

International Seminar on

**Recent Advancement in  
Chemistry and Biology**

# ABSTRACTS

14th August, 2025

Organised by

**Department of Chemistry & Botany & IQAC,  
Darjeeling Government College**

in association with  
**Department of Higher Education,  
Government of West Bengal &  
Royal Society of Chemistry,  
Local Section East India**

**ISRACB  
2025**

Abstract Book Published by Darjeeling Government College

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Memo No. 234(1)/P.C./25.....

Date : 13/5/25.....

**Message from the Officer-in-Charge**  
**Darjeeling Government College**

Greetings from Darjeeling Government College.

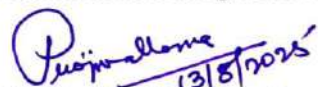
It is a great honour welcome all distinguished speakers, delegates, researchers, and participants from India and abroad to the *International seminar on "Recent advancements in Chemistry and Biology" (ISRACB-2025)*, organized by Darjeeling Government College in association with the Internal Quality Assurance Cell (IQAC).

Founded in 1948, Darjeeling Government College holds a distinguished place as a higher education Institution in West Bengal. For almost seventy five years, it has served efficiently for pursuing knowledge. The college continues to uphold this rich legacy through a strong tradition of teaching and research, while at the same time embracing change to meet the evolving challenges of higher education in global context.

The hosting of *ISRACB-2025* is an important milestone in this tradition. In today's world, where climate change, sustainability, energy security, and public health are urgent concerns, the relevance of scientific inquiry and interdisciplinary collaboration cannot be overstated.

The Abstract volume is a reflection of this shared endeavor that brings together contributions from participants across India and abroad, it offers valuable insights into current research and future directions.

I sincerely thank the Department of Higher Education, Government of West Bengal and Royal Society of Chemistry, East India section for their support in making this initiative possible and I also extend my deep appreciation to the Organizing Committee, whose dedication and tireless efforts have shaped this conference. Finally, I am grateful to the speakers, contributors, and participants for enriching the event with their presence. I hope *ISRACB-2025* will open new avenues of collaboration and inspire meaningful contributions to the global scientific community.

  
13/5/2025

**Dr. Prajjawal Chandra Lama**  
Officer – in – Charge

&  
Assistant Professor, Department of Botany  
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**Officer-in-Charge**  
**Darjeeling Government College**  
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**Government of West Bengal  
Darjeeling Government College  
Darjeeling- 734101, West Bengal, INDIA**

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*Memo No. ....*

*Date :12/08/2025*

**Message from the Desk of the IQAC Coordinator**

**Darjeeling Government College**

It gives me immense pleasure to extend my warm greetings to all the participants, researchers, academicians, and distinguished speakers of this International Seminar. At the heart of IQAC's mission lies the commitment to continuous improvement in the quality of education and research. Such type of conferences serve as dynamic platforms for the exchange of knowledge and interdisciplinary dialogue—key elements that contribute to development of our academic ecosystem.

I congratulate the organizing committee for their dedication and efforts in bringing together such a diverse work, as reflected in this abstract volume and I am confident that the deliberations and insights shared during the conference will inspire new ideas and open pathways for impactful research and learning.

Wishing all participants a meaningful and intellectually stimulating experience.

  
12/8/2025

**Dr. Sherap Bhutia**

**IQAC Coordinator,**

**&**

**Associate Professor and Head, Department of Geography**

**Darjeeling Government College**

**Darjeeling - 734101, West Bengal, India**

**Government of West Bengal  
Darjeeling Government College  
Darjeeling- 734101, West Bengal, INDIA**

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*Memo No. ....*

*Date :13/08/2025*

**Message from Convenors**

**Darjeeling Government College**

It is our immense pleasure to organize the one-day International seminar entitled "*Recent advancements in Chemistry and Biology*" (ISRACB-2025), organized by Darjeeling Government College in association with the IQAC, Higher Education Department, West Bengal and Royal Society of Chemistry, East India section, on 14<sup>th</sup> August 2025. Our aim is to provide a dynamic platform where both students and researchers can benefit from exposure to diverse methodologies, perspectives, and emerging innovations—each playing a vital role in addressing the global challenges of recent time. We are deeply honored by the commitment of our distinguished keynote speakers and resource persons, whose expertise and insight continue to elevate the academic rigor and inspiration of our event. Our heartfelt congratulations go to all contributors featured in this Book of Abstracts, which encompasses almost 56 abstracts spanning over different scientific domains. This compilation offers a rich glimpse into the innovative research carried out by our esteemed participants.

We are sincerely grateful to the Higher Education Department, West Bengal and Royal Society of Chemistry, East India section for their untiring support. Our deepest appreciation goes to the Officer-in-Charge of Darjeeling Government College for his continued cooperation and guidance, as well as to the IQAC Coordinator for his valuable suggestions and inputs.

A special note of thanks to the dedicated members of the Organizing Committee, whose commitment, hard work, and enthusiasm have been instrumental in making this conference a meaningful and impactful academic endeavor.

**Dr. Arabinda Mandal**

(Associate Professor & Head, Department of Chemistry) and

**Satyam Tamang** (Assistant Professor & Head, Department of Botany)

*[Signature]* 13/08/2025  
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Memo No. ....

Date :13/08/2025

**Message from the Organizing Secretaries & Joint Convenors**

**Darjeeling Government College**

It is our privilege to extend a warm welcome to you to the International Seminar on "*Recent advancements in Chemistry and Biology*" (ISRACB-2025), organized by Darjeeling Government College in association with the IQAC, on 14<sup>th</sup> August 2025. Designed as a dynamic forum for intellectual exchange, this conference convenes scientists, researchers, educators, industry professionals, and students to engage with the urgent global challenges of climate change, sustainability, energy security. We are pleased to present the Abstract Book of ISRACB-2025, which compiles the scholarly contributions of distinguished participants from India and abroad. Each abstract embodies rigorous academic effort and creative inquiry, offering both a glimpse into contemporary research and a window to future directions. This volume will not only serve as a valuable companion to the conference proceedings but also as a useful reference for researchers and students in the years to come.

We express our sincere gratitude to the Department of Higher Education, Royal Society of Chemistry, East India section and the University of North Bengal for their support and cooperation. We also gratefully acknowledge our patrons, advisory committee members, distinguished speakers, and contributors, whose encouragement and engagement have been invaluable. Special appreciation is extended to the faculty colleagues and volunteers, whose unwavering commitment ensured the flawless execution of the conference and this publication, without whose support the accomplishment of this mission would have been impossible. We extend our best wishes to all participants for an intellectually stimulating and gratifying experience.

With warm regards,

Mr. Surajit Saha (Assistant Professor, Department of Chemistry)

Dr. Abdul Ashik Khan (Assistant Professor, Department of Chemistry)

Dr. Sandip Mondal (Assistant Professor, Department of Chemistry)

Dr. Sourav Basu Neogi (Assistant Professor, Department of Chemistry)

Dr. Dipayan Roy (Assistant Professor, Department of Chemistry)

Dr. Gautam Ganguly (Associate Professor, Department of Botany)

Dr. Sourav Chakraborty (Assistant Professor, Department of Botany)

Mr. Chandan Naskar (Assistant Professor, Department of Botany)

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*Sherap Bhutia*



# Supramolecular Host-Guest Interaction Of $\beta$ -Cyclodextrin with Drug Molecules in Formation of Inclusion Complexes – A Theoretical Approach

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## Abstract:

Supramolecular host-guest interaction between drug molecules (Olutasidenib and Mavacamten) and  $\beta$ -Cyclodextrin ( $\beta$ -CD) have been performed using the first principle calculations. The strong binding energies of 1:1 complexes, Olutasidenib- $\beta$ -CD and Mavacamten- $\beta$ -CD indicate the formation of a stable complex in aqueous medium. From the analysis of the charge density, electrostatic potential, global reactivity parameter, it confirms the formation of a stable complex between  $\beta$ -CD and the drug. The stability of the complexes has also been confirmed by atom-centered density matrix propagation calculations. From non-covalent interaction (NCI) analysis and reduced density gradient (RDG) plots show sufficient intermolecular forces of attractions is supported for both the complexes. These results showed that hydrogen bonding and van der Waals interactions stabilize the inclusion complexes. The formation of these host-guest inclusion complexes suggests an effective strategy for minimizing the adverse effects of specific drugs.

**Keywords:** Inclusion complex, charge density, global reactivity parameters, non-covalent interactions, electrostatic potential map.

## References:

- 1) Schneider, Hans-Jörg, and Anatoly K. Yatsimirsky. "Selectivity in supramolecular host–guest complexes." *Chemical Society Reviews* 37.2 (2008): 263-277.
- 2) Zhan, Wenjun, et al. "Fabrication of supramolecular bioactive surfaces via  $\beta$ -cyclodextrin-based host–guest interactions." *ACS Applied Materials & Interfaces* 10.43 (2018): 36585-36601.
- 3) Harada, Akira, Yoshinori Takashima, and Masaki Nakahata. "Supramolecular polymeric materials via cyclodextrin–guest interactions." *Accounts of chemical research* 47.7 (2014): 2128-2140.

# High Performance NIR Light Detection of Nitrogen Functionalized p-Type Graphene Window & Silicon Nanowire Heterostructure Through Fermi Level Tuning and Structural Optimization

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## Abstract:

The type of dopants, strain, vacancies, and structural effect in reduced graphene oxide can control the electrical, optical, chemical, and transport properties. In this work, we delineate structural effects, in-plane hopping defects and vacancies that enhance p-type behavior of nitrogen/oxygen functionalized reduced graphene oxide (NORG). The NORG-6/30 has been prepared from pyrazole, which is functionalized at the edge and basal plane in the NORG lattice with increasing reduction time (6-30 hours). A combined spectroscopic approach and ab initio calculation implies pyrazole-based 4 pyrrole unit complex macrocyclic unit formation, i.e. in-plane hopping defect and vacancies at local sites in graphene lattice (i.e. graphene window) increases with reduction time (maximum for NORG-30) which can regulate the band gap opening, Fermi level position, hole doping concentrations and work function. Such modification and layer numbers of NORG-30 on Silicon nanowire substrates show remarkable NIR-based photodetector devices having maximum responsivity and detectivity as high as 50 mA W<sup>-1</sup> and 2.2 × 10<sup>11</sup> Jones at -2 V. The temperature-dependent Thermionic and Cheung's models are introduced to estimate Schottky barrier height of 0.98 eV and diode ideality factor of 2.92 which are well corroborated with UPS analysis. The high photocurrent from photoexcited high charge carrier formation of NORG-30/SiNW device is 2 orders higher in magnitude than other NORG/SiNW and ORG/SiNW (without using any nitrogen precursors) devices. Finally, the hybrid NORG-30/SiNW device rapidly quantifies the alcohol content and has excellent potential for application in the food industries.

**Keywords:** Graphene, pyrazole, Fermi level, vacancies, work function, Photo detectivity

## References:

1. Feng, B.; Zhu, J.; Lu, B.; Liu, F.; Zhou, L.; Chen, Y. Achieving Infrared Detection by All-Si Plasmonic Hot-Electron Detectors with High Detectivity. *ACS Nano* **2019**, *13* (7), 8433–8441. <https://doi.org/10.1021/acsnano.9b04236>.

# **Micromorphological Study of Floral Nectary in *Rhododendron barbatum* Wallich ex G. Don (Ericaceae)**

**Sulaxana Baraily\***

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## **Abstract:**

In this study, the floral nectary of *Rhododendron barbatum* Wallich ex G. Don was examined using scanning electron microscopy (SEM), while the floral anatomy was analysed through light microscopy (LM). As the superior position of the ovary, the nectary gland is located beneath it and is said to be an intrastaminal receptacular nectary (Nicolson et al., 2007). The nectary is characterised by a greenish ribbed ring with eight pinkish-pointed outgrowths at its base, which alternately adjoin the filament. The parenchyma cells of the nectary consist of 7-8 layers, with trichomes or hairs present on the epidermal surface. Consequently, *Rhododendron barbatum* exhibits trichomatous nectaries. The nectary height measures 390-400 µm. Nectar is secreted through anomocytic stomata, which are uniformly distributed. Notably, guard cells are predominantly located on the outgrowths of the nectary.

**Keywords:** *Rhododendron barbatum*, Micromorphology, Floral Nectary, Position

## **Reference**

1. Nicolson S.W., Nepi M., Pacini E., (2007). Nectaries and nectar. (eds). Springer, Pp 77.

# Broadband Spatial Self-Phase Modulation and All-Optical Diodes and Switching Applications Using 1D Copper Phthalocyanine Nanotubes

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## Abstract:

Cu-Phthalocyanine (CuPc) nanotubes are planar aromatic molecules with a conjugated  $\pi$ -electron system, and they are prepared by solvothermal route for studying the nonlinear optical properties by spatial self-phase modulation (SSPM) technique. The large nonlinear refractive index ( $n_2$ ) and the third-order nonlinear electric susceptibility ( $\chi^{(3)}$ ) are determined for three wavelengths 671 nm, 532 nm and 405 nm. Intense laser light produces concentric diffraction ring patterns at the far field due to the strong light-matter interaction based on the optical Kerr effect. From the linear variation of diffraction ring numbers with laser intensities, the  $n_2$  and the  $\chi^{(3)}$  values are determined. The highest  $n_2$  and  $\chi^{(3)}$  values,  $3.667 \times 10^{-5} \text{ cm}^2/\text{W}$  and  $2 \times 10^{-3} \text{ esu}$ , respectively, are reported for 405 nm laser that show a significantly strong third-order nonlinear optical response of CuPc. The nonreciprocal light propagation through CuPc/SnS<sub>2</sub> hybrid structure is formed to realize the all-optical photonic diode by taking the advantage of reverse saturable absorption of 2D SnS<sub>2</sub> nanosheet. In addition, the all-optical switching is presented using CuPc nanotubes based on the spatial cross-phase modulation technique. In this technique a phase change is induced in the weak signal beam modulated by the strong controlling light beam, which helps to produce all-optical logic gates and all-optical switching device. The experimental findings of this work unravel the great potential applications of CuPc nanotubes in all-optical information transmission and all-optical photonic devices.

**Keywords:** spatial self-phase modulation; copper phthalocyanine; all-optical logic gates; all-optical diodes.



# Advances in Supramolecular Chemistry: From Molecular Design To Functional Applications

Dr. Subhadeep Saha\*

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## Abstract:

Supramolecular chemistry investigates non-covalent assemblies in which large host molecules encapsulate smaller guests, a process increasingly important in pharmacology and targeted drug delivery. Macrocyclic hosts such as calixarenes, pillararenes, cucurbiturils, and cyclodextrins offer exceptional molecular recognition and form stable host–guest complexes. These systems can be engineered into stimuli-responsive materials, where external triggers—enzyme activation, light, temperature, pH shifts, or competitive binding—control guest release.

Cyclodextrins are particularly significant due to their amphiphilic nature, enabling self-assembly in aqueous media into nanostructures such as micelles, nanotubes, nanorods, nanosheets, and vesicles. These architectures have applications in nanomedicine, drug delivery, and bioimaging. Cyclodextrin-functionalized nanoparticles further enhance electronic, thermal, fluorescence, and catalytic properties, expanding their utility in nanosensors, targeted therapeutics, and smart materials.

Recent advances in supramolecular design have yielded functional constructs including molecular switches, artificial machines, supramolecular polymers, chemosensors, transmembrane channels, and molecular logic gates. These developments highlight the central role of supramolecular chemistry in creating next-generation functional materials with precision-controlled properties and broad technological impact.

**Keywords:** Host–Guest Chemistry, Stimuli-Responsive Materials, Cyclodextrin Nanostructures, Targeted Drug Delivery.

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# Metabolism of Cypermethrin by Hepatic Cytochrome P450 in Freshwater Teleost, *Clarias batrachus*

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## Abstract:

Cypermethrin, a synthetic pyrethroid, is increasingly used as an alternative to organochlorine and organophosphate insecticides due to its low environmental persistence. However, its toxicity to fish is substantially higher than to mammals and birds, posing ecological risks. Cytochrome P450 (CYP 450) enzymes, a diverse group of Phase I metabolic proteins, play a critical role in detoxifying xenobiotics as the body's first line of defense. This study investigated the response of hepatic cytochrome P450 (CYP 450) isoforms in *Clarias batrachus* exposed to 1/3 sub-lethal concentration (1.9 µg/L; LC<sub>50</sub>) of cypermethrin for 5, 10, and 15 days. CYP 450 content was measured, alongside activities of CYP1A (EROD), CYP2E1 (aniline hydroxylase), CYP2B (N,N-dimethylaniline demethylase), and CYP3A4 (erythromycin demethylase). Exposure caused a significant elevation ( $p < 0.05$ – $0.01$ ) in total CYP 450 content. CYP1A activity increased markedly ( $p < 0.01$ ) in all treatments, while CYP2E1 and CYP2B activities rose significantly after 10 and 15 days, respectively. In contrast, CYP3A4 activity declined significantly in all groups. CYP1A emerged as the most sensitive isoform, supporting its potential as a biomarker of cypermethrin exposure. Suppression of CYP3A4 may contribute to cypermethrin's high toxicity in fish. These findings highlight that pyrethroid-induced modulation of CYP 450 enzymes can significantly affect the physiological fitness of aquatic organisms.

**Keywords:** cypermethrin, cytochrome P450, *Clarias batrachus*, CYP1A, CYP2B, CYP2E1, CYP3A4

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# Role of Hemocytes and Hepatopancreas of Molluscs in Environmental Health

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## Abstract:

Molluscs' hemocytes (immune cells) and hepatopancreas (detoxification organ) are crucial for monitoring aquatic environmental health. Human effluent discharge into the ecosystem has raised environmental issues and create significant stress on the aquatic ecosystem. This work presented an overall abridgment of the effects of effluent on aquatic animals. Freshwater molluscs *Bellamya bengalensis* and *Pila* sp. were manually collected from the selected aquatic bodies of Nadia district of West Bengal. Hemolymph was collected and hemocytes were stained by Giemsa, methylene blue. Tissues of hepatopancreas were removed and mashed through the cell strainer into the petridish in presence of trypsin- EDTA. Cell suspension was smeared on glass slides, fixed by methanol and stained by Giemsa. The mean percentage of Trypan Blue (TB) positive cells (mortality index) was significantly increased in in the specimens collected from the sites associated with human effluents. Mean number of hemocyte aggregates and cells within aggregates were found to be less and rupture of cell membrane was noted in the cells from hepatopancreas in the specimens from the sites associated with human effluents. Studies of the hemocytes and hepatopancreas of molluscs are especially interesting because that can be useful in ecotoxicology research and biomarker for environmental health.

**Keywords:** Freshwater molluscs, Hemocytes, Hepatopancreas, Human Effluents

# Physicochemical Characterization, Molecular Docking and ADMET Analysis of Two Flavonoid Biomolecules 4H-Pyran-4-One,2,3-Dihydro-3,5-Dihydroxy-6-Methyl and Flavone 4'-OH,5-OH,7-Di-O-Glucoside Against a Range of Coronaviruses, HIV-AIDS and Hepatitis-B Virus

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## Abstract:

Viruses cause diverse types of infectious diseases and illness like COVID-19, HIV-AIDS, Hepatitis-B etc. They badly affect humans by causing various syndromes like respiratory issues and flu. Molecular docking, a method which anticipates the favored orientation of ligand (biomolecules) against receptor (protein) to make a stable complex aid in identifying prospective drug molecules. Natural bioactive compounds like flavonoids are well known for their anti-viral property. Therefore, prime flavonoid molecules identified by GC-MS analysis in *Herpetospermum darjeelingense* (C.B.Clarke) H. Schaef. & S.S. Renner encouraged *in silico* study towards investigating the possible inhibitory effect of viral replication of SARS-CoV-1, SARS-CoV-2, MERS-CoV, AIDS and Hepatitis-B. The results of *in-silico* study revealed Flavone 4'-OH,5-OH,7-di-o-glucoside inhibited the replication of all five viruses with greater binding affinity compared to the control drug Remdesivir, Atripla and Entecavir in multiple instances. However, 4H-Pyran-4-one,2,3-dihydro-3,5-dihydroxy-6-methyl was not found to possess analogous binding affinity as that of Flavone 4'-OH,5-OH,7-di-o-glucoside. Physicochemical characterization of the compounds by following Lipinski's rule of five and ADMET study have helped recognize these compounds as a probable natural therapeutic drug against Coronaviruses, HIV-AIDS and Hepatitis-B. The present study exhibits the potential of alternative drug molecules as anti-viral compounds against these three types of Coronaviruses, AIDS and Hepatitis-B. Further *in vitro* and *in vivo* evaluation followed by clinical trials for developing and successfully implementing the Flavone 4'-OH,5-OH,7-di-o-glucoside compound as an effective inhibitory agent against all three viruses can be initiated. The compound has the potential to serve as an all-rounder medicine with wide range of pharmaceutical applications.

**Keywords:** *Herpetospermum darjeelingense*, *in silico*, infectious diseases, bioactive molecules, natural remedy



# Physicochemical Exploration of Some Biologically Potent Molecules Prevailing in Aqueous Solution of an Anticoagulant Drug with The Manifestation of Solvation Consequences

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## Abstract:

**Aims:** Our research aims to uncover how solute-solvent and solute-solute interactions behave in aqueous solutions, exploring how temperature variations and concentration changes influence these interactions. This can provide deeper insights into the behavior of molecules in different environments, potentially leading to applications in fields such as drug delivery, chemical reactions, and material science. In the aqueous ternary system, the physicochemical interactions between a medically powerful pharmacological molecule and two naturally occurring amino acids were explored. The investigations were performed in a dilute to infinite dilute medium to study the interactions between the solutes and solvent extensively. The objective of this research is to systematically investigate the nature of solute-solvent and solute-solute interactions in aqueous solutions across a range of temperatures and concentrations. By doing so, we aim to elucidate the underlying principles governing these interactions, which could contribute to a deeper understanding of solution chemistry. This knowledge is intended to inform the development of more efficient and effective applications in various scientific and industrial fields, including drug formulation, catalysis, and material design. To characterize and calculate the interactions in the ternary system, various models and formulas were considered and applied. Based on various parameters, including viscosity-B coefficient, apparent molar volume, and molar conductance from viscosity, density, and conductance studies, varying temperatures and concentrations were used to elucidate the molecular interactions. To elucidate the interactions between solute with co-solute and with solvent, the limiting apparent molar volumes and the experimental slopes, derived from the Masson equation, and the Viscosity constants A and B, obtained via the Jones-Doles equation, were examined. To illustrate the structure-breaking/making character of the solutes in the solution, Hepler's method and  $\text{dB/dT}$  values were applied. The results indicated that hydrophobic-hydrophobic interaction plays a significant role in the system. These amino acid interaction models may explain the properties of a variety of physiologically active compounds, and the mechanism can be expanded to comprehend the nature of similar systems. Furthermore, the research could lead to advancements in areas such as pharmaceutical sciences, where controlling solute interactions is crucial for drug delivery systems, and in environmental chemistry, where understanding pollutant behavior in water is essential for remediation efforts.

**Keywords:** Apparent molar volume, viscosity coefficient, ticlopidine hydrochloride, drug-amino acid interaction, thermodynamics, hydrophobic-hydrophobic interaction

## References:

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# Comparative Metabolomics of Flavour-Associated Metabolites in The Ts569 and P312 Chinese Tea Varieties

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## Abstract:

Tea flavour is one of the most important attributes that define consumer preference and thus, market value; it is regulated by complex interactions of primary and secondary metabolites. The major contributors among the amino acids, polyphenols, and volatile aromatic compounds are significant contributors to characteristic flavour in the various varieties of teas. We carried out a comparative metabolomics study of differences in flavour-associated metabolites between two major varieties of Chinese tea cultivation: TS569 and P312. Using the most advanced analytical platforms gas chromatography-mass spectrometry (GC-MS), we completely described metabolite composition for each variety. Obviously, the level of some metabolites significantly differs between TS569 and P312; indeed, they possessed elevated levels of the compounds contributing to flavour traits umami and sweetness. Such variability might reflect varietally specific metabolic pathways in flavour profile differences between the two types of tea. Pathway enrichment analysis also found differences in secondary metabolite biosynthesis, especially for the phenylpropanoid, terpenoid, and alkaloid biosynthetic pathways; all critical for flavour. Higher contents of theanine in TS569 contribute to astringent taste profile. P312 has complex volatile profiles that enhance their aromatic complexity. Such results are foundational to the molecular basis of tea flavour and are useful in breeding, cultivation, and processing for maximal flavour characteristics consistent with consumers' preferences. In this way, the metabolic basis of this diversity in the flavours of tea is elucidated, pointing out the potential of metabolomics-guided strategies in Chinese tea for improving quality and consistency of flavour.

**Keywords:** GC-MS, metabolite profiling, aroma, biosynthesis, bio-energetics

# Repurposing of Anti-Lung Cancer Drugs as Multi-Target Inhibitors of SARS-CoV-2 Proteins: An Insight from Molecular Docking and MD-Simulation Study

Abdul Ashik Khan\*

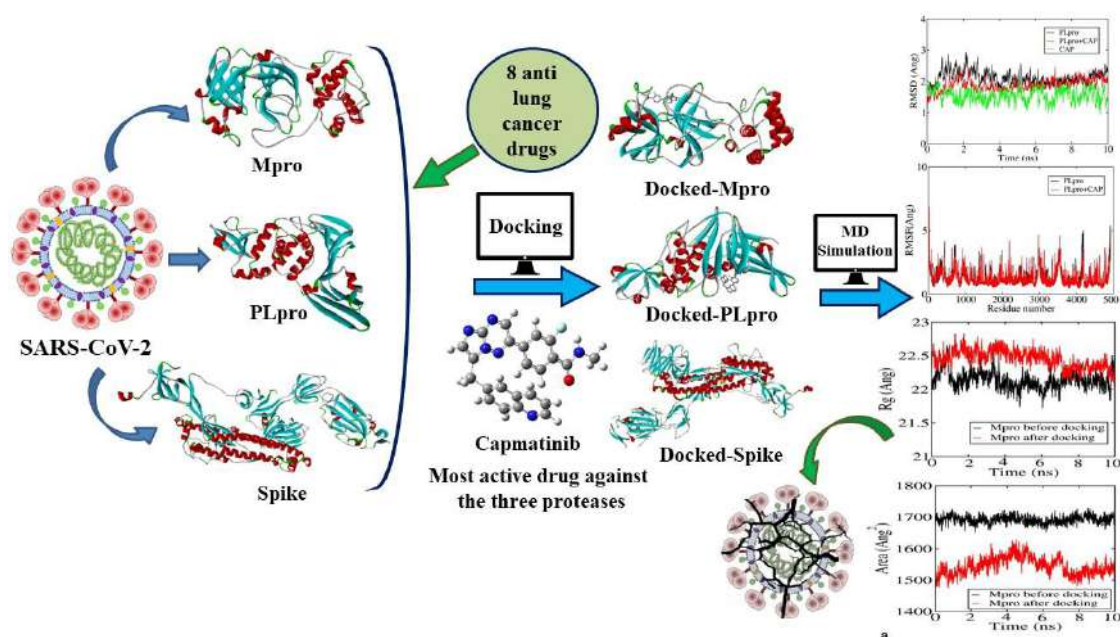
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## Abstract:

Herein we have selected seventeen anti-lung cancer drugs to screen against Mpro, PLpro and spike glycoproteins of SARS-CoV-2 to ascertain the potential therapeutic agent against COVID-19. ADMET profiling were employed to evaluate their pharmacokinetic properties. Molecular docking studies revealed that Capmatinib (CAP) showed highest binding affinity against the selected proteins of SARS-CoV-2. Molecular Dynamics (MD) simulation and the analysis of RMSD, RMSF, and binding energy confirmed the abrupt conformational changes of the proteins due to the presence of this drug. These findings provide an opportunity for doing advanced experimental research to evaluate the potential drug to combat COVID-19.

**Keywords:** SARS-CoV-2; Capmatinib; Molecular Dynamics Simulation; Mpro; PLpro; Spike protein.



# Designing Safer Cancer Drugs: Hydroxy-9,10-Anthraquinones and Its Metal Complexes as Promising Anthracycline Alternatives

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## Abstract

Anthracyclines such as doxorubicin and daunomycin are highly effective anticancer agents but their benefits are often overshadowed by serious heart-related side effects and high costs. Their effectiveness comes from their ability to insert into DNA, block essential enzymes like topoisomerases, and generate reactive oxygen species (ROS). Unfortunately, ROS also contribute to cardiotoxicity. This research explores Quinalizarin(1,2,5,8-tetrahydroxy-9,10-anthraquinone), a less costly simple structural analogue to Anthracycline anticancer drugs—as potential safer replacements. Physicochemical and biophysical interactions of Quinalizarin (THAQ) were studied. Comparative studies with anthracyclines suggested that the biophysical interactions with DNA were somewhat weaker probably due to the absence of sugar part. However, as lower binding is not desirable, metal complexes of THAQ with Co(II) and Cu(II) were prepared and characterized. The complexes showed comparable stability constant values with that of different anthracyclines. Co(II)(THAQ)<sub>2</sub> showed enhanced binding towards calf thymus DNA and Cu(II)(THAQ)<sub>2</sub> was found comparable with that of THAQ. Like anthracyclines, formation of the superoxide radical anion was identified for THAQ and its metal complexes and the study revealed that both complexes showed a decrease in superoxide formation compared to THAQ. Reduced ROS generation suggests these complexes could maintain anticancer potency while lowering the risk of heart damage. Results also suggested that complexes are effective than the parent compound in case of the inhibition of human DNA topoisomerase I and human DNA topoisomerase II. Cell line studies were also performed on JURKAT T lymphocyte cells & acute lymphoblastic leukemia (ALL) MOLT-4 cells. Together, these findings point to THAQ and its metal complexes as exciting candidates for developing next-generation, cost-effective chemotherapy drugs.

**Keywords:** Anthracyclines, Hydroxy-9,10-anthraquinones, THAQ, DNA binding, topoisomerase inhibition, superoxide radical

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3. H. Beraldo, A. Gurnier-Suillerot, L. Tosi, F. Lavelle, *Biochemistry* 24 (1985) 284.



# Regulating Population Fluctuations in Food Chains Through Threshold Harvesting

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## Abstract:

In this study, we propose a novel harvesting strategy-**threshold harvesting** for controlling chaotic dynamics in ecological systems. Specifically, we apply this approach to the well-known **three-species Hastings–Powell food chain model**, which is known to exhibit complex and chaotic population behavior. By implementing harvesting only when the prey (fish) population exceeds a specified threshold, we demonstrate that it is possible to regulate the system's dynamics, transforming chaotic trajectories into stable equilibrium, limit cycles, and periodic orbits (including period-2 and period-4 behaviors). Our results reveal that both the **frequency** and **intensity** of harvesting play crucial roles in achieving desired population dynamics. Numerical simulations validate the effectiveness of the proposed method.

**Keywords:** Chaos; Chaos control; Threshold mechanism; Hastings and Powell model.

# An Eco-Friendly Method of Synthesizing Bismuth Oxyiodide Nanocrystals for Wastewater Remediation

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## Abstract:

Bismuth oxyhalides [BiOX, X = Cl, Br, I] have emerged as promising photocatalysts due to their unique layered structures and strong visible-light absorption. In this work, bismuth oxyiodide (BiOI) nanocrystals were synthesized via a sonochemical route using Bi<sub>2</sub>O<sub>3</sub> and iodide salts, with citric acid and polyvinylpyrrolidone serving as capping agents to control crystal growth and prevent agglomeration. The structural, morphological, and optical properties of the prepared samples were examined through X-ray diffraction (XRD), UV-visible diffuse reflectance spectroscopy (UV-Vis DRS), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), high-resolution transmission electron microscopy (HRTEM), and photoluminescence (PL) analyses. The photocatalytic activity of the BiOI nanocrystals was evaluated by degrading model textile dyes, including Rhodamine B (RhB) and Methyl Orange (MO), under visible-light irradiation. The results revealed that the optimized BiOI nanostructures could degrade up to 95% of RhB within minutes, highlighting their high efficiency in removing hazardous organic pollutants. This study demonstrates that sonochemically synthesized BiOI nanocrystals, enhanced by suitable capping agents, hold significant potential for environmental remediation applications, particularly in the treatment of dye-contaminated wastewater.

**Keywords:** Bismuth oxyiodide, sonochemical synthesis, photocatalysis, capping agent, dye degradation, wastewater treatment.

# Co-Ordination and Redox Chemistry of 9,10-Phenanthreneiminoquinone(PIQ) with Heavier Metal Ions

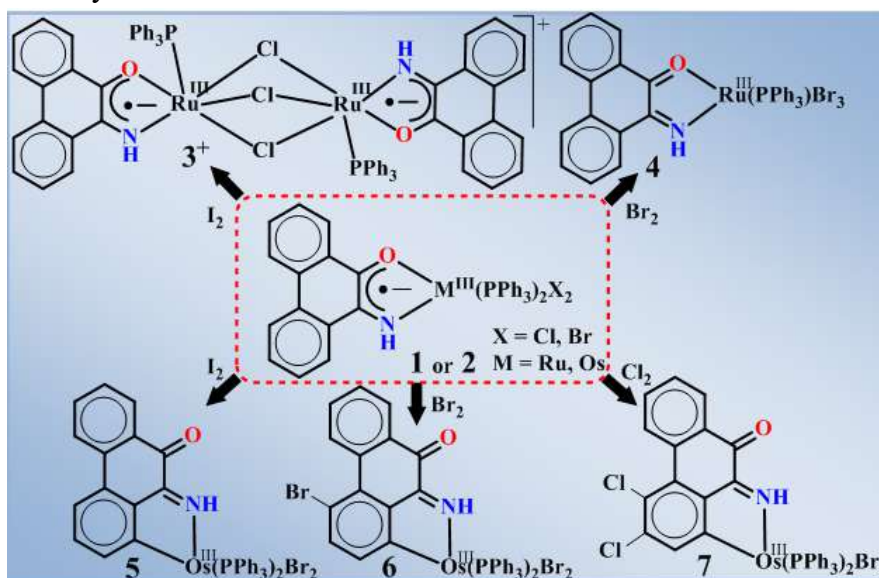
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## Abstract:

Co-ordination and redox chemistry of semiquinonate anion radical is an important area of study in light of biochemical transformation and catalytic perspective. In this work, we represented the chemistry of 9,10-phenanthreneiminosemiquinonate anion radical (PIQ<sup>•-</sup>) complexes of ruthenium and osmium metal ions. The reaction of PIQ with [Ru<sup>II</sup>(PPh<sub>3</sub>)<sub>3</sub>Cl<sub>2</sub>] and [Os<sup>II</sup>(PPh<sub>3</sub>)<sub>3</sub>Br<sub>2</sub>] afforded PIQ<sup>•-</sup> complexes of types, [Ru<sup>III</sup>(PIQ<sup>•-</sup>)(PPh<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>] (**1**) and [Os<sup>III</sup>(PIQ<sup>•-</sup>)(PPh<sub>3</sub>)<sub>2</sub>Br<sub>2</sub>] (**2**) respectively but they behave differently with halogens (I<sub>2</sub>, Br<sub>2</sub>, Cl<sub>2</sub>). Reactions of **1** with I<sub>2</sub> afforded chloro bridged complex, [Ru<sup>III</sup>(PIQ<sup>•-</sup>)(PPh<sub>3</sub>)( $\mu$ -Cl<sub>3</sub>)(PPh<sub>3</sub>)(PIQ<sup>•-</sup>)Ru<sup>III</sup>]<sup>3+</sup>I<sub>3</sub><sup>-</sup> (**3**<sup>+</sup>I<sub>3</sub><sup>-</sup>) while with Br<sub>2</sub> resulted [Ru<sup>III</sup>(PIQ)(PPh<sub>3</sub>)Br<sub>3</sub>] (**4**). Interestingly, the reaction of **2** with halogens results *ortho*-metalation producing [Os<sup>III</sup>(C,N-PIQ)(PPh<sub>3</sub>)<sub>2</sub>Br<sub>2</sub>] (**5**), [Os<sup>III</sup>(C,N-PIQ<sup>Br</sup>)(PPh<sub>3</sub>)<sub>2</sub>Br<sub>2</sub>] (**6**), [Os<sup>III</sup>(C,N-PIQ<sup>Cl2</sup>)(PPh<sub>3</sub>)<sub>2</sub>Br<sub>2</sub>] (**7**), where C,N-PIQ = *ortho*-metalated PIQ. The molecular and electronic structures of the complexes were established by different spectra, single-crystal X-ray structure, cyclic voltammetry and DFT calculations. The redox potentials were in range of +0.50 to -1.50V and the average C-O and C-N bond lengths were in the range of 1.27±0.01 and 1.30±0.01 Å as obtained from X-ray structures.



**Keywords:** Iminosemiquinonate anion radical, Chloro bridge complex, *ortho*-metalation

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# Smart Authentication Solutions: Harnessing Machine Learning to Combat Counterfeiting with $\text{Mn}^{2+}$ Co-Doped $\text{Y}_4\text{Al}_2\text{O}_9\text{:Eu}^{3+}$ Ink

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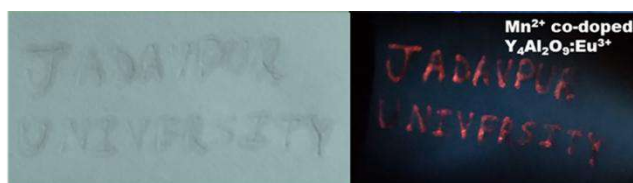
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**Abstract:** Counterfeiting is a global problem that creates difficulties for governments, businesses, and consumers [1]. Anti-counterfeiting strategies are developed to combat the rapid growth of counterfeit goods in various markets, such as luxury goods, brands, currency, and pharmaceuticals. There is a pressing need for anti-counterfeiting tags that possess high density, security, and storage capacity. These tags have attracted significant attention [2,3]. Utilizing functional materials with the ability to rapidly switch between various states, such as efficient label recording and document encryption systems, is a crucial method to enhance the data security and storage capacity of these tags. In order to investigate the potential of utilizing a solvothermal reaction technique at a temperature of 180°C for a duration of 4 hours,  $\text{Mn}^{2+}$  co-doped in  $\text{Eu}^{3+}$  doped- $\text{Y}_4\text{Al}_2\text{O}_9$  nano phosphors were synthesized. Following this, the powders underwent a calcination process at a temperature of 1050°C for 4 hours. The security ink was formulated by utilizing poly-methyl methacrylate (PMMA) as the binder, sodium dodecyl sulfate (SDS) as an additive, and dimethyl sulfoxide (DMSO) as the solvent. The design was rendered on paper substrates and illuminated with UV light to observe the pattern. The image pattern was identified through the application of machine learning techniques in image processing.



**Figure:** Hand-written pattern on paper substrates of prepared security ink under room light and excitation of UV light.

**Keywords:** Nano phosphor, Security Ink, Anti-counterfeiting, Machine Learning, Image processing

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# Diatom-Based Diets of Different Fish Species of Indian Sundarbans as Influencers of Taste and Nutraceutical Properties

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## Abstract:

Diatoms are well-recognized producers of polyunsaturated fatty acids (PUFAs) and essential amino acids (EAAs). Fish, like all other faunal components do not possess required enzymes for *de novo* synthesis of PUFAs and EAAs and procure these important bio-molecules from their algal diet, primarily diatoms. PUFAs, along with amino-acids are the precursor molecules necessary for production of flavour-enhancing compounds in fish which renders them commercially sought after and economically valuable. This study takes into account the fatty-acid and amino-acid composition of 10 diatoms obtained from the gut of two fish species *Tenualosa ilisha* (Hilsa) and *Osteobroma cotio* (Dhela). *Tenualosa ilisha*, is an exorbitantly priced shad owing to its scrumptious taste and is restricted by its seasonal availability in the estuaries of Indian Sundarbans and similar habitats elsewhere. While, *O. cotio* is a taxonomically unrelated cyprinid, abundantly found in brackish waters of Indian Sundarbans. The present study reveals the SFA and UFA content of *T. ilisha* as 48.05% and 51.62% respectively, quite similar to 45.03% SFA and 53.62% UFA content of *O. cotio* and hence advocates this species as an affordable alternative of Hilsa. The Bray-Curtis Similarity Coefficient indicates a relatively high similarity coefficient of 0.477 between *T. ilisha* and *O. cotio* which was based on results of 'Fish Consumption and Taste Perception Tool' developed and applied on the fish consuming population of West Bengal. This study further validates the similarity in diatom diet of the fish species and the relatedness in fatty-acid and amino-acid compositions of the two fish species with the diatoms present in their gut. This advocates the hypothesis that the fatty-acid and amino-acid profiles of diatom-based diet influence the fatty-acid and amino-acid profiles of fish species in a synergistic way. The results obtained have been further corroborated by means of WA-PLS statistical analyses.

**Keywords:** Diatoms, PUFA, EAA, *Tenualosa ilisha* (Hilsa), *Osteobroma cotio* (Dhela).



# 1,3-Diphenylisobenzofuran (DPBF) Arylsilane Derivatives for Improved Organic Transistor Applications and Photophysical Characteristics

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We have proposed and carefully investigated [1,2] arylsilanes based on 1,3-diphenylisobenzofuran (DPBF) as potential new organic semiconductor candidates. To determine their band gaps, excitation energies, hole- ( $\lambda_H$ ) and electron- ( $\lambda_E$ ) reorganization energies, etc., of the modeled arylsilanes, the DFT calculations are performed at B3LYP/6-311++G level. The results reveal that these suggested arylsilanes have superior properties compared to several other well-known semiconductor materials. The geometric and electronic structures and absorption/emission spectra of these 42 molecules are calculated at PBE0/Def2-TZVP level. Ground and excited state properties of these arylsilanes in gas phase and in different organic solvents are studied. Compounds with  $\lambda_H > \lambda_E$  are better electron transport materials (ETMs), and those with  $\lambda_H < \lambda_E$  are better hole transport materials (HTMs). Furthermore, the study shows that these molecules can be employed as effective trifunctional materials, i.e., emitter, hole, and electron transporters in OLEDs due to their improved electron injection and transport balance.

**Keywords:** organic semiconductor, arylsilane, diphenylisobenzofuran

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# Allelopathic Effect of *Cryptomeria Japonica* (Thunb. Ex L.F) D. Don Bark and Leaf Extracts on Seed Vigor and Metabolite Content in *Cicer Arietinum*

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## Abstract:

The allelopathic effects of *Cryptomeria japonica* on seed germination and early seedling growth of *Cicer arietinum* were investigated. Aqueous extracts of *C. japonica* bark and leaves at concentrations (0%, 15%, 25%, 50%, and 75%) were applied to *C. arietinum* seeds. Germination percentage, root and shoot length, and inhibition percentage were measured after 4 and 14 days. Tests assessed the impact on carbohydrate, protein, phenol, and amino acid content in treated seeds. Results showed concentration-dependent inhibitory effects on germination and growth. Germination decreased significantly with increasing concentrations, with strongest inhibition at 75% for bark (66.68%) and leaf (63.34%) extracts. Root and shoot lengths declined as extract concentrations increased, with highest inhibition at 75% concentration. Biochemical tests revealed reduced carbohydrate, protein, and amino acid content in treated seeds, while phenolic content increased. ANOVA showed significant differences in protein and phenol content among treatments. These findings demonstrate *C. japonica*'s allelopathic influence on *C. arietinum*, affecting growth and biochemical composition, highlighting the importance of allelopathic interactions in agriculture. Future studies could focus on identifying the specific allelopathic compounds involved and their mechanisms of action, providing further insight into their potential applications in sustainable farming.

**Keywords:** Allelopathic, Germination percentage, *Cryptomeria japonica*, Inhibitory effect.

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# Redox-Active (NNO) Ligands Enable Stabilization of M<sub>2</sub>-Oxido-Bridged Dinuclear VO<sup>3+</sup> Units

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## Abstract:

The evaluation of the dynamic activity of vanadium compounds, in particular mononuclear oxovanadium (V<sup>IV</sup>O), (V<sup>V</sup>O) and dioxovanadium (V<sup>V</sup>O<sub>2</sub>) species, represents a fascinating area in coordination chemistry. Two diamagnetic dinuclear  $\mu_2$ -oxido-bridged oxovanadium(V) complexes, [V<sup>V</sup><sub>2</sub>O<sub>4</sub>(L<sub>1</sub>)<sub>2</sub>] (**I**), and [V<sup>V</sup><sub>2</sub>O<sub>4</sub>(L<sub>2</sub>)<sub>2</sub>] (**II**), have been synthesised using different redox-active tridentate NNO-donor ligands, (L<sub>1</sub>H = (*E*)-1-(pyridin-2-yl diazenyl)naphthalen-2-ol, and L<sub>2</sub>H = (*E*)-4-methyl-2-(thiazol-2-yl diazenyl)phenol), respectively, in reaction with VO(acac)<sub>2</sub>. Both complexes were comprehensively characterised by different spectroscopy methods. The molecular geometries of **I** and **II** were confirmed by single-crystal X-ray crystallography, revealing two symmetrical oxovanadium cores in anti-angular configurations. Cyclic voltammetry studies reveal that the first reduction, observed at –0.70 V, corresponds to the (L<sub>azo</sub><sup>–</sup>/L<sub>azo</sub><sup>•2–</sup>) (L = L<sub>1</sub>(**I**) and L = L<sub>2</sub>(**II**)), while the second reduction, occurring at approximately –1.30 V, is attributed to the V<sup>V</sup>/V<sup>IV</sup> redox couple. Chemically generated in-situ produced **I**<sup>–</sup> and **II**<sup>–</sup>, exhibit single-line isotropic EPR spectra with g-values of 2.003 and 2.006, respectively, indicative of the presence of organic radicals within the systems. Mulliken spin density plots and EPR spectra of the compounds confirm that the mono-reduced analogues can be described as azo-anion radical–coupled oxovanadium (V) species, namely [V<sup>V</sup><sub>2</sub>O<sub>4</sub>(L<sub>1</sub><sup>–</sup>)<sub>2</sub><sup>•–</sup>] (**I**<sup>–</sup>) and [V<sup>V</sup><sub>2</sub>O<sub>4</sub>(L<sub>2</sub><sup>–</sup>)<sub>2</sub><sup>•–</sup>] (**II**<sup>–</sup>).

**Keywords:**  $\mu_2$ -oxido bridged vanadium, redox active tridentate NNO-donor ligands, azo anion radical, electronic structure

## Reference:

1. A. S. Roy, S. Ghosh, S. Bera and S. Maity, *Russ. J. Coord. Chem.* **50**, 11, 987–1000 (2024)

# Seasonal Variation in Avifaunal Diversity in an Iba Corridor of Darjeeling Himalaya

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## **Abstract:**

The Darjeeling part of the Eastern Himalaya is recognized as an Important bird and biodiversity area and endemic bird area. The region harbours over 43% of the 986 bird species found in the Himalaya hotspots, many of which are globally threatened and endemic. Birds provides various ecosystem services and are key indicators of ecosystem health. However, these birds are facing significant threats from anthropogenic activities and climate change in recent years. The present study documents avifauna diversity in Gangamaya Park area along the IBA corridors in the Darjeeling Hills, India. A seasonal variation in the bird community across four different habitats were examined through point count method. The study area harboured 93 species, with high species richness during the dry season. Passerines comprised of 80.6% of the bird species, 58.09% were found in forest habitats, and 61.29% were insectivores. Although all the species found were under the LC category, 10.75% are listed in CITES appendices, 15% are listed in Convention on Migratory Species appendix II, and as much as 20% were full migratory. Across season and habitat, Shannon-Weiner index and Simpson's index were consistently higher in the dry season. However, the rainy season showed better species evenness and dominance. Significantly higher species abundance was observed in habitats along the streams in the dry seasons. These findings highlight rich bird species diversity with distinct seasonal variations in the Darjeeling Hills. Despite having high species richness, researches on bird community outside protected areas is very limited. This study will serve as baseline information on seasonal variation in bird species and further the cause for conservation efforts.

**Keywords:** Bird species diversity, Darjeeling Himalaya, IBA, seasonal variation.

# Co-Exsolution Mediated *In Situ* Alloying: An Approach for Sustainable Catalytic Dry (CO<sub>2</sub>) Reforming of CH<sub>4</sub>

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## Abstract

The dry reforming of methane (DRM:  $\text{CH}_4 + \text{CO}_2 \rightleftharpoons 2\text{H}_2 + 2\text{CO}$ ) to produce synthesis gas not only bears a significant relevance in Fischer-Tropsch synthesis it has the advantage of mitigating global warming issues through natural gas valorization. Ni-based DRM catalysts go through sintering of the active phase(s) leading to coke deposition and deactivation. To address these issues, Ni and Cu co-doped hercynites ( $\text{FeAl}_2\text{O}_4$ ) have been synthesized following solution combustion synthesis and the optimized sample,  $\text{Ni}_{0.08}\text{Cu}_{0.07}\text{Fe}_{0.85}\text{Al}_2\text{O}_4$ , is reported to exhibit noteworthy coke-free conversions of 97% and 99% for  $\text{CH}_4$  and  $\text{CO}_2$ , respectively with  $\text{H}_2/\text{CO}$  ratio of  $\sim 0.80$ . Thorough characterizations suggest *in situ* co-exsolution mediated formation of NiCuFe termetallic alloy and  $\gamma\text{-Al}_2\text{O}_3$  along with retention of pristine hercynite phase. Alloying of the active components (Ni, Cu and host Fe) is shown to be beneficial in circumventing the difficulties of Ni-only catalysts in DRM. Interestingly, the residual carbon, present initially in the combustion-synthesized catalyst gets diminished in the course of reaction. Instead of coke deposition, substantial removal of the residual carbon in the DRM environment suggests  $\text{Ni}_{0.08}\text{Cu}_{0.07}\text{Fe}_{0.85}\text{Al}_2\text{O}_4$ , a promising next generation catalyst for DRM with sustainable coke resistant ability, which can be further extrapolated to simulated bio-gas reforming.

## Keywords

Sustainable coke-free DRM, NiCuFe alloy, hercynite engineering and solution combustion synthesis

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# Synthesis of Phospholipids and Its Derivatives: Their Role in Activation of Blood Coagulation

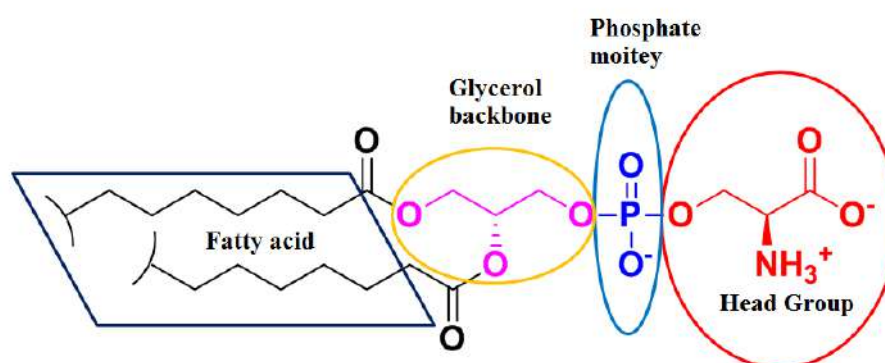
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## Abstract

Phosphatidylcholine (PC), Phosphatidyl ethanolamine (PE), Phosphatidyl serine (PS) and Sphingomyeline (SM) are main phospholipid constituents which are differentially distributed on cell membrane. PC and SM remain at outer leaflet whereas PS and PE at inner leaflet of cell membrane. Contributions of lipids in blood coagulation are known but involvement of its specific functional group is elusive. It is known till now that PS can enhance the TF-FVIIa complex activity several fold due to its negative charge. Through this project we are trying to biochemically understand the interaction of TF –FVII with different phospholipids at molecular levels and to elucidate the modulation in coagulation activity due to change of phospholipids environment. For this purpose, we have prepared different phospholipid (PL) derivatives in a novel synthetic method. We will further use this PL to understand the effect of PL in blood coagulation



**Figure:** Structural analysis of phospholipids at molecular level

**Keywords:** Blood coagulation, Phosphatidylcholine (PC), Phosphatidyl ethanolamine (PE), Phosphatidyl serine (PS)



## Allelopathic Effect of *Dryopteris* Sp. Leaf Extracts on Mung Bean Seeds

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### Abstract

An investigation was carried out to evaluate the allelopathic effect of *Dryopteris* leaf extracts on mung bean seeds. Results shows that *Dryopteris* leaf extracts (1:1, w/v) shows significantly reduced percentage germination.  $T_{50}$  values (h) were concomitantly higher in 1:1 leaf extract treated mung bean seeds. In case of TTC stainability, seeds treated with *Dryopteris* leaf extracts (1:1) showed reduced effect as well as dehydrogenase activity of mung bean seeds. Protein contents of seeds in case of control (distilled water) seeds, shows higher than the leaf extracts. Free amino acid and soluble carbohydrate leaching of mung bean seeds shows profuse leaching in case of leaf extracts (1:1) treated seeds. Thus, due to inhibitory effects of *Dryopteris* leaf extracts on mung bean seed germination behaviour, the plant extract (1:1) may use as bioherbicide purposes.

**Keywords:** Allelopathy, leaf extract, bioherbicide.

# Exploration of EMS Mutant Population of Two Local Rice Cultivars of North Bengal Revealed High Extent of Variations in Grain Quality And Yield Contributing Traits

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## Abstract:

Rice is one of the most important staple food crop consumed by half of the human civilization. Local rice cultivars consist of unrevealed genetic potentials, remarkable for rice improvement program. In this study, two local rice cultivars namely Beto and Malsira of Alipurduar district of North Bengal was assessed for promising mutant lines developed through EMS (Ethyl Methane Sulphonate), which is a potent alkylating chemical mutagen. A resource of around 2,000 M<sub>1</sub> plants of both the cultivars were screened for important agro-morphological, physico-chemical and biochemical traits following DUS guidelines (PPV & FRA), Govt. of India. Among the mutant populations of Beto and Malsira 46 and 59 M<sub>2</sub> mutant lines were identified respectively with wide range of variations in key traits associated with grain quality and yield traits. Beto revealed 13 M<sub>2</sub> lines with improved ECQ (Eating and Cooking Quality), 6 M<sub>2</sub> lines with high protein and antioxidant content and 11 M<sub>2</sub> lines with high grains per panicle. Malsira showed 9 M<sub>2</sub> lines with high ECQ and biochemical contents, 8 M<sub>2</sub> lines with long panicles and high grain weight. Therefore, these identified mutant lines having better performance than their wild-type cultivars, would be promising for rice enhancement research in near future.

**Keywords:** Eating and Cooking Quality (ECQ), Ethyl Methane Sulphonate (EMS), Local rice, Mutagen, Mutation.

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# Induction and Enhancement of the Superconductivity in $\text{BaFe}_2\text{As}_2$ by Ar Ion Implantation from Electrical and Magnetic Measurements

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## Abstract

Iron pnictide / chalcogenide superconductors(SCs) with superconducting critical temperature( $T_c$ ) reaching 58 K are promising engineering materials, particularly for making superconducting magnets. Our  $2.5 \times 10^{15} \text{Ar/cm}^2$  irradiation by 1.5MeV  $\text{Ar}^{6+}$  surprisingly enhanced  $T_c$  of underdoped  $\text{Ba}(\text{Fe}_{0.943}\text{Co}_{0.057})_2\text{As}_2$  single crystals by  $\sim 8.3\text{K}$  from its initial onset  $T_c$  of  $\sim 16.9\text{K}$  as measured from the real part of magnetic susceptibility. It matches well with 8.1K increase determined from the imaginary part, and 7.8K increase from electrical resistivity. This is in strong contrast to the earlier reported irradiation-induced  $T_c$  increases by marginal amounts [1] in different SCs. Ozaki et al(2016)-explained [2] their minor  $T_c$  increase of 0.5K in their SC samples of thickness( $t$ ) less than the ion range ( $R$ ) by assuming a nanoscale compressive strain developed from ion induced lattice modification. We have a new explanation of our large ( $\sim 49\%$ ) increase of  $T_c$ . Present  $t \gg R$  condition creates an Ar implantation layer up to a depth  $R$ , forming high pressure Ar microbubbles to provide large compressive strain on the SC lattice [3]. We discuss that such additional compressive pressure on the SC increases  $T_c$  to the extent we observe. We also discovered this pressure induced  $T_c$  in undoped and hence non-SC  $\text{BaFe}_2\text{As}_2$ .

**Keywords:** Fe-HTSC, irradiation enhancement of superconducting critical temperature, ion implantation, radiation damage.

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# High-Throughput Crystal Engineering Based Synthesis of Supramolecular Gels Capable of Synthesizing and Stabilizing Blue-Emitting Fluorescent Gold Clusters

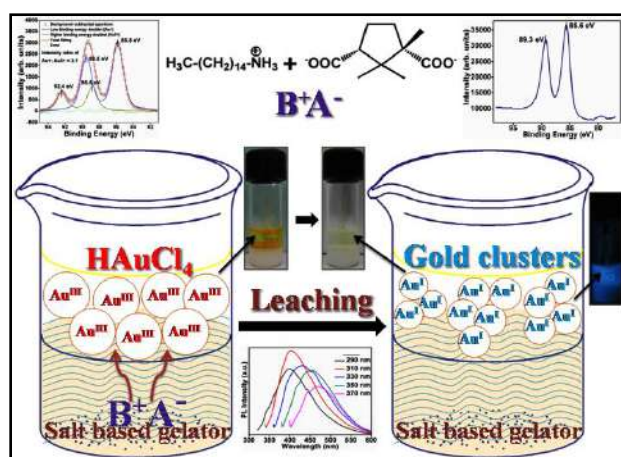
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## Abstract:

Gels are a colloidal state of matter in which a small amount of a solid-like network (gelator) is able to immobilize the bulk flow of a larger amount of liquid phase. Among different types of gelling agents, the two components low molecular weight gelators (LMWG's) are now a days a focused area of interest. This is mainly due to the reversible nature of gel forming network and their various potential applications. However, designing LMWGs is ever challenging as the mechanistic insights of gelation is poorly understood. Crystal engineering approach has been successfully exploited in designing a new series of two component supramolecular gelators derived from (1R,3S)-(+)-camphoric acid (CA) and long chain primary amines capable of synthesizing and stabilizing blue-emitting gold clusters without the use of any external reducing and capping agents.



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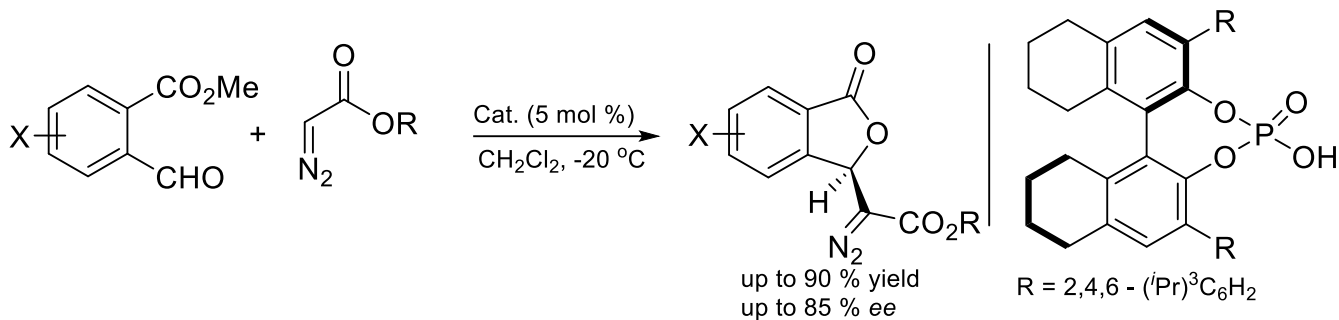
# Chiral Bronsted Acid Catalysed Enantioselective Syntheses of Phthalides: Application in The Synthesis of Herbaric Acid

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## Abstract:



Optically active phthalides, also known as isobenzofuranones, are widely found in both natural and synthetic compounds of considerable synthetic relevance and are associated with diverse biological activities. Many of these synthetic products display important pharmacological effects. The diverse pharmaceutical properties of these compounds are highlighted by their demonstrated anticonvulsant, antibacterial, anti-HIV, and anticancer activities. For instance, 3-butylphthalide has anticonvulsant properties; isochracinc acid and herbaric acid have antibacterial properties. Over the past few years, many efforts have been directed toward the asymmetric synthesis of phthalides or isobenzofuranones. Herein, we have reported a chiral Bronsted acid catalysed enantioselective syntheses of phthalides *via* aldol-lactonization reactions. A variety of enantioenriched phthalides containing  $\alpha$ -diazoesters were afforded in excellent yields and with excellent enantioselectivities. The catalytic system is amenable to gram-scale synthesis of phthalides. The synthetic potential of this methodology has also been demonstrated by exploiting the reactivity of diazo functionality in the product. Additionally, a concise synthesis of herbaric acid has been accomplished by using this protocol.

**Keywords:** Chiral Bronsted Acid Catalyst, Phthalides, Aldol-lactonisation. Herbaric acid.

# Radical Intermediates and Redox Cascades Based on 1,4-Naphthoquinone Derivatives

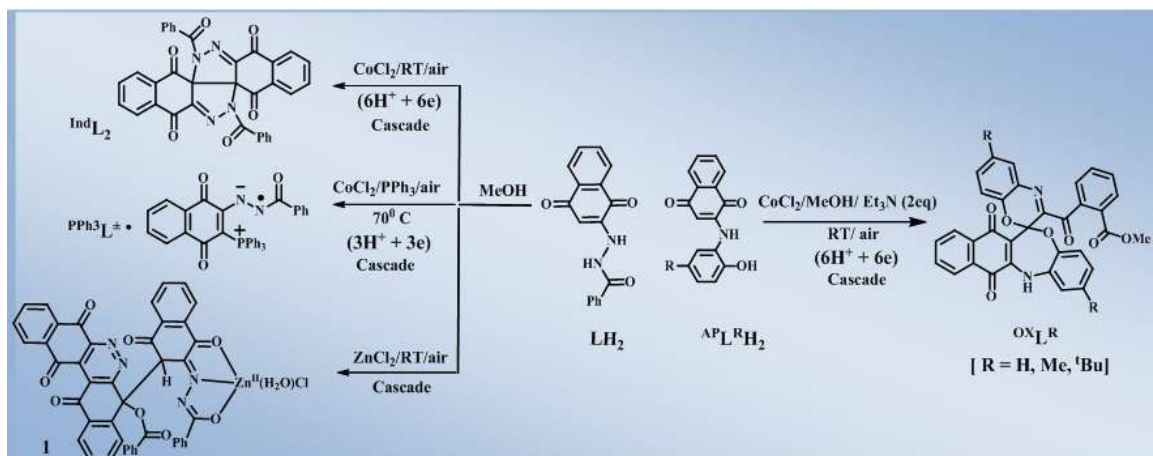
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## Abstract:

In coordination chemistry Stabilization of organic radical is significant role due to their unique bonding and reactivities in synthetic chemistry, biology as well as diverse redox reactions. Cascade reactions are worthy in synthetic organic chemistry because of their higher atom economy *vis-a-vis* reduced chemical waste that is the primary requirement of green chemistry. Herein, we disclose transition metal promoted redox cascades via organic radical intermediates and producing functional molecules that are important in pharmacy and not isolated by schematic routes. In this work, N'-(1,4-naphthoquinone-2-yl) benzhydrazide ( $LH_2$ ) is a precursor of redox cascades that undergoes transition metal promoted multicomponent redox reaction via radical intermediates involving C-N and C-C bond formations and affording diarylindazolo[3a,3-c]indazole ( $IndL_2$ ) in air is overall a ( $6H^+ + 6e$ ) oxidation reaction, in presence of  $PPh_3$ , produces a isolating chromatographically stable zwitterionic triphenylphosphonio-hydrazyl radical ( $^{PPh_3}L^{\pm\bullet}$ ) by ( $3H^+ + 3e$ ) oxidation reaction and produces pyridazine derivatives (**1**). Similarly, another naphthoquinone derivative of 2-((2-hydroxy-5R-phenyl)amino)-1,4-naphthoquinone ( $^{AP}L^R H_2$ ) is a precursor of a cascade to produce spiro oxazine-oxazepine derivative ( $^{OX}L^R$ ) in good yields. These multi-electron oxidative redox cascades of  $LH_2$  and  $^{AP}L^R H_2$  promoted by cobalt(II) or zinc(II) ions. The molecular and electronic structures of  $IndL_2$ ,  $^{PPh_3}L^{\pm\bullet}$ , **1** and  $^{OX}L^R$  were confirmed by different spectra, single-crystal X-ray crystallography, cyclic voltammetry and density functional theory calculations.



**Keywords:** Redox cascade, C-C & C-N oxidative radical coupling, chromatographically stable hydrazyl radical.

**References:** (1) S. Mondal, S. Maity and P. Ghosh, Inorg. Chem., 2017, 56, 8878-8888.

(2) S. Mondal, S. Bera, S. Maity and P. Ghosh, Inorg. Chem., 2017, 56, 13194-13204.

# Reduction of CO<sub>2</sub> to the Valuable Fuels on the Surface of Mg<sub>n</sub> (N=4 To 17) Clusters: An Insight from DFT Study

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## Abstract:

Magnesium cluster exhibits unique catalytic properties towards different organometallic and coordinating agents in different reactions. Herein we have made a comprehensive analysis of a series of twelve selected Mg<sub>n</sub> clusters to explore activation and reduction of CO<sub>2</sub> to value added fuels like formic acid, methanol and methane. Highest E<sub>ads</sub> is occurred by Mg<sub>8</sub> and lowest by Mg<sub>4</sub>. Of the twelve clusters that were chosen, only nine of them have the ability to activate CO<sub>2</sub>. The reactivity order among the clusters is found to be increased as the size of the clusters increase. Furthermore, activation energy calculation showed that Mg<sub>8</sub> has lowest energy in the transition state which also interpret with the analysis of Gibbs free energy and enthalpy change. During the reduction of CO<sub>2</sub>, we find several fuels like formate, methanol and methane; although in major portion methane will be produced. Additionally, a molecular dynamics analysis showed that CO<sub>2</sub> is significantly adsorbed on Mg<sub>8</sub> and that, at normal temperature, it does not migrate from its adsorption. These results are crucial because they offer fresh perspectives on how to create magnesium cluster catalysts that convert CO<sub>2</sub> into useful fuels.

**Keywords:** DFT, CO<sub>2</sub> activation & reduction, Mg clusters.

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1. C. Sikorska, Magnesium-Based Oxyfluoride Superatoms: Design, Structure, and Electronic Properties, Journal of Chemical Information and Modeling, 59 (2019) 2175-2189.
2. K. Li, B. Peng, T. Peng, Recent advances in heterogeneous photocatalytic CO<sub>2</sub> conversion to solar fuels, ACS Catalysis, 6 (2016) 7485-7527.



# Structure-Property Relationships of Post-Synthetically Functionalised Fluorophoric [2]Rotaxanes: Conformational Fluxionality and Metal Ion Chelation

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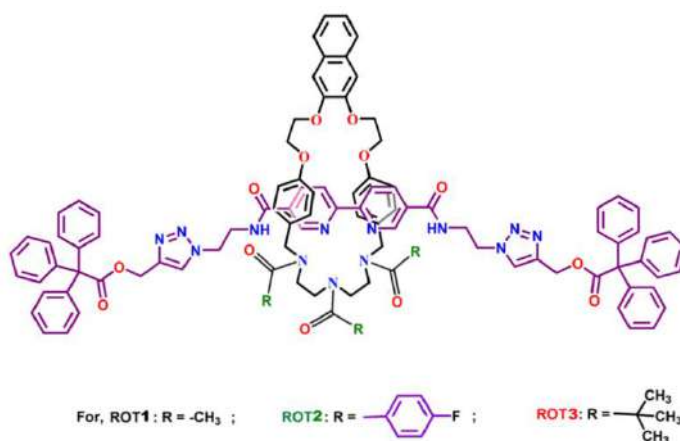
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## Abstract:

A multi-functional, metal-ion-free [2]rotaxane, built on an amino-ether fluorophoric macrocyclic wheel, was synthesized. The synthesis proceeded via passive metal-ion templation, followed by capping through click chemistry and subsequent demetallation of the templating ion. This rotaxane was further functionalized post-synthesis to yield three distinct analogues by the attachment of three different amide groups [-NC(O)R, where R = -CH<sub>3</sub>, 4-fluorophenyl, and tert-butyl].

The structural and spectroscopic properties of these post-synthetically modified analogues were characterized using mass spectrometry, 1D/2D NMR, and optical spectroscopy. The tertiary amide groups in the functionalized rotaxanes induce multiple conformers (or rotamers) due to rotation around the N-C(O) bonds. This rotational dynamic property is observed to a different extent in each analogue, with the steric bulk of the R groups playing a significant role. While the tri-acetylated and tri-aryl substituted interlocked molecules exhibit multiple conformational diversities at room temperature, the tri-tert-butyl appended rotaxane shows a predominant single conformer under the same conditions. This is attributed to the restricted rotation caused by the bulky tert-butyl groups. Notably, detailed solution-state emission studies established the presence of intramolecular exciplex formation between the wheel and the axle in ROT1,2,3. Finally, the ability of these fluorophoric rotaxanes to chelate transition metal ions was explored through absorption and emission spectroscopy.



**Keywords:** Rotaxane, Post-synthetic functionalisation, Rotamer, Tertiary amide, Exciplex

## References:

1. S. Santra, P. Ghosh, *New J. Chem.*, **2020**, 44, 5947-5964.

# **Comparative Study of the Reproductive Success in Three Species of *Arthromeris* J.Sm. from Sikkim in Relation to Leaf Architecture, Venation Pattern, Soral Position and Soral Size**

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## **Abstract:**

To elucidate the reproductive success in relation to leaf architecture, venation pattern, soral position soral size of three species of *Arthromeris* J.Sm. (*Arthromeris wallichiana* (Spreng.) Ching *Arthromeris mairei* Ching and *Arthromeris himalayensis* (Hook.) Ching) of Sikkim, the leaf sizes, leaf morphology, venation architecture, soral position, soral size were examined. There are fifteen parameters were taken into consideration for co-relating reproductive success with the venation architecture, soral position and soral size. Here reproductive success of the three species of *Arthromeris* J.Sm. were also tried to co-relate with frequency of distribution of these ferns in different altitudinal regions and climatic parameters of Sikkim. Among the parameters taken into consideration, the leaf midvein, leaf area and soral size shows strongest co-relation with increasing fertility index. Among the three species examined, *Arthromeris himalayensis* (Hook.), Ching, shows largest highest number of vein areole, highest number of sorus but *Arthromeris wallichiana* (Spreng.) Ching shows largest leaf area, sporangia and spores produced in it. This genus also shows large percentage of spore germination. In present study all these data also co-relates significantly with its frequency of distribution of these three species in the mountains of Sikkim. From the above study it is found that the reproductive success of the three species of *Arthromeris* J.Sm. were directly related to leaf architecture, number of vein areoles present, distance of the sorus from mid vein and size of the sorus along with climatic conditions.

**Keywords:** *Arthromeris*, Reproductive success, leaf architecture, venation pattern, soral position, frequency distribution, Sikkim.

## Effect of Catechol on Seed Germination Behaviour of Black Gram

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### **Abstract:**

An investigation was carried out to evaluate the effect of catechol on black gram seeds. Two concentrations *i.e.* 100 and 500 µg/ml was prepared (using distilled water) for the physiological and biochemical analysis. Results shows that reduced percentage germination was found in case of 500 µg/ml catechol solution treated seeds.  $T_{50}$  values (h) were concomitantly higher in 500 µg/ml treated black gram seeds over control (distilled water). In case of TTC stainability, seeds treated with 100 and 500 µg/ml showed reduced effect as well as dehydrogenase activity of black gram seeds. Protein contents of seeds in case of control (distilled water) seeds, shows higher than the catechol treated seeds. Leaching of free amino acids and soluble carbohydrates of black gram seeds shows higher in case of catechol treated seeds. It can be concluded from the experimental results that, the effect of catechol on black gram seeds is concentration dependent with respect to germination behaviour and metabolism. Thus, catechol shows inhibitory effects on black gram seed germination behaviour.

**Keywords:** Catechol, seed germination, black gram.

# Optimisation of Chemical Scarification for Enhanced Asymbiotic Seed Germination and *In Vitro* Propagation of *Dendrobium Gibsonii* Paxton

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## Abstract:

*Dendrobium gibsonii*, an orchid species, has seeds with unique morphology, including a thin transparent testa and an elliptical to fusiform embryo. This study aimed to investigate the effects of sodium hypochlorite treatment on seed viability and permeability in *D. gibsonii*. Seeds were treated with varying concentrations of sodium hypochlorite solution (1-10%) for different exposure times (1-10 minutes). The results showed that lower concentrations of sodium hypochlorite with minimal exposure time enhanced seed viability (86-93%), while higher concentrations with shorter exposure times (5% for 5 minutes) resulted in maximum viability. Permeability tests revealed that sodium hypochlorite treatment drastically increased seed permeability (99-100%) compared to the control (18%). Two-way ANOVA analysis confirmed significant differences in seed viability and permeability among treatments. This study provides insights into the optimisation of seed germination in *D. gibsonii* through sodium hypochlorite treatment, highlighting the importance of concentration and exposure time. The findings have implications for the conservation and cultivation of this orchid species.

**Keywords:** *Dendrobium gibsonii*, scarification, asymbiotic germination, *in vitro* propagation, permeability, sodium hypochlorite

## References:

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4. Deswal, D.P., & Chand, U. (1997). Standardization of the tetrazolium test for viability estimation in ricebean (*Vigna umbellata* (Thunb.) Ohwi & Ohashi) Seeds. *Seed Sci Technol.* 25:409–417.

# Antimicrobial and Anticarcinogenic Properties of Water Lily (*Nymphaea Nouchali*)

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## Abstract:

*Nymphaea nouchali* flower extracts and its solvent fractionates were exposed to physicochemical and fundamental phytochemical screening utilizing standard tests. The present study includes physicochemical and phytochemical examinations of the *N. nouchali* flower. The plant's flower extracts were subjected to a variety of qualitative chemical analyses, which revealed the presence of various phytoconstituents such as flavanoids, terpenoids, saponins, phenolic compounds, carbohydrates, tannins, and glycosides. Column chromatography of the DCM and CHCl<sub>3</sub> extracts was finished by solvent eluting strategies, and separated fractions were exposed to TLC study, where two compounds have been isolated as flavonoids with R<sub>f</sub> values of 0.80 and 0.74, respectively. The existence of different bioactive segments confirms the use of *N. nouchali* for different diseases by conventional experts. *In-vitro* radical scavenging actions of the various flower extracts of *N. nouchali* were executed, and the methanol extract uncovered the most scavenging power owing to polyphenolic cell reinforcement action, while pet. ether showed the least activity. The IC<sub>50</sub> Value of the extracts pet. ether, CHCl<sub>3</sub>, EtOAc, Me<sub>2</sub>CO, EtOH, MeOH and H<sub>2</sub>O were found to be 53.243 µg/ml, 62.647 µg/ml, 60.056 µg/ml, 57.728 µg/ml, 58.941 µg/ml, 69.611 µg/ml and 65.742 µg/ml respectively. The free radical scavenging properties of different extracts were in the order of: Methanol > Water > Chloroform > Ethyl acetate > Ethanol > Acetone > Pet. Ether. The investigation exposed explicit individualities for the specific herbal medication which will be helpful in distinguishing proof and quality control of the herbal drug. Experiment have indicated that these extracts can inhibit the growth of certain cancer cell lines, such as breast cancer cells (MCF-7).

**Keywords:** *Nymphaea nouchali*, physicochemical analysis, extraction techniques, phytochemical screening, anticarcinogenic activity.

## The Genus *Hypericum* L. of Darjeeling Hills

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### Abstract:

The genus *Hypericum* L. was created by Carolus Linnaeus in 1753 in his book Species Plantarum and the first detailed enumeration of the genus *Hypericum* L. was published by Choisy as a monograph, *Prodromus d'unemonographie de la famille des Hypericinees* in the year 1821. Subsequently, N. K. B. Robson described more than 457 species from 1977 to 2012. As detailed enumeration of the genus *Hypericum* L. (Hypericaceae) is not available for Darjeeling Himalaya, one of the important portions of Himalaya Hotspot of Biodiversity Conservation recognized by IUCN, the present work was planned to study and enumerate the Genus in this area. This work embodies extensive field surveys at different places of Darjeeling Hills and herbarium consultation in Lloyd Botanic Garden Herbarium. The present work describes field and herbarium specimens of 9 species of *Hypericum*, their distribution, phenology, population status and descriptions, Pollen morphology etc. The recorded species are *Hypericum himalaicum* N. Robson, *Hypericu melodeoides* Choisy, *Hypericum petiolulatum* Hook. f. & Thomson ex Dyer, *Hypericum hookerianum* Wight & Arn., *Hypericum tenuicaule* Hook. f. & Thomson ex Dyer, *Hypericum uralum* Buch.-Ham. ex D. Don, *Hypericum wightianum* Wallich ex Wight & Arn., *Hypericum japonicum* Thunb. ex Murray, *Hypericum gramineum* G. Forster. The presents study concluded with richness of species of *Hypericum* and indicated different kind of threats to them, and recommended a further details study on the genus with their population structure, ecological, ethnobotanical and pharmacological aspects as well as their conservational aspects.

**Keywords:** *Hypericum*, Darjeeling Hills, Taxonomic review, Himalaya Hotspot

# **Avian Composition of Manju Park in The Mid-Hills of Darjeeling Himalaya**

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## **Abstract:**

The mid-hill region of Darjeeling, characterized by tea gardens, forests, agricultural farmlands and ravines, provides diverse habitats that supports a variety of bird species. The region is also part of the Himalaya Biodiversity Hotspot, renowned for its rich flora that supports exceptionally high bird diversity of international significance, including threatened and migratory species. The present study was conducted in diverse land-use setting in and around Manju Park to document bird species. The study recorded a total of 31 species, representing 29 genera and 24 families under 8 orders. Among these, the order Passeriformes dominated with 18 species (17 genera, 16 families), followed by Cuculiformes (3 genera, 2 families) and Galliformes (3 genera, 1 families) with 3 species each. Accipitriformes and Strigiformes contributed 2 species each, while Columbiformes, Psittaciformes, and Piciformes were represented by a single species each. All the species recorded were categorized as Least Concerned by IUCN. These findings provide a baseline understanding of bird diversity at Manju Park and contribute to future monitoring and conservation efforts in the mid-hill region of the Darjeeling Himalaya.



# Are We on the Verge of Sixth Mass Extinction?

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## Abstract:

The Earth's history is punctuated by five major mass extinction events, each characterized by a rapid and significant loss of global biodiversity caused by catastrophic natural phenomena. Today, a growing body of scientific evidence suggests that the planet is entering, or has already entered, a sixth such event, often referred to as the Holocene or Anthropocene extinction. Unlike previous extinctions driven by asteroid impacts or volcanic activity, this ongoing crisis is attributed almost entirely to human activities. Current extinction rates are estimated to be hundreds to thousands of times higher than the natural background rate, with a significant number of species, particularly invertebrates, amphibians, and mammals, facing imminent threats. The primary drivers include habitat destruction and degradation, climate change, pollution, invasive species, and the over-exploitation of natural resources. This abstract reviews the scientific consensus, highlighting the unprecedented speed and human-driven nature of this biodiversity loss. It argues that the evidence points to a critical and accelerating trend that could have profound, irreversible consequences for global ecosystems and human well-being, underscoring the urgency for global conservation efforts.

**Keywords:** *Catastrophic, Anthropocene, Biodiversity loss, Extinction rate*

# Exploring The Molecular Interactions of Amino Acids and a Drug in Aqueous Solutions Across Various Temperatures: A Comparative Physicochemical and Theoretical Analysis

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## Abstract:

We conducted a complete chemical analysis of the significant molecular interactions for mixtures of aqueous Mephenesin (solvent) with two amino acids (as solute), L-Valine and L-Phenylalanine separately, by evaluating physicochemical parameters such as density, viscosity, and refractive index at various temperatures from 298.15 K to 313.15 K at an interval of 5K. The strong solute-solvent interaction existed in the solution have been ascertained with the help of some derived parameters such as the limiting apparent molar volume ( $\phi_v^0$ ), viscosity  $B$ -coefficient and limiting molar refraction ( $R_M^0$ ) obtained from Masson equation, Jones-Doles equation and the Lorentz-Lorenz equation respectively. Hepler's method and positive value of  $(dB/dT)$  data suggest that both the solutes (amino acids) are structure-breaking (chaotropic) in nature. The experimental findings are further authenticated by Density functional theory (DFT) calculations, such as adsorption energies, electrostatic potential maps (ESP), and reduced density gradient plots. The L-Phenylalanine-MEPN system exhibits more pronounced interactions than the L-Valine-MEPN system, as evidenced by both theoretical and experimental investigations.

**Keywords:** Mephenesin; L-Valine; L-Phenylalanine; Density functional theory.

## References:

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4. M. Mondal, S. Basak, B. Rajbanshi, S. Choudhury, N.N. Ghosh, M.N. Roy, *J. Mol. Struct.* 1257 (2022), 132571.

# PEG-Capped Silver Nano-Particle as Colorimetric Sensor for Fluoride Ion Sensing in Aqueous Medium

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## Abstract

The rapid detection of fluoride ions in aqueous solutions is very important due to the widespread contamination of groundwater and drinking water by naturally occurring fluoride ion which poses significant risks to human health. Addressing this need, poly(ethylene glycol)-400 (PEG-400) functionalized silver nanoparticles (Ag NPs) was synthesized and used for the selective detection of fluoride ions in water. The PEG-400-capped silver nanoparticles were synthesized as colloidal dispersions by heating an aqueous mixture of silver nitrate, PEG-400, and trisodium citrate. Key parameters such as temperature, silver nitrate concentration, and trisodium citrate concentration were systematically studied and optimized. The structure and morphology of the synthesized PEG-400-crowned Ag NPs were characterized by using UV-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, and field emission scanning electron microscopy (FESEM). The prepared Ag NPs exhibited high selectivity for fluoride ions in aqueous media, detecting concentrations as low as 0.098 mg/L through measurable changes in optical properties. These changes were analyzed using UV-visible spectroscopy, while morphological transformations were examined via FESEM. The results confirmed that fluoride ions induce rapid aggregation of the Ag NPs, accompanied by discharge of visible yellow.

**Keywords:** Fluoride ions; PEG-400; Silver nanoparticles

# An Asymmetric Dihydroxylation Route to (-)-Bulgecinine

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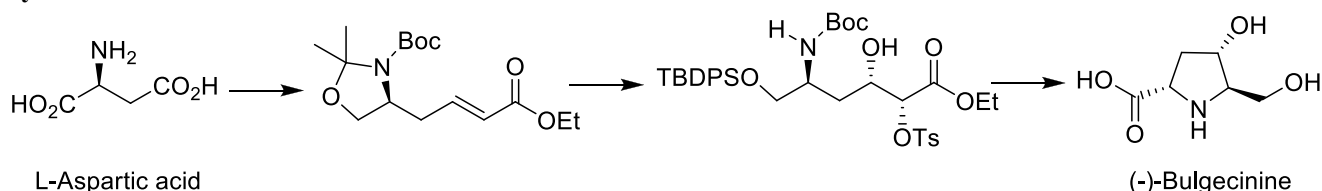
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## Abstract:

(-)-Bulgecinine is a constituent non-proteinogenic amino acid of the novel glycopeptide bulgecins, potent  $\beta$ -lactam synergists found in the culture broth of *Pseudomonas acidophila* and of *Pseudomonas mesoacidophila* (Fig.1). <sup>1</sup>Bulgecins A & B induce a characteristic morphological change called bulge formation in Gram-negative bacteria in cooperation with  $\beta$ -lactam antibiotics such as sulfazecin or isosulfazecin which is also produced by *P. acidophila* and *P. mesoacidophila*, respectively. As a result of bulge formation, the activity of these antibiotics is effectively enhanced. The structure of the new amino acid in bulgecins named (-) bulgecinine (**3**)<sup>2</sup>, has been determined chemically and crystallographically to be (2*S*,4*S*,5*R*)-4-hydroxy-5-hydroxymethyl proline.

Stereoselective synthesis of (-)-bulgecinine is reported from L-aspartic acid using Sharpless asymmetric dihydroxylation (SAD) and intramolecular cyclization via nucleophilic displacement of  $\alpha$ -tosylate as key steps.

## Synthetic Route:



**Keywords:** L-Aspartic Acid; (-)-Bulgecinine; Sharpless asymmetric dihydroxylation

## References:

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# Polymer Based Metal–Organic Framework Membranes

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## Abstract:

Polymer based metal–organic framework (MOF) membranes combine the tunable porosity and selective transport properties of MOFs with the mechanical strength and scalability of polymers, enabling next-generation separation technologies. By integrating MOFs into polymer matrices through mixed-matrix or thin-film composite designs, these membranes overcome conventional permeability–selectivity trade-offs, offering enhanced molecular sieving and improved stability. Advances in MOF–polymer interfacial engineering, nanoscale dispersion, and defect minimization have expanded applications in gas separation, water treatment, and solvent nanofiltration. Ongoing efforts focus on scalable fabrication, cost reduction, and long-term operational stability, positioning polymer-based MOF membranes as promising candidates for energy-efficient industrial separations.

**Keywords:** Polymer, MOF, Membranes

## References:

- [1] D. Bradshaw, A. Garai and J. Huo Chemical Society Reviews, 2012, 41, 2344–2381.
- [2] V. F. Yusuf, N. I. Malek and S. K. Kailasa ACS Omega 2022, 7, 49, 44507–44531.

# Temperature Compensation of Circadian Oscillations

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## **Abstract:**

Dynamics is a subject that explains how a physical variable of interest changes with time. Harmonic oscillation is a typical paradigm of linear motion. A conspicuous feature of this motion is that the frequency of the oscillator is independent of its amplitude. When the system is nonlinear its motion is more complicated because of the dependence of frequency on amplitude as a result of which the motion may vary from purely periodic to aperiodic manner. Based on the distribution of activation energies around the experimental mean and averaging of rate constants we propose a theoretical scheme to examine the temperature dependence and temperature compensation of time periods of chemical oscillations. The critical width of the distribution is characteristic of endogeneous oscillations for compensating kinetics as observed in circadian oscillations, while the vanishing width corresponds to Arrhenius temperature dependent kinetics of non-endogeneous chemical oscillation in Belousov-Zhabotinskii reaction in a CSTR or glycolysis in cell-free yeast extracts. Our theoretical analysis is corroborated with experimental data.

# Exploration of Actinobacteria as Effective Biocontrol Agents Against Phytopathogens

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## Abstract

Actinobacteria are a diverse group of Gram-positive bacteria known for their high G+C content in DNA, including *Streptomyces* and non-*Streptomyces* taxa, and are a rich and versatile source of biocontrol agents against phytopathogens. Their robust in vitro antagonism, production of antimicrobial metabolites and lytic enzymes, and multiple plant-growth-promoting traits translate into meaningful disease suppression and improved plant growth, development and disease suppression. Omics-guided screening further highlights diverse biosynthetic potential (NRPS/PKS clusters) that underpins biocontrol activity and offers opportunities to discover novel bioactive compound. Actinobacteria include a large portion of microbial rhizosphere communities and colonizers of plant tissues that not only produce pest-antagonistic secondary metabolites and enzymes but also stimulate plant growth. Non-pathogenic Actinobacteria can also induce systemic resistance against pathogens, but the mechanisms are still poorly described. In the absence of a pathogen, a mild defense response is elicited under jasmonic acid and salicylic acid signaling that involves pathogenesis-related proteins and secondary plant metabolites. Priming response partly includes the same compounds as the response to a sole actinobacterium, and the additional involvement of ethylene signaling has been suggested. Recent amplicon sequencing studies on bacterial communities suggest that future work may reveal how biocontrol active strains of plant associated Actinobacteria can be enriched. Collectively, these traits position Actinobacteria as sustainable alternatives or complements to chemical pesticides in integrated disease management.

**Keywords:** actinobacteria, biocontrol, induced systemic resistance, plant defense

# Legitimacy and Modus Operandi of Plant Music Therapy

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## Abstract:

Idea that plants are influenced by sound and music in positive and negative ways has been narrated by ancient literature, now the fact has been demonstrated by several scientists. In our country, experiments prove that raags *viz.* Maya-malav-gaul, Khara-hara-priya, Charukeshi etc., instruments such as flute, violin, harmonium, veena and Bharat Natyam have profound impact on different stages of plants' life processes *viz.* vernalization, germination, seedling physiology and growth, morphogenesis, anthesis, fruiting and seed-yields, protoplasmic streaming, oozing *etc.* Relationship might be between plant biological clock and time cycle of different raags. Western scientists observe similar botanical effects of different chords, rock, compositions of Haydn, Beethoven, Brahms, Schubert, Bach and Indian Sitar. Therapeutic value of music against pathological as well as physiological or systemic ailments of plants is now authentic.

Mode of action of sound and music on plants is more or less hypothetical. Clues, opinions and inferences are as follows: effect through soil, effects on stomata, metabolism, hormones, enzymes, respiration, photosynthesis and transpiration, RNA and soluble protein synthesis, gene regulation, resonance of cell organelles, cavitation, pressure variations, scale resonance and so on. Some botanical 'organ of Corti' and/or 'chakra' might be. So far understood from membrane permeability, potential and bioelectricity and signal transduction that sound and music perception site is plasmalemma.



# Supramolecular Aspects and Their Applications in Field of Photophysical and Bioactivity of Dicyanosubstituted 4-Pyridinyl-2-Pyridone Derivatives

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## Abstract:

Perchloric acid, hydrobromic acid, hydrochloric acid, tetrafluoroboric acid are used on dicyanosubstituted 4-(4 or 3-pyridinyl)-2-pyridone derivatives to make organic salts. The synthesized compounds were fully characterized by <sup>1</sup>H NMR, IR and single XRD. Various noncovalent interactions were thoroughly explored involving the aromatic rings, anions, and water molecules. 3-D architectures were built by using various noncovalent interactions like hydrogen bonds, halogen bonds, cation•••π, anion•••π, π•••π stacking, lone pair•••π, and C–H•••π interactions. Optical band gaps of some of the synthesized compounds were measured by using solid-state UV-vis spectrum data. Electrical conductivity and photosensitivity were examined and the results showed that they can be possible optoelectronic devices. The numerical quantities of the electrical factors change several times when the experiments were carried out in presence of visible light in place of dark conditions. These experimental outcomes have been proved by theoretical calculations. Moreover, the DNA binding ability of some of the symbolic salts was studied to find out the biological significance of the salts.

**Keywords:** 2-pyridone, Supramolecule, Photophysical Property

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# A Short and Generalized Route for The Synthesis of Polynuclear Aromatic Hydroxy Compounds by Intramolecular Gold (III) Catalyzed Diels-Alder Reaction

Khokan Samanta\*

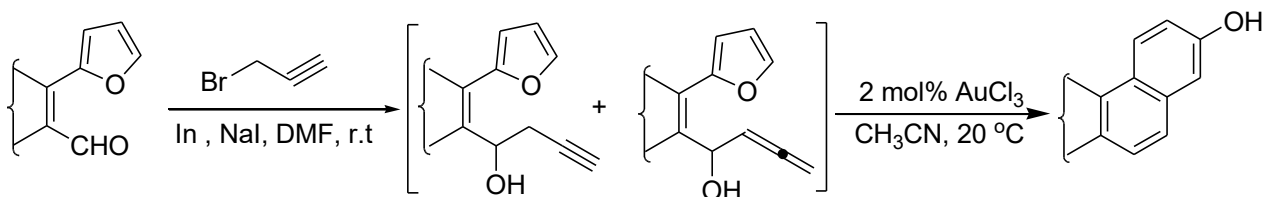
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## Abstract:

Naturally occurring different polyoxygenated phenanthrene derivatives was established as potential antimitotic compounds<sup>1</sup>, while some of these were found to be endogenous plant growth regulators. Several of the 9,10-dihydrophenanthrene derivatives were also found to exhibit pronounced phytoalexin properties.<sup>1</sup>

In this connection, Gold (III) catalysed intramolecular Diels–Alder reaction<sup>2</sup> of various 1-(2-furyl)-hex-1-en-5-yn-3-ol derivatives has been established to synthesise hydroxyphenanthrenes and other polynuclear aromatic hydroxyl compounds. The required precursors were prepared by indium catalysed propargylation<sup>3</sup> of suitable  $\beta$ -furyl- $\alpha,\beta$ -unsaturated aldehydes.



**Keywords:** Hydroxyphenanthrene, Gold(III) catalysed, Diels-Alder reaction, Propargylation

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# Nickel Catalyzed Acceptorless Dehydrogenative Annulation of 1,3-Aminoalcohols to Access 2-Amino Quinolines and Norcrypto-Tackiene Drugs

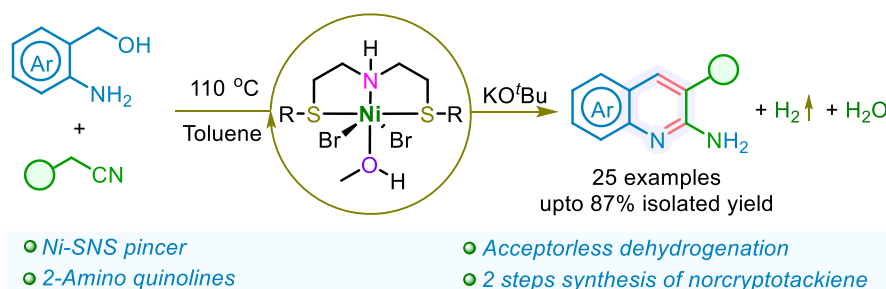
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## Abstract:

We report a phosphine-free, nickel(II)-catalyzed acceptorless dehydrogenative annulation (ADA) strategy for the selective synthesis of 2-aminoquinolines from feedstock 2-aminobenzyl alcohols and phenylacetonitriles. The well-defined Ni-SNS pincer catalyst enables a sustainable, atom-efficient process, releasing only H<sub>2</sub> and H<sub>2</sub>O as byproducts. Mechanistic studies reveal a nickel-mediated aldehyde intermediate, facilitating tandem C-C/C-N bond formation. Broad substrate scope, functional group tolerance, and scalability are demonstrated, including a streamlined synthesis of bioactive norcryptotackiene analogues *via* sequential Cu-catalyzed C-N coupling. Overall, this method offers a practical and eco-benign platform for constructing structurally diverse 2-aminoquinoline and norcryptotackiene frameworks.



**Keywords:** Acceptorless Dehydrogenative Annulation (ADA); Tandem Catalysis; Ni-SNS pincer, C-C/C-N bond formation C-O Coupling and C-C Coupling; Green and sustainable methodology

## References:

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# An Air-Stable Oxorhenium(V) Complex as a Catalyst for The Efficient Conversion of Aldehydes to Esters

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## Abstract:

The reactions of equimolar amounts of *trans*-[ReOC1<sub>3</sub>(PPh<sub>3</sub>)<sub>2</sub>] (**1**) with a Schiff base (H<sub>2</sub>L) synthesis by condensation of 2-aminophenol and 4-diethylamino salicylaldehyde result in the formation of [ReOCl(MeOH)L] in good yields. The compound (**1**) was characterized by analytical as well as spectroscopic techniques. The **1** crystallized as monoclinic crystal system with space group P2<sub>1</sub>/n. The X-ray crystal structures of **1** revealed that the molecule containing one tridentate anionic ligand (L<sup>2-</sup>) of ONO donors, one methanol, and one Chloro ligand with (ReO<sup>3+</sup>) core, adopting a distorted octahedral geometry. The **1** serves as a catalyst for the reduction of various aldehydes and ketones to their corresponding primary and secondary alcohols by phenylsilane yielding good yield. Moreover, **1** also acts as a catalyst to convert 4-nitrobenzaldehyde aldehydes or 3-nitrobenzaldehyde aldehydes to their corresponding esters in methanol with good yield. All products obtained from the catalytic reaction are isolated and purified using chromatography, and their structures are characterized by <sup>1</sup>H NMR and <sup>13</sup>C NMR spectroscopy. The structural parameters of **1** as obtained from X-ray crystal studies have been compared with the computed structure parameter. The observed outcomes are in good agreement with theoretical outcomes. The vibration frequencies, electronic transitions of **1** has been computed and compared with the experimental results. The global chemical reactivity descriptors based on conceptual density functional theory have also been calculated for a set of analogous systems derived from **1** and compare.

# Structural, Catalytic, And DFT Studies of Oxo-Rhenium(V) Complexes with N, O-Donor Schiff Base Ligands

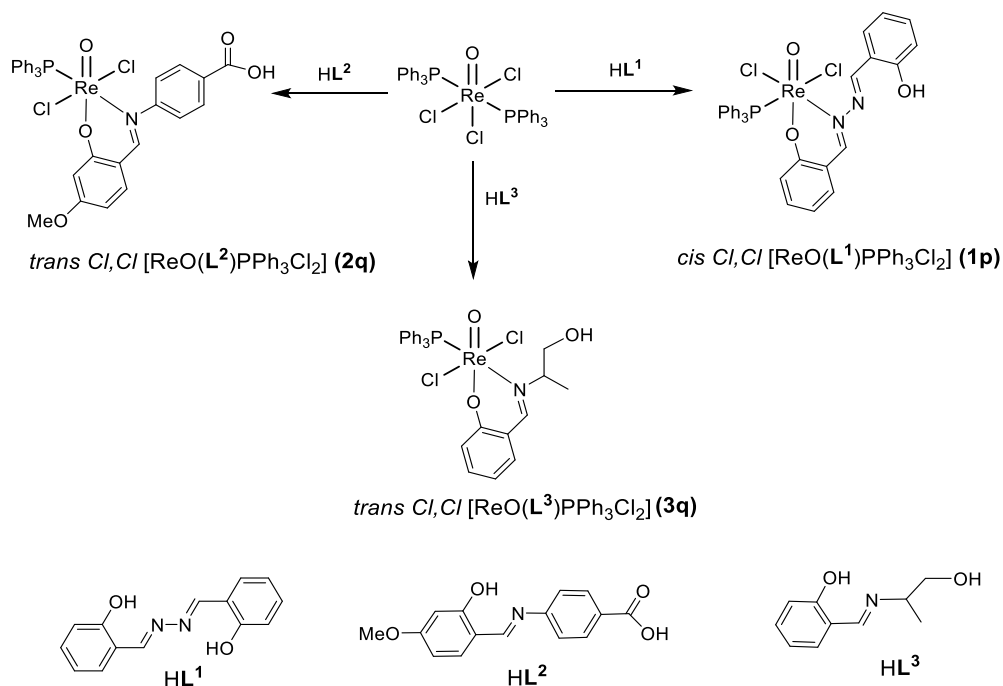
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## Abstract:

Reactions of  $[\text{ReOCl}_3(\text{PPh}_3)_2]$  with N,O-donor bidentate Schiff base ligands bis [2-(iminomethyl)phenol] ( $\text{HL}^1$ ), 4-(2-hydroxy-4-methoxybenzylideneamino)benzoic acid ( $\text{HL}^2$ ) and 2-(((1-hydroxypropan-2-yl)imino)methyl)phenol ( $\text{HL}^3$ ) resulted in the solid state isolation of the complexes *cis*- $\text{Cl,Cl} [\text{ReOCl}_2(\text{L}^1)(\text{PPh}_3)]$  (**1p**), *trans*- $\text{Cl,Cl} [\text{ReOCl}_2(\text{L}^2)(\text{PPh}_3)]$  (**2q**), and *trans*- $\text{Cl,Cl} [\text{ReOCl}_2(\text{L}^3)(\text{PPh}_3)]$  (**3q**) respectively. We have examined *cis* and *trans* isomers of all three compounds by computational method at DFT BP86/LANL2DZ. The computed geometry parameters are extremely close to the experimental values. The stabilisation energies and hardness calculation result strongly support the higher stabilities of the isomers **1p**, **2q** and **3q** over their counterparts **1q**, **2p** and **3p**. Thus, the results agree with the experimental findings of the isomers. The compounds **1p**, **2q** and **3q** were applied as catalysts for the reduction of various aldehydes to their corresponding primary alcohols in good yields and chemoselectivity.



**Keywords:** Oxo-rhenium(V) complex, Catalytic activity, DFT calculation.

# From Water Chemistry to Community Structure: Exploring Zooplankton as Sentinels of Ecosystem Health in a Wetland of Nadia District, West Bengal

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## Abstract:

Wetlands are among the most productive ecosystems, providing vital habitat for diverse aquatic organisms and sustaining ecological balance. This study investigates the relationship between water chemistry and zooplankton community structure in Bhaluka beel, a floodplain wetland of Nadia district, West Bengal, India. Zooplankton, occupying a key position in the second trophic level, play a central role in nutrient cycling and serve as an important food base for fish populations. Sampling was conducted during the monsoon season across multiple sites experiencing varying degrees of anthropogenic influence. Water quality parameters—temperature, pH, dissolved oxygen, free carbon dioxide, alkalinity, hardness, and primary productivity—were measured following standard protocols. Zooplankton were identified to Genus level, and community attributes were quantified using Shannon–Weaver diversity, Margalef's richness, Pielou's evenness, and Simpson's dominance indices. Analysis revealed clear associations between physicochemical characteristics and species composition, with certain taxa serving as reliable indicators of organic pollution. The findings highlight the importance of maintaining balanced physicochemical conditions to support stable and diverse zooplankton populations, which in turn safeguard the ecological integrity of wetland ecosystems. This work underscores the value of zooplankton-based monitoring as a practical tool for wetland health assessment.

**Keywords:** Aquatic bioindicators, Community stability, Organic pollution assessment, Trophic dynamics

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# Negative Differential Resistance Characteristics of Typical Square Graphynes

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## Abstract:

This study is based on combined Density functional theory and tight-binding calculations. Stable 4-12-2 and 4-12-4 graphynes are square symmetric, topologically equivalent containing one C-4 and one C-12 ring in the unit cell. The two probe model for the study of electrical transport are based on Landauer formalism. Density functional theory is combined with the nonequilibrium Green's function, whereas tight-binding calculations follow the wave function formulation. Results following both the procedure are equivalent, both the graphynes exhibit negative differential resistance in their current-voltage characteristics, with 4-12-2 graphynes showing superiority.

**Keywords:** Graphynes, square symmetry, transport properties.

# Generation and Evaluation of F<sub>1</sub> Hybrids Derived from Aus and Basmati-Type Rice Varieties

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## Abstract

Rice (*Oryza sativa* L.) is a nutritionally important cereal and the primary staple for more than half of the global population, sustaining human civilization since the advent of agriculture. To enhance yield potential and stress resilience, hybrid breeding is a key approach. The F<sub>1</sub> generation, obtained through controlled cross-pollination between genetically diverse parental lines, enables the integration of complementary traits. In this study, crosses were made between the high-yielding Basmati-type variety PB 1509 and the stress-tolerant Aus (Bhadoi) variety. The resulting F<sub>1</sub> progeny were evaluated under controlled conditions for critical agronomic traits, including plant height, grain yield, and tolerance to abiotic stresses. The hybrids displayed notable heterosis, with plant height increasing by approximately 20–30% compared to both parents. Additionally, grain size was improved relative to the donor parent, indicating potential enhancements in both productivity and grain quality. These results highlight the potential of Aus × Basmati-type F<sub>1</sub> hybrids to improve rice production in stress-prone environments and provide a basis for further studies on their stability, adaptability, and large-scale application in breeding programs.

**Keywords:** Abiotic stress tolerance, aus type, basmati, and F<sub>1</sub> hybrids.

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# A Green Solvent Catalyst for Many Organic Transformations

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## Abstract:

Agro-waste derived catalysts are gaining significant attention in green chemistry due to their eco-friendliness, low cost, and efficiency. This study presents the development and application of WELFSA (Water Extract of Lemon Fruit Shell Ash) as a versatile green solvent catalyst for various multicomponent reactions (MCRs), including the synthesis of benzyldinemalononitriles, 3-carboxy coumarins, 2-amino-4H-chromenes, 2-aryl substituted benzimidazoles, 2-amino-4H-pyrans, tetrahydrobenzo[b]pyrans, and pyrano[2,3-d]pyrimidine derivatives. The catalyst is prepared by burning dried lemon shells to ash, followed by aqueous extraction, yielding a basic solution (pH 11.50). These derivatives, known for promising bioactivity, were synthesized under mild reaction conditions using a few drops of ethanol without the need for chromatographic purification—pure products were obtained via simple recrystallization. Structural characterization was carried out using  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR, LC-MS, and melting point analysis. The findings indicate that WELFSA facilitates high yields and operational simplicity while aligning with the principles of green chemistry. Its scalability, cost-effectiveness, and environmental safety underscore its potential for widespread application in pharmaceutical and fine chemical synthesis. This work contributes to the advancement of sustainable catalysts in organic transformations, reducing both energy consumption and chemical waste.

**Keywords:** WELFSA, Green Catalyst, Agro-waste Utilization, Multicomponent Reactions, Sustainable Organic Synthesis

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# Diversity and Distribution Pattern of Epiphytic Bryophytes on *Cryptomeria Japonica* (Thunb. Ex L.f.) D.Don: A Case Study at Mirik, Darjeeling Hills

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## **Abstract:**

Epiphytic bryophytes play a significant role in maintaining the forest ecosystems. These species are important for biodiversity protection and conservation under sustainable forest management. The diversity and distribution pattern of these epiphytic species varies extensively among different host trees and geographical locations. This study aims to evaluate the diversity and abundance of epiphytic bryophytes on *Cryptomeria japonica*, a predominant conifer of the Darjeeling hills, and to investigate the role of microclimatic factors in shaping variations in their distribution patterns. The field surveys were conducted at Mirik and its surrounding forest areas, located within the 1500–1600 m asl elevation zone of Darjeeling, using 20 cm × 20 cm micro-plots. On each tree, field measurements and sampling were performed in eighteen quadrats, at six height zones up to 1.2 m of tree trunk from the base. Epiphytic community was mostly represented by mosses and leafy liverworts. The species accumulation curve indicated sufficient sampling effort, as it nearly reached a plateau. Among the sixteen identified taxa, fifteen were mosses, mostly belonging to the Dicranales and Hypnales, and one was Jungermanniales member. *Syrrhopodon confertus* was the most frequently observed bryophyte, showing maximum coverage, followed by *Heterophyllum amblyostegum*. The abundance-based species diversity was determined by calculating discrete Hill numbers. A Sharp decline with increasing coefficient of q (from order q=0 to q=1) indicated the presence of rarely abundant species in the studied area. The statistical evaluation predicted the influence of climatic parameters such as precipitation, temperature and solar radiation on bryophyte assemblage. The results are helpful in understanding the community structure of the conifer forests and may be further used for developing strategies for the management of such forests.

**Keywords:** Bryophytes, *Cryptomeria japonica*, Diversity, Epiphytes, *Syrrhopodon confertus*

# Unveiling the Functional Molecules of Mushrooms: Bioactivity and Therapeutic Potential

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## **Abstract:**

Mushrooms are nowadays increasingly studied for their bioactive compounds, substances that affect biological or chemical processes in the body and health. Mushrooms represent a prolific source of chemicals that provide a uniform raw material for manufacturing products in pharmaceutical, food, cosmetic, textile, environmental, and other industries. Bioactive molecules derived from mushrooms have attracted increasing attention due to their structural diversity and biological activity, including anti-inflammatory, antioxidant, antimicrobial, cytotoxic, neuroprotective, renoprotective, and immunomodulatory properties. The full potential of mushroom-based chemicals has yet to be realized. Research efforts have focused on identification of bioactive compounds and applications in medicine, food, and industry. Innovative approaches leverage the materials and chemicals inherent in mushroom mycelium for next-generation biomaterials with a range of tuneable properties.

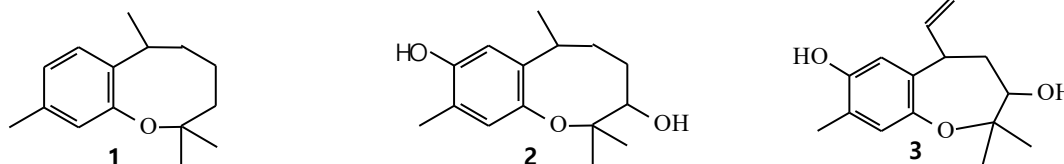
**Keywords:** Mushroom, Bioactive compounds, Antimicrobial activity, Antioxidant, Mycotoxin

# Approach Towards the Total Synthesis of Heliannane - Application of Unprecedented Selective Enol-Ether Preparation of 7-Ethoxy-2, 8, 8-Trimethyl-8, 9-Dihydro-Benzocyclohepten-5-One From 2, 2, 8-Trimethyl-Benzo [B] Oxepane-3, 5-Dione

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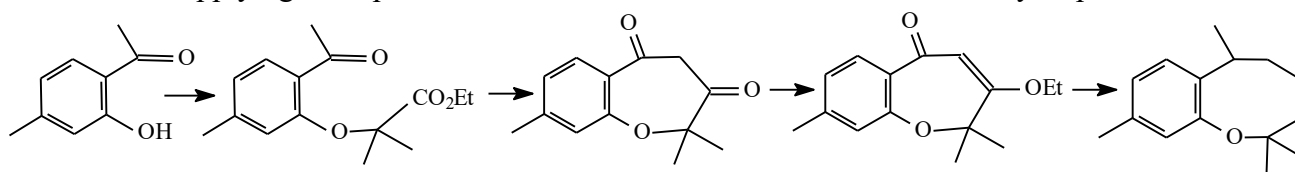
## Abstract:

Heliannane (**1**) constitutes a novel heterocyclic sesquiterpene isolated from the marine sponge<sup>1</sup>. Although marine sponges have been known to be a rich source of functionalised aromatic bisabolene sesquiterpenes, this is the first report of existence of benzofused heterocyclic ring system, with additional specialty being a benzoxocane ring system as present in (**2**).



Despite the seemingly simple structural network present in (**1**), the construction of the benzofused oxacyclic eight-membered ring is not an easily surmountable task. Snieckus<sup>2</sup> reported the first synthesis of heliannane (**1**) employing the very popular and well entrenched ring closing metathesis reaction for developing the benzoxocane ring system of (**1**). After that a number of conceptually different approaches has been initiated for the generation of the benzocyclooctane network of (**1**)<sup>3</sup>.

We are engaged for the synthesis of benzoxocane ring systems<sup>4</sup>. The synthesis of (**1**) will be demonstrated applying an unprecedented enol-ether formation reaction<sup>5</sup> as a key step.



**Keywords:** Heliannane, Wittig reaction, Enol ether formation

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- b. A. Roy, B. Biswas and Prabir K. Sen. *Syn. Comm.* 1692-1701, **2017**.
- Organic Reactions, vol-14, page-349.

# **Sustainable Use and Management of Biodiversity in Darjeeling-Sikkim Himalaya**

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## **Abstract:**

As the human population increases, so does the pressure on ecosystems, since we draw ever more resources from them. Our ecological footprint on the planet is unsustainable and will become unbearable unless we change our consumption patterns and our behaviour in general. In the past, humans have adapted to changing conditions by increasing productivity, but now we have reached the limits of the Earth's capacity. To use biodiversity in a sustainable manner means to use natural resources at a rate that the Earth can renew them. It's a way to ensure that we meet the needs of both present and future generations. The Darjeeling–Sikkim Himalaya, part of the Eastern Himalayas, is a global biodiversity hotspot. The region hosts diverse ecosystems ranging from tropical forests to alpine meadows, harboring rare and endemic species such as the red panda, Himalayan salamander, snow leopard, and numerous medicinal plants. However, this biodiversity faces growing threats from deforestation, overharvesting, climate change, unsustainable tourism, and invasive species. Sustainable use and management strategies—such as community-based resource management, regulated harvesting of medicinal plants, organic farming, ecotourism, and protected area networks—are essential to balance conservation goals with local livelihood needs. Integrating traditional ecological knowledge with scientific approaches, strengthening legal frameworks like the Biological Diversity Act (2002), and fostering active community participation are critical for long-term ecological resilience. The future of biodiversity in this fragile mountain region depends on coordinated efforts that ensure both environmental integrity and socio-economic well-being. The biodiversity of the Darjeeling–Sikkim Himalaya is both a natural treasure and a vital foundation for local culture, livelihoods, and climate resilience. Sustainable use and effective management demand a balanced approach that conserves fragile ecosystems while meeting the socio-economic needs of mountain communities. Strengthening community stewardship, promoting eco-friendly livelihoods, enhancing protected area networks, and integrating traditional knowledge with modern conservation science are essential to address current threats. With coordinated action among governments, researchers, NGOs, and local people, it is possible to safeguard this unique Himalayan biodiversity for present and future generations.

**Keywords:** *Biodiversity, sustainable, ecosystem, biological, mountain*