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P M USHA sponsored Two days International Seminar on Research and Innovations in Chemical Sciences

12th & 13th January, 2026

Organized By

Department of Chemistry,
M G Science Institute
Opp. Gujarat University, Navarangpura
Ahmedabad 380 009, Gujarat (India)

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M. G. Science Institute has been a premier center for scientific learning and inquiry for nearly seven decades. Established in 1946 by visionary educators committed to providing quality science education, the college is managed by the Ahmedabad Education Society. The institute offers the largest number of undergraduate and several postgraduate science programs in the region.

Situated in the heart of Ahmedabad, its spacious campus provides a serene environment conducive to academic growth. The college is affiliated with Gujarat University, the largest university in the state, and has been accredited with an 'A' Grade by NAAC in 2007, 2014, and 2022. In 2024,

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it achieved an Autonomous status. The institute is also the recipient of several prestigious grants, including the DBT Star College grant, DST-FIST grant, RUSA 1.0, RUSA 2.0, and the PM-USHA grant. The Chemistry Department, established alongside the college in 1946, is both the oldest and the largest department on campus. It currently offers B.Sc., M.Sc., and Ph.D. programs in Chemistry. Supported by a highly qualified and experienced faculty, the department has produced numerous researchers, industrialists, academicians, and entrepreneurs who contribute significantly to India and the global scientific community.

Theme of the Seminar

The seminar aims to explore emerging research areas and innovations in chemical sciences. The central theme **"Addressing Global Challenges through Synergistic Integration of Fundamental and Interdisciplinary Chemical Knowledge"**—highlights the need to combine core chemical principles with cross-disciplinary insights to foster innovative solutions for sustainable development. Our objective is to provide a common platform for chemists across all disciplines, along with experts from allied fields, to exchange transformative ideas that strengthen scientific and technological expertise.

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Abstract for Oral Paper

OP1

Synthesis and Molecular Docking Studies of Novel Adamantane Schiff Base Derivatives

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Abstract
The study describes the synthesis of novel adamantane-based Schiff base derivatives and their evaluation through molecular docking against the estrogen receptor alpha ligand-binding domain (PDB ID: 5U2B). Ligands were docked using the Glide module of the Schrödinger molecular modelling suite to predict binding modes, docking scores, and key receptor–ligand interactions. Several derivatives showed favourable Glide Scores with hydrophobic engagement of the adamantane core and hydrogen bonding by the azomethine group in the receptor pocket, suggesting promising ERα-targeted activity relevant to hormone-dependent cancers. These in silico findings provide a rational basis for prioritizing selected adamantane Schiff bases for further in vitroanti-cancer evaluation on ER-positive breast cancer models

Keywords: Adamantane Schiff base, 5U2B, Molecular docking, Estrogen receptor, Anti-cancer potential

OP2

Design, Synthesis and Evaluation of 3,4-Dihydroquinolin-2(1*H*)-one Derivatives as Antiplatelet Agents

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Abstract
Thrombosis refers to the formation of a blood clot that partially or entirely blocks a blood vessel, thereby disrupting normal blood flow. This impairment in circulation can lead to serious clinical outcomes such as ischemia, stroke, myocardial infarction, and other cardiovascular disorders. During the COVID-19 pandemic, a markedly increased prevalence of prothrombotic complications was reported among infected patients. Notably, individuals aged 85 years and older exhibited significantly higher mortality rates. Within platelets, three major phosphodiesterase (PDE) isoforms—PDE2, PDE3, and PDE5—play a critical role in regulating platelet function. Among the platelet phosphodiesterase, PDE3 is the most dominant, accounting for approximately 80–90% of the total PDE activity. It exhibits a low Km for cyclic AMP (cAMP) and is capable of competitively inhibiting cyclic GMP (cGMP), thereby producing a pronounced antiplatelet effect. Initially, it was believed that cGMP directly inhibits PDE3; however, subsequent studies revealed that cGMP suppresses cAMP hydrolysis by competing at the enzyme's catalytic site. Cilostazol is a selective PDE3 inhibitor known to exert antiplatelet activity by increasing intracellular cAMP levels in smooth muscle cells. During the investigation of enzyme–ligand interactions, the 3,4-dihydroquinolin-2(1H)-one scaffold was identified as forming key interactions with critical amino acid residues. Guided by these findings, a series of novel compounds was rationally designed and subjected to molecular docking studies. Their drug-likeness was assessed using ADME and TOPKAT modules available in BIOVIA Discovery Studio. Compounds that satisfied the drug-likeness criteria were subsequently synthesized and structurally confirmed through mass spectrometry, infrared spectroscopy, and nuclear magnetic

resonance analysis. These synthesized compounds will be further evaluated for their antiplatelet activity.

Key words: Thrombosis, PDE3, Cilostazol, 3,4-dihydroquinolin-2(1*H*)-one

OP3

Synthesis, characterization and phase behavior with ester of terminal alkoxy chains and methoxy substituent

Gita Zala and Pramodkumar Mahour
Department of Chemistry, Monark University, Ahmedabad

Abstract
A series of calamitic phenyl ester-aromatic imine derived from the reaction of 4-(N'-(4-methoxyphenyl)acetimidamido)phenyl 4-alkoxybenzoate by condensing 0.1 Mole of 4-acetamidophenyl -4-*n*-alkoxy benzoates [B] with 0.1 mole of 4-anisidine exhibited mesomorphic and present series compared with other structure related series have been successfully synthesized and characterized. The general molecular structures of ultimate compounds show the central fragment made up by a hybrid core of phenyl ester-aromatic imine in which the terminal alkoxy(-OR) chains, $C_n H_{2n+1}$ in which n = 1 to 8, 10,12,14 and 16 were connected to phenyl while the other end consists of methoxy moiety attached to a phenyl ring. All the target compounds under polarized lights exhibit enantiotropic nematic phase of which the temperature range was further supported by DSC analysis. It can be summarized that the lengthening of terminal alkoxy (-OR) chains has contributed to the lowering of melting and clearing temperatures as well as the thermal stability of nematic phase.

Keywords: Aromatic imine, central fragment, enantiotropic, polarized, nematic

OP4

Synthesis And Characterization Of Chitin Nanoparticles and their Application for Different Color Dye Removal from Wastewater

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Abstract
The release of dyestuffs into water resources poses significant environmental harm, necessitating effective and cost-efficient removal methods. Adsorption using biodegradable and renewable biopolymers like chitin offers a promising solution. Chitin nanoparticles, extracted from sea shells and subjected to acid hydrolysis, were investigated for their adsorption efficiency of Congo red dye ($C_{32}H_{22}N_6Na_2O_6S_2$) and antibacterial activity against Bacillus cereus. The compositional and morphological properties of the chitin nanoparticles were characterized using SEM, FTIR Spectroscopy and UV-Visible Spectroscopy. The results demonstrate the potential of chitin nanoparticles as an adsorbent for Congo red dye removal, highlighting their feasibility for environmental remediation applications. The studyreveals that the -NH_2 and -OH groups of chitosan enhance the adsorption capacity of the nanoparticles, while their low surface area and crystalline nature contribute to efficient dye removal. The findings suggest that chitin nanoparticles could be a viable alternative to traditional adsorbents, offering a sustainable and eco-friendly solution for textile wastewater treatment. Moreover, the nanoparticles exhibited significant antibacterial activity,

inhibiting the growth of Bacillus cereus, making them a promising material for water purification and biomedical applications.

Keywords: Chitin, Chitosan, SEM Morphology, FTIR, UV

OP5

Natural Antioxidant Resveratrol: In-Silico Evidence of Its Therapeutic Promise

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Abstract:
Resveratrol is a naturally occurring polyphenolic stilbene predominantly found in grapes and has been extensively investigated for its potent anti-inflammatory properties. Persistent inflammation plays a central role in the development and progression of various chronic and degenerative diseases, emphasizing the need for effective anti-inflammatory agents with minimal side effects. Resveratrol has demonstrated the ability to regulate inflammatory responses through antioxidant activity and interaction with key inflammation-associated molecular targets.
In the present study, the molecular basis of resveratrol's anti-inflammatory potential was explored using in silico molecular docking analysis against the inflammation-related protein target 5KIR. Docking simulations revealed a favorable binding affinity of resveratrol within the active site of 5KIR, indicating stable ligand–protein complex formation. Detailed interaction analysis showed the involvement of hydrogen bonding and hydrophobic interactions, which are critical for binding stability and functional modulation of the target protein. These interactions suggest that resveratrol may influence inflammatory signaling pathways mediated by 5KIR.
Overall, the docking results provide mechanistic insights into the anti-inflammatory action of resveratrol at the molecular level. The findings support the potential of resveratrol as a natural lead compound for the development of inflammation-targeted therapeutic agents. Further experimental and biological validation is required to corroborate these computational predictions and advance resveratrol toward clinical relevance.

Keywords: Resveratrol, Molecular Docking, 5KIR, anti-inflammatory potential

OP6

Light-Modulated, Color-Transformed Chemobrionic Tubes for Memristive Device and Neuromorphic/Bio-Inspired Computing Applications

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Abstract
Chemobrionically prepared inorganic tubular architectures were developed through far-from-equilibrium growth processes, enabling controlled modulation of structural and electronic characteristics arising intrinsically during material formation. The self-organized growth environment promotes the development of complex morphologies with defect-rich frameworks, nonstoichiometric regions, and heterogeneous conduction pathways within films derived from these architectures. These synthesis-induced features play a key role in governing charge transport and interfacial dynamics in the resulting electronic devices. Electrical characterization reveals reproducible and robust resistive switching behavior, characterized by well-defined resistance states, stable cycling endurance, and reliable data retention. The memristive response originates from defect-mediated conduction mechanisms within the active layer combined with interfacial barrier modulation at the memristor film–electrode interface, rather than from any external post-fabrication stimulus. Furthermore, the devices exhibit nonlinear and history-dependent electrical responses, where the present resistance state depends on prior electrical biasing, closely resembling synaptic information processing. These characteristics highlight the suitability of chemobrionic-derived systems for neuromorphic and bio-inspired computing applications, particularly as artificial synaptic elements. The inherent structural tunability afforded by chemobrionic growth, together with stable memristive performance, positions these materials as a versatile and scalable platform for next-generation adaptive and energy-efficient electronics. Overall, this work demonstrates the potential of chemobrionic synthesis as an effective strategy for engineering functional memristive systems through growth-controlled material design, enabling the development of neuromorphic device architectures without reliance on complex fabrication techniques.

Keywords: Memristive Device, Chemobrionic Tubes, Neuromorphic application

OP7

From Fallen Leaves to Soil Nourishment: Microbial Conversion of Dry Leaves into Organic Fertilizer

Vishakha Hingu
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Abstract
Dry leaves are generated in large quantities in residential areas, roadsides, parks, agricultural lands, and public spaces, and are often treated as waste. Improper disposal practices, including open burning of dry leaves, contribute to air pollution, smoke generation, and loss of valuable organic resources that could otherwise enhance soil fertility. Sustainable utilization of this biodegradable waste is therefore essential for effective waste management and environmental protection.
The aim of the present study is to develop an eco-friendly organic fertilizer from dry leaves through biological treatment and microbial activation.
The objectives include the collection and processing of dry leaves, enrichment with organic additives such as cow dung, neem leaf powder, and moringa (drumstick) leaf powder as a natural source of calcium, maintenance of a balanced nitrogen–phosphorus–potassium (NPK) composition, and enhancement of beneficial microbial activity to accelerate decomposition and improve nutrient availability. The prepared fertilizer is intended for soil application to support plant growth, restore soil nutrients, and reduce environmental pollution associated with dry leaf disposal.
The results indicate that microbial treatment significantly improves the decomposition rate of dry leaves and enhances organic matter content and nutrient release. Application of the fertilizer improves soil structure, microbial activity, and overall soil fertility while reducing dry leaf waste and associated pollution.

In conclusion, this study demonstrates a sustainable, cost-effective, and environmentally friendly approach to converting dry leaf waste into a valuable organic fertilizer, promoting waste recycling, pollution control, and sustainable soil and ecosystem management.

Ke words: Dry leaves, Fertilizers, waste management, microbial activation

OP8

Synthesis and study of mesomorphic state of matter through new homologous series

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Abstract
The mesomorphic state of matter intermediate to crystalline solid and isotropic liquid was discovered in 1888. Synthesis of a new azoester homologous series is carried out with a view to understand and establish the effect of molecular structure on Liquid crystal (LC) behaviours of a substance. All the homologues are enantiotropically nematogenic without exhibition of smectic property. Transition and melting temperatures, textures of LC are determined by an optical polarizing microscopy equipped with a heating stage. Textures of nematic phase are threaded or schlieren. Transition curves of a phase diagram behaved in normal manner. Nematic-Isotropic transition curve exhibited odd-even effect.Analytical and spectral data supported and confirmed the structures of homologues. New azoester homologous series is entirely nematogenic without exhibition of smectogenic character and the middle ordered melting type. My aim is to synthesize low temperature liquid crystalline compounds to get desired results and also to establish structure-property relationship.

Keywords: Smectic, Nematic, Mesogen, Liquid Crystals, Azoester

OP9

Exploration of a Newly Synthesized Benzothiazole-Based Pd (II) Complex as a Catalyst in the Suzuki Reaction

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Abstract
A new ligand was synthesized by the condensation of 2-hydrazino benzothiazole with different aromatic aldehydes. This ligand was then used to makePalladium metal complexes that were stable

in both air and water. The effect of different base ratios on the coupling reaction's performance was analyzed. This method is a very simple, efficient and mild protocol for the cross-coupling of aryl bromides with aryl boronic acids and the reactions proceededeffortlessly in excellent yields within short reaction times. All reactions were carried out in anhydrous condition.

Keywords: N, O, O-donating ligand, Palladium complex, Suzuki coupling, Schiff base

OP10

Zn/Mo nanocomposite: An efficient and reusable catalyst for the synthesis of 4-H Pyran derivatives

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Abstract
This study reports the synthesis of an efficient, novel, and cost-effective Zn/Mo nanocomposite via Sol-Gel method, characterized using Powder XRD, FT-IR, FE-SEM, and EDS techniques. The resulting nanomaterial serves as a heterogeneous catalyst for the rapid production of tetrahydrobenzo[b]pyran derivatives under mild conditions. Optimal synthesis conditions were determined, achieving a remarkable yield of 92% using ethanol as a solvent, 0.03 g of Zn/Mo nanocomposites, and a reaction time of just 7 minutes at 80°C. The composite oxide catalyst demonstrated excellent catalytic efficiency, and its recyclability was confirmed, maintaining activity over four cycles. The protocol highlights the advantages of a unique recyclable nanocatalyst, high yields of products, and safe reaction conditions, making it a promising approach for synthesizing tetrahydrobenzo[b]pyrans.

Keywords: Sol-gel synthesis,ZnO–MoO_3, P-XRD, SEM,Nanocatalyst

OP11

Influence of Ortho-Trifluoromethyl Substitution on the Mesomorphic and Thermal Behavior of Azo-Ester Liquid Crystals: Experimental and DFT Insights

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Abstract

A new homologous series of azo-ester-based liquid crystals bearing an ortho-trifluoromethyl (–CF_3) substituent has been synthesized and characterized to explore the influence of lateral fluorination on mesomorphic and thermal behavior. The series comprises derivatives with varying alkoxy chain lengths (C_3-C_8, C_{10}, C_{12}, and C_{14}). Structural confirmation was achieved through FT-IR, ^{1}H NMR, and mass spectrometric analyses. Differential scanning calorimetry (DSC) and polarizing optical microscopy (POM) studies revealed that the first four members (C_3–C_6) are non-mesomorphic, while the higher homologues (C_7–C_{14}) exhibit monotropic smectic phases, indicating that the elongation of the terminal alkyl chain favors mesophase formation. Thermogravimetric analysis (TGA) demonstrated good thermal stability of the compounds. Density functional theory (DFT) calculations provided optimized geometries, HOMO–LUMO distributions, molecular electrostatic potential (MEP) maps, and dipole moments, supporting the experimental findings and elucidating the effect of the ortho–CF_3 group on molecular polarity and planarity. The combined experimental and computational results highlight how ortho-trifluoromethyl substitution affects both the mesomorphic and thermal properties of azo-ester-based liquid crystals.

Keywords: Mesomorphism, Smectic, Monotropic, Trifluoromethyl, DFT

OP12

Synthesis and Antimicrobial Evaluation of some 4-Alkoxybenzoic Acid Piperidine-2-yl Methyl Ester and 1-(4-Propoxyphenyl)-N-(3H-1,2,4-triazol-4-yl)methanimine

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Abstract
The escalating challenge of microbial resistance necessitates the development ofnovel bioactive molecules. This study details the multi-step synthesis of two distinctheterocyclic derivatives: an ester, some 4-alkoxybenzoic acid piperidine-2-yl methyl ester, anda Schiff base, 1-(4-alkoxyphenyl)-N-(3H1,2,4-triazol-4-yl) methanimine. The ester wassynthesized via the DCC/DMAP-mediated coupling of 4-n-alkoxybenzoic acid with 2-piperidinemethanol, yielding 70–75%. The triazole derivative was prepared through the condensation of4-n-alkoxybenzaldehyde with 4-amino-1,2,4-triazole in the presence of an acid catalyst,achieving high yields of 80–85%. Both compounds were characterized and evaluated for their antimicrobial potential against a panel of bacterial (e.g., S. aureus, E. coli) and fungal strains using the agar well diffusion method and Minimum Inhibitory Concentration (MIC) assays. The incorporation of the piperidine and triazole moieties—common pharmacophores in medicinal chemistry wasintended to enhance bio-reactivity. Preliminary results indicate that the triazole-basedmethanimine exhibited superior inhibitory activity compared to the ester derivative, likely due tothe presence of the azomethine (-CH=N-) linkage and the triazole ring's ability to formhydrogen bonds with microbial enzymes. This study concludes that these synthesized derivatives serve as promising lead compounds for further structural optimization in the quest for potent antimicrobial agents.

Keywords: piperidine, 1,2,4-triazole, antimicrobial activity, synthesized, medicinal chemistry

Abstract for Poster paper

PP01

Stimuli-Responsive "Smart" Hydrogels: A Dynamic Scaffold for Enhanced Tissue Engineering

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Abstract
Regenerative medicine has emerged as a promising interdisciplinary field aimed at restoring, maintaining, and enhancing damaged tissues and organs. Advances in bioengineering have significantly accelerated the development of biomimetic materials capable of supporting cell growth and tissue regeneration. Among these materials, hydrogels have gained considerable attention due to their three-dimensional network structure, high water content, and resemblance to the native extracellular matrix. Smart hydrogels, in particular, exhibit stimuli-responsive behavior and are capable of responding to environmental changes such as pH, temperature, and biochemical signals, making them highly suitable for tissue engineering applications. The aim of this study is to highlight the role of smart hydrogels as advanced scaffold materials for tissue engineering and regenerative medicine. The objectives of this work are to describe the structural and physicochemical properties of smart hydrogels, discuss their synthesis and fabrication methods, and explore their applications in tissue regeneration, cell immobilization, and controlled delivery of bioactive molecules evaluating their responsiveness and functionality, and discussing their applications in cell encapsulation, growth factor delivery. To conclude, Smart hydrogels, provide an ideal microenvironment for cell survival, proliferation, and differentiation due to their tunable mechanical properties and biomimetic nature. Their ability to function as supportive scaffolds and delivery systems for growth factors makes them highly promising materials in tissue engineering. Future research focusing on scalability, long-term biocompatibility, and clinical translation will further enhance their industrial and biomedical relevance.

Keywords: regenerative medicine; hydrogels; tissue engineering; smart hydrogels.

PP02

Design and *in-silico* Evaluation of Novel 1,3,4-Oxadiazoles as Potential Antitubercular Agents Targeting Polyketide Synthase 13 (Pks13) Thioesterase

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Abstract
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The escalating threat of multidrug-resistant (MDR) and extensively drug-resistant (XDR) tuberculosis necessitates the discovery of novel antitubercular agents targeting unexplored molecular pathways. Polyketide Synthase 13 (Pks13) thioesterase plays a pivotal role in mycolic acid biosynthesis and the maintenance of mycobacterial cell-wall integrity, rendering it an attractive target for antitubercular drug development. This study employed structure based drug design to develop novel 1,3,4-oxadiazole derivatives as Pks13 thioesterase inhibitors. The 1,3,4-oxadiazole scaffold was selected for its favorable physicochemical properties, metabolic stability, and capacity for hydrophobic interactions within the enzyme's binding pocket. Molecular docking studies were performed to optimize ligand–protein interactions within the hydrophobic cavity of the thioesterase domain. Furthermore, molecular dynamics simulations were conducted to assess the conformational stability of the lead ligand–protein complexes over time. Drug-likeness and pharmacokinetic suitability were evaluated through ADME profiling in accordance with Lipinski's Rule of Five. The integrated computational approach identified several promising 1,3,4-oxadiazole derivatives exhibiting strong binding affinity and high structural stability within the Pks13 active site. These findings highlight the potential of the identified compounds as next-generation antitubercular candidates capable of overcoming existing drug-resistance mechanisms. Overall, this study provides

a robust computational foundation for subsequent experimental validation and further lead optimization in tuberculosis drug discovery.

Keywords: Tuberculosis; Pks13 Thioesterase; 1,3,4-Oxadiazoles; Molecular Docking; Molecular Dynamics; Structure-Based Drug Design.

PP03

Comparative Studies on Preparation and Physicochemical Properties of MOTF (Melamine, o-toluidine, Formaldehyde) and MPTF (Melamine, p-toluidine, Formaldehyde) Anion Exchanger

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Abstract

Ion – exchange resins comprise one of the most important scientific developments of the 21st century. Their applicability to water softening, environmental remediation, waste water treatment, hydrometallurgy, chromatography, biomolecular separations and catalysis was recognized in numerous publications. The principal of covalently bonding to cross- linked polymer networks became the basis for the area of polymer supported reagents. For the synthesis of ion-exchange resins Melamine, o-toluidine, Formaldehyde (MOTF) and Melamine, p-toluidine and Formaldehyde (MPTF), o-toluidine and *p-toluidine* was reacted with formaldehyde and melamine using hydrochloric acid as a catalyst. These resins were characterized by elemental analysis. Synthesized resin shows ion exchange capability. Ion exchange resin also showed reusability and stability at an elevated temperature. The synthetic resin is used primarily for purifying water but also for various other applications including separating out some elements. Ion exchange materials are insoluble substances containing loosely held ions which can exchange with other ions in solutions which come in contact with them. These exchanges take place without any physical alteration to the ion exchange material. Ion exchangers are insoluble acids or bases which have salts which are also insoluble, and this enables them to exchange either positively charged ions (cation exchangers) or negatively charged ions (anion exchangers).

Keywords: melamine, formaldehyde, o-toluidine, p-toluidine

PP04

Synthesis of 1,3,5-Triazine-2,4,6-Triamine as Biological Active and Antiinfective Agents

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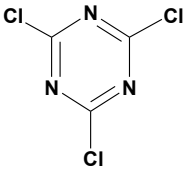
Abstract: Some novel1,3,5-triazine-2,4,6-triamine have been synthesized (1-14). The products tested for their antibacterial activity against gram (+)ve and gram (-)ve bacteria. Introduction of –OH, -NO_2, -Cl and –Br groups to the heterocyclic frame work enhanced antibacterial activities and antifungal activities.



Keywords: 1, 3, 5-triazine-2, 4, 6-triamines; Antibacterial activity, antifungal activities.

PP05

PTC-Assisted Synthesis of Bio-Active Pyrazolopyrimidines Supported by Molecular Docking and ADME Studies

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Abstract
Phase Transfer Catalysis (PTC) is an efficient and green synthetic strategy known for improving reaction rates, yields, and operational simplicity under mild conditions. In this study, PTC-assisted coupling reactions have been successfully employed for the synthesis of biologically important pyrazolopyrimidine derivatives. The study focuses on PTC-assisted C–O and C-N coupling reactions in biphasic systems, enabling mild conditions, facile work-up, and high yields. To evaluate their biological potential, molecular docking and ADME studies were performed. The results indicate favorable binding interactions, suggesting promising activity profiles. In addition, ADME studies for drug-likeness and pharmacokinetic properties, with some compounds showing compliance with standard criteria.Overall, this work demonstrates the utility of phase transfer catalysis in coupling reactions for the efficient construction of pyrazolopyrimidine frameworks, supported by computational studies that highlight their potential as drug-like molecules.

Keywords: PTC, Pyrazolopyrimidines, C–O/ C-N coupling reactions, Molecular docking, ADME

PP06

Solubility Behavior of 1-H Indole in Mono-Organic Solvents: Experimental Study and Model Correlation

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Abstract
Determining the solubility of organic compounds is crucial in fields such as pharmaceuticals, agrochemicals, and environmental science, as solubility strongly influences drug formulation, synthesis, purification, and crystallization processes. In this study, the solid–liquid solubility of 1-H indole was experimentally measured in pure methanol, ethanol, isopropanol, *n*-butanol and acetone using the isothermal saturation method over a range of temperatures. The experimental solubility data were compared with values predicted by machine learning models, namely Fusion Cycle, FastSolv, and SolProp to evaluate their predictive performance. Additionally, the modified Apelblat equation and the λh thermodynamic model were applied to correlate the experimental solubility data of 1-H indole in the selected mono-organic solvents. The results demonstrate that both thermodynamic models provide satisfactory correlations with the experimental data, while the machine learning models show promising capability in predicting solubility trends. This combined experimental, thermodynamic, and machine learning approach offers valuable insights for solubility prediction and solvent selection in chemical and pharmaceutical applications.

Key Words: 1-H Indole, Solid–liquid solubility, Organic solvents, Machine learning models, Thermodynamic modelling

PP07

In silico Design and Synthetic Planning of Potential ULK1 Inhibitors as Autophagy Modulators for Lung Cancer

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Abstract
Autophagy plays a crucial role in cancer cell survival and therapeutic resistance, particularly in lung cancer. Unc-51 Like Autophagy Activating Kinase 1 (ULK1), a key regulator of autophagy initiation, has emerged as a promising molecular target for anticancer therapy. The present study focuses on the in-silico design of potential ULK1 inhibitors as autophagy modulators for the treatment of lung cancer. Pharmacophore-based modelling was employed to identify essential features required for ULK1 inhibition, followed by molecular docking studies to evaluate binding affinity and key interactions within the ULK1 active site. Molecular dynamics simulations were carried out to assess the stability of the selected ligand–protein complexes. Drug-likeness, ADMET properties, and synthetic feasibility of the lead compounds were also analysed, and plausible synthetic routes were proposed. The computational findings revealed novel scaffolds with favourable binding interactions and stable conformational behaviour, warranting further chemical synthesis and biological evaluation.

Key words: Lung Cancer, Autophagy Modulators, ULK1 Inhibitors

PP08

Transition Metal Complexes of an Adamantane-Containing Schiff Base Ligand: Synthesis, Structural Characterization and Bioactivity

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Abstract
Novel adamantane-based Schiff base ligands, *(E)-N'-(2-hydroxybenzylidene)adamantane-1-carbohydrazides*, and their Cu(II), Co(II), Ni(II), Fe(II), Mn(II), Zn(II), Cr(III), and Ce(III) complexes were synthesized and characterized by FT-IR, UV–Vis, NMR, mass spectrometry, elemental analysis, and magnetic measurements. Spectral data confirmed bidentate coordination through phenolic oxygen and azomethine nitrogen atoms. The ligand and its metal complexes were evaluated for antibacterial and antifungal activities, showing enhanced biological activity upon metal coordination compared to the free ligand. The results demonstrate the potential of adamantane-based metal complexes as multifunctional candidates for medicinal and materials chemistry applications.

Key words: adamantane-based Schiff base, adamantane-based metal complexes

PP09

The Synthesis, Characterization and Application of Reactive Dyes Based on 4,4'-Methylene Bis-5-Nitro-O-Toluidine on Silk, Wool and Cotton Fibres

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Abstract

Ten hot-brand bisazo reactive dyes were synthesized via coupling of tetrazotised 4,4'-methylene bis-5-nitro-o-toluidine with a series of cyanurated coupling components. The structures and purity of the dyes were confirmed by thin-layer chromatography, infrared spectroscopy, and proton magnetic resonance spectroscopy. Dyeing performance was assessed on silk, wool, and cotton, with percentage dye bath exhaustion values indicating good uptake across all fibres. The dyed materials exhibited moderate to very good fastness to light, washing, and rubbing, demonstrating the potential of these bisazo reactive dyes for application in natural fibre coloration.

Keywords: 4,4'-methylene bis-5-nitro-o-toluidine, bis azo reactive dyes, cyanuric chloride, 4-chloro aniline, Dyeing, Silk, Wool and Cotton

PP10

Development and Validation of a Stability-Indicating HPLC Method for the Quantitative Estimation of Resmetirom

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Abstract

The present paper describes the development and validation of a simple, precise, and stability-indicating reverse-phase high-performance liquid chromatographic (RP-HPLC) method for the quantitative estimation of Resmetirom in bulk and pharmaceutical formulations. Chromatographic separation was achieved using a C18 column with a mobile phase consisting of acetonitrile and phosphate buffer in an optimized ratio under isocratic conditions. The flow rate, detection wavelength, and injection volume were systematically optimized to provide sharp, symmetrical peaks with adequate resolution. Resmetirom exhibited a retention time that ensured effective separation from degradation products and excipients. The method was validated in accordance with ICH Q2(R1) guidelines for specificity, linearity, accuracy, precision, limit of detection (LOD), and limit of quantification (LOQ). Linearity was observed over a suitable concentration range with a correlation

coefficient (R^2) greater than 0.999, demonstrating excellent proportionality between peak area and analyte concentration.

Keywords: Resmetirom, Sensitivity, Selectivity, Reverse phase HPLC and Validation

PP11

Analytical Method Development, Validation and Force Degradation Study for Estimation of Evogliptin Using Liquid Chromatography-Tandem Mass Spectrometry

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Abstract
The current study uses LC-MS/MS to conduct a quantitative analysis of Evogliptin after it has been exposed to various types of force degradation conditions. The goal was to create a rapid and highly selective drug detection method using liquid chromatography-tandem mass spectrometry. Before using LC-MS/MS for force degradation studies, the method was thoroughly validated. This study will be useful in determining Evogliptin's selflife under various conditions. The method for determining stability was validated in accordance with International Conference on Harmonization (ICH) guidelines. The force degradation study was carried out to evaluate Evogliptin's stability in drugs and their products.

Keywords: Evogliptin, Force Degradation Study, Tandem Mass Spectrometry

PP12

Solvent extraction and trace analysis of As (III) in alloys, biological, and environmental samples by spectrophotometry and ICP-MS.

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A novel method for the simple and selective separation and trace detection of arsenic is described. Arsenic is efficiently extracted at pH 5.5 using 7-hydroxy-4-methylcoumarin hydroxyl amine (HMCHA) in dichloromethane, showing maximum absorbance at 395 nm with a molar absorptivity (c) of 1.21× 104 L mol-1 cm-1. The method follows Beer's law for concentrations between 0.99 and 8.916 µg L-1. Sensitivity is enhanced 60-fold by directly injecting the extract into the plasma for ICP-MS analysis, allowing accurate estimation of trivalent arsenic. The extraction is unaffected by the presence of other ions, with no interference observed. The method's effectiveness is confirmed through the analysis of arsenic in alloys, water, biological, and environmental samples.

Key words: **As (III) analysis in alloys**, ICP-MS analysis

PP13

How to Reduce Air Pollutants

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Abstract
The rapidly deteriorating Air Quality Index (AQI), primarily due to rising levels of Nitrogen Oxides (NOx) and Volatile Organic Compounds (VOCs), demands innovative and sustainable chemical interventions. This presentation explores the "Q-Technique," an advanced passive air-purification strategy utilizing Heterogeneous Photocatalysis. The core of this technology involves applying semiconductor catalysts, specifically modified Titanium Dioxide (TiO2), onto urban infrastructure such as building facades and road pavements. The mechanism centers on the photo-excitation of electrons from the valence band to the conduction band, generating reactive electron-hole (e-)(h+) pairs. These charges react with atmospheric moisture and oxygen to produce potent Hydroxyl (•OH) and Superoxide (O2-) radicals. These radicals effectively mineralize harmful gaseous pollutants into benign substances like nitrates and CO2.To optimize performance for Ahmedabad's high solar intensity, the study emphasizes non-metal doping (e.g., Nitrogen) to narrow the catalyst's band gap, enabling activation under visible light rather than just UV. While challenges like catalyst deactivation and charge recombination exist, the Q-Technique represents a scalable, "smog-eating" solution to transform the city's infrastructure into an active air-cleaning system.

Keywords: Air Quality Index (AQI); Volatile Organic Compounds (VOCs); NOx Remidiation; advanced Oxidation Process; Visible light Activation; Band gap Engineering; TiO_2Heterogeneous Photocatalysis

PP14

Extraction and Determination of Vanadium in Food, Biological, Alloy, Water and Environmental Samples

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Abstract
A novel reagent, N,N′-diphenyl sebacoyl dihydroxamic acid (DPSDHA), has been developed for the extraction and trace determination of vanadium(V) in different matrices. The extraction behavior ofvanadium(V) from 6 M HCl medium has been systematically investigated. Key parameters such as solventchoice, reagent concentration, effect of pH and the effect of interfering ions were optimized. The vanadiumN,N′-diphenyl sebacoyl dihydroxamic acid complex forms a violet colored species

with a maximum absorbance (λmax) at 520 nm and a molar absorptivity of 7.96 × 103 L mol-1 cm-1. The free reagent N,N′-diphenylsebacoyldihydroxamicacid does not absorb at this wavelength. The complex obeys Beer's law in the concentration range of 6.28 × 10-8 M -1.26 × 10-6 M (0.0032-0.064 ppm). The method exhibits a limit of detection (LOD) of 6.0 × 10-7 ppm and a limit of quantification (LOQ) of 5.0 × 10-6 ppm. Ten replicate measurement of a 0.010 ppm vanadium(V) solution yielded a relative standard deviation (RSD) of 1.1%, confirminghigh precision. The dichloromethane extract of the vanadium complex was directly introduced into inductively coupled plasma – mass spectrometry (ICP-MS), enhancing sensitivity by 60 fold. The method was successfully applied to the analysis of standard reference materials, as well as water, biological, and environmental samples.

Key words: extraction of Vanadium, DPSDHA

PP15

Corrosion Inhibitors

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Abstract
Corrosion is a major challenge in the petroleum industry due to the continuous exposure of metallic structures to aggressive environments containing water, carbon dioxide, hydrogen sulfide, acids, and salts. These corrosive conditions can lead to severe material degradation, equipment failure, economic losses, and safety hazards. Corrosion inhibitors are widely used as an effective and economical method to control corrosion in oil and gas production, transportation, and storage systems. This study presents an overview of corrosion inhibitors used in the petroleum industry, focusing on their types, working principles, and applications for the protection of metallic structures. Corrosion inhibitors are broadly classified into organic and inorganic inhibitors based on their chemical composition. Organic inhibitors, such as amines, imidazolines, and azoles, act mainly through adsorption on the metal surface, forming a protective film that reduces corrosion reactions. Inorganic inhibitors, including chromates, phosphates, molybdates, and nitrites, inhibit corrosion by passivation or electrochemical control of anodic and cathodic reactions. The working principles of anodic, cathodic, and mixed-type inhibitors are discussed. Additionally, methods for evaluating inhibitor performance, such as weight loss measurements, electrochemical techniques, and surface analysis, are highlighted. The effective selection and evaluation of corrosion inhibitors play a crucial role in extending the service life of metallic structures and ensuring safe and sustainable operations in the petroleum industry.

Key words: Corrosion inhibitors, electrochemical method, Inorganic/ organic inhibitors

PP16

Design, Synthesis and Biological Evaluation of Novel Thiazole Derivatives as Direct InhA Inhibitors against *MycobacteriumTuberculosis*

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Abstract
Tuberculosis (TB) remains a major global health concern, aggravated by the increasing emergence of multidrug-resistant (MDR) and extensively drug-resistant (XDR) strains of *Mycobacterium tuberculosis*. The limitations of existing anti-tubercular drugs, particularly resistance associated with isoniazid activation via KatG, necessitate the development of novel therapeutic agents targeting

alternative mechanisms. Enoyl-acyl carrier protein reductase (InhA), a key enzyme of the mycobacterial fatty acid synthesis II (FAS-II) pathway, represents a clinically validated and selective drug target, as this pathway is absent in humans.

In the present study, a structure-based drug design approach was employed to identify novel thiazole derivatives as potential direct InhA inhibitors. Virtual screening of the Enamine Hit Locator Library containing 460,000 diversified compounds was carried out using BIOVIA Discovery Studio 2023. Sequential screening using LibDock and CDOCKER algorithms led to the identification of a phenyl thiazole hit with a favorable binding affinity (–CDOCKER energy: 31 kcal/mol). Structural optimization of this hit resulted in the design of 200 thiazole derivatives, of which five compounds were shortlisted based on docking scores, key enzyme interactions, ADMET predictions, and synthetic feasibility.

The selected compounds were synthesized and characterized using IR, mass spectrometry, and NMR techniques. Biological evaluation using the Microplate Alamar Blue Assay (MABA) against *M. tuberculosis* H37Rv strain revealed that compound LMKR-1 exhibited the most promising anti-tubercular activity with a minimum inhibitory concentration (MIC) of 6.25 µg/mL. Overall, this study highlights thiazole derivatives, particularly LMKR-1, as promising lead candidates for further development in anti-tubercular drug discovery.

Keywords
Tuberculosis; Thiazole derivatives; InhA inhibitor; Molecular docking; Anti-tubercular activity

PP17

Phycocyanin: A Bioactive Blue Pigment from Spirulina

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Abstract
Phycocyanin is a naturally occurring blue phycobiliprotein derived from Spirulina (Arthrospira platensis) that has gained considerable attention due to its unique organic chemical structure and multifunctional bioactivity. Structurally, it is a protein–chromophore complex composed of α- and β-subunits covalently linked to phycocyanobilin, an open-chain tetrapyrrole biosynthesized via the heme degradation pathway. The extended conjugated system and thioether linkage are responsible for its intense blue coloration and strong antioxidant properties. Phycocyanin exhibits broad therapeutic potential, including antioxidant, anti-inflammatory, anticancer, hepatoprotective, neuroprotective, antidiabetic, and antimicrobial activities, primarily through reactive oxygen and nitrogen species scavenging, enzyme inhibition, and apoptosis induction. Compared to synthetic blue dyes and conventional antioxidants, phycocyanin offers superior biocompatibility, multifunctionality, and sustainability while providing both coloring and therapeutic benefits. Its applications span nutraceuticals, pharmaceuticals, functional foods, cosmetics, and biomedical research. However, challenges such as instability to heat, light, and pH, along with high production costs, limit large-scale utilization, necessitating advanced extraction and stabilization strategies.

Keywords: Natural blue pigment, Strong antioxidant, anti-inflammatory, anticancer properts.

PP18

NANO-PROTACS FOR CANCER THERAPY

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Abstract

Proteolysis Targeting Chimeras (PROTACs) are bifunctional small molecules that induce targeted protein degradation through formation of a ternary complex between a protein of interest (POI) and an E3 ubiquitin ligase.This interaction promotes POI polyubiquitination and proteasomal degradation, enabling event-driven suppression rather than occupancy-based inhibition.PROTACs effectively degrade proteins that are difficult to target with classical inhibitors, including transcription factors,epigenetic regulators (BRD2/3/4), nuclear receptors (ERα, AR), kinases (BTK, CDKs), and anti-apoptotic proteins such as BCL-XL. By eliminating the full protein and its non-enzymatic functions, PROTACs achieve sustained biological effects at sub-stoichiometric concentrations. Advances in ligand design, linker optimization, and E3 ligase utilization (CRBN, VHL) have improved potency and selectivity, leading to clinically advanced candidates such as vepdegestrant (ARV-471) and ARV-110/ARV-766.Although challenges remain—particularly cell permeability, bioavailability, and tissue-specific E3 expression—PROTACs represent a refined strategy for expanding the druggable proteome and enabling next-generation therapeutic interventions.

Keywords: Ubiquitin proteasome pathway,anti apoptotic proteins

PP19

Green Hydrogen As A Fuel

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Abstract

Green hydrogen is emerging as a clean and sustainable fuel for future transportation systems. It is produced by electrolysis of water using renewable energy sources such as solar and wind power, ensuring near-zero carbon emissions. In hydrogen fuel cell vehicles (HFCVs), hydrogen undergoes oxidation at the anode to generate protons and electrons. The electrons flow through an external circuit to produce electricity, while protons migrate through the electrolyte and react with oxygen at the cathode to form water as the only by-product. Compared to petrol vehicles, hydrogen vehicles eliminate tailpipe emissions and reduce dependence on fossil fuels, offering significant environmental benefits. When compared with battery electric vehicles (EVs), hydrogen vehicles provide faster refueling times and longer driving ranges, making them suitable for long-distance and heavy-duty applications. However, EVs exhibit higher energy efficiency and are more practical for short-distance and light-duty transport. Despite challenges such as storage, infrastructure, and cost, green hydrogen holds strong potential for decarbonizing sectors where battery-based solutions are limited.

Keywords : Green hydrogen; zero carbon emissions; Renewable energy; electrolysis of water; Hydrogen Storage and Infrastructure; water as Byproduct; Decarbonizing sectors.

PP20

Bioorthogonal Chemistry As An Innovative Synthetic Tool

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Abstract
Bioorthogonal chemistry is a unique technique that allows chemical reactions to occur inside living systems, such as cells and organisms, without disturbing theirnaturalbiological processes. This poster focuses on SPAAC (Strain-Promoted Azide-Alkyne Cycloaddition), which is a metal free click reaction. Previously, Click Chemistry required a Copper (Cu) catalyst to work. However, copper is toxic to living cells, making it unsafe for use in humans or animals. SPAAC solved this problem by removing the need for copper. Instead, it uses the concept of "Ring Strain." While normal alkynes are straight, SPAAC uses a bent ring called Cyclooctyne. The bond angle in this ring is forced to bend, creating stored energy. This "strain" energy forces the reaction to happen automatically and quickly with Azides. Because it is safe for living things (biocompatible), SPAAC is widely used today for Live Cell Imaging to visualize sugars on cancer cells and for Targeted Drug Delivery to activate drugs specifically at tumour sites.

Keywords: Bioorthogonal chemistry, SPAAC, Click Chemistry, Drug Delivery

PP21

Azobenzene Photoswitches for Precision Cancer Therapy

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Abstract
Conventional cancer chemotherapy often suffers from poor selectivity, leading to severe side effects due to damage to healthy tissues. To overcome these limitations, light-responsive drug delivery systems have gained significant attention. Azobenzene-based photo switches offer a promising strategy for precision drug delivery in cancer therapy due to their reversible trans–cis photo isomerization upon light irradiation. In this approach, Azobenzene molecules act as molecular gates that control the release of anticancer drugs from carriers such as nano particles, polymers, or hydrogels. Upon exposure to specific wavelengths of light, controlled and site-specific drug release is achieved, minimizing off-target toxicity and improving therapeutic efficacy. The non-invasive nature of light activation enables spatiotemporal control over drug release, allowing repeated and on-demand dosing. Although challenges such as limited tissue penetration of UV light remain, recent developments in visible-light-responsive azobenzene derivatives and nanocarrier systems show strong potential for clinical translation. Overall, azobenzene-based photoswitches represent a powerful and innovative platform for targeted cancer therapy.

Keywords: Target cancer therapy, light-responsive drug delivery, trans–cis photo isomerization, azobenzene derivatives, Nano particles as a carrier

PP22

Docking and Simulation of Protein

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Abstract

Molecular docking and protein simulation are important computational tools used to study interactions between bio molecules at the molecular level. Molecular docking predicts the most favourable orientation and binding position of a ligand when it interacts with a target protein, helping to understand binding affinity and molecular recognition. It is mainly applied in protein–ligand and protein–protein interaction studies and is widely used in drug discovery to design more effective and selective compounds. Docking analysis evaluates interactions such as hydrogen bonding, electrostatic forces, hydrophobic interactions, and van der Waals forces using scoring functions based on free energy calculations. Protein simulation, especially molecular dynamics (MD) simulation, complements docking by analyzing the stability and flexibility of protein–ligand complexes over time under near-physiological conditions. Simulation helps to observe conformational changes, binding stability, and dynamic behaviour that cannot be captured by static docking results alone. The accuracy of docking and simulation depends on efficient search algorithms and reliable scoring methods. Overall, molecular docking combined with protein simulation provides valuable insights into bio molecular interactions, accelerates drug development, and supports structure-based research in pharmaceutical and biomedical sciences.

Keywords : Molecular Docking; Protein–Ligand Interaction; Computational Biology; Molecular Dynamics Simulation; Binding Affinity; Drug Discovery; Structure-Based Drug Design

PP23

Self-Assembling Peptides for Next-Generation Vaccine Delivery

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Abstract

Self-assembling peptide systems have emerged as promising platforms for nextgeneration vaccine delivery due to their biocompatibility, structural versatility, and tunable molecular interactions. These systems are based on short peptides that spontaneously organize into nanostructures such as fibers, micelles, or hydrogels through non-covalent interactions including hydrogen bonding, π–π stacking, hydrophobic interactions, and electrostatic forces. From an organic and supramolecular chemistry perspective, peptide self-assembly is governed by amino acid sequence, functional groups, and secondary structure formation. In vaccine delivery, self-assembling peptides act as both antigen carriers and immune adjuvants, enabling controlled antigen presentation and enhancedimmune response. Their nanoscale architecture protects antigens from degradation and facilitates uptake by antigen-presenting cells. Additionally, chemical modification of peptide sequences allows precise control over stability, responsiveness and immunogenicity.

Keywords: Self-assembling peptides, Vaccine delivery, Non-covalent interaction,
Peptide nanostructure.

PP24

Click Chemistry: Small Click, Big Impact In Modern Chemical Science

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Abstract
Click chemistry is a **Nobel Prize–winning chemical strategy** that allows the **fast, selective, and high-yield formation of molecular bonds under mild conditions**. Due to its simplicity and reliability, it is **widely used in the pharmaceutical industry**. A key industrial application of click chemistry is in the **development of antibody–drug conjugates (ADCs)** for **targeted cancer therapy**. Click reactions enable the **precise attachment of potent anticancer drugs to antibodies**, producing **stable and reproducible conjugates**. This improves **drug targeting efficiency** and **reduces toxicity**, making click chemistry highly suitable for large-scale drug manufacturing. Click chemistry is also used in **bioconjugation and bioimaging**, where biomolecules are selectively labeled for **cellular studies**. For example, click-based fluorescent labeling is applied to **4T1 mouse breast cancer cells** to visualize cancer behavior and assess therapeutic response. Overall, click chemistry provides a **clean, efficient, and industry-friendly platform** for modern drug development.

Keywords: Click chemistry, cancer therapy, bioimaging

PP25

Nanotechnology leading in modern chemistry

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Abstract:
Nanotechnology has emerged as a transformative force in modern chemistry by enabling the manipulation of matter at the nanoscale (1–100 nm), where materials exhibit unique physical, chemical, and biological properties due to quantum effects and large surface-to-volume ratios. Advances in nanochemistry have led to the design and synthesis of nanomaterials with enhanced reactivity, selectivity, and functionality compared to their bulk counterparts. These novel properties have revolutionized diverse fields including catalysis, medicine, energy storage, environmental remediation, and materials science.In modern chemistry, nanotechnology plays a crucial role in developing efficient catalysts, targeted drug delivery systems, high-performance sensors, and sustainable energy solutions such as nanostructured batteries and solar cells. Techniques such as bottom-up synthesis, surface functionalization, and self-assembly allow precise control over nanoparticle size, shape, and surface chemistry. Furthermore, nanotechnology contributes significantly to green chemistry by minimizing waste, improving reaction efficiency, and enabling eco-friendly processes.Despite challenges related to scalability,toxicity, environmental concern, and ethical considerations, nanotechnology continues to redefine chemical research and industrial practices.

PP26

Microwave Synthesis

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Abstract

Microwave synthesis is an advanced and efficient technique in which chemical reactions are performed using microwave irradiation instead of conventional heating methods. Microwaves typically operate at a frequency of 2.45 GHz, enabling rapid and uniform heating through dipolar polarization and ionic conduction mechanisms. This method generally works within a temperature range of 50–300 °C and pressures up to 10–30 bar, significantly reducing reaction times from hours to a few minutes. Microwave-assisted synthesis offers several advantages such as enhanced reaction rates, higher product yields, improved selectivity, reduced solvent usage, and lower energy consumption. Due to these benefits, it is considered an important approach in green chemistry. The technique allows precise control over reaction parameters, leading to reproducible and efficient synthesis. Microwave synthesis is widely used in organic and inorganic chemistry, including the preparation of pharmaceutical compounds, nanomaterials, polymers, catalysts, and metal–organic frameworks (MOFs). It is particularly effective for solvent-free reactions and aqueous systems, making it safer and more environmentally friendly. Additionally, microwave synthesis improves crystal quality and particle size control in material science applications.

Overall, microwave-assisted synthesis is a powerful, economical, and sustainable method that supports rapid chemical development in laboratory research and industrial-scale production.

Keywords: Microwave technology, Green tool

PP27

Surface-Modified Mesoporous Materials: Progress and Prospects in CO_2 Conversion

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Abstract

Mesoporous materials have emerged as highly versatile platforms across a wide spectrum of research domains, including carbon capture and conversion, energy storage, biomedical applications, photocatalysis, optics, and magnetism, leading to an expanding body of literature. In particular, porous heterogeneous catalysts, such as zeolites, clays, and mesoporous frameworks have gained considerable attention for CO_2 conversion, owing to their potential role in mitigating global warming. Among these materials, mesoporous structures are especially noteworthy due to their large specific surface area, substantial pore volume, and tunable pore dimensions. These attributes enable the formation of well-dispersed metal or metal oxide active sites, which are essential for enhancing catalytic efficiency in CO_2 transformation. Numerous studies have reported the direct application of mesoporous metal oxides, sulfides, and phosphides, demonstrating promising performance that arises from the synergistic presence of metal centers and mesoporosity. Continued progress in this field requires advanced research efforts and the application of sophisticated characterization techniques to elucidate their yet-unexplored properties. This review therefore focuses on the various classes of mesoporous materials and their functionalized derivatives developed for CO_2 conversion, particularly toward methane and methanol. By surveying this diverse set of materials, we aim to provide insights

into how their structural and chemical features govern catalytic performance in CO_2 conversion processes.

Keywords: Mesoporous materials, CO_2 conversion, Metal species.

PP28

Synthesis and Characterization (Thermogravimrtric Analisis) of Glass Reinforcement Matirials (Non-Conducting Matirials)

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Abstract

Reinforsement Matirials: Poly (urethane-imide)s (PUIs) were prepared by the by the intermolecular Diels-Alder (DA) Reaction of Hexamethylene bis(2-Furanylmethythioethyl carbamate) (HMFTC) with various bismaleimides. The DA reaction was carried out in 1, 4 dioxane as a solved as well as in bulk, followed by aromatization of tetrahydrophthalimideintermidiates in the presence of acitic anhydride. All the polymers were characterized by elemental analysys, IR spectral studies and thermogravimetry. The PUIs exhibit moderate thermal stability. HMFTC and bismaleimides were polymerized (at 145 + 10 0C) by DA intermolecular reaction into moderately thermally stable PUIs glass-fibre composite (i.e. laminates) and were characterized by their chemical resistance and mechanical properties.

Keywords: Poly (urethane-imide)s (PUIs); bismaleimides; IR spectroscopy; TGA Glass-fiber reinforced composites

PP29

Efficient Synthesis of 1,5-Disubstituted Tetrazoles via TMS-N_3 Based Ugi Reaction and Their Anticancer Potential

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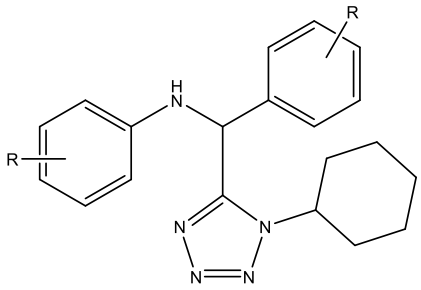
Abstract

An efficient, catalyst-free protocol has been developed for the synthesis of 1,5-disubstituted tetrazole derivatives via a TMS-N_3-based Ugi multicomponent reaction at room temperature. The method utilizes aromatic aldehydes, aryl amines, cyclohexyl isocyanide, and TMS-N_3 to afford target compounds in high yields. Structures were confirmed by MS, IR, NMR, and single-crystal XRD analysis. The synthesized compounds were evaluated for anticancer activity under the NCI-60 human tumor cell line panel, representing nine cancer types. This work demonstrates the utility of Ugi-MCR strategies in designing novel heterocyclic frameworks with promising pharmacological profiles.



Keywords: Tetrazole derivatives, Ugi multicomponent reaction, TMS-N_3, anticancer activity, heterocyclic synthesis.

PP30

Mesomorphism Dependence on Chalconyl Derivative with Heterocyclic Tail and Methoxy Lateral Group

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Abstract
A new homologous series of liquid crystal (LC) materials incorporating a heterocyclic ring was synthesized to investigate and establish the relationship between molecular structure and liquid crystal properties. The series comprises 12 members, labelled A1 to A12. Among them, A8 to A12 exhibit monotropic nematic phases. Comparative studies between mesomorphic and non-mesomorphic members were conducted, leading to several important conclusions. Transition temperatures were measured using a polarizing optical microscope equipped with a heating stage. Analytical and spectral analyses confirmed the molecular structures of the homologues. This series is classified as having middleordered melting characteristics. The LC properties of this new series were also compared with those of structurally related known series.

Keywords: Mesomorphic, Homologues, Nematic, Monotropic

PP31

Synthesis and Mesomorphic Phase Behavior of Terminal Benzo [1,3] Dioxole Ring

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Abstract
A new homologous series has been synthesized and studied to explore the impact of adding alkyl chains and a fused heterocyclic ring on mesomorphic properties. The series includes 12 homologues (G_1-G_{12}), all of which exhibit smectic mesophase. Textural analysis and phase transition temperatures were measured using polarizing optical microscopy with a heating stage. The molecular structures were confirmed using ^{1}HNMR, FTIR, and mass spectrometry. The incorporation of the 5-amino benzo [1,3] dioxole ring into the molecular structure improved thermal stability, with all derivatives maintaining stability between 48.3°C and 140.4°C. The average thermal stabilities for the smectic

was significantly higher than those commonly seen in similar compounds, offering valuable insights for the development of liquid crystalline materials.

Keywords: Homologues, Smectic, Mesomorphic, Liquid crystal.

PP32

Designing of Some Novel Casein Kinase-2 (Ck-2) Inhibitors

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Cancer is a group of diseases that are driven by progressive genetic abnormalities that includes mutations in tumor-suppressor genes, oncogenes and chromosomal abnormalities. Later, the role of epigenetic alterations was identified referring to functionally relevant modifications to the genome that do not change the nucleotide sequence. Casein Kinase-2 (CK-2) is a (second

messenger-independent nuclear) cyclic nucleotide and calcium independent serine/threonine-specific protein kinase. CK-2 levels is abnormally high in cancer cells where it is believed to

generate an environment favourable to the development of malignancies through a mechanism denoted as “non-oncogene addiction”. This makes CK-2 an appealing target to counteract different kinds of tumors. The structural basis for selectivity of the molecules resides in the shape and size of the hydrophobic pocket adjacent to the ATP binding site where the ATP competitive ligands are entrapped. We planned to screen some molecular libraries with the application of the Computer Aided Drug Design (CADD) tool like Molecular Docking to identify the CK-2 inhibitors. The retrieved hits being further docked using the Maestro software package (Maestro ver10.1, Schrodinger, LLC, New York) taking the X-ray structure of CK-2 with bound ligand (PDB code- 3BQC) as the protein structure.
The present project aims to identify the novel molecules as potent CK-2 inhibitors.

Keywords: Casein Kinase-2 (CK-2) inhibitors, CADD, Nematic, Monotropic, Cancer therapy

PP33

Green Chemistry: Sustainable Strategies for Modern Chemical Synthesis

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Abstract

Green chemistry is an innovative approach in chemical science that aims to design products and processes which reduce or eliminate the use and generation of hazardous substances. It emphasizes sustainable development by minimizing waste, conserving energy, and using environmentally benign reagents and solvents. Green chemistry is guided by twelve fundamental principles, including prevention of waste, atom economy, use of renewable resources, and safer chemical synthesis. By replacing toxic chemicals with eco-friendly alternatives, green chemistry helps reduce environmental pollution and health risks. Applications of green chemistry are found in pharmaceuticals, agriculture, energy production, and industrial manufacturing. The adoption of green chemistry reactions not only protects the environment but also improves economic efficiency and promotes sustainable industrial growth. Thus, green chemistry plays a crucial role in achieving a cleaner, safer, and more sustainable future.

Keyword: Toxic chemical, eco-friendly

PP34

"Synthesis, Characterization and Anticancer activity of novel synthesised triazole derivatives via click chemistry approach"

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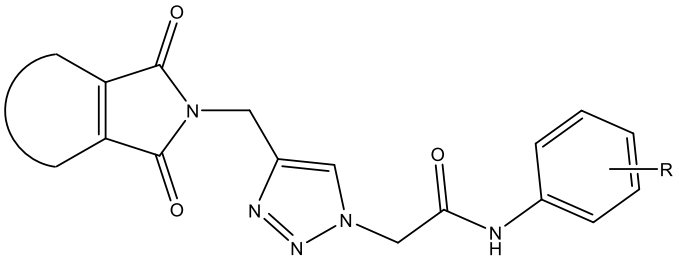
Abstract:

A highly efficient and economical synthetic protocol leveraging copper(I)-catalyzed Huisgen-Sharpless 1,3-dipolar cycloaddition ("click chemistry") has been developed for the preparation of a library of biologically important 1,4-disubstituted 1,2,3-triazoles using a phthalimide-functionalized core moiety. This facile CuAAC method exclusively yields 1,4-disubstituted triazoles by coupling azides and terminal alkynes, demonstrating complete specificity and broad functional group tolerance. The versatility of triazole linkages as bridging units, especially in carbohydrate chemistry, highlights their growing significance in medicinal chemistry. Applying this approach, a series of fifteen novel triazole derivatives were synthesized and screened for anticancer activity, showcasing promising potential for further pharmaceutical development.



Keywords: Click chemistry, 1,2,3 – triazole, drug discovery, anticancer activity, medicinal chemistry

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