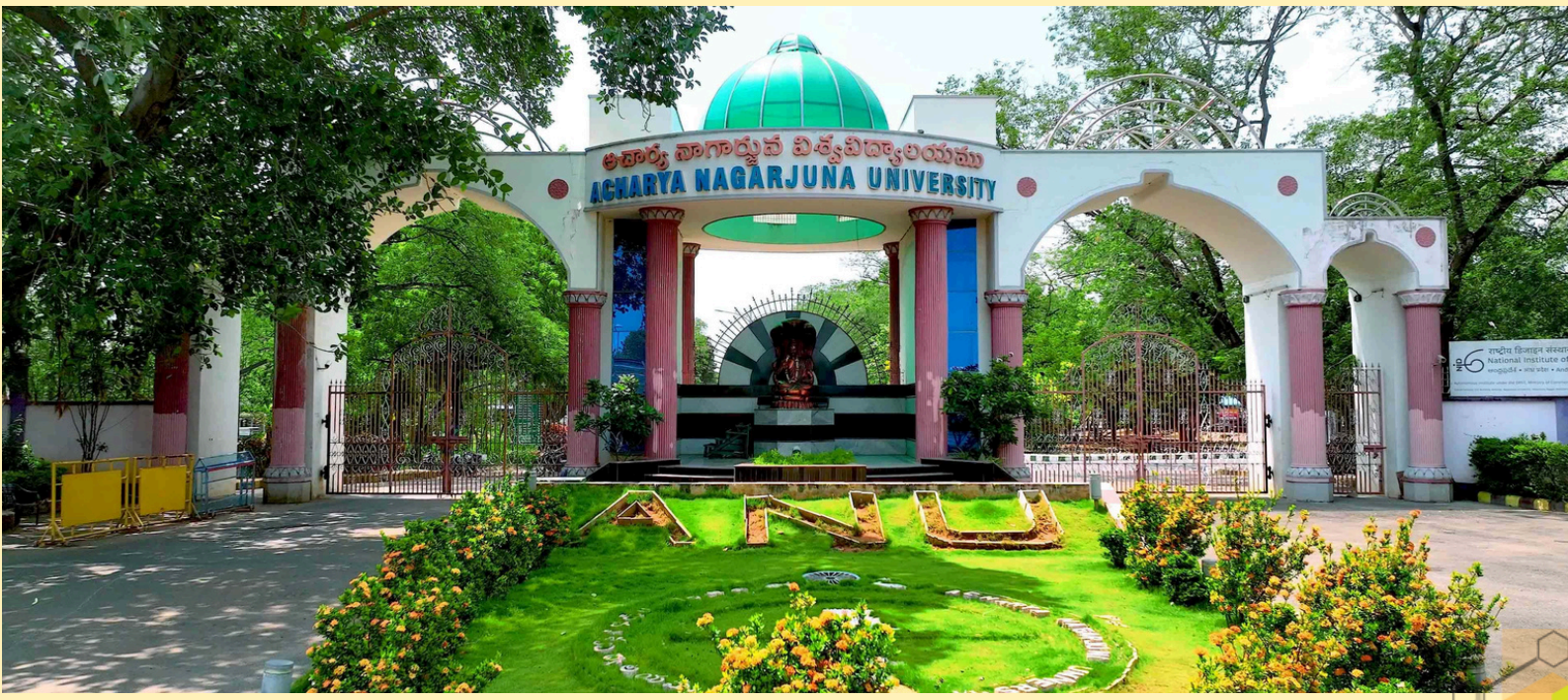
UGC Sponsored
Two day
National Seminar on

Recent Advances in Chemical Sciences for Sustainable Development

(RACSSD-2025)

3rd and 4th March 2025

SOUVENIR



Organized by

Department of Chemistry
University College of Sciences
Acharya Nagarjuna University

Edited by

Dr. M Subbarao
Professor
Director, RACSSD-2025
Head, Chairman-BOS(PG)
Coordinator (Exams)-PG & Professional Courses
Acharya Nagarjuna University

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Acharya Nagarjuna University, Nagarjuna Nagar, Guntur,

Andhra Pradesh 522510

Foreword

It is with great honor and enthusiasm that we welcome you to the UGC-sponsored National Seminar on **Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025),** organized by the Department of Chemistry, Acharya Nagarjuna University, on 3rd and 4th March 2025.

In today's world, sustainable development is a critical priority, and chemical sciences play a vital role in addressing environmental, industrial, and societal challenges. This seminar aims to bring together distinguished academicians, researchers, industry professionals, and young scholars to exchange ideas, share innovative research, and explore advancements in green chemistry, nanotechnology, renewable energy, and sustainable materials.

We are confident that RACSSD-2025 will serve as a dynamic platform for fostering collaboration, inspiring future research, and contributing to scientific progress. We sincerely thank the University Grants Commission (UGC) for its support and extend our gratitude to all esteemed speakers, participants, and organizers for their contributions in making this event a success.

We look forward to insightful discussions and meaningful outcomes that will drive advancements in chemical sciences for a sustainable future.
With best regards,

Prof. D. Ramachandran
Convener

Prof. M. Subbarao
Director

Profile of the Department of Chemistry

The Department of Chemistry at Acharya Nagarjuna University originated as the Department of Chemistry at the Andhra University Post Graduate Centre, which was established in 1967. Since its inception, the Department has been guided by eminent professors who have led it to great heights. The Department has published nearly 1,000 research articles in esteemed national and international journals. Additionally, approximately 200 research students have earned Ph.D. degrees, while around 250 students have received M.Phil. degrees. Faculty members have also presented several papers at various seminars and conferences, further contributing to the academic community.

The Department has organized numerous seminars, workshops, and conferences, with notable events such as the 39th Annual Convention of Chemists, held from December 23rd to 26th, 2002. Faculty members are actively involved in handling projects funded by prominent organizations such as UGC, DST, CSIR, and others.

Prof. B. Syama Sundar (Retd) has been honored with the prestigious title of Fellow of the Royal Society of Chemistry (FRSC-London). He was also appointed as the Vice-Chancellor of Yogi Vemana University, Kadapa, by the Government of Andhra Pradesh in 2013. Additionally, **Prof. B. Sivarama Sarma, Prof. PVV Satyanarayana, Prof. C. Rambabu, Prof. N.S. Prakasa Rao, Prof. B. Syama Sundar, Prof. B. Hari Babu and Dr. D Ramachandran** have all received the State Best Teacher Award.

The Department has also been awarded a DST-FIST Level 1 project with a grant of ₹228 lakhs. It currently offers **four M.Sc. specializations: Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, and Forensic Science**, each designed to provide students with both theoretical knowledge and practical experience to pursue careers in research, industry, and academia. Furthermore, a new course on **Oils, Fats, and Petrochemicals** has been approved and is set to begin in the 2025-2026 academic year.

Raghu Ramakrishna Raju K (RRR)
MLA, Undi Constituency
Former Member of Parliament (17th Lok Sabha)

सत्यमेव जयते

DEPUTY SPEAKER
ANDHRA PRADESH LEGISLATIVE ASSEMBLY

Message

I am pleased to extend my heartfelt congratulations to the **Department of Chemistry, Acharya Nagarjuna University**, for organizing the **UGC-sponsored National Seminar on "Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)"** on **3rd and 4th March 2025.** This seminar serves as an excellent platform for **academicians, researchers, and industry professionals** to exchange knowledge and explore innovations that contribute to **scientific advancements and sustainability.**

The **Government of Andhra Pradesh**is committed to strengthening **higher education, scientific research, and technological innovation** through initiatives such as the **National Education Policy (NEP 2020), increased research funding, and skill development programs.** These policies aim to enhance **industry-academia collaboration, innovation, and global competitiveness.** Chemistry, as a fundamental science, plays a crucial role in addressing **climate change, renewable energy, pollution control, and sustainable industrial practices.**

I deeply appreciate the efforts of **Acharya Nagarjuna University and the Department of Chemistry** in creating a platform that fosters **knowledge-sharing, academic excellence, and industry-academia collaborations.** Such initiatives strengthen our scientific ecosystem and contribute to the **nation's overall development by integrating research with real-world applications.**

I extend my best wishes to all the **distinguished speakers, scholars, and students** participating in this seminar. May this event lead to **meaningful discussions, transformative research, and impactful contributions** that drive progress for a better and more sustainable future.

Raghu Rama Krishna Raju K
Honorable Deputy Speaker
Andhra Pradesh Legislative Assembly

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ANDHRA PRADESH STATE COUNCIL OF HIGHER EDUCATION

(A Statutory Body of the Government of A.P.)

PROF. K.MADHU MURTHY
CHAIRMAN

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6th Battalion Road, Atmakur (V), Mangalagiri (M)
Guntur - 522 503, Andhra Pradesh

MESSAGE

Greetings to all distinguished academicians, researchers, industry experts, and students attending the National Seminar on Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025), organized by Acharya Nagarjuna University.

The field of chemical sciences has always been a cornerstone of scientific progress, driving transformative innovations across industries, healthcare, environmental stewardship, and energy systems. In our rapidly evolving world, sustainability has emerged as a defining global priority, and chemical sciences are uniquely positioned to address critical challenges such as pollution mitigation, circular waste management, renewable energy generation, and the development of green technologies. Recent advances in the discipline—from breakthroughs in biodegradable materials and carbon capture technologies to advancements in catalysis, nanotechnology, and AI-driven molecular design—underscore its pivotal role in shaping a sustainable future. Innovations such as green synthesis methods, energy-efficient electrochemical systems, and smart materials for environmental remediation highlight how chemical sciences are redefining industrial processes to minimize ecological footprints while maximizing efficiency.

This seminar need to serve as a vital platform for scholars and practitioners to exchange cutting-edge knowledge, deliberate on emerging trends, and forge collaborative pathways toward sustainability-driven solutions. I applaud the Department of Chemistry, Acharya Nagarjuna University for organizing this timely event, uniting thought leaders with student community, to explore and to elucidate how chemical sciences can accelerate progress toward global sustainability goals, including clean energy access, responsible consumption, and climate action. I urge all participants to engage actively in dialogues, share insights, and catalyze research initiatives that bridge scientific discovery with societal impact. The convergence of diverse expertise at RACSSD-2025 promises to spark innovative strategies and scalable solutions for the challenges ahead.

With every confidence that this seminar will yield transformative ideas and foster partnerships for a greener, more equitable world, I extend my best wishes for a successful and inspiring event!

(Prof.K.Madhu Murthy)

ACHARYA NAGARJUNA UNIVERSITY

The National Assessment and Accreditation Council (NAAC) Awarded ANU as 'A+' Grade University

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VICE-CHNCELLOR'S - MESSAGE

It is with great pleasure and pride that I extend my heartfelt greetings to all the distinguished scientists, researchers, academicians, industry professionals, and students participating in the *National Seminar on Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)*, organized by Department of Chemistry, Acharya Nagarjuna University.

Scientific progress in the field of chemical sciences has played a transformative role in shaping modern society. Today, as the world faces pressing challenges such as climate change, environmental degradation, energy crises, and resource management, the role of chemistry in developing sustainable solutions has become more crucial than ever. Innovations in green chemistry, renewable energy, and eco-friendly materials are driving the transition toward a more sustainable future. This seminar serves as a crucial platform for experts and young researchers to engage in meaningful discussions, exchange groundbreaking ideas, and collaborate on solutions that can lead to scientific and societal advancements.

Acharya Nagarjuna University has always been committed to fostering research and academic excellence. Hosting this national seminar is a testament to our dedication to promoting knowledge-sharing and interdisciplinary collaboration. I deeply appreciate the efforts of the organizing committee, faculty members, and research scholars who have worked tirelessly to make this event possible.

I encourage all participants to make the most of this opportunity by engaging in discussions, networking with peers, and contributing their insights to the ever-evolving field of chemical sciences. I am confident that the deliberations and research presented in RACSSD-2025 will inspire new ideas and pave the way for impactful advancements in sustainable development.

I extend my best wishes to the organizers and participants for a successful and intellectually enriching seminar. May RACSSD-2025 be a milestone in the pursuit of scientific innovation for a better and sustainable world.

K. Gangadhara Rao 28.2.25

VICE-CHANCELLOR

DHULIPALLA NARENDRA KUMAR
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Message

I am delighted to extend my heartfelt congratulations to the **Department of Chemistry, Acharya Nagarjuna University** for organizing the **UGC-sponsored National Seminar on "Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)"** on **3rd and 4th March 2025.** This seminar serves as an essential platform for **academicians, researchers, and industry professionals** to exchange knowledge, discuss pioneering innovations, and explore the role of chemical sciences in **sustainable development and societal progress.**

Scientific research and technological advancements are the cornerstones of progress, and **chemistry plays a crucial role** in shaping a more sustainable future. From **renewable energy and environmental protection to green materials and sustainable industrial practices,** the contributions of chemical sciences are vital in addressing global challenges. The topics covered in this seminar, including **green chemistry, nanotechnology, computational chemistry, and sustainable materials,** align with **India's sustainability goals** and reflect the **university's commitment to academic excellence and research-driven innovation.**

I deeply appreciate the efforts of **Acharya Nagarjuna University and the Department of Chemistry** in creating a platform that fosters **knowledge-sharing, academic excellence, and industry-academia collaborations.** Such initiatives not only strengthen our **scientific ecosystem** but also contribute to the **nation's overall development by integrating research with real-world applications.** By bridging the gap between **academia and industry,** this seminar paves the way for practical solutions that benefit both **science and society.**

I extend my **special congratulations to Dr. M. Subbarao, Director of RACSSD-2025, and Professor & Head of the Department of Chemistry, Acharya Nagarjuna University,** for his exemplary leadership in organizing this seminar. His dedication to **promoting research excellence, fostering collaborations, and advancing scientific innovation** is truly commendable.

I extend my **best wishes to all the distinguished speakers, scholars, and students** participating in this seminar. May this event lead to **meaningful discussions, transformative research, and impactful contributions** that drive progress toward a **better, more sustainable future.**

Sri Dhulipalla Narendra Kumar
Hon'ble Member of Legislative Assembly
Ponnur Assembly Constituency

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ACHARYA NAGARJUNA UNIVERSITY

The National Assessment and Accreditation Council (NAAC) Awarded ANU as 'A+' Grade University

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Message

It is with great pleasure that I extend my warmest greetings to all participants of the National Seminar on "**Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)**", organized by the **Department of Chemistry, Acharya Nagarjuna University**, on 3rd and 4th March 2025. This seminar serves as a vital platform for researchers, academicians, and industry professionals to exchange knowledge, present pioneering research, and explore advancements in chemical sciences that contribute to global sustainability efforts.

As environmental challenges continue to rise, the significance of chemical sciences in addressing sustainability has become more pronounced than ever. The need for innovative solutions in green chemistry, renewable energy, and eco-friendly industrial processes is essential to balancing technological growth with environmental responsibility. This seminar will facilitate discussions that not only advance scientific knowledge but also influence industry practices and policymaking, ultimately fostering a more sustainable future. The transition towards responsible chemical processes is imperative for ensuring a greener and healthier planet, and RACSSD-2025 plays a key role in accelerating this progress.

I sincerely appreciate the efforts of the Department of Chemistry, Acharya Nagarjuna University, for organizing this significant seminar and creating a platform for meaningful discussions on sustainable advancements in chemical sciences. My heartfelt gratitude goes to all contributors and supporters for their dedication to fostering research and academic excellence. I am confident that **RACSSD-2025** will pave the way for innovative discoveries, enhance academic collaborations, and drive progress toward a more sustainable future. Wishing all participants a productive and insightful seminar experience.

Prof.K.Ratna Shiela Mani

ACHARYA NAGARJUNA UNIVERSITY

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MESSAGE

I am delighted to extend my warm greetings to all the distinguished participants of the *National Seminar on Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)*, organized by Acharya Nagarjuna University.

This seminar serves as a vital platform for researchers, academicians, and industry experts to exchange knowledge and innovative ideas in the field of chemical sciences, focusing on sustainable solutions for a better future. In an era where environmental concerns and resource management are critical, scientific advancements in chemistry play a pivotal role in shaping a sustainable world.

I congratulate the organizers for their efforts in bringing together experts from various domains to discuss groundbreaking research and its practical applications. I am confident that the deliberations in this seminar will contribute significantly to the scientific community and society at large.

Wishing RACSSD-2025 great success!

G. S

REGISTRAR

ACHARYA NAGARJUNA UNIVERSITY

Nagarjuna Nagar – 522 510, Guntur (Dt), Andhra Pradesh, India.

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DEPARTMENT OF CHEMISTRY

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Message

It is with great pleasure and enthusiasm that I welcome you all to the UGC-sponsored National Seminar on "**Recent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025),**" scheduled for 3rd and 4th March 2025, organized by the Department of Chemistry, Acharya Nagarjuna University. This seminar provides a platform for researchers, academicians, and industry professionals to exchange ideas, showcase research, and explore advancements in chemical sciences that contribute to global sustainability.

Chemical sciences are at the forefront of addressing major global challenges such as climate change, pollution, resource depletion, and energy crises. Chemistry plays a vital role in renewable energy, green materials, pollution control, and sustainable industrial processes. Innovations in green chemistry, nanotechnology, catalysis, and advanced materials are transforming industries, creating sustainable solutions that balance progress with environmental responsibility.
Recent advancements in chemical sciences have driven groundbreaking innovations in organic and perovskite solar cells, hydrogen fuel cells, and next-generation batteries, revolutionizing clean energy. Computational quantum chemistry is enabling precise molecular modeling, optimizing chemical reactions, and designing green catalysts to make industrial processes more sustainable. Sustainable chemistry practices, such as biodegradable plastics, carbon capture technologies, and waste-to-energy solutions, are shaping a cleaner future.

Computational quantum chemistry, in particular, is revolutionizing sustainability efforts. High-performance computing and AI-driven simulations allow researchers to develop eco-friendly catalysts, enhance energy efficiency, and reduce hazardous waste. By bridging research and industry, computational chemistry helps policymakers and industries adopt low-impact technologies and make data-driven sustainability decisions.

The RACSSD-2025 seminar brings together leading experts, scholars, and young researchers to exchange knowledge, inspire innovation, and promote real-world applications of sustainable chemistry. I extend my sincere gratitude to the University Grants Commission (UGC) and Acharya Nagarjuna University authorities for their invaluable support. My heartfelt thanks to our distinguished speakers, researchers, and participants for their contributions to this important event.

I am confident that this seminar will catalyze groundbreaking research, foster collaborations, and contribute to the advancement of chemical sciences for a sustainable future. Let us engage in insightful discussions, embrace innovation, and work collectively toward a future where science and sustainability go hand in hand.
Wishing you all a successful and enriching seminar experience!

Dr. M. Subbarao
Director, RACSSD-2025
Professor & Head, Department of Chemistry
Acharya Nagarjuna University

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Invited
TALKS

Keynote Address

The Role of Computational Quantum Chemistry methods in designing Organic Solar Cells for Sustainable Renewable Energy

Prof. Nambury SB
Full Professor,
Department of Chemistry
University of Dodoma, Tanzania
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Abstract

The transition to sustainable renewable energy sources is a global imperative, and organic solar cells (OSCs) have emerged as a promising alternative due to their lightweight, flexible, and cost-effective nature. However, optimizing their efficiency and stability remains a significant challenge. Computational Quantum Chemistry has emerged as a powerful tool for designing and optimizing organic solar cells (OSCs), offering precise insights into molecular properties, electronic structures, and charge transport mechanisms. Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) provide reliable computational frameworks for predicting energy levels, absorption spectra, and donor-acceptor interactions, essential for enhancing OSC efficiency. This talk explores the pivotal role of computational methods in designing high-performance organic photovoltaic materials. By analyzing molecular orbitals, absorption spectra, donor-acceptor interactions, and solvent effects, researchers can systematically tailor materials to enhance light-harvesting capabilities and charge carrier mobility. Additionally, quantum chemical approaches facilitate the screening of novel materials, reducing experimental trial-and-error efforts and accelerating the discovery of sustainable energy solutions.

Invited Talk-1

Opportunities and Challenges in Natural Products Research for Drug Discovery

Dr. K. Suresh Babu
Senior Principal Scientist
Division of Natural Products and Medicinal Chemistry
CSIR-Indian Institute of Chemical Technology,
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Abstract

The Indian subcontinent has a vast costal belt along with the wide range of forest environment, which host large number of un explored plant/marine species. This diversity has been the source of unique chemical compounds with the potential for industrial development as pharmaceuticals, cosmetics, nutritional supplements, fine chemicals and agrochemicals. In recent years, a significant number of novel metabolites with potent pharmacological properties have been discovered from the natural sources including marine and terrestrial plants. Recent move of society towards nature for the treatment of various diseases where there is no satisfactory cure in modern medicine has diverted the attention of natural/medicinal chemists and biologists to unravel their chemical characteristics and biological activities together in order to define their therapeutic potential in the light of modern pathobiological understandings. This move has led collectively to rediscover, design and refine the therapeutic application of medicinal plants/marine sources.

During last fifteen years, we have studied several medicinal plants and marine organisms guided by in vitro based bioassays to delineate the chemistry of natural products responsible for biological activities.This effort has led to identify several potent multiple active medicinal plants/marine sponges, their active fractions and synergistic molecular compositions. We have identified particularly, several free radical scavengers, anti-cancer, anti-viral, xanthine oxidase and α-glucosidase inhibitory principles present in substantial yields. Presence of multiple active phytochemicals in rich concentrations in some of the medicinal plants therefore offers exciting opportunity for development of novel therapeutics and also provides scientific justification for their use in traditional medicines. Therefore, biologically activity based chemical characterization of these medicinal plants may provide scientific explanation for their use in traditional medicines and also redesign and develop preparations for novel therapeutic applications.

Invited Talk-2

DNA-targeted Cytotoxic Agents in Cancer Drug Discovery: Molecular Hybridization Approach

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Abstract

Over the past four decades, the prevalent global threat posed by cancer has prompted an urgent quest for alternative therapeutic avenues. In recent years, a wide range of strategies have been meticulously reviewed and investigated in an effort to create an effective therapy, to slow the concerning rise in the number of cancer cases worldwide. This can be attributed to the rapid proliferation of cancer cells and the multi-drug resistance.1 In this endeavour, DNA has emerged as a highly promising and pivotal biological target for the development of potent anticancer agents. The pursuit of cancer treatments has led to a strategic exploration of molecular structural modifications and the integration of pharmacophoric elements into these frameworks. This strategic amalgamation, as illustrated in Figure 12, entails a novel paradigm in drug design and development. It involves ingeniously fusing two distinct pharmacophores, giving rise to new hybrid scaffolds that might exhibit enhanced affinity and efficacy compared to their parent compounds.

In continuation of our efforts in the design, development and synthesis of new chemical entities (NCEs) of anticancer agentsthrough this pioneering approach, our research team has methodically curated a versatile collection of compounds by employing different heterocyclics such as β-carbolines, isatin, benzimidazoles, 3-alkenyl oxindoles, 1,2,3-triazoles/tetrazoles, chalcones, podophyllotoxins, phenanthrenes, thiazolidinediones, etc. Furthermore, with the aid of molecular docking studies, we explored the interaction of these designed molecules with various key protein targets specifically, tubulin and topoisomerases accounting for its ability to be involved in various DNA-dependent processes.3 This detailed analysis offers insights into the potential mode of action, shedding light on the binding interactions that underlie their potency against cancer cells. Selected compounds from this library have demonstrated noteworthy anticancer efficacy within the sub-micromolar scale across specific human cancer cell lines.

Figure 1. Molecular hybridization approach.

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Invited Talk-3

The Efficient Construction of Functionalized Heterocyclic Compounds

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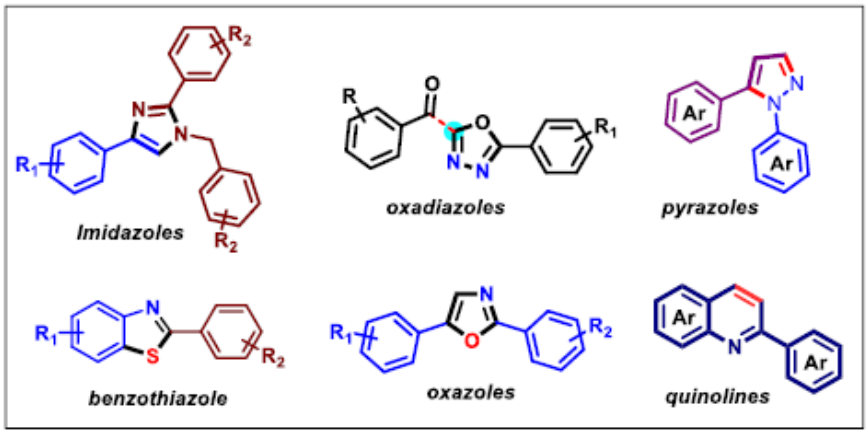
Abstract

Heterocyclic compounds are intriguing structures that include one or more heteroatoms—like nitrogen, oxygen, or sulfur—within a ring. This inclusion of heteroatoms affects the compound's properties compared to all-carbon rings. The most common heterocycles feature five- or sixmembered rings that include heteroatoms such as nitrogen (N), oxygen (O), or sulfur (S). Some of the best-known simple heterocyclic compounds are pyridine, pyrrole, furan, and thiophene. A key aspect of many heterocyclic compounds is their structural versatility, allowing for the incorporation of functional groups either as substituent or as part of the ring itself. This flexibility enables these compounds to effectively provide or mimic various functional groups, enhancing their utility in a wide range of chemical applications. Considering all aspect of having significant properties and applications, here in, we have effectively engaged to develop a list heterocyclic valuable scaffold like 1,5-disubstituted pyrazoles, 3,3-diindolyl derivatives, 1,3,4-oxadiazoles, 2,5-disubstituted oxazoles, 2,4,6-triarylpyridines, 2-(dimethylamino) pyrimidine, 2-substituted benzimidazoles, substituted imidazoles, 2-arylquinolines, etc, which is shown in Scheme 1.



Scheme 1. Development of various important heterocyclic moieties

Invited Talk-4

Hydrogels for Sustainable Development

Prof. Anitha C Kumar
Director, School of Chemical Sciences Mahatma Gandhi University, Kerala.

Abstract

Hydrogels are three-dimensional networks of polymer chains capable of absorbing and retaining substantial amounts of water. They have garnered significant interest across diverse scientific fields due to their remarkable swelling behavior. This unique characteristic, driven by the hydrophilic nature of their constituent polymers, enables hydrogels to expand in response to environmental stimuli such as changes in pH, temperature, or solute concentration. Their versatility makes them invaluable materials in applications ranging from biomedical engineering to environmental science. Hydrogels can be made from a variety of materials including synthetic polymers, naturally occurring biopolymers, and low molecular weight gelators (LMWG). LMWG are small molecules like amino acids, peptides, etc (typically with a molecular weight < 1000 Da) that self-assemble in water to form a hydrogel. Understanding the physical and chemical properties of polymeric hydrogels is paramount for harnessing their potential. These hydrogels exhibit a wide range of characteristics influenced by factors such as polymer composition, cross-linking density, and fabrication techniques. Notably, they possess excellent biocompatibility, making them ideal for various biomedical applications without triggering adverse reactions. Additionally, their mechanical properties can be finely tuned to match those of biological tissues, facilitating their use as scaffolds in tissue engineering. Moreover, their porous structure and high water content enable efficient diffusion of solutes, making them promising candidates for controlled drug delivery systems. In biological applications, in general, the polymer backbone and its degradation products have to be biodegradable and biocompatible. The major limitations with polymeric hydrogels when the desired applications are biological are that the presence of radical materials from the polymerization process can damage cells and if a controlled release application is desired, encapsulation of the drug material may also be affected by the presence of these radical materials. In this talk, the characteristics, properties, and applications of natural polymeric hydrogels will be discussed.

Invited Talk-5

Long-Lived Charge Separated Donor-π-Acceoptor Porphyrin Sensitizers For Dye-Sensitized Solar cells

Lingamallu Giribabu
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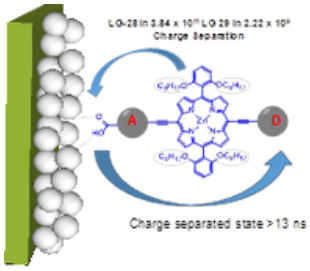
Abstract

Creation of long-lived charge separated species in Donor-π-Acceptor porphyrins (milli to nano seconds) is a challenging task. This will not only useful to understand the initial events of natural photosynthesis but also one can design efficient materials for optoelectronic applications. The sensitizer is one of the essential components of the dye-sensitized solar cells (DSSCs) in achieving high efficiency and durability. The widely used sensitizers in these devices are Ru(II) polypyridyl complexes with certified efficiencies of >11%. In spite of this, the main drawbacks of these sensitizers are lack absorption in near-IR region and also expensive due to rarity of the metal in earth's crust that hamper further improvement of the device. In this regard, porphyrins are found to be alternatives to Ru(II) polypyridyl complexes based on their optical, electrochemical and thermal properties. A great variety of porphyrin based sensitizers have been reported but their efficiency remains at around 7%. Recently, porphyrins using donor-π-acceptor (D-π-A) approach have reached an efficiency of 13%. This opens a new window porphyrin sensitizers for DSSC applications. Our groups also involved in the design of new efficient porphyrin sensitizers using D-π-A approach by varying donor and acceptor groups to understand the structure and efficiency relation. The details of molecular design, synthesis, characterization and device evaluation will be present.



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Invited Talk-6

Forensic Aspects of Drugs of Abuse

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Abstract

Globally **Drug abuse & Drug Addiction** has emerged as a significant social threat, contributing to crime, economic burden, and public health crises. Drug abuse refers to the misuse of substances like illegal & prescription drugs for non-medical purposes. Drug addiction is a chronic condition where a person becomes physically and psychologically dependent on these substances, leading to harmful consequences. In India, drug abuse is a growing concern, particularly among the youth. The easy availability of drugs like Ganja (cannabis), Opiods, and synthetic substances has worsened the situation. It affects individuals, families, and society in multiple ways. To combat drug abuse, the Indian government has implemented strict Narcotics laws, awareness campaigns, and rehabilitation programs. However, collective efforts from families, schools, colleges, and society are necessary to prevent and control drug addiction effectively.

Narcotic & Psychotropic substances (NDPS) can be categorized into Narcotics, stimulants, depressants, hallucinogens, and synthetic drugs. In India, commonly abused substances include opioids, cannabis, cocaine, amphetamine-type stimulants, and novel psychoactive substances (NPS). **Forensic Chemistry** plays a crucial role in investigating NDPS-related cases by using advanced instrumental techniques such as HPTLC, FT-IR GC-MS, and LC-MS (QTOF) with Drug spectral database for accurate identification and quantification of controlled NDPS substances. **Forensic science laboratory (FSL)** reports serve as critical evidence in the criminal justice system, aiding in the prosecution and adjudication of NDPS cases. A collaborative approach between forensic scientists, legal experts, and law enforcement authorities is essential in the fight against drug abuse, which remains a global threat.

This talk will primarily highlights the Forensic aspects of NDPS, focusing on their classification, sources, symptoms, and effects of addiction, forensic analysis of NDPS drugs and some of the case studies related to NDPS Drugs.

Invited Talk-7

Superhydrophobic Nano-Structured Porous Coordination Polymer-based Electro-Catalysts for Water Splitting

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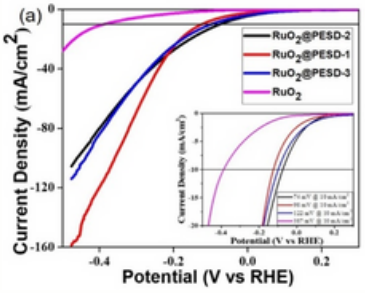
Abstract

Porous coordination polymers (PCPs), also known as metal-organic frameworks (MOFs), have emerged as potential materials of the decade, particularly for gas storage, separation, catalysts, sensors, etc. However, PCPs in the literature were mostly unstable regarding moisture and bulk water. Besides these traditional PCPs, we have designed and synthesized an organic-rich, low-density-based ligand and converted them into MOFs showing exceptional superhydrophobic properties.1-4 In the present study, we achieved PCPs/nanosheet-based superhydrophobic PCPs and nanoparticle-embedded superhydrophobic PCPs for electro-catalytical water-splitting applications.5 Here we report on metallic and bimetallic PCP-based electro-catalysts, achieved by the solvothermal method. All of them were characterized by PXRD, SEM, TEM, EDX, etc. The electro-catalytical analyses of water splitting studies on these PCPs demonstrate strong electro-catalytic capabilities for hydrogen evolution reactions (HERs)6 and oxygen evaluation reactions (OER). This study presents a simple approach for producing high-performance PCP-based electro-catalysts with numerous exposed active sites derived from metallic and bimetallic PCPs.



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Invited Talk-8

Hydrogen : The Sustainable Energy Source for Future

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Abstract

Problems associated with burning fossil fuels will be reviewed. Types of renewable energy sources will be listed and discussed. Hydrogen, the 'forever fuel', that we can never run out of as it is so important and the usage is environmental friendly.
The methods of chemical production of hydrogen, hydrogen storage and the innovative perspectives of hydrogen fuel technology will be summarized.
Recent advances in the potential use of hydrogen as green fuel for transportation will be presented. Hydrogen fuel economy, sustainability of hydrogen and newer applications will also be discussed.

Keywords: Fossil fuels, Renewable energy sources, Hydrogen, Fuel-cell, Sustainable materials, Eco-friendly methods, Future perspectives.

Invited Talk-9

Diversity Oriented Synthetic Methodologies for The Next Generation Therapeutics

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Abstract

Scientific advancement from Stone Age to Nano Era, there is a competition between construction and destruction. There is a growing demand for the methodologies of green in design and implementation. Methodologies to synthesize molecules of commercial value and their derivatives of biological importance is the attractive area of research, thereby creating library of known and unknown molecules having potential applications. Synthetic methods that allow rapid access to large number of diverse structural arrays is growing constantly, which served as a new driving force for the new innovations. In order to synthesize large number of molecules with high level of diversity and complexity, In addition to developing new synthetic techniques and reagents, organic chemists are exploring new methods to design and to evolve new molecules, strategies for new molecules leading to new source of diversity and improving the quality of compound libraries of natural product origin. This diverse new methodologies that will create structurally diverse compounds efficiently in high yields and with excellent purity and with wide range of functional groups as handles to expand them further. One of the richest source of diversity in drug discovery are development of synthetic routes for the natural products and their derivatives. Natural products isolated from marine and terrestrial origins, in addition to exhibiting biological activity, also serve as rapid scaffolds for further display of broad range of functionalities. M.V. Basaveswara Rao have been engaged in design and development of new efficient methodologies for a wide variety of heterocycles, displaying a range of skeletal and functional group diversity. The biological properties of heterocycles in general make them one of the prime interests of the pharmaceutical industry, storage device platforms for opto-electronic industry. We have synthesized various heterocyclic skeletons initially and utilized them for making other heterocycles.

All the synthetic methodologies reported by us are simple efficient and does not involve hitherto costlier chemicals, circuitous reaction pathways, drastic reaction conditions and corrosive molecules. We have exploited [4+2]cycloaddition reactions, [3+3]Cycloaddition reactions, indolo[2,3]quinodimethanes and dienolates, anion assisted aromatic annulations, heteroaromatic annulations and doubly handled reactions. Our aromatic and heteroaromatic annulation strategies are highly efficient, simple and results in variety of molecules with quantitative yields. More focus needs to be placed on building blocks for the translation of materials from laboratory scale to market. We made successful attempts on synthesis of Ammonium persulphate mediated polyaniline, Natural gum mediated catalysts, FeCo Nanoparticles by one pot polyol process, Reusable Nano Zirconia Catalysis, Cellulose and Pectin with Incorporated Zinc Oxide Nanoparticles, Ferrous Doped Titanium Dioxide Nanoparticles, ZnO nanoparticles, Ni Doping by Sol-gel Process, FeTiO2 Nanopaticles, Cu doped ZnO nano particles, hydrothermal Synthesis of Magnetite Nanoparticles, FeCo luminescence of AgGd(MoO4)2:Er3+/Yb3+@mSi core-shell up conversion nanoplates, Selenium Enriched Cobalt Selenide Nanotube for Super capacitor Application, warm white light emission from Gd2TiO5:Dy3+/Eu3+ nanophosphors. Design of shape-engineered visible light (silica) based materials (nanowires and nanorods) for decontamination of pesticides as a novel eco-friendly photo catalyst. Artificial rain is a perennial task for sustainable future Water scarcity. Hygroscopic cloud seeding - NaCl crystals as conventional hygroscopic material - attract water droplets and promote collision-coalescence process to form bigger droplets. The daunting task of the 21st Century is to clean up the contaminants of not only the environment but also the soil with viable technologies with features of eco-friendly and sustainable materials. Design of shape-engineered Fe based Materials for detoxification of soil Wet chemical methods for synthesis of targeted materials. Development of fullerene/poly-anyline (PANI) nanocomposite materials-based sensors for soil moisture detection. For the cancer treatment the Surgery became invasive, Chemotherapy multidrug resistance problems arise, Radiotherapy higher risk of damage to normal tissues, Boron Neutron Capture Therapy (BNCT) – boron enriched reagent & neutron irradiation, Phototherapy – minimally-invasive, need light, oxygen and a photosensitizing dye molecule. Iron Encapsulated carbon nanoparticles with lipid dyes make a path for the singlet oxygen generation useful for photo dynamic therapy there by finding better way of cancer treatment.

Oral

PRESENTATIONS

OP-1 Oral Presentation

Green Chemistry and Sustainable Manufacturing

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ABSTRACT

Advances in chemical sciences have made significant strides toward supporting sustainable development in various ways. These innovations have focused on addressing environmental challenges, reducing waste, and developing cleaner technologies, there has been a significant push towards replacing traditional petroleum-based plastics with biodegradable alternatives. Researchers have developed new types of biodegradable polymers from renewable sources, such as starch, polylactic acid (PLA), and polyhydroxyalkanoates (PHA). Innovations in using more environmentally friendly solvents in chemical processes have been a major focus. Ionic liquids, supercritical CO_2, and water are examples of solvents that reduce toxicity and the environmental footprint of industrial chemical processes. Advances in catalytic processes, such as using non-toxic metals (like iron or copper) in place of more hazardous heavy metals, help reduce environmental contamination. Enzyme-based catalysis also shows promise for reducing energy consumption in manufacturing (1). The development of high-performance, sustainable energy storage devices is crucial for a clean energy transition. Researchers are exploring novel battery technologies like solid-state lithium batteries, sodium-ion batteries, and organic redox flow batteries, which offer more sustainable alternatives to traditional lithium-ion batteries. Solar energy has benefited from breakthroughs in organic photovoltaics (OPVs) and perovskite solar cells, which are cost-effective and can be produced with less energy-intensive processes. Efforts to scale up production and improve the efficiency of these solar cells are contributing to the global shift toward renewable energy. Sustainable hydrogen production methods, like electrolysis powered by renewable energy, are being refined to replace fossil fuel-based methods. Research is focused on improving the efficiency and reducing the cost of electrolyzers (2). Traditional mechanical recycling methods often result in a loss of quality of materials. Chemical recycling, which breaks plastics down to their chemical building blocks to create new products, is seen as a potential solution to plastic waste. Chemists are developing innovative ways to upcycle waste materials (like plastic waste, agricultural waste, and food scraps) into higher-value products, reducing the need for virgin resources and minimizing waste. The development of advanced membrane materials, including those made from nanomaterials, has revolutionized water filtration and desalination processes. These materials are more efficient at removing contaminants from

water, helping address water scarcity and improving access to clean water. The use of photocatalysts (materials that use light to accelerate chemical reactions) in water purification has emerged as a promising solution for removing pollutants, including heavy metals, organic contaminants, and pathogens, from water sources (3). Sustainable chemistry is making strides toward replacing petrochemical-based raw materials with renewable feedstocks. This involves using plant-based materials (such as sugars, oils, and lignocellulose) as the starting point for producing chemicals, reducing dependency on fossil fuels. Advances in sustainable chemistry have led to the development of textiles made from renewable or recycled fibers and the creation of environmentally friendly dyes and treatments. This contributes to reducing the fashion industry's impact on the environment.

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OP–2 Oral Presentation

Green Chemistry for Sustainable Development

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ABSTRACT

Green chemistry is an innovative field that promotes Eco friendly and sustainable practices in chemical processes to revolutionize chemical processes by emphasizing environmental stewardship, energy efficiency, and resource conservation to minimize environmental impact, reduce energy consumption, and promote resource efficiency. This interdisciplinary approach aims to create safer, more efficient methods of producing chemicals while minimizing waste, toxicity, hazardous materials and improve the overall sustainability of chemical production.

Key strategies and innovations include the use of implementation of biocatalysis, green solvents, renewable feed stocks, energy integration, and advanced recycling techniques are path ways. Moreover, the adoption of sustainable manufacturing practices, such as modular and continuous flow systems, offers enhanced control over reaction conditions, leading to higher efficiency and lower environmental impact.

This paper explores the advances in green chemistry, highlighting the role of sustainable practices in the chemical industry, and the importance of lifecycle assessments and circular economy principles in shaping future innovations. Cutting-edge green technologies and their potential to drive sustainable chemistry across various sectors, from pharmaceuticals to materials production. Challenges and opportunities for integrating sustainability into chemical research and manufacturing processes, emphasizing the need for collaboration across science, policy, and industry to foster a sustainable future.

The core concepts of green chemistry and its applications across various industries, including pharmaceuticals, agriculture, and materials science. The integration of green chemistry principles into industrial practices is vital for creating sustainable solutions and addressing the global challenges of climate change and resource depletion.

Keywords: Green chemistry, Eco friendly, interdisciplinary, hazardous materials, implementation, environmental impact, Cutting-edge, sustainable practices, collaboration, pharmaceuticals, challenges, depletion.

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OP–3 Oral Presentation

Nanocatalysis In Environmental Remediation and Sustainable Pollution Control

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ABSTRACT

Environmental remediation and sustainable pollution control are critical to mitigating the harmful effects of industrialization, urbanization, and increasing human activities on ecosystems. The growing concerns over air, water, and soil contamination have driven the search for innovative, cost-effective, and efficient solutions for pollution management. Recent advancements in nanotechnology, particularly in the field of nanocatalysis, have shown great promise in addressing these challenges. Nanocatalysts, with their unique properties such as high surface area, enhanced reactivity, and tunable function, can facilitate the degradation of organic pollutants, removal of heavy metals, and the treatment of industrial effluents and wastewater. Nanocatalysis has changed perspectives and expectations and provides the capability to resolve global issues.

Nanocatalysts, typically composed of metals, metal oxides, and carbon-based materials, are highly effective in breaking down pollutants such as organic contaminants, heavy metals, and greenhouse gases through processes like catalytic oxidation, reduction, and photocatalysis. Their small size enables them to interact efficiently with pollutants at the molecular level, promoting faster reaction rates and improved degradation. In addition, the use of nanocatalysts can reduce the energy required for conventional treatment processes, offering a more sustainable and cost-effective solution.

This article focuses on the process of cleaning up, removing, or neutralizing pollutants from the environment, typically to restore contaminated land, water, and air to a healthier state by synthesizing novel nanocatalyst solutions such as NiCoFe-NPs, CoFe-NPs, etc. The reduction or elimination of the harmful effects of pollution on ecosystems, human health, and natural resources has been detailed.

OP–4 Oral Presentation

Recent Advances in Chemical Sciences for Sustainable Development
Green and Sustainable Medicinal Chemistry

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ABSTRACT

That's a great summary of how recent advances in chemical sciences have contributed to sustainable development in medicinal chemistry. Green chemistry approaches, renewable resources, and innovative drug design strategies are indeed revolutionizing the field and leading to more environmentally friendly and efficient processes. The use of bio-based solvents, catalytic processes, and eco-friendly synthesis methods is helping to reduce the environmental impact of drug production. Computational chemistry and AI-driven drug discovery are also playing crucial roles in speeding up drug development and improving safety profiles. The integration of biotechnology, especially enzyme-based synthesis and biocatalysis, is enabling the production of pharmaceuticals with reduced waste and energy consumption. It's truly impressive to see how these advancements are shaping the future of medicinal chemistry in a more sustainable and efficient manner. Absolutely, the recent progress in sustainable medicinal chemistry aligns well with several United Nations Sustainable Development Goals (SDGs) related to responsible consumption and production, good health and well-being, and environmental sustainability. By adopting green chemistry approaches, utilizing renewable resources, and implementing eco-friendly synthesis methods, the field is contributing to the SDGs by reducing waste, minimizing environmental impact, and promoting more sustainable practices in drug development and production. These advancements also have the potential to improve healthcare by accelerating the discovery and development of safer and more effective drugs. Overall, the progress in sustainable medicinal chemistry holds significant promise for achieving a more sustainable future in drug development while supporting the broader objectives of the SDGs.

Keywords: Green chemistry, Sustainable drug synthesis, Biocatalysis, Computational drug discovery, Renewable resources

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OP–5 Oral Presentation

Enaminone-Based Synthesis of α,β-Unsaturated β-Amino Ketones: A CSA-Catalyzed Approach

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ABSTRACT

A novel synthesis protocol has been developed for producing (α,β-unsaturated)-β-amino ketones from enaminone and aromatic amines, utilizing (±)-10-camphor sulfonic acid (CSA) as a catalyst. This method is efficient, convenient, and employs an inexpensive and non-toxic catalyst. Twelve (α,β-unsaturated)-β-amino ketones were successfully synthesized using this protocol, yielding excellent results. The methodology demonstrates broad applicability, accommodating various substituted aromatic amines. The use of CSA as a catalyst enhances the reaction's efficiency and sustainability. Overall, this new protocol offers a valuable addition to existing synthetic strategies, providing a reliable and efficient means of producing (α,β-unsaturated)-β-amino ketones.

Key words: (α,β -unsaturated)- β -amino ketones; enaminone; (±)-10-camphor sulfonic acid (CSA), aromatic amines.

OP-6

Oral Presentation

A Validated stability-indicating UPLC method for Nirogacestat was developed by separating its related impurities.

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ABSTRACT

Objective: Nirogacestat, sold under the brand name Ogsiveo, is an anti-cancer [1] medication used for the treatment of desmoid tumors. It is a selective gamma secretase inhibitor that is taken by mouth. The most common side effects include diarrhea [2], ovarian toxicity, rash, nausea, fatigue, stomatitis, headache, abdominal pain, cough [3], alopecia, upper respiratory tract infection and dyspnea.

Methods: By using Waters Acquity UPLC system with a PDA detector of 2998 instrument the chromatographic separation of Nirogacestat and its related impurities was achieved on the column of Phenomenex C18, (50 mm x 2.1mm, 1.6 pm) using isocratic elution of (60+40) with a buffer containing 0.1% Formic acid and acetonitrile as a mobile phase with a flow rate of 0.3 ml/min at ambient temperature. A detector wavelength of 232 nm utilizing the PDA detector were given in the instrumental settings. Validation of the proposed method was carried out according to an International Conference on Harmonization (ICH) guidelines.

Results: LOD and LOQ for the Nirogacestat and its impurities were established with respect to test concentration. The plotted calibration curves were linear with a regression coefficient of R2 0.999, indicates that the linearity was within the limit. As a part of method validation the parameters like specificity, linearity, accuracy, ruggedness, robustness were determined and the results were found to be within the allowable limit.

Conclusion: The method developed was found to be applicable to routine analysis and to be used for the measurement of active pharmaceutical ingredients (i.e, Nirogacestat and its related impurities). Since, there is no UPLC method reported in the literature for the estimation of Nirogacestat and its related impurities, there is a need to develop quantitative methods under different conditions to achieve improvement in specificity, selectivity etc.

***Key words*:** Nirogacestat, Related impurities, UPLC, Development, Validation.

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Investigating the Synergistic Effects of *Crotalaria pallida* Fibers on PVA Composite Performance

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ABSTRACT

The incorporation of natural fibers into polymer composites has gained significant attention due to their sustainability, cost-effectiveness, and potential to enhance material performance. This study investigates the synergistic effects of *Crotalaria pallida* fibers on the mechanical, thermal, and morphological properties of polyvinyl alcohol (PVA) composites. *Crotalaria pallida* fibers were extracted, chemically treated, and integrated into a PVA matrix at varying concentrations to evaluate their impact. Mechanical testing revealed improvements in tensile strength, modulus, and impact resistance, demonstrating enhanced load-bearing capabilities. Thermal analysis indicated increased thermal stability and reduced degradation rates, attributed to strong interfacial adhesion between the fiber and matrix. Morphological characterization through scanning electron microscopy (SEM) confirmed uniform fiber dispersion and reduced void content, contributing to improved composite integrity. The findings suggest that *Crotalaria pallida* fibers serve as an effective reinforcement for PVA-based composites, offering a promising pathway toward sustainable and high-performance biomaterials. These PVA composite films exhibit enhanced mechanical properties, biodegradability, and potential for various applications, including packaging, biomedical devices, and agricultural films

Keywords: Ssustainable materials, Biocomposites, *Crotalaria pallida* fibers, Polyvinyl alcohol (PVA)

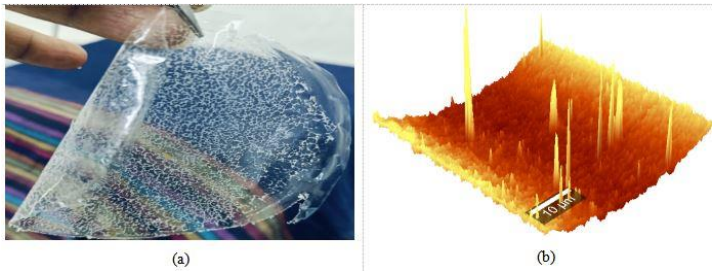

Fig.1. PVA composite film formation and characterization

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OP-8 Oral Presentation

Redefining Chemistry: Advanced Computational Strategies for Tackling Intractable Challenges and Driving Innovation

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ABSTRACT

Computational chemistry is revolutionizing science by integrating quantum mechanical (QM) methods with advanced computational models to study and predict chemical behavior. By employing mathematical algorithms at the atomistic level, it overcomes the limitations of experimental approaches restricted by cost, complexity, and time constraints. This field encompasses molecular mechanics, ab initio QM methods, semi-empirical techniques, and machine learning (ML)-assisted modeling, enhancing computational precision.

Expanding beyond density functional theory (DFT), hybrid QM/MM approaches provide deeper insights into molecular geometry, electronic structures, activation energies, and stability. These methodologies enable accurate predictions of reaction pathways, thermodynamics, and kinetics, supporting applications such as process optimization, molecular energy calculations, ligand-based and structure-based drug design, molecular docking, and virtual screening.

The implementation of computational chemistry involves method selection, basis set optimization, and software tools like Gaussian and ORCA. The accuracy of these approaches depends on parametrization databases, ranging from experimental datasets to high-level quantum data. Core principles such as stability, symmetry, quantization, and homogeneity underpin molecular and material behavior.

Advancements in computational and quantum chemistry are transforming fields such as materials science, catalysis, and direct air capture (DAC) technologies. The integration of AI and ML provides innovative solutions to intractable chemical problems, bridging theoretical research with industrial-scale applications. This interdisciplinary approach underscores the transformative potential of computational chemistry in shaping science, technology, and sustainability, reinforcing its indispensable role in addressing global challenges.

Key Words: QM- Quantum Mechanical; MM-Molecular Mechanics; ORCA-Optimized Really Fast Computational Applications; DFT-Density Functional Theory; DAC-Direct Air Capture; AI- Artificial Intelligence; ML-Machine Leaning

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OP-9

Oral Presentation

Bioactivity and mechanical properties of CaO-Na_2O-SiO_2-B_2O_3-P_2O_5 modified glasses with Al_2O_3

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ABSTRACT

Research works have carried out on the bioactivite glasses studying their bond to soft or hard tissues. The primary indicator of bioactivity in these glasses is their ability to form a hydroxyapatite (HA) layer on their surface when exposed to simulated body fluids (SBF). Hence chemical bonding implant and certain glass composition is possible so called bioactive glasses. The repair and reconstructions of diseased and damaged tissues (hard one). Both B_2O_3 and Al_2O_3 act as network modifiers, changing the structure of the glass. This, in turn, affects its mechanical and biological properties. The "acceptable amount" of Al_2O_3 is not a fixed value. It varies significantly depending on the concentrations of other oxides in the glass, such as CaO, Na_2O, SiO_2,B_2O_3 and P_2O_5. The ability to tailor the composition of bioactive glasses allows for the development of materials with specific properties for different clinical applications. The surface structure changes were examined by SEM-EDX line scan X-ray microanalysis and calcium deposition. It was found that all composition of glasses forming a rich layer.

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OP-10

Oral Presentation

Ultrasound mediated nano ZnO catalyzed synthesis of new *a*-aminophosphonates as potential anti-diabetic agents; An *In silico* ADMET, molecular docking study, *a*-amylase and *a*-glucosidase inhibitory activity

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ABSTRACT

Diabetes is a chronic condition resulting from insufficient insulin production or ineffective insulin utilization by the body, often leading to elevated post-meal blood sugar levels. A key strategy in managing early-stage diabetes is the reduction of postprandial hyperglycemia, achieved by inhibiting carbohydrate-hydrolyzing enzymes like α-amylase and α-glucosidase in the digestive tract, which hinders glucose absorption and moderates the rise in post-meal blood sugar levels.[1-3] In the present work, more efficient and environmentally friendly method has been devised for the preparation of α-amino phosphonates by Kabachnik-Fields (K-F) reaction in a solvent-free environment using an ultrasonication technique catalyzed by nano ZnO. Primarily, an in silico ADMET and molecular docking analysis was carried out on each molecule prior to synthesis to get insight into drug-likeliness behaviour and their capacity to inhibit α-amylase and α-glucosidase. The structure of the newly synthesized compounds was confirmed using spectroscopic analysis, and each one's in vitro inhibitory action against α-amylase and α-glucosidase was evaluated. Majority of the compounds exhibited good inhibitory activity against α-amylase and α-glucosidase in comparison to the reference substance acarbose. The remaining compounds have shown equipotent to good inhibitory activity against both the tested enzymes.

Keywords: *a*-aminophosphonates, Kabachnik-Fields reaction, ultrasonication, molecular docking, *a*-amylase and *a*-glucosidase

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OP-11 Oral Presentation

Diffusion of Tracer Particle in Microbial Suspension

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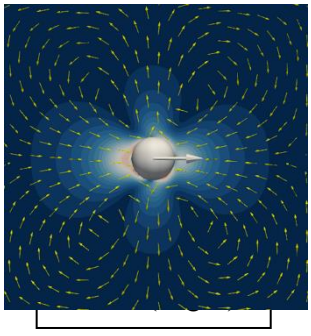
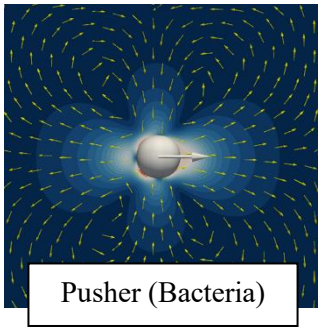
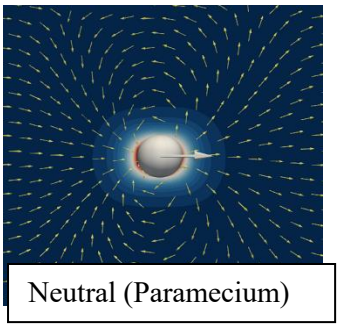
ABSTRACT

This work investigates the diffusion of tracer particles in microbial suspensions composed of bacteria, algae, and paramecia, examining single-species configurations. By introducing tracer particles, the aim is to characterize the flow patterns emerging from microbial motility and activity under the influence of Brownian motion and principles of fluid mechanics. Using numerical simulations, we analyze the interactions between tracer particles and microbial-induced flow fields, focusing on the distinct swimming behaviors of microorganisms, such as pushers, pullers, and neutral swimmers. The study explores confined settings, providing a detailed understanding of how environmental constraints and interspecies interactions influence particle trajectories and diffusion dynamics. Results highlight the role of hydrodynamic interactions and confinement geometry in shaping diffusion patterns, offering novel insights into micro scale transport phenomena. This research has broad applications in biophysics, environmental science, and the development of advanced microfluidic systems, as well as in understanding biological transport mechanisms in natural and artificial environments.

RESULTS:







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OP-12

Oral Presentation

SEPARATION AND CHARACTERIZATION OF GENTAMICIN AND DEXAMETHASONE USING HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)

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ABSTRACT

This study presents a validated method for the separation and analysis of Gentamicin and Dexamethasone using High-Performance Liquid Chromatography (HPLC) with a Waters e-2695 instrument, incorporating a Photodiode Array (PDA) detector. A precise, selective, and stability-indicating isocratic RP-HPLC method was developed for the quantification of these compounds.

The chromatographic process was carried out using a **Symmetry C-18 column** (150 × 4.6 mm, 3.5 µm) with an isocratic mobile phase consisting of **acetonitrile and 0.1% formic acid (50:50).** The flow rate was **1 mL/min**, and detection was performed at **286 nm** using the PDA detector. Method validation adhered to **International Conference on Harmonization (ICH) guidelines.** The **limits of detection (LOD) and quantification (LOQ)** for Gentamicin and Dexamethasone were determined as **0.6 µg/mL and 0.2 µg/mL,** and **1.8 µg/mL and 0.6 µg/mL**, respectively. Calibration curves were established within the concentration range of **5–30 µg/mL** for Dexamethasone and **15–90 µg/mL** for Gentamicin, with a **regression coefficient (R^2) exceeding 0.999.**

The validation process examined parameters such as **recovery, specificity, linearity, accuracy, robustness, and ruggedness**, all of which were found to be within acceptable limits. The proposed method is **efficient, straightforward, practical, and cost-effective** for quantitative analysis.

KEYWORDS: **Gentamicin, Dexamethasone, RP-HPLC, Method Development, Validation.**

OP–13 Oral Presentation

SEPARATION AND VALIDATION OF POTENTIAL ANTI-CANCER DRUGS, AMBROXOL HCL AND SALBUTAMOL, USING HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)

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ABSTRACT

This study focuses on the separation and validation of potential cancer-healing drugs, Ambroxol HCl and Salbutamol, using High-Performance Liquid Chromatography (HPLC) with a Waters e-2695 system equipped with a Photodiode Array (PDA) detector. A precise, selective, and validated isocratic Reverse Phase HPLC (RP-HPLC) method was developed to quantitatively analyze these compounds with enhanced stability.

Chromatographic separation was performed on a Phenyl column (250 × 4.6 mm, 5 µm) under isocratic elution conditions. The mobile phase consisted of acetonitrile and 0.1% trifluoroacetic acid (40:60), with a flow rate of 1.0 mL/min. Detection was carried out at a wavelength of 236 nm using a PDA detector. The method was validated in accordance with the guidelines established by the International Conference on Harmonization (ICH).

The limits of detection (LOD) and quantification (LOQ) for Ambroxol HCl were determined as 0.45 µg/mL and 1.5 µg/mL, respectively, while for Salbutamol, they were 0.3 µg/mL and 1.0 µg/mL. Calibration curves were constructed over a concentration range of 2.5–15 µg/mL for Salbutamol and 37.5–225 µg/mL for Ambroxol, showing excellent linearity with a regression coefficient (R^2) greater than 0.999.

The method was assessed for key validation parameters, including accuracy, precision, specificity, robustness, and ruggedness, with all results falling within acceptable limits. This optimized RP-HPLC method is efficient, straightforward, cost-effective, and suitable for routine analysis of Ambroxol HCl and Salbutamol in pharmaceutical applications.

KEY WORDS: **Ambroxol HCl, Salbutamol, RP-HPLC, Development, Validation.**

Ultrasound-assisted multicomponent reactions for the synthesis of indole tethered 4H-chromene under mild conditions

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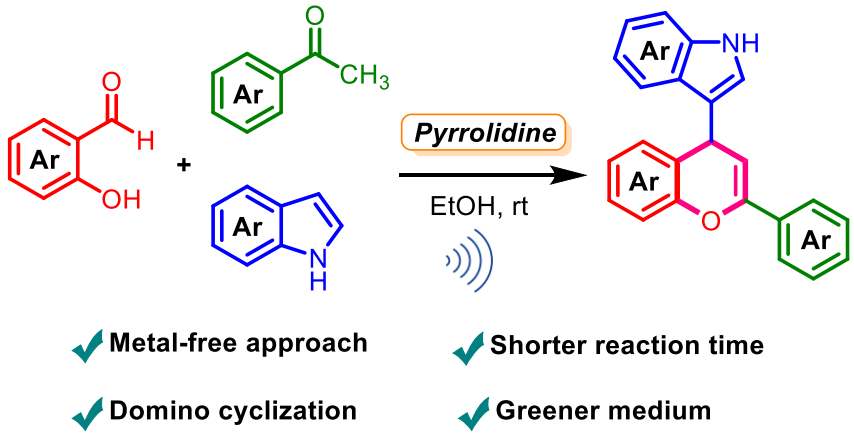
ABSTRACT

An efficient and practical approach has been developed for the rapid synthesis of indolyl-chromene derivatives. Ultrasound-assisted three-component reaction of salicylaldehyde, acetophenone and indole leads to the indolyl 4H-chromene products in good yields. Pyrrolidine base and ethanol medium are employed to achieve desired compounds within short time and at room temperature. Besides, the present method includes a metal-free process, greener solvent, broad range of substrate scope, and mild conditions.

GRAPHICAL ABSTRACT



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OP-15

Oral Presentation

Stability Indicating Method Development for the Separation and Assay of Pibrentasvir and Glecaprevir

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ABSTRACT

Objective: To develop and validate a simple, fast and efficient stability indicating high performance liquid chromatographic method for simultaneous determination of Pibrentasvir (PBVR) and Glecaprevir (GCVR) in bulk and pharmaceutical formulation.

Methods: PBVR and GCVR were separated within 6 Min on Cosmicsil C18 analytical column with 0.1M Na_2HPO_4: acetonitrile (60:40 v/v) with pH 4.5 at a flow rate of 1.0 mL/min. Validation was performed with respect to system suitability, linearity, sensitivity, selectivity, precision, accuracy and robustness. PBVR and GCVR combined tablet sample was subjected to stress degradation in 0.1N HCl for 30 min, 0.1 N NaOH for 30 min, 30% H_2O_2 for 30 min, water for 30 min, in oven at 105 °C for 30 min and in sunlight for 24 hr.

Results: The linearity for PBVR and GCVR were 5-80 and 12.5-200 µg/mL with regression coefficients of 0.9995 and 0.9997, respectively. Stability indicating ability of the developed method was shown by stress degradation studies. The proposed method was effectively applied for simultaneous determination of PBVR and GCVR in available tablet dosage form with good accuracy and precision.

Conclusion: The developed method is apt for the assay of PBVR and GCVR in the presence of their degradation products.

Key words: Pibrentasvir, Glecaprevir, Antiviral combination, Hepatitis C virus, Method development, Validation

OP-16 Oral Presentation

Corrosion resistance studies of aluminium 7075 / SiC composites materials in an acidic environment

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ABSTRACT

The aluminium and silicon carbide-based composite (Al-SiC) material was prepared using commercially available analytical grade Al7075 alloy and SiC. Here the silicon carbide is used as reinforcement particles in the composites. The metal composites were developed using liquid melt techniques (Vortex method). The reinforcement material is introduced in different weight fractions in the range of 0 to 10% in this process. These Al-SiC specimens were used for assessment of its corrosion properties. The acid corrosion experiments were carried out at room temperature (30±°C). The corrosion characteristics were estimated using the conventional weight loss method according to the procedure of ASTM G69-80. The composites performance was evaluated using microstructural analysis and the corrosion resistance tendency in different acidic environmental conditions. The SEM micrographs picture reveals that reinforcement particle was distributed uniformly. The corrosion test was conducted in HCl medium from 0.25N, 0.5N, 1M and 1.5 M respectively. The Al-SiC specimens were dipped in different HCl medium for four days in six experimental baths. Specimens were taken out from each test medium for every 24 hours and tested for its corrosion characteristics. It is observed that the corrosion rate in all HCl medium decreases with an increase in exposure time. This is due to the passivation of the Al-SiC surface induced by aluminium. It was observed that at the 10 w/w % of the aluminium metal matrix composite have higher corrosion resistance than the base alloy.

Keywords: Aluminium, Composites, Corrosion, Acidic medium, Particle reinforcement.

OP-17

Oral Presentation

Phytochemical-derived TiO_2-doped ZrO_2 for gate dielectrics

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ABSTRACT

In this abstarct, annealing temperature dependence on the structure, band gap energy and electrical properties of TiO_2 doped ZrO_2 gate dielectrics deposited by green leaf extract method at certain temperature were systemically investigated. The crystalline temperature of TiO_2 doped ZrO_2 is up to 600^0C. The transmittance and band gap value of the $ZrTiO_x$ film were about 75% and 4.0 eV, respectively. 300 C-annealed $ZrTiO_x$ MOS capacitor with high dielectric constant of 34.9, a small hysteresis value of 0.004 and low leakage current density of $2.7*10^4$ A/cm^2 were obtained. The dominant conduction mechanisms of Al/ $ZrTiO_4$/n-Si MOS structures were schottky emission and ohmic conduction in the low electric field and direct tunneling in the high electric field. As a result, it can be concluded that green leaf extract derived $ZrTiO_x$ gate dielectric displays potential application as is a promising candidate in future MOS electronic devices.

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OP-18 Oral Presentation

Electrochemical Impedance Studies of Al-8088/Al_2O_3/SiC Hybrid composites

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ABSTRACT

Aluminium alloys are employed in aerospace, automotive, and other structural uses due to their high strength and lightweight qualities. Moreover, when aluminum alloys are exposed to different conditions at different temperatures, corrosion becomes a life-limiting problem. In this study Alumina (Al_2O_3) and palm kernel shell ash (SiC) were used as reinforcement particles in Al 8088 matrix alloy, this work examines the corrosion behaviour of Nano Nano Hybrid composites at various mix ratios. The method of double stir casting was employed to develop the composites. Both gravimetric analysis and electrochemical measurements were used to examine the corrosion behaviours of the composites in NaCl solutions. The results obtained by the gravimetric analysis, suggested that the composite film was defective and that corrosion products were forming on the specimens' surface. Pitting and general corrosion were the mechanisms of corrosion that were detected in the samples. The Al8088 matrix's reinforcements served as active locations for the onset of corrosion. E Corr and I corr in 3.5% NaCl varied from −220.62 to −899.46 mV and 5.45 to 40.87 µA/cm2, respectively, at 24 hours. At 72 hours, E Corr values were between 255.88 and −887.28 mV, while I corr values were between 7.19 and 16.85 µA/cm2. The samples under investigation's electrochemical corrosion behaviour were shown by the Nyquist and Bode plots, which connected the main surface responses to processes related to charge transfer. The samples' relative resistance to corrosion is determined by the thin oxide layer that develops on their surface.

Keywords: Hybrid composites, EIS, NaCl, Al2O3, SiC, SEM.

OP-19

Oral Presentation

Composite materials of Aluminium 6061 for Green Environment

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ABSTRACT

Composite materials are gaining importance since 1990 for their excellent and improved corrosion and electrochemical properties. Due to the use of these materials the wastage, wear, tear and corrosion are reduced which leads to the decrease of environmental hazards. Composite materials are very popular in aerospace, aviation and industries because of their improved mechanical properties. In this paper electrochemical properties like corrosion resistance of composite materials made up of Aluminium 6061 reinforced with haematite ore particulates are studied. Composite materials of Aluminium 6061 containing 3,6 and 9 weight percentage of haematite ore particulates are fabricated by employing liquid melt metallurgy technique using vortex method. Aluminium 6061 without any reinforcement was also casted in the same way to compare the results at the end. Electrochemical behaviour of the composites with respect to corrosion resistance was studied by static weight loss corrosion test, potentiodynamic polarization test using electrochemical work station. The tests were conducted in three different concentrated solutions of sodium hydroxide. Scanning electron microstructures were taken before and after static weight loss corrosion tests. The results revealed that the composite materials exhibit increased corrosion resistance with increase in reinforcement content.

Key words: Aluminium 6061, Composite, Electrochemical, Polarization, Vortex, Weight loss

OP-20 Oral Presentation

Green Toxicology: A Sustainable Advancement in Forensic Toxicology

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ABSTRACT

Green toxicology is an emerging field that aims to minimize the negative impacts of chemicals on human health and the environment. It is grounded on the principle of designing safer chemicals and processes from the outset, rather than relying on traditional methods of risk assessment that often involve animal testing and can be time-consuming as well as expensive. In forensic science, green toxicology has the potential to revolutionize the approach of chemical analysis. By using green methods, we can minimize the negative environmental impact of forensic investigations, while improving the accuracy and reliability of our results. Some of the latest advances in green toxicology that are being applied to forensic science include i) the development of new in vitro and in silico methods for toxicity testing for assessing the potential toxicity of chemicals without the need for animal testing, ii) using greener reagents and solvents for forensic analysis, reducing the impact on the environment, iii) developing sensitive and specific methods for detecting and identifying toxins accurately. The present study explores the principles of green toxicology, applications of green toxicology in forensic toxicology, and methods involved in it.

Keywords: Green Toxicology, Forensic Toxicology, in vitro method, in silico method

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OP-21

Oral Presentation

Fluorescence studies on swelling behavior of poly (vinyl alcohol) (PVA) hydrogel film using fluorescein as a probe

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ABSTRACT

The swelling behavior of poly (vinyl alcohol) (PVA) hydrogels was investigated using fluorescein as a fluorescent probe and fluorescence spectroscopy. This study aimed to monitor water uptake and polymer expansion in real time. Fluorescein is incorporated in 4 wt% PVA hydrogel film and is immersed in phosphate-buffered saline (PBS, P^H 7.4) at room temperature; fluorescence was recorded at different time intervals. Results of measurements using ultraviolet-visible spectroscopy (UV-Vis) and fluorescence spectroscopy show a significant increase in fluorescence intensity, indicating progressive hydration and polymer relaxation. Spectral shifts suggested microenvironmental changes affecting fluorescein behavior. The kinetic analysis confirmed that swelling is initially diffusion-driven, transitioning to PVA relaxation. These findings are valuable for biomedical applications, particularly in drug delivery systems, tissue engineering, and responsive hydrogels.

Keywords: Poly (vinyl alcohol) (PVA), fluorescein, swelling, fluorescence spectroscopy.

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OP-22

Oral Presentation

GREEN NANOCHEMICAL PRODUCTS FOR INDUSTRIAL POLLUTION AND WATER POLLUTION

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ABSTRACT

Globally, industrial and water pollution are serious threats to human health and the environment. Conventional pollution control techniques frequently depend on risky or energy-intensive procedures that could lead to secondary pollution. By creating ecologically friendly chemical processes and materials, green chemistry provides a creative and sustainable way to address these problems. In order to reduce trash and hazardous emissions, this method places a strong emphasis on using non-toxic, biodegradable, and renewable materials. Eco-friendly synthesis methods, bio-based solvents, and catalysis are among strategies that can cut industrial pollutants right at their source.

Through adsorption, photocatalysis, and bio-remediation employing green nanoparticles, natural coagulants, and enzymatic degradation, green chemistry helps remove heavy metals, organic pollutants, and microplastics from wastewater. This strategy lowers the ecological footprint of companies while ensuring environmental sustainability, conserving natural resources, and fostering a circular economy through the incorporation of green chemistry principles into water treatment and industrial operations.

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OP-23

Oral Presentation

I_2 promoted synthesis of 2,4,6-trisubstituted pyridines from arylidene meldrum's acids via oxidative cleavage of C=C double bond

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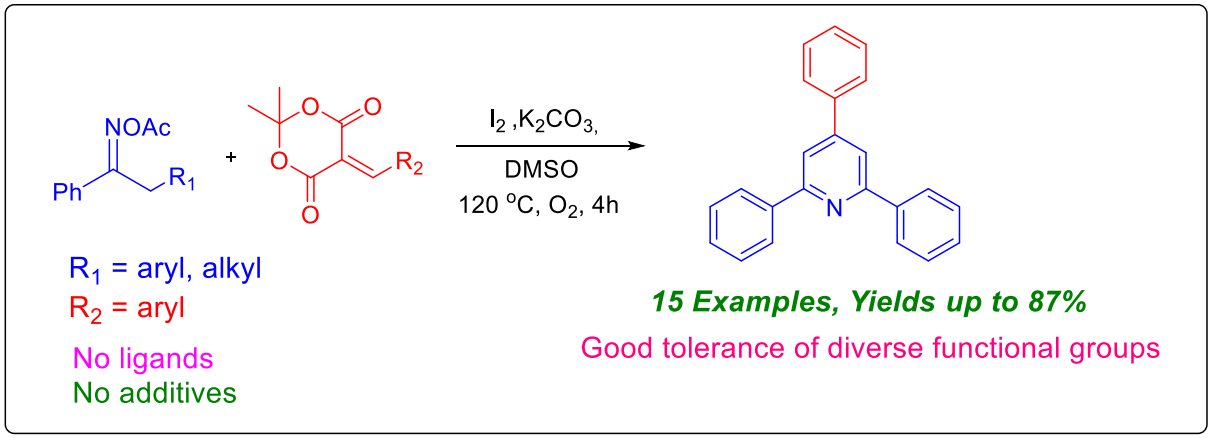
ABSTRACT

Pyridines are important class of N-hetero aromatic compounds and recognized as privileged scaffolds due to their various applications in medicinal chemistry, agro-chemistry and Natural products [1-3]. Moreover, pyridines exhibit wide range of biological activities such as anti-diabetic, anti-HIV, anti-inflammatory, anti-tubercolosis, anti-cancer, insecticidal, anti-bacterial, anti-convulsant, anti-malarial, anti-epileleptic, analgesic, pesticidal and herbicidal, fungicidal, activities etc.,. In view of the application in various fields, copious methods have been developed for the synthesis of pyridines. However, they have some setbacks such as long reaction times, low yields and usage of expensive catalysts, ligands and reagents. Therefore, there is a need to develop a new and efficient method for the synthesis of pyridines. On the other hand, transition metal or metal-free catalysed oxidative cleavage of carbon-carbon double bond of arylidene meldrum's acids has received significant attention in organic synthesis as it generates in situ aldehyde for the construction of various heterocyclic compounds. Moreover, oxime acetates have recently been used as building blocks for the synthesis of various nitrogen heterocycles such as pyrroles, pyridines, isoxazoles etc. via N-O bond cleavage. To the best of our knowledge, no precedent has been reported for the synthesis 2, 4, 6- trisubstituted pyridines from arylidene meldrum's acids and oximeacetates. So, herein we report an efficient protocol for the synthesis of 2, 4, 6- trisubstituted pyridines from ketoxime acetates and arylidene meldrum's acids in presence of I_2 and K_2CO_3 as a base in DMSO at 120 ^oC for 4 h under oxygen atmosphere(**Scheme 1**).

Key words: N-O bond cleavage, ketoxime acetates, arylidene meldrum's acids, 2, 4, 6-trisubstituted pyridines.



Scheme 1: Synthesis of 2,4,6-trisubstituted pyridines

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OP-24

Oral Presentation

Luminescent, vibrational and optical studies of Europium (Eu^{3+}) doped lithium cadmium orthophosphate nanopowders

Shaik Azad Basha[1], G. Rebbeca Rani[1,2], S.V. Balasubramanyam[1], Sandhya Cole[1*]

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ABSTRACT

The well-known solid-state reaction method was used to synthesize Eu^{3+} doped lithium cadmium orthophosphate ($Li_2Cd_2(PO_4)_2$) nanopowders. Analytical methods such as FT-IR, Raman, DRS and Photoluminescence studies were used to characterize these nanopowders. The $(PO_4)^{3-}$ vibrational modes were identified by FT-IR and Raman investigation. Eu^{3+} doping resulted in the variations of optical bandgap in the range 5.38 – 5.73 eV. PL spectra shows an emission at 591 nm, when excited at 392 nm. Color qualities viz. CIE, CCT, CRI and CP were calculated by photometric study. The PL spectra of prepared samples reveal reddish orange emission at 591 nm ($^5D_0 \rightarrow {}^7F_1$). These findings show that the prepared samples have promising advantages in the fabrication of commercial LEDs and solid state lighting devices [1, 2].

Keywords: FT-IR; Raman; DRS; Photoluminescence; Nanopowder.

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OP-25

Oral Presentation

An efficient electrocatalyst for the hydrogen evolution reaction using palladium nanoparticles supported on Nafion-functionalized Vulcan carbon black

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ABSTRACT

The development of alternative techniques for generating clean and sustainable energy has been driven by a gradual increase in global energy usage, the depletion of fossil fuels, and the rise of environmental issues including pollution, has spurred the development of alternative methodologies for generating sustainable and clean energy. Hydrogen has a high energy density and is the ideal energy carrier for developing a clean and sustainable energy system to address global warming caused using other fuels, particularly fossil fuels. Hydrogen Can be produced from Various methods. But, a sustainable method of producing hydrogen using energy from clean energy sources is water electrolysis. However, to ensure economic viability, it is crucial to reduce production costs while improving the electrocatalyst particular performance and stability in the hydrogen evolution reaction (HER). To address these issues, we have developed perfluoro sulfonic acid (Nafion) functionalised Vulcan carbon supported Palladium (Pd) nanoparticles via chemical reduction method. The Developed electrocatalyst was investigated as cathode for the hydrogen evolution reaction (HER) in water electrolysis. The resulting Pd/ Nafion-C electrocatalyst was characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS) and X-ray diffraction (XRD). SEM indicates the Pd nanoparticles on the Nafion-C support are small and more uniformly dispersed. XRD analysis further revealed a face centered cubic crystallite structure and an average crystallite particle size of ~ 10 nm. Also, the electrocatalytic activity of the developed electrocatalyst for HER was evaluated by electrochemical characterization techniques such as CV, LSV and EIS. The prepared electrocatalyst exhibited high electrochemical surface area ($132 m^2 g^{-1}$), low charge transfer resistance (9 Ω) and long-term stability. It was observed that the current density of Pd/ Nafion -C had a little decrease after continues 50 cycling, which shows the catalyst presents high stability in the recycling process. The good catalytic activity suggests that the Pd/ Nafion -C can be a promising electrocatalyst in hydrogen production process.

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OP-26

Oral Presentation

Soil Assessment for Agricultural Suitability in Devarakonda Revenue Division

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ABSTRACT

Soil analysis informs crop selection and fertilizer management by revealing chemical and physical properties that determine soil quality and fertility, ultimately maximizing yield and product quality. Local farmers in the study area, often bypass government soil testing laboratories due to perceived time constraints and accessibility issues, relying instead on experiential knowledge. Therefore a comparative study of the physico-chemical properties and nutrient content of soil is carried out in the present study from Devarakonda farmlands in the district. The study area has arid to semi-arid climate and the area witnesses an average rainfall of about 600mm from southwest monsoon during the months of June-September. All the soils tested were growing cotton as the chief crop. Standard methods were used to conduct the research and analyze the findings of the research [1]. The soil testing programme involved 1) Collection of soil samples 2) Chemical analysis of samples 3) Calibration and interpretation of the results of chemical analysis 4) Recommendations. The findings made during the study are that the pH of the farm samples collected is in the range of slightly acidic to slightly basic. The available Nitrogen in the samples was in the range of 138-287 Kg Ha^{-1} indicating nitrogen deficiency in 92% of the samples tested. All the soils showed medium to high levels of phosphorus and potassium [2, 3] attributed to the over application of DAP and potassium fertilizers. Organic carbon levels were optimum but 15.3% of the soils tested exhibited zinc deficiency, 30.75% of soils exhibited manganese deficiency and 34.6% soils have shown iron deficiency. None of the samples were deficient in copper. Based on the findings, the farmers were suggested to use green manure crops to increase microbial activity so that the fixed Phosphorous and Potassium is converted in available form for plant growth. We also suggested the farmers to compulsorily practice crop rotation and shift to organic farming in future. They were suggested to immediately discontinue the use of DAP and instead supplement it with urea.

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OP-27

Oral Presentation

SIMULTANEOUS DETERMINATION OF PROBENECID AND SULOPENEM ETZADROXIL USING RP-UPLC WITH PDA DETECTOR

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ABSTRACT

Objective: In the current investigation, to separate and validate the cancer healing drugs (Probenecid and Sulopenem Etzadroxil) through the UPLC (Water Acquity) instrument containing a PDA detector.

Methods: A simple, selective, validated and well-defined stability that shows isocratic RP-UPLC methodology for the quantitative determination of Probenecid and Sulopenem Etzadroxil. The chromatographic strategy utilized Acquity UPLC BEH chemistry Shield RP-18 column of dimensions 50x2.1 mm, 1.7 micron, using isocratic elution with a mobile phase of Acetonitrile and 0.1% Perchloric acid (30:70). A flow rate of 0.2 ml/min and a detector wavelength of 272 nm utilizing the PDA detector were given in the instrumental settings.

Results: LOD and LOQ concentrations for Sulopenem Etzadroxil were 0.5 µg/ml, 2.0 µg/ml and for Probenecid were 0.5 µg/ml, 2.0 µg/ml. The calibration charts plotted were linear with a regression coefficient of $R^2 > 0.999$. Recovery, specificity, linearity, accuracy, robustness, ruggedness were determined as a part of method validation and the results were found to be within the acceptable range. Validation of the proposed method was carried out according to an international conference on harmonization (ICH) guidelines.

Conclusion: The proposed method to be fast, simple, feasible and affordable in assay condition. During stability tests, it can be used for routine analysis of production samples and to verify the quality of drug samples during stability studies.

Key words: Probenecid, Sulopenem Etzadroxil, RP-UPLC, Development, Validation.

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OP-28

Oral Presentation

Synthesis of AgNPs & AuNPs for Environmental Catalysis

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Abstract

A laboratory experiment was conducted to evaluate the impact of silver aqueous solution, gold aqueous solution, Aristolochia littoralis-based silver nanoparticles (AL-AgNPs) and Aristolochia littoralis -based gold nanoparticles (AL-AuNPs), development and gravimetric analyses. The results showed that Ag^{+} aqueous solution as well as Au^{+3} aqueous solutions with AL extract-based nanoparticles caused more significantly in catalysis and biological activity. Aqueous solutions of Ag^{+} and Au^{+3} drastically reduced as Ag and AuNPs. AL-AgNPs and AL-AuNPs treatment drastically enhanced removal of the food contaminated dyes. Aristolochia littoralis is a traditional medicinal plant that can be used to synthesize nanoparticles for a variety of potential applications, including medicine and environmental sciences.

Keywords: AuNPs, AgNPs, Aristolochia littoralis, Environmental Catalysis.

OP–29

Oral Presentation

STABILITY INDICATING AND COST-EFFECTIVE ANALYTICAL METHOD DEVELOPMENT AND VALIDATION OF SOTORASIB BY USING RP-HPLC

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ABSTRACT

Objective: The current investigation was pointed at developing and progressively validating novel, simple, responsive and stable RP-HPLC method for the measurement of active pharmaceutical ingredient of Sotorasib**.**

Methods: A simple, selective, validated and well-defined stability that shows isocratic RP-HPLC methodology for the quantitative determination of Sotorasib. The chromatographic strategy utilized symmetry C18 column of dimensions 150x4.6 mm, 3.5 µ, using isocratic elution with a mobile phase of acetonitrile and 0.1% orthophosphoric acid (70:30). A flow rate of 1 ml/min and a detector wavelength of 221 nm utilizing the PDA detector were given in the instrumental settings. Validation of the proposed method was carried out according to an international conference on harmonization (ICH) guidelines.

Results: LOD and LOQ for the active ingredient were established with respect to test concentration. The calibration chart plotted was linear with a regression coefficient of R2>0.999, means the linearity was within the limit. Recovery, specificity, linearity, accuracy, robustness, ruggedness were determined as a part of method validation and the results were found to be within the acceptable range.

Conclusion: The proposed method to be fast, simple, feasible and affordable in assay condition. During stability tests, it can be used for routine analysis of the selected drug.

Keywords: Sotorasib, RP-HPLC, Development, Validation, Stability.

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OP-30

Oral Presentation

Unveiling the Invisible with Artificial Intelligence in Forensic Science

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ABSTRACT

Artificial intelligence (AI) is a technology that allows computers to perform tasks that typically require human intelligence. It can learn, solve problems, and make decisions. In forensic science there are different subjects like crime scene management, Fingerprints and impressions, Questioned documents, Ballistics, Toxicology, Serology, Forensic Medicine and Anthropology, digital forensics and psychology etc. In every subject artificial intelligence play very important role to analyse evidences, identify suspects, reconstruction of crime scenes, face and object recognition, video enhancement and pattern recognition. Artificial intelligence can help forensic experts work more efficiently and reduce the risk of error. Forensic toxicology is a scientific field which applies toxicology to legal investigation which involves analyses of body fluids and tissues to identify poison, drugs and other harmful substances in forensic toxicology artificial intelligence will help to analyse the chemical structure of toxic substances and predict their toxicity and can help in the identification of unknown poisons and the development of new antidotes.AI can help identify potential drug interactions that may not be immediately apparent to human analysis. Fingerprints are unique and most important evidence in different types of crimes, AI can use for fingerprints recognition, personal identification, access control, and criminal identification. There are some benefits of AI in Fingerprint recognition like Accuracy, Adaptability, Robustness, speed and ease to use. Traditionally forensic experts meticulously examined handwriting charactertics, signature and other type of textual evidences to establish authenticity or to detect forgery, AI will help in document examination like handwriting analysis, automated alteration detection, natural language processing, optical character recognition and forgery detection.AI is applied in forensic medicine like medical image analyses, postmortem interval estimation, cause of death determination and virtual autopsy. In crime prevention AI will help in many ways like predictive policing, anomaly detection, cybersecurity, early intervention and resource optimization.

Keywords: Artificial Intelligence, Forensic Science, Detection.

OP–31

Oral Presentation

Transforming Science Education- Global Shifts in Green Chemistry

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ABSTRACT

The purpose of this paper is to present the progress and development of a fundamental field that aims to design chemical processes with as little adverse effect on the environment as possible. The paper discusses the relevance of changes in industries considering the impact of the conventional chemical industry on the environment, people, and resources, with pollution, toxicity, and depletion of the resources being alarming effects. Waste minimization as one of the ten principles of green chemistry, atom economy and safer solvents and auxiliaries, is also described in detail. In the best practice examples drawn from key industries such as Unilever and BASF, a positive approach toward integrating biodegradable materials and renewable resources is evident. Furthermore, new developments in the catalysis and bio-catalysts techniques as well as innovative methods of carbon dioxide conversion are also explored to demonstrate that sustainability is a core direction of chemical transformations. Nevertheless, prospects are evident albeit constrained in economic, regulatory, and technical sectors. Overcoming these barriers is crucial to the complete realization of green chemistry in the industry and the scale-back of environmental harm. It is for this reason that the present review offers a final reflection on how both green chemistry and a circular economy can change various sectors and offer more sustainable solutions.

Key words: chemical waste, Green Chemistry,

OP–32

Oral Presentation

Iron-catalyzed environmentally benevolent construction of 2-iodo aroylguanidines

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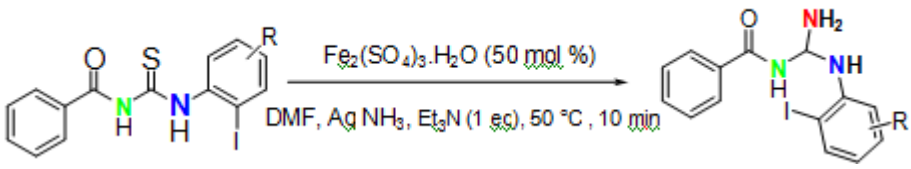
ABSTRACT

An efficient approach to access 2-iodo aroylguanidines starting from readily accessible thioureas has been established. Furthermore, desulphurisation process has been identified by Iron catalysis at 50 C. This is the first example of the synthesis of 2-iodo aroylguanidines involving Iron catalysis in the presence of a green solvent. Hence, the reaction is in line with the requirements of green chemistry by virtue of mild conditions, environmentally benign, short reaction time, and good selectivity. We have presented a new and environmentally benign method for the synthesis of aroylguanidines using Iron source under mild reaction conditions. Compared to other reported methods using $HgCl_2$ or $Bi(NO_3)_3.5H_2O$ the new method distinguishes itself by milder reaction conditions and shorter reaction times.

Keywords. Iron; Aroylguanidines; Mild reaction; Desulphurization.



OP-33

Oral Presentation

Solvent dependent structural, electronic, and optical properties of ureido peptidomimetics: a DFT and TD-DFT study on the effects of donor and acceptor functional groups

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ABSTRACT

This study provides a comprehensive examination of the structural, electronic, optical, and reactivity properties of ureido peptidomimetics (UPMs) featuring various donor and acceptor functional groups using density functional theory (DFT) and time-dependent DFT (TD-DFT). To systematically explore their effects on charge transfer, HOMO-LUMO energy gaps, and molecular stability, the molecular models were intentionally designed with both electron-donating groups (-CH_3, -OCH_3, -OH, -NH_2) and electron-accepting groups (-SH, -COCl, -CF_3). A detailed analysis of the bond lengths confirmed the electron-rich nature of the substituents, revealing that the introduction of electron-donating groups at the ureido and carboxylate terminals of the UPMs decreased the C-O and C-N bond lengths by 0.005 Å and 0.0003 Å, respectively, compared to the unsubstituted UPM. Polar solvents, notably water and DMSO, enhance the stabilization of HOMO and LUMO energy levels, thus improving the electronic stability and reactivity of UPM molecules, as demonstrated by DFT and TD-DFT calculations. In the case of UPM, the molecular orbitals (HOMO: -6.8646 eV to -6.9027 eV, LUMO: -0.3957 eV to -0.4248 eV) experienced slight stabilization as it transitioned from the gas phase to the aqueous phase. This transition increased the chemical potential (χ) and global hardness (η), signifying enhanced electronic stability. UV-Vis experiments revealed that UPM's λmax values remained around 218.6 nm across various solvents, with polar solvents, particularly water, exhibiting more robust oscillators. In water, λ_{max} decreased to 207.58 nm for D2-UPM-A2 and shifted to 227.86 nm for D1-UPM-A1. For D3-UPM-A3, λ_{max} in water exhibited a redshift to 249.28 nm along with reduced absorption. Specifically, for A1-UPM-D1 and A2-UPM-D2, the polarity of the solvent influenced transitions and increased transition probabilities, indicating their potential in optoelectronic applications.

Keywords: Ureidopeptidomimetics; Density Functional Theory (DFT); HOMO-LUMO Gap; Optical Properties and Global Reactivity Descriptors.

OP–34

Oral Presentation

The Green (Chemistry) Environment: Developing and Assessing Green Chemistry Curricula and Student Outcomes in the Chemistry Laboratory

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ABSTRACT

Climate change and its environmental and humanitarian impacts are significant challenges in the 21st century. Green chemistry, a recent addition to the chemistry family, aims to ethically and responsibly address these impacts, contributing to sustainable development and innovation within and outside chemistry.Green chemistry integration in undergraduate education offers students an ethical framework, enhances chemical learning, introduces new approaches to chemical problems, and encourages authentic problem-solving and inquiry.This research aimed to create a comprehensive green chemistry curriculum for the general chemistry laboratory course at UC Berkeley, focusing on non-chemistry majors who may not pursue further chemistry courses, thereby enhancing the effectiveness of the course.The green chemistry curriculum was designed using a constructivist learning science framework, knowledge integration, to incorporate explicit content and practices into the general chemistry laboratory, addressing both content and pedagogy.The Berkeley general chemistry laboratory structure was used for iterative curriculum revision, focusing on utilization-focused evaluation design. This work contributes to understanding how to develop coherent green chemistry materials and efficiently assess and revise curriculum by evaluating implementation processes and student outcomes.

Green chemistry student learning outcomes are often not fully assessed using self-reported items like achievement tests and course assignments, focusing on general science or lab technique/skill outcomes. For large enrollment courses, alternative assessment modes like short answer and multiple-choice content questions are needed.A study involving nearly a dozen green chemistry items was conducted to assess students' ability to define, use, and make decisions in this field. Iterative Likert and Guttman items were also used to measure self-reported green chemistry abilities and students' values towards it.The research reveals that both general and organic chemistry students demonstrate sophisticated green chemistry reasoning when presented with traditional and green data and metrics. They use the data to justify their choice, demonstrating their green chemistry knowledge and reasoning modes.Both general and organic chemistry students demonstrated similar value and ability in making green chemistry decisions, especially when organic chemistry students received no additional green chemistry instruction after general chemistry.Organic chemistry students demonstrated a strong commitment to green chemistry, choosing it on a high-stake summative exam, indicating their confidence in understanding and applying green chemistry principles and practices even after two or more semesters of learning.

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OP–35

Oral Presentation

Co-doping of Fe_2O_3 nanoparticles with yttrium and zirconium using *Dillenia indica* leaf extract

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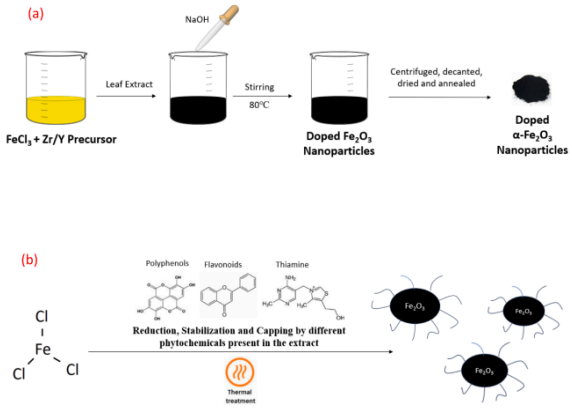
ABSTRACT

This study explores the co-doping of iron oxide nanoparticles with yttrium and zirconium using a one-pot green synthesis method, employing freshly plucked Dillenia indica leaves as a natural reducing and stabilizing agent. The synthesized nanoparticles were subjected to different annealing durations (2–4 h) at a constant temperature of 600°C to investigate their structural, optical, and antibacterial properties. Characterization techniques such as Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Ultraviolet-visible Spectroscopy (UV-Vis), Raman Spectroscopy, and Fourier Transform Infrared Spectroscopy (FT-IR) were employed.

UV-Vis spectroscopy confirmed modifications in **optical absorption**, with **yttrium and zirconium doping reducing the bandgap**, thereby enhancing **photocatalytic activity**. Additionally, co-doping influenced surface charge, stability, and bacterial interactions, potentially improving antibacterial effects. The catalytic properties of the nanoparticles were evaluated through methylene blue degradation, where co-doping modified electron transfer properties, influencing degradation efficiency. The presence of phytochemicals from Dillenia indica facilitated an eco-friendly, cost-effective, and scalable nanoparticle synthesis process. This study highlights the significance of green synthesis in developing functional nanomaterials for antibacterial and catalytic applications.

Keywords: Green synthesis, Dillenia indica, iron oxide nanoparticles, co-doping, yttrium, zirconium, photocatalysis, antibacterial properties



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OP-36

Oral Presentation

Determination of TAPENTADOL in tablet dosage form by Spectrophotometric Method

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ABSTRACT

Four simple, accurate, sensitive, precise and economical spectrophotometric methods have been developed for the determination of Tapentadol in the tablet formulations. The developed methods were based on the formulation of Method A is simple and direct UV spectrophotometric method and is based on determination of Tapentadol in 01N HCl, Method B is based on development of yellow chromogen due to reaction of Tapentadol diazotized sulphanilic acid, Method C id based on development of orange-red complex between Tapentadol and Method D is based on devolvement of Bromothymol blue in chloroform and blue color chromogen of Tapentadol with Folin-Ciocalteu reagent. UV spectroscopic methods with absorption maximum of 273.3nm (Method A), the yellow colored dye stuff show absorption maximum at 494.6nm (Method B), the orange-red complex shows absorption maximum at 414.6nm (Method C), and blue color chromogen shows absorption maximum at 773.3nm (Method D). The proposed methods showed good linearity in the concentration range of 5-25 µg/ml for all the methods. The results of analysis for all the methods are validated statistically by recovery studies.

Key Words

Tapentadol, Bromothymol blue, Folin-Ciocalteu reagent.

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OP-37

Oral Presentation

Mechanochemical synthesis of phosphoryl amides and esters from diphenylphosphoryl azides under mild conditions.

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Graphical Abstract:

Abstract:

The mechanochemical synthesis of phosphoryl amides and esters from diphenylphosphoryl azides (DPPA) is presented as a highly efficient, mild, and sustainable method, performed under solvent-free conditions. This process harnesses the mechanical energy provided by ball milling to activate and promote the nucleophilic substitution reactions, facilitating the formation of phosphoryl derivatives without the requirement for high temperatures or aggressive reagents. The reaction involves the nucleophilic attack of amines or alcohols on the diphenylphosphoryl azide, leading to the selective formation of phosphoryl amides and esters, respectively. The ability of mechanochemical methods to proceed under mild, solvent-free conditions significantly reduces environmental impact while maintaining high product yields and reaction efficiency. The reaction conditions, including milling time, reagent ratios, and the nature of the nucleophile, were systematically investigated to optimize the reaction outcomes. Furthermore, the robustness of the reaction conditions was demonstrated, as a wide range of nucleophiles with varying functional groups were compatible, showing excellent tolerance to diverse structural motifs. This is particularly advantageous for the synthesis of bioactive molecules, pharmaceuticals, and materials that often require preservation of sensitive functional groups.

The mechanochemical process benefits from short reaction times (minutes to hours), high yields, and minimal need for post-synthetic purification, offering significant operational

simplicity. The ability to scale up the reaction was also demonstrated with consistent results, reinforcing the practicality and versatility of the method. The formation mechanism is elucidated through experimental studies and the effect of different milling parameters on the reaction efficiency is discussed. The results reveal that mechanochemical activation not only provides a green alternative to conventional liquid-phase synthesis but also delivers a highly efficient, cost-effective pathway for the preparation of phosphoryl derivatives. The method, by avoiding the use of toxic solvents and harsh reagents, represents an environmentally friendly and sustainable approach for the synthesis of phosphoryl amides and esters, positioning it as an attractive alternative in both academic and industrial applications.

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OP-38

Oral Presentation

Development and Validation of a Simple and Rapid RP-HPLC Method for the Quantitative Analysis of Givosiran in Pharmaceutical Dosage Form

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ABSTRACT:

A simple, rapid, precise, sensitive, and reproducible reverse-phase high-performance liquid chromatography (RP-HPLC) method was developed for the quantitative analysis of Givosiran in pharmaceutical dosage form. The chromatographic separation was performed using a Waters Alliance-e2695 system with a Waters Symmetry C18 column (150 mm × 4.6 mm, 3.5 µm). The mobile phase consisted of 0.1% orthophosphoric acid (OPA) and acetonitrile (ACN) in an 80:20% v/v ratio, delivered at a flow rate of 1.0 mL/min. Detection was carried out at 247 nm using a photodiode array (PDA) detector under ambient temperature conditions. The method ensured a theoretical plate count of at least 2000 and a tailing factor not exceeding 2. The % relative standard deviation (RSD) of peak area measurements remained below 2.0%, demonstrating method precision. Validation was performed in accordance with ICH guidelines, confirming the method's simplicity, cost-effectiveness, suitability, precision, accuracy, and robustness for the quantitative analysis and stability study of Givosiran.

Keywords: RP-HPLC, Givosiran, Method Validation, Stability Study, Quantitative Analysis.

OP-39

Oral Presentation

Quantification of the Extracted Natural Products from Nilavemu Powder (Swertia Chirata) with different solvents

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ABSTRACT

Chirata is an excellent remedy for strengthening the stomach and promoting its action.It is used in the treatment of dyspepsia and diarrhea. Chirata stimulates the digestion and helps to normalize blood sugar,which makes it useful for diabetics.Studies with animals suggest that this herb reduces the sugar levels only when they are high,which lowers the risk of hypoglycemia.

The bitterness of the herb stimulates salvia and gastric juices, which help stop nausea, bloating, indigestion and hiccups.It is also used for fever and to rid the body of parasites.It is a tonic for the heart, liver and eyes, and can be useful to relieve sciatica, cough, scanty urine and melancholia. Chirata is used as a preventative measure for malaria during epidemics.It is given as a tonic to people convalescinmg from a ling illness.This herb is antimicrobial.Studies are underway to see if this herb continues to offer a reduction in cancer cells when tken to fight cancer.

Chirata decoction can be added to a bath to help skin rashes.Skin diseases with burning sensations, oozing and itching respond well to this herb. The traditional uses of medicinal plants in healthcare practices are providing clues to new areas of research; hence its importance is now well recognized.Swertiachirata is widely demanded for its unmatched medicinal properties to the gentian.Swertiachirata provided by us is valued as a febrifuge and tonic. Perfect for various diseases like diarrhea, fever and weakness.Our Swertiachirata is available at very affordble prices.We are well reckoned as the most preeminent chirata manufacturer and exporter based in India.

Key Words: Chirata, Traditional and medicinal uses,gentian.

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OP–40

Oral Presentation

BIOPLASTICS AND THEIR ROLE IN ACHIEVING ENVIRONMENTAL SUSTAINABILITY

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ABSTRACT

Plastic is a material that is used to great extent. Most plastics that are commercially used today are petroleum based, meaning that they can take more than a century to degrade. Nothing in our natural environment is capable of easily breaking them down since polyurethane and polyethylene are manmade polymers that microorganisms don't recognize as food. When burned, plastics release carcinogenic chemicals that are equally harmful to people and the environment. In recent years, plastic pollution has become the biggest environmental concern globally. The best eco-friendly alternative to the current commercial plastic is bioplastics. Bioplastics are plastics made from renewable resources like corn, sugarcane or microbes like yeast. Their polymers are easily decay and blend harmlessly with soil. Bioplastics have several advantages over traditional plastics in terms of low carbon footprint, energy efficiency, biodegradability and versatility. They can be used in many industries, including food packaging, agriculture and medicine.

The present paper is focused on definition and basic facts as well as the major advantages of bioplastics, then the main differences between plastics and bioplastics are briefly reviewed. It also highlights types of bioplastics based on various sources and a variety of bioplastic materials such as starch, cellulose etc., Finally, possible future developments of bioplastics are prospected.

Keywords: Bioplastics, Biodegradable, Polymers, Environment.

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OP–41

Oral Presentation

THE IMPORTANCE OF RENEWABLE FEEDSTOCKS IN GREEN CHEMISTRY

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ABSTRACT

In addition to addressing today's urgent issues, Agenda 21 and the objectives of the Rio Conference (1992) seek to prepare the world for the challenges of the twenty-first century. The primary areas of interest are resource management and conservation for development, to which chemistry will need to contribute significantly. Resource-efficient production of basic chemicals is particularly crucial for sustainable development since they are generated in huge quantities and are used to synthesis significant product lines. Here, new methods based on renewable feedstocks are important. The majority of items made from renewable raw materials might not be able to compete with the petrochemical industry's products right now, but this will change as oil becomes more scarce and costs rise. The Chemical product design should prevent bioaccumulation and enable sustainable processing and recycling. Techniques and standards are required to evaluate their role in sustainable development. It is imperative to combine the creation of new, more sustainable processes and products with effective environmental-political control procedures and operational innovation management in order to reduce the time required to introduce them.

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OP-42

Oral Presentation

Estimation of Benzyl Cyanide as a Genotoxic impurity in Primidone API and its pharmaceutical dosage forms by using GC-FID

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ABSTRACT

Objective: To develop a Sensitive, accurate, precise and linear GC-FID method for quantitate estimation of Benzyl Cyanide as an impurity in Primidone API at ppm level and validated as per ICH guidelines.
Methods: This GC-FID method was developed and validated for the trace level analysis of an impurity by using Column: VF-624ms, 30m*0.32mm ID*1.8µm. Carrier Gas: Nitrogen. Flow: 1.0 mL/min. Injector temperature: 200°C. Detector temperature: 250°C. Split ratio: 10. GC Oven program: Initial temperature 100°C hold for 2.0 min and then increase the temperature up to 200°C at Ramp rate 10°C/min hold for 10.0 min and then increase the temperature up to 240°C at Ramp rate 20°C/min hold for 36.0 min.
Results: The method was linear for Benzyl Cyanide as an impurity in Primidone 2.5 ppm to 15 ppm respectively. The coefficient of correlation (r) not less than 0.999. The limit of detection and limit of quantification obtained were 0.76 ppm and 2.5 ppm with respect to Sample concentration. The method was fully validated, complying FDA and ICH guidelines and obtained results were within acceptance criteria.
Conclusion: The method was successfully validated to determination and quantification of Benzyl Cyanide impurity in Primidone API. Hence, the method holds good for the routine trace analysis of Benzyl Cyanide impurity in Primidone API and its pharmaceutical dosage forms in pharmaceutical industries.

Key words: Benzyl Cyanide, Primidone, GC-FID, Method development, Method validation.

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OP-43

Oral Presentation

A Developed method for the determination of Ritonavir and nirmatrelvir by using HPLC in bulk and pharmaceutical forms

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ABSTRACT

A simple, rapid, precise, sensitive and reproducible reverse phase high performance liquid chromatography (RP-HPLC) method has been developed for the quantitative analysis of Ritonavir and Nirmatrelvir in pharmaceutical dosage form. Chromatographic separation of Ritonavir and Nirmatrelvir was achieved on Waters Alliance-e2695 by using Luna Phenyl Hexyl (250x 4.6mm, 5µ) column and the mobile phase containing Acetonitrile: Ammonium acetate pH-3.0/OPA in the ratio of **40:60% v/v**. The flow rate was 1.0 ml/min; detection was carried out by absorption at **266nm** using a photodiode array detector at ambient temperature. The number of theoretical plates and tailing factor for Ritonavir and Nirmatrelvir were NLT 2000 and should not more than **2** respectively. % Relative standard deviation of peak areas of all measurements always less than **2.0.** The proposed method was validated according to ICH guidelines. The method was found to be simple, economical, suitable, precise, accurate & robust method for quantitative analysis of Ritonavir and Nirmatrelvir study of its stability.

Key words: HPLC, Ritonavir and Nirmatrelvir

OP–44

Oral Presentation

STUDY OF OPTICAL PROPERTIES FOR DIVALENT CATION DOPPED LITHIUM PHOSPHATE NANO POWDERS

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ABSTRACT

Alkaline phosphates exhibits important nonlinear optical properties has become a special attention in the research groups. The phosphate is taken as a composition of $ABPO_4$. A is a monovalent cation and B is a divalent cation. The AlO_6 octahedra and PO_4 tetrahedra are tilted cooperatively to form an anionic, corrugated, two-dimensional $Al(PO_4)^{3-}$ frame work that can be regarded as a "distorted-glaserite" structure. The $[LiBaPO_4]$ sublattice is that of a layered block containing a six-membered ring formed from alternating linkages of LiO_4 and PO_4 tetrahedra. The six- membered rings show a boat-type arrangement with the up(U) or down(D) pointing sequence. Li ions can not only enhance the emission intensity but also extend the luminescence lifetime, which is probably attributed to the suitable Li^+ contents that reduce the crystal defects of phosphors. Divalent cation is taken in different proportions with divalent metal ions and they are synthesized. The phosphates were synthesized with Solid State Reaction method. The studies of optical properties and FT-IR are done for the samples. The compositions have exhibited very good optical properties which can be used as LEDs.

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OP-45

Oral Presentation

A NEW RP-HPLC METHOD FOR SIMULTANEOUS DETERMINATION OF OFLOXACIN AND CEFIXIMEIN PHARMACEUTICAL FORMULATIONS

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ABSTRACT

The aim of the study was to develop and validate high performance liquid chromatography (HPLC) assay for the simultaneous determination of **ofloxacin and cefixiein** in multicomponent tablet dosage form. Ofloxacin[60] is a fluoroquinolone subsidiary. Synthetically, it is(±)-9-fluoro-2,3-dihydro-3-methyl-10-(4-methyl-1-piperazinyl)-7-oxo-7H-pyrido-[1,2,3-de]-1,4-benzoxazine-6-carboxylicacid.It is primarily utilized as antibacterial for the management of urinary tract contamination, explicitly spreaded illnesses. Ofloxacinis utilized in the management of urinary tract, prostate, skin, urinary and respiratory tract contaminations. It is like wise used to treat certain explicitly transmitted ailments and is additionally utilized as an antibacterial operator in the treatment of diseases brought about by extensive scope of both Gram-positive and Gram-negative microscopic organisms. **The method was validated with respect to specificity,precision, accuracy and linearity. Due to its simplicity and accuracy, the assay method is suitable for routine analysis of multi-component tablet formulation.**

KEY WORDS: HPLC, ofloxacin and cefiximein, **multi-component tablet formulation.**

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OP–46

Oral Presentation

Structural, vibrational, and photocatalysis properties of $Nd_{0.7}Bi_{0.3}Fe_{0.7}Sc_{0.3}O_3$ rare-earth orthoferrite nanoparticles synthesized by the sol-gel method

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ABSTRACT

To synthesize the rare earth orthoferrite $Nd_{0.7}Bi_{0.3}Fe_{0.7}Sc_{0.3}O_3$ nanopowder, a perovskite, a sol-gel technique was employed. The resulting particles were characterized using SEM, XRD, and UV-visible absorption spectroscopy. The perovskite structure of $Nd_{0.7}Bi_{0.3}Fe_{0.7}Sc_{0.3}O_3$ (with La having an ionic radius of 1.36 Å) exhibits internal deformation due to the large ionic radii of the elements occupying the A-site. This deformation affects several of its desirable properties. Notably, there is a reduction in lattice parameters and an increase in octahedral distortion. Deviations in the Raman modes can indicate spin-phonon coupling in $Nd_{0.7}Bi_{0.3}Fe_{0.7}Sc_{0.3}O_3$ additionally, increased crystalline distortions can hinder the spin-lattice interactions, leading to adverse effects. The particles were found to be uniformly spherical, with an average size of 80 nm. The optical energy band gap of $Nd_{0.7}Bi_{0.3}Fe_{0.7}Sc_{0.3}O_3$ at the nanoscale was measured to be 2.1 eV. This structure was further confirmed through optical absorbance and Raman spectroscopy measurements, aided by spin-phonon coupling. The optical characteristics exhibit intriguing variations that correlate with the expected photocatalytic activities. The photocatalytic activity of $LaFeO_3$ nanoparticles was evaluated through the UV degradation of various organic dyes, including acid fuchsine (AF), methyl orange (MO), rhodamine B (RhB), and methylene blue (MB). Notably, the dyes underwent substantial photocatalytic degradation when exposed to visible light.

Keywords: X-ray diffraction, Surface morphology, Photocatalysis, Raman Spectroscopy, Sol-gel.

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OP–47

Oral Presentation

Cu, Ag, and Au doped Graphene Oxide-CdS NPs synthesis and investigation of photocatalytic degradation of dyes and pesticides for wastewater treatment

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ABSTRACT

The Cu, Ag and Au doped GO-CdS NPs are prepared through the hydrothermal method under temperature and pressure controlled conditions. The samples are characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), high-resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED) and UV-vis diffused reflectance spectra (UV-DRS). The photodegradation performances of the Cu, Ag and Au doped GO-CdS samples are mainly investigated using the mixture wastewater containing both rhodamine B (RhB) and methyl orange (MO) as the simulated industry wastewater. The photocatalytic action of the dyes is tested in photodegradation of the commercial organic dyes RhB and MO as well as pesticides in aqueous solutions under sunlight irradiation. Moreover, the doped GO-CdS NPs as photocatalysts exhibit the unexpectedly higher efficiencies than the bare GO-CdS NPs. The apparent rate constants of the process are determined from the kinetic curves using appropriate models. Importantly, the highly efficient, inexpensive doped CdS NPs are expected to be applied in practical industry wastewater that containing complicated toxic components.

Keywords

Doped CdS NPs, Hydrothermal method, Mixture dyes, Photodegradation, Rate constants

OP–48

Oral Presentation

Thermo physical Properties of binary liquid systems at various temperatures (2-methyl-2,4-pentanediol with 3-chloroaniline, m-methyl aniline and m-methoxy aniline)

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ABSTRACT

Excess molar volume, excess isentropic compressibility, deviation in viscosity and excess Gibbs free energy for activation of viscous flow for binary mixtures of 2-methyl-2,4-pentanediol with meta-substituted aniline (3-chloroaniline, 3-methoxyaniline and 3-methylaniline) at selected compositions were determined from the measured values of densities (ρ), viscosities (η), and speeds of sound (u) of pure components and their mixtures at from 303.15 K to 313.15 K. The results are analyzed in terms of interactions arising due to hydrogen bond forces in the binary mixtures. Prigogine-Flory-Patterson (PFP) theory is applied to identify the predominant molecular interaction. Jouyban-Acree model, results are discussed in terms of mean relative deviation (MRDs) and individual relative deviation (IRD) between calculate and experimental densities and speeds of sound as an accuracy criterion.

Keywords: 2-methyl-2,4-pentanediol, meta-substituent aniline, Jouyban-Acree model, PFP Theory

OP–49

Oral Presentation

Marine Natural Products to be Anti-cancer agents

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ABSTRACT

Marine sponges and tunicates are an excellent source of unexploited pharmaceuticals due to their structural diversity and biological activities. These chemicals are created in response to the hard and competitive circumstances present in the maritime environment. Invertebrates are regarded as one of the most diverse groupings. A large number of marine natural products(MNPs) have been identified as antineoplastic medicines. The abstract provides the overview of marine natural products, both in the research and clinical stages, from various organisms that have been shown to be active or potentially useful in cancer treatment. The structural variety of MNPs is additionally highlighted and compared to small molecule anticancer medicines currently in clinical use. Furthermore, this research investigates the use of virtual screening for MNPbased drug development and demonstrates that traditional approaches to drug candidate selection still effective. This study summarises the synthesized marine sponges will give potent anticancer drugs which are useful for mankind.

Keywords: Marine natural products,cancer,invertebrates

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OP–50

Oral Presentation

Synthesis of new derivatives of 5-((Dimethylcarbamoyl)methyl)-2-butyl-N-alkyl / aryl-4-methyl-6-oxopyrimidine-1(6H)-carboxamides and their biological evaluation of antimicrobial and anticancer activity

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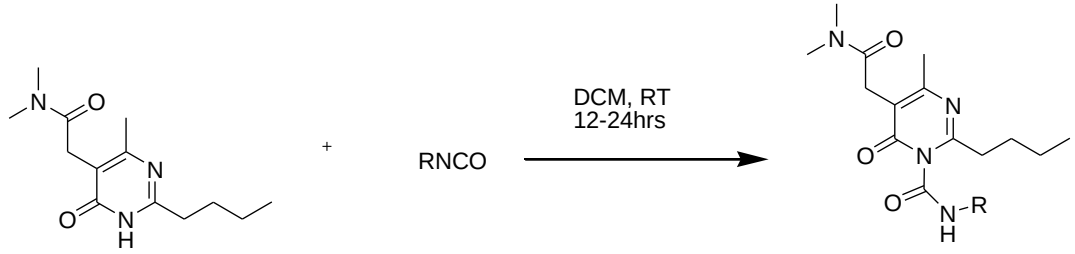
Abstract

P-heterocyclic pyridine urea derivatives showed significant anti-inflammatory activities both in vivo and vitro and also acts as antiviral especially piperazine doped with febuxostat urea and thiourea derivatives found to be promising antiviral agents against Tobacco Mosaic Virus. Ten new derivatives of 5-((dimethylcabamoyl)methyl)-2-butyl-N-alkyl/aryl-4-methyl-6-oxopyrimidine-1(6H)-carboxamide (**3a-l**) have been synthesized, and most of the derivatives were promisingly active towards antibacterial and antifungal strains as compared with Ampicilin and flconazole as positive controls due to the presence of pyrimidine heterocyclic ring system. All the new derivatives were prepared from 2-(2-butyl-1,6-dihydro-4-methyl-6-oxopyrimidin-5-yl)-N,N-dimethylacetamide (**1**) is reacted with alkyl / arylisocyanate (**2a-l)** in dichloromethane at room temperature. The structures of newly synthesized derivatives were confirmed by IR, 1H NMR, MS spectral data and elemental analysis.



2-(2-Butyl-1,6-dihydro-4-methyl-6-oxopyrimidin-5-yl)-*N*,*N*-dimethylacetamide(**1**)

Alkyl /Arylisocyanates(**2a-l**)

5-((Dimethylcarbamoyl)methyl)-2-butyl-*N*-alkyl /aryl -4-methyl-6-oxopyrimidine-1(6*H*)-carboxamide (**3a-l**)

Scheme: Synthesis of new conjugative derivatives of 5-((dimethylcarbamoyl)methyl)-2-butyl-N-alkyl/aryl-4-methyl-6-oxopyrimidine-1(6H)-carboxamides (**3a-l**).

Key words: 2-(2-butyl-1,6-dihydro-4-methyl-6-oxopyrimidin-5-yl)-N,N-dimethylacetamide; alkyl / arylisocyanate; 5-((dimethylcabamoyl)methyl)-2-butyl-N-alkyl / aryl-4-methyl-6-oxopyrimidine-1(6H)-carboxamide; antibacterial activity; antifungal activity.

OP–51

Oral Presentation

Determination of genotoxic impurities in paracetamol by LC-MS/MS

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ABSTRACT

Paracetamol is a well-known analgesic and antipyretic agent. It is employed in the treatment of fever and mild to moderate pain. It is an extensively accessible drug that is marketed under various brand names. Genotoxic impurities are a distinct case of compounds that exhibit a high potential for health risks, even at lower concentrations in pharmaceutical products. These impurities are substantially mutagenic and can potentially damage the DNA at different levels. It indicates that the limitation of these genotoxic impurities is the need of the hour. Hence, the present study focuses on the development of a simple and reliable LC-MS/MS method for the determination of the selected four genotoxic impurities in paracetamol, where the run time is shorter. The developed method was validated as per the existing ICH Q2 (R2) guidelines.

KEYWORDS: Paracetamol, Determination, Method development, Validation, Genotoxic impurities, LC-MS/MS

OP-52

Oral Presentation

Synthesis of 1,2,4-Oxadiazole from amidoximes and TBHP as a methyl free radical

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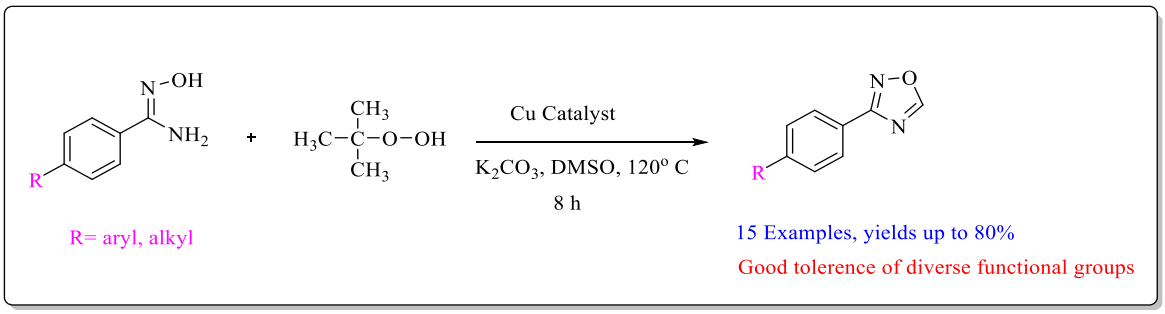
ABSTRACT

Oxadiazoles are a fascinating class of heterocyclic aromatic compounds. These compounds are known for their diverse biological and pharmaceutical applications like Anticancer [1], antimicrobial [2], anticonvulsant, antiviral [1], antioxidant, antitubercular [2], insecticides [3], etc. various pharmaceutical drugs like raltegravir, butalamine, fasiplon, oxolamine, and pleconaril has oxadiazole moieties. **1**,2,4-Oxadiazole Linked 5-Fluorouracil Derivatives have shown promising results on human breast cancer cell lines.

On the other hand, amidoximes can act as a valuable building blocks for the synthesis of various heterocyclic compounds like 1,2,4-oxadiazole, quinolinones, imidazole, etc. whereas *tert*-Butyl hydroperoxide, which has been widely used as an oxidant, has also been employed as a source of a methyl radical [4] in the presence of a copper catalyst. In this reaction TBHP acts as a methyl free radical source which is formed as an intermediate and further reacts with amidoximes to give oxadiazoles. To the best our knowledge no reaction has been reported for the synthesis of 1,2,4-Oxadiazoles from Amidoximes and TBHP as a methyl source. Therefore, herein, we report an efficient and facile method for the synthesis of 1,2,4-Oxadiazoles from amidoximes and TBHP in the presence of copper catalyst, K_2CO_3 as a base, DMSO as a solvent at 120 ^oC for 8 h.



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OP–53

Oral Presentation

Study of the physicochemical stability, followed by a comparative study of the dissolution kinetics of a generic drug Amisulpride (200mg) and its original drug Solian (200 mg) Case

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ABSTRACT

The activity of the pharmaceutical industry and development has improved since the evolution of generic drugs worldwide to obtain a therapeutic action identical to the same pharmaceutical product, which must present constant characteristics and comply with strictly rigorous regulations to ensure their quality and effectiveness. Dissolution kinetics is essential for the quality control and performance evaluation of drug products, and the drug's registration—the objective is to be achieved by taking the sample from the Sanofi-Synthelabo (India) laboratory, to carry out, according to the recommendations of the American Pharmacopoeia, a comparative study of the dissolution profiles of the princeps Solian tablet dosed at 200 mg and Amisulpride 200mg in three buffer environments (pH = 1.2, 4.6 and 6.8), using the method of direct comparison of dissolution profiles (dissolution percentage greater than 90%). Through the exploratory analysis of the dissolution profiles, it was shown that the kinetic mechanisms that best fit were zero-order. These models describe the drug release process by diffusion and are therefore more suitable for dissolution profiles of slow-release drugs. This study concluded that Amisulpride 200 mg is similar to the Princeps and has good pharmaceutical quality. Still, for the moment, the bioequivalence of these generic drugs must be discussed through clinical studies.

KEYWORDS: dissolution kinetics, generic drug, original drug, drug registration, bioequivalence, Amisulpride 200mg, Solian 200mg.

OP–54

Oral Presentation

Advancements in Sustainable Chemistry: Nanoadsorption Techniques for Biomedical Remediation

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ABSTRACT

Sustainable chemistry focuses on minimizing environmental and health impacts through green and efficient methods, and in recent years, nanotechnology has emerged as a promising field in biomedical applications. Among the various nanotechnological advancements, nanoadsorption has shown great potential for the remediation of biomedical contaminants, including toxins, drugs, and pathogens. This review highlights the development of nanoadsorption techniques for biomedical applications, including drug delivery systems, toxin removal, and pathogen capture. Special emphasis is placed on biocompatible and sustainable nanomaterials such as graphene oxide, carbon nanotubes, metal-organic frameworks (MOFs), and nanoparticles that exhibit high adsorption capacities and selectivity. The article explores the principles behind nanoadsorption, such as surface functionalization, adsorption kinetics, and interaction mechanisms, and discusses the role of these materials in biomedicine for detoxification, targeted therapy, and pathogen deactivation. Additionally, the article considers the challenges of integrating nanoadsorption into clinical settings, including safety, biocompatibility, and regulatory concerns, while suggesting future directions for research in this emerging field of biomedical remediation.

Keywords: Sustainable chemistry, nanoadsorption, biomedical remediation, nanomaterials, drug delivery, toxin removal, pathogen capture, biocompatibility, environmental impact.

Poster

PRESENTATIONS

Design, Synthesis and Biological Evaluation of Imidazo[1,2-a]pyridin-3-yl) cinnamamide Derivatives as Novel Anti-Cancer Agents

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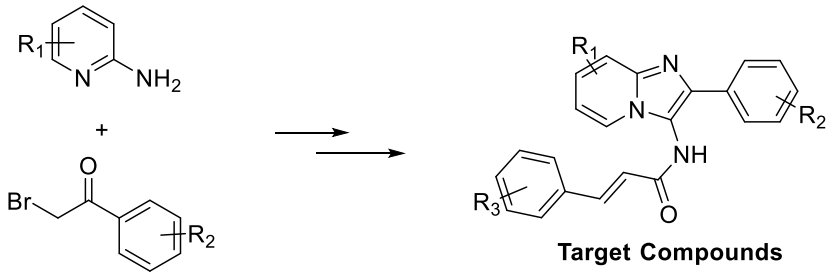
ABSTRACT

Despite tremendous scientific efforts and advancements in treatment options, cancer continues to be a major global health concern. It remains one of the leading causes of morbidity and mortality worldwide, with its complex and multi-factorial nature. As researchers, we are focused on exploring new strategies to synthesize molecules that could serve as promising scaffolds in the development of novel bio-active compounds offering hope for cancer patients while deepening our understanding of the disease's underlying mechanisms. In the present work, a series of new 20 imidazo[1,2-a] pyridin-3-yl) cinnamamide derivatives have been synthesized using an easy and conventional synthetic route in three stages allowing large-scale production using the commercially available key starting materials. All the synthesized compounds were characterized by using ^{1}H, ^{13}C NMR, LC-MS, & FT-IR spectroscopic techniques.

Compounds were tested for anticancer activity in three cancer cell lines, SCC-25 (Oral squamous cell carcinoma), U87-MG (glioblastoma), MCF-7 (breast cancer), and one normal cell line (HEK-293T) using WST-1 assay. Out of 20 compounds, two compounds **(PBC3)** and **(PBC14)** demonstrated potent activity against cancer cell lines, with IC_{50} values ranging from 5 to 10 µM. Additionally, fourteen compounds exhibited IC_{50} values from 2-10 µM against SCC-25 cell line. **(PBC3)** emerged as the most potent against the SCC-25 cell line with IC_{50} of 2 µM compared to camptothecin **(standard drug)**, showing IC50 of ≅1 µM. Additionally, in-silico ADME properties are carrying out for the most active molecules, aiding in assessing their pharmacokinetic profiles.



Target Compounds

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Ring-opening polymerisation (ROP)-induced catalytic activity of the zinc metal complex to lower the curing temperature of bisphenol-A/F benzoxazines

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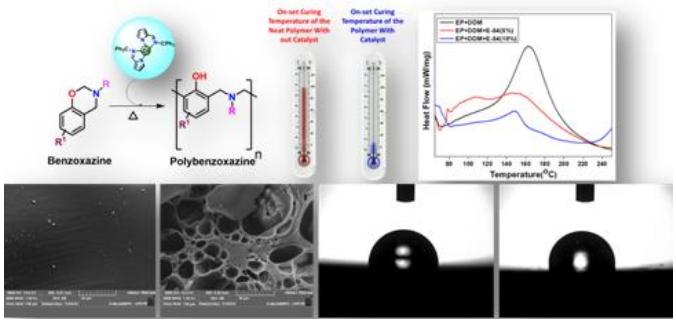
Here we report the synthesis of Zn(II) complex stabilized by flexible donor bidentate Schiff's base ligands such as [2-(Ph_3CN=CH)–C_4H_3NH] by salt metathesis route. The obtained zinc complexes [Zn(2-(Ph_3CNH-CH)=$C_4H_3N)_2$] were preliminarily characterized by using FT-IR and NMR spectroscopic techniques. Furthermore, also report the curing behaviour of benzoxazines (B.Z-a, B.F-a) and Epoxy resins via ring-opening polymerization using zinc catalysts with use of DSC analysis results. Results of curing investigations showed that, without compromising intrinsic properties of the polymer, such as thermal stability, all zinc are efficient in lowering the ring-opening polymerization curing temperature through the coordination–insertion process. We observed that, reduction of curing temperature was achieved up to 20% once we use 10% catalyst loading and there is no considerable activity at room temperature. This indicates that, Metal cations which are surrounded by sterically bulky ancillary ligands are capable of converting benzoxazines into PBZs relatively at lower temperatures via controlled ring-opening polymerization process. Zinc complex was exhibited high catalytic activity towards ring-opening polymerization of benzoxazine monomers at different catalyst/monomer ratio. The obtained polymers were initially characterized by using NMR spectroscopic studies. However, the solid-state structures of zinc complex are confirmed by X-ray crystallographic.



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DETERMINATION OF TIME SINCE DEATH FROM HAIR ROOT BANDING

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ABSTRACT

DNA is a molecule that carries the genetic information of an organism's development and functioning. It is passed from one generation to the other i.e., from the adult organism to their offsprings. It varies from person to person. It is double-stranded and helical in structure. DNA is involved in the replication, transcription, cellular metabolism, DNA fingerprinting and gene therapy etc., It is located inside the nucleus. DNA helps in the development of organisms, survival, reproduction, building and maintaining structure, passing on the genetic information to the next generations, making proteins, determining the physical characteristics etc., DNA is present nearly in every body sample like; blood, hair, saliva, skin cells, semen, tissue, bone, teeth, fingernails and even bodily fluids like sweat and mucus. Here, in this we talk about the hair sample. Hair root banding is a visible, microscopic band that can appear near the root of a hair follicle. It is typically observed in the forensic investigations. It is considered as a sign of postmortem decomposition; means it occurs after the death of a person. It is a visible indication of hair degradation during the process of decomposition. It helps to estimate the time since death of a person. It is only visible under the microscope and appears as an opaque area near the hair root. The exact cause of this formation of the banding of hair root is not known yet, it is believed that it might be due to the breakdown of the proteins within hair root causing definite band pattern. It appears as a dark band around the hair near the root where the skin surface meets the hair shaft.

Keywords: DNA, genetic information, transcription, DNA fingerprinting, gene therapy, root banding, time since death, hair shaft.

Green Synthesis of Silver Nanoparticles Using *Panisea uniflora* Leaf Extract: A Comparative Study of Antibacterial Efficacy

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ABSTRACT

Panisea uniflora (Lindl.) Lindl (Orchidaceae) commonly known as One-flowered Panisea is an important ethnomedicinal plant used to treat various ailments by tribal healers of Darjeeling Himalaya. The increasing resistance of bacteria to conventional antibiotics has led to the exploration of plant-derived antimicrobials and nanotechnology-based solutions. This study compares the antibacterial activity of crude *Panisea uniflora* leaf extract (PU), prepared using aqueous extraction, and its synthesised silver nanoparticles (PU-AgNPs), produced using aqueous extracts as both the reducing and stabilizing agents. The antibacterial efficacy of PU and PU-AgNPs was evaluated against two Gram-positive bacteria (*Bacillus subtilis* and *Staphylococcus aureus*) and two Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*) using Agar well diffusion method. The zone of inhibition was measured at three different concentrations (10 µg/mL, 20 µg/mL, and 30 µg/mL).

The results revealed that while the crude extract of *Panisea uniflora* (PU) exhibited minimal antibacterial activity, the silver nanoparticles synthesized from this extract (PU-AgNPs) displayed a significant, dose-dependent inhibition of bacterial growth. Notably, at a concentration of 30 µg/mL, *Escherichia coli* exhibited the largest inhibition zone of 12.52 ± 0.15 mm, with *Bacillus subtilis* and *Pseudomonas aeruginosa* also showing increased susceptibility. For comparison, the positive control, chloramphenicol (10 µg/mL), produced a 15 mm inhibition zone, whereas the negative control, sterile distilled water, showed no inhibitory effect. The increased antibacterial potency of PU-AgNPs can be attributed to their nanoscale size, enhanced silver ion release, and synergistic interactions with bioactive plant compounds. These findings suggest that silver nanoparticle synthesis significantly enhances the antibacterial properties of *Panisea* leaf extract, making PU-AgNPs a promising candidate for natural antimicrobial applications.

Keywords: *Panisea uniflora*, Aqueous leaf extract, Silver nanoparticles (AgNPs) and Antibacterial activity.

Vitrimers trigger covalent bonded bio-silica fused composite materials for recycling, reshaping and self-healing applications

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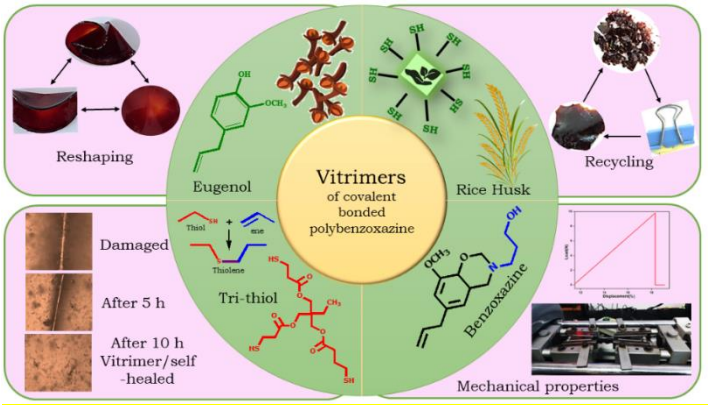
ABSTRACT

In this work, a recycling, reshaping and self-healing strategy was followed for polybenzoxazine through Vitrimers of S-S bond cleavage reformation and supramolecular interactions were described. The E-ap benzoxazine monomer has been synthesized through Mannich condensation reaction by using a renewable Eugenol, 3-amino-1-propanol and paraformaldehyde. Further, E-3ap monomer was reinforced with various weight percentages (5, 10 & 15 wt.%) of thiol-ene group. Followed by various weight percentages of functionalized bio-silica (BS) has been copolymerized with E-3ap(10%-SH) for to improve the thermal stability. The structure of the monomers was confirmed by NMR and FT-IR analysis, Thermal properties of the cured materials were analyzed by DSC and TGA. Tensile test was used to study the mechanical property of the poly(E-3ap-*co*-SH)/BS material. The SEM and Optical microscope were characterized on the film for to investigate the self-healing properties of the poly(E-3ap-*co*-thiol-ene)/BS. Moreover, the self-healing ability of a test specimen was shown by using photo and video clippings. The results of Vitrimer based renewable polybenzoxazine showed good recycling, reshaping and self-healing abilities and have several industrial and engineering applications.



Keywords: Thiolene, bio-silica, shape memory, self-healing, Vitrimers

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Unveiling the Pharmacological Paradox: A Comparative Analysis of 5F-ADB and 5F-MDMB, Two Prominent Synthetic Cannabinoids

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ABSTRACT

Synthetic cannabinoids, such as 5F-ADB and 5F-MDMB, have gained notoriety for their potent psychoactive effects and potential for abuse. These compounds, often marketed as "legal highs," have been linked to numerous adverse health effects, including seizures, psychosis, and even death. This study aims to provide a comprehensive comparison of 5F-ADB and 5F-MDMB, including their chemical structures, pharmacological effects, and toxicological profiles. A review of existing literature was conducted, including scientific studies, case reports, and forensic analysis. Chemical structures were analyzed using molecular modeling software, and pharmacological effects were compared using in vitro and in vivo studies. Our analysis reveals significant differences in the chemical structures and pharmacological effects of 5F-ADB and 5F-MDMB. Toxicological profiles also differed, with 5F-ADB linked to more severe adverse effects. This study highlights the importance of understanding the distinct properties of synthetic cannabinoids, such as 5F-ADB and 5F-MDMB. Our findings have significant implications for forensic science, toxicology, and public health, and underscore the need for continued research into the effects of these substances.

Keywords: Synthetic Cannabinoids, 5F-ADB, 5F-MDMB, Forensic Science, Toxicology

Vacutainer Systems: A Cornerstone of Forensic Science for Secure and Efficient Biological Evidence Collection

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ABSTRACT

Vacutainer systems have transformed the collection and handling of biological evidence in forensic science. This study aims to highlight the significance of Vacutainer in forensic investigations, emphasizing its reliability, efficiency, and accuracy in collecting and preserving biological samples. The Vacutainer system ensures a closed, sterile environment for sample collection, minimizing contamination risks and preserving evidence integrity. Its evacuated tubes facilitate smooth blood draw and separation, enabling accurate analysis and interpretation of results. This is particularly crucial in forensic toxicology, serology, and DNA analysis, where even minute contaminants can compromise the integrity of the evidence. This study demonstrates the critical role of Vacutainer in forensic science, showcasing its benefits in maintaining the chain of custody, preventing sample degradation, and ensuring the accuracy of test results. By utilizing Vacutainer systems, forensic experts can ensure the integrity and reliability of biological evidence, ultimately contributing to the delivery of justice. The findings of this study underscore the importance of adopting standardized protocols for biological evidence collection and handling, with Vacutainer systems at the forefront of this effort.

Keywords: Vacutainer, Blood, Evacuated tubes, Forensic Science, Biological evidence

Hierarchy of Police and Emerging Legal Frameworks in India: A Critical Analysis of Recent Legislative Development

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ABSTRACT

Police badges represent authority, accountability, and identity within the law enforcement agencies. In India, recent legislative changes have impacted the design, significance, and regulatory framework of police insignia. This study delves into the evolution of police badges in India, emphasizing their role in law enforcement, security, and public perception amid new laws. It provides a comprehensive overview of key new laws introduced in India, analysing their objectives, implications, and potential challenges. The study also examines the socio-legal impact of these changes on policing and citizen interactions, discussing reforms in areas such as data protection, labour laws, environmental regulations, and digital transactions. The presentation aims to offer insights into the broader impact of these changes on industries, legal practitioners, and policymakers, ultimately fostering a deeper understanding of India's dynamic legal system within a global context. The study concludes that recent legislative developments in India have made incremental progress in addressing police accountability and reform, but more robust measures are required to tackle entrenched systemic issues.

Keywords*:* Police badges, legal reforms, policy changes, law enforcement, policy makers

Green synthesis of silver nano particles from custard apple seeds and study of their antimicrobial activity and anticancer properties

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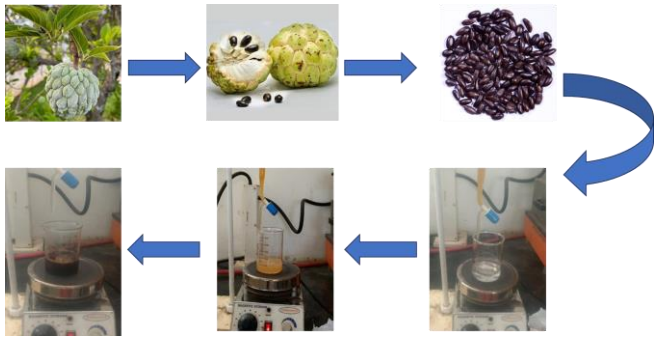
ABSTRACT

Nanotechnology is developing field of science in which particle size vary from 1 – 100 nanometers. Nanoparticles can be synthesized by physical, chemical and biological route of synthesis. This study focused on biological synthesis of nanoparticles. Silver has very different and unique properties like antimicrobial activity, protection against cancer cells, anti-viral activity etc. Biological way of silver nanoparticles synthesis is cost effective and eco-friendly. Also biosynthesis is very simplest way to produce nanoparticles. Now-a-day's food waste utilization is important to minimizing generated waste and waste related problems.

Our aim is the green synthesis of silver nanoparticles from custard apple seeds and study of its antibacterial and anticancer activities. Bio-synthetic route is used for production of non-toxic, eco-friendly particles. Biosynthesis (Green synthesis) of silver nanoparticles was studied using Annona Squamosa (Custard Apple) seeds. Silver nanoparticles were characterized by UV-visible and X-ray diffraction spectroscopic techniques. Finally, the biological activities of nanoparticles also studied. Antimicrobial activity was checked against E-coli and to study of anticancer activity of silver nanoparticles of different sizes.



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Optical and vibrational studies of Cu^{2+} ions doped $Li_2Zn_2Al(PO_4)_3$ nanopowders

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ABSTRACT

In this study Cu^{2+} doped $Li_2Zn_2Al(PO_4)_3$ was synthesized by using Wet chemical method. The optical absorption and Fourier transform infrared spectroscopy (FTIR) are systematically investigated. From optical absorption spectrum characteristics bands indicating the presence of Cu^{2+} ions are found. By using Optical absorption data band gap energies were determined. The fundamental vibrational modes are studied from Raman & FTIR spectra. The combined results suggest that Cu^{2+} doping effectively tailors the structural and optical properties of $Li_2Zn_2Al(PO_4)_3$ making it a promising candidate for advanced material applications.

Keywords: Cu^{2+}, Optical Absorption, FTIR , Nanopowders.

Determination of Limit of Detection (LOD) and Limit of Quantification (LOQ) of Doripenem by High-Performance Liquid Chromatography (HPLC)

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ABSTRACT

Doripenem, a broad-spectrum carbapenem antibiotic, plays a crucial role in the treatment of complex bacterial infections, particularly those resistant to conventional antibiotics. Its effectiveness against a wide array of Gram-positive and Gram-negative bacteria, including *Pseudomonas aeruginosa*, makes it a valuable asset in the clinical arsenal. Given its clinical importance, the accurate and sensitive detection and quantification of doripenem in biological matrices (such as plasma, serum, and urine) and pharmaceutical formulations are paramount for both therapeutic drug monitoring (TDM) and quality control purposes. The concepts of the limit of detection (LOD) and the limit of quantification (LOQ) are fundamental in analytical chemistry, ensuring that methods used for the detection and quantification of substances like doripenem are both sensitive and reliable. The LOD refers to the lowest concentration of the substance that can be detected but not necessarily quantitated as an exact value, while the LOQ is the lowest concentration that can be quantitatively determined with acceptable precision and accuracy. Establishing these parameters for doripenem is essential to ensure the reliability of pharmacokinetic studies, therapeutic monitoring, and ensuring the efficacy and safety of the drug in treatment protocols. This introduction sets the stage for a detailed exploration of the methodologies and technologies employed in determining the LOD and LOQ for doripenem, discussing their implications for clinical practice and pharmaceutical quality assurance. The development and validation of analytical methods, including chromatography, mass spectrometry, and other innovative techniques, are critical for achieving the sensitivity and specificity required for effective monitoring and quality control of this vital antibiotic.

Keywords: Doripenem, High-Performance Liquid Chromatography (HPLC), UV Detection, Limit of Detection (LOD), Limit of Quantification (LOQ), Pharmaceutical Quality Control, Pharmacokinetic Studies, Regulatory Compliance.

Synthesis and optical properties of Li_2Co_3 electrode material

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ABSTRACT

Transition metal oxides promised as electrode materials for supercapacitors have received much interest, the combination of lithium carbonate (Li_2Co_3) with cobalt chloride hexahydrate ($CoCl_2.6H_2O$) nanoparticles, which is the simplest, most cost-effective solution and combustion for producing electrode material. The present study describes the preparing of electrode powder by synthesizing of transition metal oxide with Urea (NH_2CONH_2) in deionized water. Urea is rich source of nitrogen which is essential element and it decomposes easily when they can react with metals to form electrode materials under thermal treatment. Further this solution treating with sintered at 300 ^{0}C to produce desired material. Raman and FTIR study shows the modes of vibrations of obtained material and Optical Absorption characteristics are studied.

 ISBN:978-93-92760-51-8

Synthesis of Schiszandrin derivatives and evaluation of their Anti-cancer Activity

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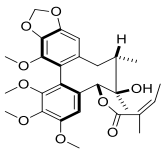
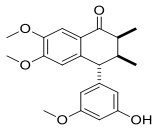
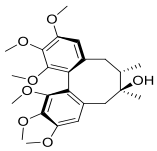
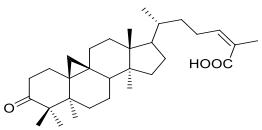
ABSTRACT

Schisandra grandiflora belongs to the Magnoliaceae family and grown in Far East Asia and its cultivation requires moderate humidity and wet soil. In Chinese and Korean traditional medicine, *Schisandra species* has been used to treat diabetes, palpitation, insomnia, nocturnal enuresis, dysentery, cough, asthma, phlegm, and jaundice.[1] Recent studies have demonstrated its effects on the cardiovascular system, gastrointestinal system, anti-inflammatory, central nervous system, endocrine system, and stress protect.[2] Phytochemical investigation of chloroform extract from fruits of *Schisandra grandiflora* resulted in the isolation of known compounds (**1-5**). Their structures were elucidated on the basis of the extensive spectroscopic analyses (IR, Mass and NMR) and by comparison of the data with those reported in the literature. Further, we also prepared the derivatives of Schiszandrin *via* esterification reaction and all the derivatives were tested for their cytotoxic activities.

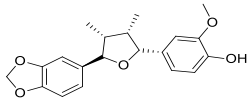

GOMISIN B(1)


ARISANTETRALONE(2)


SCHISZANDRINE

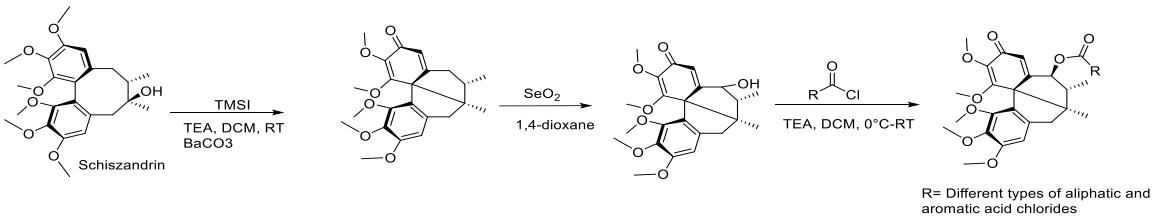


SCHIZADRNIC ACID(4)



(-) CHICANINE(5)

Semi Synthetic Derivatives:



R= Different types of aliphatic and aromatic acid chlorides

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Ultrasound-assisted synthesis of α – aminophosphonates using nano ZnO catalyst: evaluation of their anti-diabetic activity

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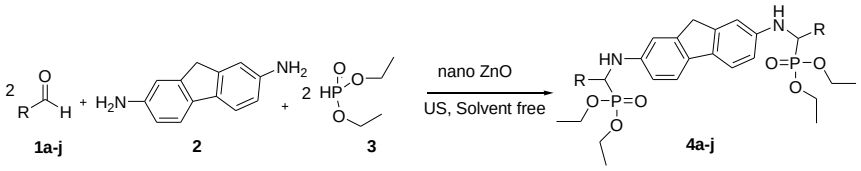
ABSTRACT

Diabetes mellitus (DM) has emerged as a serious global health concern, with an estimated 537 million individuals living with the condition by 2021. This figure is expected to rise to 783 million by 2045, placing a substantial economic and social strain on global healthcare systems.[1] Notable biological properties of bis(α-aminophosphonates) include antioxidant, anti-tubercular, anti-diabetic, and anti-proliferative activity against human tumor cells from colon carcinoma. Among the various synthetic techniques suggested for the production of α-Aps, the Kabachnik-Fields (K-F) reaction-the nucleophilic addition of phosphites to imines was demonstrated to be a practical method.[2]

In the present work, a more efficient and environmentally friendly way of synthesizing α-aminophosphonates is achieved by employing nano-ZnO to catalyze the Kabachnik-Fields reaction under ultrasonication within a solvent-free environment. Before synthesis, molecular docking and in silico ADME analysis were used to assess each molecule's drug-like characteristics and ability to inhibit α-amylase and α-glucosidase. The newly synthesized compounds' in vitro inhibitory effects on α-amylase and α-glucosidase were also evaluated, and their structure was confirmed using spectroscopic investigation. The target enzyme was effectively inhibited by most of the substances. In comparison to the reference drug, acarbose (IC_{50}, 106.5±0.6 µg/mL), compounds 4d (IC_{50}, 102.2±0.3 µg/mL), 4h (IC_{50}, 102.9±0.4 µg/mL), which contained a 2H-1,3-benzodioxol-5-yl moiety, and 4i (IC_{50}, 103.9±0.5 µg/mL) showed the strongest inhibitory activity. The enzyme inhibition of the remaining compounds ranged from moderate to good.



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Corrosion Studies of Al-6063/TiB2/SiC Nano Hybrid composites

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ABSTRACT

Aluminium alloys are employed in aerospace, automotive, and other structural uses due to their high strength and lightweight qualities. Moreover, when aluminum alloys are exposed to different conditions at different temperatures, corrosion becomes a life-limiting problem. In this study Alumina (TiB2) and palm kernel shell ash (SiC) were used as reinforcement particles in Al 6063 matrix alloy, this work examines the corrosion behaviour of Nano Nano Hybrid composites at various mix ratios. The method of double stir casting was employed to develop the composites. Both gravimetric analysis and electrochemical measurements were used to examine the corrosion behaviours of the composites in NaCl solutions. The results obtained by the gravimetric analysis, suggested that the composite film was defective and that corrosion products were forming on the specimens' surface. Pitting and general corrosion were the mechanisms of corrosion that were detected in the samples. The Al8088 matrix's reinforcements served as active locations for the onset of corrosion. E Corr and I corr in 3.5% NaCl varied from −220.62 to −899.46 mV and 5.45 to 40.87 µA/cm2, respectively, at 24 hours. At 72 hours, E Corr values were between 255.88 and −887.28 mV, while I corr values were between 7.19 and 16.85 µA/cm2. The samples under investigation's electrochemical corrosion behaviour were shown by the Nyquist and Bode plots, which connected the main surface responses to processes related to charge transfer. The samples' relative resistance to corrosion is determined by the thin oxide layer that develops on their surface.

Keywords: Nano Hybrid composites, NaCl, TiB2, SiC, Electrochemical studies, SEM.

The Role of Biocarbon on the Removal of Cu (II) and Cr (VI) ions from Synthetic Wastewater

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ABSTRACT

Most of the heavy metals are toxic in nature. It may contribute variety of adverse environmental and human health effects due to their acute and chronic exposure through air, water and food chain. They are released into the aquatic environment from many industrial activities. Particularly cadmium, lead, chromium, nickel and copper are the most toxic metals of widespread in industrial wastewater. Hence, treatment water and wastewater and possible removal of toxic pollutants are very essential before discharge into receiving environmental systems. There are number of adsorbents are used in water treatment process. Most of the conventional treatment methods of metal removal are often limited by their operational cost and ineffectiveness at low concentrations. In this respect, a new search is in progress to identify cheap materials which may have potential adsorption capacity for the removal of pollutants in water. The use of activated biocarbon as adsorbents offers an attractive alternative to the conventional chemical materials used in water and wastewater treatment. In the current investigation, a new biocarbon material is introduced, which are produced from a medicinal plant *Lantana camara*, for the metal removal. In a model trial, 2.5g/100mL of biocarbon is used as adsorbent to the removal of Cu (II) and Cr (VI) ions with the initial concentration of 100mg/L. At the equilibrium time of 180min, at the working pH of 5.0, it is noticed that 96.30% and 95.80% removal of Cu (II) and Cr (VI) ions are observed. The removal process of selected heavy metal ion on the biocarbon matrix is an ion-exchange mechanism and also mainly depends on the physical characteristics of the materials.

Keywords: Biocarbon, adsorption, toxic pollutants, copper, chromium, wastewater

GREEN CHEMICAL APPROACHES FOR INDUSTRIAL CHEMICAL PROCESSING

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ABSTRACT

One or more chemical processes are used in the majority of manufactured goods. We can't even begin to picture our lives without the goods that the chemical industry produces. However, present chemical processes typically only transform a small percentage of the resources we take from the Earth into the needed products, resulting in a substantial number of toxic compounds and waste. The question of how to sustainably provide enough food, energy, chemicals, and materials to civilization without endangering the environment is inevitable. Since its establishment roughly twenty years ago, green chemistry has garnered a lot of interest.

It shows how academia and industry are working to solve the issues surrounding the chemical industry's sustainable growth, and both sectors are making steady strides. In a nutshell, green chemistry is the use of a set of guidelines to minimize or completely do away with the use or production of hazardous materials in the creation, production, and usage of chemical goods. The broad field of "green chemistry" includes topics including synthesis, solvents, catalysis, raw materials, products, and effective procedures.

GREEN FUELS FOR SUSTAINABLE DEVELOPMENT IN CLEAN TECHNOLOGY

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ABSTRACT

Cleaner fuels (free or aromatics, with low sulfur content) or those that convert chemical energy directly to electricity without producing harmful oxides or particulates, silently, and without the use of solvents; chemical, petrochemical, and pharmaceutical processes that can be carried out in a single step without the use of solvents and that use air as the preferred oxidant; and industrial processes that reduce energy consumption, waste production, or the use of corrosive, explosive, volatile, and nonbiodegradable materials.

By designing the right heterogeneous inorganic catalyst, which should ideally be inexpensive, easily prepared, and fully characterized, preferably under in situ reaction conditions, all of these needs and other desirable outcomes, such as the in-situ production and containment of aggressive and hazardous reagents and the avoidance of the use of ecologically harmful elements, can be met. The article describes a variety of nanoporous and nanoparticle catalysts that satisfy the majority of the strict requirements of responsible (clean) technology and sustainable development.

The manufacturing of caprolactam, the precursor of nylon, without the use of oleum and hydroxylamine sulfate; the terminal oxy-functionalization of linear alkanes in air; and the production of adipic acid, the precursor of polyamides and urethanes, without the use of concentrated nitric acid or greenhouse gases like nitrous oxide are some specific examples that are highlighted. The manufacture of 1,3-propanediol from corn, the epoxidation of terpenes and fatty acid methyl esters, the creation of polymers, polylactides, and polyesters, and biocatalysis and sustainable development are also briefly covered.

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Determination of Caffeine in coffee beverage by HPLC

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ABSTRACT

Caffeine, a stimulant found naturally in coffee, tea, and other beverages, is commonly quantified to assess its concentration in various products. HPLC is a highly effective technique for this purpose because it allows for accurate separation and quantification of caffeine, even in complex mixtures like coffee. The principle behind the determination of caffeine in a coffee beverage using **High-Performance Liquid Chromatography (HPLC)** is based on **separation, detection,** and **quantification** of caffeine from other compounds in the sample**.**

Quantitative analysis was done by HPLC method with methanol-water (95:5v/v) as mobile phase and ODS as stationary phase with flow rate 1 ml/min and UV 272 nm as the detector. The level of caffeine data was statistically analyzed using Anova at 95% confidence level. The Qualitative analysis showed that the three samples contained caffeine. The average of caffeine level in coffee bottles of X, Y, and Z were 138.048 mg/bottle, 109.699 mg/bottle, and 147.669 mg/bottle, respectively. The caffeine content of the three coffee beverage samples are statistically different ($p<0.05$). The levels of caffeine contained in X, Y, and Z coffee beverage samples were not meet the requirements set by the Indonesian Standard Agency of 50 mg/serving.

Key Words: Caffeine, Indonesian Standard Agency, High Performance Liquid Chromatography (HPLC), methanol-water(Mobile Phase), ODS- Octadecylsilyl(Stationary Phase).

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Anti-microbial constituents from the flowers of *Centratherum punctatum.*

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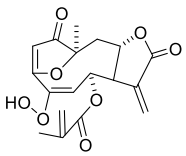
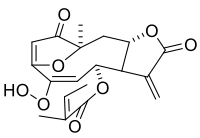
ABSTRACT

Nature has been a valuable source of medicine and has helped human in the mainte nance of his health since time immemorial1. According to the World Health Organizatio n (WHO), almost 80% of
the world's population relies on traditional medicines for their health needs due to b etter cultural acceptability, fewer side effects and better compatibility with the human bo dy. *Centratherum punctatum* (Astraceae) is well known medicinal plant and almost all part of this plant are renowned in traditional systems of medicine. As part of our programme to identify bio-active constituents from the Indian medicinal plants used in traditional systems of medicine, we have investigated the chloroform extract from the flowers of *Centratherum punctatum* which resulted in the isolation of four compounds (1-4). The structures of all the isolates were established by the interpretation of NMR and Mass spectral data. The isolates were screened against bacterial and fungal strains for their efficacy. The result indicated that all the compounds shown good activity against the bacterial strains.

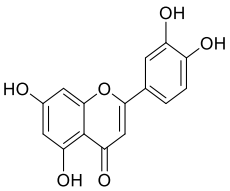
Centratherum punctatum.



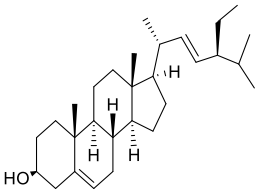
Goyazensolide (**1**)



IsoCentratherine (**2**)



Luteoline (**3**)



Stigmasterol(**4**)

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Phytochemical and synthetic studies on phenolic compounds isolated from Indian Lichen *Parmoterma tinctorum* (Despr.ex Nyl.) Hale

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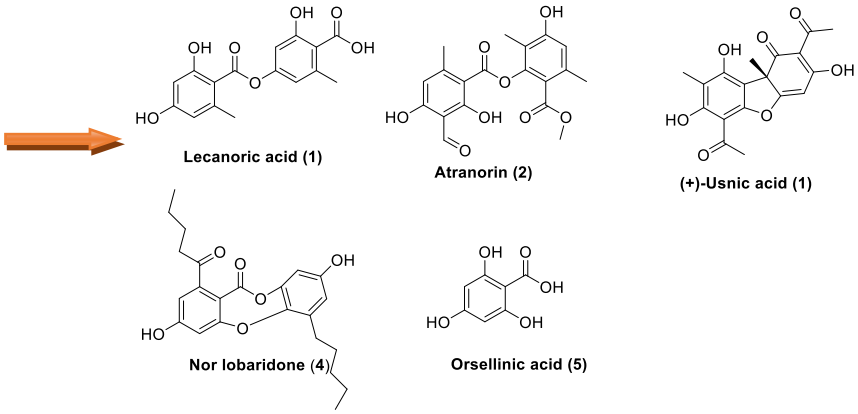
ABSTRACT

Lichens are symbiotic combination of algae and fungi. *Parmoterma tinctorum* (Despr. ex Nyl.) Hale of Parmeliaceae family got considerable attention from medicinal chemists as well as chemical biologists because of their important biological activities. *Parmoterma tinctorum* (Despr. ex Nyl.) Hale is a widely distributed in India which can grow on rocks and trees in moist areas. This lichen has been used in folk medicine for the treatment of blurred vision, bleeding from uterus, bleeding from external injuries, sores and swelling, chronic dermatitis and localized swelling diseases. As part of our continuous endeavours of phytochemical–pharmacological integrated studies on the Indian flora, we were attracted to the fascinating structural features and significant biological activities of polyphenolic compounds from lichens, which have prompted us to investigate lichens of Indian origin. Thus, our studies led the isolation of polyphenols (**1-5**) and the structures of these known compounds (**1-5**) were elucidated on the basis of extensive spectroscopic techniques, especially 2D-NMR and mass spectral data.



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Molecular docking and Swiss ADME studies of novel pyrimidopyrimidine derivatives with Human Topoisomerase IIβ receptor

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ABSTRACT

Molecular docking and evaluation of physicochemical properties, drug likeliness and pharmacokinetics were performed on a library of novel substituted pyrimido pyrimidine derivatives for their anticancer activity against human topoisomerase IIβ. All the ligand structures were drawn using chem3d and the receptor protein preparation was done using USCF Chimerax dockprep, followed by followed by Molecular docking studies performed using autodock vina integrated with PyRx 0.8 virtual screening tool. Post docking visualization was done on Biovia DS 2024 and UCSF Chimerax. The results have shown that the compound with 4-bromo styryl substituent has better binding affinity (-7.7k.cal/mole) than the standard etoposide ligand. The swiss ADME studies show that the top compound cannot cross the blood brain barrier, and has remarkably good gastrointestinal tract absorption with TPSA 91 Å2 indicating favourable pharmacokinetics, balancing permeability and bioavailability with minimal side effects, complies with Lipinski rule for drug likeliness.

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AuNPs: A Greener Approach for High Performance in Catalysis

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ABSTRACT

A traditional synthetic strategies for nanoparticles (NPs) synthesis involves toxic chemicals that are harmful to humans as well as the environment. The green chemistry method for NP synthesis is rapid, eco-friendly, and less toxic as compared to the traditional methods. In the present research, the synthesized gold nanoparticles (AuNPs) employing *via* greener approach from *Soymida febrifuga* bark extract (SFBE). The protocol was achieved by the preparation of the NPs using dried SF bark materials were taken as fine powder about 1.5g in 120mL in deionized water boiled at 60^{o}C for 30 min. After that the wine-red color crude extract was filtered. By taking 30ml of extract in 100mL round bottom flask equipped with stirring adding a freshly prepared 0.1M $AuCl_3$ in 20mL dd water maintaining 60-80^{o}C for 4 h. After that the deep brownish content was filtered and dried at 200^{o}C in hot air oven for 2h. Finally, the SFBE-AuNPs was obtained with 90 mg of brown colour powder. The physicochemical characterization of optimized SFBE-AuNPs was done by UV, FT-IR. SFBE-AuNPs have been shown to have catalytic activity employed for the treatment of waste water and dye degradation and so on.

Keywords: *Soymida febrifuga* Bark Extract, AuNPs, Greener Approach, Characterization, Catalyst.

Design of RuNPs for Biological Study and Forensic Application

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ABSTRACT

Phytochemical compounds are found in plants that are not required for normal functioning of the body, but have a beneficial effect on health or play an active role in amelioration of diseases. This is due to increased awareness of the limited ability of synthetic pharmaceutical products to control major diseases and the need to discover new molecular structures as lead compounds from the plant kingdom. Plants are the basic source of knowledge of modern medicine. Mulberry trees produce flavorful berries that are enjoyed around the world. For centuries, its leaves have been used in traditional medicine as a natural treatment for a variety of conditions. Mulberry leaves are rich in plant compounds like polyphenol antioxidants, as well as vitamin C, zinc, calcium, iron, potassium, phosphorus, and magnesium. In this Protocol, using the Mulberry leaves as a reducing and stabilizing agent for the synthesis of Ruthenium nanoparticles (RuNPs) *via* a greener tactic. Simply, dried Mulberry leaves taken as fine powder about 1g/100 mL in deionised water boiled for 30 min at 60 ^{o}C. At that time of brown color extract was filter and taking 30 mL extract stirred in 100 mL RB flaks equipped with stirrer and adding freshly prepared 0.1 M $RuCl_3$ in 20 mL distilled water maintaining at 60-85 ^{o}C for 2 h. After black color content was filtered with centrifuged at 1000 rpm and dried in hot air oven at 80 ^{o}C for 2 h. Finally, RuNPs were obtained with 80 mg as black color powder. Further, the RuNPs was characterized by UV-Visible and FT-IR spectroscopic analysis. Optimized RuNPs will be used to visualize latent fingerprints (LFPs) and shows antibacterial activity.

Keywords: RuNP, Mulberry Leaves, Forensic Application, Biological studies.

An autonomous Self-Healing ability of Polyurethane Co-polymerized with Bio-based Polybenzoxazine through Hydrogen-Bonding

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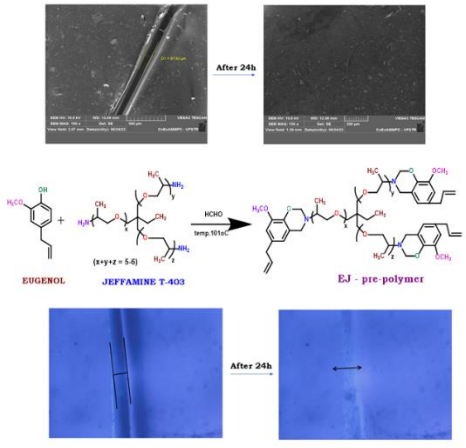
ABSTRACT

Thermal stability and autonomous self-healing abilities identified in the bio-based pre-polymer, was synthesised from naturally occurring Eugenol (4-allyl-2-methoxyphenol) and commercially available JEFFAMINE T -403 (Trimethylolpropane tris [poly (propylene glycol), amine terminated] ether), Para-formaldehyde through the Mannich condensation reaction. In the present work, the synthesised pre-polymer was polymerized thermally with the addition of Thiol (SH) and Polyurethane (PU) at different weight ratios (0.25,0.5) or (25%, 50%). The chemical structure or structural determination of the EJ-polymer was studied by NMR and FTIR spectroscopies. Thermal properties were studied by thermal gravimetric analysis (TGA) and differential scanning colorimetry (DSC). Self-healing property of the polymer was examined by the Scanning Electron Microscopy (SEM) and also optical microscopy (OM) and it was clearly shown in photos. Contact angle (CA) measurement also taken for the EJ-polymers and shown in photos, shows the hydrophilic nature of EJ-polymers. The polymer of EJ shows the good shape memory property and also show good anti-microbial activity.



Self-Healable Polymers

Key words: Eugenol, JEFFAMINE T -403, self-repairing, Shape memory, Polyurethane (PU), Wettability, Hydrophobicity, Hydrophilicity, Anti-microbial activity.

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Structural and Optical properties of Nickel Oxide nanopowder

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ABSTRACT

Nickel Oxide (NiO) is synthesized via Urea (NH_2CONH_2) in 100ml of double distilled water or deionized water. This transition metal oxide is used for electrode nanopowder as super capacitors. The NiO nanoparticles limit their electrochemical performance and impede the commercialization of these electrodes. The solution is stirring at room temperature for half an hour, further the effect of annealing combustion at 300 ^{0}C approaches for producing the nano structural samples of potential electrode material. This synthesis of electrode powder is the simplest, most cost-effective and commercially used for charge-discharge and long charging time without degradation. Characteristic modes of fundamental vibrations of functional group are observed in the FTIR spectrum and Optical Absorption technique characterises the molecular structure of the material.

A study on the quality of drinking water supply by the Chennai Metropolitan water supply system

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ABSTRACT

Water has become an essential commodity for the development of industrials and agriculture. It is absolutely essential not only for survival of human beings, but also for animals, plants and all other living things. It is also crucial for the quality of life. The ecological balance maintained by the quantity and quality of water determines the way of life of a people. On the other hand, polluted water is the greatest source of disease and besides debasing the land also becomes unfit to sustain life. The main problem today is not only of fresh water availability but of environmental quality and ecological balance. With increasing industrialization, urbanization and technological advance in all fields, sources of water are getting more and more seriously polluted. Natural waters are afflicted with a wide variety of inorganic, organic, and biological pollutants. The current research study was conducted to assess the physical and chemical water quality parameters of drinking water supply system of Chennai Metropolitan Water and Sewage Board. The water samples were collected in plastic container of 1liter capacity from three different geographic locations such as Kilpauk, Koyambedu and Chembarambakkam water treatment plants. A number of physiochemical water quality parameters including Temperature, pH, EC, TDS, DO, BOD, COD, Nitrate, Ammonia, Sulphates, Chlorides, and Calcium were measured in laboratory. The mean value of such respective parameters was compared with the water quality standards as set by the WHO and ICMR guidelines.

Keywords: Drinking water quality, Chemical parameters, Pollution.

Design, Synthesis and Biological Evaluation of New Tetrazol-1-yl imidazo[1,2-a] pyridine Derivatives

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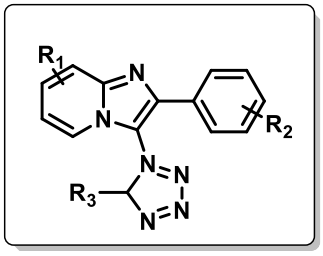
ABSTRACT

Imidazopyridine is a heterocyclic compound formed by the fusion of an imidazole ring with a pyridine ring. Imidazopyridines have been expeditiously used for the rationale design and development of novel synthetic analogs for various therapeutic disorders. A wide variety of imidazopyridine derivatives have been developed as potential anti-cancer, anti-diabetic, anti-tubercular, anti-microbial, anti-viral, anti-inflammatory, central nervous system (CNS) agents besides other chemotherapeutic agents. Imidazopyridine heterocyclic system acts as a key pharmacophore motif for the identification and optimization of lead structures to increase medicinal chemistry toolbox. In view of this, it has gained tremendous importance over the past few decades.

Derivatives of tetrazoles are screened for various biological activities such as antiviral, antibacterial, antifungal, antiallergic, anticonvulsant and anti-inflammatory properties. In drug design, tetrazoles are regarded as an isostere for the carboxylate group. Tetrazoles are medicinally important heterocycles that are incorporated in a large number of drugs approved by the FDA. Losartan, irbesartan, and valsartan are famous antihypertensive drugs belonging to the class of nonpeptide angiotensin-II inhibitors, and have a biphenyl tetrazolyl moiety in their structure. One of the antifungal agents, TAK-456 also carries a tetrazole ring. This initiated us constructing a system containing a tetrazole ring in the imidazopyridine skeleton to serve as a new scaffold for the synthesis of possible anticancer/ antimicrobial agents. In continuation of our ongoing efforts endowed with the discovery of nitrogenated heterocycles with potential biological activities, herein we delineated a synthesis of new series of tetrazolyl imidazopyridine derivatives and investigated the biological activity.



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Metal-free efficient synthesis of unsymmetrical thiosulfonates from N-hydroxy aryl sulfonamides and disulfides.

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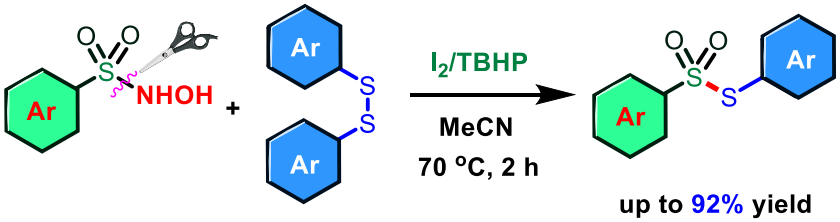

- S-S bond formation
- Highly stable materials
- Metal-free approach
- Broad substrate scope

The development of a metal-free, iodine/tert-butyl hydroperoxide (TBHP)-promoted cross-coupling reaction between *N*-hydroxy aryl sulfonamides and disulfides provides an efficient strategy for the synthesis of unsymmetrical thiosulfonates. This transformation proceeds under mild conditions at room temperature, utilizing iodine as a catalyst and TBHP as an oxidant, eliminating the need for transition metal catalysts or expensive ligands. Mechanistic investigations suggest that TBHP undergoes homolytic cleavage in the presence of iodine, generating tert-butoxy and hydroxyl radicals, which subsequently facilitate the oxidation of *N*-hydroxy aryl sulfonamides to form sulfonyl radicals. Concurrently, disulfides undergo homolytic cleavage to generate thiol radicals, which then couple with the sulfonyl radicals to afford the desired thiosulfonates. The reaction exhibits a broad substrate scope, accommodating various electron-donating and electron-withdrawing groups on both *N*-hydroxy aryl sulfonamides and disulfides, affording the products in moderate to excellent yields. Additionally, the protocol is environmentally benign, operationally simple, and highly selective, tolerating a wide range of functional groups, including halogens, nitro, cyano, and alkyl substituents. Given the biological significance of thiosulfonates in medicinal chemistry, agrochemicals, and materials science, this methodology provides a valuable synthetic tool for accessing diverse sulfur-containing compounds with potential pharmaceutical and industrial applications.

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Design, Synthesis and Biological Evaluation of 1,3,4-Oxadiazole-oxazole-pyrimidine Derivatives as Anticancer Agents

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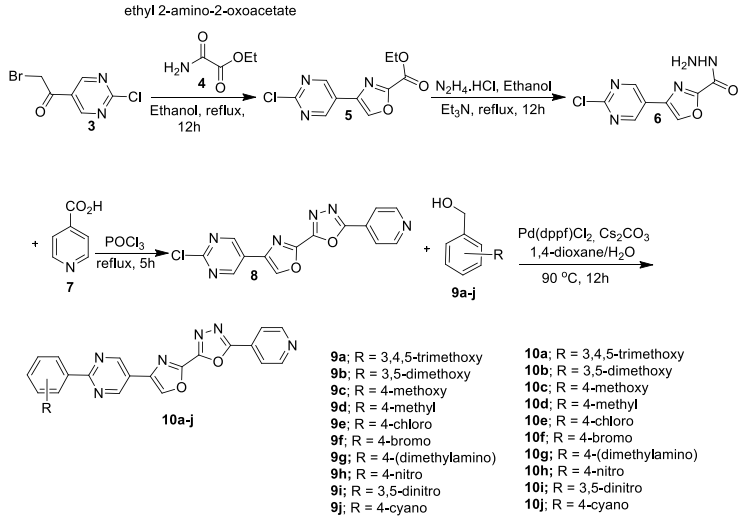
ABSTRACT

A new series of 1,3,4-oxadiazole-oxazole-pyrimidine compounds (**10a-j**) and determined their structures using ^{1}H NMR, ^{13}C NMR and mass spectral data. Further, all compounds were examined for their preliminary anticancer properties against four types of cancer cell lines, such as breast cancer (MCF-7), lung cancer (A549), colon cancer (Colo-205) & ovarian cancer (A2780) by using of the MTT method. The obtained IC_{50} values were compared with the known standard etoposide used as a positive control. The investigation of anticancer testing indicated that all derivatives displayed moderate to good anticancer activities. Among them, these compounds **10a, 10b, 10c, 10d** and **10g** displayed more potent activity than the positive control. Predominantly, one compound **10a** showed superior activity.



Scheme

Conclusions

In conclusion, a new series of 1,3,4-oxadiazole-oxazole-pyrimidine compounds (**10a-j**) and determined their structures using ^{1}HNMR, ^{13}CNMR and mass spectral data. Further, all compounds were examined for their preliminary anticancer properties against four types of cancer cell lines, such as breast cancer (MCF-7), lung cancer (A549), colon cancer (Colo-205) and ovarian cancer (A2780) by using the MTT method. The obtained IC_{50} values were compared with the known standard etoposide used as a positive control. The investigation of anticancer testing indicated that all derivatives displayed moderate to good anticancer activities. Among them, these compounds **10a, 10b, 10c, 10d** and **10g** were displayed more potent activity than the positive control. Particularly, compound **10a** showed superior activity.

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THE ROLE OF GREEN CHEMISTRY FOR CHEMICAL ENGINEERING

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ABSTRACT

The challenge of sustainable development is to live in ways that are compatible with the long-term limitations imposed by the closed system's limited carrying capacity, which is the Earth. In order to handle the challenge, the management of complex systems including material and energy flows will require a chemical engineering approach. Chemical engineering concepts are already present in system-based tools for environmental management, but they are used in broader systems than are typically covered by chemical engineering. A fascinating new avenue in the use of chemical engineering to create more sustainable processes is clean technology, which is an approach to process selection, design, and operation that blends traditional chemical engineering with some of these system-based environmental management tools.

Chemical engineering is used in less common ways in public sector decisions, where it is referred to as "post-normal science." Chemical engineers must assume a very different role in these applications, collaborating with individuals from other fields and the general public while utilizing their technical experience. An illustration of the significance of this position is the role that chemical engineering played in the development of UK energy policy. A different set of abilities is implied by acknowledging engineers' role as social change agents, which may increase the profession's appeal to prospective new hires.

Development and Validation of a Simple Isocratic RP-HPLC Method for the Quantitative Determination of Levodopa and Benserazide HCl

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ABSTRACT

In the current investigation, to separated and validate the cancer healing drugs (Levodopa and Benserazide HCl) through the HPLC (Waters e-2695) instrument containing a PDA detector. A simple, selective, validated and well-defined stability that shows isocratic RP-HPLC methodology for the quantitative determination of Levodopa and Benserazide HCl. The chromatographic strategy utilized Kromasil C-18 column of dimensions (150x4.6 mm, 3.5µm), using isocratic elution with a mobile phase of acetonitrile and Ammonium formate pH-2.5/Ortho Phosphoric acid (40:60). A flow rate of 1 ml/min and a detector wavelength of 228 nm utilizing the PDA detector were given in the instrumental settings. Validation of the proposed method was carried out according to an international conference on harmonization (ICH) guidelines. LOD and LOQ concentrations for Levodopa and Benserazide HCl were 0.6 µg/ml, 0.15 µg/ml and 2.0 µg/ml, 0.5 µg/ml. The calibration charts were plotted in the concentration range of 50-300 µg/ml for Levodopa and 12.5-75 µg/ml for Benserazide with a regression coefficient of $R^2 > 0.999$ was observed. Recovery, specificity, linearity, accuracy, robustness, ruggedness were determined as a part of method validation and the results were found to be within the acceptable range. The proposed method to be fast, simple, feasible and affordable in assay condition.

Key words: Levodopa, Benserazide HCl, RP-HPLC, Development, Validation.

Density functional theory study of the optoelectronic properties of new D′-D-π-A type organic dyes for dye-sensitized solar cells

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ABSTRACT

Density functional theory and time-dependent approaches are used for the theoretical investigation of a new class of novel carbazole-based D′-D-π-A type dyes. For all the dyes under study, the primary electron donor is the carbazole moiety, with 4H-cyclopenta[c]thiophene acting as a π-bridge and cyanoacrylic acid serving as the electron acceptor. The effect of the terminal electron donor on the optoelectronic properties is examined for the dyes in their isolated condition and the acetonitrile solvent. Their electronic and structural characteristics, as well as their absorption spectra, are analyzed and explained. All of the dyes showed good optoelectronic capabilities, according to the theoretical findings. Based on its red-shifted absorption spectrum, smaller energy gap, lowest total value, and higher G_inject and G_Reg, D5 with methyl-substituted thiophene as the terminal electron donor moiety, in particular, has the potential to be used as a sensitizer for nanocrystalline TiO_2 solar cells.

Keywords: 9-vinyl-9H-carbazole, D′–D–π–A structure, optoelectronic properties, HOMO-LUMO, DFT, and TD-DFT methods.

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ALCOHOL-INDUCED ALTERATIONS IN LIPID PROFILE PARAMETERS: A COMPARATIVE ANALYSIS OF HEALTHY AND ALCOHOLIC MALE ADULTS AGED 25-40 YEARS

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ABSTRACT

Alcohol consumption has been identified as a major risk factor for cardiovascular diseases, primarily due to its detrimental impact on lipid metabolism. Lipid profile alterations are among the key mechanisms by which alcohol contributes to cardiovascular risks. This study was conducted to assess and compare the lipid profile parameters of healthy and alcoholic adults between the ages of 25 and 40 years to better understand these associations.

A total of 50 participants were recruited for this study, comprising 25 healthy individuals and 25 alcoholic individuals. The lipid profile parameters analyzed included total cholesterol, triglycerides, high-density lipoprotein (HDL), low-density lipoprotein (LDL), and very low-density lipoprotein (VLDL). These parameters were measured using standardized biochemical techniques, and statistical comparisons were performed using ANOVA to determine significant differences between the groups.

The results of the study indicated substantial differences in lipid profile parameters between the two groups. Alcoholic individuals exhibited significantly higher levels of total cholesterol, triglycerides, LDL, and VLDL compared to their healthy counterparts. Conversely, their HDL levels were markedly lower, suggesting impaired lipid metabolism. These findings emphasize the adverse effects of chronic alcohol consumption on lipid homeostasis, further strengthening the link between alcohol abuse and increased cardiovascular disease risk.

In conclusion, this study highlights the impact of alcohol consumption on lipid profiles and, consequently, on cardiovascular health. Elevated levels of atherogenic lipids and reduced HDL levels in alcoholic individuals suggest a heightened risk for developing cardiovascular conditions such as atherosclerosis, coronary artery disease, and stroke. The findings underscore the importance of public health initiatives aimed at reducing excessive alcohol intake to mitigate the risk of cardiovascular complications.

KEYWORDS: Alcohol consumption, Lipid profile, ANOVA.

COMPARISON OF LIPID PROFILE PARAMETERS BETWEEN SMOKERS AND NON-SMOKERS: AN ANALYSIS USING ANOVA AND REGRESSION MODELS

A.Divya[1], Chandramouli V Sastry[2] and S.V.M.Vardhan[*1]

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[2]Department of Statistics, Krishna University Dr.M.R.A.R.College of Post Graduation Studies, Nuzvid, AP,India

ABSTRACT

This study was conducted to assess and compare the lipid profile parameters between smokers and non-smokers to determine the impact of smoking on cardiovascular health. A total of 50 participants were included in the study, consisting of 25 smokers and 25 non-smokers. The lipid profile, which includes critical indicators such as total cholesterol, triglycerides, low-density lipoprotein (LDL), and high-density lipoprotein (HDL), was analyzed to identify any significant differences between the two groups.

Statistical analysis using ANOVA revealed that all lipid profile parameters exhibited significant differences between smokers and non-smokers, indicating that smoking has a measurable impact on lipid metabolism. Additionally, regression analysis demonstrated that smoking status was a significant predictor of lipid profile variations, further emphasizing the strong association between smoking and adverse lipid changes.

The findings suggest that smoking contributes to detrimental alterations in lipid levels, including increased LDL and triglyceride levels and decreased HDL levels, which are well-established risk factors for cardiovascular disease. These results highlight the potential long-term health risks associated with smoking and reinforce the need for effective smoking cessation programs and public health initiatives aimed at reducing smoking-related cardiovascular complications.

KEYWORDS: Lipid Profile, ANOVA, Cardiovascular Disease

IN-DEPTH ANALYSIS OF WATER QUALITY IN PORANKI VILLAGE, KRISHNA DISTRICT, AP, INDIA

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[1]Department of Biochemistry, Krishna University Dr.M.R.A.R.College of Post Graduation Studies, Nuzvid,AP,India

[*2]Department of Biosciences & Biotechnology, Krishna University, Machilipatnam, AP,India

ABSTRACT

Water quality analysis plays a crucial role in safeguarding public health and preserving environmental integrity by ensuring that water sources meet the required standards for consumption and other uses. This study focuses on evaluating the physicochemical and microbial characteristics of water sources in Poranki Village, Krishna District, to determine their suitability for drinking and domestic purposes. Three water samples, designated as S1, S2, and S3, were systematically collected from different sources and analyzed for a range of key parameters, including temperature, pH, turbidity, total dissolved solids (TDS), total hardness, major cations and anions, electrical conductivity (EC), and microbial contamination.

The results of the analysis revealed that while most physicochemical parameters remained within permissible limits prescribed by regulatory standards, certain concerns were identified, particularly the presence of microbial contamination and elevated concentrations of nitrate and fluoride in some samples. The presence of these contaminants, particularly microbial pollutants, suggests a strong influence of domestic sewage intrusion, which could pose potential health risks if left unaddressed.

These findings highlight the urgent need for continuous water quality monitoring, improved wastewater management practices, and the implementation of effective water treatment solutions to ensure the availability of safe and clean drinking water for the residents of Poranki Village. Strengthening public awareness and infrastructure development for water sanitation and hygiene measures will be critical in mitigating the risks associated with waterborne diseases and long-term exposure to chemical contaminants.

KEYWORDS: Water quality, Poranki Village, microbial contamination, physicochemical analysis, domestic sewage, Bureau of Indian Standards (BIS), Physicochemical Analysis

Study on the molecular interactions of some binary mixtures through Thermodynamic properties and FT-IR spectra and correlation with the Jouyban–Acree model (Propargyl alcohol with tetra chloromethane, trichloromethane and Dichloromethane)

B. SivaParvathi, E Ramanjaneyulu, M. Gowrisankar, and V.Anuradha
Department of Chemistry, Acharya Nagarjuna University, Guntur,

ABSTRACT

Densities (ρ), speeds of sound (u), and viscosities (η) were measured for three binary mixtures of propargyl alcohol with tetrachloromethane, trichloromethane, and dichloromethane from 303.15 K to 313.15 K at atmospheric pressure across the composition range. Excess molar volume, excess isentropic compressibility, deviation in viscosity, and excess Gibbs free energy of activation of viscous flow were calculated. Partial molar properties and infinite dilution molar partial properties were also determined for each system. Results suggest heteroassociates forming cross-complexes and chemical forces with specific interactions. PFP theory was used to identify the predominant molecular interactions. The Jouyban–Acree model findings were discussed, considering mean relative deviation (MRDs) and individual relative deviation (IRD) between calculated and experimental data. FTIR studies were included to corroborate the experimental findings.

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Ultrasound-assisted synthesis of α – aminophosphonates using nano ZnO catalyst: evaluation of their anti-diabetic activity

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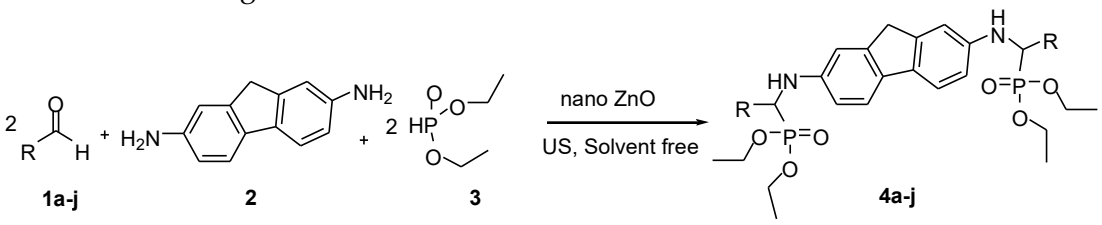
ABSTRACT

Diabetes mellitus (DM) has emerged as a serious global health concern, with an estimated 537 million individuals living with the condition by 2021. This figure is expected to rise to 783 million by 2045, placing a substantial economic and social strain on global healthcare systems.[1] Notable biological properties of bis(αaminophosphonates) include antioxidant, anti-tubercular, anti-diabetic, and antiproliferative activity against human tumor cells from colon carcinoma. Among the various synthetic techniques suggested for the production of α-Aps, the KabachnikFields (K-F) reaction-the nucleophilic addition of phosphites to imines was demonstrated to be a practical method.[2]

In the present work, a more efficient and environmentally friendly way of synthesizing α-aminophosphonates is achieved by employing nano-ZnO to catalyze the Kabachnik-Fields reaction under ultrasonication within a solvent-free environment. Before synthesis, molecular docking and in silico ADME analysis were used to assess each molecule's drug-like characteristics and ability to inhibit αamylase and α-glucosidase. The newly synthesized compounds' in vitro inhibitory effects on α-amylase and α-glucosidase were also evaluated, and their structure was confirmed using spectroscopic investigation. The target enzyme was effectively inhibited by most of the substances. In comparison to the reference drug, acarbose (IC_{50}, 106.5±0.6 µg/mL), compounds 4d (IC_{50}, 102.2±0.3 µg/mL), 4h (IC_{50}, 102.9±0.4 µg/mL), which contained a 2H-1,3-benzodioxol-5-yl moiety, and 4i (IC_{50}, 103.9±0.5 µg/mL) showed the strongest inhibitory activity. The enzyme inhibition of the remaining compounds ranged from moderate to good.



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Role of Entomology in Estimating time of Death

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ABSTRACT

Entomology is a branch of zoology dealing with the scientific study of insects. The zoological categories of genetics, taxonomy, morphology, physiology, behavior, and ecology are included in this field of study. Right from the early stages, insects are attracted to the decomposing body and may lay eggs in it. By studying the insect population and the developing larval stages, forensic scientists can estimate the postmortem interval, any change in the position of the corpse, as well as the cause of death. Forensic odontologists are called upon more frequently to collaborate in criminal investigations and hence should be aware of the possibilities that forensic entomology has to offer and use it as an adjunct to conventional means of forensic investigation.

Keywords: Insects, larvae, maggots, postmortem interval, entomology

ROLE OF DRUG DESIGN AND DEVELOPMENT IN PREDICTION OF NOVEL MEDICINAL COMPOUNDS FROM GREEN AND SUSTAINABLE METHODS

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ABSTRACT

The advancement of science in research is not only to identify new molecules but also to synthesize bioactive molecules efficiently using sustainable methods. Especially, the isolation, purification, and characterization of the medicinal value constituents from various medicinal plants have led to the development of such bioactive molecules through synthetic methods. Nowadays, in drug design and development, many approaches are being implemented for the synthesis of newer drug molecules by utilizing green synthetic routes. Over the past few decades, research has been focusing on producing safer, more efficient, and less side-effect-prone drugs by using molecular modeling techniques, computational-aided drug design (CADD), quantitative structure-activity relationship (QSAR) studies, and ligand-based drug design.

Keywords: Bioactive, medicinal value, molecular modeling techniques, green synthesis, ligand-based drug design.

Program Schedule

UGC Sponsored Two Day National Seminar on

"Recent Advances in Chemical Sciences for Sustainable Development"

(RACSSD-2025)

Date: 3rd – 4th March 2025

Venue: Prof. L. Venugopal Reddy Seminar Hall, Dr. H. H. Deichmann Auditorium, ANU

Day 1: 3rd March 2025

Time	Technical Session	Event
09:00 AM – 09:30 AM	-	Registration
09:30 AM – 10:30 AM	-	Inaugural Function
10:30 AM – 11:15 AM	-	**Keynote Address** – **Prof. S. B. Nambury**, Department of Chemistry, College of Natural and Mathematical Science, The University of Dodoma, Tanzania
11:15 AM – 11:30 AM	-	**Tea Break**
11:30 AM – 12:15 PM	**Technical Session-I**	**Invited Talk** – **Dr. K. Suresh Babu**, Senior Principal Scientist, Department of Natural Products and Medicinal Chemistry, CSIR-Indian Institute of Chemical Technology, Hyderabad, Telangana
12:15 PM – 01:00 PM	**Technical Session-I**	**Invited Talk** – **Dr. N. Shankaraiah**, Associate Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, Telangana
01:00 PM – 02:00 PM	-	**Lunch Break**
02:00 PM – 02:45 PM	**Technical Session-II**	**Invited Talk** – **Dr. D. Rambabu**, Assistant Professor, Institute of Chemical Technology (ICT), Bhubaneswar, Odisha
02:45 PM – 03:30 PM	**Technical Session-II**	**Invited Talk** – **Prof. Anitha C. Kumar**, Director, School of Chemical Sciences, Mahatma Gandhi University, Kerala
03:30 PM – 04:00 PM	-	Oral/Poster Presentation Session
04:00 PM – 04:15 PM	-	**Tea Break**
04:15 PM – 05:00 PM	-	Oral/Poster Presentation Session
05:00 PM Onwards	-	Cultural Program

Program Schedule

UGC Sponsored Two Day National Seminar on

"Recent Advances in Chemical Sciences for Sustainable Development"

(RACSSD-2025)

Day 2: 4th March 2025

Time	Technical Session	Event
09:30 AM – 10:15 AM	**Technical Session-III**	**Plenary Lecture** – **Dr. L. Giri Babu**, Chief Scientist, Department of Polymers & Functional Materials, CSIR-Indian Institute of Chemical Technology, Hyderabad, Telangana
10:15 AM – 11:00 AM	**Technical Session-III**	**Invited Talk** – **Mr. A. Vamsi Krishna**, Assistant Director, Narcotics, Andhra Pradesh State Forensic Science Laboratory (APFSL), Mangalagiri, Andhra Pradesh
11:00 AM – 11:30 AM	-	Tea Break
11:30 AM – 12:15 PM	**Technical Session-IV**	**Invited Talk** – **Prof. Koya Prabhakara Rao**, Head, Department of Chemistry, Vignan University, Vadlamudi, Guntur
12:15 PM – 01:00 PM	**Technical Session-IV**	**Invited Talk** – **Prof. M. Krishna Murthy**, CEO, Varsity Education Management Limited, Hyderabad
01:00 PM – 02:00 PM	-	Lunch Break
02:00 PM – 02:45 PM	**Technical Session-V**	**Invited Talk** – **Prof. M. V. Basaveswara Rao**, Rector, Krishna University, Machilipatnam
02:45 PM – 03:15 PM	**Technical Session-V**	**Invited Talk** – **Dr. P. Sudhakar**, Associate Professor, Department of Biotechnology, Acharya Nagarjuna University
03:15 PM – 03:45 PM	-	Oral/Poster Presentation Session
03:45 PM – 04:00 PM	-	Tea Break
04:00 PM Onwards	-	**Valedictory Function**

Prof. R. Ramesh Raju
Organizing Secretary, RACSSD-2025
Department of Chemistry, University College of Sciences, ANU

Important Notes:

✅ Participants must arrive at least **30 minutes before the scheduled sessions**.
✅ Oral & Poster Presentation participants must confirm their participation at the registration desk.
✅ Certificates will be distributed during the Valedictory Function.

About the Two-Day National Seminar

The Department of Chemistry, Acharya Nagarjuna University is honored to organize the UGC-sponsored Two-Day National Seminar on "R**ecent Advances in Chemical Sciences for Sustainable Development (RACSSD-2025)**" on 3rd and 4th March 2025. This seminar serves as a dynamic platform for researchers, academicians, industry professionals, and students to exchange knowledge, present innovative research, and explore the latest advancements in chemical sciences that contribute to global sustainability.

Over these two days, the seminar will feature keynote addresses, invited talks, technical sessions, and research presentations covering a wide range of cutting-edge topics such as green chemistry, nanotechnology, catalysis, computational chemistry, renewable energy, sustainable materials, and pollution control. Experts and scholars from various institutions will discuss scientific breakthroughs, industrial applications, and innovative solutions that align chemical sciences with sustainable development goals.

The Department of Chemistry at Acharya Nagarjuna University has always been at the forefront of academic excellence and scientific research. This seminar reflects the department's commitment to fostering interdisciplinary collaboration, industry-academia partnerships, and research-driven innovation that addresses global challenges such as climate change, resource conservation, and environmental protection.

With the active participation of renowned scientists, researchers, faculty members, and young scholars, this event aims to bridge the gap between theoretical research and practical applications. The discussions and knowledge shared during these two days will not only advance scientific understanding but also inspire future generations of researchers to contribute to sustainable advancements in chemical sciences.

We extend our sincere gratitude to the University Grants Commission (UGC), the authorities of Acharya Nagarjuna University, distinguished speakers, scholars, and all participants for their support and enthusiasm in making this event a success. May this two-day seminar pave the way for transformative research, impactful collaborations, and groundbreaking innovations that benefit both science and society.

Wishing all participants a fruitful, engaging, and intellectually enriching seminar experience!

-Dr. M. Subbarao
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Director, RACSSD-2025
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