



3rd INTERNATIONAL CONFERENCE IN CHEMISTRY-2026

(3rd ICC-2026)

ON

**CHEMISTRY FOR A SUSTAINABLE FUTURE: DISCOVERY,
INNOVATION AND IMPACT**

ABSTRACTS

Chief Patron

**Prof. Syed Ainul Hasan
Hon'ble Vice Chancellor
MANUU, Hyderabad**

Patron

**Prof. Sk. Ishtiaque Ahmed
Registrar
MANUU, Hyderabad**

Conference Chairman

**Prof. H. Aleem Basha
Dean, School of Sciences,
MANUU**

Conference Director

**Prof. Salman A. Khan
Head, Chemistry Section,
MANUU**

Convener

**Dr. Syed Salahuddin
Assoc. Professor, Chemistry
Section, MANUU**

Organized by

**Chemistry Section, School of Sciences,
Maulana Azad National Urdu University, Hyderabad-
500032, Telangana, India**

Under the Auspices of

- Chief Patron :** ***Prof. Syed Ainul Hasan***
(Hon'ble Vice-Chancellor, MANUU)
- Patron :** ***Prof. Sk. Ishtiaque Ahmed***
(Registrar, MANUU)
- Chairman :** ***Prof. H. Aleem Basha***
(Dean, School of Sciences, MANUU)
- Director :** ***Prof. Salman Ahmad Khan***
(HOD, Department of Chemistry, MANUU)
- Convener :** ***Dr. Syed Salahuddin***
(Department of Chemistry, MANUU)

Advisory Committee International

- Prof. Jean Louis Reymond, Department of Chemistry and Biochemistry, University of Bern, Switzerland
- Prof. Syed Kaleem Ahmed, Associate Director of Medicinal Chemistry, School of Pharmacy, University of Southern California
- Prof. Farooq Adil Syed, Department of Chemistry, College of Science, King Saud University Riyadh
- Prof. Ajay Kumar Mishra, Department of Chemistry, University of the Western Cape, South Africa
- Prof. Shaik Manirul Haque, Department of Chemical Engineering Jubail Industrial College, Saudi Arabia
- Prof. Zainab Binti Ngaini, Department of Chemistry, University of Malaysia Sarawak (UNIMAS), Malaysia
- Prof. Shivani, Department of Chemistry, Hebei University of Science and Technology, China

National

- Prof. Athar Adil Hashmi, Department of Chemistry, Jamia Millia Islamia, New Delhi
- Prof. Ramendra K. Singh, Department of Chemistry, University of Allahabad, Prayagraj, UP
- Prof. Gurjaspreet Singh, Department of Chemistry, Panjab University Chandigarh
- Prof. Naseem Ahmed, Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee
- Dr. S Sridhar, Chief Scientist at CSIR-IICT, CSIR-IICT Hyderabad, Telangana
- Dr. Abdul Rasheed Mohammed, Associate Vice president, Suven Life Sciences Ltd., Hyderabad, Telangana
- Dr. Ajaz Ahmed, Scientist, Organic Synthesis and Process Chemistry, CSIR-IICT Hyderabad, Telangana

About MANUU

Maulana Azad National Urdu University (MANUU) is a Central University, proudly accredited with an A⁺ grade by NAAC. Established in 1998 by an Act of Parliament, its mission is to promote and advance the Urdu language while providing vocational and technical education through both traditional and distance learning formats. MANUU operates across 11 states in India, encompassing eight schools, 20 departments and offering 96 programs up to the Ph.D. level. The University's headquarters are situated in Gachibowli, Hyderabad, spanning 200 acres of a centrally located, lush green campus. With state-of-the-art educational infrastructure, MANUU fosters a conducive environment for academic and research excellence. Its serene surroundings offer an ideal atmosphere for students to pursue professional courses, ensuring holistic development.

About the School of Sciences(SOS)

The School of Sciences (SoS) was established in 2006 to offer educational programs that complement the humanities and social sciences, recognizing the crucial role of Science Education in the nation's development. The School currently offers B.Sc., M.Sc. and Ph.D. programs in Mathematics, Physics, Chemistry, Botany and Zoology, along with B.Voc. in Medical Laboratory Technology (MLT), Medical Imaging Technology (MIT) and Emergency & Trauma Care Technology (ETT) and M.Voc. in (MIT & MLT) programs. Since its inception, the School of Sciences has made remarkable strides in fostering academic and research excellence. Our outcome based academic model integrates theoretical coursework, research projects, seminars, resource-based learning, and practical laboratory work, ensuring a strong foundation for students. This holistic approach enhances students' knowledge and skills, preparing them for future challenges in the field of science.

About Department of Chemistry

The Chemistry Department, SoS, established in 2014, offers B.Sc., M.Sc. and Ph.D. programs supported by cutting-edge laboratory and classroom facilities equipped with modern teaching and learning tools. The Chemistry Department, boasts a diverse and highly qualified faculty with national and international teaching and research experience and their work is regularly published in reputable journals. We emphasize the collaborative and interdisciplinary nature of science in both teaching and research. Faculty members are actively engaged in exploring frontier areas of chemistry and its intersections with related disciplines while maintaining their teaching responsibilities. The Chemistry Department, SoS offers comprehensive core courses in both theoretical and practical laboratory work, covering essential topics in Organic, Inorganic, Physical and Analytical Chemistry.

About 3rd ICC - 2026

The International Conference on “Chemistry for a Sustainable Future: Discovery, Innovation and Impact”

" serves as a platform to unite academicians, scientists, researchers, chemists, and industry professionals to exchange and share their research insights across various domains of Chemical Sciences. The Chemistry Section, School of Sciences, is pleased to invite distinguished Speakers, Delegates, Researchers, Students, and Industry Experts to participate in this prestigious event.

This two-day conference, scheduled for February 13–14, 2026, will take place at Maulana Azad National Urdu University, Gachibowli, Hyderabad. It will feature Keynote and Plenary Sessions, Speaker Presentations, a Young Researchers' Forum, Video Presentations, Poster Displays, E-Posters, and networking opportunities to explore the latest advancements in Chemistry. To achieve a sustainable future, transformative changes in the chemical industry and its underlying principles are essential. The Chemistry Section, School of Sciences, MANUU, is committed to facilitating this transformation by organizing an event that bridges diverse disciplines and provides a glimpse into the potential of a sustainable future in Chemistry. Additionally, the conference will address the opportunities and challenges linked to various sustainable approaches. Its primary objective is to deepen participants' understanding of the principles and methodologies essential for sustainable innovation in the field of Chemistry.



مولانا آزاد نیشنل اردو یونیورسٹی
MAULANA AZAD NATIONAL URDU UNIVERSITY

A Central University under Ministry of Education
Government of India



پرو. سید عین الحسن، کولپتی

پروفیسر سید عین الحسن، شیخ الجامعہ

Prof. Syed Ainul Hasan, Vice-Chancellor



MESSAGE

Dear Scholars, Researchers, and Esteemed Participants,

It is my pleasure to welcome you to the release of the abstract book for the 3rd International Conference in Chemistry, themed "Chemistry for a Sustainable Future: Discovery, Innovation and Impact", hosted by Chemistry Section, School of Sciences, at Maulana Azad National Urdu University, Hyderabad. This milestone event builds on the successes of our previous gatherings, reinforcing our dedication to cutting-edge research and societal progress.

This conference unites global experts, academics, and innovators to exchange insights and collaborative strategies in chemical sciences. Our theme highlights the key role of discovery, innovation, and real impact in addressing sustainability challenges, from resource conservation to eco-friendly technologies.

The abstract book captures the strength of your submissions forward thinking research set to drive real-world changes. It shows the passion and expertise of every contributor. My sincere thanks go to the organizing committee, faculty, and all the participants for their efforts in making this conference a great success.

May this event lead to major progress in chemistry and shaping the better world for tomorrow.

Prof. Syed Ainul Hasan

Gachibowli, Hyderabad-500 032 Telangana, India,

Contact : 9313336337, (040) 23006601

mail - vc@manuu.edu.in, sahasan14@hotmail.com

f manuuhydoofficial officialmanuu imcmanuu manuuhyd
www.manuu.edu.in



مولانا آزاد نیشنل اردو یونیورسٹی
MAULANA AZAD NATIONAL URDU UNIVERSITY
A Central University under Ministry of Education
Government of India



پرو. اسکے. اشتیاق احمد، کولسچیف
پروفیسر ایس کے اشتیاق احمد، رجسٹرار
Prof. Sk. Ishtiaque Ahmed, Registrar



Message from the Registrar

It is a privilege to offer warm greetings to all distinguished participants, esteemed speakers, and the organizing committee of the 3rd International Conference in Chemistry focusing on the theme "Chemistry for a Sustainable Future: Discovery, Innovation and Impact", hosted by the Chemistry Section, School of Sciences, Maulana Azad National Urdu University, Hyderabad.

This conference provides a key platform for building interdisciplinary ties and sharing fresh ideas to meet sustainability challenges. Chemistry, at the heart of science, plays a vital role in creating sustainable technologies, advancing green practices, and delivering practical solutions for a healthier planet.

The hybrid format of this event welcomes researchers, scholars, and professionals from diverse regions and fields, sparking lively exchanges of knowledge and skills. Events like this fuel important discussions and support progress toward sustainable development goals.

I praise the organizing team of the Chemistry Section, School of Sciences, MANUU, for their clear vision and strong effort in hosting this gathering. I am sure the talks and sessions will make a real difference in academic and research circles, opening doors to new advances in chemical sciences.

Best wishes for a successful and fruitful conference.


Prof. Sk. Ishtiaque Ahmed



Conference Chairman

Prof. H. Aleem Basha

Dean, School of Sciences, MANUU



MESSAGE

Dear Participants,

It is with great pride and energy that I offer my heartfelt welcome to all participants of the 3rd International Chemistry Conference 2026 on Chemistry For a Sustainable Future: Discovery, Innovation and Impact. This important event, organized by the Chemistry Section, School of Sciences, Maulana Azad National Urdu University, acts as a strong platform for sharing ideas and examining new progress in chemical sciences.

The conference theme highlights chemistry's central part in solving global issues and supporting sustainable growth. The wide variety of abstracts here shows the skill, hard work, and teamwork of researchers from around the world. I am sure the ideas and talks in this hybrid conference will lead to solid solutions and open paths for real progress in chemical sciences.

I give my sincere thanks to all authors, speakers, and organizers whose work has made this event possible. Your efforts prove the shared drive of the scientific community to build a better future through sustainable methods.

Wishing you all a lively, insightful, and rewarding conference.

Prof. H. Aleem Basha

Dean

School of Sciences

Maulana Azad National Urdu University

Conference Director

Prof. Salman Ahmad Khan

Head

Chemistry Section, SoS, MANUU



MESSAGE

Dear Participants

With great honor and energy, I offer my heartfelt thanks to all of you for joining the 3rd International Chemistry Conference 2026, held under the theme "Chemistry For a Sustainable Future: Discovery, Innovation and Impact." Hosted by the Chemistry Section, School of Sciences, Maulana Azad National Urdu University, this conference gathered researchers, scholars, and innovators from around the world to exchange knowledge, build ties, and tackle key global challenges through the strength of chemical sciences.

The theme of this conference points to chemistry's main role in reaching sustainable development goals and fixing real problems. The range of abstracts and talks here shows the skill, effort, and fresh thinking of the scientific community. It is exciting to see such strong research and ideas that can truly help society.

I am especially thankful to all contributors—authors, speakers, and organizers for your steady work and dedication that made this event a clear success. Your efforts reflect the shared goal of the global scientific community to shape a sustainable and thriving future through progress in chemical sciences.

As we share this abstract book, a permanent record of the strong contributions to the conference, I hope it sparks new talks and ongoing partnerships.

Wishing you all continued success in your work.



Prof. Salman Ahmad Khan
Head, Department of Chemistry
School of Sciences
Maulana Azad National Urdu University

Convener

Dr. Syed Salahuddin

Chemistry Section, SoS, MANUU



MESSAGE

On behalf of the Organizing Committee, it is my honor to welcome our distinguished Chief Guest, Guest of Honour, keynote speakers, and participants from around the world. Your presence at the 3rd International Conference in Chemistry (3rd ICC-2026) reflects a shared dedication to advancing chemical sciences.

Centered on the theme “Chemistry for a Sustainable Future: Discovery, Innovation and Impact,” this forum brings together academic and industrial leaders. We are aligned in our mission to position chemistry as a transformative force for global sustainability driving green, scalable, and equitable solutions.

Over two days in hybrid format, the conference will feature keynote and plenary sessions, specialized speaker presentations, and a Young Researcher Forum. Discussions will span critical areas including Organic Synthesis, Medicinal Chemistry, Advanced Materials, Environmental Remediation, and AI-driven Molecular Design, all aimed at decoding the molecular foundations of a sustainable planet.

We extend sincere thanks to our Hon’ble Vice Chancellor, Prof. Syed Anjul Hasan; Registrar, Prof. Sk. Ishtiaque Ahmed; Head of Chemistry, Prof. Salman Ahmad Khan; and Dean, School of Sciences, Prof. H. Aleem Basha, for their unwavering support and resources.

Your engagement is vital to fostering discovery, partnership, and translational impact. Welcome to 3rd ICC-2026, let us collaborate to design tomorrow’s molecular solutions.



Dr. Syed Salahuddin
Convener, 3rd ICC-2026
SoS, MANUU

Dr. D. Srinivasa Reddy
Director
CSIR-IICT, Hyderabad



Role of Chemistry in Society: Case Studies from Our Research Group

Dr. D. Srinivasa Reddy

*Council of Scientific & Industrial Research, Indian Institute of Chemical Technology,
Hyderabad, Telangana-500007*

Abstract

Chemistry impacts human welfare and sustainable development by turning molecular innovations into real-world solutions. This work is a case study from our research group that show how basic discoveries tackle key challenges in India and beyond, linking lab work to public good. We created low-cost, reusable nanomaterial adsorbents to remove heavy metals and organic pollutants from industrial wastewater selectively; field-ready cartridges are in pilot tests, drawn from India's polluted rivers. For treatments, we built prodrug structures for targeted anti-TB delivery, cutting side effects and improving drug uptake against a big health issue. In energy, we use catalysts to turn biomass into aviation fuel building blocks; studies of C–C bonds and hydrogen shifts led to a patent-pending process for carbon recycling at scale. These cases prove that research fueled by curiosity and real needs creates solid science and useful results. Chemists should explain their work's worth to leaders, businesses, and people, matching studies to sustainability aims. This study urges students to use chemistry for change, bringing clean water, health gains, and green energy from current labs.

Dr. Nanduri Srinivas

I/c Director

NIPER, Hyderabad



Bridging Molecules and Medicine: Sustainable Strategies in Drug Discovery and Development

Dr. Srinivas Nanduri

I/c Director, NIPER Hyderabad

Drug discovery today stands at the critical intersection of therapeutic innovation and environmental stewardship. This keynote will chart the strategic evolution from lead identification to clinical candidate, highlighting recent breakthroughs and future directions in synthetic organic and medicinal chemistry.

The presentation will address three major therapeutic frontiers: novel synthetic strategies against antimicrobial resistance targeting biofilms and metallo- β -lactamases; precision small-molecule inhibitors and improved metal-based chemotherapeutics for cancer; and multi-target directed ligands (MTDLs) for neurodegenerative disorders that simultaneously modulate cholinergic, glutamatergic, and amyloidogenic pathways.

A dedicated segment on process optimization and green chemistry will feature contemporary case studies, continuous flow photochemistry, solvent-free synthesis, and biocatalytic cascades, demonstrating that sustainability drives cost reduction, scalability, and intellectual property creation, rather than serving as mere regulatory compliance.

The final segment traverses natural product-based discovery: from isolation and spectroscopic characterization of bioactive metabolites from underexplored flora, to strategic total synthesis and chemo-enzymatic semi-synthesis. Emphasizing late-stage functionalization, this address positions nature as the ultimate medicinal chemist and envisions a future where synthetic ingenuity, biological insight, and green principles converge to meet global therapeutic needs.



Dr. Syed Kaleem Ahmed
Associate Director of
Medicinal Chemistry
University of Southern California



Design, Optimize, Deliver: Medicinal Chemistry from Hit to Lead

Dr. Syed Kaleem Ahmed

Associate Director of Medicinal Chemistry Keck School of Medicine, University of Southern California (USC), Los Angeles

Abstract

Drug discovery is increasingly driven by the integration of ligand- and structure-based design to efficiently identify and advance small-molecule therapeutics from initial hits to optimized leads. Following hit identification, candidates undergo iterative cycles of molecular design, chemical synthesis, and biological evaluation to enhance potency, target selectivity, and developability. Medicinal chemistry efforts focus on refining target engagement while optimizing physicochemical properties, pharmacokinetics, and safety profiles. Computational and AI-enabled tools support these efforts by guiding structure–property relationships, predicting

ADME/toxicity liabilities, and informing rational decision-making. Integrating classical design principles with robust lead optimization strategies provides a powerful framework for generating high-quality development candidates, improving efficiency, reducing attrition, and enabling the delivery of hits as optimized leads with strong clinical potential.

Dr. Nazar Hussain
Assistant Professor,
Dept. of Medicinal Chemistry,
BHU



Lewis Acid-Mediated Transformations of Glycals to Annulated Glycosides

Ram Pratap Pandey, Bindu Tiwari, M. Ansari and Nazar Hussain*

*Department of Medicinal Chemistry, Institute of Medical Sciences
Banaras Hindu University, Varanasi-221005, India*

E-mail: nazar10@bhu.ac.in

Abstract

C-glycosides are a privileged class of organic compounds involved in many biological processes and prevalent in various natural products. Their enhanced importance over O glycosides stems from their greater chemical and enzymatic stability. Among C-glycosides, annulated C-glycosides are a notable subclass where glycosyl donors different positions participate in a cyclic structure. This subclass is prominent in many biologically active molecules and includes major natural products such as bergenin, chafuroside, and bradyrhizose. Traditional synthesis emphasizes stereoselective α/β C-glycoside formation, but efficiently engaging both reactive carbons of glycosyl donors remains challenging. This study introduces a novel domino sequence using glycals and substituted glycals and naphthols under Lewis acid catalysis, generating glycosylated intermediates that undergo cascade reactions to yield annulated 1,2/1,3- annulated glycosides. The method features broad substrate scope, mild conditions, and versatility. Notably, annulation type varies with substituted glycals, yielding [3+2] or [3+3] fused pyran systems. Control experiments and DFT calculations provide mechanistic insights into the substrate-specific formation of products.



**Dr. Mohammad Mujahid
Ali Khan**
Faculty of Engineering
and Technology, AMU



Fabrication, structural crystallinity, and electrochemical behaviour of organic-inorganic nano-coated ion-exchange composite membranes for desalination applications

Mohammad Mujhaid Ali Khan*

Applied Science and Humanities Section, University Polytechnic, Faculty of Engineering and Technology, Aligarh Muslim University, Aligarh, 202002

Corresponding author email id: mujahidchemistry@gmail.com

Abstract

In this paper, we present an overview of an innovative approach based on the observation of chemical, surface and electrochemical studies of nano coated membrane. The polymer based new inorganic-organic composite ion-exchange membrane has been prepared by sol-gel and characterized by SEM, TEM, XRD, EDX, FTIR and TGA. The organic and inorganic matrix enhanced the properties of membrane such as chemical stability, flexibility, thickness, water uptake, swelling, mobility, surface morphology and further more improved the electrochemical properties. It is clear that surfaces, interfaces and electrochemical parameters play important roles in the preparation and application of the hybrid multifunctional nanocoated membrane.

Furthermore, results of degree of crystallinity, morphology, membrane potential, transport number, mobility ratio, charge effectiveness and surface charge density give better efficiency for desalination of hyper saline water, making it a promising candidate for treating high-salinity brines.

Keywords: Sol gel method; membrane matrix; Structural properties; Percentage crystallinity; Electrochemistry



**Dr. Pathan Mohd
Arif Ali Khan**
Head of the Dept.
Maulana Azad College of Arts,
Science and Commerce,
Aurangabad



Microwave Assisted Synthesis of Fluorinated triazolo[3,4-b]-1,3,4-thiadiazoles under Solvent Free Condition

Bharat Dhotre a, Sabreena Yameen b, Arif Pathan b

*a Department of Chemistry, Swami Vivekanand Senior College Mantha, Maharashtra, 431504
India*

b Department of Chemistry, Maulana Azad College Aurangabad, Maharashtra, 431001 India

E-mail id: bharatd219@gmail.com

Abstract

A convenient and efficient one-pot synthetic protocol for the preparation of fluorinated triazolo[3,4-b]-1,3,4-thiadiazoles has been developed using microwave irradiation under solvent free conditions. The method involves the cyclocondensation of 4-amino-5-fluoro-1,2,4-triazole-3-thiol with various substituted fluorinated benzoic acid in the presence Phosphorus oxychloride under microwave conditions, resulting in the formation of the desired heterocyclic scaffolds. Microwave irradiation significantly reduces reaction times compared to conventional heating methods, offering enhanced reaction rates and product selectivity. Maximum Yield, and Short reaction time are merits of the developed protocol. This eco-friendly approach eliminates the need for excess solvents and harsh reagents, aligning with green chemistry principles. Synthesized compounds were characterized by a spectroscopic technique like IR, ¹H NMR, and Mass spectra.

Keywords: Triazolo, 1,3,4-thiadiazoles, Fluorinated acid, cyclization, Microwave Irradiation.



मौलाना आज़ाद नेशनल उर्दू यूनिवर्सिटी
MAULANA AZAD NATIONAL URDU UNIVERSITY

(A Central University established by an Act of Parliament in 1998 .Accredited with 'A+' Grade by NAAC)



Dr. Saif Ali Chaudhry
Director
Centre for Nanoscience and
Nanotechnology, JMI



Water treatment through nanocomposites: A facile, inexpensive and advance technique

Saif Ali Chaudhry

*Professor, Department of Chemistry, Faculty of Sciences, Hony. Director
Centre for Nanoscience and Nanotechnology, Jamia Millia Islamia, New Delhi -110025,
India*

Email: schaudhry@jmi.ac.in

Abstract

The synthetic dyes, toxic heavy metal ions, pesticides, pharmaceuticals are released from tannery, textile and other industries which cause severe water pollution. These pollutants are toxic and highly stable so persist for long time in water resources and on consumption by human being lead to different water borne diseases. Therefore, wastewater from these mentioned industries must be treated before discharging into the water bodies. Various methods are in use for wastewater treatment but photocatalysis and adsorption are considered economical and eco friendly. Numerous types of materials including nanoparticles have been extensively investigated for these two methods. However, nanocomposites are relatively new player in the water treatment field because of their porous structure, high surface area, and having almost all other desirable properties. We have prepared and investigated various types of materials for adsorptive removal of toxic heavy metals, synthetic dyes and photocatalytically degraded dyes, pesticides, antibiotics etc. and the talk will discuss few of these.



Dr. Syeda Sameena Aziz
Assoc. Professor of Chemistry,
Anwarul Uloom College, Hyderabad



Exploring Electro and Thermal Analytical Techniques as Essential Tools for Modern Research

Syeda Sameena Aziz

Department of Chemistry, Anwarul Uloom College, New Mallepally, Hyderabad, Telangana-500001

*Corresponding author: Syeda Sameena Aziz. Email: ssaauc@gmail.com

Abstract

Electro and thermal analytical techniques are essential tools for the identification, quantification, and characterization of chemical substances. Electroanalytical techniques are based on the interaction between electrical parameters and chemical reactions occurring at electrode surfaces. Polarography is a classical electroanalytical method that employs a dropping mercury electrode and a reference electrode to record current–voltage curves known as polarograms. The half-wave potential obtained from polarograms is characteristic of a particular element or functional group and is used for qualitative analysis, while the diffusion current is proportional to concentration. Various factors, such as temperature, viscosity, capillary characteristics, and the presence of maximum suppressors, influence polarographic measurements. Advanced techniques, such as AC polarography, square wave, normal pulse, and differential pulse polarography, offer higher sensitivity and lower detection limits for trace analysis. Amperometric titrations, carried out at a constant applied potential, are used for quantitative determination of electroreducible and non-electroreducible species and are widely applied in redox, precipitation, and complexometric titrations. Cyclic voltammetry is another important electrochemical technique used to study redox mechanisms, electron-transfer kinetics, reaction intermediates, and electrochemical reversibility.



Dr. Rehana Anjum

Associate Dean Student Affairs
Lords Institute of Engineering
and Technology, Hyderabad



**Next-Generation Environmental, Energy and Fuel Chemistry: From Green
Molecules to Global Solutions**

Dr. Rehana Anjum*

**Lord Institute of Engineering and Technology, Himayath Sagar, Hyderabad, 500091,
Telangana*

Abstract

Environmental, Energy and Fuel Chemistry represents a vital interdisciplinary area of chemical sciences dedicated to addressing climate change, environmental contamination, and the growing global demand for sustainable energy. The field integrates green chemistry, catalysis, materials engineering, and thermodynamic principles to design cleaner fuels, high-efficiency energy conversion systems, and environmentally responsible industrial processes. It spans renewable energy technologies including solar cells, fuel cells, hydrogen production, and biofuels while advancing carbon capture, utilization, and storage (CCUS) strategies to reduce greenhouse gas emissions. A key focus is the development of earth-abundant and cost-effective catalysts, nanostructured functional materials, and low-carbon fuel alternatives that decrease reliance on fossil resources. Environmental chemistry within this framework investigates pollutant transport, atmospheric transformations, water purification, soil remediation, and waste valorisation, promoting sustainable resource management under circular economy principles. Simultaneously, fuel chemistry drives innovation in alternative fuel formulations and optimized combustion technologies aimed at lowering emissions and enhancing energy efficiency. By connecting fundamental chemical research with scalable technological applications, Environmental, Energy and Fuel Chemistry support the transition to carbon-neutral and energy-secure systems.

Keywords: Environmental chemistry; Renewable energy; Green chemistry; Fuel chemistry; Catalysis; Carbon capture; Sustainable fuels; Hydrogen energy.

Table of Content

S. No.	Author's Name	Title	Page no
Organic and Bioorganic Chemistry			ICC/OBC/001 to 016
1	Md. Musawwer Khan and Anam Arif	TfOH- Catalyzed Knoevenagel /Michael/Intramolecular Cyclization Cascade Synthesis of Coumarin-1,4-Dihydropyridine Derivatives	1
2	Dr. Yogesh Kumar	Novel Tyrosine and Pectin-based Nanoparticles for Anticancer Application	2
3	Humaira Parveen	A Sustainable, Mild, and Green NIS-Mediated Methodology for the Room-Temperature Synthesis of Quinoxalines	3
4	Trupti Subhash Pawal and Vasundhara Sawant	Computationally Guided Design, Optimization and Synthesis of Multi-targeted Antifungal Agents	4
5	Yata Sravan kumar, Salman A. Khan	Synthesis Approaches and Biological Applications of Novel Aficamten Derivative	5
6	Jeba Aslam Mulani and Vasundhara Sawant	Structure-guided development of amino-pyrazole derivatives as selective C-terminal HSP90 inhibitors	6
7	Kahkashan Sarfaraz, Saif Ali Chaudhry	GAAL@ZFT Nanocomposite Hydrogel as a High-Performance Adsorbent for Cationic Dye Removal	7
8	Yerrabelly Hemasri	Synthesis of New 4-[1-(1-Phenyl-1H-[1,2,3]Iriazole-4-ylmethyl)-1H-benzoimidazol-2-yl]-piperidine-1-carboxylic ester Derivatives-Evaluation of Anti-Cancer and Anti-Bacterial Activity/Docking studies	8
9	Zeenathunnisa Begum, Qasimullah	Development of Novel Quinoline incorporated Chalcones as potential therapeutic agents	9
10	Abul Hasnat	Utilization of triglycerides in the synthesis of useful polymers: A greener approach	10
11	Gourav Arora, Priya, Arif Ali Khan	Selective Synthesis of two isomeric Oxazines and their characteristion	11
12	Noorunnisa Begum, Salahuddin Syed, Mohammed Arifuddin Qasimullah and Salman	Development of novel Immidazole chalcones as potential therapeutic agents	12

	Ahmad Khan		
13	Zuverya Zareen, Aram Rahman, Anzar Jahan, Ariffuddin Mohammed, Syed Salahuddin	Synthesis and invitro Antimicrobial Evaluation of Novel Heterocyclic Schiffs base and their corresponding 3-Chloro-2-Azetidinones and 4-Thiazolidinone derivatives	13
14	Azra Soban, Sohra Tabassum, Qasim Ullah	Efficient and Facile Synthesis of Maleic anhydride ring opening reaction with anilines under Bio-Catalytical Condition by Employing Baker's Yeast as Biocatalyst	14
15	Khutubuddin, Md. Mohasin, Zafir Aribuddin Baag, Salahuddin Syed, Salman A. Khan	Recent Advances in Coumarin-Schiff Base Fluorescent Chemosensors for the Detection of Al ³⁺ and Cu ²⁺ Ions	15
16	Umme Salma, Salman A. Khan	Synthesis of Triazole based Schiff base: A Highly Selective and Sensitive Fluorescent Chemosensor for the Detection of Cu ²⁺ Metal Ion	16
17	Sushil Kumar, Maneesha D. Sati and S. C. Sati	Synthesis and determination of antibacterial activity of Benzimidazole derivatives	17
18	Kahkashan Begum	1,25- Dihydroxycholecalciferol: A Biological Imperative for Human Health and Immune Regulation	18
19	Kiran Naykodi and Vasundhara Sawant	Design and Development of Oxadiazole-based Derivatives as Histone Deacetylase (HDAC) Inhibitors	19
<i>Inorganic and Bioinorganic Chemistry</i>		<i>ICC/IBC/017 to 041</i>	
20	Md. Ghaznafar Alam	Synthesis and Characterization of Ni (II) Schiff-Base Complexes: Structural and Biological Insights	20
21	Imtiyaz Ahmad Mantoo, Ilma Tarannum, Imtiyaz Yousuf	Mononuclear and dinuclear cobalt (II) complexes: Structural insights and evaluation of biomolecular interaction, catecholase activity and <i>in vitro</i> cytotoxic activity	21
22	Nadeem Ahmad	Development of Bioadsorbents from Chenopodium album Leaves and Manilkara zapota Seeds for the Removal of Heavy Metals from Water Samples	22
23	Priyanka S Thakur and	Synthesis and Spectral Studies of New	23

	Manohar V Lokhande	Organometallic Schiff Base Complexes and Their Anti-fungal Activity	
24	Gurjaspreet Singh, Komal	Pyrrolidine derived 1,2,3-triazolyl organosilane as “Turn on” fluorescence sensor for Zn (II) ion: synthesis, antioxidant, molecular docking and DFT studies	24
25	Gurjaspreet Singh, Parul	A multifunctional Schiff base: Investigating its Zirconium sensing and antiproliferative effects	25
26	Priyanka R. Kokate and Manohar V. Lokhande	Green Synthesis of AgNPs and CuNPs using Schleicheria oleosa bark Extract and its Application	26
27	Ruheen Khan, M. Shahid	A Cd (II)-Pyrazine Dicarboxylate Metal-Organic Framework as a High-Performance Adsorbent for Dye Removal	27
28	Gurjaspreet Singh, Jyoti	Benzimidazole appended 1,2,3-Triazole Chemosensor: Selective Zr (IV) Sensing Coupled with Anticancer and Antioxidant Potency	28
29	Gurjaspreet Singh, Poonam	Silatrane-Chalcone-Triazole Hybrid for Selective Zr (IV) Detection via Naked-Eye and Turn-on Fluorescence: Anticancer Evaluation	29
30	Gurjaspreet Singh, Anurag Dalal	Design and Synthesis of Symmetric bis Schiff Base as Potential Anti-Cancer Agent and Selective Chemosensor for Sn (II) Detection	30
31	Gurjaspreet Singh, Priyanka	Fluorescent and Colorimetric Schiff Base Allied Organosilane-Iron Nanoparticles for Ni (II) Detection with Anticancer Potential Backed by Docking and DFT Investigations	31
32	Gurjaspreet Singh, Vinit Yadav	Investigating 1,2,3-Bistriazole-Functionalized Sn (II) Chemosensors for COX-2 Detection	32
33	Dr. Maqdoom Farooqui, Dr. Uzma Parveen Shaikh, Siddiqui Alima Fatema	Catalytic Applications of Mixed Transition Metal Oxides: A Review	33
34	Dr. Rasika C. Torane, Dr. Gayatri S. Kamble	Synthesis, Characterization and Non-Isothermal Study of Bioactive transition Metal Complex, dichloro [(E)-3-	34

		[(4''dimethylamino) phenyl]-1-phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III)	
35	Mohd Yaseen Sirwal, Amit Kumar	Assessing Spatio-Temporal Water Quality Variations in Rural and Urban Zones of Kishtwar Valley	35
36	Raza Rasool	Antimicrobial Schiff Base Polymers Containing Transition Metals: Synthesis, Characterization and Their Applications	36
37	Siddiqui Alima Fatema, Dr. Maqdoom Farooqui, Dr. Uzma Parveen Shaikh	Catalytic Applications of Mixed Transition Metal Oxides: A Review	37
38	NazmaTabassum, Nouman, Suman Maji, Rahisuddin	Synthesis, Characterization, and Catalytic Studies of Transition Metal Complexes derived from heterocyclic ligand system	38
39	Harshada Katkar, Padekar Akshada, Dinesh Garud, Sudhir Arbuj	Synthesis and Characterization of HZSM-5 for Carbon-Carbon coupling Reactions	39
40	Rehana Farooq	Sustainable Green-Synthesized Nanomaterials for Enhanced Photocatalytic Degradation and Reusability in Wastewater Treatment	40
41	Mohd Shahab, Afroz Khan, Sameera Mujahid, Asad U. Khan and Faiyazur Rahman	Photoactivated antibacterial activity of eco-friendly synthesized ZnO and ZnO/GO nanocomposites	41
42	Md. Shahid, Md. Zafer Alam, Salman A. Khan	A colorimetric and fluorometric sensor based on Thiazole Schiff base use as a sensor for the detection of Fe ³⁺ and Hg ²⁺ ions	42
43	Zeeshan Ahamad	Synergistic Fe-Sn-Ni ternary metal oxide nanocomposite for Congo red adsorption: Synthesis, characterization, and Box-Behnken optimization	43
44	Dr. Gayatri S. Kamble, Dr. Rasika C. Torane	Synthesis, Characterization and Non-Isothermal Study of Bioactive transition Metal Complex, dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1-phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III)	44
Physical and Material Chemistry			ICC/PMC/042 to 067

45	Prashnasa Tiwari, Vivek Sharma	Facile Microwave Assisted Synthesis of Covalent Triazine Framework for Exceptional Iodine Capture	45
46	Subiya Nasir	Effect of surfactants and polymers on the kinetics of Hydrolysis of Cefuroxime Axetil and the Resulting Degradation Pathways	46
47	Md Naseem Ansari, Md Naseem Ansari, Alimuddin, Salman A. Khan and Neha Maheen	Synthesis, Characterization and Analytical applications of Polyaniline Zr (IV) Iodovanadate nanocomposite	47
48	Nuzhat Fatma, Alimuddin and Salahuddin Syed	Development of Poly-O-toluidine Zr (IV) iodotungstate nanocomposite for removal of heavy metals from wastewater	48
49	Ruby Ahmed	Volatile Organic Compounds (Vocs) Sensing Studies on Electrically Conductive Polyaniline@Mos ₂ Nanocomposites	49
50	Meraj Madani, H. Aleem Basha, Md Shareefuddin	FTIR and Raman Spectroscopic Investigation of Alkaline Earth Modified Bismuth Borate Glasses	50
51	Muhammad Bilal Ahmad and Arifa Shaheen	L-Tryptophan and Gemini Surfactant-Based Fluorescent Ionic Liquid Crystals for Dual Detection of Cu (II) and Ascorbic Acid in Real Samples	51
52	Surjit Kaur and Mithu Maiti Jana	Synthesis of Rice Husk-Based Green Biodegradable Composites Reinforced with <i>Yucca filamentosa</i> Fiber and its Graft Copolymers	52
53	Kapilkumar Dattatraya Randhir	Green Photodegradation of Xylenol Orange Dye Under Solar Light using Metal and Non-Metal Modified ZnO-G-C ₃ N ₄ Nanocomposites Synthesized by an Ultrasound-Assisted Route	53
54	Sarvani Jowhar Khanam	Recent Advancements in n-i-p Perovskites Solar Cells	54
55	Mohammad Shafi Sheikh, Nusrat Shafi	Zwitter ionic Surfactants under the impact of short chain Surfactants	55

56	Chandan Kumar Singh and Angad Kumar Singh	Synthesis, Characterization, and Optoelectronic Studies of Schiff Base Lanthanide (III) Complexes	56
57	Mohd Amil Usmani	Vegetable Oil Based Eco-Friendly Biopolymers	57
58	Juveria Iram, Aleem Basha, Kaleem Ahmed Jaleeli	A Non-Invasive, Conductivity-Based Sensing Principle for Automated Grading of Egg Fertility and Freshness Using Terahertz Spectroscopy	58
59	Deepika Nanaware, Dr. K. S. Munde	Preparation of activated nano carbon from Leucaena leucocephala biomass for dye removal from wastewater	59
60	Saif Uz Zafar, Mohd. Akram	Synthesis and Applications of C ₁₂ -E2O2-C ₁₂ Assisted Bioactive Silver Nanoparticles	60
61	Zakiya Tazeen, Md. Shadab, Salman Ahmad Khan, Shahjahan	Molecular Interactions of Paracetamol with Ionic Surfactants: A Conductometric Study of CTAB and SDS in Aqueous Media	61
62	Nizamul Haque Ansari	Physicochemical studies on interactions between bio surfactants derived from natural oil with pesticides	62
63	Anwar Ali and Shahjahan	Investigation of Interactions of Proline with Non-aqueous SDS, CTAB and TX-100 at 298.15 K, 303.15 K, 308.15 K, and 313.15 K	63
64	Sadiya Mushtaq, Tayyaba Naaz, Md. Mohasin, Prof. Salman Khan	A Comprehensive Review of Mercury (II) Ion Detection via Rhodamine Schiff Base Fluorescent Sensors	64
65	Chitra Devi Palanichamy, Lakshmi Prabha Krishnamoorthy, Maadathi Sivakumar, Prabakaran Panchanathan, Devi Selvaraj, Sivasankari Gnanam, Boobalan Sivalingam and Shenbagam Kanagaraj	Eco-Friendly Biosynthesis of Cobalt Oxide Nanoparticles Mediated by Boerhavia diffusa and Evaluation of Their Antimicrobial Potential	65
66	Riyaj Mohammad	Role of Gemini Surfactants in Green Chemistry and their Interfacial behavior in the presence of additives	66

67	Vishal Pardeshia, Vijay Naukudkara	Eco-friendly synthesis of highly efficient Nickel-doped Fe ₂ O ₃ -g-C ₃ N ₄ photocatalyst for solar-driven degradation of anionic dyes in water	67
68	Md Sameer Ahmed, Anjum Begum	Multifunctional Ni-Al/Chitosan Composite Spheres for Integrated Antibacterial and Photocatalytic Water Treatment	68
69	Anjum Begum, Md Sameer Ahmed	Electrochemical Sensing of Ascorbic Acid Using Silica-Coated ZnO Nanospheres on Gold Electrode	69
70	Md. Mohasin, Salman A. Khan	Synthesis of thiophene based chalcone derivative as selective fluorescent chemosensor for the detection of Fe ³⁺ metal ions	70
71	Juveria Iram Aleem Basha, Kaleem Ahmed Jaleeli	A Non-Invasive, Conductivity-Based Sensing Principle for Automated Grading of Egg Fertility and Freshness Using Terahertz Spectroscopy	71
Analytical and Industrial Chemistry ICC/AIC/068 to 79			
72	Habibur Rahman	Green Analytical Chemistry: Recent Trends and Greenness Assessment Methods	72
73	Babla V Pendam, Amol S Gaikwad, Manohar V. Lokhande	Identification of Process-related Genotoxic Impurities of 3,7-Dimethyl-1-(5-oxohexyl) purine-2,6-dione by GC-HS Method	73
74	Sushil Kumar R Singh, Manohar V Lokhande	Development and Evaluation of NDBA as a Genotoxic Impurity in Dapagliflozin Drug Substance by using Liquid Chromatography-Mass Spectrometry	74
75	Ibrahim baje Syed, Radhakrishnan.Sivaprakasam	Synthetic Strategy, Mechanistic Insight, and Analytical Evaluation of Vildagliptin	75
76	Shaikh Manirul Haque, Sirhan Al-Batty, Abdullah Al-Sultan, Abdulrahman Ali Alkhaldi, Yunusa Umar	Optimized and Validated RSM-BBD Model for the Determination of Residual Solvent Acetic Acid in Empagliflozin	76
77	Amol S Gaikwad and Manohar V. Lokhande	Validation of a Gas Chromatography Method for Determination of Residual Solvents in 1-(p-bromophenyl)-1-(2-pyridyl)-3-dimethylaminopropane	77

		maleate Active Pharmaceutical Ingredient	
78	Mahfoozurrahman Khan, S. Md Wazed Ali, Md Shahadat	Efficient Removal of Organic Dyes from Wastewater Using Polyaniline-Impregnated Silica Gel Nanocomposites	78
79	Dr. Narjis Fatima, Syeda Ayesha Fatima, Maseerah Nazneen Osman	Development of an Eco-Friendly Paper-Based Colourimetric Indicator for Monitoring Humidity Exposure in Dry Food Commodities	79
80	Shumaila Hasan, Mohammad Zain Khan	Polycarbazole-Integrated BiCe-MOF Hybrid for Electrochemical Detection of Azithromycin toward Antibiotic Monitoring	80
81	Md. Zafer Alam, Salman A. Khan	Multifunctional Chalcone Probe for Sensitive Fe ³⁺ Sensing and Mechanistic Insights into Silver Nanoparticle-Induced Quenching	81
82	Suhail Ahmad, Salman A. Khan	Design, Synthesis, and Photophysical investigation of a Novel Tetrahydrobenzo[h]quinoline Derivative: A Turn-ON Fluorescent Sensor for Zn ²⁺ Ion	82
83	Priyanka S Thakur and Manohar V Lokhande	Spectroscopic Studies On Organometallic Schiff Base, Some Transition Metal Ion Complexes: Structural Insights and Anti-Microbial Activity	83
Environmental, Energy and Fuel Chemistry			ICC/EEFC/80 to 95
84	Nazifa Noor, Abu Nasar	Adsorptive Removal of Methylene Blue from Aqueous Solution using Magnetically Modified Shorea Robusta (SAL) Sawdust: Transforming Waste into Resources	84
85	Zoha Maqsood, Dr Shahid Pervez Ansari, and Dr Shahabuddin	Conductive Nanocomposite Hydrogel for Photocatalytic Dye Removal from Wastewater	85
86	Nandkishor B. Shirsath	Rational Design, Synthesis, and Advanced Characterization of Titanium Dioxide Nanoparticles for Sustainable Applications	86
87	Amit Kumar	Public Health Implications of Dung Cake Combustion in Households	87
88	Dharpawar Unnati	Environmental, Energy and Fuel	88

	Suresh, Dr. Aditi Kulakrni	Chemistry	
89	Mohsina Ahmed, Abu Nasar	Magnetized waste-peel-derived adsorbents: synthesis, characterization, and application for the removal of a cationic dye from artificially contaminated water	89
90	Aiman Khan, Mohd Arsalan	Polysulfone supported zinc oxide thin film composite membrane-fabrication, characterization and applications for metal ion removal	90
91	Mohd Arshad, Dr. Mohd Yusuf Ansari and Dr. Arham Shareef Ahmed	Structural and Electrochemical Investigation of Green-Synthesized CuO-RGO Nanocomposites for Energy Storage Devices	91
92	Nowsheenah Farooq and Athar Adil Hashmi	Nitrogen-Rich Porous Organic Polymer (SB-NRPOP) for High-Capacity Iodine Capture toward a Sustainable Future	92
93	Uqba Rashid, Mohd Arsalan	Removal of Microplastics in Water bodies through Composite Membranes	93
94	Abhishek Solanki and Vikal Gupta	Bio-inspired zinc remediation: Tamarind kernel polysaccharide and Amino acid-based resin for Removal of Zn (II) Ions from Aqueous Solutions	94
95	Shabana Sajid	Green Chemistry Initiatives for a Sustainable Development	95
96	Arisha Bi, Zeba Haque	Polyindole/Copper oxide Composite: A Highly Efficient Multi-Cyclic Photocatalyst	96
97	Mohd Suhail Chaudhary, Mohammad Zain Khan	Nanostructuring Materials to Overcome Performance Challenges in Flexible Solid-State Supercapacitors for Next-Generation Portable and Wearable Energy Storage Systems	97
98	Vidya Singh	An Analysis of Hydrothermal Biomass Processing for Sustainable Energy and Fuels	98
99	Kahkashan Sarfaraz, Saif Ali Chaudhry	GAAL@ZFT Nanocomposite Hydrogel as a High-Performance Adsorbent for Cationic Dye Removal	99
Medicinal and Drug Delivery			ICC/MDD/096 to 104
100	Dr. Uzma Faridi	Mechanistic Insights into the Anticancer	100

		Activity of Phenyl-1,3,5-Heptatriyne from <i>Bidens pilosa</i>	
101	Mohd Nadeem, Abul Kalam Najmi	Receptor Pharmacology of Phytochemicals in Alzheimer's Disease: Multi-Target Modulation of Neurodegenerative Pathways	101
102	Daniya Ikram, Prof M. Z. A. Rafiquee	Sodium Alginate-Based Delivery Systems for Tetracycline Hydrochloride: Encapsulation and Release Profiles	102
103	Aaishwarya Deepak Bansode, Dr. Madhuri Deshmukh	Design and Optimization of a Dual-Polymer Mucoadhesive Microsphere System for Controlled Neuroactive Drug Delivery	103
104	Ahmed Helmi Billo, Abdullah Saad Al-Bogami, Mohmmad Younus Wani	<i>In Silico</i> Screening of Newly Designed Azole-Based Derivatives as Prospective Antimicrobial Leads	104
105	Reyaz Ahmad, Mukesh Choudhary	Copper (II) complex as SARS-CoV-2 inhibitor: Synthesis, crystal structure, antiviral and anticancer properties	105
106	Sohera Tabassum, Azra Soban, Qasim Ullah	Synthesis of Benzenesulfonamides under Biocatalytic Conditions by Employing Baker's Yeast as a Biocatalyst	106
107	Touseef Begum and Suroor A. Khan	Design, Synthesis, and Biological Evaluation of Innovative 1,2,4-Triazine Derivatives Exhibiting Anxiolytic and Anti-Inflammatory Activity	107
108	Anzar Jahan, Aram Rahman, Syed Salahuddin, Arifuddin Mohammad	Design, Synthesis, Biological Evaluation, and Molecular Docking Studies of Novel Quinoline-Incorporated 4-Thiazolidinone Derivatives as Potential Anticancer Agents	108
109	Dr. Akanksha Gupta, Dr. Atul Kumar and Dr. Rajeev Gupta	Spiro-Pyrollidine-Oxiindole Derivatives: Novel Molecular Scaffolds as an Anti-Cancer Agent	109
Computational, Theoretical, and AI-Driven Chemistry			ICC/CTAIC/106 to 120
110	Shaيدا Khan, Abu Nasar	Magnetically Modified Pomegranate Peel for Methylene Blue Removal: Process Optimization by Response Surface Methodology and Prediction via Machine Learning	110

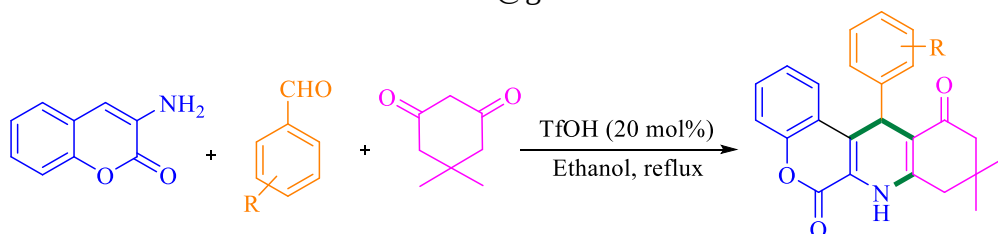
111	Omkesh Vyankatesh Aghav	Computational Deconvolution of Ligand-Macromolecular Recognition and Binding Energetics at an Insomnia-Associated Molecular Target	111
112	Fathima Dilruba Rasheed, Dr. Anoop Ayyappan	Donor-Acceptor Stenhouse Adduct (DASA): A computational investigation on molecular orbital, solvation and cyclization	112
113	Abdul Moheman	Advances in High Performance Thin Layer Chromatography (HPTLC) Using Artificial Intelligence (AI) and Machine Learning (ML) Tools	113
114	Saiyyad Mohammedzaid, Adiba Zohra, Saleem Javed	Integrated quantum chemical computational studies of 4,7-dichloroquinoline as a potential lead for PPAR γ activation as Anticancer Agents	114
115	Mohd. Zaid, Md Wasee Murtuza, Manoj Sharma, Saleem Javed	A reproducible multi-scale computational workflow for DL-methionine in breast cancer targets: DFT, data-driven docking, MD and MM-PBSA validation	115
116	Manoj Sharma, Md Wasee Murtuza, Mohd Zaid and Saleem Javed	Quantum Computational, Spectroscopic, Topological, Molecular Docking, and Dynamics Studies of 2-Amino-3-Hydroxypyridine (2A3HP): A Potential Antimicrobial Agent	116
117	Adiba Zohra, Saiyyad Mohammedzaid, Saleem Javed	Bridging electronic structure and binding stability: DFT, docking and MD investigations of Ninhydrin as a Promising AChE Inhibitor Lead	117
118	Neha Tarase	Comparative Molecular Docking Analysis Targeting HER2 and ROR Gamma Receptors in Breast Cancer Progression	118
119	Fatima Zahra, Shaikh Sana Naeem, Zeeshan Ahamad	Role of Advanced and Sustainable Nanomaterials in Water and Wastewater Treatment: Mechanisms, Applications, and AI-Aided Insights	119
120	Md Wasee Murtuza, Ayesha Parveen, Saleem Javed	In silico studies on Fenamic Acid as a potential human dihydroorotate dehydrogenase (DHODH) inhibitor employing molecular docking, molecular dynamics, MM-PBSA, PCA, FEL and ADME analysis	120
121	Aram Rahman, Anzar Jahan, Salahuddin	Quinoline-Pyridine Schiff Bases Hybrids as Potential Anticancer Agents	121

	Syed, Juveria Zareen, Salman Ahmed Khan, Mohammad Ariffuddin		
122	Dr. Rehana Anjum and Arshiya Anjum	Nanoengineered Biodegradable Polymers for Targeted Cancer Therapy	122
123	Afreen, Amarnath Velidandi	Preparation of Thiazole Schiff bases by grinding method	123
124	Dr. Afreen	Thiazole, Coumarin conjugated (β -lactam scaffold) Azetidinones Synthesis and their substitution effect	124

TfOH- Catalyzed Knoevenagel/Michael/Intramolecular Cyclization Cascade Synthesis of Coumarin-1,4-Dihydropyridine Derivatives

Md. Musawwer Khan and Anam Arif

Department of Chemistry, Aligarh Muslim University (AMU), Aligarh-202002, India
musawwer@gmail.com



1,4-Dihydropyridine (1,4-DHP) is a well-known class of pyridine derivatives with a biochemically active nucleus. Apart from drugs like Nifedipine and Felodipine, some second-generation antagonists namely Elgodipine, Furnidipine, and Darodipine are also used to treat congestive heart issues. Being highly bio-active, attempts are in progress to identify and generate the cancer pharmacophores in 1,4-DHP moieties.

Since our group is working on synthesis of heterocycles for medicinal importance using MCRs, here, we would like to present an efficient method of coumarin 1,4-DHP hybrid synthesis through a triflic acid (TfOH) catalyzed reaction of aromatic aldehyde, dimedone and 3-aminocoumarin in ethanol under reflux followed by alkylation at the free N-H site, in vitro cytotoxic study against A549 cell line along with molecular docking and molecular dynamic simulations.

Keywords: TfOH, Coumarin, 1,4-Dihydropyridine, Multicomponent Reaction

Novel Tyrosine and Pectin-based Nanoparticles for Anticancer

Application

Dr. Yogesh Kumar

*Department of Chemistry, Centre of Excellence Government college Sanjauli Shimla
Himachal Pradesh, India-171006*

E-mail: sood05yogesh@gmail.com

Abstract

A novel class of anticancer therapies may be developed with the aid of nanotechnology. These compounds medicinal qualities are improved and their toxicity is decreased using nanotechnology. A nanoparticle is an extremely small particle that can be produced artificially or organically, and depending on its intended application, it can have many different forms. Nanoparticles with particle size capable of penetration into deep-seated body tissue are excellent candidates for site-specific therapeutic applications. The present work focuses on the synthesis, characterisation and in vitro MTT assay of novel tyrosine-pectin-based nanoparticles against HeLa Cells. The nanoparticles were synthesized under ultrasonication at 75°C employing citric acid as crosslinker and acrylamide as co-monomer. The synthesized tyrosine-pectin-*cl*-citric acid-poly (acryl amide) nanoparticle [(Ty-Pc-*cl*-CA-poly (AAM))] were characterised using techniques such as FT-IR and FESEM to get evidence of successful nanoparticle synthesis. The characterization results indicated that the nanoparticles of size below 100nm were successfully synthesised. These nanoparticles were employed for anticancer study against HeLa cells and proved to be better cytotoxic agents than the control. They exhibited the IC_{50} value ($\mu\text{g/ml}$) of 359.8 ± 0.14 .

Keywords: Anti-cancer, Citric acid, Pectin, Nanoparticle, Tyrosine

A Sustainable, Mild, and Green NIS-Mediated Methodology for the Room-Temperature Synthesis of Quinoxalines

Humaira Parveen

Organic and Medicinal Chemistry Research Lab., Department of Chemistry, Faculty of Science, University of Tabuk, Tabuk-71491, Kingdom of Saudi Arabia.

E-mail: h.nabi@ut.edu.sa

Abstract

Quinoxaline is a renowned and significant class of nitrogen-containing heterocyclic compounds that display broad pharmaceutical and biological properties. Compounds possessing a quinoxaline framework exhibit a range of pharmaceutical and biological activities such as anti-HIV, anticancer, antileishmanial, antiproliferative, antitumor, etc. Moreover, quinoxaline framework is also an active essential unit of numerous advanced functional materials, herbicides, antibiotics, fungicides, and pesticides. Previously, quinoxalines were synthesized through hazardous metal catalysts or oxidants. Moreover, other methods also utilized expensive metal catalysts or oxidants for the reactions. In our present invention, we have established a green, environmentally benign, efficient, mild, and metal-free N-iodosuccinimide mediated approach for the synthesis of quinoxalines from o-phenylenediamines and sulfoxonium ylides at room temperature. Moreover, we have not utilized expensive and hazardous metal catalysts or oxidants for the reactions. In our present invention we observed that, sulfoxonium ylides and o-phenylenediamines decorated with several functional groups were well tolerated during the reactions and produced desired products with good to excellent yields through a simple and trivial procedure. We also executed gram-scale reaction to validate the practicality of this method. Metal-free, operational simplicity, mild reaction conditions, atom economy, and high yields are some significant features of this present invention which supports the environmental sustainability. This invention can be implemented in a wide range of products and services across several key industries such as pharmaceutical industry, chemical industry, biotechnology, material science, and agriculture etc.

Computationally Guided Design, Optimization and Synthesis of Multi-targeted Antifungal Agents

Trupti Subhash Pawal^{1*} and Vasundhara Sawant²

¹PG. Scholar, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.

²Assistant Professor, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.

E-mail: truptipawal54@gmail.com

Abstract

Heat shock protein 90 (HSP90), VEGFR2, acyltransferase GWT1 and lanosterol 14 α -demethylase plays a pivotal role in antifungal a multi-targeted therapeutic strategy aims to concurrently inhibit several critical enzymes within the ergosterol biosynthesis and associated metabolic pathways, thereby increasing antifungal efficacy and reducing the potential for the development of drug resistance. In this study, a structure-guided computational approach was employed to design and evaluate a focused library of amino-pyrazole derivatives (TP01-TP16) bearing diverse substituents on the amino-pyrazole core as multi-targeted antifungal inhibitors. The designed derivatives established key hydrogen-bonding interactions with conserved the each protein residues such as Glu, Lys, and Asp, alongside hydrophobic and π - π interactions involving residues in the helix-loop-helix region (e.g., Phe/Ile/Leu-rich motifs) that are critical for chaperone regulation. Substituent variation on the amino-pyrazole moiety markedly influenced binding orientation and affinity, providing clear structure-activity relationships governing antifungal activity. Several compounds within the TP01-TP16 series demonstrated superior docking scores and well-balanced interaction profiles, consistent with effective binding. In silico drug-likeness and ADMET analysis indicated favourable oral bioavailability, compliance with Lipinski's rule and low predicted toxicity, supporting their suitability as lead-like molecules. Overall, this study highlights amino-pyrazole scaffolds as inhibitors offer a strategic pathway to discover potent, selective and safe antifungal agents capable of overcoming current therapeutic limitations.

Synthesis Approaches and Biological Applications of Novel Aficamten Derivative

Yata Sravan kumar¹, Salman A. Khan*

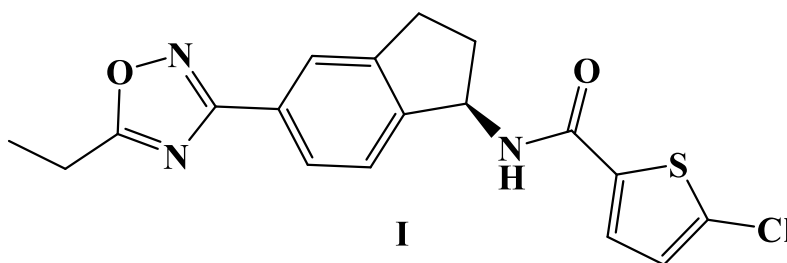
Physical Sciences (Chemistry), School of Sciences, Maulana Azad National Urdu University, Hyderabad 500032, Telangana, India

*Correspondence Author e-mail address: sahmad_phd@yahoo.co.in (S. A. Khan)

Abstract

In this work, multi step synthesis and Biological applications of novel Aficamten Derivatives (I) .It has been prepared by using of Bromophenyl propionicacid, with suitable dehydration reagents such EDC.HCl/TEA, and Cyanation by Coppercyanide were used in preparation. Based on the molecule functional group may its shows biological activity. We sent the sample for biological activity and are awaiting the results of the Anti-Cancer or Ant-viral. The mass, H1-NMR, and C13 spectra of the synthesized compounds (I) were used to confirm their structure. TLC indicated a single spot for these compounds.

Keywords: Biological activity of novel Aficamten derivatives.



C F: C₁₈H₁₆ClN₃O₂S

M Wt: 373.86

Structure-guided development of amino-pyrazole derivatives as selective C-terminal HSP90 inhibitors

Jeba Aslam Mulani^{1*} and Vasundhara Sawant²

¹PG. Scholar, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.

²Assistant Professor, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.
jebamulani786@gmail.com

Abstract

Heat shock protein 90 (HSP90) plays a pivotal role in cancer progression by stabilizing oncogenic client proteins involved in cell proliferation, survival, and drug resistance. While N-terminal HSP90 inhibitors have shown clinical limitations due to induction of the heat shock response, selective targeting of the C-terminal domain (CTD) represents a promising alternative therapeutic strategy. In this study, a structure-guided computational approach was employed to design and evaluate a focused library of amino-pyrazole derivatives (JM01–JM16) bearing diverse substituents on the amino-pyrazole core as selective HSP90 CTD inhibitors. The designed derivatives established key hydrogen-bonding interactions with conserved CTD residues such as **Glu, Lys, and Asp**, alongside hydrophobic and π – π interactions involving residues in the **helix loop-helix region (e.g., Phe/Ile/Leu-rich motifs)** that are critical for chaperone regulation. Substituent variation on the amino-pyrazole moiety markedly influenced binding orientation and affinity, providing clear structure-activity relationships governing CTD selectivity and potency. In silico drug-likeness and ADMET analysis indicated favourable oral bioavailability, compliance with Lipinski's criteria, and low predicted toxicity, supporting their suitability as lead-like molecules. Given the conserved role of HSP90 in both oncogenic signaling and fungal stress response pathways, these findings also suggest potential translational relevance in antifungal drug discovery.

Keywords: HSP90 C-terminal inhibition, Amino-pyrazole scaffold

GAAL@ZFT Nanocomposite Hydrogel as a High-Performance Adsorbent for Cationic Dye Removal

Kahkashan Sarfaraz, Saif Ali Chaudhry

Department of Chemistry, Jamia Millia Islamia, New Delhi-110025, India

Email: kahkashans31@gmail.com

Abstract

The development of smart, super-adsorbent nanocomposite hydrogel materials with biodegradability and biocompatibility is decisive in the material world to address the major shortcomings associated with the sustainability issues of ecological footprints. Further, the massive applicability of nanocomposite hydrogels in the modern world has drawn huge interest in the development of high-performing materials. On the practical applicability, the absorption experiments were performed using the Yamuna water, Sewage wastewater and tap water spiked with a 10 mg/L JG-B, 10 mg/L VB and 20 mg/L AZ-A. The results show a significant removal of 95.66% JG-B, 84.27% VB and 81.29% AZ-A in Yamuna water, which is slightly lower than the result observed in the synthetic dye solutions due to the presence of competing ions. The fabrication of GAAL and its interaction with cationic dyes were characterized via FT-IR, PXRD, FE-SEM, TEM, SAED, BET, TGA and ZPC techniques. Batch adsorption experiments were performed to examine the influence of pH (2-10), adsorbent dosage (0.2-1 g/L), contact time (15-120 min), initial dye concentration (10-30 mg L⁻¹), and temperature (303-323 K) on adsorption efficiency. The adsorption kinetics followed the pseudo-second-order model ($R^2 > 0.99$), while the equilibrium data conformed well to the Langmuir isotherm ($R^2 = 0.998$), suggesting monolayer chemisorption on a homogeneous surface. Henceforth, the demonstrated works provide several mechanistic ways to achieve high-performing nanocomposite hydrogel.

Keywords: Nanocomposite hydrogel, Gum Arabic, Zinc ferrite, Cationic dye adsorption, Batch adsorption, Isotherm and kinetic modeling, Wastewater treatment, Biopolymer-based adsorbent

**Synthesis of New 4-[1-(1-Phenyl-1H-[1,2,3] triazol-4-ylmethyl)-1H-benzoimidazol-2-yl]-piperidine-1-carboxylic ester Derivatives-
Evaluation of Anti Cancer and Anti-Bacterial Activity/Docking studies**

Yerrabelly Hemasri^{a*}

*^aDepartment of chemistry, Nizam College, Osmania University, Hyderabad-500004,
India*

Abstract

A straightforward and effective method for the synthesis of new series of Benzimidazole-Triazole hybrids developed by adopting Click Cu(I) catalyzed [1,3] dipolar cycloaddition. Alkyne tethered benzimidazole carboxylates treated with various aromatic azides using sodium ascorbate and copper sulphate as catalytic medium. The resulting series of novel benzimidazole-linked 1,2,3-triazole analogues were characterized using spectral data. All the compounds screened for Anti cancer and Anti bacterial activity. The docking study was conducted to evaluate the interaction modes of the synthesized compounds within the active site of α -glucosidase. Three compounds exhibited good Anti cancer as well as antibacterial activity.

Development of Novel Quinoline incorporated Chalcones as potential therapeutic agents

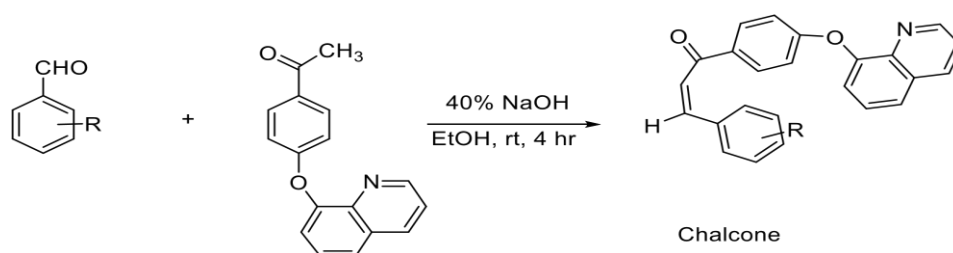
Zeenathunnisa Begum¹ and Qasimullah¹

¹Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Gachibowli, Hyderabad 500032, TS, India.

Email: drqasimullah@manuu.edu.in

Abstract

Quinoline derivatives are highly significant heterocyclic compounds in medicinal chemistry, recognized for a broad spectrum of biological activities. They are extensively studied for their potent anticancer, antimalarial, antimicrobial, anti-inflammatory, and anti-tubercular properties. Chalcone is a class of compounds that contain aromatic ketone and an enone and forms the central core for a number of important biological compounds called as chalcones or chalconoids. Chalcones are found in many naturally occurring compounds and many chalcone derivatives are prepared due to their simple synthesis. Chalcones are considered as synthons and bio-active scaffolds of wide medicinal interest as they have many pharmacological and biological activities such as antimicrobial, anticancer, antitubercular, antioxidant, antiinflammatory, antileishmanial, and other important biological activities. In the present study the new quinoline incorporated chalcones derivatives were synthesized (**Scheme-1**) and will be evaluated for their biological activities in particularly for antimicrobial.



Scheme-1: Synthesis of new quinoline incorporated chalcones derivatives

Keywords: Quinoline, Chalcones, Biological Activities, Antimicrobial Agents, Antileishmanial Agents

Utilization of triglycerides in the synthesis of useful polymers: A greener approach

Abul Hasnat

Department of Chemistry, Gandhi Faiz-e-Aam College (Affiliated to MJP Rohilkhand University, Bareilly), Shahjahanpur, U.P., India

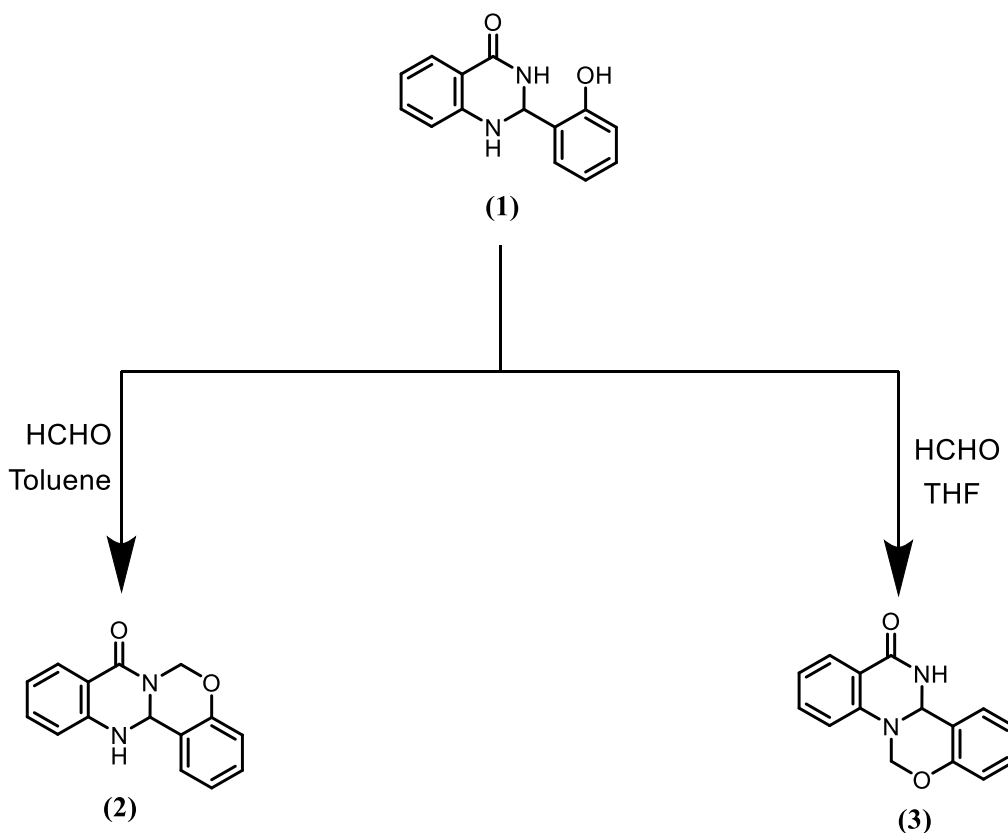
Abstract

In the recent past, vigorous efforts have been made to synthesize the polymeric materials from renewable resources with the objective to reduce the dependency on petrochemicals and different environment issues. The petrochemicals are going to deplete with fast rate day by day and hence resulting in a hike in prices. Numerous renewable resources of natural spectrum like lignin, chitosan, wool fiber, proteins, carbohydrates, vegetable oils and many others have been successfully used for the synthesis of different polymeric materials of versatile applications. Among them, vegetable oils, especially extracted from different seeds, opens an enormous potential to develop different polymeric recipes. Different functional groups present provide suitable sites for chemical transformation. Double bonds present in the fatty acid chain provides centre for hydroxylation, epoxidation, acrylation, cyclizations, metathesis and many others. Furthermore, unsaturation facilitates the film formation through the unsaturation. Polyols generated through double bonds and glyceride linkages, and used in different polyesters of significance. In present communication, efforts have been made to overview the different synthetic aspects and future prospective of applications.

Keywords: Triglycerides, Fatty Acid, Polyester, Polyol.

Selective Synthesis of two isomeric Oxazines and their characterisation**Gourav Arora, Priya, Arif Ali Khan****Guru Gobind Singh Indraprastha University, New Delhi*E-mail: gouravarora9336@gmail.com**Abstract**

A novel series of oxazine-quinazoline compounds was designed and synthesized via the cyclization of 2-(2-hydroxyphenyl)-2,3-dihydro-1H-quinazolin-4-one (1) with formaldehyde, affording 12,12a-dihydro-5-oxa-6a,12-diaza-benzo[a]anthracen-7-one (2) and 10b,11-dihydro-6-oxa-4b,11-diaza-chrysen-12-one (3) in toluene and tetrahydrofuran, respectively. After the products were isolated, elemental analysis, GC-MS, ¹H and ¹³C NMR spectroscopy were used to confirm their chemical structures.



Development of novel Imidazole chalcones as potential therapeutic agents

Noorunnisa Begum¹, Salahuddin Syed^{1*}, Mohammed Arifuddin² Qasimullah¹ and
Salman Ahmad Khan¹

¹Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Hyderabad-India.

²Department of Chemistry, Centre for Distance and Online Education (CDOE), Maulana
Azad National Urdu University, Hyderabad-India.

Corresponding Author: salahuddinsyed@manuu.edu.in

Abstract

Chalcone is a privileged species with medicinal significance as it consists of reactive ketoethylenic moiety –CO–CH=CH– belonging to flavonoids. The presence of a reactive α , β -unsaturated carbonyl function in chalcone and its derivatives is the reason for its pharmacological activities. Chalcones exhibit a wide spectrum of pharmacological effects such as antioxidant, antibacterial, anthelmintic, antiulcer, antiviral, insecticidal, antiprotozoal, anticancer, antiinflammatory, antidiabetic, etc. Chalcones can be synthesized by Claisen–Schmidt's condensation, Heck's reaction, Suzuki's reaction, etc. The heterocyclic compound family is the most prevalent category of organic compounds and plays indispensable roles in our daily lives. These compounds have demonstrated efficacy in treating conditions ranging from hypertension and neuropathic pain to infectious diseases and cancer. The imidazole scaffold serves as a key building block in drug design and discovery. These compounds can be synthesized using various techniques and their diverse structural reactions provide a wealth of opportunities in medicinal chemistry. In view of the importance of Imidazole and chalcone scaffolds as potential biological agents the present work is undertaken to development of novel imidazole based chalcones as potential therapeutic agents. In the present study the imidazole-4-carboxaldehyde (1) are reacted with the substituted-acetophenones (2) to obtain the target novel imidazole based chalcones (3).

Keywords: Imidazole-4-carbaldehyde, Acetophenones, Chalcones.

**Synthesis and invitro Antimicrobial Evaluation of Novel Heterocyclic
Schiffs base and their corresponding 3-Chloro-2-Azetidinones and 4-
Thiazolidinone derivatives**

**Zuverya Zareen, Aram Rahman, Anzar Jahan, Ariffuddin Mohammed, Syed
Salahuddin**

Department of Chemistry, School of Science, MANUU, Hyderabad - 500032, India

E- mail: zareenayaan2017@gmail.com

Abstract

In the present study, we synthesized and evaluated the antimicrobial activity of (4-aminophenyl) benzimidazoles Schiff bases and their corresponding 2-azetidinones and 4-thiazolidinone derivatives. These compounds were obtained from the condensation of 2-chloro-3-formylquinolines and 2-(4-aminophenyl) benzimidazoles and their condensation with chloroacetyl chloride and thioglycolic acid. The structures of the synthesized compounds were confirmed using spectroscopic techniques such as FT-IR, ¹H-NMR, and mass spectrometry analysis. The antibacterial activity of all these compounds were tested against Staphylococcus Aureus, Bacillus Subtilis, Escherichia Coli and Pseudomonas Aeruginosa. The antibacterial results in terms of zone of inhibition revealed that these compounds are more active against S. aureus in comparison to B. subtilis, E. coli and P. aeruginosa. It is also found that the antibacterial activities of 2-(4-aminophenyl) benzimidazoles Schiff bases, 3-chloro-2-azetidinones and 4-thiazolidinones are showing the same trends against other three bacterial strains i.e., B. subtilis, E. coli and P. aeruginosa. The Molecular docking studies were conducted to show the interaction of the molecules with the protein by using the crystal structure of S. aureus DNA gyrase (PDB ID:3TTZ). Further, exploration of these compounds will be definitely will emerge as lead molecules as selective antibacterial agent for S. aureus.

Keywords: Schiffs base, 3-chloro-2-azetidinones, 4-Thiazolidinones, anti-bacterial activity.

Efficient and Facile Synthesis of Maleic anhydride ring opening reaction with anilines under Bio-Catalytical Condition by Employing Baker's Yeast as Biocatalyst

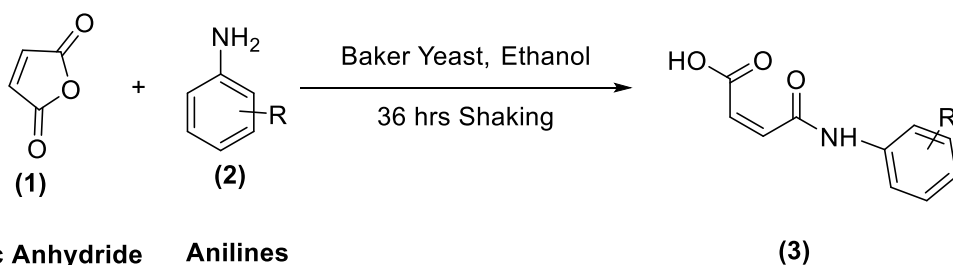
Azra Soban¹, Sohra Tabassum¹, Qasim Ullah^{1*}

¹Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Gachibowli, Hyderabad 500032, TS, India

Email: drqasimullah@manuu.edu.in

Abstract

Biocatalysis is an approach to green chemistry. A crucial step in the synthesis of organic compounds is the reduction of aldehydes and ketones to secondary alcohols. The use of a biocatalyst, such as enzymes or entire cells, has not affected this process. It offers great selectivity, high specificity, and an environmentally friendly approach to synthesis. *Dried Baker's Yeast* is used in various organic transformations as a bio-catalyst. Maleic anhydride ring-opening reaction with aniline is a nucleophilic acyl substitution reaction where the amino group of aniline acts as a nucleophile, attacking one of the carbonyl carbons of the Maleic anhydride. This attack opens the ring, resulting in the formation of an amide bond and a free carboxylic acid group i.e., *Maleanilic acids* (carboxylic acid amides). In the present study the Maleic anhydride (**1**) ring-opening reactions with anilines (**2**) to give the corresponding maleanilic acids (carboxylic acid amides) (**3**), under bio-catalytic conditions by using baker's yeast as bio-catalyst to afford the corresponding ring opened *Maleanilic acids* (Carboxylic Acid Amides) (**3**) in good to excellent yield.



Keywords: Anhydrides, Anilines, Maleanilic acids (carboxylic acid amides), Baker's Yeast

**Recent Advances in Coumarin–Schiff Base Fluorescent Chemosensors
for the Detection of Al³⁺ and Cu²⁺ Ions**

Khutubuddin, Md. Mohasin, Zafir Aribuddin Baag, Salahuddin Syed, Salman A. Khan*

*Department of Chemistry, School of Sciences, Maulana Azad National Urdu University,
Hyderabad 500032, Telangana, India*

*Correspondence Author e-mail adders: sahmad_phd@yahoo.co.in (S. A. Khan)

Abstract

Coumarin–Schiff base hybrids have gained significant interest as fluorescent derivative for the selective and sensitive detection of metal ions particularly Al³⁺ and Cu²⁺ ions. The azomethine (C=N) moiety provides effective metal-binding sites, while the coumarin core functions as a strong fluorophoric platform with favorable photophysical characteristics. Despite the difficulty in sensing Al³⁺ due to its high hydration energy in aqueous systems, numerous coumarin-based derivatives have achieved remarkable selectivity, typically forming 1:1 metal–ligand complexes accompanied by pronounced fluorescence enhancement, large Stokes shifts, and low detection limits extending from micromolar to nanomolar ranges. Monitoring Cu²⁺ is equally important because of its dual role as an essential micronutrient and a toxic ion at elevated concentrations. Overall, coumarin-Schiff base systems represent a promising class of fluorescent chemosensors for Al³⁺ and Cu²⁺ detection, offering valuable applications in environmental monitoring and bioimaging studies.

Keywords: Coumarin; Schiff base; Photophysical; Fluorescent; Chemosensor

Synthesis of Triazole based Schiff base: A Highly Selective and Sensitive Fluorescent Chemosensor for the Detection of Cu²⁺ Metal Ion

Umme Salma, Salman A. Khan*

Department of Chemistry, School of Sciences, Maulana Azad National Urdu University,
Hyderabad 500032, Telangana, India

*Correspondence Author e-mail address: sahmad_phd@yahoo.co.in (S. A. Khan)

Abstract

A specific fluorescent chemosensor triazole based schiff base was developed via condensation of triazole hydrazide and diphenyl-amino-benzaldehyde. The structure of compound (TSB) was confirmed by Mass spectrometry, ¹H-NMR and ¹³C-NMR spectral techniques. The solvent interaction between TSB and various solvents were investigated by UV-vis and fluorescence titration studies, revealing a bathochromic shift (red shift) of 11 nm in the absorption and emission spectra, when the solvent polarity shifted (from n-hexane to DMSO). Fluorescence spectrometry titration was used to assess the specificity and selectivity of TSB for the identification of the Cu (II) ion. The results showed that there was a discernible decrease in fluorescence when 0.5×10^{-2} M of aqueous Cu²⁺ ions solution was added to the 0.1×10^{-4} M of TSB in acetonitrile. Several photophysical techniques were used to analyze the fluorescence quenching process, such as spectroscopic titration, Benesi-Hildebrand analysis, Job's plot graph that confirming a 1:1 stoichiometry ratio between TSB and Cu²⁺ ions. The association constant (K_a) of TSB for Cu²⁺ ion was determined to be $1.83 \times 10^4 \text{ M}^{-1}$.

Keywords: Triazole schiff base, dipole moment, stoke shift, Fluorescence chemosensor, Cu²⁺

Synthesis and determination of antibacterial activity of Benzimidazole derivatives

Sushil Kumar, Maneesha D. Sati² and S. C. Sati¹

¹Department of Chemistry, H.N.B.Garhwal University (A Central University) Srinagar
Garhwal, Uttarakhand, India .246174

²Department of Chemistry, Govt. PG College Augustyamuni, Rudra Prayag, India

Corresponding author: Sati_2009@rediffmail.com

Abstract

The synthesised benzimidazole compounds were prepared by condensing o-Phenylenediamine with various carbonyl compounds. The present paper deals with a series of benzimidazole derivatives synthesised in a single step by reacting o-phenylenediamine with benzoic acid. The structures of all the synthesised compounds were elucidated using IR, ¹H-NMR, and ¹³C-NMR. The synthesised target compounds were evaluated for in vitro antibacterial activity against three bacterial strains by employing the disc diffusion method, using Ciprofloxacin as a standard drug.

1,25- Dihydroxycholecalciferol: A Biological Imperative for Human Health and Immune Regulation

Kahkashan Begum*

Department of Chemistry, Gandhi Faiz-E-Aam College (Affiliated to MJP Rohilkhand University, Bareilly), Shahjahanpur, UP, India

*Email: apkahkashanbegum@gmail.com

Abstract

Vitamin D is a fat-soluble secosteroid hormone that plays a fundamental role in maintaining human health. Traditionally recognized for its importance in calcium and phosphorus homeostasis and skeletal integrity, vitamin D is now acknowledged as a multifunctional nutrient influencing diverse physiological systems. Endogenously synthesized in the skin upon exposure to ultraviolet B radiation and obtained from limited dietary sources, vitamin D undergoes hepatic and renal hydroxylation to form its biologically active metabolite, calcitriol (1,25- Dihydroxycholecalciferol). The primary biological necessity of vitamin D lies in its regulation of mineral absorption, bone mineralization and prevention of disorders such as rickets in children and osteomalacia and osteoporosis in adults. Emerging evidence also highlights its involvement in muscle function, cardiovascular regulation, insulin sensitivity, and neurocognitive processes. Given its broad biological significance, maintaining adequate vitamin D levels is essential for overall health and disease prevention. Strategies such as sensible sun exposure, dietary supplementation, and food fortification are crucial public health measures to combat widespread deficiency. Continued research is warranted to further elucidate optimal vitamin D requirements and its therapeutic potential in human health management.

Key Words: Vitamin D, Human Health, Secosteroid Hormone, Cause of Bone Disorder

Design and Development of Oxadiazole-based Derivatives as Histone Deacetylase (HDAC) Inhibitors

Kiran Naykodi^{1*} and Vasundhara Sawant²

¹PG. Scholar, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.

²Assistant Professor, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune, Maharashtra-411 048, India.

E-mail: kirann8997@gmail.com

Abstract

The present study aimed to identify anti-oxidant leads by rational design, synthesis, and biological evaluation of a focused library of Oxadiazole derivatives (NK0–NK17) targeting Histone deacetylase (HDAC), a key enzyme implicated in disorders.

A structure-based drug design strategy was adopted, employing molecular docking to elucidate the binding mode and interaction profile of the designed compounds within the HDAC active site. A series of Oxadiazole derivatives (NK0–NK17) were synthesized via oxidative cyclization of hydrazide with carbonyl compounds in polar solvent system. Comprehensive structural characterization was performed using IR spectroscopy. The antioxidant potential will be evaluated *in vitro* using the DPPH radical scavenging assay.

Docking analysis revealed consistent and energetically favourable interactions of the synthesized oxadiazole derivatives with critical residues in the HDAC-6 binding pocket, supporting the proposed target engagement. Notably, compounds NK4 and NK7 displayed superior affinity during computational screening indicating a clear structure–activity relationship governed by substituent effects on the oxadiazole scaffold. The designed derivatives established key hydrogen-bonding interactions with PHE A:504, HIS A :75, ARG A:499. Several compounds within the NK0–NK17 series demonstrated superior docking scores and well-balanced interaction profiles. *In silico* drug-likeness and ADMET analysis indicated favourable oral bioavailability, compliance with Lipinski's criteria, and low predicted toxicity, supporting their suitability as lead-like molecules.

The convergence of *in silico* predictions and experimental outcomes establishes the Oxadiazole nucleus as a promising pharmacophoric platform for HDAC-6-directed anti-oxidant agents. Compounds NK4 and NK7 emerge as credible lead candidates for further optimization and mechanistic exploration.

Synthesis and Characterization of Ni (II) Schiff-Base Complexes: Structural and Biological Insights

Md. Ghaznafar Alam

Ph.D. Research Scholar, Dept. of Chemistry, Patna University, Bihar

Abstract

Nickel (II) Schiff-base complexes are interesting because variations in the design of the ligands can greatly impact their coordination geometry, stability and biological response. In this study, selected aldehydes were condensed with different primary amines under reflux conditions to prepare a set of Schiff-base ligands which the imine scaffolds were obtained in good purity. The transformed ligands reacted with Ni (II) salts in an alcoholic medium to give coloured, air-stable Ni (II) complexes. The products were isolated by filtration, washed free of unreacted starting materials, and recrystallized to give analytically pure solids. The FTIR spectra show presence of azomethine (C=N) band which is the characteristic band that may be observed in the spectra and this band is shifted on complexation due to the involvement of imine nitrogen in binding while the emergence of additional bands and weakening of other bands in the regions are attributed to donor-atom related chelation. Thermal studies showed that the complexes were stable enough for further tests in downstream. In vitro assays took place to screen the ligands and complexes for their antimicrobial activity against representative bacteria for biological insights. Usually, the Ni (II) complexes exhibited improved inhibition in comparison with the free ligands, which is consistent with chelation-driven lipophilicity enhancement and better interaction with cellular targets. The research reliably synthesized and characterized Ni (II) Schiff-base complexes and presented a first estimate of their structure activity trend to warrant further mechanistic and cytotoxicity studies.

Keywords: Nickel (II) complexes, Schiff-base ligands, Spectroscopic characterization, Coordination geometry, Antimicrobial activity

Mononuclear and dinuclear cobalt (II) complexes: Structural insights and evaluation of biomolecular interaction, catecholase activity and *in vitro* cytotoxic activity

Imtiyaz Ahmad Mantoo, Ilma Tarannum, Imtiyaz Yousuf*

Department of Chemistry, Aligarh Muslim University, Uttar Pradesh, 202002

**Corresponding author E-mail address: imtiyazchm@gmail.com (I. Yousuf).*

Abstract

A mononuclear and a dinuclear cobalt (II) complexes **C1** and **C2** were synthesized, characterized and examined for their potential biological studies. The structural validation of **C1** and **C2** was ascertained by various analytical and spectral methods which corroborated well with single crystal X-ray diffraction studies. The DFT/TD-DFT investigations of **C1** and **C2** were performed to understand their electronic and structural properties. *In vitro* DNA/BSA interactions of synthesized complexes were conducted by a range of biophysical techniques including UV-vis, fluorescence, circular dichroism (CD), cyclic voltammetry (CV) and electron paramagnetic resonance (EPR). The binding strength of complexes **C1** and **C2** with DNA was calculated to be $8.06(\pm 0.84) \times 10^4$ and $8.63(\pm 1.03) \times 10^5 \text{ M}^{-1}$ and with BSA was found to be $2.8(\pm 0.31) \times 10^4$ and $6.7(\pm 0.54) \times 10^4 \text{ M}^{-1}$, respectively. Catechol oxidase activity of complexes **C1** and **C2** were explored employing 3,5-di-tert-butylcatechol (3,5-DTBC) as a substrate and its subsequent conversion to 3,5-di-tert-butylquinone (3,5-DTBQ) product was validated. We have also validated the antioxidant potential of **C1** and **C2** via DPPH assay. Furthermore, cytotoxic activity of **C1** and **C2** was carried out against A549 (lung), MCF-7 & MDA-MB-231 (breast), MIA-Pa-Ca-2 (pancreas) and Hep-G2 (liver) employing ADR (adriamycin) as a standard and the results specified that the complexes **C1** and **C2** demonstrated cytotoxicity against A549 cell lines with a relatively low GI_{50} values (8–10 $\mu\text{g mL}^{-1}$).

Keywords: Mononuclear and dinuclear cobalt (II) complexes, DFT and TD-DFT, DNA/BSA interaction studies, catecholase activity, cytotoxic assessment

Development of Bioadsorbents from *Chenopodium album* Leaves and *Manilkara zapota* Seeds for the Removal of Heavy Metals from Water Samples

Nadeem Ahmad

*Department of Chemistry, Faculty of Science, Mohammad Ali Jauhar University,
Rampur-244901, India*

Emails: nadeemahmad9639@gmail.com; drgulrez2@gmail.com

Abstract

The contamination of water resources by toxic heavy metals has become a critical environmental concern, prompting the search for low-cost, sustainable, and efficient remediation materials. In the present work, bioadsorbents were developed from *Chenopodium album* leaves and *Manilkara zapota* seeds and investigated for their ability to remove heavy metal ions from aqueous water samples. The biomass materials were washed, dried, pulverized, and chemically activated to enhance their adsorption performance. The prepared bioadsorbents were characterized using FTIR, SEM, and Brunauer–Emmett–Teller (BET) surface area analysis. FTIR spectra confirmed the presence of hydroxyl, carboxyl, and amine functional groups responsible for metal ion binding, while SEM images revealed a porous and heterogeneous surface morphology. BET analysis showed surface areas of $48.6\text{ m}^2\text{ g}^{-1}$ for *Chenopodium album* and $36.2\text{ m}^2\text{ g}^{-1}$ for *Manilkara zapota* bioadsorbents. Maximum removal efficiencies were observed at pH 5-6, with equilibrium attained within 60 minutes. The maximum adsorption capacities, calculated using the Langmuir isotherm model, were found to be 112.4 mg g^{-1} and 95.7 mg g^{-1} for Pb^{2+} ions using *Chenopodium album* and *Manilkara zapota* bioadsorbents, respectively. Kinetic studies indicated that the adsorption process followed a pseudo-second-order model, suggesting chemisorption as the dominant mechanism. The results demonstrate that these plant-based bioadsorbents are effective, economical, and environmentally friendly materials for heavy metal removal from contaminated water, offering strong potential for application in wastewater treatment systems.

Synthesis and Spectral Studies of New Organometallic Schiff Base Complexes and Their Anti-fungal Activity

Priyanka S Thakur and Manohar V Lokhande

Department of Chemistry, Sathaye College (Autonomous), Mumbai-400057

Abstract

Synthesis of new organometallic Schiff bases complexes with general formula $[ML]_xH_2O$ [where M = Mn(II), Ni(II), Cu(II) Pd(II) and Pt(II), L=2,2'-{(1R,1'S)-1,1'-Ferrocen-2,4-dien-1-yl-2,2'-diyl bis [(Z)methyl[1]ylidenenitrilo}}bis(3-iodophenol)] have been prepared and characterized by elemental analysis, magnetic susceptibility, Conductivity IR, UV-Visible, Mass spectra and TGA/DTA. Organometallic Schiff base is tetradentate and co-ordination through nitrogen of azomethine ($>C=N-$) and oxygen of Hydroxyl group. The complexes have octahedral geometry with six coordination number. Electronic spectra of the complexes were recorded and its parameters like Nephelauxetic effect (β), bonding parameter ($b_1/2$) and Sinha's parameter (δ %) are calculated. TGA and DTA results of $[Pt(C_{24}H_{16}FeI_2N_2O_2).2H_2O]$ and $[Pd(C_{24}H_{16}FeI_2N_2O_2).2H_2O]$ are reported, Complexes were losing weight due to exothermic and endothermic process. The mass spectra of prepared ligand ($C_{24}H_{16}FeI_2N_2O_2$) and its complex such as $[Mn(C_{24}H_{16}FeI_2N_2O_2).2H_2O]$ were used to compare their stoichiometric composition and it found that near about equal to the theoretical mass of the complex and prepared ligand. Synthesis of nanoparticles of OMNPs (organometallic Nanoparticles) of Cu (II) Complex with SEM and EDX were recorded and particle size is in between 52-60nm. The ligand and complexes have been screened for its anti-fungal activities against three fungi *Alternaria brassicae*, *Aspergillus niger*, *Fusarium oxysporum*.

Keywords: Mass, IR, UV-Visible, SEM, EDX, TGA/DTA, Anti-Fungal activities.

**Pyrrolidine derived 1,2,3-triazolyl organosilane as “Turn on”
fluorescence sensor for Zn (II) ion: synthesis, antioxidant, molecular
docking and DFT studies**

Gurjaspreet Singh^{a*}, Komal^{a*}

^aDepartment of Chemistry, Panjab University, Chandigarh, 160014, India.

Email: komalkalwan09@gmail.com

Abstract

The article emphasizes the synthesis of pyrrolidine derived 1,2,3-triazolyl organosilane 5 which was well characterized by utilizing spectroscopic techniques such as NMR (¹H and ¹³C), UV-visible, fluorescence and mass spectrometry. The molecule exhibits exceptional sensitivity to Zn²⁺ in comparison to other ions, which is demonstrated by fluorescence spectroscopy and UV-visible and with detection limits of 3.622×10^{-7} M and 1.893×10^{-7} M, respectively. The binding stoichiometry comes out to be 1:1 by using Job's plot approach and accordingly metal-ligand complex was synthesised and then characterised. Further, the molecule exhibits notable antioxidant property examined with DPPH assay. 'Molecular docking' was used to determine the binding interactions of molecule with Superoxide Dismutase (SOD) (PDB ID-1Z9P).

A multifunctional Schiff base: Investigating its Zirconium sensing and antiproliferative effects

Gurjaspreet Singh^{a*}, Parul^{a*},

^aDepartment of Chemistry, Panjab University, Chandigarh, 160014, India

Email: parul029r@gmail.com

Abstract

The current investigation is focused on the synthesis of Schiff base 5, which was characterized via X-ray crystallographic study, ¹H NMR spectroscopy, ¹³C NMR spectroscopy, FT-IR spectroscopy, mass spectrometry (LCMS) and thermal gravimetric analysis (TGA). Compound 5 has been identified as an effective and highly selective Zr (IV) sensor using UV–Visible spectroscopy with a limit of detection (LOD) 3.7×10^{-7} M. Compound 5 exhibited the most significant anticancer activity, reducing cell viability by upto 67.67 % compared to untreated control cells. Experiments on *Cajanus cajan* (pigeon pea) seeds revealed its efficacy as a good plant growth regulator. Molecular docking studies further supported its therapeutic potential by revealing strong interactions with both an anticancer target protein and a plant gibberellin protein, indicating its dual role as potential anticancer agent and a plant growth regulator. The finding from the study provides the foundation for future research into zirconium sensing and anticancer applications, potentially leading to the development of new sensors and anticancer drugs.

Green Synthesis of AgNPs and CuNPs using *Schleichera oleosa* bark Extract and its Application

Priyanka R. Kokate and Manohar V. Lokhande

*PG-Research Centre, Department of Chemistry, Sathaye College (Autonomous),
Mumbai-400057, Maharashtra, India*

Corresponding Email: manohar2210@gmail.com/kokatepriyanka753@gmail.com

Abstract

This study explores the eco-friendly synthesis of silver (AgNPs) and copper nanoparticles (CuNPs) using the aqueous bark extract of *Schleichera oleosa*. The plant extract is a natural reducing and stabilizing agent, enabling a green synthesis process. The nanoparticles were characterized using advanced techniques, including FTIR, UV-visible spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy-dispersive X-ray analysis (EDX). UV-visible spectroscopy revealed a surface plasmon resonance (SPR) peak at 421 nm for AgNPs, confirming their formation. TEM analysis showed that AgNPs and CuNPs were spherical, with sizes ranging from 1-10 nm and 9-17 nm, respectively, while XRD confirmed their face-centered cubic (FCC) structure. Both nanoparticles demonstrated notable antimicrobial activity against various bacterial strains, and their catalytic potential was evaluated in the degradation of 4-nitrophenol, following pseudo-first-order kinetics. The antimicrobial efficacy was assessed using the agar well diffusion method, revealing high toxicity against tested microbial strains. These findings underscore the potential of green-synthesized AgNPs and CuNPs in biomedical applications and environmental remediation.

Keywords: SEM, TEM, EDX, XRD, FTIR, UV-VIS, Microbial and catalytic activity.

A Cd (II)-Pyrazine Dicarboxylate Metal-Organic Framework as a High-Performance Adsorbent for Dye Removal

Ruheen Khan^a, M. Shahid^{a*}

^aFunctional Inorganic Materials Lab (FIML), Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India

*Corresponding author: shahid81chem@gmail.com

Abstract

Metal-organic frameworks (MOFs) are highly tunable porous materials that have shown great promise in applications such as gas storage, chemical sensing, and wastewater treatment. In this study, a novel Cd (II)-based MOF was rationally synthesized using 2,3-pyrazine dicarboxylic acid via a solvothermal route at 120 °C. Single-crystal X-ray diffraction revealed the formation of a three-dimensional framework in which the Cd (II) ions exhibit distorted octahedral coordination environments. Structural features and ligand coordination modes were further confirmed by Fourier transform infrared spectroscopy, while thermogravimetric analysis demonstrated good thermal stability of the material. The adsorption performance of the synthesized MOF was evaluated using methylene blue and methyl orange as model organic dyes. The framework showed significantly higher affinity and selectivity toward the cationic dye methylene blue compared to methyl orange. These results demonstrate the potential of this Cd (II)-based MOF as an efficient and selective adsorbent for dye removal, highlighting its applicability in environmental remediation.

Keywords: Metal-organic framework, Dye adsorption, Separation, Adsorption kinetics, Wastewater treatment.

**Benzimidazole appended 1,2,3-Triazole Chemosensor: Selective Zr (IV)
Sensing Coupled with Anticancer and Antioxidant Potency**

Gurjaspreet Singh^{a*}, Jyoti^{a*}

^aDepartment of chemistry, Panjab University, Chandigarh, 160014, India

Email- jyotinain66@gmail.com

Abstract

Benzimidazole appended 1,2,3-triazole was synthesized and highlighting the Zr (IV) sensing, antioxidant and anticancer properties. The characterization of the probe (Bentz) was executed via ¹H and ¹³C NMR, mass spectrum analysis, Infrared spectroscopy (FT). The Bentz shows good sensitivity and selectivity towards Zr (IV) in contrast to other various metal ions through UV-Visible spectrophotometer. The LOD and binding constant was figured out as 0.349 ppm and 5.32×10⁴ M⁻¹. Job's plot confirms that the binding ratio between Bentz and Zr (IV) comes out to be 1:1. The interaction between Bentz and Zr (IV) was verified through ¹H NMR, mass spectrum analysis and Fourier transform infrared spectroscopy. The Bentz showed antioxidant and anticancer activity which has been checked through experimental method and molecular docking analysis. The binding energies of Bentz with proteins human papillomavirus 31 and cyclooxygenase-2 comes out to be -10.43 and -11.27 kcal/mol respectively.

Silatrane-Chalcone-Triazole Hybrid for Selective Zr (IV) Detection via Naked-Eye and Turn-on Fluorescence: Anticancer Evaluation

Gurjaspreet Singh^{a*}, Poonam^{a*}

^a*Department of Chemistry, Panjab University, Chandigarh, 160014, India.*

E-mail: poonam17011994@gmail.com

Abstract

This poster presents a Silatrane-Chalcone-Triazole conjugate (6) synthesized via Cu(I)-catalysed azide-alkyne cycloaddition and evaluated as a selective colorimetric and fluorescent probe for Zr (IV). Compound (6) exhibited excellent selectivity toward Zr (IV), with a detection limit of 2.7×10^{-7} M. Titration analysis showed a strong linear correlation, indicating a 1:1 binding stoichiometry. The coordination mode was investigated using ¹H NMR, FT-IR, and mass spectrometry. Biological studies revealed pronounced anticancer activity, with a 94.81% decrease in cell viability. The probe was successfully applied for real sample analysis in wheat flour. Furthermore, molecular docking with 5HU9 showed a favorable binding energy of -12.66 kcal/mol.

Design and Synthesis of Symmetric Bis Schiff Base as Potential Anti-Cancer Agent and Selective Chemosensor for Sn (II) Detection

Gurjaspreet Singh¹ Anurag Dalal¹

Abstract

In this research article, we have successfully synthesized a symmetric bis Schiff Base compound and it was thoroughly characterized utilizing various spectroscopic techniques such as proton (¹H) NMR, carbon (¹³C) NMR, and mass spectrometry. Compound DSB was found to detect very selectivity Sn (II) as determined through UV-visible spectroscopy. The greater sensitivity of DSB toward Sn (II) was evident as the value of limit of detection (LOD) came out to be 82.31nM. Additionally, Job's plot supported 1:1stoichiometric binding of DSB and Sn (II). In addition to its sensing ability, the compound demonstrated noteworthy anti-cancer activity, evaluated through both in vitro experiments and molecular docking studies. This versatile strategy, encompassing Sn (II) detection, and anti-cancer potential, highlights the promise of this Symmetric bis Schiff Base chemosensor as an effective tool for applications in both environmental monitoring and biomedical research.

Fluorescent and Colorimetric Schiff Base Allied Organosilane-Iron Nanoparticles for Ni (II) Detection with Anticancer Potential Backed by Docking and DFT Investigations

Gurjaspreet Singh^{a*}, Priyanka^{a*}

^a*Department of chemistry, Panjab University, Chandigarh, 160014, India*

Email- kundup149@gmail.com

Abstract

In this present study, we report the design and synthesis of a new Schiff base-linked silane derivative (Compound 7) via an efficient click reaction, fully characterized by ¹H and ¹³C NMR, mass spectrometry, and FT- IR spectroscopy. The triazole moiety of Compound 7 exhibited exceptional selectivity for Ni (II), achieving impressively low detection limits (LOD) of 5.2×10^{-7} M (UV Vis) and 6.37×10^{-8} M (fluorescence). When immobilized on iron nanoparticles via the Stöber method, the resulting hybrid nanoparticle complex (H- NPs) demonstrated enhanced sensing performance, with LODs of 5.5×10^{-8} M (UV-Vis) and 1.68×10^{-8} M (fluorescence). The Stern-Volmer constants were determined to be 2.796×10^8 for Compound 7 and 8.15×10^7 for H- NPs, highlighting the superior quenching efficiency of the hybrid system. Beyond sensing, Compound 7 displayed significant anticancer activity against the HeLa cell line, while molecular docking studies revealed strong interactions with the 3HB4 protein (binding energy -8.04 kcal/mol), indicating a stable ligand-protein complex. Overall, these findings showcase Compound 7 as a versatile chemosensor with remarkable potential for Ni (II) detection in environmental, agricultural, and biomedical applications, combining sensitive detection, nanoparticle hybridization, and therapeutic potential in a single platform.

Investigating 1,2,3-Bistriazole-Functionalized Sn (II) Chemosensors for COX-2 Detection

Gurjaspreet Singh^a, Vinit Yadav^a

^aDepartment of Chemistry, Panjab University, Chandigarh, India

Email: vinit041997@gmail.com

Abstract

This article, describe the synthesis of 4-ethynylaniline derived 1,2,3- bis-triazole (**3**) via Cu(I) catalyzed click reaction and various spectroscopic methods such as FT-IR, TGA, ¹H and ¹³C NMR, and mass spectrometry are used for characterization. The probe **3** exhibits high sensitivity and selectivity to Sn (II) in UV-visible spectroscopy, with a limit of detection of 27μM and association constant 8.32 MM⁻¹, respectively. The synthetic sensor practical application was further explored by detecting Sn (II) in real sample analysis. The computational analysis using the DFT techniques shows the binding mechanism of sensor with Sn (II). Additionally, molecular docking investigation was conducted against cyclooxygenase-2 to shows the anti-inflammatory properties of the synthesized ligand having a good binding energy -10.26Kcal/mol.

Catalytic Applications of Mixed Transition Metal Oxides: A Review

Dr. Maqdoom Farooqui¹, Dr. Uzma Parveen Shaikh, Siddiqui Alima Fatema

Dr. Rafiq Zakaria College for Women

¹*Principal of Dr. Rafiq Zakaria College for Women*

alima15102000@gmail.com

Abstract

Mixed transition metal oxides (MTMOs) are an important class of heterogeneous catalysts, offering tunable electronic structures, redox flexibility, thermal stability, and strong synergistic metal–metal interactions. Incorporating two or more transition metals into a single oxide lattice creates cooperative active sites that often outperform single-metal oxides in catalytic activity, selectivity, and durability.

This review highlights spinel ferrites and multimetal nanocomposites, focusing on synthesis strategies such as co-precipitation, sol–gel, hydrothermal, and combustion methods. These approaches allow control over particle size, cation distribution, defect density, and surface characteristics, all of which strongly influence catalytic behavior. Structure–activity relationships are discussed, emphasizing the roles of mixed valence states, oxygen vacancies, and exposed crystal facets in enhancing redox cycling, oxygen mobility, and reactant adsorption.

MTMOs exhibit wide-ranging applications in oxidation and reduction reactions, multicomponent organic transformations, environmental remediation, and energy-related processes. Magnetically recoverable catalysts, including NiFe₂O₄ and Ag/Cu–Fe₂O₄ systems, demonstrate excellent recyclability and operational stability, supporting sustainable catalytic processes.

Mechanistic aspects such as electron transfer, lattice oxygen participation, and synergistic metal interactions are examined. Challenges related to selectivity, stability, and scalability are identified, along with future opportunities in rational catalyst design, defect engineering, and green synthesis. Overall, MTMOs provide a robust platform for high-performance and industrially relevant catalysis.

Keywords: Mixed transition metal oxides; spinel ferrites; nanocatalysis; heterogeneous catalysis; green chemistry; magnetic catalysts

Synthesis, Characterization and Non Isothermal Study of Bioactive transition Metal Complex, dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1- phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III)

Dr. Rasika C. Torane^{*1}, Dr. Gayatri S. Kamble²

^{1*}Dr. T. R. Ingale Research Laboratory, Department of Chemistry, Sir Parashurambhau College, Pune 411030, Maharashtra, India

² ABMSP's Anantrao Pawar College of Engineering and Research, Parvati, Pune 411009, Maharashtra, India

*Corresponding author e-mail: toranerasika@gmail.com

Abstract

The bioactive transition Metal Complex, dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1-phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III) (**Compound 1**) was synthesized and characterized by modern spectral techniques like Mass, IR, ESR etc. which are in accordance with Thermo Gravimetric Analysis (TG) and Differential Thermal Analysis (DTA). The synthesized **Compound 1** was tested for their antimicrobial and anthelmintic activities. The results obtained were in harmony as compared to standard. Results indicate activation energy is highest for third step decomposition of **Compound 1** (59.16 KJ/mol) Thermal and kinetic study of the compound confirms its stability. The yield of the product is good to excellent and purity is high. The study is having a great value as it is also confirmed by biological assays resembling antimicrobial and anthelmintic activities **Compound 1** has noticed potent antimicrobial and specifically anthelmintic activity. The results confirm the use of the synthesized bioactive ligand in pharmaceutical/ biochemical industries.

Keywords: Dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1- phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III) (**Compound 1**), ESR, TG, DTA and Bioactivities.

Assessing Spatio-Temporal Water Quality Variations in Rural and Urban Zones of Kishtwar Valley

Mohd Yaseen Sirwal^{1*}, Amit Kumar²

¹*PhD Scholar, Department of Chemistry, School of Applied Sciences, Shri Venkateshwara University, Gajraula, UP, India*

²*Assistant Professor, Department of Chemistry, School of Applied Sciences, Shri Venkateshwara University, Gajraula, UP, India*

E-mail: yaseensirwal@gmail.com

Abstract

The Kishtwar Valley in Jammu and Kashmir, India, presents complex hydro-ecological dynamics, with both urban and rural communities reliant on surface and groundwater resources. This study investigates spatial and temporal variations in water quality through seasonal sampling of physicochemical parameters, including pH, dissolved oxygen (DO), biological oxygen demand (BOD), chemical oxygen demand (COD), turbidity, nitrates, phosphates, and heavy metals. Comparative analysis revealed distinct pollution profiles: urban sources exhibited elevated organic and industrial contaminants, while rural sources were primarily influenced by agricultural runoff and seasonal erosion. Temporal assessment revealed deterioration during the summer months due to reduced dilution capacity, followed by improvement during the monsoon periods. The findings underscore the necessity of integrated water management strategies to mitigate pollution, protect public health, and sustain ecological integrity. Water quality evaluation was further supported by analysis of parameters such as colour, cation–anion composition, total suspended solids (TSS), and total dissolved solids (TDS).

Keywords: Analysis of variance, Water standards, Water Quality Index, Physico-chemical analysis, Spatio-temporal variation.

**Antimicrobial Schiff Base Polymers Containing Transition Metals:
Synthesis, Characterization and Their Applications**

Raza Rasool*

*Department of Chemistry, Gandhi Faiz-E-Aam College, Shahjahanpur, Uttar Pradesh,
India*

E-mail address: razarasool@gmail.com

Abstract

A new polymeric Schiff base was synthesized by the condensation of a monomeric Schiff base derived from acetophenone and diamine. Polymer-metal complexes were also synthesized by the reaction of the polymeric Schiff base with Mn (II), Co (II), Ni (II), Cu (II), and Zn (II) acetate. The polymeric Schiff base and its polymer-metal complexes were characterized with magnetic moment measurements, elemental analyses, and spectral techniques (infrared, ¹H-NMR, and ultraviolet-visible). The thermal behaviors of these coordination polymers were studied by thermogravimetric analysis in a nitrogen atmosphere up to 800°C. The thermal data revealed that all of the polymer-metal complexes showed higher thermal stabilities than the polymeric Schiff base and also ascribed that the Cu (II) polymer-metal complex showed better heat-resistant properties than the other polymer-metal complexes. All of the polymer-metal complexes demonstrated good antibacterial activity when tested against a variety of chosen pathogens using the agar well diffusion method. Among all of the complexes, the antimicrobial activity of the Cu (II) polymer-metal complex showed the highest inhibition

zone because of its higher stability constant and may be used in biomedical applications

Keywords: Polymer-metal complexes, Schiff base, Barbituric acid, Formaldehyde

Catalytic Applications of Mixed Transition Metal Oxides: A Review

Siddiqui Alima Fatema¹, Dr. Maqdoom Farooqui¹, Dr. Uzma Parveen Shaikh¹

¹Department of Chemistry Dr. Rafiq Zakaria College for Women

alima15102000@gmail.com

Abstract

Mixed transition metal oxides (MTMOs) are an important class of heterogeneous catalysts, offering tunable electronic structures, redox flexibility, thermal stability, and strong synergistic metal–metal interactions. Incorporating two or more transition metals into a single oxide lattice creates cooperative active sites that often outperform single-metal oxides in catalytic activity, selectivity, and durability. This review highlights spinel ferrites and multimetal nanocomposites, focusing on synthesis strategies such as co-precipitation, sol–gel, hydrothermal, and combustion methods. These approaches allow control over particle size, cation distribution, defect density, and surface characteristics, all of which strongly influence catalytic behavior. Structure–activity relationships are discussed, emphasizing the roles of mixed valence states, oxygen vacancies, and exposed crystal facets in enhancing redox cycling, oxygen mobility, and reactant adsorption. MTMOs exhibit wide-ranging applications in oxidation and reduction reactions, multicomponent organic transformations, environmental remediation, and energy-related processes. Magnetically recoverable catalysts, including NiFe_2O_4 and $\text{Ag/Cu-Fe}_3\text{O}_4$ systems, demonstrate excellent recyclability and operational stability, supporting sustainable catalytic processes. Mechanistic aspects such as electron transfer, lattice oxygen participation, and synergistic metal interactions are examined. Challenges related to selectivity, stability, and scalability is identified, along with future opportunities in rational catalyst design, defect engineering, and green synthesis. Overall, MTMOs provide a robust platform for high-performance and industrially relevant catalysis.

Keywords: Mixed transition metal oxides; spinel ferrites; nanocatalysis; heterogeneous catalysis; green chemistry; magnetic catalysts

Synthesis, Characterization, and Catalytic Studies of Transition Metal Complexes derived from heterocyclic ligand system

NazmaTabassum^{1,2}, Nouman², Suman Maji^{*1}, Rahisuddin^{*2}

¹*Department of Chemistry, Lovely Professional University, Phagwara (Punjab), India*

²*Molecular and Biophysical laboratory, Jamia Millia Islamia, New Delhi, India*

*Corresponding authors: suman.18432@lpu.co.in rahisuddin@jmi.ac.in

Abstract

Transition metal complexes containing heterocyclic ligands have attracted considerable interest in coordination chemistry due to their structural diversity and wide range of practical applications. In this study, a series of metal complexes was synthesized using a nitrogen-donor heterocyclic ligand exhibiting strong affinity toward various metal ions. The complexes were prepared through conventional reflux and precipitation methods, and their purity was confirmed by elemental analysis. Comprehensive structural characterization was performed using mass spectrometry, FT-IR, UV-Visible, EPR, and ¹H NMR spectroscopy. The synthesized complexes demonstrated promising potential in catalytic and biological applications, highlighting the functional versatility of heterocyclic ligand-based metal systems. Overall, the findings emphasize the role of heterocyclic ligands in tuning the physicochemical and biological properties of transition metal complexes, thereby supporting their prospective use in catalysis, medicinal chemistry, and the development of advanced functional materials.

Keywords: Transition metal complexes; Heterocyclic ligands; Nitrogen donor ligands; Coordination chemistry.

Synthesis and Characterization of HZSM-5 for Carbon-Carbon coupling Reactions

Harshada Katkar^{1,2}, Padekar Akshada^{1,2}, Dinesh Garud¹, Sudhir Arbuj^{2*}

²Center for materials for Electronics Technology (C-MET), Off Pashan road, Panchwati, Pune -411008 Maharashtra, India.

¹Department of Chemistry, Sir Parshurambhau College, Pune-411008, Maharashtra, India.

[E-mail-harshadakatkart2003@gmail.com](mailto:harshadakatkart2003@gmail.com), sudhir@cmet.gov.in

Abstract

The HZSM-5 catalyst is a highly acidic material known for having a significant number of strong Bronsted acid sites, which are primary active site for many catalyzed reactions. The strength and density of these acid sites can be tuned, but it generally exhibits high acidity compared to other zeolites. HZSM-5 Zeolites are also used in the methanol to aromatics reaction due to its unique pore structure, high specific surface area and proper acidity it is also used because of its Strong Bronsted acidity, High Thermal and Hydrothermal Stability, Petroleum Refining, Petrochemicals etc. Here in. we have prepared HZSM-5 catalyst using hydrothermal reaction technique and further heated at 1000°C for 6 h. The prepared catalyst was characterized with various spectroscopic techniques. The characterization of pyridine-IR shows the value between Lewis's acid and Bronsted acid sites. Different transition metals (Cu, Ni) will be loaded on to the catalyst and will be utilized for various carbon-carbon coupling reactions such as Suzuki, Heck, and Sonogashira cross-coupling reactions.

Keywords: HZSM-5 Zeolite, Hydrothermal Synthesis, Bronsted Acid, Lewis Acid.

Sustainable Green-Synthesized Nanomaterials for Enhanced Photocatalytic Degradation and Reusability in Wastewater Treatment

Rehana Farooq^{1*}

Department of Chemistry, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara-144411, Punjab, India.

^{*1} Corresponding Author: rehanafarooq117@gmail.com

Abstract

Endocrine-disrupting chemicals (EDCs) pose a major risk to the environment and public health when they contaminate water bodies, because of their durability and biological activity at trace levels. In this study, natural phytochemicals were used as stabilising and reducing agents to synthesise lead sulphide (PbS) quantum dots (QDs) in an environmentally friendly, plant-mediated manner. Sustainable nanotechnology principles are upheld by this environmentally friendly synthesis method, which does away with the necessity for dangerous chemicals. In order to confirm the quantum confinement properties, crystallinity, and nanoscale morphology of the resultant PbS QDs, they were extensively characterised using UV-Vis spectroscopy, photoluminescence (PL), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and transmission electron microscopy (TEM). Under visible light irradiation, the green-synthesised PbS QDs photocatalytic activity was evaluated for the degradation of model EDCs. Their effectiveness in breaking down model EDCs in the presence of light was assessed, showing great promise for environmental cleanup. This study highlights how green-synthesized PbS QDs may be used as an efficient and sustainable photocatalyst to remove newly discovered organic pollutants from wastewater.

Keywords: Quantum dots; Nano-technology; Green-synthesis; EDCs; Eco-friendly.

Photoactivated antibacterial activity of eco-friendly synthesized ZnO and ZnO/GO nanocomposites

Mohd Shahab^{1*}, Afroz Khan², Sameera Mujahid³, Asad U. Khan³ and Faiyazur Rahman¹

¹Department of Physics, Aligarh Muslim University, Aligarh, 202002, India

²Department of Bio-mechatronics Engineering, National Taiwan University, Taiwan

³Medical Microbiology and Molecular Biology Lab., Interdisciplinary Biotechnology Unit, Aligarh Muslim University, Aligarh, 202002, India

sameersayyed0101@gmail.com

Abstract

The emergence of antimicrobial resistance (AMR) among pathogens demands alternative therapeutic strategies beyond conventional antibiotics. Green nanotechnology provides dual advantages of sustainability and multifunctional antimicrobial agents to combat this concerning situation. In this context, zinc oxide nanoparticles (ZnO NPs) have been synthesized using lemon leaf extract as a reducing and capping agent, followed by their nanocomposite with graphene oxide (ZnO/GO). XRD spectra reveal the successful synthesis of ZnO and average crystallite sizes is increased from 14 nm to 19 nm. The reduction in optical band gap has been found in the case of ZnO/GO. These nanomaterials exhibit a potent antibacterial effect against *Escherichia coli*, displaying a lower minimum inhibitory concentration value of 250 µg/mL in the case of ZnO/GO, on the light irradiation. Moreover, in the presence of conventional LED light, both ZnO and ZnO/GO show excellent biofilm suppression at MIC levels. These results suggest that photoactivated ZnO/GO nanocomposite has superior antibacterial effects, which offers the development of safe and promising candidates for next-generation antimicrobial therapy.

Keywords: Zinc oxide, Green synthesis, Nanocomposite, Photoactivation, Minimum inhibitory concentration, Biofilm inhibition.

**A colorimetric and fluorometric sensor based on Thiazole Schiff base
use as a sensor for the detection of Fe³⁺ and Hg²⁺ ions**

Md. Shahid, Md. Zafer Alam, Salman A. Khan*

Corresponding Author: sahmad_phd@yahoo.co.in

Abstract

In this study, a novel thiazole-based Schiff base was designed, synthesized, and evaluated as a dual-mode colorimetric and fluorometric sensor for the selective detection of Fe³⁺ and Hg²⁺ ions. The probe exhibits pronounced optical changes upon interaction with these metal ions, including a distinct visible color transition and significant modulation in fluorescence intensity. The sensing behavior is attributed to strong coordination between the metal ions and the imine nitrogen and thiazole sulfur donor sites, resulting in alterations in intramolecular charge transfer (ICT) and possible chelation-enhanced or chelation-induced quenching effects. The sensor demonstrates high selectivity toward Fe³⁺ and Hg²⁺ over other competing metal ions, along with rapid response time and low detection limits. Spectroscopic studies using UV-Vis and fluorescence techniques confirm the formation of stable metal-ligand complexes. Furthermore, the probe shows good performance in aqueous or semi-aqueous media, indicating its practical applicability for environmental monitoring and potential biological analysis. These results highlight the effectiveness of thiazole Schiff base frameworks in developing simple, sensitive, and cost-effective optical chemosensors for toxic and environmentally relevant metal ions.

Keywords: Thiazole Schiff base; Dual-mode sensor; Colorimetric detection; Fluorometric sensing; Fe³⁺ion; Hg²⁺ ion; Intramolecular charge transfer; Metal-ligand coordination.

ICC/IBC/043

Synergistic Fe-Sn-Ni ternary metal oxide nanocomposite for Congo red adsorption: Synthesis, characterization, and Box-Behnken optimization**Zeeshan Ahamad***

Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Hyderabad, Telangana 500032, India
zahmad@manuu.edu.in

Abstract

A Fe-Sn-Ni ternary metal oxide nanocomposite (FSN-MONC) was synthesized via co-precipitation for the efficient adsorption of Congo Red (CR), an azo dye micropollutant known for persistence and toxicity. Structural and morphological analyses confirmed the irregular porous architecture and nanoscale particle aggregation, offering high surface area and abundant adsorption sites. Elemental mapping verified the homogeneous distribution of Fe, Sn, and Ni, while TEM and SAED confirmed highly crystalline nanoparticles (2–20 nm) with polycrystalline multi-phase structure. FTIR and XRD analyses identified metal–oxygen bonds and the coexistence of individual oxide phases (Fe₂O₃, SnO₂, NiO) and mixed phases (NiFe₂O₄ spinel). BET analysis revealed mesoporosity with a surface area of 243.78 m²/g. Adsorption studies achieved 87.92% CR removal under optimized conditions, fitting pseudo-second-order kinetics and Langmuir isotherm, consistent with chemisorption and monolayer coverage. Comparative analysis with literature data shows that FSN-MONC exhibits competitive performance (76.87mg/g). Box–Behnken Design systematically evaluated the effects of pH, adsorbent dosage, concentration, contact time, and temperature. The Fe-Sn-Ni combination imparted synergistic stability, surface activity, and adsorption capacity. FSN-MONC maintained excellent reusability over five cycles, underscoring its promise as a cost-effective, sustainable adsorbent for CR dye removal in wastewater treatment.

Keywords: Fe-Sn-Ni ternary metal oxide nanocomposite; Wastewater treatment; Azo dye adsorption; BBD-RSM optimization; Congo red removal.

Synthesis, Characterization and Non Isothermal Study of Bioactive transition Metal Complex, dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1- phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III)

Dr. Gayatri S. Kamble^{1*}, Dr. Rasika C. Torane²

^{1*}*ABMSP's Anantrao Pawar College of Engineering and Research, Parvati, Pune 411009, Maharashtra, India*

²*Department of Chemistry, S. P. College, Pune 411030, Maharashtra, India*

*Corresponding author e-mail: gayatri.kamble@abmspcorpune.org

Abstract

The bioactive transition Metal Complex, dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1- phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III) (Compound 1) was synthesized and characterized by modern spectral techniques like Mass, IR, ESR etc. which are in accordance with Thermo Gravimetric Analysis (TG) and Differential Thermal Analysis (DTA). The synthesized Compound 1 was tested for their antimicrobial and anthelmintic activities. The results obtained were in harmony as compared to standard. Results indicate activation energy is highest for third step decomposition of Compound 1 (59.16 KJ/mol) Thermal and kinetic study of the compound confirms its stability. The yield of the product is good to excellent and purity is high. The study is having a great value as it is also confirmed by biological assays resembling antimicrobial and anthelmintic activities Compound 1 has noticed potent antimicrobial and specifically anthelmintic activity. The results confirm the use of the synthesized bioactive ligand in pharmaceutical/ biochemical industries.

Keywords: dichloro [(E)-3-[(4''-dimethylamino) phenyl]-1- phenylprop-2-en-1-one] vanadium (III) di-μ-chloro aqua dichloro vanadium (III) (Compound 1), ESR, TG, DTA and Bioactivities.

ICC/PMC/045

Facile Microwave Assisted Synthesis of Covalent Triazine Framework for Exceptional Iodine Capture

Prashnasa Tiwari, Vivek Sharma

Department of Chemistry, Banasthali Vidyapith, Banasthali, Rajasthan-304022, India

*Email Id: prashnasatiwari1999@gmail.com

Abstract

To mitigate the environmental challenges posed by the emission of radiotoxic iodine from nuclear waste, there is an urgent need for the development of high-capacity, reusable adsorbents. However, the adsorbents reported so far do not have rapid enough iodine adsorption rates to be useful in emergency situations such as radioiodine leaking during a nuclear disaster. A simple microwave-assisted synthesis was employed to produce a nitrogen-rich covalent triazine framework (CTF-CB). This framework was then characterized with FTIR, XRD, SEM, BET and TGA, among other analytical techniques. CTF-CB was tested for its ability to adsorb iodine in both vapor and liquid phases. Results showed a 4.85 g g⁻¹ uptake of vapor iodine after 36 hours and a 96.37 mg g⁻¹ uptake of iodine from the liquid phase within 33 hours. CTF-CB can be reused by washing and heating it, and after five cycles, it still retains over 90.3% of its original iodine-capturing ability. This shows how structurally stable it is. Mechanisms and kinetic investigations indicate that the adsorption of iodine onto CTF-CB obeys the Langmuir isothermal adsorption model with a pseudo-second-order equation. The adsorption of iodine in both phases was confirmed using FTIR and Raman spectroscopy.

Effect of surfactants and polymers on the kinetics of Hydrolysis of Cefuroxime Axetil and the Resulting Degradation Pathways

Subiya Nasir

Kinetics and catalysis, Department of Applied Chemistry, Zakir Hussain College of Engineering and Technology, Aligarh Muslim University, Aligarh-202002

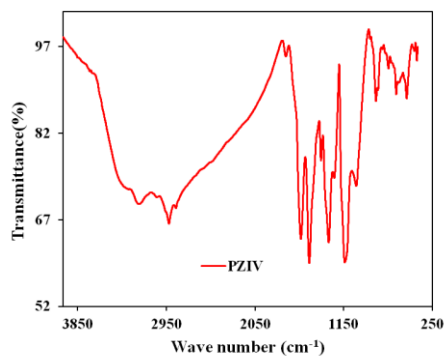
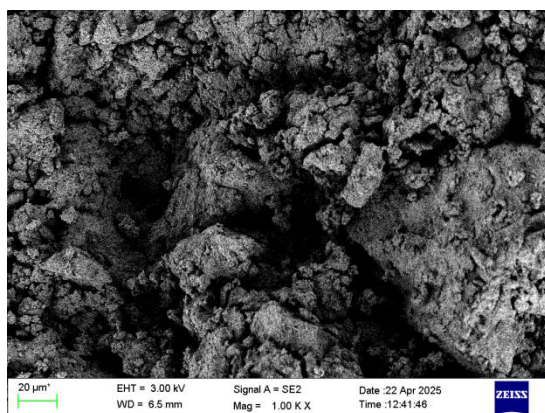
Abstract

Cefuroxime axetil, a second-generation oral cephalosporin antibiotic inhibits bacterial cell wall synthesis. As an ester prodrug, cefuroxime axetil is designed to enhance the oral bioavailability of cefuroxime. It exhibits limited aqueous solubility, however, the solubility is significantly improved under acidic or buffered conditions. The acid-catalyzed hydrolysis of the prodrug Cefuroxime Axetil (CFA) were quantitatively investigated in both homogeneous aqueous media and micro-heterogeneous structured media. The kinetics was studied in the presence of perchloric acid, which served as the proton source. To further study its solubility and dissolution profile in aqueous environments, surfactants such as sodium dodecyl sulphate (SDS) and Triton X-100 (TX100) were used. Water soluble polymers such as PEG and PVA are widely used in drug formulations and the variation in the rate of reaction is used to explain extent of association between the drug molecules and micelles/polymers. Both surfactants and certain polymers tend to self-assemble into micellar structures in aqueous solutions. Micelles of surfactants were found to inhibit the rate of hydrolysis. In contrast, water-soluble polymers accelerated the reaction rate at lower concentrations, producing a peak-like plot of the rate constant in the observed pseudo-first-order rate constant versus polymer concentration. Variation in the rate of reaction is used to explain extent of association between the drug molecules and micelles/polymers. The determination of binding constants provides critical insight into the stability and interaction mechanisms of cefuroxime axetil in surfactant/polymer media. The micellar rate constant values were treated using the pseudo phase model from which the binding constant (K_s) for CFA into the micellar pseudo-phase and the micellar rate constant values (k_m) were determined through the iterative method.

Synthesis, Characterization and Analytical applications of Polyaniline**Zr (IV) Iodovanadate nanocomposite****Md Naseem Ansari, Neha Maheen, Alimuddin[#] and Salman A. Khan****Department of Chemistry, Maulana Azad National Urdu University, Hyderabad**, [#]Correspondence Author e-mail adders: khanalim192@gmail.com (Alimuddin)[#],sahmad_phd@yahoo.co.in (Salman A Khan) ***Abstract**

In this study synthesis, characterization and analytical application of polyaniline zirconium (IV) iodovanadate, has been carried out. This material prepared by combining polyaniline gel with zirconium iodovanadate in different amounts to get the best polymer yield. Using UV-VIS spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), X-ray analysis, and X-ray Diffraction (XRD), the material has been characterized to understand its physical and chemical properties¹. The results show that polyaniline zirconium (IV) iodovanadate has good qualities for use as an electron exchanger in many fields. This work helps advance the development of better nanocomposite material showing how they might be useful in electronics and materials science.

Keywords: Synthesis, Characterization, Nanocomposite, Polyaniline, zirconium iodovanadate, Electron Exchanger



Development of Poly-O-toluidine Zr (IV) iodotungstate nanocomposite for removal of heavy metals from wastewater

Nuzhat Fatma, Alimuddin[#] and Salahuddin Syed^{*}

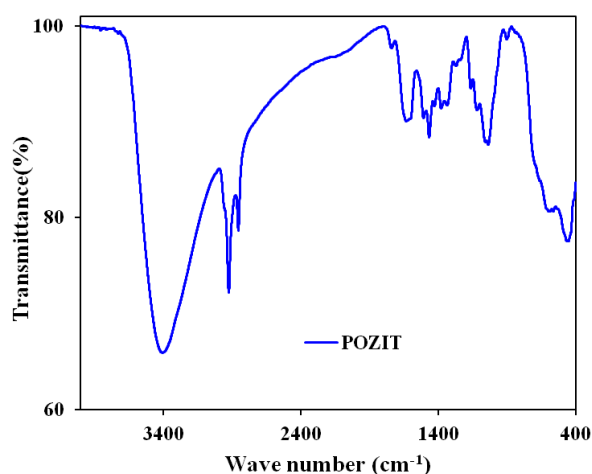
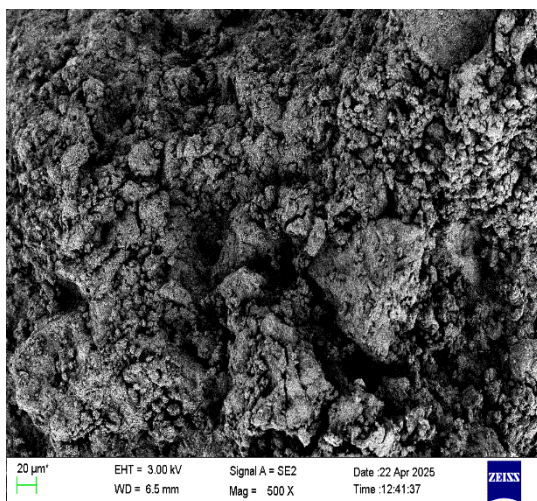
Department of Chemistry, Maulana Azad National Urdu University, Hyderabad

^{*}, [#]Correspondence authors E-mail address: alimuddin@manuu.edu.in

Abstract

In this study Development of Poly-O-toluidine zirconium (IV) iodotungustae, has been carried out. This material prepared by combining Poly-O-toluidine gel with zirconium iodotungustae in different amounts to get the best polymer yield. Using UV-VIS spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), X-ray analysis, and X-ray Diffraction (XRD), the material has been characterized to understand its physical and chemical properties. The results show that Poly-O-toluidine zirconium (IV) iodotungustae has good qualities for use as an electron exchanger in many fields. This work helps advance the development of better nanocomposite material showing how they might be useful in electronics and materials science.

Keywords: Synthesis, Characterization, Nanocomposite, Poly-O-toluidine, zirconium, iodotungustae, Electron Exchanger



Volatile Organic Compounds (Vocs) Sensing Studies On Electrically Conductive Polyaniline@Mos₂ Nanocomposites

Ruby Ahmed

Associate Professor Shibli National College, Azamgarh
ahmedruby1974@gmail.com

Abstract

Polyaniline (PANI) and molybdenum disulphide (MoS₂) were used to prepare nanocomposites by in-situ oxidative polymerization of acidified aniline in presence of dispersed MoS₂ in the reaction mixture. Electron Microscopy (SEM & TEM), Fourier Transform Infrared spectroscopy (FTIR), Ultraviolet-Visible (UV-Vis) spectroscopy, and X-ray diffraction (XRD) were used to characterize these nanocomposites. SEM micrographs showed that PANI is present on the layers of MoS₂ which were exfoliated during the preparation and the presence of MoS₂ is also confirmed by XRD peaks. The nanocomposites were studied for their electrical conductivity and stability of electrical conductivity in terms of d.c. electrical conductivity retention. Further, the nanocomposites were also studied for their sensing behavior towards alcohol, ketone, and aldehyde in ambient condition. These nanocomposites were found to be semiconducting, stable up to 100°C and exhibited good sensitivity towards volatile organic compounds (VOCs), viz. methanol, ethanol, formaldehyde, acetone and diethyl ether.

FTIR and Raman Spectroscopic Investigation of Alkaline Earth Modified Bismuth Borate Glasses

Meraj Madani¹, H. Aleem Basha¹, Md Shareefuddin²

¹*Department of Physics, Moulana Azad National Urdu University, 500032, Hyderabad, Telangana, India.*

²*Department of Physics, Osmania University, Hyderabad, 500007, Telangana, India.*

Email: merajmadani015@gmail.com

Abstract

The structural characteristics of alkaline earth oxide-modified bismuth borate (XBBC) glasses were examined utilising Fourier transform infrared (FTIR) and Raman spectroscopy. All glass samples produced with the standard melt-quenching method were verified to be amorphous, as demonstrated by X-ray diffraction examination. FTIR spectra showed distinct vibrational bands linked to borate structural units, affirming the presence of trigonal BO_3 and tetrahedral BO_4 groups within the glass matrix. Clear identification of different Bi-O vibrations of stretching and BiO_6 octahedral units indicates that Bi_2O_3 functions both as a network former and a modulator. Raman spectroscopy study further validated the FTIR results by identifying distinct bands associated with different borate groups and the emergence of non-bridging oxygens. Fluctuations in the locations and intensities of vibrational bands with various alkaline earth modifiers indicate alterations in network connection and structural disorder. The integrated FTIR and Raman investigations reveal that alkaline earth oxides strongly affect the borate glass network by facilitating the conversion of BO_3 to BO_4 and the creation of non-bridging oxygen, hence enhancing the understanding of the structural development in bismuth borate glass structures.

Keywords: FTIR spectroscopy, Raman spectroscopy, BO_3 and BO_4 units, non-bridging oxygen, Alkaline earth oxides

ICC/PMC/051

**L-Tryptophan and Gemini Surfactant-Based Fluorescent Ionic Liquid
Crystals for Dual Detection of Cu(II) and Ascorbic Acid in Real
Samples**

Muhammad Bilal Ahmad and Arifa Shaheen*

Department of Chemistry, Aligarh Muslim University, Aligarh, India
E-mail address: ashaheen.ch@amu.ac.in ; ahmadbilal4826@gmail.com

Abstract

Ionic liquid crystals (ILCs) constitute a promising and emerging subclass of ionic liquids, distinguished by their remarkable and versatile properties. This study investigates the potential of newly synthesized ILCs, featuring two imidazole rings connected by a three-carbon spacer and the groups of added amino acid L-Tryptophan (L-Trp). The ILCs were characterized using FT-IR, ¹H NMR, ¹³C NMR, mass spectral technique and XRD analysis. Circular dichroism (CD) spectroscopy was applied to examine the chiroptical properties of L-Trp and the synthesized ILCs, [C_nIm3OHImC_n]. 2Trp (n=12, 14, 16). Confocal laser scanning microscopy (CLSM) was utilized to study the morphology and luminescence of these ILCs. Three structurally distinct ionic liquid crystals (ILCs) with different alkyl chain lengths were rationally designed and synthesized, and their potential was explored as a novel fluorescent sensing platform for the detection of Cu²⁺ ions and L-ascorbic acid (AA). Practical applications were validated through the analysis of real-world samples like coffee, black tea, green tea and tomato, pomegranate, orange, human blood serum (HBS) respectively. This study highlights the potential of gemini surfactant based ILCs as efficient fluorescent sensors for Cu²⁺ and AA detection in real sample assessments.

ICC/PMC/052

Synthesis of Rice Husk-Based Green Biodegradable Composites Reinforced with *Yucca filamentosa* Fiber and Its Graft Copolymers

Surjit Kaur* and Mithu Maiti Jana

**Department of Physical Sciences, Assistant Professor, Sant Baba Bhag Singh University,
Jalandhar, Punjab, India*

*Department of Physical Sciences, Associate Professor, Sant Baba Bhag Singh University,
Jalandhar, Punjab, India*

surjitkaur1089@gmail.com

Abstract

The increasing demand for eco-friendly materials has encouraged the development and design of biodegradable composite materials. The utilization of low-value agricultural waste in composite fabrication plays a significant role in reducing the environmental problems associated with petroleum-based polymers. Green biodegradable composites derived from rice husk waste can effectively replace petro-based fiber composites due to their excellent physicochemical properties, low cost, and low density. Presently, we have developed a cross-linked rice husk matrix-based green biodegradable composites reinforced with natural *Yucca filamentosa* fiber, and its different graft copolymers. Green biodegradable composite materials have been developed by many researchers, but there have been no reports of such composites reinforced with different graft copolymers. Therefore, we have developed rice husk-based green biodegradable composites reinforced with different graft copolymers of *Yucca filamentosa* fibers by the grafting technique. With the help of graft copolymerization, we can improve the different physico-chemical and thermal properties of various graft copolymers and green biodegradable composites.

Keywords: Natural *Yucca filamentosa* fiber, ethylmethacrylate, graft copolymer, rice husk, green biodegradable composites

ICC/PMC/053

**Green Photodegradation of Xylenol Orange Dye under Solar Light
Using Metal and Non-Metal Modified ZnO-G-C₃N₄ Nanocomposites
Synthesized by an Ultrasound-Assisted Route**

Kapilkumar Dattatraya Randhir

*Research Scholar Department of Chemistry, M.S.G.College Malegaon Camp, Affiliated to
SPPU Pune University*

E-mail: kapil.randhir@yahoo.com

Abstract

A cost-effective and rapid synthesis of bismuth- and cobalt-modified ZnO-GCN nanocomposites was successfully accomplished through a simple hydrothermal co-precipitation route, followed by an ultrasound-assisted hydrothermal process for composite formation. The prepared nanocomposites were systematically characterized using SEM, TEM, XRD, EDAX, FT-IR, and UV-DRS techniques.

Their photocatalytic efficiency was assessed for wastewater treatment through the solar-driven photodegradation of xylenol orange dye. Characterization results confirmed the successful incorporation of dopants with high phase purity and well-defined particle morphology. The nanocomposites exhibited enhanced photocatalytic activity under environmentally benign solar irradiation. Optimal degradation performance was achieved at a catalyst dosage of 1.5 g L⁻¹, dye concentration of 10 mg L⁻¹, pH 8, and 180 min of solar exposure. These findings demonstrate the excellent potential of the synthesized nanocomposites for efficient organic dye degradation.

Keywords: Photocatalysis; xylenol orange; nanocomposite; carcinogen.

Recent Advancements in n-i-p Perovskites Solar Cells**Sarvani Jowhar Khanam***Department of Chemistry and Earth Science, Qatar University, Doha, Qatar***Abstract**

Perovskites solar cells (PSCs) have emerged as a highly attractive class of semiconductor materials for photovoltaics because of their superior optoelectronic properties, tunable bandgap and low defect density compared to conventional materials.¹ Some of recent applications of metal halide perovskite (MHP) materials, including solar cells,² light-emitting diodes (LEDs), and phototransistors. A key advantage of 2D MHPs lies in their inherent stability and tunable crystal thickness, a feature absent in 3D perovskites. This unique characteristic opens exciting possibilities for device design and performance optimization. This paper aims to exploit recent advancements in n-i-p PSCs for developing high-performance photovoltaic devices. We will explore various device architectures to optimize performance and functionality.

Keywords: Perovskites solar cells, metal halide perovskite, light-emitting diodes, phototransistors and Photovoltaics.

ICC/PMC/055

Zwitter ionic Surfactants under the impact of short chain Surfactants**Mohammad Shafi Sheikh^a, Nusrat Shafi^{b*}**^aDept of School Education, BHSS Beerwah, J&K India^bDept of Higher Education, HKM GDC Eidgah, Srinagar, J&K India[*nusratshafi075@gmail.com](mailto:nusratshafi075@gmail.com)**Abstract**

Addition of anionic Short chain Surfactants decreases the critical micelle concentration (cmc) of Zwitterionic surfactants than cationic one. Interaction Parameter (β) measuring the nature of interaction between monomers in the micelle were found to be negative which implies attractive interaction within the micelle. These short chain surfactants with hydrophobic moiety and hydrophilic tails interact with micellar surface by reducing surface charge and by enhancing hydrophobic interaction. Free energy micellization is negative which is followed by large negative value of ΔH^0 (enthalpy of micellization). Doping of Surfactants with short chain Surfactants (Organic salts) refine the solubilizing power, viscosity etc., acquire relevance in drug permeation and delivery due to moderate toxicity.

Keywords: Zwitterionic Surfactants, Short chain Surfactants, micelle, Interaction Parameter, free energy.

ICC/PMC/056

Synthesis, Characterization, and Optoelectronic Studies of Schiff Base Lanthanide (III) Complexes

Chandan Kumar Singh and Angad Kumar Singh

*Department of Chemistry, School of Physical and Chemical Science Central University of
South Bihar, Gaya Ji-824236*

Corresponding Author Email: chandankr994@gmail.com, angad@cusb.ac.in

Abstract

A novel multidentate Schiff base ligand, H-L, was synthesized via the condensation reaction of 5-bromosalicylaldehyde with triethylenetetramine. Five lanthanide (III) complexes of this ligand were subsequently prepared and systematically characterized. The structural features and coordination behaviour of the ligand and its metal complexes were elucidated using a combination of FT-IR, NMR, UV–Vis, TGA, CHNS elemental analysis, and molar conductance studies. In addition, density functional theory (DFT) calculations were employed to optimize the geometries of both the free ligand and its lanthanide complexes, providing insights into their electronic structures. The electronic absorption characteristics and photonic responses were further examined to evaluate their optoelectronic potential. The results demonstrate that the incorporation of lanthanide ions into the Schiff base framework significantly influences the optical and electronic properties, highlighting their promise for advanced optical and photonic material applications.

Keywords: Schiff base, Lanthanides complex, Crystal XRD, Optoelectronics.

Vegetable Oil Based Eco-Friendly Biopolymers**Mohd Amil Usmani***Department of Chemistry, Gandhi Faiz-e-Aam College (Affiliated to MJP Rohilkhand University, Bareilly), Shahjahanpur, U.P., India***Abstract**

Practicable materials derived from natural and renewable spectrums are demanded nowadays due to both environmental and ecological factors. These act also a move towards sustainability, an ethical and moral responsibility of academicians and scientific researchers. Numerous bio-based starting materials bestowed by nature have been utilized as precursors for different products of enormous potential. Among them, vegetable oils generally liquid at room temperature having inbuilt various functionalities provide avenues for suitable derivatization as per requirements. The presence of unsaturations, triglyceride linkages, epoxies, hydroxyl groups enable them to undergo into various chemical transformations. Numerous low molecular weight polymeric recipes like polyesters, polyesteramides, polyurethanes, polyetheramides, and many others have been developed and successfully utilized in different industrial arena from small household articles to magnificent machines. Furthermore, incorporation of different monomers and other reagents have been carried out to improve the performance of the final product. In the present communication, efforts have been made to enlighten the physico-chemical properties of vegetable oil and different state of art strategies of formulation of different valuable products, as well as future prospects in this line.

Keywords: Triglycerides, Physico-chemical, Polyesteramides, Polyurethanes.

ICC/PMC/058

A Non-Invasive, Conductivity-Based Sensing Principle for Automated Grading of Egg Fertility and Freshness Using Terahertz Spectroscopy

Juveria Iram^{1*}, Aleem Basha, Kaleem Ahmed Jaleeli²

¹*Department of Physics, Maulana Azad National Urdu University, Hyderabad, India, 500032*

²*Department of Physics, Nizam College, Osmania University, Hyderabad, India, 500001*
Corresponding author email: iramjuveria@gmail.com

Abstract

The absence of rapid, non-destructive, and objective methods for egg quality grading represents a significant bottleneck in industrial food processing. Here, we introduce a novel sensing principle based on terahertz-derived electrical conductivity (σ) for the automated classification of egg fertility and freshness. Using reflection-mode terahertz time-domain spectroscopy (THz-TDS), we demonstrate that fertile eggs exhibit a significant and consistent reduction in electrical conductivity (from ~ 0.70 S/m to ~ 0.55 S/m) within 24 hours of incubation. This reduction correlates with physiological water and ion mobilization during early embryonic development, quantified as a decrease in estimated shell hydration from 38.5% to 29.6%. The conductivity signal remains stable across a broad frequency range (0.1–3.0 THz), confirming its robustness for high-throughput applications. We propose that this conductivity-based biomarker can be implemented at GHz frequencies for inline, non-contact grading systems, offering a scalable engineering solution to reduce waste and enhance automation in egg processing and hatchery operations.

Keywords: Egg Fertility, Non-destructive Testing, Electrical Conductivity, Water content, Food Quality, Biomarker.

Preparation of activated nano carbon from *Leucaena leucocephala* biomass for dye removal from wastewater

Deepika Nanaware^a, Dr. K. S. Munde^b

^aAnatrao Thopate College and research centre bhor pune maharashtra ,412206 Tal - Bhor dist-Pune, maharashtra 412206

E-mail: deepikananaware17@gmail.com

^bAnatrao Thopate College and research centre bhor pune maharashtra ,412206 Tal - Bhor dist-Pune, maharashtra 412206

E-mail: mundhekavita@gmail.com

Abstract

Synthetic dyes are used in many industries, and upon mixing with wastewater, they result in serious environmental problems. These dyes do not easily degrade in nature, and once they have entered water bodies, they are very hard to remove. They can reduce sunlight in water, harm aquatic plants and animals, and even cause toxic or cancer-causing effects. Activated carbon is being prepared in this work from the biomass of a common and fast-growing plant, *Leucaena leucocephala*. Plant material was washed to remove dirt, dried well, and then heated at high temperature to form char. This char was treated with chemicals such as H₂SO₄, KOH, and NaOH to increase the number of pores which helps for better dye removal. The material was then heated again after this chemical activation to produce highly porous activated nano carbon. This activated carbon will be tested to see how well it can remove dyes from wastewater. They will study how pH, contact time, amount of carbon used, and starting dye concentration affect the dye removal process. Early observations indicated that activated carbon mixes well in dye solutions and may have good adsorption ability. The present work serves as a simple, inexpensive, and eco-friendly method for the conversion of natural plant biomass into activated carbon for cleaning wastewater. The usage of *Leucaena leucocephala* would provide a very cheap and renewable source of the raw material. Further experiments shall be completed to check the efficiency of the dye removal and compare with results of other adsorbents.

Keywords: Activated carbon; Biomass; *Leucaena leucocephala*; Dye removal; Wastewater treatment; Batch process.

Synthesis and Applications of C₁₂-E2O2-C₁₂ Assisted Bioactive Silver Nanoparticles

Saif Uz Zafar, Mohd. Akram

Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India

E-mail: Saifuzzafar9@gmail.com

Abstract

Gemini-surfactant-stabilized silver nanoparticles (C₁₂-E2O2-C₁₂-AgNPs) were synthesized using a diester-linked cationic gemini surfactant, C₁₂-E2O2-C₁₂, which served as an effective capping and stabilizing agent. The characterization of C₁₂-E2O2-C₁₂-AgNPs was systematically investigated using UV–visible spectroscopy, XRD, FT-IR, HR-TEM, SEM, EDX, DLS, zeta potential measurements, and XPS. The antibacterial efficacy of C₁₂-E2O2-C₁₂-AgNPs was evaluated against *S. aureus*, *E. coli*, and *P. aeruginosa*. A comparative investigation was carried out to understand the interaction behavior of C₁₂-E2O2-C₁₂-AgNPs with bovine serum albumin (BSA) and porcine serum albumin (PSA), representing a transport protein and a disease-related biomarker protein, respectively. Although both proteins exhibited appreciable affinity toward the prepared AgNPs, notable differences in binding strength, conformational response, and interaction mechanism were observed. PSA demonstrated a relatively stronger binding affinity toward C₁₂-E2O2-C₁₂ compared to BSA, as evidenced by higher binding constants obtained from UV–visible and fluorescence spectroscopic analyses. Fluorescence quenching studies revealed that PSA underwent more pronounced quenching upon nanoparticle addition, indicating closer proximity and stronger interaction between the C₁₂-E2O2-C₁₂-AgNPs and PSA fluorophores. FT-IR and circular dichroism measurements indicated a significant reduction in the α -helical content of PSA, confirming notable conformational rearrangements induced by nanoparticle binding. In contrast, BSA exhibited relatively less changes in its secondary structure as compared to PSA. These results highlight their potential as a suitable platform for applications in diagnostics, drug delivery, and nanobiotechnology, thus justifying further in-depth investigation.

**Molecular Interactions of Paracetamol with Ionic Surfactants: A
Conductometric Study of CTAB and SDS in Aqueous Media**

Zakiya Tazeen^a, Md. Shadab^a, Syed Salahuddin^a, Shahjahan^{a,*}

^a*Department of Chemistry, School of Sciences, Maulana Azad National Urdu University,
Gachibowli, Hyderabad-500032*

*Corresponding author: shahjahan23@gmail.com

Abstract

The present study investigates the molecular interactions between the common analgesic paracetamol (PCM) and two ionic surfactants, cetyltrimethylammonium bromide (CTAB) and sodium dodecyl sulfate (SDS), in an aqueous medium. Paracetamol, at a fixed concentration of 0.1 M, is used as the solvent for the preparation of 0.0001 M, 0.0003 M, 0.0005 M, 0.0007 M, and 0.0010 M solutions of CTAB and SDS, respectively. The conductometric method is used to examine the micellization behaviour of these surfactant systems over a range of temperatures (298 K, 303 K, 308 K, and 313 K). The present study investigates the effect of paracetamol on the properties of surfactants, such as the critical micelle concentration (CMC), and derives associated thermodynamic parameters.

Keywords: Paracetamol, Ionic Surfactants, Micellization, Conductometry, Molecular Interactions.

ICC/PMC/062

Physicochemical studies on interactions between bio surfactants derived from natural oil with pesticides

Nizamul Haque Ansari

Basic & Applied Scientific Research Center (BASRC), Environmental and Sustainable Unit, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam 31441, Saudi Arabia.

Abstract

Surfactants have lot of application in industry and are mostly petroleum-based. Petroleum-based surfactants, which are cost-effective and efficient for industrial use, have significant environmental and ecological risks as they are non-biodegradable in nature, and they have high toxicity. To overcome this problem, there is a growing trend toward environmentally friendly technologies, which has led to the search for biodegradable natural surfactant known as bio-surfactants. These bio-surfactant are produced by bacteria, fungi, yeast, and natural oil and have low toxicity, and are eco-friendly. Bio-surfactants can be used in agriculture for soil remediation, pathogen elimination, and improving soil quality. They are also important constituents of most pesticides formulations since they may function as spreaders, stickers, anti-foamers, compatibility agents or activators. They can also work as adjuvants with pesticides. Physicochemical studies provide valuable information regarding solute-solvent interactions present between surfactant and pesticides. So keeping these in mind, in the present study we have discussed physicochemical studies on interaction of bio surfactants derived from natural oil with pesticides.

Keywords: Surfactants, Bio surfactants, Adjuvant, Solute- solvent interaction and Biodegradability.

ICC/PMC/063

Investigation of Interactions of Proline with Non-aqueous SDS, CTAB and TX-100 at 298.15 K, 303.15 K, 308.15 K, and 313.15 K

Anwar Ali^a and Shahjahan^{b,*}

^aDepartment of Chemistry, Jamia Millia Islamia (Central University), New Delhi - 110025

^bDepartment of Chemistry, School of Sciences, Maulana Azad National Urdu University, Gachibowli, Hyderabad -500032

*Corresponding author: shahjahan23@gmail.com

Abstract

In the present investigation, volumetric and viscometric measurements were carried out to study the interactions between the amino acid, proline (Pro) and non-aqueous, formamide (FA) -based surfactant systems at 298.15 K, 303.15 K, 308.15 K, and 313.15 K. The anionic surfactant, sodium dodecyl sulfate (SDS), cationic, cetyltrimethylammonium bromide and non-ionic TX-100 were employed. The volumetric study results the strong interactions of Pro in SDS+FA/ CTAB+FA/ TX-100+FA systems with ion–ion and ion–hydrophilic interactions dominating over hydrophobic interactions in all three systems. Furthermore, Pro behaves as a structure-maker in these non-aqueous surfactant systems. The viscometric measurements support trends observed from volumetric parameters, except in the TX-100 system where solute–solute (Pro–Pro) interactions appear more pronounced than solute–solvent (Pro-surfactant/FA) interactions. Overall, the volumetric and viscometric studies show good agreement.

Keywords: Proline, Surfactants, Nonaqueous Solvents, Molecular Interactions.

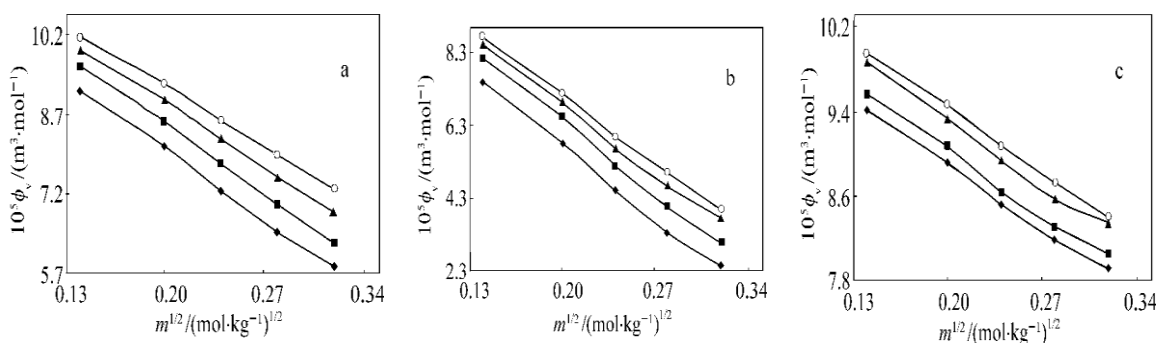


Fig. 1. Plots of apparent molar volumes vs concentration of Pro in (a) SDS+FA, (b) CTAB+FA, and (c) TX100+Fa at (♦) 298.15, (■) 303.15, (▲) 308.15, and (○) 313.15 K.

A Comprehensive Review of Mercury (II) Ion Detection via Rhodamine Schiff Base Fluorescent Sensors

Sadiya Mushtaq¹, Tayyaba Naaz², Md. Mohasin², Prof. Salman Khan^{2*}

¹*Department of Chemistry, Anwarul Uloom College, Hyderabad, Telangana, India*

²*Department of Chemistry, School of Sciences, Maulana Azad National Urdu University, Hyderabad 500032, Telangana, India*

*Correspondence Author e-mail adders: sahmad_phd@yahoo.co.in (S. A. Khan)

Abstract

Mercury (Hg^{2+}) contamination poses a critical global threat due to its extreme toxicity, persistence, and bioaccumulative nature, necessitating the development of rapid, sensitive, and cost-effective detection strategies. Among various chemical sensing platforms, rhodamine-based Schiff bases have emerged as highly efficient fluorescent chemosensors owing to their simple synthesis, excellent photophysical properties, and distinctive spirolactam ring-opening mechanism, which enables strong “off–on” fluorescence and visible colorimetric responses upon Hg^{2+} binding. This review comprehensively summarizes the progress in rhodamine Schiff base sensors reported between 2015 and 2025, highlighting their structural diversity, sensing mechanisms, analytical performance, and applications in environmental and biological systems. Most rhodamine Schiff base probes exhibit remarkable selectivity toward Hg^{2+} , low detection limits reaching nanomolar or sub-nanomolar levels, rapid response times, and compatibility with aqueous media. Several probes further show promising performance in real-sample analysis, portable test strips, and cellular/zebrafish imaging. By consolidating synthetic strategies, sensing pathways, and practical applications, this review provides an essential foundation for designing next-generation rhodamine-based Schiff base sensors for efficient mercury monitoring in environmental and biological contexts.

Keywords: Rhodamine; Schiff Base; Fluorescent; Chemosensor; Mercury

ICC/PMC/065

Eco-Friendly Biosynthesis of Cobalt Oxide Nanoparticles Mediated by *Boerhavia diffusa* and Evaluation of Their Antimicrobial Potential

Chitra Devi Palanichamy^{1*}, Lakshmi Prabha Krishnamoorthy², Maadathi Sivakumar³, Prabaharan Panchanathan⁴, Devi Selvaraj⁵, Sivasankari Gnanam⁶, Boobalan Sivalingam⁷ and Shenbagam Kanagaraj⁸

^{1*} Assistant professor of Chemistry, OASYS Institute of Technology, Pulivalam, Trichy-621006

² Assistant Professor of Chemistry, Government Arts College, Tiruchirappalli-620 022

³ Research Scholar, Department of Chemistry, Cauvery College for Women (A), Tiruchirappalli-18.

Affiliated to Bharathidasan University

⁴ Lecturer, Department of Chemistry, Government Polytechnic College, Trichy-620022.

⁷ Associate Professor of Chemistry, Indra Ganesan College of Engineering, Manikandam, Tiruchirappalli-620012

^{5,6,8} Assistant Professor of Chemistry, Cauvery College for Women (A), Trichy-18.

^{1*} corresponding author email: chitraparthi14@gmail.com

Abstract

In this study, an environmentally benign and cost-effective method for the green synthesis of cobalt oxide nanoparticles (Co-O-NPs) using *Boerhavia diffusa* leaf extract is reported, followed by an evaluation of their antimicrobial activity. The phytochemical constituents present in the leaf extract serve as natural reducing, capping, and stabilizing agents during nanoparticle formation. The antimicrobial activity of the synthesized Co-O-NPs was investigated against selected pathogenic bacterial and fungal strains using standard in vitro assays. The results revealed notable antimicrobial efficacy, which can be attributed to the nanoscale size, high surface reactivity, and the synergistic interaction between cobalt oxide nanoparticles and bioactive compounds derived from *Boerhavia diffusa*. The findings suggest that green-synthesized cobalt oxide nanoparticles hold promise as effective antimicrobial agents with potential applications in biomedical and pharmaceutical fields.

Keywords: Cobalt oxide nanoparticles; Green synthesis; *Boerhavia diffusa*; Leaf extract; Antimicrobial activity; Plant-mediated synthesis; Nanotechnology; Nanomedicine

Role of Gemini Surfactants in Green Chemistry and their Interfacial behavior in the presence of additives

Riyaj Mohammad

Department of Chemistry, Gandhi Faiz-E-Aam P. G. College (Affiliated to M.J.P. Rohilkhand University, Bareilly), Shahjahanpur-242001, U.P., India

E-mail: riyaz138@gmail.com

Abstract

It has been known for many years that amphiphiles can form aggregates of varying sizes and shapes like spherical micelles, worm-like micelles, bilayers and reverse micelles with properties different from those of unassembled molecules. This property of self-aggregation forms the basis of many biological and household applications. A long list of amphiphiles exists. However, compared to the conventional single head/single chain amphiphiles, the last decade has witnessed emergence of a new class of amphiphiles called gemini or 'next generation' surfactants. Gemini surfactants are an interesting class of surfactants whose ability to strongly reduce surface tension makes them potentially useful as detergents. They are made up of two amphiphilic moieties connected by a spacer group of varied nature at or near the polar head groups. Gemini surfactants are a big deal in green chemistry because they do more with less, which is basically the green chemistry motto. Many Gemini surfactants are being designed with biocompatible or biodegradable head groups. Green chemistry research is actively focused on bio-based Gemini surfactants made from sugars, amino acids, or fatty acids. Mixed micellization and interfacial properties of cationic gemini surfactant hexanediyl-1,6-bis(dimethyldodecylammonium bromide) have been studied in the presence and absence of various alcohols and related parameters have been calculated. The aim of this study is to find the effect of different alcohols on gemini surfactant, furthermore they can be used again for drug encapsulation and delivery. Also, amines are very good co-surfactants and they can be used in microemulsion formulation.

Keywords: Alcohols, gemini surfactant, mixed micelle.

Eco-friendly synthesis of highly efficient Nickel-doped Fe₂O₃-g-C₃N₄ photocatalyst for solar-driven degradation of anionic dyes in water

Vishal Pardeshia, Vijay Naukudkara

^aResearch Centre, KTHM College, Nashik, India-422002

Abstract

Water pollution poses a major threat due to the uncontrolled discharge of textile dyes and chemicals. This work reports the development of a cost-effective photocatalyst utilizing eco-friendly sunlight for waste water remediation. 5% Ni-doped Fe₂O₃-g-C₃N₄ nanocomposite was synthesized via an ultrasound-assisted hydrothermal co-precipitation method to degrade thymol blue dye. Comprehensive characterization using FTIR, XRD, SEM, EDS, TEM, and UV-DRS confirmed the successful synthesis and enhanced optical features of the material. The nanocomposite exhibited a reduced band gap of 3.6eV, enabling improved visible-light absorption. Under optimal conditions, it achieved 98% dye degradation within 90 minutes. The degradation process followed first-order kinetics with a rate constant of 0.01980 min⁻¹. Influence of parameters such as pH, catalyst dosage, and reusability were systematically evaluated.

Scavenger experiments identified the predominant reactive species responsible for dye degradation. Overall, the study demonstrates a sustainable and highly efficient approach for anionic dye removal from water.

Keywords: ultrasound, Photocatalysis, graphitic carbon nitride, doping, nanocomposites, Thymol blue

Multifunctional Ni-Al/Chitosan Composite Spheres for Integrated Antibacterial and Photocatalytic Water Treatment

Md Sameer Ahmed^{1*}, Anjum Begum²

¹Associate Professor, Science & Humanities Department, Lords Institute of Engineering and Technology, Hyderabad, India

²Assistant Professor, Science & Humanities Department, Lords Institute of Engineering and Technology, Hyderabad, India

*Corresponding Author: sameer.ahmed2525@gmail.com

Abstract

Ni-Al embedded chitosan nanocomposite spheres (CS-NC sphere) and sheets (CS-NC sheet) were synthesized via a simple embedding method and characterized using FE-SEM, EDS, XRD, and FTIR analyses. The prepared materials were evaluated for the removal of organic dyes, including acridine orange, cresyl blue, and methyl orange, from aqueous solutions through adsorption-assisted photocatalysis. Both nanocomposites exhibited enhanced adsorption and photocatalytic performance compared to pristine chitosan. Among the tested dyes, methyl orange showed selective and higher removal efficiency. Notably, CS-NC sphere demonstrated superior performance over CS-NC sheet, particularly under light irradiation, confirming that dye removal occurred predominantly through adsorption-coupled photodegradation. Furthermore, CS-NC sphere exhibited significant antibacterial activity against *Micrococcus luteus*, highlighting its multifunctional behavior. The combined adsorption, photocatalytic, and antibacterial properties suggest that these Ni-Al/chitosan nanocomposite spheres are promising, eco-friendly materials for wastewater treatment and environmental remediation applications.

Keywords: Ni-Al/chitosan nanocomposite, CS-NC sheet, *Micrococcus luteus*, Antibacterial activity, Photocatalysis

Electrochemical Sensing of Ascorbic Acid Using Silica-Coated ZnO Nanospheres on Gold Electrode

Anjum Begum¹, Md Sameer Ahmed²

¹Assistant Professor, Department of Chemistry, Lords Institute of Engineering and Technology, Hyderabad, India

²Associate Professor, Department of Chemistry, Lords Institute of Engineering and Technology, Hyderabad, India

Email: anjumbegum024@gmail.com¹, sameer.ahmed2525@gmail.com²

Correspondence: anjumbegum024@gmail.com¹

Abstract

Reliable and highly sensitive electrochemical detection of biomolecules is essential for biomedical diagnostics, food quality monitoring, and environmental analysis. This study presents the synthesis of core-shell ZnO@SiO₂ nanospheres and their application in amperometric sensing of ascorbic acid (AA). ZnO nanospheres were prepared through a hydrothermal route and subsequently coated with a silica shell using a sol-gel process to improve stability and interfacial electron transfer. The nanostructures were deposited onto a gold electrode to fabricate an electrochemical sensing platform. Comparative electrochemical measurements revealed that the ZnO@SiO₂ modified electrode exhibits significantly enhanced response toward AA compared with uncoated ZnO. The fabricated sensor demonstrated high sensitivity, a broad linear detection range, and a low detection limit, confirming the effectiveness of the core-shell architecture. Scanrate optimization further improved analytical performance. The proposed nanomaterialbased sensing strategy shows strong potential for accurate and rapid determination of ascorbic acid in real samples.

Keywords: Ascorbic acid sensing; Amperometric sensor; ZnO@SiO₂ Nano spheres; Gold electrode modification; Core-shell nanostructures; Electrochemical detection.

ICC/PMC/070

Synthesis of thiophene based chalcone derivative as selective fluorescent chemosensor for the detection of Fe³⁺ metal ions

Md. Mohasin, Salman A. Khan*

Department of Chemistry, School of Sciences, Maulana Azad National Urdu University,
Hyderabad 500032, Telangana, India

*Correspondence Author e-mail adders: sahmad_phd@yahoo.co.in (S. A. Khan)

Abstract

A thiophene-based aldol-derived chalcone derivative was successfully designed, synthesized, and structurally characterized using ¹H NMR, ¹³C NMR, FT-IR, and HR-MS spectroscopic techniques. The solvatochromic behavior of the chalcone derivative was systematically investigated in nonpolar, polar aprotic, and polar protic solvents. Its photophysical properties were evaluated through key parameters including Stokes shift, dipole moment, oscillator strength, and fluorescence quantum yield/quenching efficiency in different solvent environments. Furthermore, the synthesized chalcone derivative was explored as a fluorescent chemosensor for metal ions. Among the various tested cations, the chalcone derivative exhibited a highly selective fluorescence quenching response toward Fe³⁺ ions in aqueous dimethylformamide (DMF). The fluorescence intensity decreased progressively with increasing Fe³⁺ concentration, demonstrating a clear concentration-dependent quenching behavior characteristic of an “on-off” sensing mechanism. The binding interaction between the chalcone derivative and Fe³⁺ was determined to follow a 1:1 stoichiometric ratio, as confirmed by Benesi-Hildebrand analysis, Stern-Volmer plots, and Job’s method of continuous variation.

Keywords: Thiophene; chalcone; solvatochromic; fluorescent; Fe³⁺; chemosensor

ICC/PMC/071

A Non-Invasive, Conductivity-Based Sensing Principle for Automated Grading of Egg Fertility and Freshness Using Terahertz Spectroscopy

Juveria Iram* Aleem Basha, Kaleem Ahmed Jaleeli

Department of Physics, Maulana Azad National Urdu University, Hyderabad, India,
500032

Department of Physics, Nizam College, Osmania University, Hyderabad, India, 500001

Corresponding author email: iramjuveria@gmail.com

Abstract

The absence of rapid, non-destructive, and objective methods for egg quality grading represents a significant bottleneck in industrial food processing. Here, we introduce a novel sensing principle based on terahertz-derived electrical conductivity (σ) for the automated classification of egg fertility and freshness. Using reflection-mode terahertz time-domain spectroscopy (THz-TDS), we demonstrate that fertile eggs exhibit a significant and consistent reduction in electrical conductivity (from ~ 0.70 S/m to ~ 0.55 S/m) within 24 hours of incubation. This reduction correlates with physiological water and ion mobilization during early embryonic development, quantified as a decrease in estimated shell hydration from 38.5% to 29.6%. The conductivity signal remains stable across a broad frequency range (0.1–3.0 THz), confirming its robustness for high-throughput applications. We propose that this conductivity-based biomarker can be implemented at GHz frequencies for inline, non-contact grading systems, offering a scalable engineering solution to reduce waste and enhance automation in egg processing and hatchery operations.

Keywords: Egg Fertility, Non-destructive Testing, Electrical Conductivity, Water content, Food Quality, Biomarker.

ICC/AIC/072

Green Analytical Chemistry: Recent Trends and Greenness Assessment Methods

Habibur Rahman

*Department of General Studies, Jubail Industrial College, Royal Commission for Jubail,
Jubail Industrial City, 31961, Saudi Arabia*

E-mail: habibur_r@rcjy.edu.sa; habib11129@gmail.com

Abstract

Green analytical chemistry (GAC) has recently emerged as a central approach for aligning analytical science with the broader goals of environmental sustainability and human health protection. It focuses on designing and executing analytical processes that reduce or eliminate hazardous substances, minimize energy and resource consumption, and generate as little waste as possible, while preserving or enhancing method sensitivity, selectivity, accuracy, and robustness. Recent developments increasingly integrate the twelve principles of green chemistry into all stages of analytical method development, from sampling and sample preparation to detection and data handling. Initial tools, such as the National Environmental Methods Index (NEMI) and advanced NEMI, provide simple pictographic evaluations, whereas the Analytical Eco-Scale (AES) introduced a penalty-point system for quantitative scoring of reagent hazards, waste, and energy. More comprehensive, multi-parameter tools, including the Green Analytical Procedure Index (GAPI) and ComplexGAPI, expanded the assessment to cover the entire analytical workflow, yielding easily interpretable color-coded pictograms. Recently, GAC metrics such as the red-green-blue (RGB) model, the RGB 12 algorithm, the Analytical GREENness metric (AGREE), AGREEprep, the Blue Applicability Grade Index (BAGI), and the Red Analytical Performance Index (RAPI) have integrated greenness, analytical performance, and practical applicability into unified visual or numerical outputs. These trends and assessment tools provide a structured basis for designing, selecting, and continuously improving analytical methods that are not only fit for purpose but also environmentally responsible and sustainable.

Identification of Process-related Genotoxic Impurities of 3,7-Dimethyl-1-(5-oxohexyl) purine-2,6-dione by GC-HS Method

Babla V Pendam¹, Amol S Gaikwad², Manohar V. Lokhande^{2*}

¹Department of Chemistry, J. S University, Shikohabad, Uttar Pradesh 283135

²Department of Chemistry, Sathaye College, Mumbai-400057, Maharashtra, India

manohar2210@gail.com

Abstract

Three distinct types of genotoxic pollutants were present in the pentoxifylline synthesis. 3,7-dimethyl-1-(5-oxohexyl)-2,3,6,7-tetrahydro-1H-purine-2,6-dione has a structural alarm for genotoxic mutagenicity and carcinogenicity, although 6-chloro-2-hexanone may be genotoxic. The structural alert and QSTR model consensus state that 3-chloro-1-propanol and 1-bromo-3-chloropropane are both genotoxic. Gas chromatography (GC) with direct liquid injection and a flame ionisation detector (FID) is the best technique for the majority of volatile and semi volatile analytes. In monitoring three genotoxic pollutants, the proposed method was demonstrated to be very efficient, precise, linear, accurate, and specific. Pharmacological analysis of 3-chloro-1-propanol, 1-bromo-3-chloropropane, and 6-chloro-2-hexanone. These pollutants were examined using GC methods. The results of the LOQ and LOD approaches show that the method is very sensitive to assessing 6-chloro-2-hexanone, 1-bromo-3-chloropropane, and 3-chloro-1-propanol pollutants at 0.3 ppm and 0.9 ppm, respectively. Determining threshold levels and suitable techniques for measuring the three genotoxic chemicals that might be present during the manufacturing of pentoxifylline is the aim of this investigation.

Keywords: Genotoxic impurities, Gas chromatography (GC), Flame ionisation detector (FID)

Development and Evaluation of NDBA as a Genotoxic Impurity in Dapagliflozin Drug Substance by using Liquid Chromatography-Mass Spectrometry

Sushil Kumar R Singh^{1*}, Manohar V Lokhande^{2*}

PG Department of Chemistry, Sathaye College (Autonomous), Vile Parle East, Mumbai-400057, Maharashtra, India

E-mail: manohar2210@gmail.com, sushilsejal1012@gmail.com

Abstract

Dapagliflozin tablets are used with diet and exercise to lower blood sugar in people with type 2 diabetes. It is also used to reduce the risk of life-threatening events, including heart attack and stroke, in adults with type 2 diabetes and avoid heart or blood vessel disease. During analysis of drug Dapagliflozin one unknown impurity was detected which may be due to presence of Primary and Secondary amine in Final Drug substance or different stages of Synthetic route. This Impurity was Isolated and characterized by different analytical techniques like IR, NMR, GCMS and GC. NDBA having molecular weight of 158 was fragmented to 128 which was having good response to Quantify, hence it can be nominated as Quantifier ion. Chromatographic separation of NDBA and Dapagliflozin was achieved by using Acquity UPLC BEH C18, (100 mm x 2.1 mm x 1.7 μ m) column, by using carrier gas as Nitrogen and Cooling gas as Argon, Sample temperature 10°C, Flow of 0.25ml/min, Wavelength 254 nm The resolution between NDBA and Dapagliflozin was sufficient to specify both the components. The LOD Limit of detection and LOQ Limit of Quantitation were 0.02 and 0.04 ppm respectively for 15 min run time. The percentage recovery for NDBA was ranged between 99.0 to 101 % in the samples of Dapagliflozin. The developed method was validated as per International council on Harmonization guidelines in terms of Specificity, Limit of Detection (LOD), Limit of Quantitation (LOQ), Precision, Linearity, Accuracy and Ruggedness.

Keywords: LC-MS, genotoxic impurities, Dapagliflozin, N-Nitrosodibutylamine, Limit of Detection (LOD), Limit of Quantitation (LOQ), Precision, Linearity, Accuracy and Ruggedness.

Synthetic Strategy, Mechanistic Insight, and Analytical Evaluation of Vildagliptin

Ibrahim baje Syed¹, Radhakrishnan.Sivaprakasam^{2*}

¹Department of Chemistry, AM Reddy Memorial College of Engineering & Technology (Autonomous), Jawaharlal Nehru Technological University Kakinada (JNTUK)

²Department of Chemistry, School of Sciences and Humanities, SR University, Warangal, Telangana 506371, India

Abstract

Vildagliptin is a selective dipeptidyl peptidase-4 (DPP-4) inhibitor widely employed in the management of type-2 diabetes mellitus. The present study reports the synthesis, reaction mechanism, spectral characterization, and analytical method validation of vildagliptin. The synthetic route involves the construction of a cyanopyrrolidine core followed by amide bond formation with an adamantane-based amine, resulting in vildagliptin with high yield and purity. The reaction proceeds via carboxylic acid activation and subsequent nucleophilic substitution, with retention of stereochemical integrity. Structural elucidation of the synthesized compound was carried out using UV-visible spectroscopy, Fourier-transform infrared (FT-IR) spectroscopy, proton and carbon nuclear magnetic resonance (¹H-NMR and ¹³C-NMR), and mass spectrometry. Mass spectrometric analysis revealed a protonated molecular ion peak at m/z 304, consistent with the molecular mass of vildagliptin. The developed methods exhibited excellent linearity, accuracy, precision, robustness, and sensitivity. In the synthetic process, 3-aminoadamantan-1-ol was prepared by controlled nitration of 1-adamantylamine hydrochloride followed by basification and crystallization. Separately, (2S)-1-(chloroacetyl)pyrrolidine-2-carbonitrile was synthesized from L-prolinamide via acylation and dehydration. Final coupling of the intermediates yielded vildagliptin after purification. Overall, this study establishes a robust synthetic approach and validated analytical framework suitable for pharmaceutical quality control applications.

Keywords: Vildagliptin; DPP-4 inhibitor; Cyanopyrrolidine; Spectral characterization; Analytical method validation; HPLC; UPLC; LC-MS

Optimized and Validated RSM-BBD Model for the Determination of Residual Solvent Acetic Acid in Empagliflozin

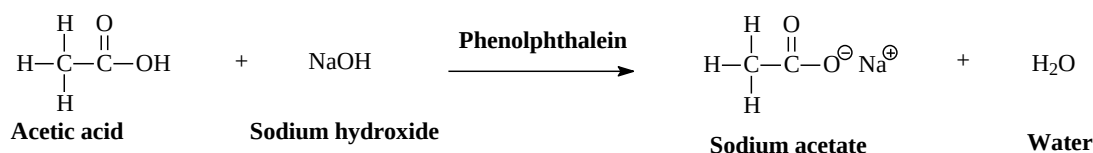
Shaikh Manirul Haque, Sirhan Al-Batty, Abdullah Al-Sultan, Abdulrahman Ali Alkhaldi, Yunusa Umar

Department of Chemical Engineering, Jubail Industrial College, Jubail Industrial City - 31961, Saudi Arabia.

*Author for correspondence e-mail: haque_m@rcjy.edu.sa; manirul1986@gmail.com

Abstract

Residual solvents are generally used or produced during the manufacturing of drugs and drug products and are organic volatile components. These are possibly toxic in nature to humans and must be controlled in the drug product. The titrimetric method is a simple and accurate procedure for quantifying acetic acid content as a residual solvent in Empagliflozin. The process is based on an acid-base reaction that produces water and salt. Sodium hydroxide acts as a base and is titrated against acetic acid (Scheme 1). The endpoint is light yellowish to pink, and phenolphthalein is used as an indicator. The Response Surface Methodology combined with the Box–Behnken Design (RSM–BBD) was applied to optimize the variables acetic acid concentration, sodium hydroxide concentration, and temperature. The method is validated in accordance with the International Conference on Harmonization (ICH) guidelines. The method is linear over the 2.25–12.5 µg/ml range, with a correlation coefficient (r^2) of 0.9999 under the optimum conditions. The developed method's limit of detection (LOD) and limit of quantitation (LOQ) are 1.45 and 4.79 µg/ml, respectively. Additionally, the reported method has a wider linear dynamic range. The technique exhibits no interference from the common excipients present in the formulations. This is a specific, precise, reproducible, and cost-effective method for determining Empagliflozin.



Scheme 1: The titrimetric method is based on the reaction between acetic acid and sodium hydroxide; the endpoint is light yellow to pink.

**Validation of a Gas Chromatography Method for Determination of
Residual Solvents in 1-(p-bromophenyl)-1-(2-pyridyl)-3-
dimethylaminopropane maleate Active Pharmaceutical Ingredient**

Amol S Gaikwad and Manohar V. Lokhande

*Department of Chemistry, Sathaye College (autonomous), Mumbai- 400057,
Maharashtra, India.*

amolgcarrers@gmail.com:manohar2210@gmail.com

Abstract

Gas chromatography was used to validate the active pharmaceutical ingredient (API) of the pharmaceutical bulk medication brompheniramine maleate (API). This article's goal was to use gas chromatography to determine the residual solvents in brompheniramine maleate (API). To verify a gas chromatographic technique for the identification and measurement of residual solvents, including methanol, isopropyl alcohol, DMSO, and -O-xylene. Accuracy, specificity, precision, linearity and range, limit of detection (LOD), limit of quantitation (LOQ), robustness, and system suitability testing are among the validation characteristics that were explained in the development of this technique. FID detector, headspace injection, and a 30m × 0.32mm ID × 1.8µm DB-624 capillary column with a temperature range of 40°C (hold 10 min) to 250°C at a rate of 40°C/minutes, with a 5-minute hold at 250°C. Methanol (2.18), isopropyl alcohol (3.37), DMSO (13.82), and -O-xylene (13.70) all had retention times that were specific. The recovery percentages for O-xylene, isopropyl alcohol, and methanol were 1.87, 2.58 and 1.27, respectively. The routine and stability analysis make use of all validation parameters.

Keywords: FID detector, headspace injection, methanol, Accuracy, specificity, precision, linearity and range, limit of detection (LOD), limit of quantitation (LOQ), robustness, and system suitability

Efficient Removal of Organic Dyes from Wastewater Using Polyaniline-Impregnated Silica Gel Nanocomposites

Mahfoozurrahman Khan^{*1,2}, S. Md Wazed Ali¹, Md Shahadat¹

¹*Department of Textile and Fibre Engineering, Indian Institute of Technology Delhi (India)*

²*Applied Sciences, Moulana Mukhtar Ahmed Nadvi Technical Campus, Malegaon Maharashtra, India*

*Corresponding author: mahfooz55@gmail.com

Abstract

New wastewater solutions are required due to a recent lack of clean water as a result of rising water demand. The removal of organic dyes from wastewater has been the subject of numerous studies, and adsorption is a simple and efficient technique for eliminating both organic and inorganic pollutants from polluted water. Conjugated modified polymers, mainly polyaniline (Pani), have been widely used in wastewater treatment because to their special qualities (simple synthesis, customizable morphology, porous structure, high electrorheological property, biodegradability, and non-toxic nature). Modified surface polymers have exceptional dye removal capabilities in wastewater treatment and are more reactive when it comes to removing dyes from wastewater. The separation of organic dyes from their mixtures is carried out using polyaniline-modified silica gel, which enables the resolution of coexisting dyes based on their migration behavior in an optimized system. This approach helps in evaluating the adsorption efficiency of various organic dyes, allowing comparison with commercially available adsorbents and optimization of experimental conditions for the effective removal of dyes. Moreover, chemical modification of the adsorbent surface, by introducing acidic or basic functional groups, significantly enhances the adsorption of charged organic species, including both cationic and anionic dyes, through improved electrostatic interactions.

Keywords: Polyaniline modified silica gel nanocomposite, Adsorption, biodegradability, organic dyes, wastewater treatment

Development of an Eco-Friendly Paper-Based Colourimetric Indicator for Monitoring Humidity Exposure in Dry Food Commodities

Dr. Narjis Fatima*, Syeda Ayesha Fatima, Maseerah Nazneen Osman

St. Ann's College for Women

*Corresponding author email – dr.narjisfatima@gmail.com

Abstract

Maintaining low humidity is essential for preserving the quality of dry food commodities such as spices, cereals, and pulses, as moisture exposure can accelerate spoilage. Existing moisture indicators used in food storage often make use of harmful chemicals, which may raise concerns related to sustainability, cost, and safety. The present study focuses on the development of a biodegradable, paper-based colourimetric indicator using anthocyanin pigments extracted from *Hibiscus sabdariffa* to detect humidity exposure in dry food environments.

Anthocyanins were extracted using three different solvent systems: distilled water, 50% ethanol, and 70% ethanol. These were embedded into a starch-based medium. Paper strips were coated with anthocyanin-starch mixture to create moisture responsive indicators. Controlled humid and dry conditions were generated using saturated salt solutions and desiccants, respectively. Indicators made from the different solvent systems were compared by observing their colour changes and quantifying the results using digital image analysis.

Upon exposure to controlled conditions, the indicator strips exhibited a noticeable colour change between humid and dry environments. Some variation in colour response was observed between different solvent systems. Image analysis confirmed changes in colour intensity of indicator strips, predominantly within the red channel, supporting the visual findings.

Overall, this study demonstrates a simple and practical approach for preliminary moisture indication in dry food products, offering a low-cost and environmentally friendly alternative for basic quality monitoring applications.

Polycarbazole-Integrated BiCe-MOF Hybrid for Electrochemical Detection of Azithromycin toward Antibiotic Monitoring

Shumaila Hasan^a, Mohammad Zain Khan^{a*}

^a*Electrochemical Research Laboratory, Department of Industrial Chemistry, Aligarh Muslim University, Aligarh, UP-202002, India.*

Corresponding Author: dr_mzain.ch@amu.ac.in

Abstract

The widespread, often uncontrolled use of antibiotics has led to their persistent release into the environment, contributing significantly to the emergence and spread of antimicrobial resistance. Consequently, the sensitive and reliable detection of trace levels of antibiotic residues has become an important analytical priority. Electrochemical sensing offers a promising approach due to its high sensitivity, rapid response, operational simplicity, and suitability for portable and on-site monitoring. A polycarbazole-supported bimetallic metal-organic framework (PCz@BiCe-MOF) was developed as an electrochemical sensing platform for the detection of the macrolide antibiotic azithromycin (AZI). The electrochemical performance of the modified electrode was systematically investigated at varying scan rates, solution pH, and analyte concentrations. The composite electrode exhibited an enhanced electrochemically active surface area with abundant accessible active sites, attributed to the high porosity of the MOF and the synergistic interaction between polycarbazole and the Bi-Ce framework. Differential pulse voltammetry studies demonstrated optimal sensing performance at pH 6.5 within the investigated pH range (5.5-7.5). The proposed sensor achieved a low detection limit of 0.75 μ M, along with excellent reproducibility, stability, and selectivity, indicating its potential for environmental monitoring of antibiotic residues.

Keywords: Bimetallic MOF; Polymer-MOF Composite, Electrochemical Sensor, Azithromycin, Environmental Monitoring

Multifunctional Chalcone Probe for Sensitive Fe³⁺ Sensing and Mechanistic Insights into Silver Nanoparticle-Induced Quenching

Md. Zafer Alam^{1,2*}, Salman A. Khan²

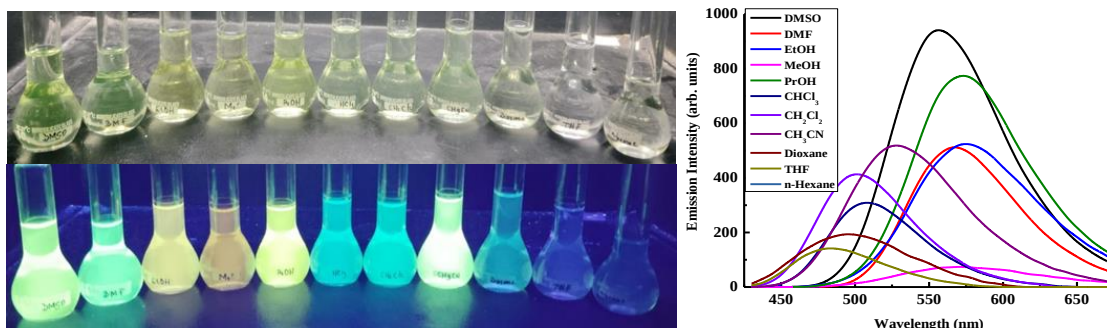
¹Lord Institute of Engineering and Technology, Hyderabad, Telangana, 500091.

²Maulana Azad National Urdu University, Hyderabad, Telangana, 500032.

Abstract

A novel chalcone-based fluorescent probe, TCPO, was successfully developed and evaluated as a dual-mode chemosensor for the selective detection of Fe³⁺ ions. The structure of the synthesized compound was confirmed through ¹H NMR, ¹³CNMR, and mass spectrometric analyses. TCPO displayed strong absorption and bright fluorescence in the visible region; however, the introduction of Fe³⁺ ions resulted in pronounced colorimetric changes accompanied by significant fluorescence quenching. This response is attributed to coordination of Fe³⁺ with the carbonyl oxygen and thiophene sulfur atoms of the probe, facilitating photoinduced electron transfer (PET) and ligand-to-metal charge transfer (LMCT) processes. Quantitative studies revealed limits of detection (LOD) and quantification (LOQ) of 9.7×10^{-7} M and 2.94×10^{-6} M, respectively, indicating high analytical sensitivity in aqueous medium. Binding analysis using Job's method and Benesi–Hildebrand plots confirmed a 1:1 complex formation with an association constant (K_a) of 6.28×10^3 M⁻¹. Additionally, fluorescence quenching was further enhanced in the presence of silver nanoparticles (AgNPs), demonstrating the probe's suitability for nanoparticle-assisted sensing strategies. Stern-Volmer analysis yielded quenching constants (K_{sv}) of 4.35×10^8 M⁻¹ in ethylene glycol and 1.07×10^8 M⁻¹ in ethanol, reflecting efficient quenching dynamics. Collectively, these findings establish TCPO as a sensitive and selective dual-mode optical sensor for Fe³⁺ detection with potential applications in environmental and nano-photonic systems.

Keywords: Dual Sensors; Fe³⁺ ions; TCPO sensor; Turn-off; Silver nanoparticle;



**Design, Synthesis, and Photophysical investigation of a Novel
Tetrahydrobenzo[h]quinoline Derivative: A Turn-ON Fluorescent
Sensor for Zn²⁺ Ion**

Suhail Ahmad, *Salman A. Khan

*Department of Chemistry, School of Sciences, Maulana Azad National Urdu University,
Hyderabad 500032, Telangana, India*

*E-mail: sahmad_phd@yahoo.co.in

Abstract

A novel tetrahydrobenzo[h]quinoline derivative (MTQC), was efficiently synthesized via a one-pot multicomponent reaction. The structure of MTQC was confirmed by FT-IR, ¹H NMR, ¹³CNMR and mass spectrometry analyses. Photophysical investigations, including UV-visible and fluorescence spectroscopy, revealed that MTQC exhibits strong absorption, intense fluorescence, pronounced solvatochromism, and a high fluorescence quantum yield. Fluorescence studies using various metal ions in acetonitrile (1×10^{-5} M) indicated that MTQC is highly selective and sensitive towards Zn²⁺ ions, acting as an efficient turn-on fluorescent sensor. The binding interaction between MTQC and Zn²⁺ follows a 1:1 stoichiometry with a marked association constant $8.04 \times 10^4 \text{ M}^{-1}$, indicating strong interaction between MTQC and Zn²⁺. The limits of detection (LOD) and quantification (LOQ) for the MTQC–Zn²⁺ complex were determined to be 3.88×10^{-7} M and 1.18×10^{-6} M, respectively. These results demonstrate the potential of MTQC as a highly sensitive and selective fluorescent chemosensor for Zn²⁺ detection.

Keywords: One-Pot Synthesis, Quinoline Derivatives, Zn²⁺ ion, Fluorescence

**Spectroscopic Studies On Organomettallic Schiff Base, Some
Transition Metal Ion Complexes: Structural Insights And Anti-
Microbial Activity**

Priyanka S Thakur and Manohar V Lokhande

Department of Chemistry, Sathaye College (Autonomous), Mumbai-400057

Abstract

Synthesis of new organometallic Schiff bases complexes with general formula $[ML]_xH_2O$ [where M = Mn(II), Ni(II), Cu(II) Pd(II) and Pt(II), L=2,2'-{(1R,1'S)-1,1'-Ferrocen-2,4-dien-1-yl-2,2'-diyl bis [(Z)methyl[1]ylidenenitrilo}}bis(3-iodophenol)] have been prepared and characterized by elemental analysis, magnetic susceptibility, Conductivity IR, UV-Visible, Mass spectra and TGA/DTA. Organometallic Schiff base is tetradentate and co-ordination through nitrogen of azomethine ($>C=N-$) and oxygen of Hydroxyl group. The complexes have octahedral geometry with six coordination number. Electronic spectra of the complexes were recorded and its parameters like Nephelauxetic effect (β), bonding parameter ($b_1/2$) and Sinha's parameter (δ %) are calculated. TGA and DTA results of $[Pt(C_{24}H_{16}FeI_2N_2O_2)_2 \cdot 2H_2O]$ and $[Pd(C_{24}H_{16}FeI_2N_2O_2)_2 \cdot 2H_2O]$ are reported, Complexes were losing weight due to exothermic and endothermic process. The mass spectra of prepared ligand ($C_{24}H_{18}FeI_2N_2O_2$) and its complex such as $[Mn(C_{24}H_{16}FeI_2N_2O_2)_2 \cdot 2H_2O]$ were used to compare their stoichiometric composition and it found that near about equal to the theoretical mass of the complex and prepared ligand. Synthesis of nanoparticles of OMNPs (organometallic Nanoparticles) of Cu (II) Complex with SEM and EDX were recorded and particle size is in between 52-60nm. The ligand and complexes have been screened for its anti-fungal activities against three fungi *Alternaria brassicae*, *Aspergillus niger*, *Fusarium oxysporum*.

Keywords: Mass, IR, UV-Visible, SEM, EDX, TGA/DTA, Anti-Fungal activities.

ICC/EEFC/084

Adsorptive Removal of Methylene Blue from Aqueous Solution using Magnetically Modified Shorea Robusta (SAL) Sawdust: Transforming Waste into Resources

Nazifa Noor*, Abu Nasar

Research Scholar, Department of Applied Chemistry, Zakir Husain college of Engineering and technology, Aligarh Muslim University, Aligarh.

Abstract

The persistent presence of synthetic dyes such as methylene blue (MB) in industrial wastewater poses serious environmental and health hazards due to their toxicity, stability, and resistance to conventional treatment methods. In this study, we report the development of a novel and eco-friendly Magnetized Shorea Robusta Sawdust (MSRS) for the effective adsorption of MB from aqueous solutions. The composite was fabricated by incorporating shorea robusta sawdust and Iron oxide nanoparticles. Comprehensive characterization using SEM confirmed the composite's hierarchical porous structure, while FTIR revealed functional group interactions among the components. XRD analysis validated the crystalline structure of MSRS, and TGA demonstrated enhanced thermal stability. BET analysis showed a high specific surface area of 25.509m²/g and mesoporous nature while VSM revealed the magnetic properties. Batch experiments were conducted to investigate the effects of various parameters, viz., adsorbent dosages, contact duration, pH, starting dye concentration, and temperature. Adsorption studies revealed the removal efficiency of 96.325% under optimized condition of 1g/L of magnetized adsorbent, 120 min contact time, pH7, and temperature of 30°C for 50 mg/L MB solution. The adsorption kinetics were best described by the pseudo-second-order (PSO) model. Similarly, equilibrium data conformed well to the Langmuir isotherm model, indicating monolayer adsorption capacity of 80.24mg/g, spontaneous and endothermic. These results highlight the MSRS composite as a promising, sustainable material for advanced wastewater treatment applications.

Keywords: Adsorption, Methylene Blue, Wastewater treatment, Magnetized Shorea robusta sawdust

ICC/EEFC/085

Conductive Nanocomposite Hydrogel for Photocatalytic Dye Removal from Wastewater

Zoha Maqsood, Dr Shahid Pervez Ansari, and Dr Shahabuddin*

Department of Applied Chemistry, Faculty of Engineering and Technology, Aligarh Muslim University, Aligarh 202002, India

*Corresponding author: drshahab786786@rediffmail.com

Abstract

The removal of toxic dyes from wastewater is a critical environmental challenge that demands stable and efficient materials. In this study, a conducting hydrogel was synthesized from polyvinyl alcohol (PVA), titanium dioxide (TiO₂) nanoparticles, and polyindole. The hydrogel combines the mechanical flexibility of PVA with the high photocatalytic activity of TiO₂ and the electrical conductivity of polyindole. The incorporation of polyindole enhances charge-carrier separation, addressing the common limitation of electron-hole recombination in pure TiO₂. Photocatalytic degradation experiments with methylene blue demonstrated promising dye removal, highlighting the hydrogel's effectiveness in degrading pollutants. Overall, these results indicate that the PVA/TiO₂/polyindole hydrogel is a promising, recyclable candidate for advanced water-remediation applications.

Keywords: Conducting Hydrogel, PVA, Titanium Dioxide, Polyindole, and Methylene Blue Dye

Rational Design, Synthesis, and Advanced Characterization of Titanium Dioxide Nanoparticles for Sustainable Applications

Nandkishor B. Shirsath

*Department of Chemistry, MGV's M.S.G. Arts, Science, and Commerce College,
Malegaon, Savitribai Pule Pune University, Pune (MH) INDIA
Corresponding Author E-mail: shirsathnandkishor91@gmail.com*

Abstract

The present study describes the development of a nano-TiO₂ based composite of starch-co-poly(acrylamide) copolymer. The graft copolymer was characterized by Fourier transform infrared (FT-IR), thermal gravimetric analysis (TGA), scanning electron microscopy (FE-SEM), and X-Ray Diffraction (XRD) confirmed that acrylamide (AM) was grafted onto starch successfully. The effects of pH, initiator dosage, temperature, and time on grafting percentage (GP) and grafting efficiency (GE) were also investigated. The synthesized TiO₂ nanoparticles have successfully enhanced the thermal and biological properties of a native copolymer which was confirmed by TGA and biological assay. This synthesized nanocomposite starch-co-poly(acrylamide) was used as a superabsorbent polymer (SAP) with great thermal property and antibacterial activity which regulates the growth of the plant. With this synthesized nano-TiO₂ of can employed in society to control mosquito larvae which show very good ant larvicidal activity against the material vector.

Keywords: TiO₂ nanocomposite; starch-co-poly(acrylamide); starch; graft polymerization; plant growth regulator, Larvicidal activity

Public Health Implications of Dung Cake Combustion in Households

Dr. Amit Kumar

*Department of Chemistry, Indira Gandhi National College, Ladwa (Dhanora),
Kurukshetra, Haryana
E-mail: amitvash76@gmail.com*

Abstract

Fuel is essential for generating energy required for cooking food. In rural areas, dung cakes are among the most commonly used and readily available solid fuels. Households that rely on dung cakes are often socially and economically marginalized, with lower levels of education and fewer physical assets. Factors such as income, educational attainment, and ethnicity have been identified as key determinants influencing the use of dung cakes as a household energy source. Poorer households, individuals with limited education, and those belonging to marginalized ethnic groups are more likely to depend on dung cakes for cooking.

The use of dung cakes for cooking is associated with a wide range of health problems, particularly respiratory illnesses such as chronic obstructive pulmonary disease (COPD). The prevalence of respiratory diseases is higher among dung cake users compared to households using other solid fuels like wood or coal. This increased health risk may be attributed to the high concentrations of toxic emissions released during dung cake combustion, including fine particulate matter in indoor environments. Additionally, elevated levels of carbon monoxide (CO) and strong oxidative activity linked to the presence of transition metals such as iron and manganese in dung may further contribute to adverse health outcomes.

Keywords: Solid cooking fuels, dung cakes, household air pollution, clean cooking

Environmental, Energy and Fuel Chemistry**Dharpawar Unnati Suresh, Dr. Aditi Kulakrni**

Sinhgad Technical Education Society, Smt. Kashibai Navale College of Pharmacy, Pune,
Savitribai Phule Pune University
udharpawar176@gmail.com

Abstract

The rapid depletion of fossil fuel reserves and increasing environmental concerns have intensified the demand for sustainable and renewable energy sources. Biofuels have emerged as a promising alternative due to their potential to reduce greenhouse gas emissions and enhance energy security. Among various biofuel feedstocks, *Jatropha curcas L.* and *corn (Zea mays)* have attracted considerable attention for biodiesel and bioethanol production, respectively. The extracted oil predominantly consists of triglycerides, which are chemically converted into biodiesel via a **base-catalyzed transesterification reaction**. In this reaction, triglycerides undergo nucleophilic substitution with short-chain alcohols (methanol or ethanol) in the presence of alkaline catalysts such as NaOH or KOH, leading to the formation of fatty acid alkyl esters as a by-product:



This conversion reduces oil viscosity, improves volatility, and enhances combustion efficiency. The produced *Jatropha* biodiesel complies with international fuel standards (ASTM 6751 and EN 14214) and demonstrates superior cetane number, high flash point, and lower exhaust emissions compared to petroleum diesel. Through enzymatic hydrolysis followed by microbial fermentation, starch is converted into fermentable sugars and subsequently into ethanol. Despite challenges related to food security and land use, continued technological advancements support its role in renewable energy production. Overall, this study highlights the chemical conversion pathways and sustainability potential of *Jatropha* and *corn*-based biofuels for a cleaner energy future.

ICC/EEFC/089

Magnetized waste-peel-derived adsorbents: synthesis, characterization, and application for the removal of a cationic dye from artificially contaminated water

Mohsina Ahmed*, Abu Nasar

Department of Applied Chemistry, Zakir Husain College of Engineering and Technology, Aligarh Muslim University, Aligarh

Abstract

The present investigation explored the adsorption characteristics of three different magnetized adsorbents, namely magnetized bentonite clay particles (MBCP), magnetized *Artocarpus heterophyllus* fruit peel particles (MAHFP), and pineapple peel iron manganese binary oxide nanoparticles (PP-IMBON) for removing the cationic dye methylene blue (MB) from artificially contaminated water. The adsorbents were characterized by VSM, SEM/EDAX, FTIR, TEM, TGA, XRD, and point of zero charge. Batch experiments were performed by varying operating parameters, including initial dye concentration, pH, adsorbent dose, and temperature. The optimal conditions for adsorption resulted in removal efficiencies of 93.97, 91.93, and 92.68% for MBCP, MAHFP, and PP-IMBON, respectively. Langmuir isotherms were well fitted to the adsorption equilibrium data for all adsorbents, and the maximum monolayer adsorption capacities were 588.23, 261.35, and 312.50 mg/g, respectively. The research adsorption data are best explained by pseudo-second-order kinetics. Adsorption was found to be thermodynamically feasible, resulting in heat absorption and an increase in entropy. In the regeneration study, the magnetized adsorbents were regenerated up to 5 times using HCl as the best desorbing agent. The various magnetically modified adsorbents offer very high adsorption affinity for dyes, easy separation, low cost, and reusability, making them an attractive option for removing MB from industrial wastewater.

Keywords: Magnetized adsorbent, Methylene Blue, Langmuir isotherm, Pseudo-second-order kinetics

Polysulfone supported zinc oxide thin film composite membrane-fabrication, characterization and applications for metal ion removal

Aiman Khan, Mohd Arsalan*

Department of Applied Chemistry, Faculty of Engineering and Technology, Aligarh Muslim University, Aligarh - 202002, India
Email address: aimansabiha03@gmail.com

Abstract

The increasing exploitation of water resources and the growing scarcity of clean water have pushed the trajectory of research to clean water generation techniques. In the given study, a novel Polysulfone and Zinc Oxide (PSf@ZnO) Thin film composite membrane is presented for the removal of heavy metal ions from wastewater. The membrane was synthesized using the phase inversion technique and then surface-modified with ZnO nanoparticles to enhance its chemical stability and filtration efficiency. FESEM, FTIR, XRD, and TGA were the characterization techniques employed to examine the membrane's morphology, chemical structure, crystallinity, and thermal degradation. The concentrations of heavy metal ions Pb^{2+} , Cu^{2+} , Cd^{2+} , Cr^{6+} , and Ni^{2+} using Atomic Absorption Spectroscopy (AAS) were analyzed. The results show that ZnO nanoparticles spread evenly throughout the polysulfone matrix. This setup boosts surface hydrophilicity and makes the membrane's pores highly uniform. Thermal tests (TGA/DTA) show the membrane stands up better to heat and resists breaking down. When it comes to removing heavy metal ions, the membrane works remarkably well across the tested range, as long as conditions are suitable. Additionally, ZnO brings strong antibacterial properties, which helps the membrane fight off fouling and keeps it running longer. In conclusion, these findings point to the PSf@ZnO composite membrane as a cost-effective and sustainable option for water purification. The ZnO nanoparticles push its performance, making it an apt choice for both environmental and industrial uses.

Keywords: Polysulfone, Zinc Oxide, Composite membranes, Membrane separation processes, Thin Film Composite membrane

Structural and Electrochemical Investigation of Green-Synthesized CuO-RGO Nanocomposites for Energy Storage Devices

Mohd Arshad¹, Dr. Mohd Yusuf Ansari² and Dr. Arham Shareef Ahmed^{1*}

¹Department of Physics, Aligarh Muslim University, Aligarh (India), 202002

²Department of Petroleum studies, Aligarh Muslim University, Aligarh (India), 202002
arham.ph@amu.ac.in

Abstract

Copper oxide (CuO) nanoparticles were synthesized via a green method utilizing lemon leaf extract, followed by the preparation of reduced graphene oxide (RGO)-based nanocomposites through ultrasonication. Structural analysis using X-ray diffraction revealed a decrease in crystallite size upon RGO incorporation as calculated by the Debye-Scherrer formula and Williamson-Hall plots, indicating high surface area and active sites, enhancing electrochemical interfaces. Raman spectra showed the signature D and G bands, revealing the presence of RGO in the synthesized nano-samples. FTIR spectra confirmed the formation of CuO-RGO nanocomposites through signature vibrational bands. The electrochemical analysis via cyclic voltammetry revealed that the nanocomposite exhibited a much higher specific capacitance (102 F/g) compared to pure CuO (44 F/g) at a scan rate of 10 mV/s. The improved performance is ascribed to enhanced charge storage and improved electrical conductivity introduced by RGO. These findings suggest that these non-toxic synthesized CuO-RGO nanocomposites are promising, sustainable alternatives for energy storage applications, combining environmental safety with enhanced performance.

Nitrogen-Rich Porous Organic Polymer (SB-NRPOP) for High-Capacity Iodine Capture toward a Sustainable Future

Nowsheenah Farooq and Athar Adil Hashmi

Jamia Millia Islamia, New Delhi, India-110025

Email id: nowsheenahfarooq@gmail.com/ ahashmi@jmi.ac.in

Abstract

The mitigation of iodine emissions is critically important for ensuring environmental safety and advancing sustainable technologies, particularly in the context of nuclear waste management and environmental remediation. In this study, we report on the synthesis of a nitrogen-rich porous organic polymer via a Schiff base polycondensation strategy and investigate its iodine capture performance. The porous framework exhibits high iodine uptake capacities of $4.1 \text{ g} \cdot \text{g}^{-1}$ from iodine vapor and $3.9 \text{ g} \cdot \text{g}^{-1}$ from iodine solution, demonstrating strong affinity toward iodine species. The efficient adsorption behavior is attributed to the synergistic effects of accessible porosity and electron-rich nitrogen sites that facilitate strong host-guest interactions. Flow-through adsorption experiments further confirm the practical applicability of the material, achieving up to 88% iodine removal under continuous conditions. Additionally, the polymer displays selective iodine adsorption in mixed-halogen systems, highlighting its potential for halogen separation. This work demonstrates that nitrogen-functionalized porous organic polymers are promising, sustainable adsorbent materials for efficient iodine capture, contributing to safer environmental practices and a sustainable future.

Keywords: Iodine capture; porous organic polymer; nitrogen-rich framework; adsorption; sustainable materials.

Removal of Microplastics in Water bodies through Composite Membranes

Uqba Rashid¹, Mohd Arsalan*¹

¹*Department of Applied Chemistry, Faculty of Engineering and Technology, Aligarh Muslim University, Aligarh –202002, India*
Email address: uqbarashid5@gmail.com

Abstract

Microplastics (MPs) have become a major worldwide hazard to ecosystem stability and human health due to their buildup in aquatic settings. As a result of the ongoing fragmentation of larger plastic trash and direct inputs from textiles, cosmetics, and industrial processes, rivers, lakes, and marine systems are now widely contaminated. This review attempts to give a thorough summary of the state of knowledge about Microplastics pollution in water bodies, with a focus on the origins, effects on the environment, and methods of removal. The most important scientific databases were thoroughly searched for pertinent research that was published between 2010 and 2025. According to the findings, the main sources of MPs are atmospheric deposition, urban runoff, and wastewater treatment plant effluents; the breakdown of used plastics is a key secondary pathway. Through ingestion, bioaccumulation, and behavioral changes, Microplastics endanger aquatic life, and their presence in human and terrestrial systems raises increasing toxicological concerns. Numerous removal techniques, such as membrane filtering, coagulation–flocculation, adsorption, biodegradation, and advanced oxidation processes, have been studied. The removal efficiency of membrane technologies and hybrid systems is the highest among them; nonetheless, fouling and cost issues are problems. In order to reduce Microplastics pollution and protect water resources for future generations, the review concludes that standardized monitoring techniques, sustainable treatment technologies, and integrated management strategies are urgently needed.

Keywords: Microplastics, Pollution, Composite Membranes, Coagulation, Flocculation.

Bio-inspired zinc remediation: Tamarind kernel polysaccharide and Amino acid-based resin for Removal of Zn (II) Ions from Aqueous Solutions

Abhishek Solanki¹, and Vikal Gupta^{1*}

¹*Department of Chemistry, Jai Narain Vyas University, Jodhpur 342 001, Rajasthan, India*

E-mail address: abhishek.solanki04@gmail.com (A. Solanki).

Abstract

The pollution of water resources by heavy metals like Zinc (II) presents serious environmental and health challenges, highlighting the urgent need for the creation of sustainable and effective remediation technologies. This research explores the creation and adsorption properties of a new bio-sorbent resin made from tamarind kernel powder that has been functionalized with aspartic acid. The resin was produced through cross-linking and was characterized using FTIR, SEM, and XRD to verify its surface morphology and the modification of functional groups. Batch adsorption tests were performed to fine-tune parameters such as pH, contact time, initial metal ion concentration, and temperature. The findings showed that the highest adsorption capacity reached 85.623 mg/g at an optimal pH of 7.8. The adsorption data fit best with the Langmuir isotherm model, indicating monolayer coverage, while kinetic analysis adhered to the Pseudo-second order model, suggesting a chemisorption mechanism. Additionally, thermodynamic evaluations indicated that the adsorption process was both spontaneous and exothermic. Desorption experiments revealed that the resin could be efficiently regenerated for up to five cycles. These results indicate that the tamarind kernel powder and aspartic acid resin is a viable, cost-effective, and biodegradable adsorbent for the extraction of Zn (II) from wastewater.

Keywords: Tamarind kernel powder, Aspartic acid, Zinc removal, Adsorption isotherm, Wastewater treatment.

Green Chemistry Initiatives for a Sustainable Development

Shabana Sajid

Department of Chemistry, Gandhi faiz-e-Aam College, Shahjahanpur-242001, Uttar Pradesh, India

E-Mail: drshabanaathar@rediffmail.com

Abstract

Green chemistry plays a pivotal role in realizing the vision of Viksit Bharat (Developed India) by promoting sustainable development, environmental protection, and economic growth simultaneously. It focuses on designing chemical products and processes that minimize the use and generation of hazardous substances, thereby safeguarding human health and natural resources. One of the primary contributions of green chemistry to Viksit Bharat is environmental sustainability. By reducing toxic waste, lowering emissions, and conserving energy and water, green chemistry helps combat pollution, climate change, and resource depletion—critical challenges faced by a rapidly developing nation like India. Green chemistry also strengthens industrial growth and innovation. Adoption of eco-friendly processes in pharmaceuticals, agrochemicals, textiles, and manufacturing enhances efficiency, reduces production costs, and improves global competitiveness of Indian industries. This supports the “Make in India” and “Atmanirbhar Bharat” initiatives by encouraging cleaner and safer technologies.

In the agricultural sector, green chemistry promotes the development of bio-fertilizers, bio-pesticides, and sustainable farming inputs, reducing dependence on harmful chemicals. This ensures soil health, food safety, and long-term agricultural productivity, which are essential for national food security. From a public health perspective, green chemistry reduces exposure to toxic chemicals in medicines, cosmetics, packaging, and household products. Safer alternatives contribute to improved quality of life and lower healthcare costs, aligning with the goals of inclusive and healthy development.

Key words: Green chemistry, environmental sustainability, eco-friendly

Polyindole/Copper oxide Composite: A Highly Efficient Multi-Cyclic Photocatalyst

Arisha Bi^a, Zeba Haque^{a*}

^aDepartment of Chemistry, Jamia Millia Islamia University, New Delhi, 110025, India

Abstract

Copper oxide (CuO) has demonstrated a great potential over last decades as photocatalyst. In the current study CuO has been doped to a conducting polymer, polyindole (PIn) to prepare an efficient photocatalyst with improved cyclic reusability and easy extraction. In-situ chemical oxidative polymerization technique was employed for the synthesis of PIn and composites using ferric chloride as an oxidant. A range of PIn/CuO nanocomposites were synthesized by varying CuO contents (%w/w) between 10 to 25. Morphological, optical and structural properties of the composites, sole CuO and PIn were investigated by various spectroscopic techniques like XRD, SEM, UV–visible, FTIR, XPS, PL etc. The photocatalytic activity of different composites was studied for the degradation of Acridine orange (AO) and Bismarck brown (BB) dyes. Photocatalytic activity of dyes was investigated separately, and various parameters such as catalytic dosage, initial dye concentration and pH were optimized in order to get the best photocatalytic efficiency. The composite showed an enhanced photocatalytic activity as compared to pure CuO and PIn and demonstrated twice the cyclic activity than CuO. Excellent results demonstrated by PIn/CuO composite makes it a promising photocatalyst for future applications.

Nanostructuring Materials to Overcome Performance Challenges in Flexible Solid-State Supercapacitors for Next-Generation Portable and Wearable Energy Storage Systems

Mohd Suhail Chaudhary^{a,b}, Mohammad Zain Khan^{a*}

^a*Electrochemical Research Laboratory, Department of Industrial Chemistry, Aligarh Muslim University, Aligarh, UP-202002, India.*

^b*Environmental Research Laboratory, Department of Chemistry, Aligarh Muslim University, Aligarh, UP-202002, India.*

Corresponding Author: dr_mzain.ch@amu.ac.in

Abstract

Flexible solid-state supercapacitors (FSSCs) have attracted significant attention as energy storage devices for next-generation wearable and portable electronics, thanks to their safety, mechanical durability, and design flexibility. Unlike liquid-electrolyte systems, solid-state supercapacitors offer leakage-free operation, enhanced stability, and improved compatibility with flexible architectures. However, maintaining high electrochemical performance under mechanical deformation remains a major challenge. Recent advances show that optimized electrode architectures and nanostructured interfaces effectively improve ion transport, increase electroactive surface area, and preserve structural integrity during bending and twisting. The use of solid or gel polymer electrolytes further enhances device safety and flexibility while ensuring stable charge storage behavior. This work highlights key design strategies governing device architecture, electrolyte selection, and mechanical reliability, providing insight into the development of efficient and durable FSSCs for emerging portable, wearable, and smart electronic applications.

Keywords: Energy Storage; Flexible Supercapacitors; Nanostructured Materials; Energy Density; Power Density; Portable and Wearable Electronics.

An Analysis of Hydrothermal Biomass Processing for Sustainable Energy and Fuels

Vidya Singh

*Assistant Professor, Department of Chemistry, Maharaja Bijli Pasi Govt. P.G. College,
Ashiana, Lucknow, U.P., India,
vidyasingh005@gmail.com*

Abstract

A revolutionary strategy for tackling the dual problems of energy sustainability and climate change is the combination of fuel synthesis and renewable energy sources. A conceptual framework for combining renewable energy technologies is present in this paper, including using fuel synthesis techniques, solar, wind, and biomass can used to create sustainable, carbon-free fuels. The framework places a strong emphasis on using renewable electricity for carbon dioxide reduction and water splitting, two essential processes in the production of hydrogen and other synthetic fuels. The conceptual framework emphasizes how crucial sophisticated catalysts are to raising these chemical processes' efficiency and selectivity. The potential of developments in bio-mimetic techniques, hybrid materials, and nano-structured catalysts to enhance the efficiency and longevity of catalytic processes is examine. Biomass currently generates 5×10^{19} kJ of energy annually, or 10% of the world's yearly energy consumption. Considering the variety of biomass resources, this number is anticipating to reach 150×10^{19} kJ by 2050. In the twenty-first century, biomass may become even more significant as a source of energy and a raw material for chemicals. Hydrothermal biomass conversion is a particularly promising alternative method. In order to reduce the expense and time associated with drying biomass, hydrothermal methods have developed. This method breaks down biomass with high moisture content into smaller molecules and lowers its oxygen concentration to produce valuable chemicals or liquid fuels. The state of energy, energy sources, biomass properties, biomass conversion technologies, and water properties in hydrothermal media are cover in this review, with a particular emphasis on hydrothermal technologies.

Keywords: Sustainable, Hydrothermal, Biomass, Energy, Fuel

GAAL@ZFT Nanocomposite Hydrogel as a High-Performance Adsorbent for Cationic Dye Removal

Kahkashan Sarfaraz, Saif Ali Chaudhry

Department of Chemistry, Jamia Millia Islamia, New Delhi-110025, India

Email: kahkashans31@gmail.com

Abstract

The development of smart, super-adsorbent nanocomposite hydrogel materials with biodegradability and biocompatibility is decisive in the material world to address the major shortcomings associated with the sustainability issues of ecological footprints. On the practical applicability, the absorption experiments were performed using the Yamuna water, Sewage wastewater and tap water spiked with a 10 mg/L JG-B, 10 mg/L VB and 20 mg/L AZ-A. The results show a significant removal of 95.66% JG-B, 84.27% VB and 81.29% AZ-A in Yamuna water, which is slightly lower than the result observed in the synthetic dye solutions due to the presence of competing ions. The fabrication of GAAL and its interaction with cationic dyes were characterized via FT-IR, PXRD, FE-SEM, TEM, SAED, BET, TGA and ZPC techniques. The prepared nanocomposite hydrogel has a high surface area. The hydrogel exhibited excellent reusability, maintaining over 90% removal efficiency after five adsorption-desorption cycles, demonstrating strong structural stability and regeneration potential. Batch adsorption experiments were performed to examine the influence of pH (2-10), adsorbent dosage (0.2-1g/L), contact time (15–120min), initial dye concentration (10-30mgL⁻¹), and temperature (303–323 K) on adsorption efficiency. The adsorption kinetics followed the pseudo-second-order model ($R^2 > 0.99$), while the equilibrium data conformed well to the Langmuir isotherm ($R^2 = 0.998$), suggesting monolayer chemisorption on a homogeneous surface. Henceforth, the demonstrated works provide several mechanistic ways to achieve high-performing nanocomposite hydrogel.

Keywords: Nanocomposite hydrogel, Gum Arabic, Zinc ferrite, Cationic dye adsorption, Batch adsorption, Isotherm and kinetic modeling, Wastewater treatment, Biopolymer-based adsorbent

Mechanistic Insights into the Anticancer Activity of Phenyl-1,3,5-Heptatriyne from *Bidens pilosa*

Dr. Uzma Faridi

Department of Biochemistry, Faculty of Science, University of Tabuk, Saudi Arabia
ufaridi@ut.edu.sa

Abstract

Bidens pilosa L. (Ottocarpedi) is a traditionally used medicinal plant rich in bioactive compounds such as polyacetylenes, flavonoids, terpenoids, and phenylpropanoids, known for their antimicrobial and anticancer activities. In this study, we investigated the anticancer mechanism of phenyl-1,3,5-heptatriyne against the human liver cancer cell line HepG-2. The mode of action was evaluated using DNA fragmentation, caspase-3 activity assay, cell cycle analysis, and fluorescence microscopy. Our results demonstrated that phenyl-1,3,5-heptatriyne induces apoptosis in HepG-2 cells through significant activation of caspase-3 and causes cell cycle arrest at the G2/M phase. Previous studies have reported that *B. pilosa* L. infusions are non-toxic following single and repeated dosing, including dermal exposure. These findings suggest that phenyl-1,3,5-heptatriyne is a promising lead compound for future anticancer drug development.

Keywords: Liver cancer; Phenyl-1,3,5-heptatriyne; Apoptosis; Anticancer

Receptor Pharmacology of Phytochemicals in Alzheimer's Disease: Multi-Target Modulation of Neurodegenerative Pathways

Mohd Nadeem¹, Abul Kalam Najmi*¹

¹*Department of Pharmacology, School of Pharmaceutical Education and Research,
Jamia Hamdard, New Delhi, India, 110062.*

Abstract

Alzheimer's disease (AD) is a progressive neurodegenerative disorder whose complex, multifactorial pathophysiology has largely evaded effective treatment by conventional single-target pharmaceuticals. The disease is characterized not only by the canonical amyloid-beta (A β) plaques and neurofibrillary tangles (NFTs) but also by a web of interconnected pathologies, including synaptic failure, neuroinflammation, oxidative stress. Current therapeutic options, such as cholinesterase inhibitors and N-methyl-D-aspartate (NMDA) receptor antagonists, offer only modest symptomatic relief and fail to halt disease progression. Bioactive compounds like curcumin, resveratrol, and ginsenosides possess the ability to simultaneously modulate multiple receptor targets and signaling pathways. This review provides a critical analysis of the receptor-based mechanisms of phytochemicals in AD. We examine key receptor systems, including those governing A β processing and clearance, tau phosphorylation cascades (e.g., GSK-3 β , PP2A), synaptic integrity, neuroinflammatory responses, and oxidative stress defenses (e.g., Nrf2, SIRT1). Evidence from preclinical and clinical studies demonstrates that herbal compounds can beneficially modulate these receptor-driven pathways. However, significant challenges in clinical translation remain, primarily concerning poor bioavailability, penetration of the blood-brain barrier, and the need for rigorous standardization. Overcoming these hurdles through advanced drug delivery systems and robust, biomarker-guided clinical trials is essential to fully integrate the multi-target potential of phytopharmacology into future AD therapeutics.

Keywords: Alzheimer's disease, phytochemicals, receptor pharmacology, neurodegeneration, multi-target therapy.

Sodium Alginate-Based Delivery Systems for Tetracycline Hydrochloride: Encapsulation and Release Profiles

Daniya Ikram, Prof M. Z. A. Rafiquee

*Department of Applied Chemistry, ZHCET Faculty of Engineering and Technology
Aligarh Muslim University, Aligarh, UP, 202002, India*

ikramdaniya5@gmail.com

Abstract

Tetracycline Hydrochloride (TCH) is a broad-spectrum antibiotic; however, its clinical efficacy is often compromised by rapid elimination, instability, and gastrointestinal side effects. This study investigates the development of a controlled release delivery system using sodium alginate hydrogel beads prepared via ionic gelation. The primary objective was to optimize formulation parameters to enhance Encapsulation Efficiency (EE) and modulate drug release kinetics.

Two encapsulation strategies were employed. In the first method, a 6% sodium alginate solution mixed with 1×10^{-2} mol dm⁻³ TCH was extruded into a 5% CaCl₂ cross-linking bath. Conversely, the second method involved adding an 8% sodium alginate solution into a 5% CaCl₂ both containing 1×10^{-2} mol dm⁻³ TCH. Fourier Transform Infrared (FTIR) spectroscopy confirmed the successful entrapment of TCH within the biopolymer matrix without adverse chemical interactions. Release profiles were evaluated in diverse media, including distilled water, varying concentrations of HCl and NaOH, as well as salt and surfactant solutions (SDS, CTAB, TX-100). The release kinetics exhibited a biphasic pattern, characterized by an initial burst effect followed by a sustained release over a 24-hour period. Results indicated that the alginate matrix significantly improved encapsulation efficiency and retarded release rates due to increased matrix density. Conclusively, calcium-alginate beads present a viable, biocompatible approach for the oral delivery of TCH, offering potential for reduced dosing frequency.

Keywords: Tetracycline Hydrochloride, Calcium-Alginate beads, Ionic Gelation, Antibiotics Encapsulation, Controlled Drug Delivery, Kinetics

ICC/MDD/103

Design and Optimization of a Dual-Polymer Mucoadhesive Microsphere System for Controlled Neuroactive Drug Delivery

Aaishwarya Deepak Bansode, Dr. Madhuri Deshmukh

*Sinhgad Technical Education Society, Smt. Kashibai Navale College of Pharmacy,
(Savitribai Phule Pune University), Pune.*

aishbansode18@gmail.com

Abstract

The present study reports the factorial design optimization and characterization of a novel dual-drug mucoadhesive microsphere-based capsule system intended for controlled gastroretentive delivery. Olanzapine microspheres were formulated using sodium alginate–carbopol polymeric networks via ionotropic gelation, where Ca²⁺-mediated crosslinking generated a dense hydrophilic matrix governing diffusion-controlled release. Fluoxetine hydrochloride microspheres were prepared using chitosan and Eudragit RS100 by using emulsion solvent evaporation. Preformulation and compatibility studies were conducted using UV spectrophotometry (λ_{max}), FTIR, DSC, and XRD to confirm drug purity, polymer compatibility, and solid-state stability. A 3² full factorial design was employed to optimize critical formulation variables, including polymer concentration and crosslinker content, with responses such as entrapment efficiency, mucoadhesive strength and *in-vitro* drug release. Statistically significant models with close agreement between predicted and experimental R² values validated the robustness of the optimization process. *In-vitro* dissolution studies revealed zero-order release kinetics for Fluoxetine HCl and Higuchi diffusion-controlled release for Olanzapine, governed by polymer swelling and matrix diffusion mechanisms. SEM analysis confirmed discrete, spherical microspheres with rough surfaces favorable for prolonged mucosal adhesion. The developed polymer-engineered, factorially optimized mucoadhesive microsphere capsule represents a stable and innovative platform for controlled oral drug delivery.

Keywords: Dual-Drug Mucoadhesive Capsule; Polymer Matrix Engineering; 3² Factorial Design; Ionic Gelation Crosslinking; Emulsion Solvent Evaporation; Zero-Order Release

***In Silico* Screening of Newly Designed Azole-Based Derivatives as Prospective Antimicrobial Leads**

Ahmed Helmi Billo, Abdullah Saad Al-Bogami, Mohmmad Younus Wani*

Department of Chemistry, College of Science, University of Jeddah, Jeddah 21589, Saudi Arabia

mwani@uj.edu.sa

Abstract

Antimicrobial resistance (AMR) is increasingly limiting the effectiveness of many current antibacterial and antifungal agents, highlighting the urgent need for new chemical scaffolds with improved target engagement and resistance-bypassing potential. In this study, we designed a series of novel azole-based derivatives, with particular emphasis on triazole-containing structures, as prospective antimicrobial leads. We performed preliminary screening using multiple computational tools and structure-based approaches to prioritize compounds with favorable drug-like characteristics and plausible target binding. Molecular docking was carried out against key microbial targets, including fungal lanosterol 14 α -demethylase (CYP51) and bacterial DNA gyrase, to evaluate predicted binding affinity, binding orientation, and key stabilizing interactions. The docking outcomes suggest that several designed derivatives can adopt reasonable binding poses within the active sites and form relevant non-covalent interactions, supporting their potential as antimicrobial candidates. These *in silico* findings are being used to shortlist and rank compounds for experimental follow-up. The next phase of this work will focus on synthesizing the top-ranked candidates (including click-chemistry-enabled triazole analogs), confirming structures through standard spectroscopic techniques, and validating the computational predictions through *in vitro* antimicrobial assays against representative bacterial and fungal strains. Overall, this study provides a docking-guided prioritization workflow to accelerate the identification of promising azole-based antimicrobial leads for experimental validation.

Keywords: antimicrobial resistance; azole derivatives; triazoles; *in silico* screening; molecular docking; DNA gyrase.

Copper(II) complex as SARS-CoV-2 inhibitor: Synthesis, crystal structure, antiviral and anticancer properties

Reyaz Ahmad^a, Mukesh Choudhary^{a*}

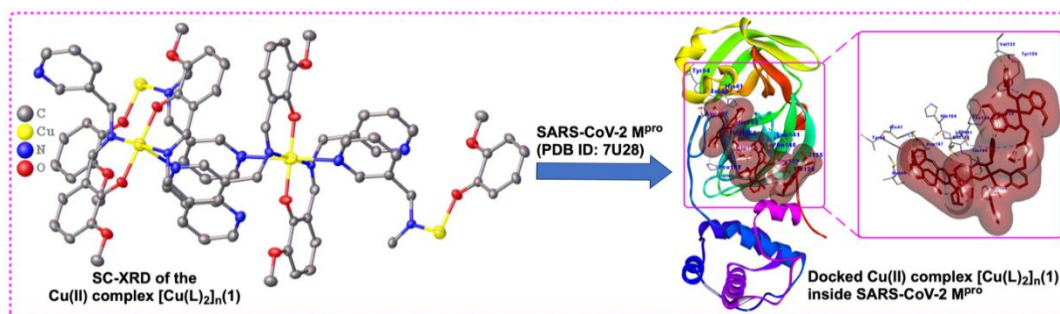
^aDepartment of Chemical Science and Technology, National Institute of Technology Patna, Patna-800005 (Bihar) India.

E-mail: reyaza.ph23.ch@nitp.ac.in

Abstract

The synthesis and theoretical/biological evaluation of a novel Cu(II) complex $[\text{Cu}(\text{L})_2]_n(\mathbf{1})$ intended as a dual function agent against SARS-CoV-2 M^{pro} and cancer cells. SC-XRD analysis of Cu(II) complex $[\text{Cu}(\text{L})_2]_n(\mathbf{1})$ revealed that the coordination geometry around Cu(II) ions is distorted octahedral. The cytotoxicity activity of the complex was investigated on HeLa and A549 cancer cells by the MTT assay. The Cu(II) complex $[\text{Cu}(\text{L})_2]_n(\mathbf{1})$ showed moderate cytotoxicity against HeLa and A549 cells with IC₅₀ values of $24.65 \pm 0.11 \mu\text{M}$ and $27.34 \pm 1.10 \mu\text{M}$, respectively, at 24h of incubation, when compared with the cisplatin under identical conditions gave IC₅₀ values of $10.31 \pm 1.63 \mu\text{M}$ (HeLa) and $11.45 \pm 1.51 \mu\text{M}$ (A549), confirming that our complex is moderately active relative to the standard. To explore potential pharmaceutical and therapeutic applications, the Cu(II) complex $[\text{Cu}(\text{L})_2]_n(\mathbf{1})$ was tested with the structure of the SARS-CoV-2 main protease (M^{pro}) Lambda (G15S) in complex with *Nirmatrelvir* (PDB ID: 7U28). The docking studies showed that Cu(II) complex had stronger binding affinity against SARS-CoV-2 M^{pro}. Our work provides theoretical evidence that Cu(II) complex $[\text{Cu}(\text{L})_2]_n(\mathbf{1})$ can be developed as antiviral drug candidate against SARS-CoV-2 M^{pro}.

Keywords: Cu(II) complex; Molecular docking; SARS-CoV-2; Anticancer.



Synthesis of Benzenesulfonamides under Biocatalytic Conditions by Employing Baker's Yeast as a Biocatalyst

Sohera Tabassum¹, Azra Soban¹, Qasim Ullah^{1*}

¹Chemistry Section, School of Sciences, Maulana Azad National Urdu University, Gachibowli, Hyderabad-500032, Telangana, India

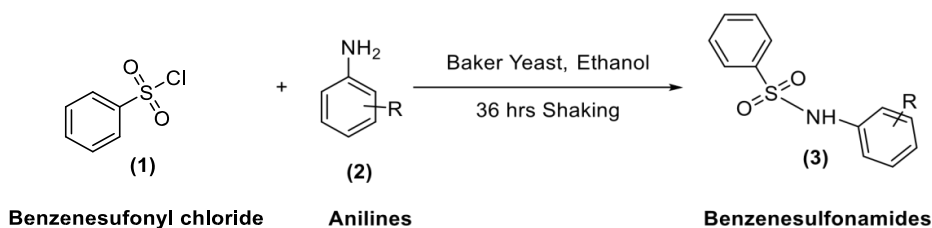
Email: drqasimullah@manuu.edu.in

Abstract

Sulfonamides are a versatile class of compounds containing the $-\text{SO}_2\text{NH}_2$ functional group and are well known for their antibacterial (bacteriostatic) activity through inhibition of dihydropteroate synthase. Beyond their antimicrobial properties, sulfonamides also exhibit diverse therapeutic activities such as anticancer, antiinflammatory, diuretic, hypoglycemic (antidiabetic), and carbonic anhydrase inhibitory effects.

Traditionally, sulfonamides are synthesized via nucleophilic substitution of sulfonyl chlorides with amines or ammonia, often in the presence of bases or metal catalysts such as copper or palladium. Common synthetic approaches include reactions using pyridine as a base, direct sulfonylation, and modern catalytic methods employing reagents such as DABCO to avoid hazardous gases.

A literature survey reveals that no direct enzymatic synthesis of sulfonamides using enzymes such as lipases or esterases has been reported so far. In the present study, benzenesulfonamides are efficiently synthesized by the reaction of benzenesulfonyl chloride (1) with anilines (2) under biocatalytical conditions using whole-cell Baker's yeast as a biocatalyst, affording the corresponding benzenesulfonamides (3) in good to excellent yields.



Keywords: Benzenesulfonyl chlorides; Anilines; Benzenesulfonamides; Baker's Yeast

Design, Synthesis, and Biological Evaluation of Innovative 1,2,4-Triazine Derivatives Exhibiting Anxiolytic and Anti-Inflammatory Activity

Touseef Begum^{a*} and Suroor A. Khan^b

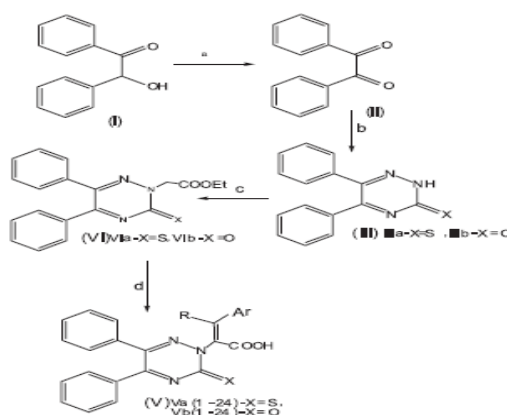
^aDepartment of Pharmaceutical Sciences, Ibn Sina National College for Medical Studies, Jeddah, Kingdom of Saudi Arabia,

^bDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Jamia Hamdard, New Delhi, India.

Abstract

A novel series of 1,2,4-triazine derivatives, designated as **Va (1-24)** and **Vb (1-24)**, were designed, synthesized, and screened for their anti-anxiety and anti-inflammatory activities. Structural confirmation of the synthesized compounds was achieved through detailed spectral characterization. Biological evaluation revealed that several derivatives exhibited promising pharmacological activity. Notably, sulfur-containing triazine analogues demonstrated superior activity compared to their oxygen-substituted counterparts, highlighting the importance of heteroatom substitution in modulating biological response. These findings suggest that 1,2,4-triazine scaffolds represent a promising framework for the development of new therapeutic agents targeting anxiety and inflammatory disorders.

Keywords: 1,2,4-triazines derivatives, anxiolytic, anti-inflammatory.



Scheme 1. (a) conc. HNO₃, (b) thiosemicarbazide/semicarbazide, acetic acid, (c) ClCH₂COOEt, pyridine, (d) substituted aldehydes/acetophenones

**Design, Synthesis, Biological Evaluation, and Molecular Docking
Studies of Novel Quinoline-Incorporated 4-Thiazolidinone Derivatives
as Potential Anticancer Agents**

Anzar Jahan¹, Aram Rahman¹, Syed Salahuddin¹, Arifuddin Mohammad²

¹*Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Gachibowli, Hyderabad-500032, Telangana, India*

²*CDOE, Maulana Azad National Urdu University, Gachibowli, Hyderabad-500032,
Telangana, India*

Corresponding Author anzar7912@gmail.com

Abstract

Cancer continues to pose a major global health burden, necessitating the development of novel chemotherapeutic agents with improved efficacy and reduced toxicity. In the present study, a series of novel quinoline-incorporated 4-thiazolidinone derivatives (AR-MANUU-01 to AR-MANUU-07) were rationally designed, synthesized, and evaluated for their anticancer potential. All synthesized derivatives were screened for in vitro cytotoxic activity against a panel of human cancer cell lines, including NCI-H460 (lung cancer), A549, BT-549, HCT-15, HCT-116, PC-3, and DU-145, using the MTT assay, with etoposide as the reference drug. Notably, compounds AR-MANUU-01 and AR-MANUU-05 demonstrated superior inhibition (93.61% and 83.97%, respectively), surpassing the reference drug. IC₅₀ studies further identified AR-MANUU-05 as the most potent derivative, with an IC₅₀ value of 4.40 ± 0.08 μM against NCI-H460 cells, outperforming etoposide. To elucidate the possible mechanism of action, molecular docking studies were performed against human DNA topoisomerase IIβ (PDB ID: 3QX3). Compound AR-MANUU-05 exhibited a strong binding affinity (-3.7 kcal/mol) and favorable interactions within the enzyme's active site, corroborating the in vitro findings. Overall, compound AR-MANUU-05 as a promising lead compound for further development as an anticancer agent, particularly for lung cancer therapy.

Keywords: Quinoline derivatives, 4-Thiazolidinone, Hybrid molecules, Anticancer activity, MTT assay, Lung cancer (NCI-H460), Molecular docking

ICC/MDD/109

Spiro-Pyrollidine-Oxiindole Derivatives: Novel Molecular Scaffolds as an Anti-Cancer Agent

Dr. Akanksha Gupta^{*a} and Dr. Atul Kumar^{*b} Dr. Rajeev Gupta^{*c}

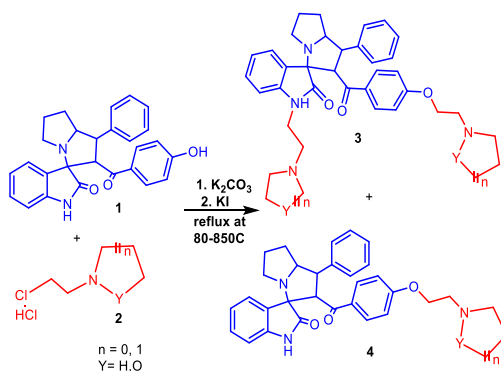
^aLords Institute of Engineering & Technology, Hyderabad, Telegana, India

^bCentral Drug Research Institute, Lucknow, Uttar Pradesh 226031

^cChhatrapati Shahu Ji Maharaj University, Kanpur, Uttar Pradesh 208024

Email: dr.akankshagupta@lords.ac.in

Today breast cancer is the most common cause of cancer death and the most common form of cancer in women with a 9% incidence of being diagnosed during a lifetime.¹ Since estrogens have a crucial role in breast cancer initiation, proliferation, and metastasis, a ligand which can compete or eliminate endogenous estrogen may offer a potent strategy for breast cancer treatment and prevention.² The SERMs are chemically diverse compounds which can be divided in steroidal and non-steroidal frame work. The non-steroidal frame work compound however dominates ER-research. It has been revealed that spiro cyclic oxindole found cytostatically active in three cancer cell lines (human breast cancer MCF-7, human lung cancer H 460, human CNS SF-268). Therefore, keeping in mind a remarkable biological significance of these spiro oxindole derivatives, we designed, rationalised and synthesized the novel **spiro-pyrollidine-oxindole** scaffolds and explored their activity in anti-cancer cell lines. The spiro-pyrollidine-oxindole scaffold, a novel central spiro core mimic estrogenic subunit with anti-estrogenic basic amino side chain of the high profile SERMs in orthogonal placement.



**Magnetically Modified Pomegranate Peel for Methylene Blue Removal:
Process Optimization by Response Surface Methodology and Prediction
via Machine Learning**

Shaida Khan*, Abu Nasar

*Department of Applied Chemistry, Faculty of Engineering and Technology, Aligarh
Muslim University, Aligarh – 202002, India*

Email address: shaidakhan9086@gmail.com

Abstract

Water pollution from dye-containing industrial effluents remains a major environmental concern. Here, a magnetic pomegranate peel-based adsorbent (MPGP) was prepared by in situ co-precipitation of Fe₃O₄ nanoparticles onto the biomass matrix, enabling rapid magnetic separation. The composite was characterized using SEM/EDS, FTIR, XRD, TGA, BET, VSM, and pH_{PZC} measurements to relate surface properties to adsorption behavior. MB removal increased with increasing dosage, with an optimum of 1.2 g/L within the studied range. Higher pH values enhanced removal, reaching ~99.9% under alkaline conditions, and the adsorption equilibrium was attained at approximately 80 min. Process optimization using response surface methodology (RSM) identified operating conditions that maximized MB removal, and model validation experiments showed close agreement with predicted values (if applicable). Equilibrium and kinetic data were fitted with common isotherm and kinetic models, yielding a maximum adsorption capacity of 166.667 mg/g (Langmuir q_{max}) under the tested conditions. Machine-learning models (random forest, XGBoost, and stacking) were trained to predict MB removal, and the stacked model achieved the best predictive performance. Overall, the magnetically separable biomass composite provides an effective route for MB removal, while combining RSM and machine learning improves process optimization and performance prediction.

Keywords: Methylene blue; Magnetic bioadsorbent; Fe₃O₄; Pomegranate peel; Adsorption isotherms; Kinetics; Response surface methodology; Machine learning

Computational Deconvolution of Ligand–Macromolecular Recognition and Binding Energetics at an Insomnia-Associated Molecular Target

Omkesh Vyankatesh Aghav

PG Scholar, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale College Pharmacy, Kondhawa (BK.) Savitribai Phule Pune University, Pune, Maharashtra, 411048, India.

Email: aghavomkesh077@gmail.com

Abstract

The use of computational chemistry in preliminary research provides an ecofriendly substitute for resource demanding experimental screening by minimizing chemical usage and laboratory waste. This work utilized molecular docking to assess the interaction profile of a plant-derived chemical with a specific biological target and to compare its binding affinity to that of a reference standard. The target protein structure was acquired from the Protein Data Bank, and ligand geometries were established prior to docking. Docking simulations were performed with AutoDock Vina to evaluate binding affinity and examine critical molecular interactions inside the binding region. Under the given docking circumstances, the plant-derived chemical showed a lower projected binding energy (–10.2 kcal/mol) than the conventional ligand (–8.8 kcal/mol), suggesting a stronger connection. According to interaction studies, complex stabilization is facilitated by hydrophobic interactions and hydrogen bonds. This work supports sustainable chemistry-driven methods in medical research by illustrating the use of molecular docking as a computational screening technique to find structurally advantageous natural molecules. The results are meant to direct future experimental research and are predictive in nature.

Keywords: Computational chemistry, molecular docking, sustainable chemistry, natural compounds, in-silico screening

Donor-Acceptor Stenhouse Adduct (DASA): A computational investigation on molecular orbital, solvation, and cyclization**Fathima Dilruba Rasheed, Dr. Anoop Ayyappan***Aligarh Muslim University*fathimadilu21@gmail.com**Abstract**

A new class of visible-light-responsive photo-switches known as Donor–acceptor Stenhouse adducts (DASAs) have been discovered in the year 2014 and have been an important subject of recent research. It exhibits a range of vital properties for photochromic materials, such as negative photochromism, visible-light activation, and modular synthesis. Hence, DASAs have found greater application in photo-responsive materials. Three structures of DASAs consisting of an N containing donor group on the left, a system of conjugated double bonds in the middle and an acceptor part on the right which is variously substituted were further investigated using computational methods. Computational methods use computer simulations to solve complex chemical problems. These methods provide a theoretical explanation using computer programs to understand the structure, interaction and to calculate various parameters.

Advances in High Performance Thin Layer Chromatography (HPTLC) Using Artificial Intelligence (AI) and Machine Learning (ML) Tools

Abdul Moheman

Department of Chemistry, Gandhi Faiz-e-Aam College, Shahjahanpur-242001, Uttar Pradesh, India

E-mail: amohemanappchem@gmail.com

Abstract

High performance thin layer chromatography (HPTLC) is a well-known technique utilized in a variety of sectors, including environmental, food analysis, forensics, pharmaceuticals, agriculture and biological research. HPTLC provides several advantages, including high sample throughput, low cost per analysis, simultaneous separation of several samples and standards, minimal sample preparation requirements, and offline zone identification using various post-chromatographic methods. It also enables the preservation of separations for later identification and quantification.

With an increasing demand for automation, precision, and high-throughput analysis, the combination of Artificial Intelligence (AI) and Machine Learning (ML) has opened up new opportunities for improving HPTLC performance. This study summarizes current achievements in the use of AI and ML approaches to HPTLC, such as digital image analysis, peak detection, compound identification, retention prediction, and pattern recognition. We explore innovative approaches, existing challenges, and future prospects, emphasizing AI's revolutionary role in chromatographic analysis.

Keywords: Artificial Intelligence (AI) in Chromatography, High Performance Thin Layer Chromatography (HPTLC), Machine Learning (ML), Separation, Retention Prediction

Integrated quantum chemical computational studies of 4,7-dichloroquinoline as a potential lead for PPAR γ activation as Anticancer Agents

Saiyyad Mohammedzaid¹, Adiba Zohra¹, Saleem Javed^{1*}

¹Department of Chemistry, Jamia Millia Islamia, New Delhi-110025
sjaved1@jmi.ac.in

Abstract

The activation of PPAR γ has been demonstrated to encourage the differentiation of cancer cells, indicating it may be a valuable approach for creating novel therapies for undifferentiated carcinomas with reduced side effects. Herein, we present a heterocyclic compound, 4,7-dichloroquinoline (4,7-DCQ), using quantum chemical calculations and molecular modelling methods. Density Functional Theory (DFT) calculations were conducted utilizing Gaussian 09W at the B3LYP/6-311G++(d,p) level to optimize molecular geometry. Electronic properties were evaluated using the HOMO-LUMO energy gap (4.6573eV) together with the topological descriptors, which included molecular electrostatic potential (MEP) mapping ($\pm 3.67 \times 10^{-2}$ a.u.) and the electron localization function (ELF). The conceptual density functional theory (CDFT) was computed to calculate the global descriptors yielding electrophilicity index of ~ 4.5 .³ The in silico ADME studies suggested strong compliance with Lipinski's Rule of Five and Veber's criteria, moderate probability of bioavailability, indicating favourable drug-likeness. PPAR γ is a nuclear receptor and its ligand-binding domain (PDB ID: 6AD9) which is a regulatory protein and 4,7-DCQ binds within its binding pocket with a binding affinity of $-7.4 \text{ kcal mol}^{-1}$, indicating a possible involvement in the activation of PPAR γ related to the differentiation of cancer cells. To validate this, GROMACS assisted molecular dynamics simulation of 500 ns was carried out which displayed the average RMSD profiles ($\sim 0.6 \text{ nm}$), constant hydrogen bonds and radius of gyration of $\sim 1.9 \text{ nm}$ during the simulation resulting into stable protein ligand complexes. Collectively, the computational studies of 4,7-DCQ indicates that it could be served as a stable and promising lead compound for PPAR γ -mediated differentiation-based cancer therapy.

A reproducible multi-scale computational workflow for DL-methionine in breast cancer targets: DFT, data-driven docking, MD and MM-PBSA validation

Mohd. Zaid¹, Md Wasee Murtuza¹, Manoj Sharma¹, Saleem Javed¹

¹*Department of Chemistry, Jamia Millia Islamia, New Delhi-110025*

Corresponding Author Email: sjaved1@jmi.ac.in

Abstract

The structural, vibrational, electronic, and biological relevance of DL-Methionine (DL-MT), a potential anti-breast cancer agent, were investigated using experimental FT-IR and UV-Vis spectra, density functional theory (DFT), molecular docking, molecular dynamics (MD) simulations, and MM-PBSA binding free-energy estimation. Harmonic vibrational wave numbers were calculated at the B3LYP/6-311++G(d,p) level for optimized geometries and vibrational spectrum assignments were obtained using normal coordinate analysis in conjunction with Pulay's SQMFF methodology, allowing for a precise correlation between simulated and experimental spectral profiles. A comparison of DL-MT frontier molecular orbital (FMO) gaps in dissimilar environments disclosed energy gap values of 5.608eV (gas), 5.586eV (water), 5.577eV (methanol) and 5.581eV (DMSO), indicating solvent-dependent modulation of reactivity. To predict electrophilic and nucleophilic reactive sites, molecular electrostatic potential (MEP) visualisations were generated in both gas and solvent phases, and Fukui function descriptors were also assessed. A comparison of DL-MT frontier molecular orbital (FMO) gaps in different settings yielded energy gap values of 5.608 eV (gas), 5.586 eV (water), 5.577 eV (methanol), and 5.581eV (DMSO), demonstrating solvent-dependent reactivity. To anticipate electrophilic and nucleophilic reactive sites, molecular electrostatic potential (MEP) visualizations were created in both gas and solvent phases, and Fukui function descriptors were evaluated. In addition, AIM, RDG/NCI, DORI, ELF, and LOL topological investigations were performed to gain a better understanding of intramolecular stabilisation and electron density localization behaviour.

**Quantum Computational, Spectroscopic, Topological, Molecular
Docking, and Dynamics Studies of 2-Amino-3-Hydroxypyridine
(2A3HP): A Potential Antimicrobial Agent**

Manoj Sharma¹, Md Wasee Murtuza¹, Mohd Zaid¹ and Saleem Javed¹

¹*Jamia Millia Islamia India*

Corresponding Author Email: sjaves1@jmi.ac.in

Abstract

Antimicrobial resistance requires computational techniques that associate molecular electronic structure to target-level binding stability. DFT geometry optimization and electronic properties calculations were performed at B3LYP/6-311++G(d,p) level and solvent effects (acetone, 1-propanol, water) were considered using IEFPCM and excited state properties were calculated using TD-DFT to interpret UV-Vis features. Reactivity and charge distribution were determined by using frontier molecular orbital (FMO) descriptor, MEP surface and Fukui functions, while noncovalent interaction patterns were studied by Hirshfeld surface analysis combined with RDG/ELF/LOL topological descriptor. The surface map of the MEP is between -7.082 and 7.082a.u in gas, -8.542 to 8.542a.u for water and -8.451 to 8.451a.u for acetone. FMO analysis shows a narrowly distributed HOMO-LUMO gap 5.104eV in gas phase and 5.116-5.118eV in solvents, which support moderate kinetic stability while enabling intramolecular charge transfer. The NBO analysis shows that the strong donor-acceptor delocalization is dominated by LP(1)N4 → $\pi^*(\text{N3-C7})$ with $E(2) = 37.47$ kcal/mol. A 100 ns MD simulation of the 1CF3-2A3HP complex further validated docking-supported binding, demonstrating stable complex behaviour with ligand RMSD observed at 0.40-0.55 nm, protein folding (Rg value 2.33-2.38 nm), consistent SASA (215-230 nm²), and persistent protein-ligand hydrogen bonding (4-8 H-bonds), confirming dynamic stability under physiological temperature (300K). The hybrid quantum calculation to dynamics simulation computational platform places 2A3HP as a currently advancing antimicrobial lead scaffold and offers the basis of quantitative reasons of future optimization and experimental screening.

Bridging electronic structure and binding stability: DFT, docking and MD investigations of Ninhydrin as a Promising AChE Inhibitor Lead

Adiba Zohra¹, Saiyyad Mohammedzaid¹, Saleem Javed^{1*}

¹*Department of Chemistry, Jamia Millia Islamia, New Delhi-110025*

* Corresponding Author Email: sjaved1@jmi.ac.in

Abstract

The acetylcholinesterase (AChE) inhibitors remain key therapeutic drugs for the treatment of Alzheimer's disease (AD). Herein, we report a multiscale computational workflow to explore ninhydrin as a potential AChE inhibitor lead through using quantum chemistry, molecular docking, and molecular dynamics simulations. Density functional theory (DFT) calculations were carried out using B3LYP/6-311G++ (d,p) level for geometry optimisation followed by frequency analysis to confirm that the optimised structure corresponds to a true minimum. Time-dependent DFT (TD-DFT) was used to examine key excited-state features, and conceptual DFT (cDFT) was employed to compute the electrophilicity index, which was found to lie in an acceptable range, supporting a reasonable balance of reactivity for further consideration.

Molecular docking was performed using AutoDock Vina with the AChE binding site models derived from the above PDB structures. The best predicted binding affinity was -8.6 kcal/mol with 7D9Q, while the other AChE conformations (4EY7, 7D9O and 7D9P) yielded consistent scores in the range of -7.6 to -8.0 kcal/mol, suggesting stable binding in the target active site. Further validation came from molecular dynamics simulations (MDS), molecular dynamics simulations were used to test the stability of the docked complex. The trajectory showed a stable behaviour with a plateau-like value around 0.85 nm, indicating that the complex remains well maintained during the simulation. These findings highlight ninhydrin's potential as a lead for AD drug design, leveraging its computational binding strength and dynamic stability.

Comparative Molecular Docking Analysis Targeting HER2 and ROR Gamma Receptors in Breast Cancer Progression

Neha Tarase

*PG. Scholar, Department of Pharmaceutical Chemistry, STES, Smt. Kashibai Navale
College of Pharmacy, Kondhwa (Bk.), Savitribai Phule Pune University, Pune,
Maharashtra-411048, India,
Email: nehatarase84@gmail.com*

Abstract

Breast cancer research increasingly utilizes computational techniques to evaluate therapeutic candidates while maintaining target confidentiality. Molecular docking serves as a reliable in-silico approach to assess binding affinity, conformational stability, and interaction strength of ligands prior to experimental validation. In the present study, a comparative docking analysis was conducted to evaluate the binding behavior of two selected ligands, referred to as Ligand-1 and Ligand-2, against a biologically relevant receptor associated with breast cancer. Docking results demonstrated that Ligand-1 exhibited strong binding affinity, with docking scores ranging from -8.5 to -8.2 kcal/mol, indicating favorable interaction strength. The RMSD values for Ligand-1 were observed between 2.615 and 3.004 Å. In contrast, Ligand-2 showed moderate binding affinity values ranging from -7.7 to -7.4 kcal/mol. Interaction analysis further revealed that Ligand-1 formed multiple stabilizing interactions, including hydrogen bonding, hydrophobic contacts, and π - π stacking, which collectively enhanced ligand-receptor complex stability. Ligand-2 primarily exhibited hydrophobic interactions with limited hydrogen bonding and lacked π - π stacking interactions, contributing to its lower binding consistency. Overall, the comparative evaluation highlights Ligand-1 as a more stable and reliable candidate based on its stronger binding affinity and lower RMSD values, whereas Ligand-2 demonstrated structural instability and variable binding behavior. This study emphasizes the importance of RMSD and interaction profiling in interpreting docking outcomes and supports the application of computational docking as an effective tool in early-stage breast cancer-oriented drug evaluation, while preserving the novelty of the biological target.

Role of Advanced and Sustainable Nanomaterials in Water and Wastewater Treatment: Mechanisms, Applications, and AI-Aided Insights

Fatima Zahra*, Shaikh Sana Naeem, Zeeshan Ahamad

*Chemistry Section, School of Sciences, Maulana Azad National Urdu University,
Hyderabad, Telangana 500032, India*

Abstract

The presence of various organic waste, heavy metals, and non-biodegradable materials present at higher concentration in wastewater necessitates the development of advanced, efficient, and sustainable treatment technologies. In this context, different methods like reverse osmosis, advanced oxidation process, ultrafiltration and nanotechnology had been applied for reducing or eliminating the toxic pollutants from wastewater. The nanomaterials have emerged as transformative agents for water and wastewater treatment due to their high surface area, low-cost, tunable surface chemistry, and enhanced selectivity. This chapter provides a comprehensive overview of advanced and sustainable nanomaterials including carbon-based nanostructures, metal and metal oxide nanoparticles, magnetic nanomaterials, polymeric nanocomposites, and hybrid systems employed for the removal of organic and inorganic contaminants from aqueous solutions. In addition to laboratory-scale applications, the chapter critically discusses performance evaluation under realistic water matrices, regeneration, reusability, and environmental safety considerations. A unique feature of this chapter is the integration of artificial intelligence (AI) and machine learning approaches to predict removal efficiencies, optimize process parameters, and accelerate material design. By bridging experimental insights with data-driven modeling, this chapter highlights emerging trends and future directions toward scalable, cost-effective, and environmentally benign nanomaterial-based water treatment technologies.

Keywords: Nanomaterials, nanocomposites, wastewater treatment, adsorption, sustainability, AI, mechanism, application

In silico studies on Fenamic Acid as a potential human dihydroorotate dehydrogenase (DHODH) inhibitor employing molecular docking, molecular dynamics, MM-PBSA, PCA, FEL and ADME analysis

Md Wasee Murtuza¹, Ayesha Parveen¹, Saleem Javed^{1*}

¹*Department of Chemistry, Jamia Millia Islamia, New Delhi-110025*

* Corresponding Author Email: sjaved1@jmi.ac.in

Abstract

Human dihydroorotate dehydrogenase (DHODH) is a key mitochondrial enzyme involved in de novo pyrimidine biosynthesis and is considered an important therapeutic target for several proliferative and inflammatory disorders¹. In the present work, an integrated in silico approach was employed to explore the potential of fenamic acid as a DHODH inhibitor using computational chemistry and molecular simulation techniques. The electronic structure and reactivity of fenamic acid were first investigated using conceptual density functional theory (cDFT) at the B3LYP/6-311++G(d,p) level. The calculated electrophilicity index was found to be within an acceptable range, indicating favorable reactivity and chemical stability. Further electronic and topological analyses using molecular electrostatic potential (MEP), electron localization function (ELF), and time-dependent DFT (TD-DFT) confirmed the stable electronic nature of the molecule. Molecular docking studies were carried out against the crystal structure of human DHODH (PDB ID: 2WV8). Fenamic acid exhibited strong binding affinity with a docking score of -9.2 kcal/mol and showed stable interactions within the catalytic ubiquinone-binding site. To validate the docking results, molecular dynamics simulations were performed, and the stability of the protein-ligand complex was assessed using RMSD and RMSF analyses, which indicated stable binding throughout the simulation period. These results supported the formation of a stable and energetically favourable DHODH-fenamic acid complex. In addition, in silico ADME analysis revealed that fenamic acid satisfies Lipinski's rule of five and shows a bioavailability score of 0.55, suggesting acceptable drug-likeness. Collectively, the present in silico study suggests that fenamic acid demonstrates strong binding affinity and stable interactions with human DHODH and may serve as a potential lead scaffold for the development of DHODH inhibitors.

Quinoline-Pyridine Schiff Bases Hybrids as Potential Anticancer Agents

Aram Rahman¹, Anzar Jahan¹, Salahuddin Syed^{1*}, Zuverya Zareen¹, Salman Ahmed Khan¹, Mohammad Ariffuddin²

¹Chemistry Section, School of Sciences, Maulana Azad National Urdu University, Hyderabad-India

²Department of Chemistry, Centre for Distance and Online Education (CDOE), Maulana Azad National Urdu University, Hyderabad-India

*Corresponding Author: Dr. Syed Salahuddin: salahuddinsyed@manuu.edu.in

Abstract

The 2-Chloroquinoline-3-carbaldehyde derivatives incorporated with pyridine derivatives with Schiff base were synthesized. The characterization of the synthesized compounds was done by IR, mass and ¹HNMR and ¹³C-NMR spectral analysis. The anticancer activities of the synthesized compounds were screened against different cancer cell line i.e., NCIH460, HCT15, HCT116, A549 and PC3. The results revealed that they are active and among them, the compounds AR-MANUU-103, 104 and 107 are showing maximum activities against all cell line, in terms of % inhibition cell viability results for the NCIH460 the compounds AR-MANUU-103 is showing the 70.32% inhibition, AR-MANUU-104 70.92 % inhibition and AR-MANUU-107 is exhibiting the 73.54% inhibition, whereas the IC₅₀ values for NCIH460 for the compounds AR-MANUU-103 is 3.75 µg/ml, AR-MANUU-104 3.73 µg/ml and AR-MANUU-107 is exhibiting the 2.58 µg/ml respectively. Thus, the compounds AR-MANUU-103, 104 and 107 are most active against cell line NCIH460 understand their binding interactions with human topoisomerase II protein. It was observed that the binding energy is ranging between -2.9 to 3.1kcal/mol. The results of the anticancer and molecular docking analysis in the present study demonstrated that the synthesized compounds are possessing potential anticancer activity. Thus it can be anticipated that AR-MANUU-107 can be emerged as a lead compound for the Large-cell lung carcinoma upon on further details anticancer studies.

Keywords: 2-Chloroquinoline-3-carbaldehyde, Ammonium Molybdate, Aminopyridine, Schiff bases, Anti-cancer activity, In-Silico studies.

Nanoengineered Biodegradable Polymers for Targeted Cancer Therapy**Dr. Rehana Anjum and Arshiya Anjum***Lords Institute of Engineering and Technology, Himayath Sagar, Hyderabad, 500091, Telangana***Abstract**

Targeted cancer therapy aims to enhance therapeutic efficacy while minimizing systemic toxicity associated with conventional chemotherapy. However, challenges such as poor tumor selectivity, multidrug resistance, rapid systemic clearance, and limited drug solubility significantly restrict clinical outcomes. This study investigates the development and mechanistic evaluation of surface-functionalized biodegradable polymeric nanoparticles for site-specific anticancer drug delivery. Biodegradable polymeric nanoparticles were synthesized using poly (lactic-co-glycolic acid) via the emulsion–solvent evaporation technique. Surface functionalization was performed through PEGylation to prolong systemic circulation and conjugation with folic acid as a targeting ligand for receptor-mediated uptake in folate-overexpressing cancer cells. Physicochemical characterization included dynamic light scattering for particle size and polydispersity index, zeta potential analysis for surface charge, transmission electron microscopy for morphology, and high-performance liquid chromatography for drug encapsulation efficiency. In vitro drug release kinetics were evaluated under physiological (pH 7.4) and tumor-mimicking acidic conditions (pH 6.5). Cellular uptake studies were performed using fluorescence microscopy, and cytotoxicity was assessed via MTT assay on human cancer cell lines.

Nanoengineered biodegradable polymeric systems provide a robust and adaptable platform for targeted cancer therapy by integrating controlled release, receptor-mediated uptake, and enhanced tumor accumulation. Their capacity to overcome pharmacokinetic limitations and improve therapeutic index underscores their potential in precision oncology. Future research should focus on in vivo pharmacokinetic validation, immunogenicity assessment, and scalable manufacturing strategies to facilitate clinical translation and commercialization.

Preparation of Thiazole Schiff bases by grinding method

^aAfreen, ^{*b}Amarnath Velidandi,

^aDepartment of S&H, Lords Institute of Engineering and technology,

Himayath sagar, Hyderabad, 500091,

^{*b} Department of Physical Sciences, Kakatiya Institute of Technology and Science,

Hanamakonda, Telangana,

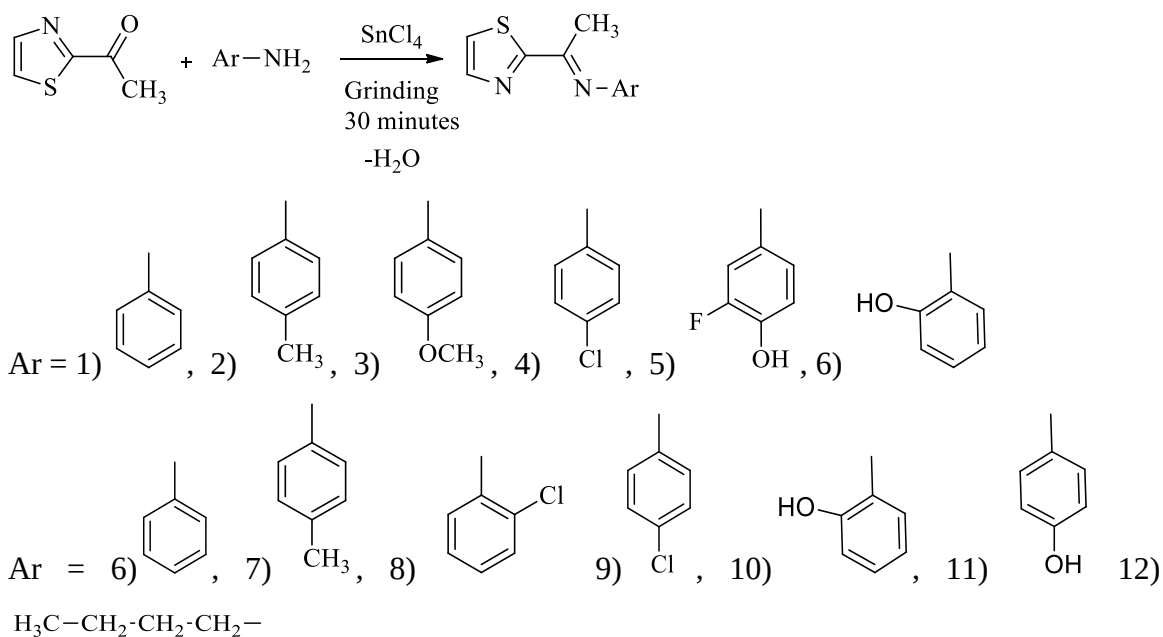
email: afreen.mohammad@gmail.com, velidandi@yahoo.co.in

Abstract

Thiazole contained based Schiff bases shows various biological activities. Herein, we discussed the simple, low cost Tin chloride mediated grinding method for the titled compounds.

Keywords: Tin chloride, Thiazole, Imidazole, Schiff bases, and herbicidal activity

(Scheme 1)



Thiazole, Coumarin conjugated (β -lactam scaffold) Azetidinones

Synthesis and their substitution effect

Dr.AFREEN

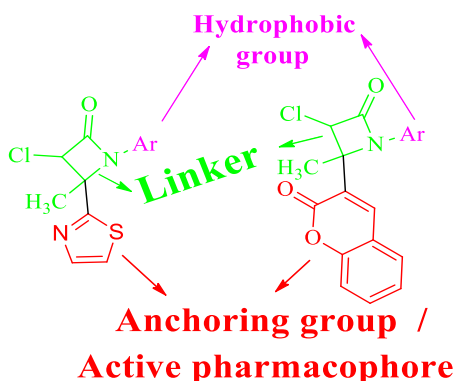
Lords Institute of Engineering and Technology, Himayath Sagar, Hyderabad, 5000091

Abstract

Thiazole, Coumarin conjugated (β -lactam scaffold) Azetidinones Synthesis and their substitution effect Azetidinones (β -lactams) and bicyclic diaza compounds are important structures found in many biologically active molecules such as antibiotics, enzyme inhibitors, and central nervous system drugs. In this work, we describe a step-by-step method for the synthesis of these compounds. In the first method, aldehydes were converted into hydrazones. These hydrazones were then cyclized to form azetidinone derivatives through Schiff base formation followed by [2+2] cyclocondensation using chloroacetyl chloride. In the second method, aldehydes were converted into chalcones. The chalcones were then transformed into pyridine derivatives, which were further converted into bicyclic diaza compounds. The 2,5-diazabicyclo [2.2.1] heptane derivatives were synthesized by double reductive amination of glutaraldehyde with ethylenediamine. All reactions were carried out under mild conditions. The synthesized compounds showed significant biological activities, including antimicrobial and antioxidant properties. These compounds can serve as useful scaffolds for drug discovery and structure–activity relationship (SAR) studies.

Graphical representation.

Conjugates role in the Azetidinone





3rd-ICC-2026

