins (Cat No: SEA563Hu, Cloud-Clone Corp, Iraq) levels in serum was estimated with ELISA test kit.

We found from the data that the subjects in the age group from 61-65 to be more susceptible to the disease ($P<0.05$) with a count of 28 out of 70 (40%). Patients had considerably greater levels of IL-2, IL-4, IL-6, IL-17A and IL-10 than healthy controls. Il-2 levels were elevated to 25.67 ± 2.132 when compared to control (12.31 ± 1.20215) and Il-4 levels were elevated to 45.63 ± 3.4512 when compared to control (20.34 ± 2.143726). Il-6 levels were elevated to 65.43 ± 1.654 when compared to control (21.34 ± 0.9342) and Il-10 levels were elevated to 12.341 ± 2.1218 when compared to control (20.34 ± 2.143726). Il-17A levels were elevated to 45.33 ± 3.121 when compared to control (16.11 ± 1.1132). This would confirm the strong association between interleukins and PC.

OP-18

Estimation and correlation studies of circulating CTRP12 and Adipsin with Chronic Kidney Disease Among Iraqi Population

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Abstract:

Background: Globally, chronic kidney disease (CKD) ranks as the 16th most common cause of years of life lost. To avoid detrimental CKD-associated outcomes, such as cardiovascular disease, end-stage kidney disease, and death, primary care physicians must perform appropriate screening, diagnosis, and therapy. Among the recently investigated families of adipokines, serum C1q/TNF-related protein-12 (CTRP12) and Adipsin are thought to be linked to type 2 diabetes. Nevertheless, it is still unknown how serum CTRP12 and Adipsin levels and CKD are related.

The purpose of this study was to examine the connection between CKD patients' serum CTRP12 and Adipsin levels. Our study's objective was to determine the serum adipsin and CTRP12 levels of CKD participants from the Iraqi community. Using the ElabScience ELISA kits, we calculated the serum Adipsin and CTRP12 levels. In addition to these protein levels, we looked for any potential links between the participants' chronic renal illness and a number of blood indicators.

Results: In comparison to controls, the individuals' serum creatinine, blood urea, serum uric acid, and CRP levels were found to be higher ($P<0.01$). When compared to the control group, the patients' group had lower calcium levels and a lower glomerular filtrate rate (GFR) ($P<0.01$). The CTRP12 levels were found to be lowered among the patients group (0.68544 ± 0.07042) when compared to control (0.98511 ± 0.2516). The Adipsin level was found to be highly lowered among the patients group (9.76 ± 1.2052) when compared to control (27.90889 ± 6.7827). This confirms the strong association of Adipsin and CTRP12 with CKD. ($y = 0.021x + 0.0915$; $R^2 = 0.9911$). We discovered through various correlation tests that there was a positive link between Adipsin and CTRP12 ($r=0.164129$) and between CRP and CTRP12 ($r=0.160291$).

OP-19

Mucoadhesive Xanthan gum-based Nanoparticle Delivery of drug for Psoriasis Treatment

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Abstract:

Psoriasis is a long-term autoimmune skin condition marked by an overabundance of keratinocytes and an overreaction by the immune system. The available therapy alternatives such as immunosuppressants, corticosteroids, and biologics are frequently linked to systemic side effects and have limited effectiveness. In order to address these issues, we created a mucoadhesive nanoparticle system based on thiolated xanthan gum (XG-SH) for the topical administration of drug that modifies illness and has strong anti-inflammatory effects. To improve mucoadhesion and drug-loading ability, XG was chemically altered by adding thiol groups and conjugating it with stearylamine (SAN). Utilizing FTIR, CHNS(O) analysis, 1H-NMR, and thiol content estimate, the synthesized XG-SH conjugate was studied. Improved stability, increased mucoadhesion, and prolonged drug release were all demonstrated by drug-loaded nanoparticles. The drug loaded topical hydrogel formulation exhibited ideal rheological characteristics enabling efficient. Effective skin application was made possible by the topical gel formulation which showed ideal rheological characteristics. Superior dermal localization of drug was validated by ex vivo permeation and retention experiments, reducing systemic exposure while optimizing therapeutic efficacy. Drug loaded gel is a prospective substitute for the treatment of psoriasis because of its sustained drug release profile, which indicates prolonged therapeutic efficacy. To prove its therapeutic effectiveness and safety more in vivo research is needed.

OP-20

Advanced Spectroscopic Insights into Organosilatranes for Selective Cu^{2+}, Hg^{2+}, and Pb^{2+} Detection

Sanchita

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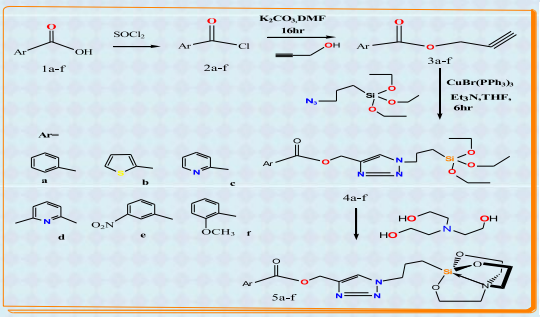
Abstract:

A novel series of organosilatranes has been synthesized for the selective and specific detection of Cu^{2+}, Hg^{2+}, and Pb^{2+}. These compounds were thoroughly characterized using various spectroscopic techniques. Their metal ion binding abilities were assessed through UV-Vis and photoluminescence spectroscopy, revealing significant interactions. The Stern-Volmer analysis further confirmed a quenching effect upon the addition of Cu^{2+}, Hg^{2+}, and Pb^{2+}. This study underscores the importance of integrating advanced spectroscopic methods into chemical sensing strategies to enhance detection efficiency and mitigate environmental risks associated with heavy metal contamination.



Scheme: Synthesis of Organosilatranes

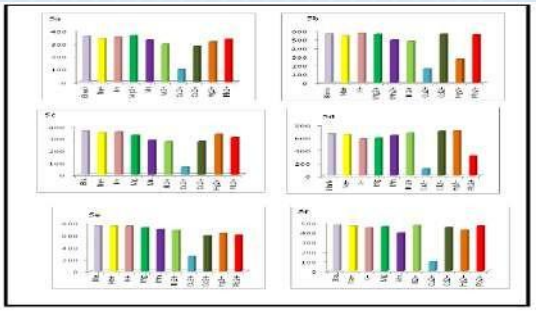


Fig: Intensity of various metal ions of silatranes

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OP-21

A Simple and Facile Conjugate Addition of Cyclic and Acyclic 1,3-Diketones to β-Nitrostyrenes

Dharti Mistry and Dandamudi V, Lenin

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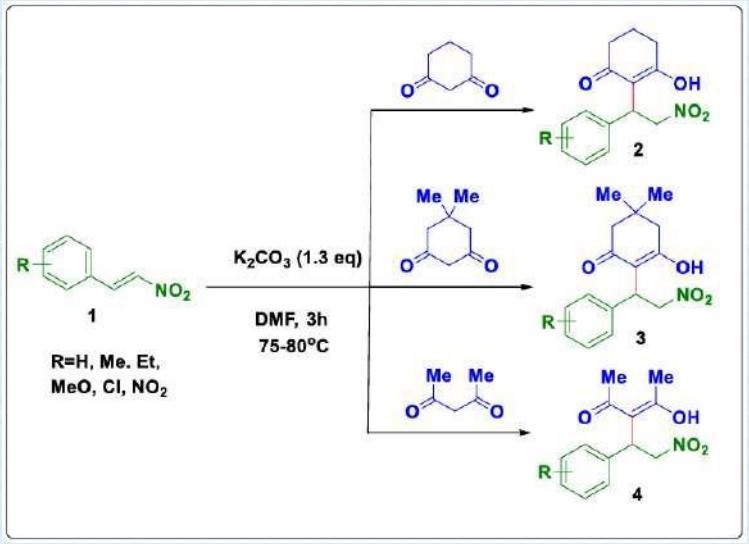
Abstract:

A simple and facile conjugate addition of cyclic and acyclic 1,3-diketones to β-nitrostyrenes Dharti Mistry and Dandamudi V, Lenin* School of Chemical Science, Central University of Gujarat, Gandhinagar, India-382030 β -Nitrostyrenes are an important class of compounds in synthetic organic chemistry and their applications are well-documented in the literature. These compounds can be used as precursor for the synthesis of various heterocyclic compounds. In this method appears to be a well-structured and scalable synthetic way for producing specific functionalized compounds using conjugate addition chemistry. The key components, like cyclic diketones as a 1,3 cyclohexanedione and 5,5-dimethyl-1,3-cyclohexanedione, and along with the acyclic diketone pentane-2,4-dione,are reaction with β-nitrostyrenes to form 3-hydroxy-2-(2-nitro-1 arylethyl)cyclohex-2-en-1-ones, 3-hydroxy-5,5-dimethyl-2-(2-nitro-1-arylethyl)cyclohex-2 en-1-ones, and 4-hydroxy-3-(2-nitro-1-arylethyl)pent-3-en-2-are provide variety of the structure. The flexibility of this reaction lies in the ability to produce both cyclic and acyclic β ketone, which are valuable desirer compound for further functionalization into more complex molecules. These compounds can be produced in gram quantities, which makes the method suitable is also an important consideration for industrial applications, where large-scale synthesis is often necessary.



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OP-22

1,2,3-Triazole Linked 1,8-Dioxooctahydroacridine Scaffold as Potential A-Glucosidase and A-Amylase Inhibitors: Design, Green Synthesis, Kinetics, and Insilico Studies

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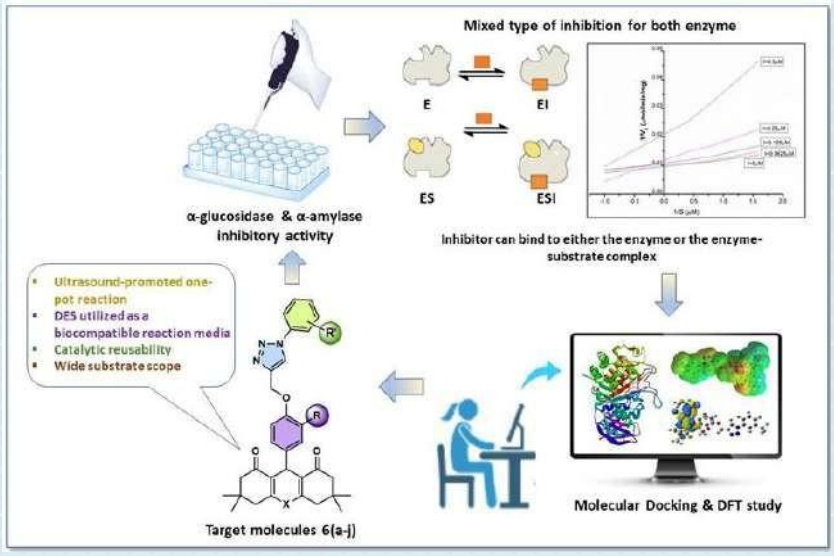
Abstract:

In an ongoing effort to discover new α-glucosidase as well as α-amylase inhibitors for the treatment of type 2 diabetes mellitus (T2DM), herein we introduced the synthesis of 1,2,3-triazole linked 1,8 dioxooctahydroacridine derivatives 6(a-j). This approach utilized ultrasound-promoted deep eutectic solvent (DES) as a biodegradable medium, resulting in a highly efficient and environmentally friendly process with high yields. Upon inhibiting α-glucosidase and α-amylase enzymes, compounds 6g, 6h, 6i, and 6j demonstrated significant inhibition, with IC50 values ranging from 3.24 ± 0.07 to 5.03 ± 0.05 µM and 3.28 ± 0.07 to 4.68 ± 0.07 µM respectively. Kinetic studies were conducted on the most effective compounds to elucidate their mechanism of action, unveiling a mixed-type inhibition mode against both enzymes Molecular docking studies have corroborated the findings, demonstrating that these compounds engage in multiple binding interactions within the active pockets of both enzymes. Additionally, density functional theory (DFT) calculations were conducted for all the synthesized molecules to enable comparisons between the biological activity of representative compounds and the theoretically derived quantum chemical descriptors.



OP-23

Microwave Assisted One-Pot Synthesis of 3-Imidazolyl Indole Linked 1,2,3-Triazole Hybrids: Antiproliferative Evaluation and DFT Study

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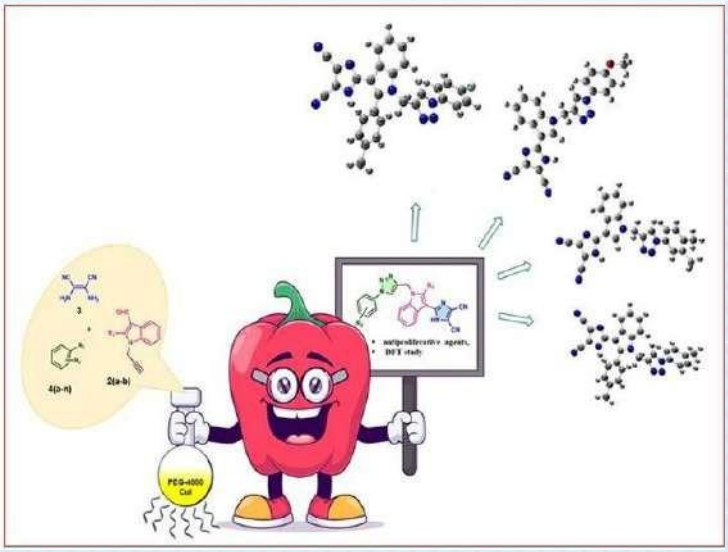
Abstract:

Herein, we present a highly efficient PEG-4000-mediated one-pot, three-component reaction for synthesizing 3-imidazolyl indole-clubbed 1,2,3-triazole derivatives 5(a-r) with yields of up to 96% as potential antiproliferative agents. This three-component approach provides an eco-friendly reaction, high yields, rapid execution, and straightforward operation, facilitated by a copper catalyst under microwave irradiation. All the synthesized compounds were tested for antiproliferative activity against six human solid tumor cell lines, namely A549 and SW1573 (nonsmall cell lung), HBL100 and T-47D (breast), HeLa (cervix), and WiDr (colon). Among them, six compounds, 5(g–j), 5m, and 5p demonstrated effective antiproliferative action with GI50 values under 10 μM. Density functional theory (DFT) calculations, including geometry optimizations, frontier molecular orbitals, and molecular electrostatic potential (MESP), were conducted to analyze synthesized molecules and compare their biological reactivity with quantum chemical descriptors. We also investigated the drug-likeness characteristic and absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction. In general, our approach enables environmentally friendly access to 3-imidazolyl indole clubbed 1,2,3-triazole derivatives as prospective antiproliferative agents.



OP-24

Studies Toward the Synthesis of Cannabinoid and Cannabinoid-like Compounds

Kumar Vijay, Anand Radhika, Singh Parvinder Pal

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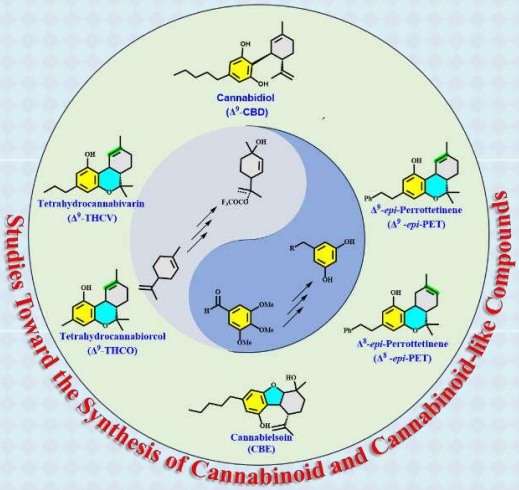
Abstract:

Cannabinoid-based therapeutics have garnered significant attention due to their diverse pharmacological properties. The term phytocannabinoid refers to meroterpenoids with a resorcinyl core, typically decorated with a *para*-positioned alkyl or aryl side chain. This group of specialized metabolites was first identified in *Cannabis sativa* (Cannabaceae). Major cannabinoids, such as cannabidiol (CBD) and cannabigerol (CBG) play crucial role in pharmacology. However, minor cannabinoids remain less explored due to their limited natural availability. In addition, the cannabinoid-like compounds have also been reported from other genera (Liverworts, Fungi, Rhododendron and Helichrysum) and being less explored. A key challenge in cannabinoid synthesis lies in the efficient construction of both the resorcinol and terpene cores. In this study, we developed an efficient synthesis of both the resorcinol and terpene cores using readily available and inexpensive precursors, 3,4,5-trimethoxybenzaldehyde and limonene. The resulting intermediates were successfully utilized for the synthesis of *epi*-perrottetinene (*epi*-PET), cannabidiol (CBD), and cannabielsoin (CBE). This streamline approach significantly enhances synthetic efficiency, making it a promising strategy for medicinal chemistry and further cannabinoid exploration.



OP-25

Repurposing FDA-Approved molecules to Combat Virulence Factors of *Porphyromonas Gingivalis*: A Synergistic *Insilico* and *In Vitro* Approach

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Abstract:

Antimicrobial resistance (AMR) poses a significant threat to public health and economic stability worldwide. Porphyromonas gingivalis, a key pathogen in periodontitis, has demonstrated resistance to major classes of antibiotics. This study aims to evaluate the potential of repurposed molecule, against P. gingivalis virulence factors through in silico analysis and to develop a nanotechnology-driven hybrid nanogel formulation for improved antibacterial efficacy. An insilico docking study was performed to evaluate the binding affinity of tigecycline against gingipain-K, a key virulence factor of P. gingivalis. The analysis revealed strong molecular interactions with the catalytic triad (Cys477, His444, and Asp388), suggesting a potential inhibitory effect of the tigecycline.These findings indicate tigecycline's stable binding to the active site, reinforcing its potential as a therapeutic candidate against P. gingivalis-mediated infections. Following computational validation, a hybrid nanogel formulation of tigecycline was developed and evaluated in vitro for its antimicrobial activity against P. gingivalis. The docking analysis revealed that tigecycline exhibited high binding affinity toward gingipain-K, suggesting strong inhibitory potential against the enzyme, which is essential for bacterial adhesion, host tissue destruction, and immune evasion. The formulated hybrid nanogel demonstrated significant antibacterial activity in vitro, effectively inhibiting key virulence factors of P. gingivalis and overcoming biofilm-related resistance. These findings highlight tigecycline as a promising repurposed therapeutic agent for targeting P. gingivalis infections. The nanogel-based formulation enhances its bioavailability and antibacterial efficacy, offering a nanotechnology-driven regenerative therapy to combat AMR in periodontal infections.

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OP-26

Ugi-Mediated Synthesis and Characterization of Nitrogen-Containing Heterocyclic Molecules as Anticancer Agents

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Abstract:

Heterocyclic compounds, particularly nitrogen-containing heterocycles, have gained significant interest in medicinal chemistry for their potential anticancer properties. These compounds exert anticancer effects by modulating key cellular mechanisms and interacting with vital biomolecules such as proteins and DNA. This study explores the synthesis of tetrazole derivatives through the Ugi multicomponent reaction and evaluates their anticancer activity against a panel of NCI-60 cancer cell lines. The results indicate that the tetrazole derivatives show promising anticancer effects, suggesting their potential as lead compounds for the development of targeted cancer therapies. These findings contribute to the ongoing search for novel, effective therapeutic agents capable of combating various forms of cancer, highlighting the relevance of heterocyclic compounds in the advancement of cancer treatment strategies. Further research is necessary to optimize the efficacy and selectivity of these compounds for clinical applications.

OP-27

Recycling Waste into Energy: Biodiesel Production from Used Cooking Oil via Alkali Metal Catalysts – Significance of Physiochemical parameters

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[a]Department of Chemistry, Swaminarayan University, Kalol Gandhinagar.
[b]Department of Chemistry, Shree Swaminarayan Science College, Swaminarayan University, Kalol Gandhinagar.

Abstract:

The constraint for sustainable energy growth has become progressively evident, chiefly due to the restricted nature of fossil fuel reserves and the correlated environmental alarms. In light of these concerns, biodiesel emerges as a fascinating alternative. Its key aspects include renewability, lowered emissions, and the capability to be produced from a variety of sources, providing it a promising candidate in addressing these energy and environmental challenges. Biodiesel holds considerable promise as an energy source appropriate to its lower environmental impact compared to traditional diesel fuels. Waste cooking oil can be used as a possible feedstock for producing biodiesel. Disposal of waste cooking oil by itself is an environmental challenge due to its adverse environmental impact. Transesterification provides a key process for biodiesel production with minimum cost and under mild reaction condition. This work explores the production of biodiesel from waste cooking oil (WCO) by utilizing alkali metal catalysts, highlighting the significance of its physicochemical properties. Fundamental parameters such as acid value, free fatty acid (FFA) content, viscosity, density, moisture content, and saponification value directly affect transesterification efficiency and biodiesel quality. High FFA and moisture levels

necessitate pre-treatment to prevent soap formation and catalyst deactivation. The study evaluates alkali catalysts such as calcium oxide (CaO) and potassium hydroxide (KOH) or their mixture for their effectiveness in optimizing yield and fuel properties. Results indicate that process optimization, including catalyst concentration, reaction time, and temperature, significantly enhances biodiesel conversion. Understanding the physicochemical characteristics of WCO ensures better process control, high-quality biodiesel production, and adherence to international fuel standards such as ASTM D6751 and EN 14214. This research highlights the potential of WCO as a sustainable feedstock, promoting waste-to-energy conversion and environmental sustainability.

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PP-28

Insilico and Invitro analysis of Syntaxin-1 Like Molecule from Pathogenic Protozoan Parasite Entamoeba Histolytica

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Abstract:

Entamoeba histolytica is the causative agent of amoebiasis, a neglected tropical disease that claims close to 50,000 lives globally each year and is a major cause of mortality in children below 5 years of age. The morbid pathology of E. histolytica is reliant on cysteine proteases and amoebopore proteins that facilitate intestinal tissue damage. The transport of these virulence factors is carried out by vesicular transport machinery that involves the SNARE complex and accessory vesicle sorting proteins. Not much is known about the vesicular membrane dynamics of E.histolytica (Eh) thus, here we have identified four proteins involved in the vesicular transport system of Eh: Syntaxin binding protein, EhSec1, small Rab GTPase, and EhRabX10. The N-ethylmaleimide-sensitive fusion protein (NSF) and soluble NSF attachment receptor (SNARE) molecules play critical roles in vesicle fusion and neurotransmitter release, with their dysfunction being implicated in various neurodegenerative diseases. Invasive amoebiasis, caused by Entamoeba histolytica, is characterized by the secretion of extracellular vesicles (EVs) that release several virulence factors. One such factor is a syntaxin 1-like molecule, a SNARE protein identified in E. histolytica. The characterization of this syntaxin 1-like molecule has been approached using both in silico and in vitro methods. BLAST analysis reveals conserved regions, which allowed for the prediction of its structure, subsequently validated through root mean square deviation (RMSD) calculations and Ramachandran plot analysis. The identification of heptad repeats indicates the presence of a coiled-coil domain, and the corresponding sequence has been amplified for further cloning. The full-length syntaxin 1B protein has been successfully expressed, and purified. Protein-protein interactions of syntaxin and its coiled-coil domain with other proteins that is mentioned above will be investigated and further used as a drug targets.

OP-29

Application of Imidazolium and Benzimidazolium Ionic liquids for Heavy Metal Ion Sensing and Green Catalysis

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Abstract:

Our group has synthesized 3 novel imidazolium/benzimidazolium based ionic liquids (ILs) namely IL1, IL2 and IL3. The two ILs IL1 and IL2 was utilized as fluorescent sensor of cadmium and mercury with remarkable selectivity and sensitivity. The limit of detection of each ionic liquid was lower than micromolar range suggesting better seletibiy and semsitivty Moreover, paper-based device was fabricated for one site and rapid detection. IL3 was utilized to synthesize Pd based metal complex which was used as green and reusable catalyst for Suzuki reaction. Totally green methodology was developed using IL3 and it was tested with different substituted Iodo benzene. Reaction was carried out in water, and at room temperature.

OP-30

Investigation of In-Vitro Interaction of BSA With Biocompatible Graphene Oxide Using Multi-Techniques Approach

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Abstract:

Graphene oxide (GO) nanomaterial have unique properties for biomedical and interaction studies. GO with higher surface area, functional groups (-COOH, -OH, -O-), and excellent dispersibility in aqueous solutions has enable it for strong interactions with BSA (bovine serum albumin). The functional groups facilitate the GO to interact with BSA via non-covalent interaction such as π-π stacking, hydrogen bonding, and electrostatic interactions. Herein, the GO is synthesized via modified Hummer's method and structurally characterized with high end equipments. The in-vitro cytotoxicity assays have demonstrated excellent biocompatibility with higher cell viability. The biocompatibility has proven a GO as potential candidate to interact with BSA. The in-silico study demonstrated good binding affinity of GO with BSA, that encouraged to investigate the interaction between aq-GO and aq-BSA via in-vitro physicochemical analysis. The physicochemical properties of aq-BSA on varying its concentration are measured with aq-GO to illustrate the interacting mechanism. Furthermore, the results of physicochemical properties are interfaced with UV-Vis and fluorescence analysis. All the studied techniques have revealed that GO have interacted with BSA without disrupting protein structure. These finding offer prospective applications in drug delivery, biosensors, or other therapeutic domains.

PP-31

Network Pharmacology Exploring the Mechanistic Role of Isorhamnetin Phytoconstituent from Opuntia Ficus-Indica Targeting Membrane Integrity-Associated Anemia

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Abstract:

Opuntia ficus-indica, frequently referred to as the Findla or prickly pear, has long been utilized in medicine because of its antibacterial, anti-inflammatory, anti-anemic, and hemoglobin-level-boosting qualities. Its active ingredients may help preserve the integrity of red blood cell (RBC) membranes and regulate hemoglobin levels. This study used network pharmacology, molecular docking, and molecular dynamic simulations to investigate potential pathways of isorhamnetin that could defend against the membrane integrity of RBCs. The Swiss target database revealed 100 isorhamnetin-associated pharmacological targets, whereas DisGeNET provided the top 30 target genes associated to anaemia. These candidate drug targets were examined in STRINGs in order to identify any potentially important drug targets linked to the membrane integrity of RBCs. Additionally, their statistical centrality metrics and biological annotations were examined in Cytoscape (Ver. 3.10.3). The range of their significance level spanned from 0.4 to 0.6. The optimal K-core network, determined by MCODE, also represented these possible therapeutic targets. Additionally, researchers considered molecular modelling and a molecular dynamics technique using isorhamnetin for these potential therapeutic targets. The results indicated a possible degree of interaction as non-bonded interactions with the protein ANK1. ADMET. Molecular dynamics represented the stability of the proteins at the cytoskeleton level. It was revealed by network analysis that disintegrated RBC membranes may be prevented by isorhamnetin through the modulation of critical signalling networks, which could be one of the molecular mechanisms underlying the effectiveness of the plant against Membrane integrity associated anemia. It was shown by molecular docking studies that strong binding abilities to key target proteins ANK1, SPTA1, and SPTAB were exhibited by isorhamnetin.

OP-32

Synthesis, Structural Analysis, DFT Study, Molecular Docking and ADMET Evaluation of Indole-Oxadiazole Derivatives for Anticancer Study

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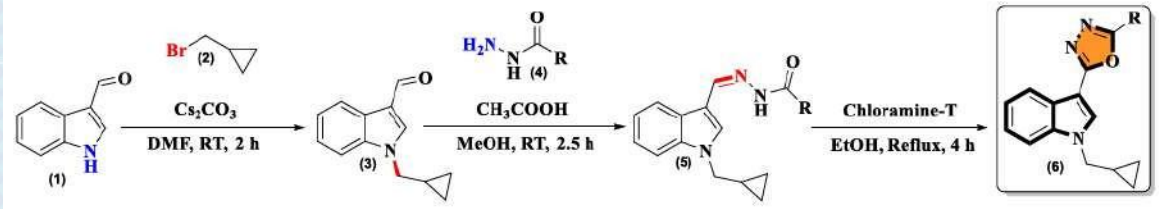
Abstract:

Indole and oxadiazole moieties have emerged as promising anticancer agents due to their unique structural framework and biological activity. In this study, we have synthesised 11 derivatives of indole-oxadiazoles using various reactions which involves N alkylation, Schiff base formation, and cyclization. The synthesized compounds were analysed using various spectroscopic techniques such as mass spectrometry, nuclear magnetic resonance (NMR) spectroscopy, IR, UV-Vis spectra. To assess their drug-likeness and pharmacokinetic properties, DFT, ADMET analysis and Molecular Docking studies were conducted to investigate their potential binding interactions. The combined experimental and computational approach provides valuable insights into the Structure-Activity Relationship (SAR) of indole-oxadiazole derivatives. These findings indicate that the compound complies with Lipinski's rule of five, suggesting favorable oral bioavailability. Additionally, its bioavailability radar supports good drug-like potential. Based on these properties, we are considering further evaluation of its anticancer activity to explore its therapeutic viability.

Reaction Scheme:



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OP-33

Precision Chemotypes for Acute Myeloid Leukemia (AML) *via* Hydroadamantylation of Quinoxalones under Metal- and Light-Free Conditions

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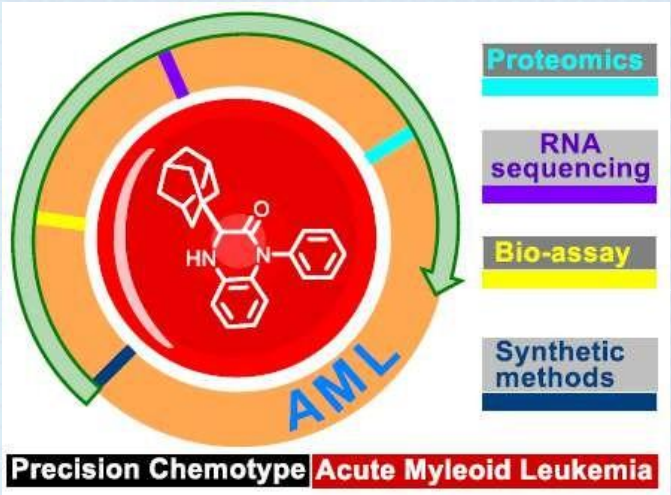
Abstract:

Acute myeloid leukemia (AML) is an aggressive blood cancer with a poor prognosis, especially when diagnosed late. Around 10–15% of cases involve the specific chromosomal abnormality t(8;21), which drives uncontrolled myeloid cell proliferation and contributes to disease onset. Despite advances in AML research and treatment protocols, outcomes for t(8;21) AML remain stagnant, as patients receive standard, non-specific chemotherapies. This one-size-fits-all approach targets both cancerous and healthy cells, leading to unwanted toxicity and highlighting the urgent need for targeted therapies. In this study, we present a precision chemotype based on a quinoxalone-tethered adamantane framework, developed via a metal- and light-free protocol. The compound selectively inhibits t(8;21) AML cell proliferation and induces cell death by disrupting growth and metabolic pathways, as demonstrated through bioassays, RNA sequencing, and proteomic analysis. Notably, it spares other leukemic and solid cancer cells, underscoring its specificity and potential as a targeted therapy for t (8;21) AML.



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OP-34

Functionalization of Alkynyl Hydroxylamines: A Gateway to 1,2-*N*/*O*-Heterocycles

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Abstract:

Metal catalyzed transformations of alkynyl hydroxylamines have gained prominence for the synthesis of 1,2-*N*-*O* heterocycles. However, their utility under metal free conditions is still under explored. In this context, we have demonstrated TMSOTf-mediated highly diastereoselective synthesis of isoxazolidine bearing three contiguous stereocentres *via* the alkyne-oximium cyclization (**Figure 1)**. The synthetic potential of methodology is demonstrated by synthesizing the corresponding 1,3-aminodiols with precise control over all stereocenters formed. On the other hand, gold-catalyzed 5-*exo*-*dig* hydroamination on *O*-homopropargylic hydroxylamine gave expeditious access to methylene isoxazolidine. Excess catalyst loading led to facile 1,3-sulfonyl migration in a cascade fashion to furnish the isoxazoline.

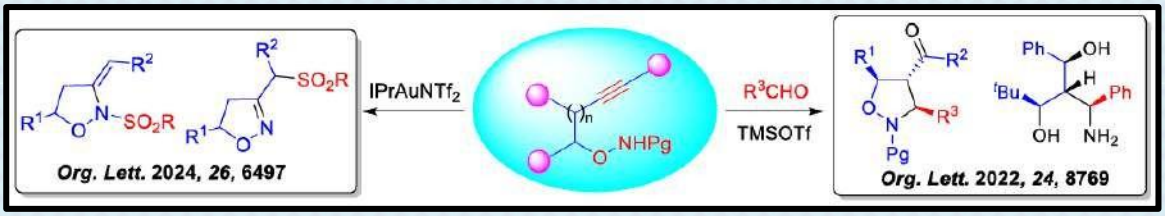

Figure 1: Alkynyl Hydroxylamines in the synthesis of 1,2-*N*-*O* heterocycles

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OP-35

Lewis Acid-Promoted Hydroalkoxylation Reduction/Cycloaddition of Cyclopropenes: A Unified Route to Synthesize THF, THP, Oxaspirolactones and Spiroketals

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Abstract:

Cyclic ethers like tetrahydrofuran's (THFs), tetrahydropyrans (THPs), oxaspirocyclic lactones and spiroketals are fundamental structural core moieties present in many natural products and bioactive compounds.1 Developing a method that enables the synthesis of these heterocycles is an important objective. Metal or acid-catalysed synthesis of these heterocycles *via* hydroalkoxylation reduction cascade of alkynes/olefins and spiroketalization of oxo diols are reported in the literature.2 To the best of our knowledge, a unified approach towards the divergent synthesis of these heterocycles from cyclopropenes is unprecedented in literature. Herein, we report the utility of hydroxy cyclopropenes in the synthesis of these heterocycles through the generation of donor-acceptor cyclopropanes as a common reactive intermediate. In the presence of an external nucleophile under Lewis acidic condition reaction furnished the desired THF and THP derivatives, whereas in the absence of an external nucleophile, the diester functionality serves as an internal nucleophile to provide access to oxaspirolactones stereoselectively. Similarly, the reactivity of donor-acceptor cyclopropanes in the cycloaddition reaction is exploited in the stereoselective synthesis of [5,5] and [6,5] spiroketals. The developed methodology was found to be general with broad range of substrate scope with good functional group tolerance. Furthermore, these heterocycles were transformed to facilitate the access of intricate polycyclic heterocycles.

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PP-36

Live Cell Imaging of Lipid Droplets: Fluorescent Chalcones as Probes for Lipophagy and Lipid-Mitochondria Interactions

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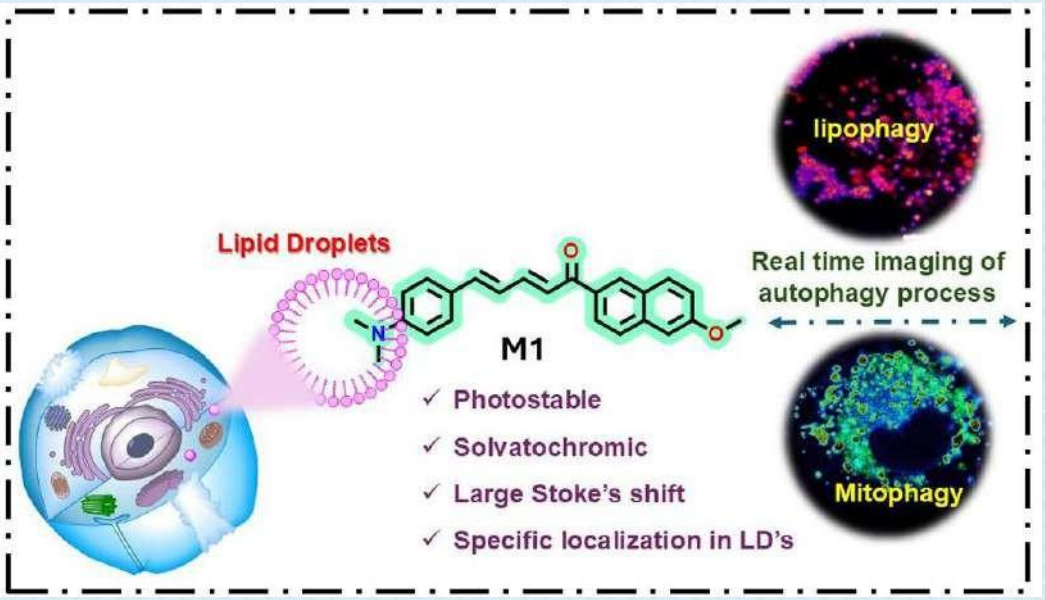
Abstract:

Lipid droplets are crucial organelles involved in cellular energy storage and metabolism, which is key in maintaining energy homeostasis through lipophagy. In this work, we successfully synthesized donor-acceptor chalcone derivatives with improved photophysical characteristics, such as significant Stokes shifts and strong emission features. These molecules show excellent selectivity in staining lipid droplets in COS-7 cells and other cell lines. The molecule M1 was also further utilized to monitor verapamil-induced lipophagy. Using M1, we also demonstrate the link between lipid droplets and mitochondria during stress, emphasizing the significance of lipophagy in cellular energy balance and metabolism. These results shed light on lipid metabolism and may have implications for researching metabolic diseases.



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PP-37

Thiamine Hydrochloride Assisted One-Pot, Multicomponent Synthesis of 1,3-Diaryl-3-Arylamino Propan-1-One Derivatives: A Sustainable and Greener Approach

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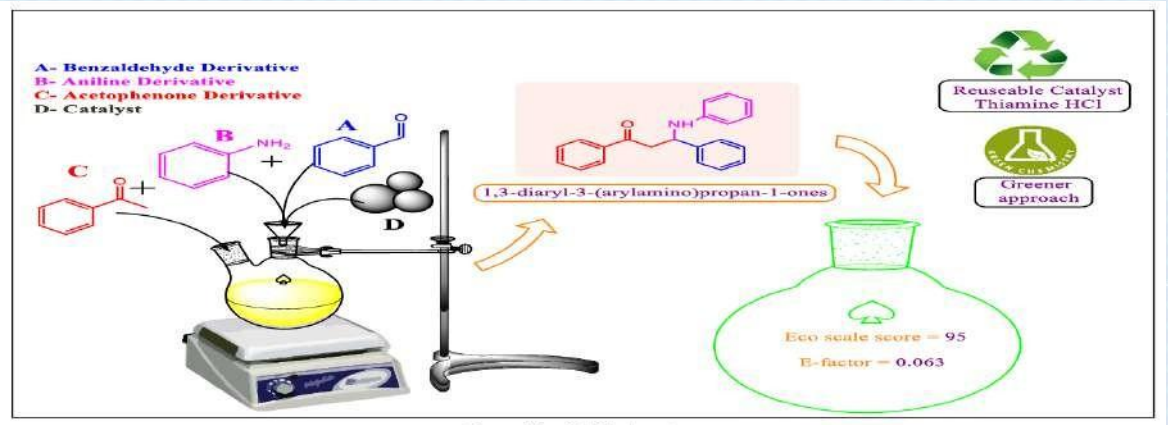
Abstract:

In this efficient approach, thiamine hydrochloride serves as an organocatalytic for the rapid synthesis of 1,3-diaryl-3-arylamino-propan-1-ones via a one-pot, multicomponent reaction (MCR). This protocol enables the production of β-amino carbonyl compounds using acetophenones with various substituted aromatic amines and aromatic aldehydes via a Manniche condensation reaction. The method offers several advantages, such as adhering to sustainable practices, following green chemistry principles, and providing an easy work-up process, yielding 1,3-diaryl-3-arylamino-propan-1-ones in moderate to excellent quantities.



Graphical Abstract

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PP-38

Styryl Benzoxazolium Salts as Fluorescent Probes for Organelle-Specific Bioimaging

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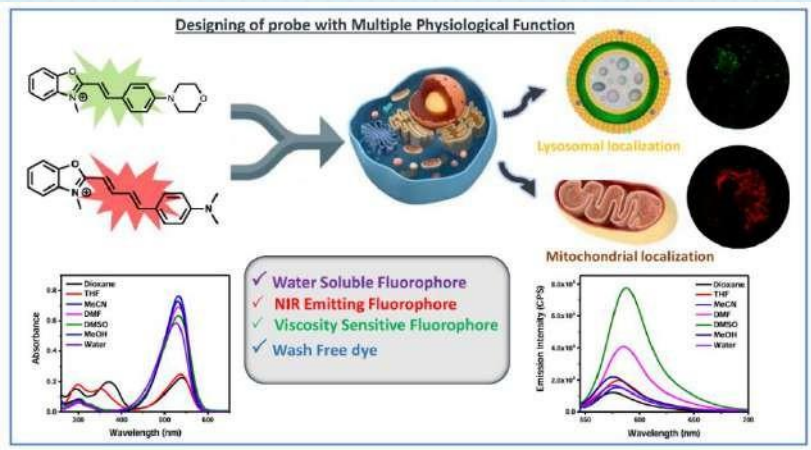
Abstract:

Fluorescent probes with tailored photophysical properties are crucial for high resolution bioimaging. We synthesized and characterized a series of styryl benzoxazolium salts as potential organelle-specific fluorescent probes. Structural modifications, especially electron-donating groups, influenced intramolecular charge transfer (ICT), affecting absorption, fluorescence, and subcellular localization. These dyes showed strong visible-region absorption, efficient fluorescence emission, and excellent biocompatibility for live-cell imaging. Most derivatives targeted mitochondria, while one with a morpholine moiety exhibited exclusive lysosomal localization, demonstrating the impact of electronic tuning on cellular uptake. Viscosity-dependent fluorescence studies confirmed ICT-mediated enhancement via restricted intramolecular rotation. Our findings establish a clear structure-property relationship in styryl benzoxazole salts, providing insights for designing next-generation fluorescent probes for cellular imaging.



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PP-39

Synthesis of *Pyrrolo-Pyridine Scaffolds*: Characterization and Biological Insights

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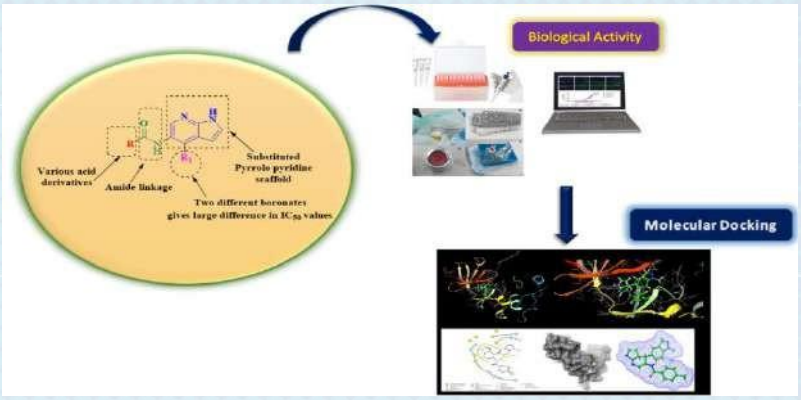
Abstract:

The work detailed acid-amine coupling chemistry with diverse reaction condition to synthesize new functionalized Pyrrolo-pyridine compounds. Synthesis of functionalized Pyrrolo-pyridine scaffold is more convenient via Acid-amine coupling chemistry which involves various aromatic acid and amine using HATU as an amide linker and DIPEA as a base, in addition to these aliphatic acids were also coupled with amine by using Pyridine as a base and $POCl_3$ as acid to generates acyl chlorides from acids. Herein, different substituted Aromatic/aliphatic acids chosen for exploring the biological potency of molecules, Future research employing cutting-edge computational technologies may increase the potency of drugs. All the synthesised compounds confirmed using TLC and various spectral analyses, such as LCMS, Mass and 1H NMR analysis.



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PP-40

Aloevera as a Natural Nano Carrier: Advancing Green Chemistry Solution

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Abstract:

Aloe Vera's Nano carrier systems have been prepared by standard method. Compound were screened for their antimicrobial –MIC-test, TEWL Test, Disinfectant effect, Biodegradability, Anti oxidation & Light Protection effect, Immuno protective effect & Bio Lubricant test. The combine elemental analysis, Electron Micrograph & Radio carbon Test data prove the authenticity of the Aloe Vera's Nano carrier systems.

PP-41

Bioactive Bile Acid Conjugates for Enhanced Drug Delivery and Real-Time Food Safety Sensing

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Abstract:

Our research explores the development of novel bioactive conjugates inspired by bile acid derivatives to enhance drug bioavailability and therapeutic properties. The amphiphilic nature of bile acids makes them ideal building blocks for drug delivery systems, improving membrane permeability and reducing side effects. Our study focuses on the synthesis of bile acid–bioactive molecular conjugates, evaluation of their hydrogelation and metal ion sensing via fluorescent probes, particularly Schiff bases of phenothiazines and carbazoles. The synthesized bile acid derivatives incorporating phenothiazine, carbazole, amide, and triazole linkers demonstrate promising applications due to their cost-effective and scalable synthesis. These molecules exhibit significant hydrogelation properties, making them valuable for biomedical applications. Additionally, their strong affinity for heavy metal ions enables efficient recognition and sensing, crucial for environmental monitoring and industrial safety. Furthermore, we explore the use of bile acid–based triazole–phenothiazine derivatives for the rapid detection of biogenic amines in spoiled foods, providing real-time monitoring for food safety applications. Future research aims to further optimize these conjugates for enhanced selectivity and sensitivity in various biomedical and environmental applications. This research is aligned with the theme of "Sustainable Innovations in Drug Development," which contributes to the fields of drug discovery, sensor technology, and industrial applications through the use of natural product-inspired bioactive molecules.

PP-42

Novel Nitrogen-Containing Heterocyclic Hybrids: Design, Synthesis and Assessment of Potential Pharmacological Activities

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Abstract:

Diverse functions of drug-driving nitrogen-containing heterocyclic molecules as scaffolds for drug discovery to achieve that, this research focuses on designed to develop and preparing a novel series of nitrogen-containing heterocyclic hybrids and assessing their potential pharmacological effects. A diverse array of nitrogenous heterocyclic moieties including pyrazole and triazole were, in one or more instances, combined through efficient synthetic procedures to afford the target libraries. The molecules that were produced were characterized using spectroscopic techniques. In vitro tests will be conducted against sixty human cancer cell lines to evaluate the synthesized hybrids pharmacologically. The efficient design and synthesis of these unique nitrogen-containing heterocyclic hybrids provide a promising framework for developing novel medicinal compounds.

PP-43

Synthesis and Characterization of New Azo Ester Derivatives: Influence of Lateral and Terminal Group Variations

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Abstract:

A new azo-ester linkage homologous series was synthesized to understand the effect of structural change on mesomorphism. This homologous series was compared with well reported similar homologous series. This series contains 12 homologues. Among 12 homologues C_5 to C_{16} homologues show smectic phase while others are non-mesomorphic in nature. The study of mesomorphism and non-mesomorphism were carried out with the comparison and some important conclusions were drawn. All homologues of the series were confirmed by different analytical techniques like ^1H NMR, ^{13}C NMR IR, and Mass spectrometry. Transition temperature of all synthesised homologues was carried out by polarizing optical microscope with hot stage and also it was confirmed by DSC analysis.

PP-44

Nutritional Values of Parsley Plant

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Abstract:

Parsley (*Petroselinum crispum*) is a biennial herb belongs to the carrot family (Apiaceae). It is well known species and vegetables. its herb and root are widely known for their effect of digestion, stomach, kidney, blood and liver. It has been cultivated throughout the world and used for thousands of years for food flavoring, essential oil applications and in traditional medicines. Mostly parsley plants are rich in carbohydrate, protein and fiber but are also rich in vitamins & minerals. *Petroselinum crispum* contains many antioxidant properties, Flavonoids, essentials oils and Phenolic compounds. Carotenoids, vitamin A, B and C and minerals like iron, zinc calcium, phosphorous are also present. An aqueous extract *Petroselinum crispum* show that the presence of steroids, alkaloids, Phytosterol, tannins, saponins and etc. Leaves, seeds and roots of *Petroselinum crispum* are used as Hepatoprotective, brain protective, anti-diabetic, anti - hypertensive effects anti platelet, anti- inflammatory, anti-tumor allergy and many more diseases. This research put a light on bioactive and nutraceuticals properties of *Petroselinum crispum*. Further research on the nutrient contains of the plant was determined by various solvents and phytochemicals screening, antioxidant & antimicrobial activities of plant.

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PP-45

Heterocyclic Compound Synthesis and Derivatives Development with Prediction of their Application

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Abstract:

Heterocyclic compounds have been a cornerstone of medicinal chemistry due to their diverse biological activities and therapeutic applications. In this study, we designed and synthesized a series of heterocyclic compounds with potential biological activity. Our approach involved the combination of molecular modeling, synthetic chemistry, and in vitro biological evaluation. The synthesized compounds were characterized by NMR, IR, and mass spectrometry. Preliminary biological screening revealed promising antimicrobial and anticancer activities in several compounds. Further optimization and structure-activity relationship (SAR) studies are underway to enhance the potency and selectivity of these compounds. Our findings demonstrate the potential of heterocyclic compounds as leads for the development of novel therapeutics.

PP-46

Estimation of Heavy Metal Accumulation and Phytochemical Profiling of Brassica juncea (L.)

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Abstract:

Heavy metal emissions into the environment are mostly caused by human activity, such as automobile emissions, industrial processes, and a rise in forest fires because of global warming (Stanton et al., 2022; Huang et al., 2020; Faizan et al., 2021). Phytoremediation, is utilizing plants to detoxify soils, emerges as a sustainable result. Understanding heavy metal accumulation in Brassica juncea (L.) Czern. and their secondary metabolites is crucial for environmental management and remediation efforts. Plant samples were collected and heavy metal element concentrations were determined using Atomic Absorption Spectroscopy. Qualitative assays were conducted to identify active compounds in alcoholic extracts. The findings indicate the existence of several bioactive substances, including carbohydrates, alkaloids, amino acids, proteins, saponins, phenolic compounds, flavonoids, and tannins, while phytosterols were found to be absent. In Brassica juncea (L.) Czern., AF value of 1.36 in control, 11.29 in 100 ppm concentration of Ni heavy metal and 6.31 in 100 ppm as heavy metal showed. Nickel absorbs heavy metal into soil more than arsenic, so nickel has a higher Accumulation value. The study demonstrated significant differences in heavy metal accumulation and chemical profiles among plant highlighting their potential for phytoremediation.

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PP-47

Evaluation of Phenolic and Flavonoid Content from Weeds

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Abstract:

Phyllanthus niruri L. and Chloris barbata Sw. are used for their allelopathic effects on various plants, both weeds produce naturally occurring chemical compounds. The current investigation focused on Phyllanthus niruri L. and Chloris barbata Sw. and measured their total phenolic and flavonoid content. Phenols and flavonoids were determined using the Folin Ciocalteau and aluminum chloride methods, respectively. Both weeds had a positive reaction to the presence of secondary metabolites, indicating it can be employed as herbal components. Both weeds have significant phenol and flavonoid values. Phyllanthus niruri L. had a higher number of phenols and flavonoids than compare to Chloris barbata Sw., making it more advantageous to employ these medicinal plants as natural medicine rather than pharmaceutical products. Both of the selected weeds grow in various parts of the world, their medicinal properties used in many kinds of applications.

PP-48

Transition Metal Catalyzed C(sp_2) Olefination of Coumarins with Activated Olefins

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Abstract:

Natural products (NPs) rich source of therapeutic agents plays an unprecedented role in drug discovery. C-H activation well flourished in last two decades has profound role in late-stage functionalization of complex NPs. Coumarin, oxygen containing nucleus consists of benzene ring fused with a lactone (a cyclic ester) well known for their numerous biological activities. The heterocyclic core containing C3 and C4 sites which were well explored for numerous nucleophilic as well as electrophilic reaction but very few advancements have been achieved on benzenoid core. To this end, we developed a novel protocol for regioselective olefination of C(sp2) position of coumarins with activated olefins under Ru(III) catalysis. The developed protocol described wide substrate scope for both coumarins and olefin coupling partners in moderate to excellent yields. Further, the cleavage of directing group under acidic conditions resulted into functionalized naturally occurring umbelliferon derivatives.

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OP-49

Characterization of Syntaxin-1 Like Molecule from Pathogenic Protozoan Parasite Entamoeba Histolytica

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Abstract:

The N-ethylmaleimide-sensitive fusion protein (NSF) and soluble NSF attachment receptor (SNARE) molecules play critical roles in vesicle fusion and neurotransmitter release, with their dysfunction being implicated in various neurodegenerative diseases. Invasive amoebiasis, caused by Entamoeba histolytica, is characterized by the secretion of extracellular vesicles (EVs) that release several virulence factors. One such factor is a syntaxin 1-like molecule, a SNARE protein identified in E. histolytica. The characterization of this syntaxin 1-like molecule has been approached using both in silico and in vitro methods. BLAST analysis reveals conserved regions, which allowed for the prediction of its structure, subsequently validated through root mean square deviation (RMSD) calculations and Ramachandran plot analysis. The identification of heptad repeats indicates the presence of a coiled-coil domain, and the corresponding sequence has been amplified for further cloning. The full-length syntaxin 1B protein has been successfully expressed, and protein purification is currently ongoing. Protein-protein interactions between syntaxin and its interacting partner will be done through invitro method.

PP-50

Development of AIE Active Pyridinium-Based Ionic Liquids for Selective Detection of Explosives

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Abstract:

In this study, we present the synthesis of a pyridinium-based ionic liquid designed for the detection of metal ions, explosives, and white light emission (WLE) properties. The unique chemical structure of the pyridinium cation, combined with the ionic liquid's inherent stability and tunability, provides a versatile platform for the selective recognition of target analytes. The ionic liquid was evaluated for its ability to detect and distinguish different metal ions, including transition and heavy metals, as well as its sensitivity to explosive compounds. This study highlights the promising prospects of pyridinium-based ionic liquids in advanced sensing technologies, offering a highly efficient and adaptable tool for real-time monitoring of hazardous materials.

PP-51

Relocating NSAID into Endoplasmic Reticulum Induces ER Stress-Mediated Apoptosis in Cancer Cells

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Abstract:

The endoplasmic reticulum (ER) is a vital subcellular organelle that orchestrates numerous essential biological processes, including protein synthesis and processing. Disruption of ER function can lead to ER stress, a condition closely associated with the progression and development of cancer. Consequently, inducing ER stress in cancer cells has emerged as an unconventional yet promising therapeutic approach. However, selectively targeting the ER within cancer cells remains a significant challenge. To address this, we have designed and synthesized a novel small molecule library composed of nonsteroidal anti-inflammatory drugs (NSAIDs), fluorescent probes, and ER-targeting moieties. Through screening the library in cancer cells, we identified a promising compound: an ibuprofen derivative conjugated with a dansyl group as dual fluorescence tag and ER-targeting moiety. This ibuprofen derivative successfully localized into the ER of HCT-116 colon cancer cells within 3h, induced ER stress by upregulating key stress markers such as CHOP, GRP94, IRE-1α, PERK, and Cas-12, while simultaneously inhibiting Cox-2. The resulting ER stress triggered autophagy by upregulating Beclin and LC3-II/LC3-I as autophagy markers, followed by apoptosis, culminating in significant cancer cell death, particularly when combined with Bafilomycin A,10hydroxycamptothecin and obatoclax. This NSAID-based ER stress inducer provides a powerful tool for exploring the chemical biology of NSAIDs in the ER and holds great potential for advancing ER-targeted cancer therapies in combination with other anti-cancer drugs.

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PP-52

Routing NSAIDs into the Golgi Apparatus Induces Autophagy and Apoptosis in Cancer Cells

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Abstract:

The Golgi apparatus (GA), a critical sub-cellular organelle, plays a pivotal role in numerous biological signaling pathways, including the post-translational modification of proteins and their secretion to various cellular destinations. Dysregulation of GA function is implicated in the development of several diseases, including cancer. As a result, detouring clinically approved drugs into the GA for enhanced anti-cancer effect remained a major challenge. To address this, herein, we designed and synthesized NSAID-based conjugates incorporating a fluorophore (1,8-naphthalimide) and a Golgi-homing moiety (phenylsulfonamide). Screening these conjugates in cervical (HeLa) and colon (HCT-116) cancer cells identified a particularly promising candidate: the Ibuprofen-1,8-naphthalimide-phenylsulfonamide conjugate (7a) which exhibited significant cytotoxicity against HCT-116 cells. Interestingly, compound 7a self-assembled into nanoscale petal-like structures in water and efficiently homed into the GA within 30 min to induce morphologiocal damage to the Golgi apparatus. Compound 7a mediated GA damage increased the expression of Beclin and LC3-I/II proteins to induce autophagy which was further inhibited by chloroquine (CQ) leading to remarkable HCT-116 cell death in combination with 7a with IC_{50} = 0.19 μM. Moreover, compound 7a triggered apoptosis by downregulating anti-apoptotic Bcl-2 and Cas-3 proteins in HCT-116 cells, while demonstrating no toxicity towards non-cancerous human retinal pigment epithelial cells (RPE-1). This Ibuprofen derivative (7a) holds promise as a valuable tool for illuminating the chemical biology of the GA in cancer cells and as a potential candidate for anti-cancer therapy.

PP-53

A Diversity-Oriented Multicomponent Approach to Novel Fused Nitrogen Heterocycles Using 6-Aminoindazole

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Abstract:

We present a novel, efficient, eco-friendly so, no chemical strategy for synthesizing fused nitrogen hetero cycles via Bronsted acid-promoted, one pot multi component reactions (MCRs). This method involves the rapid assembly of 6-aminoindazole, arylaldehydes, and 1,3-cyclodione derivatives (barbituric acid, dimedone, and 1,3-dimethyl barbituric acid) under mild and identical reaction conditions. The approach deliver sadiverserange of highly functionalized heterocyclic frameworks, including 11-phenyl-1,6,7, 11 tetrahydro-8H-pyrazolo[3,4-f]pyrimido [4,5-b]quinoline-8, 10(9H)-di one, 8,8-dimethyl-11-phenyl-1,6,7,8, 9,11 hexahydro-10H-pyrazolo[3,4-a]acridin-10-one, and 7,9-diphenyl-1,6,7,9-tetrahydro - 2'H – spiro [pyrazolo [3,4f] quinolone-8,5'-pyrimidine]-2',4',6'(1'H,3'H)–tri one derivatives. The molecular structure so of these compounds we are unambiguously confirmedthrough ^{1}H-NMR, ^{13C}-NMR spectroscopy and single – crystal X - ray diffraction (SC-XRD) analysis. Additionally, control experiments provided valuable mechanistic in sights in to the reaction pathway. This protocol stands out for its efficiency, high yields, and broad functional group tolerance, making it a versatile tool for diversity –oriented synthesis in modern heterocyclic chemistry.

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PP-54

Small Molecule-Mediated Photothermal Therapy Induces Apoptosis in Cancer Cells

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Abstract:

A small molecule library with aromatic substituted-3-methoxy-pyrrole and 2-(3-cyano-4,5,5-trimethylfuran-2(5H)-ylidene) malononitrile was synthesized. One member (7H) formed <100 nm nanoparticles, raising temperature under 740 nm NIR light. In HCT-116 colon cancer cells, 7H localized in lysosomes and lipid droplets, inducing a photothermal effect, generating ROS, and triggering apoptosis via Caspase-3/9 cleavage, offering promise for non-invasive cancer therapy.

Keywords: Photothermal effect, Lipid droplets, Lysosomes.

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PP-55

Organocatalytic Asymmetric Synthesis of α-Arylcyclohexenones from Arylacetones and α,β-Unsaturated Aldehydes

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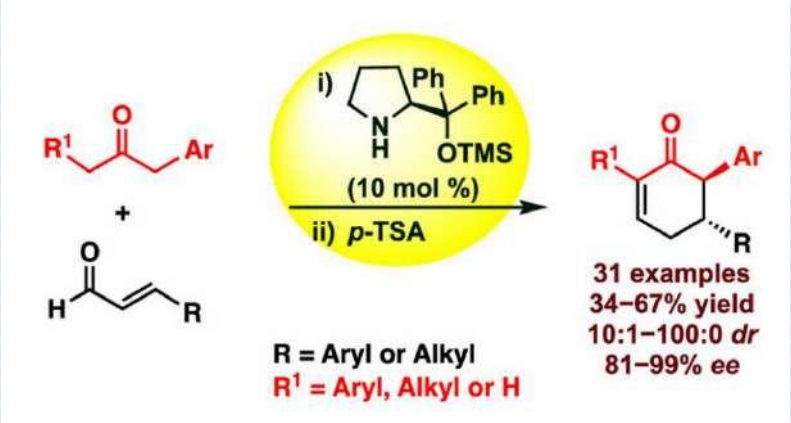
Abstract:

Chiral cyclohexenone is a common structural motif in natural products and pharmaceuticals.1 Asymmetric synthesis of cyclohexenones via Michael addition followed by aldol condensation (Robinson annulation) is mainly restricted to the reaction between ketones (a ketone and an α,β unsaturated ketone). In spite of the fact that α-arylcyclohexenones were used as an intermediate for the total synthesis of natural products,2 there are very few reports known for the racemic or asymmetric synthesis of α-arylcyclohexenones.3 Here in this, a general methodology for the asymmetric synthesis of α-arylcyclohexeneones from arylacetones and α,β-unsaturated aldehydes catalyzed by diphenylprolinol silyl ether followed by p-TSA-mediated cyclization is developed. A variety of arylacetones and α,β-unsaturated aldehydes were successfully converted to α-arylcyclohexeneones in 34–67% yield, 10:1–100:0 dr, and 81–99% ee. The scalability of this methodology by a gram-scale synthesis and their utility by converting the product to the corresponding epoxide, alcohol, and diol are demonstrated.[4]



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PP-56

Alcohol Halogenation using Thiourea: A Mild and Effective Strategy

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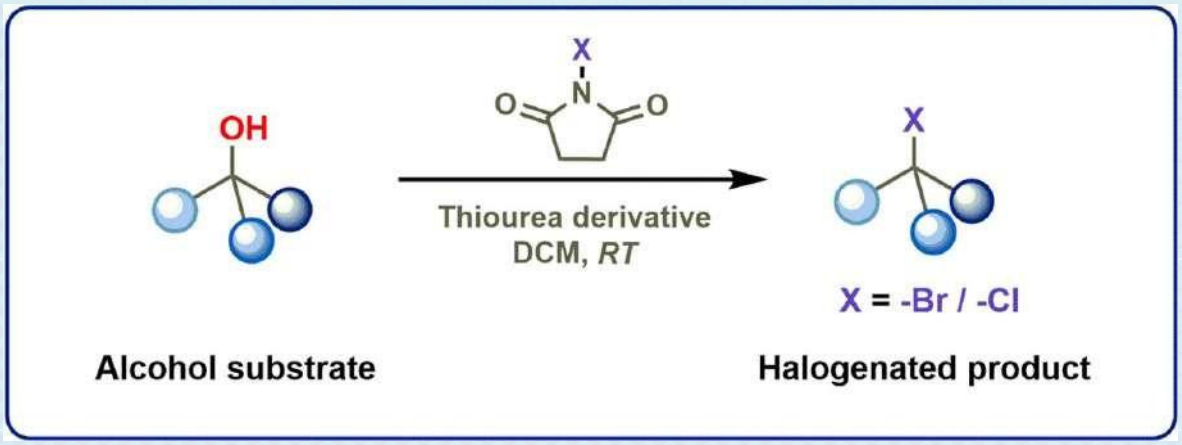
Abstract:

Halogen-containing compounds are essential in pharmaceuticals, agrochemicals, and polymer industries, yet traditional halogenation methods often suffer from sustainability and efficiency challenges. We present a direct, one-step methodology for transforming alcohols into alkyl halides (alkyl bromides and chlorides) using thioureas and N-halo-succinimides (NXS) as halogenation source under mild conditions. Critical to success is sub-stoichiometric thiourea and its derivatives, which suppresses undesired oxidation pathways while directing reactivity toward halogenation. Mechanistic studies (EPR, isotopic labeling) support a radical-based pathway, distinct from classical activation strategies. Key advantages include operational simplicity, low-cost reagents, scalability, and enhanced atom economy compared to traditional methods (e.g., Mitsu Nobu or Appel reactions). This approach offers broad substrate compatibility, including sterically hindered alcohols, while maintaining cost-effectiveness and atom efficiency. The recyclability of byproducts further enhances its environmental appeal, making this method a promising alternative for both academic research and industrial applications.



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PP-57

Synthesis and Evaluation of Hydrazides via SNAr and Cyclization: Molecular Docking, DFT, and ADMET Investigations

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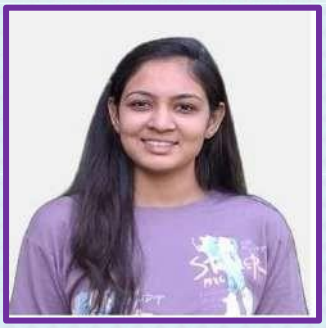
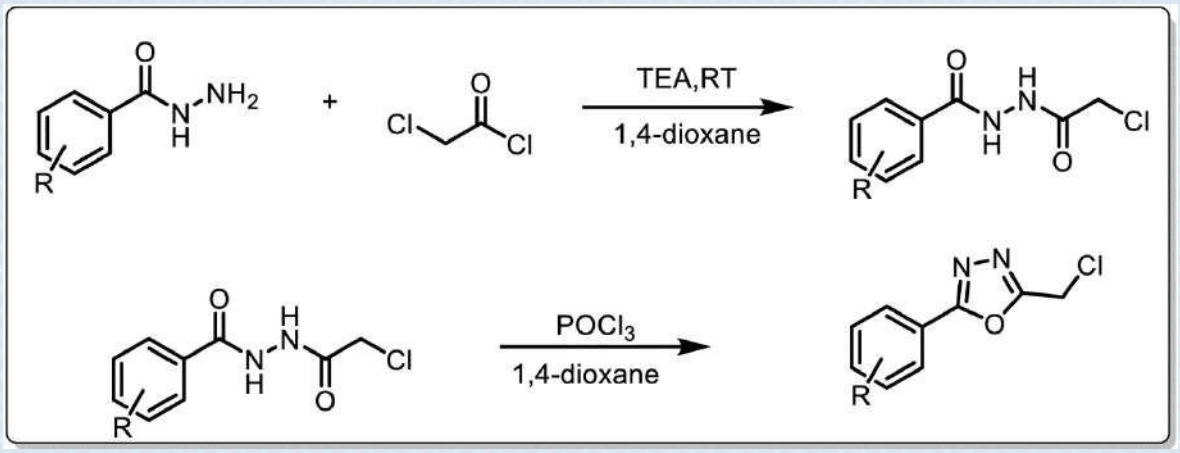
Abstract:



Oxadiazole derivatives are known for their diverse pharmacological properties, including anti-inflammatory, antiallergic, antipsychotic, antimicrobial, antitumor, and antiviral activities. In our research, we successfully synthesized oxadiazole derivatives from various hydrazides. The synthesized compounds were characterized using thin layer chromatography (TLC), UV spectroscopy, mass spectrometry, and melting point analysis to confirm their purity and structural integrity. Our synthetic approach began with the N alkylation of hydrazide using chloro-acetyl chloride (CAC) and triethylamine in dioxane solvent. This initial product was subsequently cyclized in the presence of phosphorus oxychloride using dioxane as the reaction medium to obtain the desired oxadiazole derivatives. Given the significance of oxadiazole derivatives in modern drug discovery, the development of novel synthetic strategies and the evaluation of their biological activities remain crucial areas of ongoing research.



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PP-58

Synthesis of Quinoline-Based Chalcone Derivatives via SNAr Reaction for their Potential Anticancer Activity

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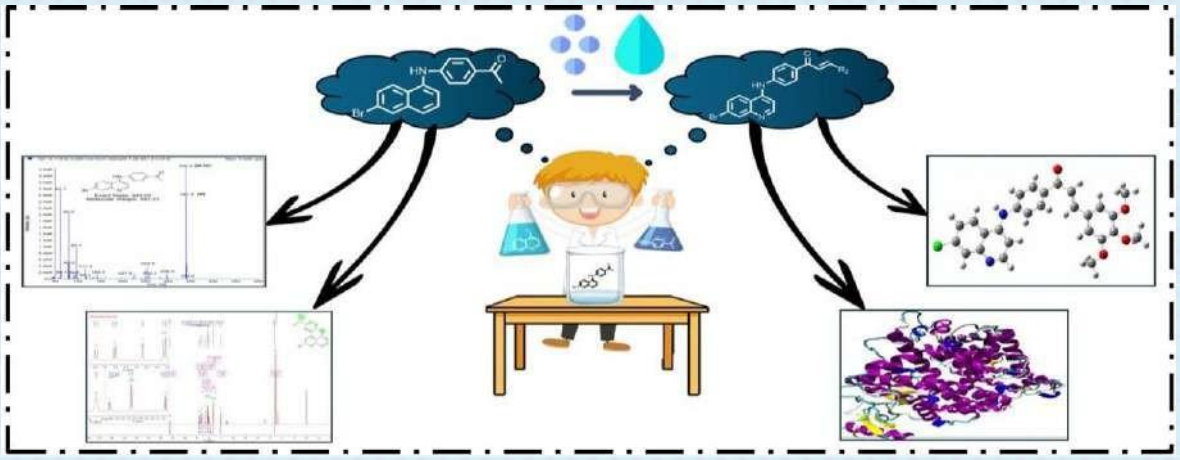
Abstract:

This study focuses on making quinoline-based chalcone compounds using a Nucleophilic Aromatic Substitution (SNAr) reaction between quinoline and aromatic amine. The resulting intermediate 1-(4-((7 bromoquinolin-4-yl)amino)phenyl)ethan-1-one was used to form 16 chalcones derivatives using various aldehydes. We have optimised the process using acidic as well as basic conditions to improve the yield. The synthesized products were characterized by mass spectrometry and nuclear magnetic resonance (NMR) spectroscopy. DFT study of the Reaction was performed, alongside to gain insight for structural relations in-silico ADMET study for product with no violation of the Lipinski's rule suggesting drug-like behavior of synthesized intermediates. The docking study of molecules provides good protein interaction compared to the standard compound. We aim to perform a biological study to predict biochemical effectiveness.



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PP-59

DFT insight and Metal Complex study on Schiff Bases of 5 Chloro-salicylaldehyde

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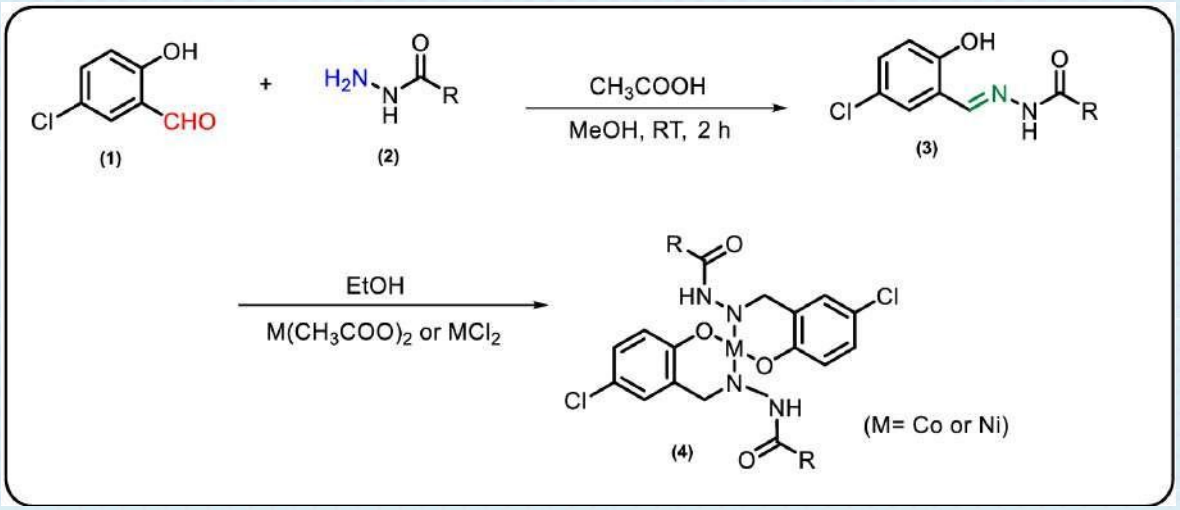
Abstract:

Schiff bases contain imine group, which serves as a strong ligand, enabling coordination with metal ions to form metal complexes, which are useful in catalysis, sensor technology, and drug development. The present work focuses on the synthesis of Schiff based derivatives followed by formation of metal complex. We have synthesized 6 Schiff bases using 5-Chlorosalicylaldehyde and combining it with various benzoic acid hydrazides. Synthesized compounds were analysed by TLC, melting point, DFT and UV spectroscopy. Additionally, we have formed metal complex using synthesized Schiff base derivatives with cadmium and other metal ions. The addition of metal ions to the Schiff base can enhance both the stability and reactivity of the compound, offering a foundation for the development of potential antifungal and antimicrobial agents. We also employed DFT study to analyse the reaction pathways.



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PP-60

Synthesis, Characterization and UV study of 5-Chloro Salicyaldehyde Based Schiff Base Metal Complexes

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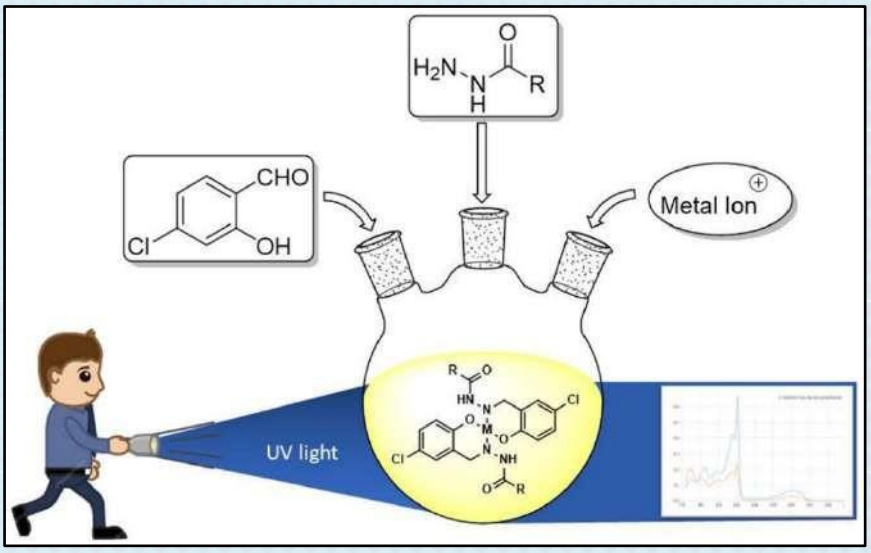
Abstract:

Schiff bases are widely known for its numerous activity such as antimicrobial, antifungal, antioxidant and anticancer. We have synthesized five Schiff base derivatives using 5 chloro-salicylaldehyade and various benzoic acid hydrazides. We characterized analyzed compounds using thin layer chromatography (TLC), UV spectroscopy, mass spectroscopy and melting point. Further, we have employed various metal ions to form metal complexes using Schiff base as ligand. The imine group in these compounds acts as a key pharmacophore, and may contributing significantly to their biological activity. The metal center in Schiff base-metal complexes may plays an essential role in enhancing the compound's stability and biological function. These complexes may have demonstrated promising potential in medicinal chemistry, with applications ranging from enzyme inhibition to targeted drug delivery systems.



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PP-61

A Complete Summary of The Present State of Heavy Metals in Groundwater in Gujarat, India.

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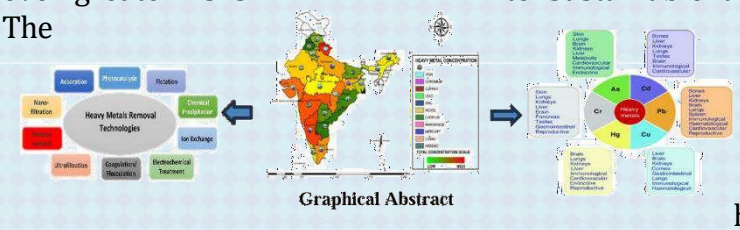
Abstract:

Gujarat's economy has grown rapidly, which has significantly increased energy consumption and thus has suffered major environmental pollution. In Gujarat, heavy metal pollution has become one of the main environmental problems among other types of pollution. In Gujarat, groundwater is primarily used for agriculture and drinking water, and metal contamination is frequently reported. The concentration of heavy metals in the environment determines their toxicity and how toxic they are; as the concentration rises, the potential of the groundwater and soil decreases. Besides natural sources, anthropogenic activities such as extensive use of fertilizers, cement and chemicals industries, oil and petroleum refineries, metal processing units, thermal power plants and port activities can be identified as prime sources of metal contamination in Gujarat. Relatively high concentrations of nutrients and metal ions indicate that the water is in very dire condition, which will ultimately affect the flora and fauna of this ecosystem. Different regions of Gujarat have been reported to have the presence of heavy metals and metalloids (As, Cd, Co, Cr, Fe, Hg, Mn, Mo, Ni, Pb, and Zn) at different concentrations. Thus, the current research offers a snapshot of the causes and conditions of heavy metal contamination in the different regions of Gujarat. However, heavy metal ion pollution has not garnered enough attention despite posing even greater risks to sustainable development and public health. The aim of the study is to investigate feasible solutions to Gujarat's heavy metal pollution. This study offers baseline information on groundwater hydrochemistry and the effects of ongoing human influence in Gujarat. Additionally, it offers some recommendations and mitigation strategies to minimize heavy metal pollution.



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PP-62

Quinoline - Chalcone Hybrids as Potential: Design, Synthesis, DFT, ADMET and Docking Study

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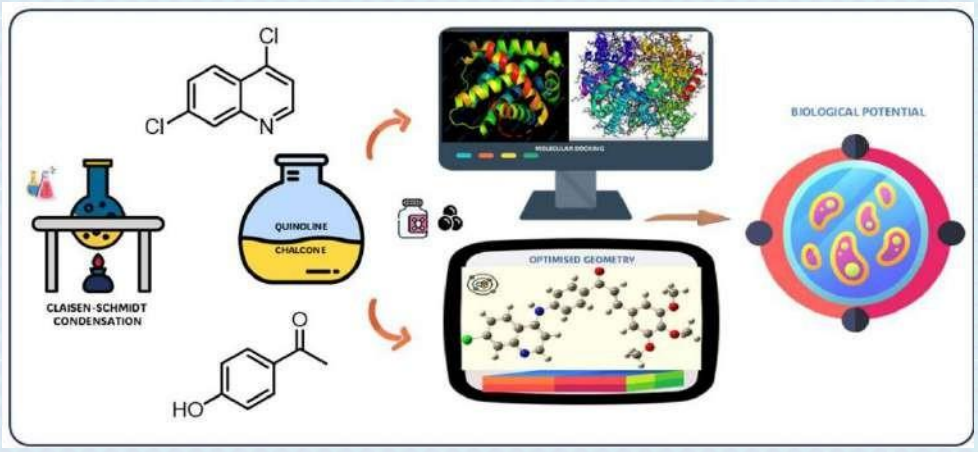
Abstract:

Chalcones are privileged scaffolds in medicinal chemistry, they have properties like fighting against cancer, bacteria, and inflammation. Our study presents the synthesis of quinoline-fused chalcones utilizing Aromatic Nucleophilic Substitution (SNAr) were step-1 followed by chalcone synthesis step-2 using both acidic/basic conditions. 4-(4 Acetylphenoxy)-7-chloroquinoline was prepared by the reaction between 4,7-Dichloro quinoline and 4- hydroxy acetophenone in KOH and DMF as polar aprotic solvent. We were synthesizing Eight chalcone derivatives. The synthesized compounds were initially Monitored by TLC and staining reagents. followed by detailed structural characterization using spectroscopy techniques such as Mass, NMR, IR, UV-Vis. To evaluate the pharmacokinetic profile and oral drug-likeness, an in-silico ADME analysis was conducted along with DFT calculations and molecular docking studies. ADMET study Revealed no violation on Lipinski's rule in over derivatives Because of their advantageous pharmacokinetic properties, The produced molecule is expected to exhibit moderate biological activity.



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PP-63

Applications of Fluorinated Benzothiazoles and Benzimidazoles Scaffolds in Drug Discovery

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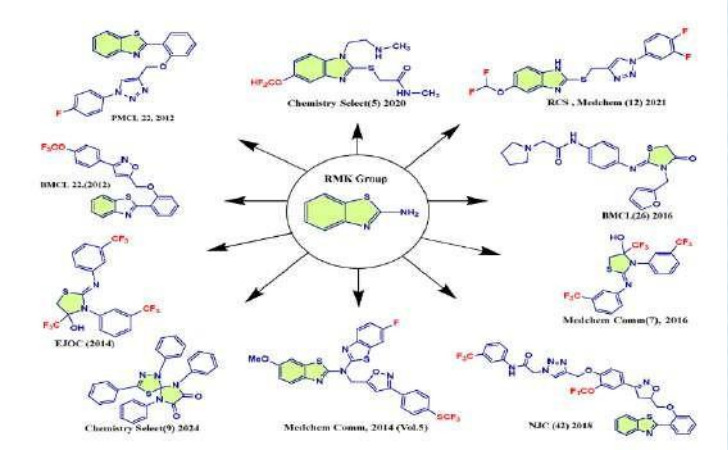
Abstract:

Fluorinated compounds are important pharmacophore due to their high electronegativity, enhancing biologically important properties like acidity, lipophilicity, binding affinity and metabolic stability. These analogs show promising activities like Broad spectrum Anti-Biofilm, Telomerase inhibitors, G-Quadruplex DNA binders along with potent Anti-Microbial agents. Pharmaceutical industry has extensive range of heterocyclic bio active molecules leading to drug discovery. These privileged scaffolds form special frame work in drug molecules that are modified to deliver its chemical applicability as a "Hit molecule". Our research group synthesized many biological active Benzothiazoles and Benzimidazoles scaffolds, which show in scheme- 1



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PP-64

Design and Synthesis of Bromo Indazole-Chalcones: Computational and Drug-Like Property Assessment

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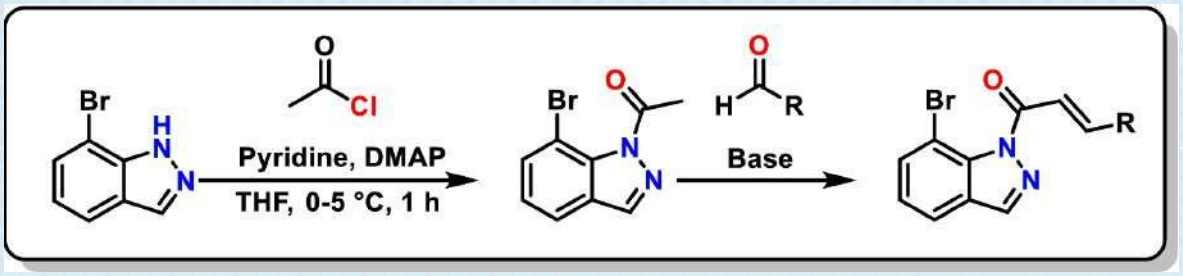
Abstract:

Indazole-based chalcones have emerged as promising scaffolds in anticancer drug discovery due to their diverse pharmacological properties. In this study, 7-bromo indazole-chalcone hybrid was designed, 7 derivatives were synthesized, and characterized using advanced spectroscopic techniques. The synthetic strategy involved the N-acetylation of 7-Bromo-1H-indazole with acetyl chloride to afford 1-(7-bromo-1H-indazol-1-yl)ethan-1-one, followed by a Claisen Schmidt condensation with a substituted aromatic aldehyde under basic conditions to yield the chalcone derivatives. Molecular docking studies revealed strong binding affinity and favorable interactions suggesting potential biological activity. Furthermore, in silico ADMET predictions indicated promising drug-like properties, including good oral bioavailability and pharmacokinetic suitability. These findings highlight the therapeutic potential of indazole-chalcone hybrids as anticancer agents. Further structural optimization and biological evaluations are warranted to enhance their efficacy and advance them toward clinical development.



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PP-65

Synthetic Strategies for Indazole-Chalcone Scaffolds: Docking, DFT, and ADMET Analysis

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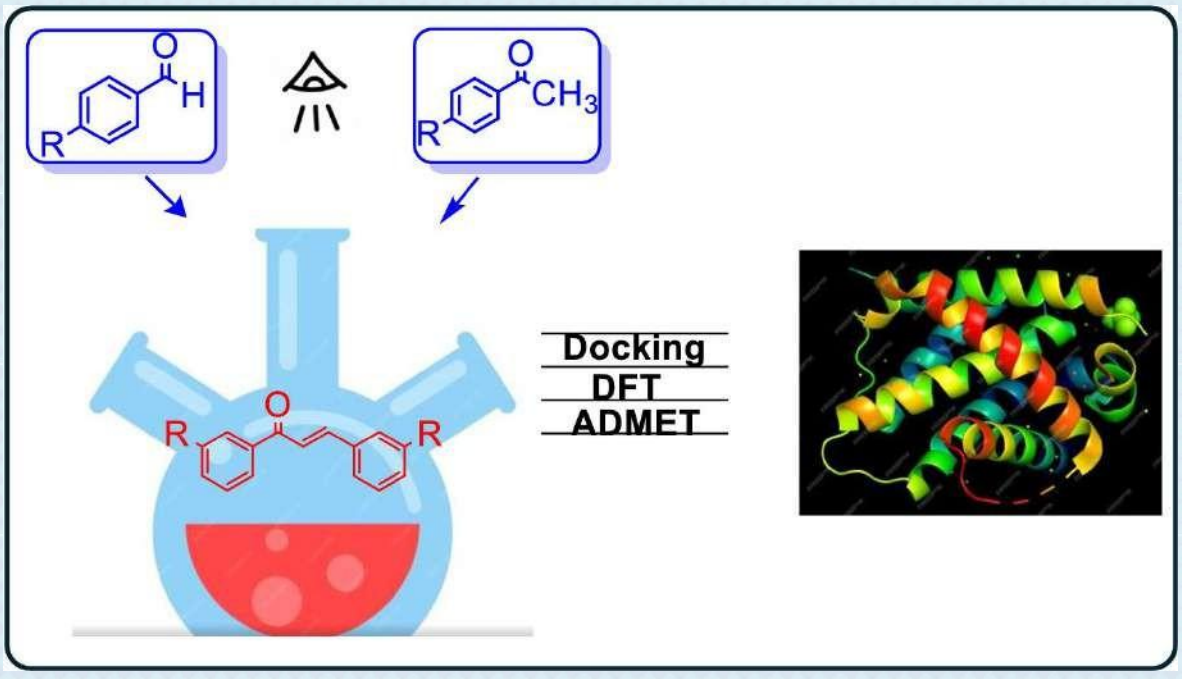
Abstract:

Indazole-based chalcone have gained significant attention due to their diverse pharmacological properties, particularly in anticancer research. In this study, a novel indazole-chalcone hybrid was synthesized and characterized using spectroscopic techniques. The synthesis involved N-acetylation of 6-iodo-1H-indazole with acetic anhydride to form 1 (6-iodo-1H-indazol-1-yl)ethan-1-one, followed by a Claisen-Schmidt condensation reaction between the indazole-containing ketone and an aromatic aldehyde under basic conditions. To further understand the molecular interactions, docking studies were conducted, revealing strong binding affinity and favorable interactions. Additionally, in silico ADMET predictions indicated good oral bioavailability and drug-like properties, suggesting its potential for further drug development. Overall, this highlights the therapeutic potential of indazole-chalcone hybrids as promising anticancer agents, warranting further exploration through advanced biological studies and structural modification to enhance efficacy.



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PP-66

Synthetic Approaches on Methyl 2-oxoindole-6-carboxylate Linked Chalcone: Computational Insight and Biological Application

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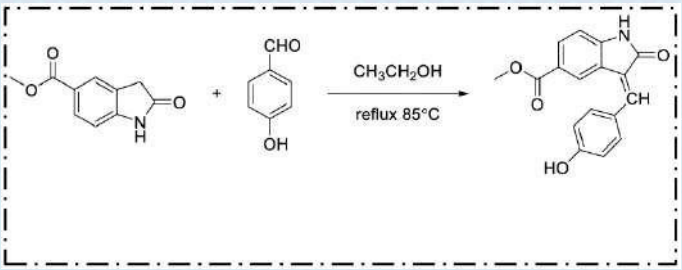
Abstract:

In the chalcone reaction of methyl 2,7-dihydro-1H-pyrrolo[1,2-a] imidazole-1-carboxylate with 4-hydroxybenzaldehyde in ethanol at 85°C through an aldol condensation occurs, resulting in the formation of an α, β-unsaturated ketone (chalcone derivative). One of the most important steps in the synthesis of chalcones is the combination of an aldehyde and a ketone, leading to the formation of a crucial carbon- carbon double bond. Chalcones, a class of aromatic ketones, serve as key intermediates in organic synthesis and exhibit various biological activities, including Anticancer, Antibacterial, Antifungal, Anti-inflammatory, Antioxidant, and Antiviral properties. These bioactivities make chalcones valuable in pharmaceutical and medicinal chemistry, contributing to the development of new therapeutic agents. It provides a 90-95% good to outstanding yield revelation. All of the produced compounds were thoroughly characterized using mass spectroscopy, TLC, and TLC spraying Reagents. A thorough investigation using Density Functional Theory (DFT) can be carried out to find out how different catalysts and solvents affect the yield of chalcone reactions.



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PP-67

An Overview of the Geochemistry of Fluoride in Groundwater from Gujarat, India

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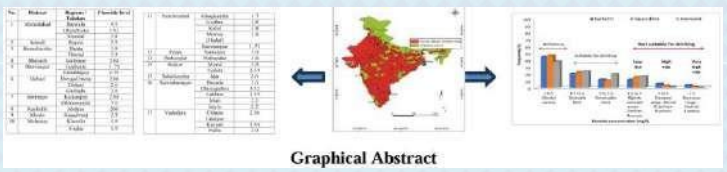
Abstract:

Extensive use of groundwater for household, agriculture, and industrial use has resulted in significant changes in its chemical composition. The state of Gujarat has witnessed rapid industrialization, urbanization, and population growth over the past few decades which has increased the environmental stress. Due to toxicity related issues, and accumulation in human bodies, fluoride contamination in groundwater has gained considerable attention in recent years. The max. amount of fluoride that is allowed in drinking water by the WHO is 1.5 mg/L, which is within the bounds of the national standard. Fluoride contamination of groundwater is understood to consist of fluoride conc. higher than 1.5 mg/L because of geogenic or anthropogenic activity. Fluorite (CaF2), cryolite (Na3AlF6), apatite, biotite, and amphiboles are some examples of F-rich minerals that are formed by geological processes, whereas industrial waste, extensive use of fertilizer, and brick kilns are examples of anthropogenic source. Fluoride is generally viewed as a substance that is essential for human health in low concentrations. Fluorosis (skeletal-dental) is a dangerous complication generated by exposure to high F- concentrations. Gujarat is one of the most severely affected states with fluorosis. This study provides a thorough overview of fluoride contamination in the groundwater resources of Gujarat. Another specific aspect covered in this study is the effect of fluoride on different human organs and systems, including the urinary, renal, central nervous, gastric, cardiovascular, brain, and reproductive systems. This study unravels several methodologies employed to remove fluoride from water, including reverse osmosis, electrocoagulation, Nano filtration, adsorbents and precipitation/coagulation. We believe this article will help to identify fluoride affected areas of Gujarat and would provide a guideline to the policymakers to consider this critical issue and adopt safe alternatives for drinking water.



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PP-68

Synthesis, Optimization and Computational Insight of Indole Acetic Acid Fused Chalcone Derivatives

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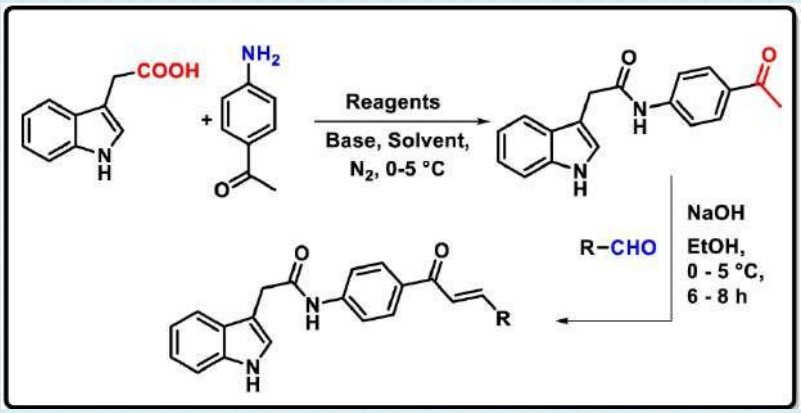
Abstract:

Chalcone derivatives fused with indole acetic acid have emerged as promising molecular frameworks due to their diverse pharmacological applications, particularly in anticancer and anti-inflammatory drug development. This study focuses on the synthesis, optimization, and computational analysis of indole acetic acid fused chalcone derivatives. The synthesis was carried out via formation of amide bond using various conditions followed by Claisen–Schmidt condensation under optimized reaction conditions to achieve higher yields and purity. The structural elucidation of the synthesized compounds was performed using spectroscopic techniques. To gain deeper insights into the stability, reactivity, and biological relevance of these compounds, computational studies were employed. Density Functional Theory (DFT) calculations provide valuable information on the electronic properties and molecular orbitals, while molecular docking studies predict potential interactions with biological targets. The ADMET study was also performed which shows good drug like properties. This work aims to contribute to the development of therapeutic agents by combining experimental and computational methodologies.



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PP-69

Discovery of Novel Small Molecule Inhibitors for Human Tousled-like Kinase 1 (hTLK1) for Prostate Cancer Therapy

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Abstract:

Kinases are essential for maintaining the genomic stability and their modifications often end up with initiation and metastasis of cancer. The Human Tousled-like kinases (TLKs) are a set of serine-threonine kinases that exhibit divergent role during the DNA damage response and repair pathway (Figure1). The TLK1>Nek1>ATR>Chk1 axis is actively involved in Androgen-deprived therapy (ADT) treated prostate cancer (PCa), thereby enhancing drug resistance and promoting tumor aggressiveness. TLK1 knockdown would eliminate the proper functioning of cells, reduced cell viability which in turn align the cell towards apoptosis. Despite being identified as a promising druggable target yet none of the molecule has received approval as a marketed drug. However, several phenothiazine and indole-based TLK1 inhibitors has been reported but lacks selectivity. To enhance their potency, using ring bioisotere strategy, we have designed novel series of indazole-based TLK1 inhibitors. Based on our previous understandings and reported crystal structure of TLK2 (shares 84% structural similarity), homology model of hTLK1 was constructed via Schrodinger software package. Based on the in-silico studies, a novel series of TLK1 inhibitors were synthesized and their in-vitro potency was checked on panel of PCa cell lines. Based on the preliminary results, further SAR was carried out on different positions of hit molecule. Furthermore, kinase assay and other cellular based studies will be conducted once the hit molecule will be identified.

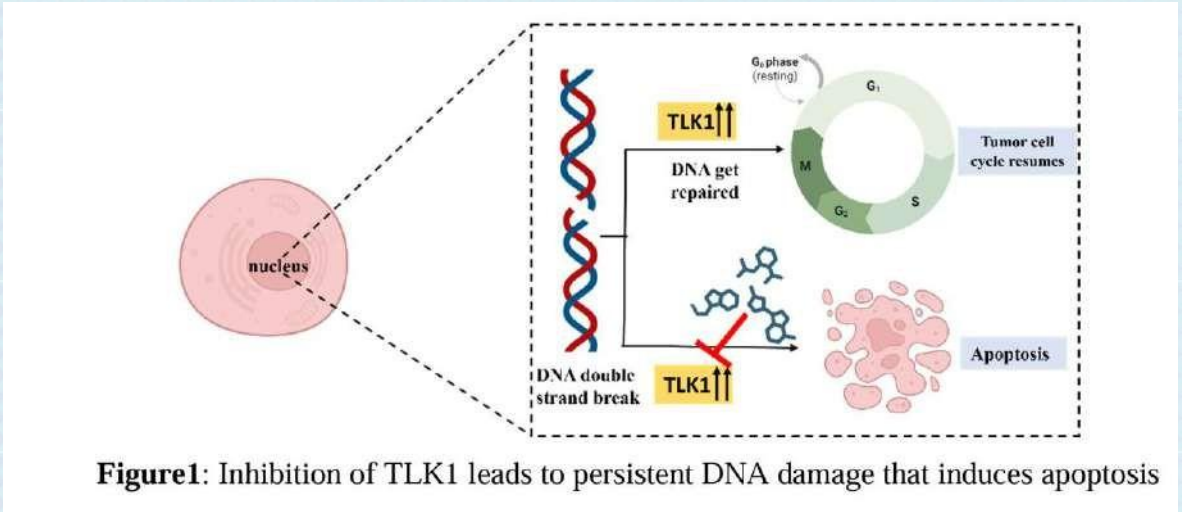

Figure1: Inhibition of TLK1 leads to persistent DNA damage that induces apoptosis

PP-70

Targeting Helicobacter Pylori IMPDH: Designing and Establishing Novel Pyrrolo Pyridine-Based Inhibitors

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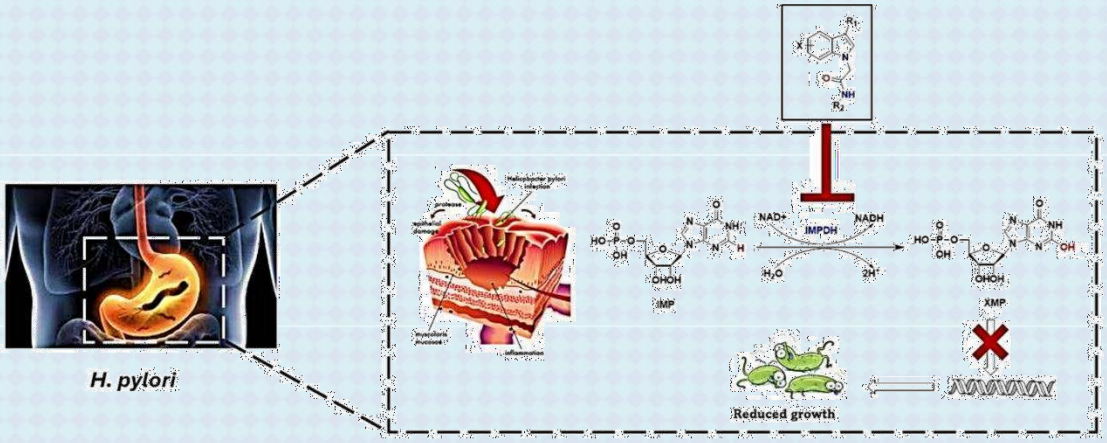
Abstract:

Helicobacter pylori is a Gram-negative bacterium that colonizes the stomach mucosa, producing urease to survive in acidic conditions. It is a major cause of peptic ulcers, and a type I carcinogen linked to gastric cancer. Prevalent in developing countries, it infects nearly 50% of the global population. Rising multidrug resistance necessitates novel therapeutic targets. Inosine-5′ monophosphate dehydrogenase (IMPDH) plays a crucial role in guanine nucleotide biosynthesis and represents a promising target for antibacterial drug development. While benzimidazole- and indole-based inhibitors have been explored for IMPDH inhibition in various species, there is a need for more selective and potent inhibitors against H. pylori IMPDH. In this study, a novel series of pyrrolopyridine scaffold was designed using scaffold hopping to enhance activity and specificity towards Hp IMPDH. The structure of H. pylori IMPDH was generated using AlphaFold based on the reported sequence of the target protein. A series of novel Hp IMPDH inhibitors were synthesized based on in-silico studies, followed by their preliminary biological testing. Structure-activity relationship (SAR) studies and in-vitro assays will be conducted to assess the inhibitory potential of the synthesized molecules after initial hit identification.

Keywords: H. pylori, IMPDH, Pyrrolopyridine, peptic ulcer.



PP-71

Design, DFT Analysis, ADMET Profiling, and Molecular Docking Studies of Pyrido [2,3 d] Pyrimidine Derivatives as ATR Kinase Inhibitors

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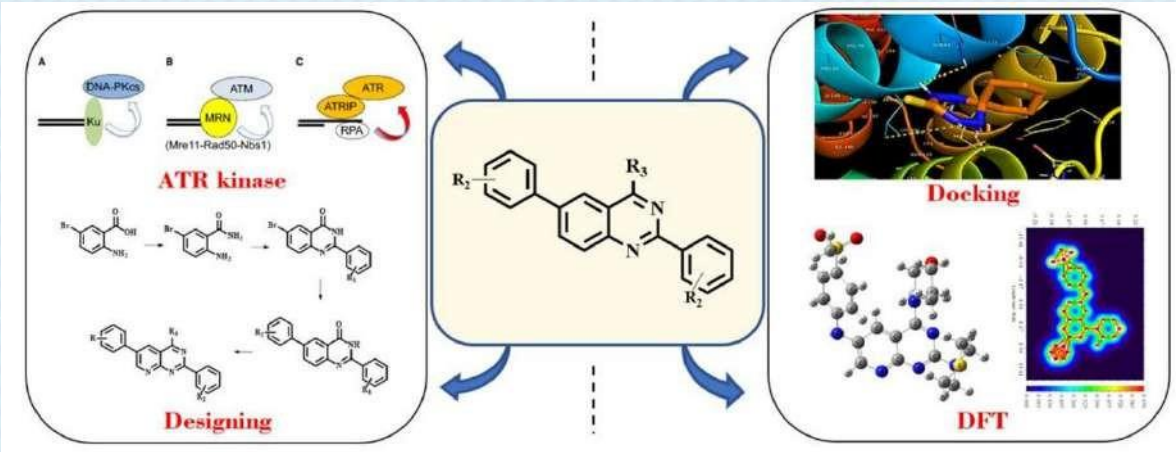
Abstract:

ATR kinase serves a key role in the DNA damage response by activating critical signaling pathways involved in DNA damage repair, particularly in response to replication stress. Since DNA damage and replication stress are primary contributors to genomic instability, selective ATR inhibition has emerged as a promising strategy in cancer therapy. In this study, we designed and synthesized potent and highly selective ATR inhibitors based on pyrido[2,3-d] pyrimidine analogues. Furthermore, density functional theory (DFT) calculations employing the B3LYP functional with the 6 311++G(d,p) basis set are utilized to determine the optimized structures of the synthesized molecules. ADMET analysis was conducted, and the resulting parameters indicated that the designed compounds under investigation exhibit favorable oral bioavailability. Additionally, an in-silico molecular docking study was performed on the designed compounds using the ATR protein homology model based on PI3Kα mutants (PDB ID: 5UK8). The most potent pyrido[2,3-d] pyrimidine analogue was found to be positioned within the active site through multiple strong hydrogen and hydrophobic interactions. The molecular docking results demonstrated that the designed compounds possess a higher binding affinity for PI3Kα mutants, compared to some Phase I, II and III ATR kinase inhibitors. The findings from ADMET and molecular docking studies suggest the potential of these analogues in the development of novel ATR kinase inhibitors.

Keywords: ATR kinase, Pyrido[2,3-d] pyrimidine, DFT, Molecular docking.



PP-72

Design, synthesis and biological evaluation of small molecule inhibitors for Salmonella typhimurium IMPDH

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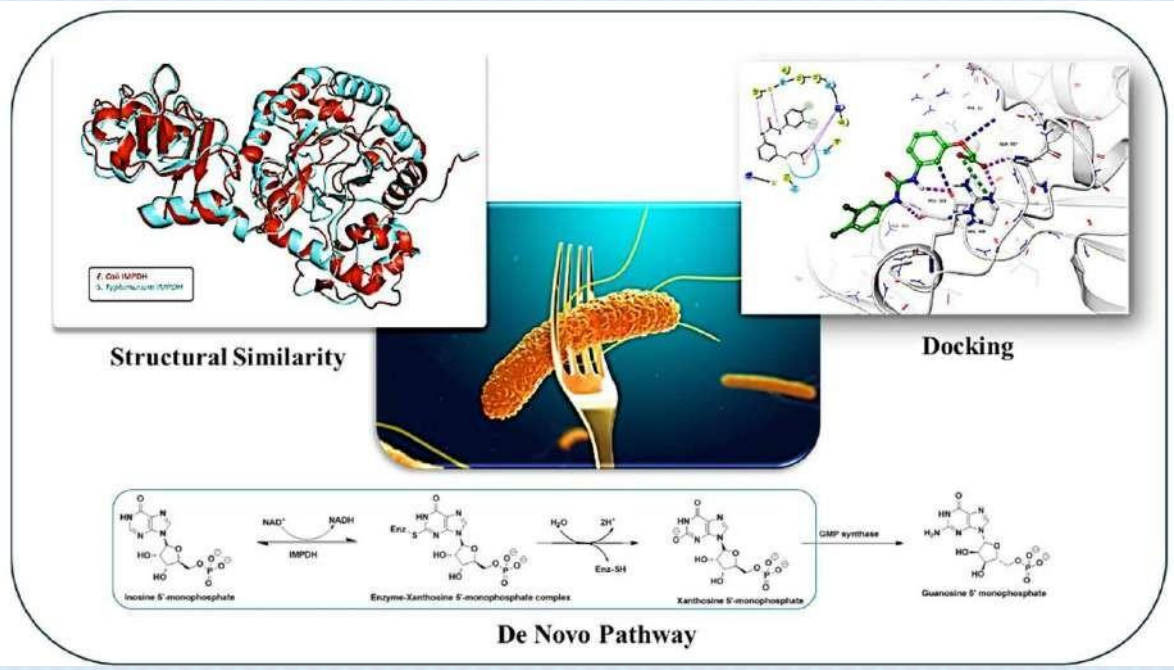
Abstract:

Salmonella typhimurium poses a significant threat to public health due to its role in foodborne illnesses and increasing antibiotic resistance. Notably, Salmonella has gained resistance to commonly used antibiotics, such as ciprofloxacin and azithromycin, underscoring the urgent need for new therapeutic strategies. Inosine-5'-monophosphate dehydrogenase (IMPDH) is a crucial enzyme in Salmonella's metabolic pathways, making it a promising target for novel antimicrobial therapies. This study is focused on the design, synthesis, and biological evaluation of small-molecule inhibitors for IMPDH in Salmonella typhimurium. Utilizing computational modelling and leveraging the high sequence similarity between Salmonella and E. coli IMPDH, potential inhibitors for St-IMPDH were developed. These compounds were synthesized, and testing for their inhibitory activity against recombinant purified St-IMPDH using enzyme assays is the next step in the research. After lead molecule identification, enzymatic characterization and crystallization screening of St-IMPDH will be performed to further understand its kinetic properties and structural dynamics. This research aims to develop innovative treatments against Salmonella infections, addressing the pressing issue of antimicrobial resistance and enhancing global public health safety.



PP-73

Photocatalyzed Organic Transformations by Iridium (III) Dipyrrinato Complexes

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Abstract:

Metal dipyrrinato complexes have been emerged as promising photocatalysts for oxidation applications.1,2 Iridium (III) dipyrrinato complexes acquire high absorption coefficients in the visible region of the electromagnetic spectrum.3 Heavy atom effect in iridium (III)dipyrrinato complexes leads to the formation of long-lived triplet excited states. Also, these complexes exhibit excellent singlet oxygen generation quantum yields.3 These attributes make them propitious photocatalysts for distinctive photochemical transformations.

In this poster, photocatalytic oxidation reactions will be presented employing iridium-dipyrrinato complexes. We developed an efficient protocol for the photocatalytic oxidations of sulfides and imines employing iridium-dipyrrinato complexes to provide sulfoxides and imines, respectively in excellent yields. Additionally, we unveiled an innovative methodology for the hydroxylation of aryl boronic acids utilizing iridium-dipyrrinato complexes as photocatalysts for synthesizing functionalized phenols in high yields. Notably, these photochemical transformations require only a minimal catalyst loading of 0.05 mol%, demonstrating their exceptional cost-effectiveness. This research aims to develop new catalytic systems that harness visible light and sunlight for challenging organic reactions and promote a green and sustainable chemical synthesis.

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PP-74

From Alkyne to Antitumor Agent: Selective [3+2] C-H/C-H Annulation *via* Dual (Distal) C ($_{b,d}$)-H Bond Activation of Aryl Alkyl Quinazolinones

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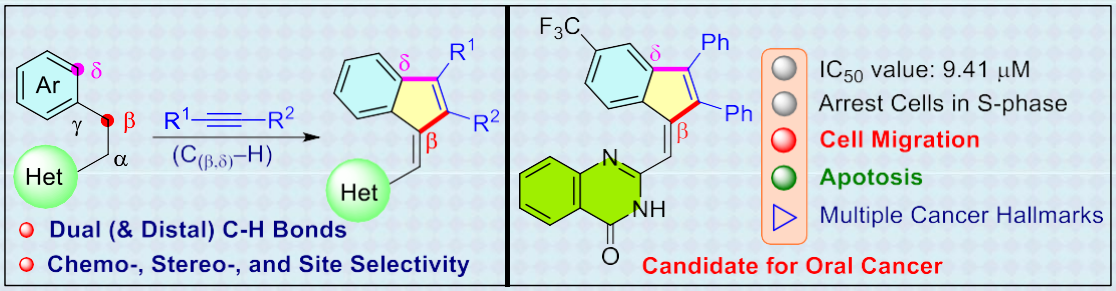
Abstract:

In contrast to proximal C-H bond activations, distal C-H bond activation is fundamentally more challenging and requires distinctly specialized directing partners or techniques. In this context, we report an unprecedented dual (distal) b-C(benzylic)–H and d-C(aryl)–H bond activation relay protocol for the chemo-, regio- and stereo-selective construction of heterocycle-tethered benzofulvenes *via* [3+2] CH/CH-alkyne annulation under palladium catalysis. The synthesized NCEs constitute a novel scaffold with favourable anti-cancer activity against oral squamous cell carcinoma (OSCC).



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Solvent-Tuned Annulation of Sulfonyl Enynals for the Synthesis of Sulfonylated Arenes and Isochromenes

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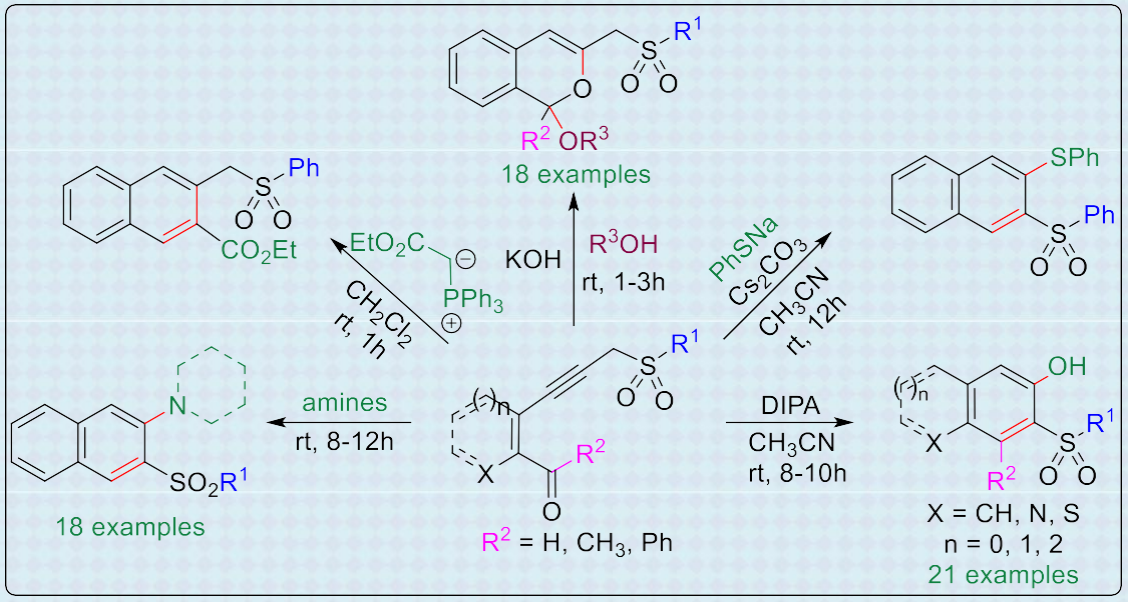
Abstract:

Arenes, particularly sulfonylated arenes, exhibit significant biological activity and are highly relevant to the pharmaceutical and agrochemical industries. Traditional approaches for arene synthesis primarily involve the functionalization of pre-existing arene moieties through electrophilic and nucleophilic aromatic substitution, directed metalation, cross-coupling reactions, and C–H activation strategies. However, a broadly applicable strategy for accessing structurally diverse arenes from a common platform remains underexplored. Herein, we developed a divergent approach for synthesizing sulfonylated arenes, including *β*-naphthylamines, *β*-naphthols, phenols, and naphthalenes, *via* a base-mediated annulation of sulfonyl enynals. This strategy is further extended to the synthesis of heterocycles such as carbazoles, quinolines, and benzothiophenes. Additionally, the method was extended to the annulation of the skeleton of natural steroidal derivatives. Notably, when the reaction was conducted in a polar protic solvent, the same precursor underwent a 1,2-addition/*oxa*-Michael reaction sequence to yield the isochromenes.



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PP-76

PIDA Mediated Keto-oximation of *O*-Alkynyl Hydroxylamines for the Synthesis of 3-Acyl Isoxazolines and 1,2-Oxazines

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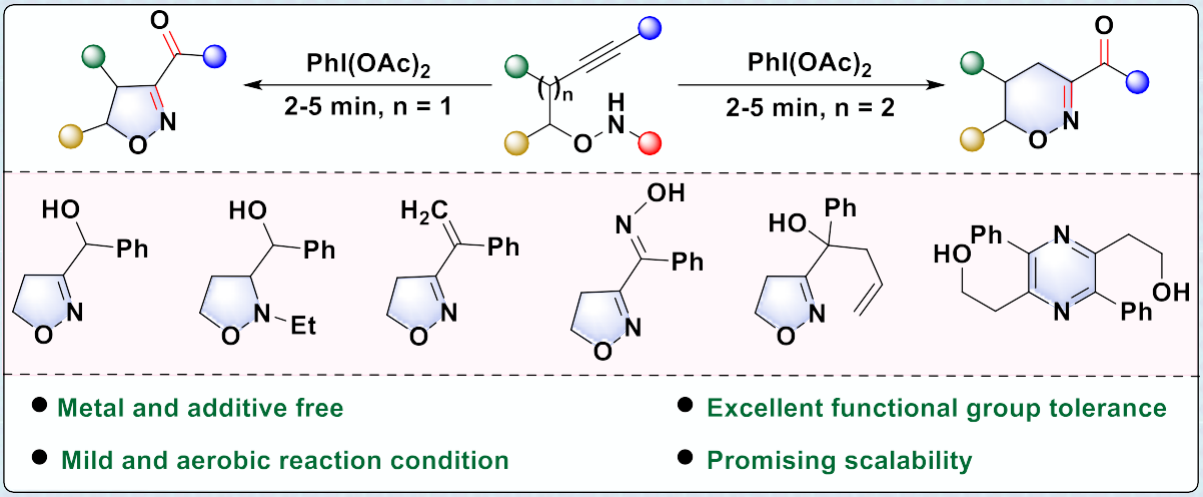
Abstract:



An intramolecular hypervalent iodine mediated keto-oximation of *O*-alkynyl hydroxylamines enables the rapid synthesis of 3-acyl Δ^2-isoxazolines and 1,2-oxazines. This method proceeds under mild, metal-free, and aerobic conditions, demonstrating remarkable tolerance for a wide range of functional groups. The synthetic flexibility of this strategy is highlighted by the creation of diverse structural motifs, including isoxazolidines, 3-vinyl isoxazolines, and 2,5-diphenylpyrazines, showcasing its broad applicability in organic chemistry.

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PP-77

Water Mediate Greener Cyclization of Novel 1*H*-1,2,3-triazol-1-yl-*N*-phenylacetamide Derivatives using Click Chemistry Via (CuAAC) Approach.

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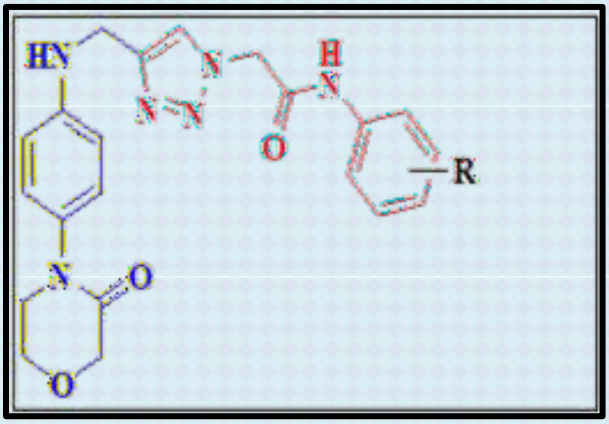
Abstract:

A series of seventeen novel analogues of 1H-1,2,3-triazol-1-yl-N-phenylacetamidederivatives were synthesized. The target compound 2-(4-(((4-oxomorpholino)phenyl)amino)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide have been synthesized by 4-(4-(prop-2-ynylamino)phenyl)morpholin-3-one and 2-azido-N-phenylacetamideaddition of catalytic amount of sodium ascorbate and copper sulphate pentahydrate. The structures of all the synthesized compounds have been characterized by using elemental analysis, FT-IR, Mass, 1HNMR spectroscopy. Purity of all the compounds has been checked on thin layer chromatographic plate and NMR analysis technique. The synthesized compounds were examined for their antibacterial and antifungal activity.



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OP-78

Sustainable Photooxidation of Organic Compounds with Metal Dipyrrin Photosensitizer

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Abstract:

Metal dipyrrinato complexes have emerged as promising candidates for photocatalytic oxidation application1. The dipyrrinato complexes with heavy metals have high absorption coefficients in the visible region of the electromagnetic spectrum2-3. The heavy atom effect in Metal dipyrrinato complexes leads to the formation of long-lived triplet excited states, and these complexes can generate singlet oxygen in excellent yields (upto84%)2-3. These distinctive features make them promising candidates for photocatalytic applications in light-induced aerobic oxidation reactions. The present study evaluates the efficacy of rhenium and palladium dipyrrinato complexes as a photocatalyst for aerobic oxidation reactions with very low catalyst loading (0.05 mole %), which improves its cost-effectiveness under white LED or sunlight. It demonstrated excellent conversion yields for photo oxidation of sulfide into sulfoxides, and oxidative coupling of amines to imines with a variety of substrates was catalyzed by rhenium(I)dipyrrinato complexes, while palladium dipyrrinato complexes were able to catalyze the oxidative cleavage of indole. These catalysts have emerged as versatile systems for the sustainable oxidation of various organic substrates under white light and sunlight, demonstrating their efficiency and broad applicability.

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Hydrogen Bond Donor (HBD) Catalyzed Domino Transformations: An Efficient Tool for the Synthesis of Biologically Prevalent Ring Systems

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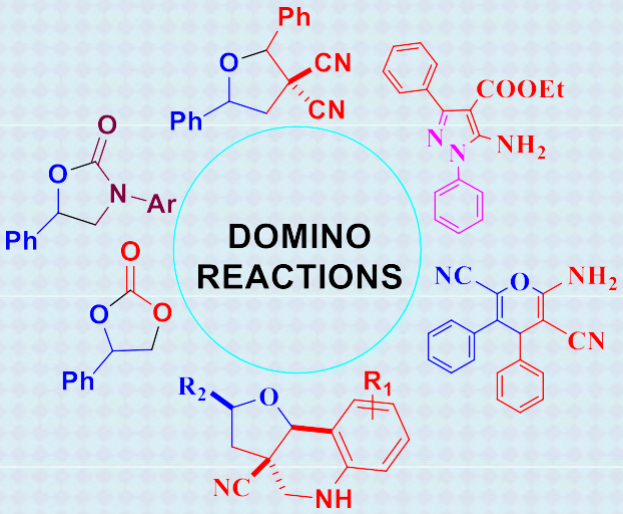
Abstract:

Domino reactions could be defined as an efficient synthetic tool for the construction of two or more chemical bonds in a single reaction step.[1] This technique has been frequenty utilized by the synthetic organic chemists for the synthesis of complex molecular entity in a very simple, and step economic ways in the presence of either a metal or organo-catalyst.[2] In this continuation, our group is focused in developing newer catalyst system for the synthesis of functionalized heterocyclic derivatives via the utilization of suitable domino reaction strategy. We have successfully installed CO_2 to obtain cyclic carbonate from epoxide in the presence of ketimine based Hydrogen Bond Donor (HBD) catalyst. This methodology has also been utilized for the synthesis of highly functionalized, tetrahydro furan isooxazolidine derivatives and pyran derivatvies.[3]



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PP-80

Machine Learning encounter with Metal Organic Framework for Gas Storage

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Abstract:

MOFs have attractive physical and chemical features and have been studied for many different areas such as gas storage and separation, bioimaging, catalysis, batteries, supercapacitors, and drug delivery. **Machine learning** (ML) aims to develop computer programs capable of learning from large data sets using **statistics and some algorithms**; it may help to identify the hidden patterns and relations in data or to construct models to correlate some input variables **(descriptors)** with the output (performance) of the system. The most common approach in ML analysis of MOFs is to acquire the MOF related information from the experimental sources such as the **computation-ready experimental (CoRE)** MOF database or computationally produced data such as hypothetical MOFs, while the applications (such as gas uptake) are usually computed in house (such as with **GCMC simulations**). The most critical issue related to the MOF data is that **HTCS and ML** on MOFs generally focus on **computation-ready databases**; however, these databases consist of different MOFs with different properties, and the range of properties in one database may have huge impacts on the transferability of results or models to other MOF databases.

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PP-81

Schiff Base Innovations Using Water as a Solvent: Green Chemistry Approaches for Sustainable Chemical Processes

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Abstract:

Schiff bases and their metal complexes, synthesized through the condensation of amino compounds with carbonyl compounds, are highly versatile entities with broad industrial applications and a wide spectrum of biological activities. In this study, a series of Schiff bases were synthesized using various substituted aromatic aldehydes and amine derivatives under mild conditions, employing Water and hydrochloric acid as green solvents. Upon completion of the reactions, the products were isolated, dried, achieving yields of 90-95%. the conventional methods of Schiff base synthesis often involve the use of toxic solvents, high temperatures, and hazardous reagents, raising concerns over environmental sustainability. In response, recent innovations in eco-friendly Schiff base chemical processes have focused on green chemistry principles such as solvent-free reactions, water as a green solvent, and the use of renewable or bio-based materials. Emphasizing the use of non-toxic, low-energy methods, the paper also explores the potential of Schiff bases in various eco-friendly applications, ranging from environmental remediation to green catalysis. By incorporating sustainable practices, these new approaches provide a promising pathway for future research and industrial applications of Schiff bases in a more sustainable and environmentally conscious manner. This approach aligns with the goals of modern synthetic organic chemistry by offering an efficient, environmentally friendly route to valuable chemical commodities, thus paving the way for future applications in drug discovery and other industries. Additionally, a comparative study involving temperature and time variations was conducted. Spectrometric analyses, including 1H NMR, 13C NMR, and LCMS, were performed to confirm the structures of the obtained target molecules, highlighting the reliability and accuracy of the presented synthetic methodology.

OP-82

Synthesis of low molecular mass-self assembled gel

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Abstract:

Designing of low molecular weight supramolecular gel is still a complicated task.On the other hand the discovery and design of small organic molecules capable of gelling aqueous solvents (hydrogelators) or organic solvents(Organogelator) is rapidly gabbing attention of researchers, in particular due to their possible practical applications1 in tissue engineering , for controlled drug delivery , pollutant capture and removal , and many more.2 Moreover two-component systems producing hydrogels or orgaganogel through supramolecular complex formation have attracted much interest recently. The bicomponent hydrogels/organogel has certain advantages over one-component small-molecular hydrogels/organogel since the supramolecular bonding between the components is very labile and can be utilized for the synthesis of the gel. We have also reported the synthesis of a novel class of one component Thiazole based organogelator 3. Lately we have investigated a new class of two component Low molecular mass gel (LMOG) based on organic salts/cocrystals. For this purpose, we have followed a combinatorial library approach. The combinatorial library was prepared by reacting different aliphatic and aromatic carboxylic acids and 2-aminothiazole derivatives. The synthesized salts/cocrystals have been characterized by various physic- chemical techniques and we also tried to establish a systematic structure-property correlation study based of gelator and non-gelator supramolecular assemblies.

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PP-83

Design, Synthesis, and Photophysical Characterization of Tetraphenyl-ethylene-Based AIE-Active Sulfone Derivatives.

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Abstract:

Aggregation-induced emission (AIE) has developed as an attractive optical phenomenon with significant implications for optoelectronics, bioimaging, and sensing applications. Tetraphenyl-ethylene (TPE) derivatives, acknowledged for their fundamental AIE characteristics, provide an outstanding foundation for the synthesis of highly emissive materials.[1] The work presents the synthesis and comprehensive photophysical analysis of novel TPE-based sulfone derivatives demonstrating prominent AIE properties. The intentional integration of electron-withdrawing sulfone groups into the TPE core was intended to improve molecular rigidity, boost photostability, and adjust electrical characteristics.[2] We produced the compounds using an efficient, high-yield method and thoroughly characterized them using NMR spectroscopy and mass spectrometry. We thoroughly evaluated the photophysical behavior in both solution and aggregated stages, revealing a significant fluorescence amplification following aggregation. UV-vis absorption and fluorescence spectroscopy validated their exceptional AIE activity.[3] Moreover, these TPE-sulfone derivatives demonstrated exceptional thermal and photostability, positioning them as viable candidates for use in organic light-emitting diodes (OLEDs), fluorescence sensors, and bioimaging probes. This research enhances the current collection of AIE-active fluorophores and offers a more profound comprehension of the structure-property link that dictates their photophysical characteristics. The findings underscore the promise of sulfone-functionalized TPE systems for next-generation luminous materials, facilitating novel applications in advanced optoelectronic technologies.[4]

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PP-84

Synthesis and characterization of Novel Sparfloxacin p-amino benzoic acid salt

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Abstract:

The design and synthesis of API (active pharmaceutical ingredient) solid forms, including polymorphs, hydrates, solvates, cocrystals, and salts, plays a crucial role in the pharmaceutical industry since it enhances their physicochemical and pharmacological behaviors without altering the molecular structure of the API.[1]The synthesis of novel multicomponent crystal forms of Sparfloxacin has been reported as an efficient for enhancing physicochemical properties, including solubility and dissolution. Sparfloxacin is a fluoroquinolone extensively utilized in the treatment of bacterial infections.[2], [3] We synthesized a new salt form of Sparfloxacin combined with para-aminobenzoic acid, classified as generally recognized as safe category . New salt forms were identified by single crystal X-ray diffraction, powder X-ray diffraction, differential scanning calorimetry, and FT-IR analysis. Sparfloxacin salt exhibits significantly better solubility in buffer solution compared to the parent drug. The salt synthesis of Sparfloxacin (NH_2^+) cation and para-aminobenzoic acid anion exhibits synthon tetramers $R_4^4(12)$ by intermolecular hydrogen bonding.

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OP-85

Exploring Triazole-Functionalized Benzamides: A Synthetic Approach Towards Effective Antimicrobial and Antifungal Compounds

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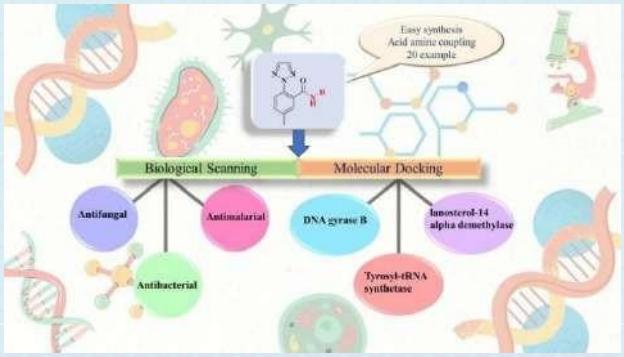
Abstract:

The global **drug resistnce crisis** demands urgent development of **new antifungal and antimicrobial agents**. This study reports the **synthesis of amide-coupled 1,2,3-triazole scaffolds** via **acid-amine coupling** of **5-methyl-2-(2H-1,2,3-triazol-2-yl) benzoic acid** with **aliphatic and aromatic amines**. The synthesized compounds (H1-H20) were **characterized spectroscopically** and evaluated for **antifungal, antibacterial, and antimalarial activities**. Notably, **H3, H7, H9, H13, H14, H17, and H19** showed strong **antifungal activity against *C. albicans*** (**MIC 250 µg/mL**) vs. **griseofulvin (MIC 500 µg/mL)**. **Antibacterial screening** against **Gram-positive (*S. pyogenes, S. aureus*)** and **Gram-negative (*E. coli, P. aeruginosa*) bacteria** showed moderate to good activity compared to **ciprofloxacin and chloramphenicol**. **H5 and H7** displayed **moderate antimalarial activity** (**IC50 = 0.67 and 0.70 µg/mL**) vs. **quinine**. **Molecular docking** confirmed strong **binding affinities** to **lanosterol-14α demethylase, DNA gyrase B, and tyrosyl-tRNA synthetase**, supporting their potential as **novel antimicrobial agents**.



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PP-86

Metabolite Assemblies and its implications in Inborn Errors of Metabolism

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Abstract:

The word "amyloid" was conventionally referred to as abnormal aggregates of proteins and peptides which produced cellular toxicities and induces pathogenesis in protein misfolding diseases like Alzheimer's and Parkinson's to name a few and and its applications in designing novel micro/nanoarchitectures for drug delivery and material science. However, recent research suggest not only proteins and peptides but metabolites like single amino acids, nucleobases, glucosyceramides too aggregate to form amyloid like toxic structures and have possible implications in the etiology of rare inborn errors of metabolism (IEM).[1] In this context, our group for the very first time reported self-assembly of non-aromatic amino acids like cysteine and methionine to amyloid-like cytotoxic structures.[1e] Further we also reported unusual aggregates formed by other amino acids proline, hydroxyproline and lysine.[1f] Herein, I will present our work on self-assemblies of metabolite of urea cycle, uric cycle pathway[2] and nonaromatic polar amino acids,[3] their characterization, and its implications in pathophysiology of inborn error of metabolism caused by excess of these metabolites along with their association to amyloid diseases and thus offering exciting insights into the development of targeted interventions for these metabolic disorders.

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PP-87

Development of Nicotinonitrile-Containing Compounds for the Treatment of Chronic Obstructive Pulmonary Disease & SARS-Cov-2

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Abstract:

Nicotinonitrile, a versatile compound with significant pharmaceutical potential, can be synthesized through catalytic conversion of nicotine extracted from tobacco waste This process involves oxidative ammonolysis using oxide catalysts, offering an economically viable method for tobacco waste utilization. Nicotinonitrile derivatives have garnered attention due to their wide range of therapeutic activities, with several drugs containing these compounds already available in the market, such as Bosutinib, Milrinone, and Neratinib Recent research has focused on developing novel nicotinonitrile-derived compounds as potential anticancer agents. A study also demonstrated that certain nicotinonitrile derivatives exhibit potent cytotoxic activity against cancer cell lines, with some compounds showing promising inhibition of Pim kinases. These findings highlight the importance of nicotinonitrile as a scaffold in medicinal chemistry and its potential for developing new therapeutic agents.

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PP-88

Investigating the Molecular Self-Assembly of Diverse Molecules and Assessing its Application

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Abstract:

The self-assembly and aggregation of biomolecules, including nucleotides, nucleobases, and metabolic intermediates, represent an emerging area of interest in disease pathophysiology. While traditionally studied in the context of proteins, recent evidence suggests that small metabolites can form supramolecular assemblies with amyloid-like characteristics. In this study, we investigate the self-assembly behavior of adenine nucleotides (AMP, ADP, ATP), nucleobases (Guanine, Cytosine, Thymine), and metabolic intermediates (Homogentisic acid, N-acetyl aspartic acid, Isovaleric acid). Using advanced microscopy, Thioflavin T (ThT) fluorescence assays, and biophysical characterization, we demonstrate that these biomolecules undergo time-dependent aggregation, forming oligomeric structures that evolve into larger, amyloidogenic fibrils. Cytotoxicity assessments in human retinal pigment epithelial (RPE-1) and colorectal carcinoma (HCT-116) cell lines reveal significant toxicity, particularly for aged aggregates, mirroring pathogenic amyloid species. Furthermore, in vivo assays in *Caenorhabditis elegans* confirm cellular stress responses and impaired proteostasis, suggesting a broader biological impact. Our findings highlight the non-canonical role of biomolecular aggregation in metabolic and nucleotide-associated disorders, drawing parallels to protein misfolding diseases and opening new avenues for therapeutic intervention.

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OP-89

Synergy between Silver Nanoparticles and Knk437 for as Antimicrobial Agents

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Abstract:

Antimicrobial resistance (AMR) is a growing global health threat, which is caused by the misuse and overuse of antibiotics. AMR is estimated to have caused 4.95 million deaths worldwide in 2019 [1]. Future solutions require the development of novel antimicrobial agents.
KNK437, a benzylidene lactam compound has a significant role in inhibiting HSPs. It has been reported to inhibit the accumulation of HSP27, HSP30, HSP70, and HSP90 leading to the significant reduction of thermotolerance during hyperthermic therapy. It has also been reported as an effective antimicrobial agent [2]. However, the minimum inhibitory concentration of an antimicrobial agent (KNK437) expressed in 250 µg/mL, which can be improved. On other hand, silver nanoparticles (AgNPs) have emerged as an excellent antimicrobial agent, capable of combating bacterial infections both in vitro and in vivo [3]. We anticipate, upon the combination of KNK437 and AgNPs the dosage can be moderated and an effective antimicrobial solution may be developed [4].
In this work, the synthesis of KNK437 and AgNPs was accomplished. The products were characterized using ^{1}H-NMR, ^{13}C-NMR, HRMS data, UV-visible spectroscopy, zeta potential analysis, and DLS. The antimicrobial properties against gram-positive bacteria *Staphylococcus aureus*, suggest that these synergistic effects hold great potential for antimicrobial applications.

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OP-90

Fluorinated Benzophenone Derivatives: A Dual In Vitro & Silico Approach to Advancing Anti-Cancer Therapy

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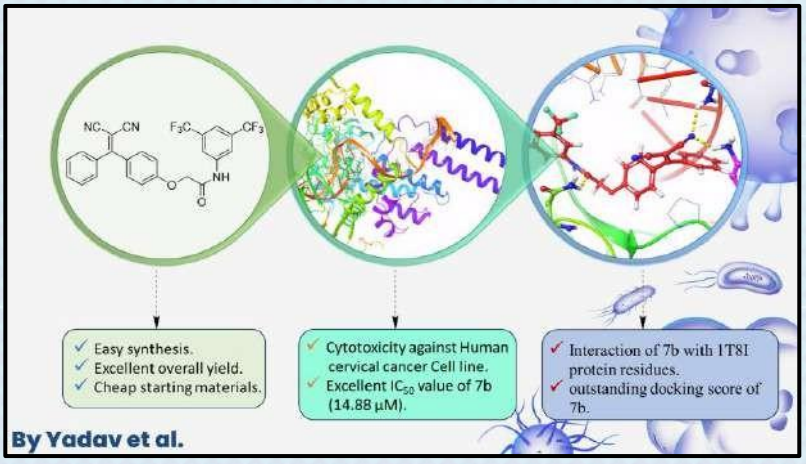
Abstract:

A series of novel fluorinated benzophenone derivatives were synthesized and evaluated for their cytotoxic and anti-proliferative effects against human MDA-MB-231 triple-negative breast cancer and KB-3-1 cervical carcinoma cell lines. The synthesized compounds were characterized using **^{1}H NMR, ^{13}C NMR, FTIR, HRMS, and XRD spectroscopy**.

Among the tested derivatives, **compounds 6a and 7a exhibited ~2.1-fold and ~13-fold higher cytotoxic activity against the KB-3-1 cell line** compared to the standard drug gemcitabine. Malononitrile-modified **fluorinated benzophenone derivatives 6b and 7b displayed remarkable cytotoxicity, surpassing the reference standard by ~3.6 and ~13.5 times, respectively**. Against the MDA-MB-231 breast cancer cell line, **compounds 6a and 7a demonstrated ~1.2-fold and ~2.5-fold greater cytotoxic activity**, while **compounds 6b and 7b outperformed the reference standard by ~2.2-fold and ~2.8-fold, respectively**. Compound **7b emerged as the most potent candidate**, exhibiting superior cytotoxic activity against the KB-3-1 cervical cancer and MDA-MB-231 breast cancer cell lines.

Furthermore, **molecular docking studies were performed to predict binding affinities and potential interactions**, offering insights into the mechanism of action of these promising fluorinated benzophenone derivatives.



PP-91

Advancing Energy Storage and Chemical Sensing with MOFs: A Computational and Experimental Perspective

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Abstract:

Metal–organic frameworks (MOFs) are widely recognized for their **tunable porosity, high surface area, and structural flexibility**, making them promising materials for **energy storage** and **chemical sensing**. However, optimizing their real-world performance requires a thorough understanding of **stability, adsorption properties, and functionalization strategies**. This study employs a combined **computational and experimental approach** to enhance MOF efficiency. **Molecular simulations, density functional theory (DFT) calculations, and machine learning techniques**, alongside **experimental validation**, are used to design **stable, high-performance MOFs** for energy and sensing applications.

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PP-92

Triphenylamine-Naphthalimide-Based "On–Off–On" AIEgen for Imaging Golgi Apparatus and Endoplasmic Reticulum

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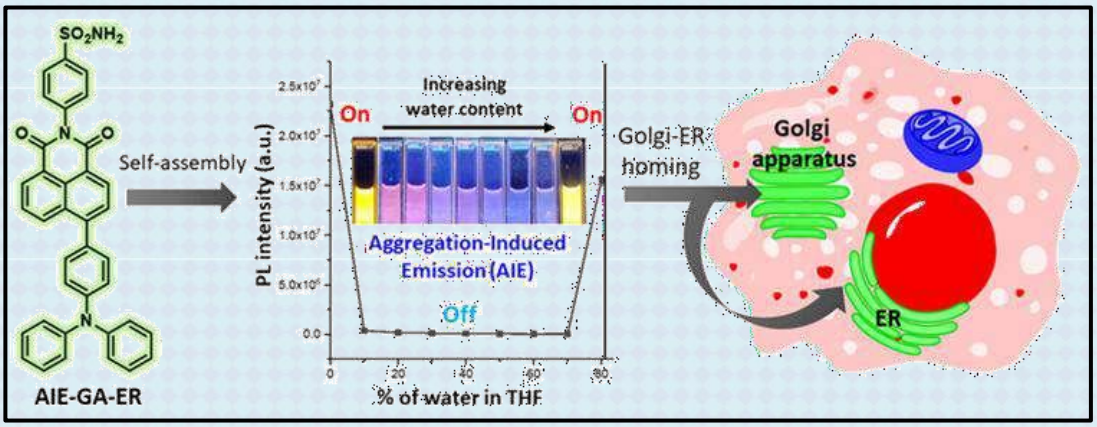
Abstract:

Golgi apparatus (GA)and endoplasmic reticulum (ER)are two of the interesting subcellular organelles that are critical for protein synthesis, folding, processing, post-translational modifications, and secretion. Consequently, dysregulation in GA and ER and cross-talk between them are implicated in numerous diseases, including cancer. As a result, simultaneous visualization of the GA and ER in cancer cells is extremely crucial for developing cancer therapeutics. To address this, herein, we have designed and synthesized a 1,8-phthalimide-based small molecule (AIE-GA-ER) consisting of phenyl sulfonamide as Golgi-ER homing and triphenylamine- naphthalimide as aggregation-induced emission (AIE) triggering moieties. AIE-GA-ER exhibited remarkable "on-off-on" AIE properties in the THF/water binary solvent system due to aggregated "on-state" in pure THF and 80%water in THF. Molecular dynamic simulations and density functional theory (DFT) calculations exhibited the underlying mechanism of the emissive property of AIE-GA-ER to be the interplay between intramolecular charge transfer (ICT)stabilization and aggregation in THF, DMSO, and water. AIE-GA-ER efficiently homed into the GA and ER of HCT-116 colon cancer cells within 15-30min as well as noncancerous human retinal epithelial pigment cells (RPE-1) within 3h with minimum toxicity. This AIEgen has the potential to illuminate the Golgi apparatus and ER simultaneously in cancer cells to understand the chemical biology of their cross-talk for next-generation cancer therapeutics.



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OP-93

Fabrication of a Polymeric Scaffold Infused with Silver Nanoparticles and Curcumin for Wound Care

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Abstract:

Cutaneous wounds are a serious problem in medical care, with roughly 300 million chronic and 100 million traumatic wound patients worldwide. In addition to it, microbial infections slow the healing process [1]. Some of the current wound dressings have interesting properties such as excellent porosity, good water-absorbing capacity, moderate water vapour transmission rate, high drug loading efficiency, and good ability to provide a moist environment, However, they are limited in antimicrobial properties. Hence, there exists a critical demand for novel and innovative antimicrobials embedded wound dressing materials [2]. Herein, we design polymeric scaffold infused with silver nanoparticles and curcumin. Curcumin, is a traditional thertaputic which has shown anticancer, antibacterial, and antioxidant properties [3]. Silver nanoparticles have inherent medicinal qualities and broad antibacterial spectrum [4]. Combination of these two on a strong polymeric support of has a potential to heal wounds efficiently.

In this work characterization of silver nanoparticles was done using UV-visible spectroscopy, zetapotential measurement and DLS. The fabricated scaffold gives magnificent antibacterial property against *E. coli, S. aureus, B. subtilis, P. aeruginosa, V. cholerae* and *E. faecalis.* Hence, these properties have potential in wound care application.

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PP-94

Development of cost-effective Synthetic Route of Rilpivirine

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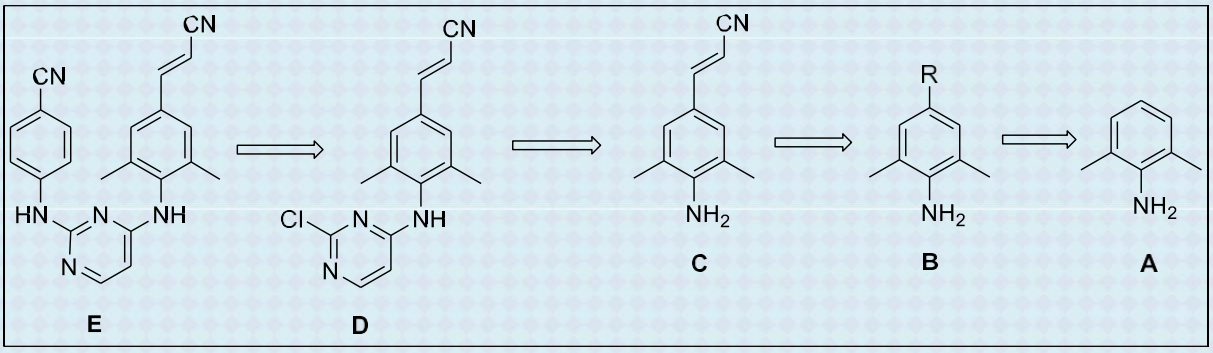
Abstract:

Globally, 39.9 million people were living with HIV by the end of 2023, with an estimated 1.3 million new infections and 630,000 AIDS-related deaths. HIV (human immunodeficiency virus) infection. Rilpivirine is a non-nucleoside reverse transcriptase inhibitor (NNRTI) that inhibits the action of the reverse transcriptase enzyme, which is required for HIV replication, making it an option to statins for HIV patients. U.S.A FDA-approved on May 20, 2011 respectively. This study focuses on developing a new, novel, cost-effective, and commercially efficient synthetic route to reducing the cost of starting raw material, reagent, reuse solvent, and time and increasing process sustainability. The synthetic route uses four steps, conducted under carefully optimized conditions to access the target and increase overall yield over two steps.

The findings of this study have significant significance for pharmaceutical producers since they may lead to a decrease in the market price of Rilpivirine, hence improving patient access. Subsequent research is going to concentrate on scaling production, assuring regulatory compliance, and further improving the process for broader industrial applications.



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PP-95

Advancing Innovative Trifluoromethylation Strategy and Their Application in Drug Synthesis

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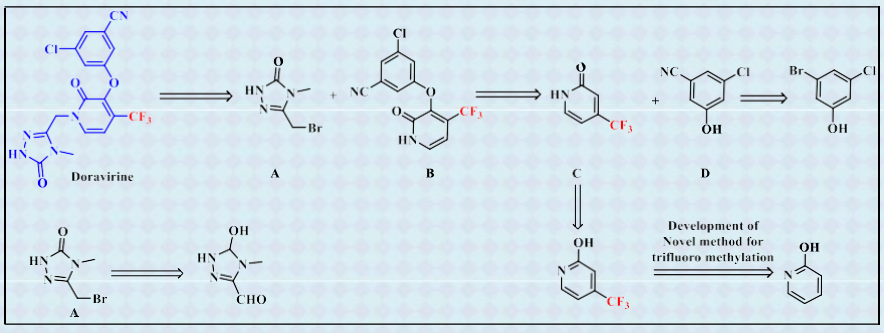
Abstract:

Trifluoromethylation is a key chemical process that can significantly influence the physical and biological properties of organic compounds. The incorporation of a trifluoromethyl (-CF_3) group enhances a molecule's lipophilicity, permeability, and metabolic stability, making it a valuable modification in medicinal chemistry and drug discovery. The trifluoromethyl group plays a crucial role in various biological activities, including antiviral, anticancer, and antibacterial effects. It can act as a bio isostere, replacing other functional groups to optimize drug properties. As a highly lipophilic structural motif, CF_3 groups are often integrated into aromatic rings, where they contribute to increased molecular potency by engaging in multipolar interactions with amide and carbonyl groups in targeted proteins. Our research focuses on developing innovative trifluoromethylation methodologies to facilitate the synthesis of CF_3-containing drug molecules, including: **Doravirine** – an antiviral drug used in combination therapies to treat HIV in adults. **Enasidenib** – a targeted therapy for acute myeloid leukemia (AML), a type of cancer that begins in the white blood cells. **Pexidartinib** – a kinase inhibitor designed for the treatment of tenosynovial giant cell tumor (TGCT). By advancing new trifluoromethylation techniques, we aim to expand the accessibility and effectiveness of CF_3-containing pharmaceuticals, contributing to the development of next-generation therapeutics.



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PP-96

Designing Novel Route to Dihydropyrimidinone and their Biological Activities

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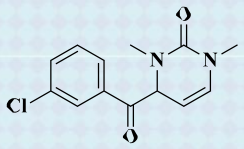
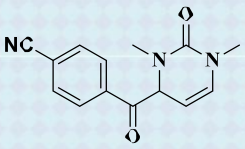
Abstract:

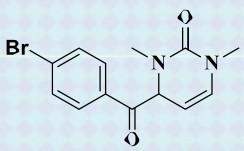
Dihydropyrimidinones are important compounds in pharmaceutical and medicinal chemistry, known for their diverse biological activities' antimicrobial, anti-cancer, anti-bacterial. The preparation of dihydropyrimidinones typically involves the combining aldehydes, β-keto esters, and urea or thiourea under basic conditions. This one-pot synthesis leads to the formation of the dihydropyrimidinone core. Key factors influencing the reaction include the choice of catalyst, solvents, and reaction conditions, which can affect yield and selectivity. Variations of the subsequent modifications can further enhance the structural diversity and biological activity of the resulting dihydropyrimidinones. This poster summarizes the novel rout significance and methods of novel rout synthesizing and characterization of dihydropyrimidinones in the context of drug development.



4-(3-chlorobenzoyl)-1,3-dimethyl-3,4-dihydropyrimidin-2(1*H*)-one



4-(1,3-dimethyl-2-oxo-1,2,3,4-tetrahydropyrimidine-4-carbonyl)benzonitrile



4-(4-bromobenzoyl)-1,3-dimethyl-3,4-dihydropyrimidin-2(1*H*)-one

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PP-97

Design, Synthesis and Biological Evaluation of Amino Acid-conjugated Benzamide Derivatives

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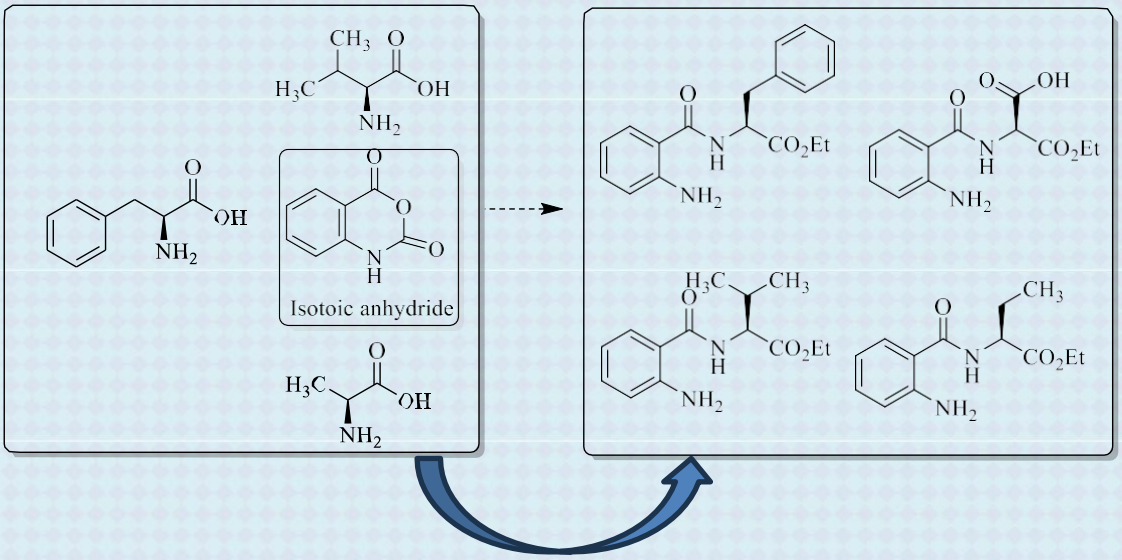
Abstract:

Benzamide derivatives have emerged as promising antimicrobial agents due to their diverse structural modifications and bioactive properties.[1] These compounds exhibit significant antibacterial and antifungal activities by targeting essential microbial processes, such as enzyme inhibition, membrane disruption, and protein synthesis interference. Structural modifications, including halogenation, hydroxylation, and heterocyclic substitutions, have been shown to enhance their potency against both Gram-positive and Gram-negative bacteria, as well as pathogenic fungi.[2] The present research work aims to synthesise amino-acid conjugated benzamide derivative and to evaluate their potential biological applications. The details of synthetic design, execution of experiments and characterization of products will be discussed during this presentation.



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PP-98

Development of Cost-effective Synthetic Route of Loratadine Drug Intermediate

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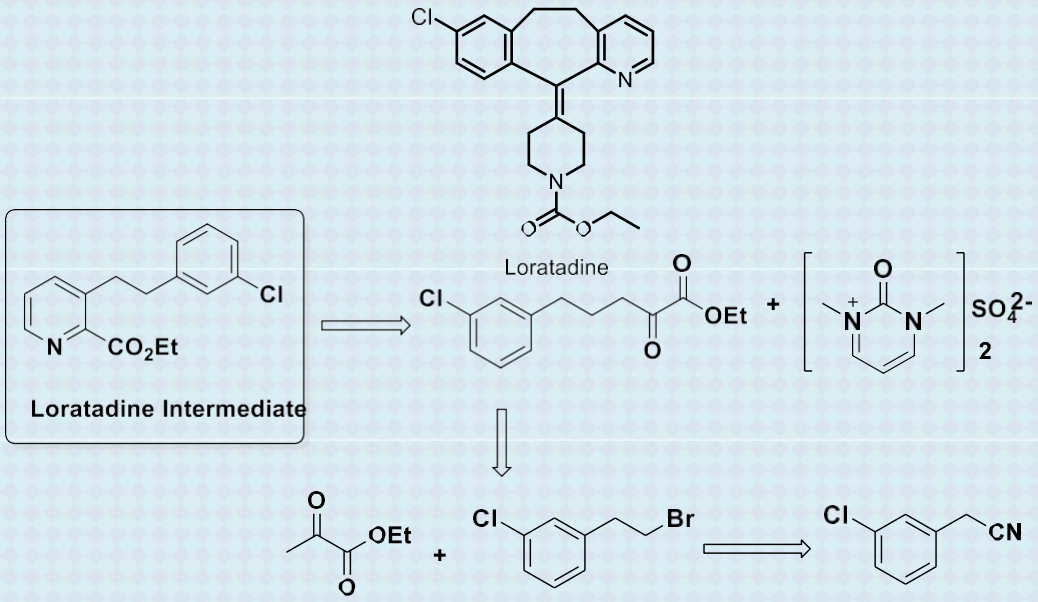
Abstract:

Loratadine is a second-generation antihistamine commonly used to treat allergic conditions such as hay fever (allergic rhinitis) and urticaria (hives). It works by selectively blocking peripheral H1 histamine receptors, reducing symptoms like sneezing, runny nose, and itching without causing significant drowsiness, a common side effect of first-generation antihistamines.[1] Several Loradatine derivatives and analogues have been synthesized and evaluated for their anti-histamine activities.[2] It is available over the counter and in prescription forms, often marketed under brand names like Claritin. Its active metabolite, desloratadine, contributes to its prolonged efficacy.[3] The present research work aims to discuss cost-effective synthetic route, optimization of reaction conditions, and characterization of synthetic products by spectroscopic techniques.



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PP-99

Development of Economical Synthetic route of Bempedoic Acid

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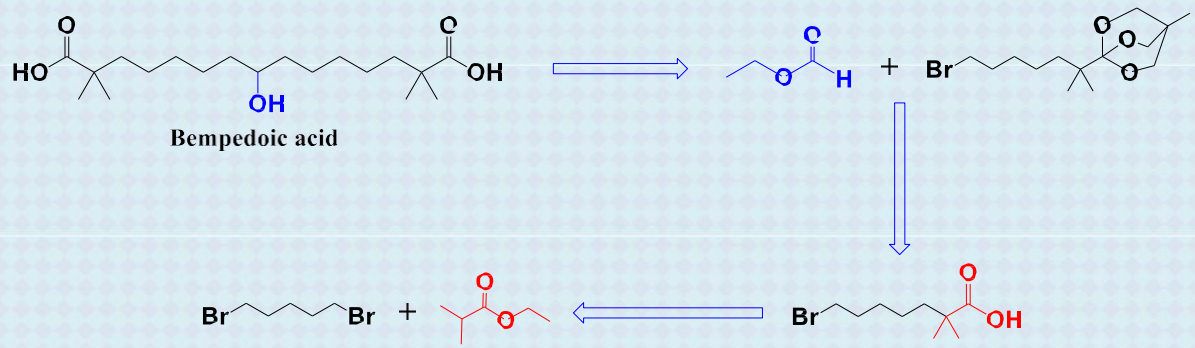
Abstract:

Nexletol (Bempedoic acid) and Nexlizet (combination of Bempedoic acid and Ezetimibe) both are approved by U.S.A FDA on 20 February 2020 and 26 February 2020 respectively. Bempedoic acid is a novel lipid-lowering agent that inhibits ATP citrate lyase, that is effective in the treatment of hypercholesterolemia and hypertension, providing an alternative to statins for patients with hypercholesterolemia. Bempedoic acid has been also identified as a histone deacetylase-6 inhibitor. This study focuses on developing a cost-effective and scalable synthetic method to improve yield, reduce raw material expenses, and enhance process sustainability. Bempedoic acid has been developed starting from 1,5- Dibromo pentane in six steps. The synthesis of key precursor i.e. Orthoester, has been accomplished through the coupling of bromo-Acid with 3-methyl 3- oxetane methanol followed by orthoester formation by BF_3:Et_2O. Ketone formation by addition of alkyl Grignard reagent with ethyl formate is introduced as the key step of this process. This study's findings have significant implications for pharmaceutical manufacturers, potentially lowering the market price of bempedoic acid and increasing patient accessibility. Future work will focus on scaling up production, ensuring regulatory compliance, and further refining the process for industrial application.



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PP-100

A Novel route for Oxidation of Aldehyde to Carboxylic Acid

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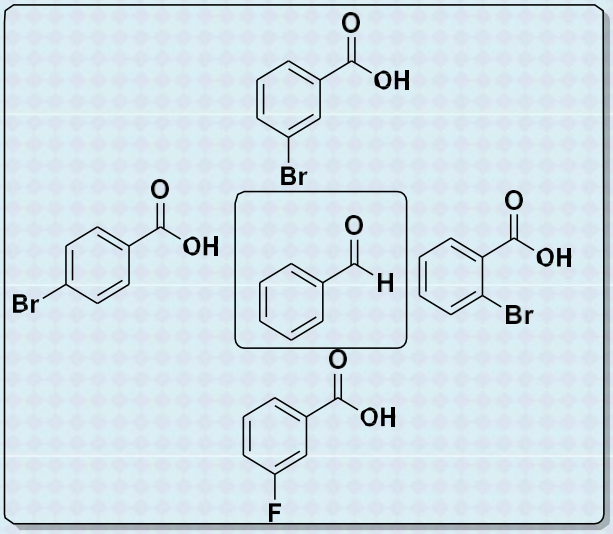
Abstract:

Aliphatic and aromatic carboxylic acids play important role as a key functionalities in several synthetic intermediates and natural products utilized in pharmaceuticals and agrochemicals.1 Furthermore, carboxylic acids are also as a synthetic precursor for the synthesis of peptides, esters, amides, and polymers.2 With highest level of oxidation, carboxylic acids can be easily reduced to be aldehyde/ketones and alcohols which act as a chemical feedstock in academic research studies as well as industrial processes. The present research work aims to discuss development of synthetic method for oxidation of aldehyde to carboxylic Acids.

Acid:



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PP-101

Unlocking Coumarin's Potential: A Computational and Experimental Approach to Combatting Microbial Resistance

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Abstract:

Researchers are investigating potential new antimicrobial drugs to combat the emergence of resistant bacterial and fungal epidemics. Researchers are looking at Coumarins for their potential to increase the effectiveness of antimicrobial, antiviral, and anti-cancer treatments. Research into bacterial killing strategies and optimization of the structure-activity relationship (SAR) is underway to make Coumarin hybrids more efficient against drug-resistant pathogens. There is a growing problem with drug-resistant bacteria, and medications are unable to stop it. The Coumarin part is what kills bacteria by stopping ATPase activity, DNA supercoiling, and the attachment of bacterial DNA gyrase.

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OP-102

Exploring the Multifunctionality of Exopolysaccharides from *Lactobacillus delbrueckii*: Structural Insights and Postbiotic Potential

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Abstract:

The evaluation of exopolysaccharides (EPS) extracted from *Lactobacillus delbrueckii*, demonstrated significant potential as a postbiotic. To determine EPS's functional characteristics, this research focuses on its extraction and comprehensive characterization. EPS were isolated from *L. delbrueckii* and subjected to structural and surface analyses using optical microscopy, bright field imaging, scanning electron microscopy (SEM), and atomic force microscopy (AFM). These studies revealed a network-like structure of EPS, which may be a prime cause to inhibit pathogen adhesion to the intestinal epithelium, thereby contributing to the protection of the human gastrointestinal tract. The physicochemical confirmation of the extracted EPS was further evaluated using ultraviolet (UV) and immunofluorescence (IF) spectroscopy, confirming its structural integrity and biological activity. The functional efficacy of EPS was assessed through a wound healing assay, which showed positive results and hence demonstrated its potential to promote tissue regeneration. Additionally, antimicrobial activity tests indicated that EPS exhibited inhibitory effects against common gastrointestinal pathogens. These findings collectively highlight the diverse functions of *L. delbrueckii*-derived EPS in enhancing gut health and preventing infections. The network-like structure, along with its antimicrobial and wound-healing properties, underscores the potential of EPS as a functional postbiotic with applications in human health. This research provides valuable insights into the structural and functional properties of EPS, establishing the framework for its use in therapeutic and preventive healthcare strategies.

OP-103

Antimicrobial smart packaging films derived from starch and aloe vera

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Abstract:

Environmental concerns over petroleum-based plastic packaging have driven interest in biodegradable alternatives. Starch is a promising substitute due to its abundance, non-toxicity, biodegradability, renewability, and edibility. Starch-based films help preserve food freshness and improve transport, storage, and display. Growing demand for sustainable, healthy foods has increased research into plant-derived materials for edible films. Aloe vera, known for its medicinal properties, is gaining attention for use in bioactive, edible coatings.
This study developed smart, active packaging films using starch, Aloe vera gel, and the pH-sensitive dye HPTS (8-hydroxypyrene-1,3,6-trisulfonic acid trisodium salt). These films detect pH changes via fluorescence shifts, enabling real-time freshness monitoring. UV-visible spectroscopy confirmed HPTS incorporation with a 407 nm absorbance peak. The films also showed antibacterial activity against Staphylococcus aureus, highlighting their potential for smart packaging that enhances food safety, shelf-life, and supports sustainability.

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