ONE DAY NATIONAL SEMINAR ON "INTERFACES OF CHEMISTRY AND BIOLOGY" (ICB-2024)

BOOK OF ABSTRACTS



11th May, 2024



Organized By

Department of Chemistry in collaboration with IQAC

Rammohan College

102/1, 85A-Raja Rammohan Sarani

Kolkata-700009

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श्रद्धावान् लभते ज्ञानम्

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Programme Schedule

May 11, 2024 (Saturday)

Registration: 09:00 a.m.-10:00 a.m.

Inaugural Function: 10:00 a.m.-11:00 a.m.

Felicitations of the Guests and Invited Speakers

Welcome Address: Dr. Saswati Sanyal, Principal, Rammohan College, Kolkata

Adress by the Chief Guest: Mrs. Tapati Ghosh, President, Governing Body, Rammohan College

Adress by the IQAC Co-Ordinator: Dr. Krishnendu Sarkar, Rammohan College

Address by HOD: Dr. Arup Mandal, HOD, Dept. of Chemistry

Convenors' Address: Dr. Samiran Mondal, Convenor, ICB-2024

Official Inauguration by Watering of Plant

Tea Break: 11:00 a.m. - 11:30 a.m.

Scientific Session 1

Plenary Lecture 1 11.30 a.m 12.30 p.m. Dr. Arpita Chandra	Plenary Lecture I	11.30 a.m 12.30 p.m. Dr. Arpita Chandra	
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Poster cum Lunch: 01:30 p.m. - 03.00 p.m.

Scientific Session 2

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Vote of Thanks

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INVITED SPEAKERS' ABSTRACT

Unveiling the chemotherapeutic potential of a novel cobalt Schiff base complex

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Discovery of cisplatin, motivated the development of metal complexes for chemotherapeutic purpose. However, the high toxicity of these platinum-containing chemotherapeutic drugs prompted the scientific community to investigate other less toxic chemotherapy drugs. In this context, we have synthesized a novel mononuclear Schiff-base base cobalt complex (III) in a single pot, characterized completely, by a wide range of physicochemical methods including X ray single crystallography and isolated > 99% purity. We tested the anticancer activity of this mononuclear cobalt complex against breast cancer cell line MCF. Cell viability was evaluated using the MTT assay. CFSE staining, PI and Annexin-PI were employed to measure cell proliferation, cell cycle arrest and apoptosis respectively using flow cytometry. Western blot analysis is used to measure the protein expression. Cell invasion was investigated using the scratch assay. MTT study revealed that 1 has IC₅₀ value 16.81 \pm 1.33 μ M and demonstrates cytotoxicity towards MCF-7 cells after 24 hours of treatment at a lower dosage than oxaliplatin with IC₅₀ value 31.4 \pm 0.69 μ M without being excessively toxic to human PBMCs ($IC_{50} > 60 \mu$ M). In vitro investigation revealed that 1 inhibits cell proliferation and invasion in MCF-7 cells while promoting apoptosis by G2-M phase cell cycle arrest. The relatively simple to synthesize, non-toxic mono-nuclear cobalt complex indicates that it may be a promising candidate for novel anti-cancer therapies in future [1]. References

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In-silico and Immunopharmacological targeting of TLR4 for the Therapeutic Intervention of

Infectious and Inflammatory diseases

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Toll-like receptor-4 (TLR4) is an innate Immune receptor that plays pivotal roles in recognizing pathogenassociated molecular patterns and governs induction of Innate Immune responses. TLR4 activation can lead to the activation of both proinflammatory as well as anti-inflammatory cytokines. This functional peculiarity designates TLR4 as one of the crucial mediators of host immunity and immunopathogenesis in many infectious and inflammatory diseases of mankind. Till date, I have worked on understanding the critical roles of TLR4 in some of the prevalent infectious (lymphatic filariasis and COVID-19) and inflammatory diseases (Ulcerative colitis and colorectal cancer).

In our work on lymphatic filarial immunology, TLR4 was identified as the cognate receptor for binding surface antigen of the filarial parasite, Wuchereria bancrofti and inducing proinflammatory responses in host macrophages and dendritic cells. Therefore, human TLR4 was selected for designing anti-filarial agents. Eventually, a quinolone-fused cyclic sulfonamide was found as an active moiety while its derivative was found as a far better compound.

Our next finding demonstrated spike protein of SARS-COV-2 as the ligand of human TLR4 in the context of immunopathogenesis of COVID-19. This indeed opened a door to design a series of phytochemicals as well as a universal vaccine, AbhiSCoVac for intervening SARS-COV-2 induced immunopathological manifestations.

In our recent studies, TLR4 was critically examined for its association in two common gut-associated diseases viz. Ulcerative colitis (UC,) and colitis-associated colorectal cancer (CAC). TLR4 activation was found to be instrumental in the pathogenesis of UC as well as progression of CAC from UC. Considering the impact of TLR4 in these two pathological conditions, phytomedicines were screened and eventually IBIL-AR1 was found an excellent anticancer formulation with no apparent toxic effects on non-targeted cells and tissues.

Collectively, our research findings as well as other research works in the similar domain endorses TLR4targeted therapies as effective strategy to combat the aforementioned diseases if human.

Keywords: TLR4, Infectious diseases, COVID-19, Inflammatory diseases, Ulcerative colitis, Therapeutic intervention.

Ir(III) and Ru(II)-Based Photo-catalysts for Catalytic Cancer Therapy

Dr. Samya Banerjee

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Currently, the market available cancer chemotherapeutics are facing major problems like severe side effects and various types of cancer-producing resistances.^[1] These problems have limited the clinical application of chemotherapy.^[1,2] The worldwide burden of cancer could rise by 47% in 2040 with respect to 2020.^[2] Thus, a new generation of cancer drugs that can overcome the drawbacks of chemotherapy with a novel mechanism of action is urgently needed to save the cancer-affected population of the globe. Importantly, metal complexes possess the largely unexplored potential to enhance the immunomodulatory effects of chemotherapeutic agents.^[3] The design concepts for metallodrugs are in their infancy and need to be more widely explored.

The talk highlights the development of metal-based photocatalytic anticancer drugs, which is the core focus of our lab.^[4-12] Recently, our group has pursued the concept of photocatalytic cancer therapy as an alternative to chemotherapy with a novel mechanism of action and target site.^[4-12] This therapy provides spatiotemporal control over the activation of catalytic amounts of drugs at the target cancer site.^[4-12] This new concept of "photocatalytic cancer therapy" can overcome cis-platin resistance with no harmful effects on normal cells in vivo and in vitro.^[4-12] Ir(III) and Ru(II)-based photocatalysts^[4-11] induced intracellular NADH or NAD(P)H photo-oxidation in cancer cells at catalytic concentrations to create in-cell redox imbalance and metabolic disorder, which leads to cell death.^[4-11] Moreover, these Ir(III) and Ru(II)-based photocatalysts were also able to overcome the hypoxia-related cancer drug resistance problems.^[4-12] Overall, these Ir(III) and Ru(II)-based photocatalysts have the potential to emerge as next-generation clinical cancer therapeutics.

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PRESENTING AUTHORS' ABSTRACT

Kinetics and Mechanism of Lactic Acid by Hexavalent chromic acid in the Presence of 1,10-Phenanthroline Catalyst in Aqueous –Micellar Sulfuric Acid Media Monirul Islam* Seth Anandram Jaipuria College

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Hetero-aromatic N-base ligand like 1,10-phenanthroline (phen) catalysed chromic acid oxidation of Lactic acid in aqueous sulfuric acid media have been studied under the experimental conditions, [Lactic acid] $\tau >>$ [Cr(VI)-] at different temperatures. Under the kinetic conditions, HCrO₄ has been found kinetically active in the absence of phen catalyst while in the phen catalyzed path Cr (VI)-phen complex has been suggested in the active oxidant. In the catalysed path, Cr (VI)-phen complex neceives a nucleophilic attack by the substrate to form a ternary complex which subsequently experiences a two-electron transfer redox decomposition leading to Cr(IV)-phen complex. Then Cr (IV)-phen complex participates further in the oxidation of Lactic acid and ultimately is converted into Cr (III)-phen complex. Both the paths show first-order dependence on [Lactic acid] τ and [Cr (VI]) τ . The phen catalyzed path is first-order in [phen] τ . These observations remain unaltered in the presence of externally added surfactants. Effect of anionic surfactant sodium dodecyl sulfate (SDS) on the Phen-catalysed path has been studied. SDS accelerates the phen-catalysed path on the path. The observes micellar effects have been explained by considering the hydrophobic and electrostatic interaction between the surfactants and reactants.

Keywords: kinetics; catalysis; Lactic acid; Chromium (VI); 1,10-phenanthroline; surfactants.

New Aspects of Gold Catalyzed Benzannulation Reactions

Biswajit Panda

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Gold catalysis has emerged as an important tool in the field of synthetic organic chemistry for the selective functionalization of C–C multiple bonds. Previously, we have reported the gold-catalyzed benzannulation of pyridine-containing oxo-alkynes with alkynes for the synthesis of a variety of quinoline and isoquinoline derivatives in good to excellent yields. In this poster, we will discuss some reactivity and selectivity issues faced in our previous work and describe how we solved all these issues through the modification of reaction parameters. We also observed a hitherto unreported self-benzannulation reaction of oxo-alkynes, which will be discussed as well.

Enteropathogenic Bacterial Diversity as Alarming Indicator of Subhas Sarobar Lake, Kolkata:

Concerning public health

Jyoti Choudhury, Priya Mandal, Koena Sarkar, Misha Parveen Sk, Disha Bhagat,

Srijoni Basak and Dr. Sanjib Saha*

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Subhas Sarobar is a medium-sized man-made lake located in the north-eastern part of Kolkata, WB, and the water body supports diverse flora and fauna including phytoplankton, zooplankton, benthos, nekton, and bacteria, contributing to an interdependent and balanced ecosystem. Seasonal changes like temperature, rainfall, and humidity affect the water's physic-chemical parameters, which may contribute to the change in the faunal population. Also, this aquatic system is subjected to the use of domestic effluents. So along with seasonal changes, domestic discharges, washing cloth, utensils, bathing, and dumping of plastic wastes beside the lake water contribute to the changes in the physico-chemical properties of the water. All these anthropogenic activities ultimately deteriorate the lake water quality. These changes (low DO, high nutrient content) make a suitable environment for bacterial growth in the lake system, including the infectious bacteria that may affect aquatic animals and public health. Water contains bacteria species (Vibrio, Salmonella, Shigella, Enterobacter, Yersinia, Escherichia, Tetanus, etc.) that are harmful and can pose serious health issues in humans. Several health problems such as gastroenteritis and diarrhea featuring fever, chills, nausea, hypertensive septic shock, secondary lesions, and infection. Through the food chain, such bacteria are also transmitted in aquatic and terrestrial animals. Experimentally we have proved that the lake water bacteria (Vibrio, Salmonella, Shigella, Enterobacter, Yersinia) have a dose-dependent lethal effect on people by using a mice model (using live and heat-killed bacteria). Through our findings, we have identified, isolated, and purified different enteropathogenic bacteria like Salmonella sp., Vibrio sp., Shigella sp., Enterobacter sp., and Yersinia sp., and their role in the transmission of waterborne diseases among aquatic animals and surrounding people that cause serious health problems in near future.

Kew words: Subhas Sarobar, Bacterial diversity, Enteropathogenic bacteria, Public Health

Small-Molecule modulation of Protein-Protein interactions to treat cancer: Emerging Concept in

Drug Discovery

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Protein-protein interactions (PPIs) are intriguing targets for drug development since they are involved in the majority of crucial biological functions, such as DNA replication and cell motility. They are nevertheless regarded as difficult targets and frequently brushed off as "undruggable" due to the lack of deep pockets and the substantial contact surfaces involved in these interactions. Finding innovative therapeutic targets for a wide range of disorders with significant unmet medical needs is driving an increase in interest in researching the untapped potential of PPIs in drug discovery. Small molecule PPI (SMPPIs) inhibition has, to date, been the mechanism most frequently investigated, leading to substantial advancements in medication development. The main general strategies for finding small-molecule inhibitors of protein-protein interactions are described in this article, including high-throughput screening (HTS), fragment-based drug discovery. For this approaches, successful instances of the discovery of modifiers of protein-protein interactions are also highlighted.

Nanoparticles in Cancer Therapy

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Nanotechnology and nanomedicine are rapidly developing biomedical approaches in cancer diagnosing and treatment. These are the single agents capable of seeking the cancer cells and destroys them efficiently without harming normal surrounding cells. It can also simultaneously monitor the response to treatment. This technology encompasses the creation of materials and devices at atomic, molecular and supramolecular level for application in clinical use potentially. These nanomaterials have high therapeutic efficiency due to high surface to volume ratio. It enables them to tie, absorb and convey small bio molecules such as DNA, RNA, proteins, drugs and other molecules to targeted site. Targeted chemotherapy also minimizes systemic side effects. This write up elaborates the use of different nanomedicines in cancer therapy and imaging applications using radio labeled nanomaterials.

Plant growth-promoting Bacillus cereus MCC3402 facilitates rice seedling growth under

arsenic-spiked soil

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Arsenic (As) is a dangerous class-I non-threshold carcinogen in humans and a toxic metalloid that causes significant environmental contamination (classified by the International Agency for Research on Cancer). An arsenic-resistant bacterial strains were isolated from the agricultural field near industrial belt and identified as Bacillus cereus MCC3402. based on phenotypic characteristics, FAME analysis and 16SrDNA sequence-based homology. These strains were found to exhibit more resistance to arsenate than arsenite. The arsenic resistance was positively correlated to its ability in arsenate reduction and presence of arsB gene suggested its role in arsenic cycling. The bioaccumulation of arsenic was evidenced by AAS, FTIR, XRD, XRF, SEM, TEM and EDAX studies. Moreover, this strain also exhibited important PGP traits and found to enhance rice seedlings growth in terms of morphological, biochemical changes and reduces oxidative stress under arsenic stress in inoculated seedlings compared with un-inoculated experiments. Therefore, strain PMM6 holds the potential as bioremediator to restore As-contaminated agricultural lands while also promoting the growth of rice seedlings. It could thus be utilized in the bioremediation of As-contaminated agricultural lands in the near future.

Key words:

Bioremediation; Bioaccumulation; ACC deaminase; Arsenic toxicity; Antioxidant activity; Plant growth promotion

A zwitterionic probe for ratiometric fluorescent detection of aluminium(III) ion in aqueous

medium and bioimaging study

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The development of a fluorescent method for the selective ratiometric fluorescent detection of AI^{3+} ions in pure aqueous solutions and live cells is still a significant challenge. In the present study, we have synthesized an aminobenzoic acid containing Schiff base 2-((2-hydroxybenzylidene) amino) benzoic acid (compound 1) and its structure was confirmed through single crystal X-ray study. Compound 1 is highly soluble in water The sensing property of compound 1 towards different metal ions has been demonstrated using different analytical techniques. In fact, compound 1 acts as a ratiometric fluorescent probe for the selective detection AI^{3+} ion in aqueous solution without organic cosolvent. Moreover, test strips based on compound 1 were fabricated, which were found to act as a convenient and efficient AI^{3+} ion detection "Test Kit". In addition, compound 1 was successfully applied to detect AI^{3+} in RAW 264.7 murine macrophage cell line.

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Synthesis, characterization and spectrochemical studies on a few binuclear µ-oxo molybdenum(V)

complexes of pyrimidine derived Schiff base ligands

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Ten new binuclear singly oxo-bridged Molybdenum complexes (complexes 1–10) were prepared using five pyrimidine derived Schiff base ligands and two Mo(V) precursors (NH₄)₂MoOCl₅ and (NH₄)₂MoOBr₅. The ligands are prepared by the condensation of 4,6-dimethyl 2-hydrazino pyrimidine with salicylaldehyde (for HL1), o-hydroxy acetophenone (for HL2) and substituted salicylaldehydes (for HL3, HL4 and HL5) respectively. These ligands are already reported as good donors for Mo(VI) state. The μ -oxo Mo(V) complexes reported here bears a distorted octahedral geometry around each Mo atom with either N₂O₂Cl or N₂O₂Br chromophores. Fine variations in the spectroscopic behaviour of the complexes are observed in accordance with the varying electron donating properties of the ligands. All the complexes are unstable in solution and X-ray quality crystal of complex 1 could be isolated. All the complexes are characterized by IR and UV-Vis spectra.



Importance of solubility and solvation thermodynamics for understanding biological functions of

I-histidine in electrolytic environment

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L-histidine plays a crucial role in oxygen transportation, reversible CO₂ hydrolysis and prevention of inflammation in gastrointestinal tract in human body. The transportation hydrolysis and inflammatory phenomenon depend on solvation thermodynamics of concerned amino acid. In aqueous solution l-histidine exist as zwitterionic form and this regulate all interactions and changes occur in solution which in turn very much crucial for understanding the knowledge of their working mechanism as well as solvation phenomenon in biological system. All those biological processes must occur in aqueous solution as well as in aqua-electrolytic environment. Thus, profound knowledge of solution chemistry is very much essential to proper understanding of complex biological reactions. So, this investigation primarily examines the solubility at equilibrium and the dissolution thermodynamics of essential amino acid, I-histidine, a scavenger of reactive oxygen [1], in aqueous solutions containing **sodium chloride**, blood pressure controller and **potassium chloride**, a major nerve function helper [2]. The solubilities were measured from 288.15 K to 328.15 K using the analytical gravimetric method [3]. Salting in/out effect [4] is one the crucial factor responsible for solubility variation here. The resulting solubilities were then used to deduce the thermodynamics of the solutions. Subsequently, the free energies associated with solvation through transfer were examined.

Keywords: I-Histidine, Potassium Chloride, Sodium Chloride, Solubility, Solvation Thermodynamics, biological Processes

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<u>P-10</u>

Tailoring the Synthesis and Characterization of Graphene Oxide Thin Films with a Focus on

Electronic Properties

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A novel approach to synthesizing graphene oxide (GO) thin film was employed, beginning with an enhanced Hummers method to oxidize purified natural graphite flake, followed by solvothermal treatment. This method facilitated the introduction of oxygen-containing functional groups onto the graphene surface, enhancing its solubility, dispersibility, and reactivity. The resulting GO was characterized using various techniques including X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and ultraviolet-visible spectroscopy (UV-Vis). XRD analysis revealed a characteristic peak at $2\theta = 10.05^\circ$, corresponding to an inter-layer spacing of 0.83 nm. FTIR and Raman spectroscopy confirmed the presence of various oxygen-containing functional groups incorporated into the graphene structure, including C-H, OH, C=O, C-O-C, and COOH. SEM images depicted the formation of ultrathin and homogeneous graphene films. UV-Vis spectroscopy of the synthesized GO exhibited absorption peaks at approximately 239 nm, corresponding to the π - π^* transition of atomic C-C bonds, and at 301 nm, corresponding to the n- π^* transition of aromatic C-C bonds. Furthermore, the electrochemical behavior of glassy carbon electrodes modified with GO was investigated using the K_3 [Fe(CN)₆] redox couple system. The results suggested that the electron transfer process governed the electrochemical behavior of the modified electrodes. This study presents a comprehensive analysis of the structural and physicochemical characteristics of GO synthesized via an enhanced Hummers method, providing valuable insights into its potential applications in various fields.

Keywords: Graphene oxide, Thin films, Synthesis, Characterization, Electronic behavior

<u>P-11</u>

Progress of Rhodamine based Chromium Sensors - A decade

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Chemical sensors provide a rational approach in molecular recognition, molecular signaling, and optoelectronics leading to their usage in monitoring neutral and ionic species. Due to its rapidity and sophisticated instrumentation, the fluorogenic technique along with an appropriate probe might be a great strategy for sensing and/ detecting different *in vitro/ in vivo* cations in biological and environmental samples.

Rhodamine dyes, owing to their excellent photo-stability and photophysical properties along with high quantum yield, are excellent fluorophores. Spirolactam or spirolactone derivatives of rhodamine are not luminous and are colourless, but when the ring of the corresponding spirolactam or lactone is opened, a bright pink fluorescence is generated. Rhodamine derivatives are crucial for this application, as recently been demonstrated by the fluorescent labelling of biomolecules and the development of chemically driven logic gate devices using rhodamine organic probes.

Despite the fact that Cr³⁺ is an effective nutrient that offers immune power to the human body, its over dose disrupts glucose levels and lipid metabolism and imposes noxious effects on the usual enzymatic activities, cellular structure and function through non-specifically binding itself to DNA, ultimately leading to mutation and cancer. Moreover, Cr³⁺ deficiency in humans causes maturity-onset diabetes, cardiovascular disease and nervous system disorders.

The focus of this study is to explore and understand the published fluorescence sensors for Al³⁺ ions using Rhodamine fluorophore by ring opening along with various type of process such as FRET-based 'ratiometric', 'OFF-ON' fluorescent responses, FRET (Fluorescence Resonance Energy Transfer) coupled with ICT (Intramolecular Charge Transfer) etc.

Schematic presentat rhodamine 6G deriva

Fluorescence OFF Spirolactam Form

form of the

Fluorescence ON Non-Spirolactam Form

<u>P-12</u>

Dynamics and stabiliy

Khushi Agarwal UG student, Rammohan College, 102/1, Raja Rammohan Sarani, Kolkata-09

How do you judge the stability of a particle or an object? Does just by visual representation one can define a particle to be stable or unstable? Here our objective will be to study or to discuss how to consider a particle or an object to be stable or unstable using some graphical analysis as well as numerical methods. The poster explores fundamental concepts of dynamics and stability in various systems. Dynamics refers to the study of how objects or systems change over time, influenced by forces and interactions. Stability, on the other hand, concerns the behaviour of these systems and their tendency to return to equilibrium after disturbances. Chemical dynamics involves studying the rates and pathways of chemical reactions. This encompasses the exploration of reaction mechanisms, energy landscapes, and kinetic processes. By investigating how molecules interact and transform over time, chemists can uncover the underlying principles governing reactivity. Dynamic systems exhibit varying levels of stability depending on factors such as temperature, pressure, and concentration. For instance, the stability of a reaction intermediate can dictate the overall pathway and efficiency of a chemical transformation. Conversely, the kinetics of a reaction can be influenced by the stability of intermediates along the reaction coordinate. The poster delves into key aspects of dynamics, highlighting concepts such as motion, acceleration, and at the same time the oscillatory motion of molecules within a chemical reaction. It examines equilibrium states and their stability properties, including stable, unstable and neutral equilibrium. Examples and applications from physics, engineering, and other disciplines are incorporated to demonstrate the significance of dynamics and stability in real-world scenarios. The poster aims to provide a comprehensive overview of these concepts, aiding in the understanding and analysis of dynamic systems for researchers and enthusiasts alike.

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Comprehensive Intervention to Address Physiological Risk Factors in Type 2 Diabetes Patients

of West Bengal: A Pilot Study

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Background: Diabetes is a medical condition that occurs when the body either doesn't produce enough insulin or can't use it properly. This results in high blood sugar levels that fail to reach the cells. In India, it is predicted that by 2025, approximately 98 million people may develop diabetes. The people of West Bengal are also at risk of this condition.

Objective: The aim is to identify and evaluate the physiological risks and morbidity associated with Type 2 diabetes patients. This involves reviewing and quantifying the health status of local diabetic patients. Additionally, recommendations for remedial measures will be suggested to improve the health and wellbeing of diabetic patients.

Method: The study included 75 male patients suffering from type 2 diabetes mellitus for a minimum of 5 years, between the ages of 30 to 42, residing in Burdwan and Hooghly districts of West Bengal, India. All the patients' physical parameters and physiological parameters such as **blood sugar levels**, **HbA1c**, **triglycerides**, **LDL/HDL ratio**, **vitamin D**, **HS-CRP**, and **LP** (a) were assessed using standardized procedures. Some clinical compounds: 'Empagliflozin (25mg) + Linagliptin (5mg)', daily 1 tablet before the meal, 'Metformin (1000mg)', daily 2 tablets after lunch and dinner, and 'Vitamin D3 (60000IU)' once in a week; were introduced for 24 weeks as advised by clinicians.

Results: All the mentioned parameters were found to be significantly improved in the intervention-phase. **Conclusion:** Taking together all the clinical compounds, the results of this study suggest that the mentioned compounds are the evidence to mitigate the physiological risk factors of Type 2 Diabetes.

Keywords: Type 2 Diabetes Mellitus, Vitamin D, Triglyceride, Glycated Haemoglobin, Blood glucose, Cardiovascular risk.

A natural flavonoid, Rutin rescues immunopathological consequences in an experimental model

of Lymphatic Filariasis

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Lymphatic filariasis (LF) is a widely recognized parasitic disease that has inflicted significant suffering on individuals globally, leading to a considerable social burden (WHO, 2023). The clinical manifestations associated with LF, including lymphedema, lymphangitis, and elephantiasis, are a result of the inflammatory responses triggered by interactions between the host and the pathogen. Upon recognition of antigenic surface proteins from the nematodes, pattern recognition receptors (PRRs) such as toll-like receptor (TLR)-4 play a crucial role in initiating the release of pro-inflammatory cytokines like TNFα, IL-6, and IL-1B, subsequently promoting the upregulation of co-stimulatory molecules on macrophages ($M\Phi$) and dendritic cells (DCs). This cascade of events can ultimately lead to exaggerated immunopathological responses associated with LF (Mukherjee et al., 2017). The persistent release of TNF α and other proinflammatory cytokines can perpetuate a cycle of chronic inflammation, primarily driven by the interaction between TNF α and its receptor TNFR1. To address this issue, a screening of natural anti-inflammatory compounds was conducted to identify potential candidates capable of inhibiting TNFR1 and TLR4 receptors, thereby restoring immune homeostasis. Through the utilization of an in silico methodology, a comprehensive analysis of 100 phytocompounds renowned for their anti-inflammatory properties was carried out. This investigation reported Rutin, a flavonoid compound known for its non-toxic nature, as exhibiting the highest binding affinity towards both TNFR1 and TLR4 receptors. In summary, the findings suggest a robust binding interaction between rutin and TNFR1 as well as TLR4 (in silico), indicating the potential of rutin to be explored further as a therapeutic agent for the management of LF.

<u>P-15</u>

Electron transfer between CT DNA and ternary copper complexes containing tyrosine and

tryptophan

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Electron transfer between small molecules and large macromolecules has been widely studied in recent days mainly for drug designing. In such systems beside the covalent bonding, noncovalent weak interactions play vital roles. Among the four amino acids with an aromatic side chain, phenyl alanine, tryptophan, tyrosine and histidine, phenyl alanine contributes mainly to the stabilization of proteins through hydrophobic interactions whereas tryptophan has an electron rich indole ring which has an excellent electron donating property. Further aromatic amino acid residues preferably engaged in stacking with nucleic acid bases and could represent a possible target for oxidative damage through radical migration.

The copper ternary complexes containing tyrosine and tryptophan undergo intramolecular photoinduced electron transfer. The amino acids are acting as electron donor while the other ligand present accepts the electron. In presence of CT DNA the guanine base present in the nucleic acid acts as electron donor. In presence of an external magnetic field the radicals generated are increased in population because their geminate characteristics is preserved due to electrostatic interaction between the complexes and the nucleic acid.
Replacement of classical experiments by experiments involving nanomaterials as greener

alternatives

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Chemistry is indissolubly linked to our daily life. There are lot of classical experiments or conventional methods are available to synthesize chemical compounds or products. But the traditional or classical experiments has many disadvantages like air pollution, expensive, toxic to human health etc. Mainly, hazardous side products are responsible for the environmental pollution which is the most worrying issue now a days. To solve this problem scientists introduced greener methods which can avoid such difficulties. Replacement of classical experiments by experimental methods involving nanoparticles are environment friendly as well as cost effective. This poster discusses some key examples of nanomaterial-based experiments and emphasize on adopting such environment friendly practices in research for more environmentally conscious future.

<u>P-17</u>

Flavonoid-based small-molecule drugs development against COVID-19

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By the end of 2019, scientists came to know about a novel Corona virus, SARS-CoV-2 [severe acute respiratory syndrome-Corona virus-2] causing COVID-19 (Corona Virus Disease-19). This initially affected people of Wuhan city of China. Later, this virus became the root cause of deaths and untold sufferings of millions of people around the globe due to the unavailability of specific medicine or therapeutic strategies. Although several effective vaccines were developed to prevent COVID-19 spreading and infections. Natural products and their derivatives especially flavonoids showed immense therapeutic potential early in the pandemic and thus attracted particular attention. Quercetin, baicalein, and luteolin are among the most studied flavonoids in this field. Flavonoids can directly or indirectly exert antiviral activities, such as the inhibition of virus invasion and the replication and proinflammatory factors in the body and improve inflammation in COVID-19 patients. It is hoped that this will provide ideas for the development of flavonoid drugs.

Non-linear dynamics & vanderpol oscillator

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Many problems in physics, chemistry, biology are related to nonlinear self-excited oscillators. We have to learn about them and about their stability. Firstly, we have to know that what is non linear dynamics? Secondly about its application in various fields. The importance of being non-linear is very much essential as it will give us about the characteristics of various classification of non linear dynamics. The poster will deal with many types of examples with graphical illustrations. How will you judge the stability of an object just by visual representation? Here our objective is to learn or to discuss how will a particle be stable or unstable just by using some graphical analysis. We will also learn about some methods like EULER method & RUNGE-KUTTA method which are used to solve a differential equation and also illustrate them with some special type of examples. Our next discussion will be about bifurcations. Lastly, the poster explores about the VANDERPOL OSCILLATOR which is a nonconservative oscillating system and about its characteristics through graphical analysis.

<u>P-19</u>

Computational insights into the ion channel architecture of the Dengue Virus M protein

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Dengue virus, an arbovirus belongs to the Flavivirus genus and is the causative agent of Dengue fever, Dengue Hemorrhagic fever and Dengue Shock Syndrome, thus accounting for thousands of lives every year. Very less information regarding the Dengue virus viroporins makes studies on the structural, mechanistic and functional aspect on these porins important. In this study we have characterized the M protein ion channel of Dengue virus which have been previously shown to possess porin like functions. The pore forming segments of the protein were identified using exhaustive literature survey and several in silico methods. The possible oligomeric status of the pore forming segments were ascertained using independent sets of MD simulations and post simulation analyses followed by hydration analysis of the channel interiors. The ion conductivity mechanism of the different oligomeric architectures were studied making use of computational electrophysiology MD simulations leading to the selection of the most probable ion conducting conformation and oligomeric status. The ion channel architectures were characterized in depth based on their structural organization and their electrical properties like current through channel and conductance. This study also sheds light into the conductance mechanism of the ion channel architectures. This study helps to provide detailed information into the structure-function relationship into the porin activity of M protein. The information obtained from this study may aid further studies on the ion channel activity of the Dengue virus proteins in near future and help to target these proteins for therapeutic intervention leading to decrease in the number of casualties as a result of Dengue infection.

<u>P-20</u>

An in-silico analysis of 3-dimensional structure of fish proteins: An interface of zoology and

chemistry

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In-silico analysis of proteins by various bioinformatics tools via different computer-assisted procedure and web programmes like: analysis of physiochemical properties of proteins, 3-dimensional structural prediction by homology modelling, drug designing etc. are very recent advanced interface areas of biology with structural chemistry. Implementation of such an emerging area in zoology, especially in fisheries can be useful for betterment of fishery sciences. Goldfish (Carassius auratus) is an ornamental fish consisting melanocortin system. Various researches in several fish species presented melanocortin receptors $\overline{4}$ (MC4R) is involved in different functions in fish body. Therefore, an *in-silico* analysis of MC4R of gold fish has been presented in the study via implementing bioinformatics tools to know the physicochemical properties and 3D structural confirmation of the protein. Sequence containing accession number XM_026207258.1 was taken from National Center for Biotechnology Information (NCBI) and then processed by various web-servers to analyse its physicochemical characterization, secondary and 3D structural prediction of the concerned protein. The results suggested MC4R is a stable, hydrophobic and slightly basic nature of protein. The secondary structure of the analyzed MC4R protein suggested presence of 50.77% alpha helix, 19.69% extended strands and 3.38% beta turns along with 26.15% random coils. Moreover, it might be resolved from the Ramachandran plot that the structural prediction of MC4R is correct in prediction. Further, predicted 3D structure of MC4R protein can also be utilized for docking and simulation studies in future. Moreover, such studies reduces the gap between the sequence data and solved structures by X-ray crystallography and NMR spectroscopy, which are also tedious and expensive chemistry laboratory techniques as well.

Key words: Bioinformatics, Proteins 3D Structural Prediction, Utility in fisheries.

Synthesis of amino ester embedded benzimidazoles: A one-pot sequential protocol under metal-

free neutral conditions

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The benzimidazole structural motif has been of great interest in many applications, especially in pharmaceuticals, owing to its broad range of biological functions. Because of our recent interest in the synthesis of benzimidazole derivatives of potential pharmacological interest we decided to explore the synthesis of amino acid embedded benzimidazoles. This initiative was based on the assumption that both the benzimidazole and the amino acid moiety would be responsible for enhanced anabolic activity of the individual parent compounds. However, such a study has not been examined previously, which might be due to the lack of general methods for the synthesis of amino acid embedded benzimidazoles.



Recognition of Cyanide Ion by Functionalized Indole Derivative

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An amide indole based triazole functionalized chemosensor (L) has been synthesized and characterized. This can selectively sense cyanide (CN^-) in acetonitrile medium through changes in its fluorescence profile. The 1H-NMR spectroscopic data exhibits significant changes to establish the sensing mechanism. The four indolic and amide protons were deprotonated in presence of cyanide anion as confirmed through 1H-NMR tritration forming 1:1 aduct with ligand and cyanide anion. Jobs plot also confirmed this aduct formation. Computational studies are carrying to have a deep insite into the mechanism. Reference:

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Study of Antimicrobial Activity of Natural Surfactant-Saponin Extracted from Acacia concinna

(Shikakai)

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Primarily the extraction of the natural surfactant-saponin was done from Acacia concinna (native name shikakai or soap-pod) fruit-pericarp [1]. After isolation and purification, characterization of the saponin (NS) was performed by employing HR-ESI-TOF-MS (ES+), ¹H-NMR, ¹³C-NMR, FT-IR, HR-TEM, HR-SEM and UV-Vis spectroscopic methods. The CMC value of the NS was recorded to be 4.67×10⁻⁴ M, which indeed is much lower in value with respect to most of the commercially available surfactants [2].

In present era antimicrobial resistance to commercially available medications has become a global issue, though there is still the possibility of developing new antimicrobial formulation from bio-origin [3]. The aim of the present study is thus to investigate antimicrobial activity of natural surfactant extracted from shikakai plant.

To screen the antimicrobial activity of saponin samples against bacteria and fungi, the agar diffusion method has been followed. Gram-negative bacterial strains *Pseudomonas aeruginosa, E. coli* and Grampositive strains *Staphylococcus aureus* and *Bacillus subtilis* have been taken for screening. In the case of fungus, pathogenic fungus *Aspergillus flavus* and *Candida albicans* have been used. Conventional broad-spectrum antibiotic Streptomycin and fungal antibiotic Amphotericin B has been used as positive control respectively [4].

The saponin sample was able to inhibit the growth of Gram-negative bacteria *Pseudomonas aeruginosa*, but insensitive to other three bacteria e.g., *E. coli, S, aureus* and *B, subtilis*. In the case of fungus, it has been found to inhibit both the fungus *Aspergillus flavus* and *Candida albicans* with significant inhibition zones. The extracted saponin formed a mean zone of inhibition of 14.9 ± 0.2 mm and 26 ± 0.15 mm, respectively, against *Aspergillus flavus* and *Candida albicans* at a concentration of 50 mg/mL, whereas it formed a 14 ± 0.15 mm inhibition zone only against *Pseudomonas aeruginosa* at 50 mg/mL.

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Selective Detection of Environmentally Hazardous Mercury ions by Bio-Functionalized Reusable

Silver Nanoparticles

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Abstract: We have synthesized silver nanoparticles (AgNPs) by the aqueous extract of leaves of phyllanthus acidus: phyllanthus family. The biosynthesized AgNPs exhibits excellent efficiency towards detection of Hg^{2+i} ons by the naked-eye color change in aqueous medium. It has to be mentioned that this is highly selective and sensitive for Hg^{2+i} ons in presence of other cations. Interestingly, the detection process is almost reversible even after two cycles.

Transition Metal Complexes: Catalysts Enabling Water Oxidation

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The urgent need for sustainable energy sources has prompted extensive research into renewable energy technologies, particularly those harnessing the power of sunlight to drive chemical reactions for energy conversion. Among these, water oxidation stands as a pivotal step in artificial photosynthesis, aiming to produce clean and renewable fuels such as hydrogen. Transition metal-based complexes have emerged as promising catalysts for water oxidation due to their tunable redox properties and catalytic activity.

This article delves into the foundational principles that underpin the design, synthesis, and application of transition metal-based complexes for water oxidation. It expounds upon the crucial role of water oxidation within renewable energy systems, exploring the intricate electronic structures and reactivity of transition metal complexes. Through this exploration, the key factors that shape their catalytic performance are illuminated, providing invaluable insights into the mechanisms driving their efficacy.

Furthermore, the article highlights recent advancements in the field, encompassing novel synthetic methodologies, mechanistic insights, and innovative catalyst architectures. Through case studies of representative transition metal complexes, the structure-activity relationships and the underlying mechanisms governing water oxidation catalysis is discussed here. Moreover, the manuscript discusses the challenges and future prospects in the development of transition metal-based catalysts for water oxidation, addressing issues such as scalability, cost-effectiveness, and long-term stability. By fostering a deeper understanding of the intricate chemistry behind these catalysts, this article aims to inspire further research endeavors aimed at realizing efficient and sustainable water oxidation catalysts for renewable energy applications.

Transition-Metal-Free Direct Oxidative 3-Arylation of Quinoxalin-2(H)-ones with

Arylhydrazines

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A PhIO-promoted direct oxidative 3-arylation of quinoxalinone is developed using arylhydrazines as an arylating agent. This protocol affords the various and diverse 3-arylquinoxalin-2(*H*)-one derivatives in moderate to good yield. A wide range of functionality in the quinoxalinone ring and arylhydrazine are well tolerated under mild arylation conditions. This direct arylation allows the rapid access to biologically interesting benzo[g]quinoxalinones and pyrido[3,4-*b*]pyrazinones.



Metal-free synthetic rout for the 3-arylation of quinoxalin-2(H)-ones

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<u>P-27</u>

Stability, Oscillation..An Essence towards Circadian Rhythm

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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.

Anti-cancer potential of small molecule flavonoids

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Cancer is one of the leading causes of death now-a-days and the worst nightmare among human being. Cancer become one of the leading causes of death globally, accounting for an estimated 10 million deaths, and International Agency for Research on Cancer (IARC) provided estimates of 18.1 million new cases worldwide. There are various treatments of cancer. Treatment of cancer depends on the type of cancer the person has and how advance is it. Some people have cancer with only one type of treatment and some have to go through combinations of treatment. Surgical treatment, chemotherapy, radiotherapy, etc. are the main approaches of cancer treatment. The biggest disadvantage of Chemotherapy is that its inability to distinguish between cancer cell and normal cell hence causing significant toxicity and side effects. Amidst various treatment of Cancer role of small molecule have been very effective. The main mechanism of the small molecule inhibitor is to inhibit the function of the targeted proteins by binding to the pocket on their surface. Due to their smaller size, they can bind a wider range of extracellular and intracellular targets. Flavonoids are polyphenolic compounds synthesized in plants as bioactive secondary metabolites responsible for their colour, flavour and pharmacological activities. The anticancer activity of flavonoids is related to their modulation of signal transduction pathways within cancer cells. As a result, flavonoids can inhibit cell proliferation, angiogenesis, and metastasis, while also promoting apoptosis. Flavonoids have dual action regarding ROS homeostasis-they act as antioxidants under normal conditions and are potent pro-oxidants in cancer cells triggering the apoptotic pathways and downregulating pro-inflammatory signalling pathways.

<u>P-29</u>

Impact of Arsenic Exposure on Antibiotic Resistance of Mammalian Gut Bacteria

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Antibiotic resistance compromises the efficacy of antibiotics and is emerging as a global public health concern. Overuse of antibiotics may accelerate antibiotic resistance but more seriously, the universality and environmental pressure of heavy metals may facilitate the proliferation of antibiotic resistance in bacteria. Arsenic (As) is one of the major heavy ubiquitous metal pollutants of wastewater. In this study, the impact of arsenic shock on antibiotic resistance of mammalian gut prokaryotes is under investigation to determine its contribution to the same.

Wistar rats were exposed to sub-chronic doses of Sodium Arsenite (NaAsO₂), keeping proper vehicular control. As-treated rats exhibited health deterioration, evidenced by reduced body weight and altered organ indices. Quantification by Atomic Absorption Spectroscopy (AAS) confirmed arsenic deposition in the gut of treated animals.

From the gut samples of the model animals, 79 As-resistant bacterial strains were isolated and characterized in terms of morphology and biochemical tests. The proportion of As-resistant strains was 35.88% in the control group, whereas, the same was 59.62% in the treated group. Bacterial isolates from the treated group were resistant to all the 27 antibiotics tested, but the control group isolates were resistant to only 16. Multiple Antibiotic Resistance (MAR) index was nearly tripled in the As-treated group (0.211) compared to the control group (0.076).

The outcomes of this study demonstrate a significant alteration in the antibiotic resistance profiles of mammalian gut bacteria, potentially opening a novel avenue for understanding arsenic toxicity and its interplay with antibiotic resistance.

Keywords: Arsenic, mammal, gut, bacteria, antibiotic-resistance.

Zinc embedded over covalent organic framework for the carbamates production under

sustainable pathway

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Recent trends in synthesis of organic fine chemicals using metal incorporated covalent organic frameworks as heterogeneous catalyst clinching appreciable attentions towards researchers. Permanent porosity, high surface area and extremely thermal stable nature makes those covalent organic frameworks (COFs) based materials as appropriate heterogeneous catalyst. Therefore, the amine-aldehyde modified covalent organic framework constructed zinc catalyst; Zn@DBPG is synthesized and characterized properly. The synthesized material is utilized as an efficient catalyst for the production of organic carbamates. It was very much efficient for carbamate synthesise ven after sixth cycle of reaction for both CO₂ pathways



<u>P-31</u>

Biomedical applications of nanofluids

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Now a day's technological trend of increasing speed and decreasing size is going on as an interesting research topic. And for that reason nanotechnology is more important, nanofluid term even withdraws tremendous attention for its extensive applications. Dilute liquid suspensions of Nanoparticles with at least one major dimension less than 100 nm are called Nanofluids. Nanofluids are a new magnificence of fluid designed by dispersing Nano-sized materials (Nanoparticles ,Nanofibers, Nanotubes, Nanowires, Nanorods, Nanosheets or Droplets) into a base fluid. In general, nanofluids are colloidal combinations of metal or ceramic nanoparticles in a liquid containing water, glycol, or oil. This poster presentation highlights the important biomedical applications of nanofluids in drug delivery, analysis, and disease functioning. Nanofluids can also be used as antibiotics that can defeat the immune system.

Resorcinol Bridged Dinuclear Copper (II) Complexes: Syntheses, Structural, Spectroscopic and

Magnetic Studies

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A new C₂-symmetric Schiff base ligand featuring a core resorcinol bridging unit has been created, utilizing the Duff formylation reaction followed by Schiff base condensation reaction. Cu(II) salts with varying anions in methanol were allowed directly to react with the preformed ligand (H₂L) in a 2:1 molar ratio to create dinuclear Cu(II) complexes. The free ligand is neutral, but in presence of NEt₃ a mild base, it tends to lose both the phenolic hydrogen and coordinates to metal centre as dianionic moiety resulting the formation of dinuclear metal complexes. X-ray analysis discloses that both complexes are dinuclear Cu(II) complexes where the ligand (H₂L) being tridentate in nature coordinates through its two N donor atoms and one O donor atom in the equatorial positions. The fourth position being coordinated by different anions. Temperature dependent magnetic susceptibility measurements indicate that both complexes show antiferromagnetic interactions through resorcinol bridge.

Keywords: Copper (II) complexes; resorcinol; Schiff base ligand; X-Ray crystallography; magneto structural correlation

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Surface Water and Ground Water

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Surface water and groundwater are vital resources supporting various ecosystems and human activities. This abstract explores their intricate interactions, management strategies, and the challenges posed by anthropogenic activities and climate change. Surface water and groundwater often interact, influencing each other's quality and availability. Understanding these interactions is crucial for sustainable water management. Surface water replenishes groundwater through infiltration, while groundwater discharges into surface water bodies, maintaining flow and water quality. Effective management of surface water and groundwater requires integrated approaches considering their interconnectedness. Strategies such as conjunctive use management, groundwater recharge, and surface water storage aim to optimize water availability and mitigate risks of overexploitation and depletion. However, managing these resources faces challenges exacerbated by human activities and climate change. Overextraction of groundwater for agricultural, industrial, and domestic purposes leads to depletion and subsidence, threatening water security and ecosystem health. Pollution from urban runoff, industrial discharge, and agricultural practices further degrades water quality, compromising human health and aquatic habitats. Climate change exacerbates these challenges by altering precipitation patterns, increasing evaporation rates, and intensifying extreme weather events. Shifts in hydrological regimes impact water availability and quality, exacerbating competition and conflicts over limited water resources. Addressing these challenges requires a holistic approach integrating scientific research, policy interventions, and community engagement. Sustainable water management practices, coupled with adaptive strategies to mitigate and adapt to climate change, are essential for ensuring water security and preserving the integrity of surface water and groundwater systems.

Surface water includes any freshwater that is sent into wetlands, stream systems, and lakes. On the other hand, groundwater exists in subterranean aquifers that are situated underground. Most groundwater is obtained from snowmelt and rainfall that gets into the bedrock via the surrounding soil.

<u>P-34</u>

An experimental study on Xenohormesis as a driving force for interspecific signaling between

plants and animals at perceived adversities in colonies of Amano shrimps (Caridina sp.) in

Coleochaete rich medium under induced heat stress.

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Xenohormesis refers to a phenomenon when an animal acclimates to an environmental stress without being directly exposed to it but by consuming organisms that have been exposed. An experiment was conducted to study the role of xenohormesis as a factor of growth and longevity in colonies of Amano shrimp grown in Coleochaete rich medium treated at various temperatures. Results indicate that consuming heat acclimated algae facilitates significantly better survival rate in Amano shrimps. Thus foreign molecules that seem unrelated to any endogenous molecule triggers some similar pathways that mediate an immediate response to a perceived adversity. This inevitably raises a concern with excessive anthropogenic manipulations in agricultural practices- whether we are losing some important health and nutritional benefits by consuming agricultural products grown in extreme artificial conditions that may maximize the crop yield but definitely minimize the abiotic and biotic stress factors that would have existed in natural environments otherwise.

Synthesis and Resolution of An Axially Chiral, Fluorinated 1,8-DiaryInaphthalene Scaffold with

Catechol Unit

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We have demonstrated a successful synthetic technique for the synthesis of a fluorinated, axially chiral 1,8-diarylnaphthalene ligand via a consecutive Ullmann and Suzuki coupling reaction-based strategy. A practical methodology for the successful chiral resolution of the newly synthesized catechol based moiety has also been achieved. Most interestingly, we disclose the preliminary application of these axially chiral molecules as ligands in asymmetric Mukaiyama Aldol transformation reactions where the fluorinated ligand induced up to 28% ee in the aldol product.¹

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Ionic Liquid Cross-Linked Multifunctional Cationic Polymer Nanobeads: Applications in Anion

Exchange, Templates for Palladium, and Fluorescent Carbon Nanoparticles

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An ionic liquid based cross-linker is synthesized by simple nucleophilic substitution reaction of 4vinylbenzyl chloride and N-vinylimidazole. This ionic liquid is utilized as cross-linker for dispersion polymerization of acrylamide in the presence of poly(vinyl methyl ether) (PVME) stabilizer, which produces water-friendly cationic cross-linked poly(acrylamide) (CPAAm) beads. Morphology investigation reveals that these beads are nanosized and spherical and their size varies with the amount of cross-linker and PVME used. The ionic cross-linker imparts ionic nature in these beads, where anion is mobile and areeventually exchangeable. Consequently, anion exchange capacity is checked using an anionic dye Eosin B via UV-vis spectroscopy. Subsequently, the release of dye is monitored on addition of a pinch of sodium acetate. Analogous anion exchange with [PdCI4]²⁻ results in the formation of palladium (Pd) nanoparticles (NPs) inside the cross-linked poly(acrylamide) beads due to in situ reduction by imidazolium cation present in CPAAm. The carbonization of the CPAAm nanobeads produces nitrogen-doped carbon nanoparticles of comparable morphology and sizes. The resultant carbon nanoparticles emit blue fluorescence under irradiation of UV light. Similarly, Pd NPs embedded carbon nanoparticles are easily prepared by carbonization of the Pd NPs loaded CPAAm nanobeads.



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Capsaicin content of chilli (*Capsicum annuum* L.) of West Bengal and the structure prediction of Capsaicin synthase of *Capsicum annuum*.

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In West Bengal, chilli (*Capsicum annuum* L.) a spice in many dishes, adding both flavour and hot taste to traditional Bengali cuisine. The capsaicin content in chilli can vary depending on factors such as the variety of chilli pepper and growing conditions. Generally, the spiciness of chilli is measured on the Scoville scale, which quantifies the concentration of capsaicinoids, including capsaicin, the primary compound responsible for the hot sensation. In the present study, colorimetric estimation of capsaicin from *Capsicum annuum* has done. Capsaicin synthase is the enzyme responsible for the biosynthesis of capsaicin in chilli. Understanding Capsaicin synthase (ABC74559.1) structure from *Capsicum annuum* is crucial for elucidating the biochemical pathways involved in capsaicin production. For predicting the structure of capsaicin synthase from *Capsicum annuum*, homologous protein (A1XEH0.1.A) serve as templates for modeling. Swiss model (software tool) is used to generate a three-dimensional model of capsaicin synthase from *Capsicum annuum*. Computational method for structure prediction plays a crucial role in elucidating the structure and function of capsaicin synthase in *Capsicum annuum*. Understanding the architecture of capsaicin synthase from *Capsicum annuum* provides insights into the biochemical pathways underlying capsaicinoid production and can inform efforts to manipulate chilli (*Capsicum annuum*) spiciness through breeding and genetic engineering.

Synthesis and Crystal Structures of a mixed bridged trinuclear and a 1-D polynuclear Ni(II) complexes derived from a tridentate NNO donor Schiff base ligand

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One mixed bridged trinuclear Ni(II) complex $[Ni_3L_2(o-(NO_2)C_6H_4COO)_2(\mu_{1,1}-N_3)_2(CH_3OH)_2]\cdot 2H_2O$ (1) and a 1D polynuclear Ni(II) chain $[Ni_2L_2(\mu_{1,1}-N_3)(\mu_{1,3}-N_3)]_n$ (2) have been synthesized using a tridentate NNO donor Schiff base ligand, 1-[(3-dimethylamino-propylimino)-methyl]-naphthalen-2-ol (HL). Complex 1 has been formed by allowing the Schiff base ligand HL to react with the methanolic solution of nickel(II) o-nitro benzoate salt in presence of an aqueous solution of NaN₃ in 2:3:2 molar ratio. Complex 2 was obtained through the reaction of the Schiff base ligand (HL) and the perchlorate salt of nickel (II) in the presence of pseudohalide azide as a coligand. Both the complexes are characterized by elemental analyses. FT-IR and UV-Vis spectroscopic techniques. Single crystal X-ray structure shows that complex 1 is a linear trinuclear Ni(II) complex which may be assumed to be composed of two terminal mononuclear units of [NiL(N₃)(CH₃OH)] connected by a central [Ni(o-(NO₂)C₆H₄COO)₂] unit through $\mu_{1,1}$ -azido. μ_{2-} phenoxido and syn-syn o-nitrobenzoato bridges. Single crystal X-ray result reveals that complex 2 is a one-dimensional chain in which the neighboring dimeric units are further connected by $\mu_{1,3}$ -azido bridges in a zig-zag fashion. In the dinuclear $[Ni_2(\mu_2-phenoxido)_2(\mu_{1,2}-N_3)]$ cores two Ni(II) centers are triply bridged by two μ_2 phenoxido oxygen atoms and one bridging nitrogen atom of $\mu_{L,L}$ -azido co-ligand. Finally the dimeric building blocks are coupled through $\mu_{i,i}$ -azido linkers and the chain propagates. The cooperative participation of N···H hydrogen bonding, π ··· π stacking and C-H··· π interactions occur during crystal packing. Complex 2 gives rise to 2-D supramolecular architecture with the formation of star shaped voids via C–H··· π stacking interactions.



Exploring 2,5-diphenyl furan derivative as promising inhibitor of p53-MDM2 interaction for cancer therapy

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P53-MDM2 protein-protein interaction (PPI) is one of the most crucial and intensively studied PPIs involved in human cancer. Importantly, cell cycle and apoptosis are potentially regulated by the p53 protein. The negative regulator of p53, minute double minute 2 (MDM2), induces p53 degradation and modulates its tumour-suppressing activity. Hence, regain of p53 function by targeting and inhibiting the p53-MDM2 interaction for the treatment of cancer is a unique approach. In this present study, one of the important furan-based scaffolds, 2,5-diphenyl furan derivative, 2,5-diphenyl-furan 3,4-dimethyl dicarboxylate (DPFDCA) was synthesized and used as MDM2 inhibitors. Molecular docking studies were done to show the p53-MDM2 inhibitory effect of this furan-based small-molecule and determined the various possible conformations and binding affinity value. Lastly, investigation of the dynamic behaviour of MDM2-DPFDCA complexes through molecular dynamics (MD) simulation showed similar RMSD, RMSF, RoG and SASA profile compared to the reference inhibitor nutlin-3, suggesting stability throughout the simulation time. DPFDCA potentially inhibit p53-MDM2 interaction by blocking the p53-binding domain of MDM2 and was found to be the strong binding affinity comparable to the reference compound nutlin-3 towards MDM2 protein. These results indicate the 2,5-diphenyl furan-based derivative, DPFDCA might be the promising early lead compounds for the development of new anticancer agents targeting p53-MDM2 interaction, which to our knowledge has never been reported to disrupt p53-MDM2 interaction.

<u>P-40</u>

Single crystal: An Aspect in Undergraduate Chemistry

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Single crystal is a 3D solid object of the atoms, ions, or molecules of continuous and unbroken to the edges of the sample, with no grain boundaries. Schiff bases compounds¹ are one type of single-crystal formed by the presence of a double bond linking carbon and nitrogen atoms and are both found in nature and synthesized in the laboratory². Schiff base compounds are seen in flexible organic crystals because of their good mechanical strength, high yield, stimulus responsiveness, and ease of synthesis. Calcium fluoride (CaF₂), a single-crystal fluorite is extensively researched for its potential uses in materials science, electronics, and optics. CaF₂ is a body-centred structure and a cubic crystal system. It comes in a variety of colours, ranging from colourless to green, yellow, bluish-green, or purple, and is typically translucent to transparent. To synthesis single-crystal fluorite, Bridgman-Stockbarger method, chemical vapour transport, or hydrothermal synthesis techniques are used. Primary amine and an aldehyde or ketone usually undergo a condensation process to produce Schiff bases compound of single-crystal fluorite. The Schiff base ligand can be utilised in coordination chemistry with metal ions to create complex molecules. Most Schiff base single-crystals are effective antibacterial and antifungal drugs³. Thus, these compounds are interesting both for academician and industrialist.



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<u>P-41</u>

Synthesis of Nano-dimensional Polyaniline

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Tuning of polymer morphology has high impact for its applications. When the morphologies are in the nano-scale region attract special interest. Here we report matrix assist tuning of morphologies of polyaniline. The matrix can remain either in sol state or in gel state depending on its temperature. Depending of the state of the matrix, physical state of initiator, synthesized polyaniline nanostructure obtained nanotube to nanofiber to three-dimensional network morphologies. Synthesis of nanostructured polyaniline is of great interest because it can be used to enhance sensor properties for its large surface area and low dimensional conductivity [1,2]. Depending on the morphology and electronic state of polyaniline it is used in chemical and biological sensors [3], gas separation membranes [4], electronic devices [5], light weight battery electrodes [6], anticorrosion coatings [7], etc. It is a cheap, one-step synthesis with high reproducibility in large scale.

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Exploration of the solubility, stability and biological activity of biologically important amino acids L-

cysteine and L-tyrosine in aqua organic solvent mixtures

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The regulation of the different functions required for the proper sustainability of life is heavily dependent on proteins. They are not only important for the growth and development of the body but also helps in multiple functions including transport of nutrients and oxygen and even boosts digestion. As our body contains various solvent systems in which the proteins are supposed to function, study of dissolution and thermodynamic behaviour of proteins in diverse solvent systems are of immense importance. The solubility, thermodynamic behaviour along and biological activity of two biologically important amino acids Lcysteine and L-tyrosine are investigated in this study. Both the amino acids were found to be more soluble in aqueous solvents compared to organic environments. The extent of solubilities were measured using the standard Gibbs energy measurements. L-cysteine serves a vital role in treatment of arthritis, bronchitis, emphysema, and tuberculosis. It is also important for the normal growth rate of hair. L-tyrosine is known to regulate important neurotransmitters, including epinephrine, norepinephrine, and dopamine. L-tyrosine also helps produce melanin, the pigment responsible for hair and skin colour. This study will hence enrich the understanding about the importance of L-cysteine and L-tyrosine in different living systems and will provide information about the impediments that may arise in case of modifications of their extent in the living systems.

Keywords

Amino acids, L-cysteine, L-tyrosine, organic solvents, biological importance

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Cyanide Selective Off-On Fluorescent Chemo-sensor with in-vivo Bio-imaging in Water

P-43

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The design and development of chemosensor capable of detecting selective toxic and lethal anionic species are of current research interest in chemistry, biology, medicine and relation to environmental issues. Among various biological hazardous anions, cyanide (CN⁻) is considered to be most potent one. The widespread use of CN- in industries and their waste effluents impose serious threat to aquatic environment. Hence intensive effort should be given for the development of water soluble selective and sensitive CNchemosensor with rapid response for effective in-vivo detection. We report the design and synthesis along with detailed structural analysis of a solid fluorescent chemosensor $[Cu(BP)HMB]_2(ClO_4)_2$ (Probe) (BP = 2,2'-bipyridine), based on а tiny organic chromophore, 2-hydroxy-3-(hydroxymethyl)-5methylbenzaldehyde (HHMB), operating in "turn off-on" mode with high selectivity and sensitivity for recognizing the CN⁻ in 100% aqueous medium. It is noteworthy that in aqueous medium, the dimeric solid probe undergoes irreversible change to its monomeric form of probe $[Cu(BP)HMB(H_2O)_2](CIO_4)$ which is actually responsible for cyanide attack. To demonstrate the bio-applicability of sensor Probe for CNdetection, nematode C. elegance was used to in-vivo imaging. It is most suitable living organism for testing the cyanide toxicity for municipal and industrial waste water. Below, μM detection limit instantaneous and excellent radiometric responses are also beneficial to detect trace amount of anthropogenic and biogenic cyanide.

In silico identification of potential inhibitors of filarial intracellular steroid hormone binding receptor

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Lymphatic filariasis is one of the debilitating diseases of the tropical countries, targeting the global population with India contributing to highest disease burden. The current elimination programs rely upon the mass distribution of selected number of drugs that have been in use for decades, and show limited efficacy with adverse side-effects. A shortcoming of these drugs is their inability to target the infective stages of the parasites. Thus, there is a critical need for novel therapeutic agents to supplement the current scanario. Here, we have screened some botanical compounds of different groups with antiparasitic, anthelmintic and anti-microbial properties which are abundant, inexpensive, and non-toxic, that may be a promising alternative in this context. Nuclear hormone receptors have begun to be studied in parasitic worms, where they are widely distributed and play key roles in governing metabolic and developmental transcriptional networks. One such nuclear receptor is intracellular steroid hormone binding receptor (ISHBR) of *Wuchereria bancrofti* that is required for molting of the parasites. In our study, we have selected ganoderic acid, a triterpenoid as a potential phytocompound on the basis of binding affinity with ISHBR that is predicted to interact with ISHBR. However experimental validation is still needed especially in animal models and if successful, in clinical trials.

-NH-Dansyl Isocolchicine Exhibits a Significantly Improved Tubulin-Binding Affinity and Microtubule Inhibition to Tubulin

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Structure activity relationship studies have established that the A and C ring of colchicine comprise the minimum structural feature necessary for high affinity drug-tubulin binding. Thus, colchicine acts as a bifunctional ligand by making two points of attachment to the protein. Furthermore, analogs belonging to the iso series of colchicine are virtually inactive in binding to tubulin and inhibiting microtubule assembly. In the present study, we found that the substitution of a hydrophobic dansyl group on the B-ring side chain (C-7 position) of isocolchicine reverses the structural alterations at the C-ring and the newly synthesized – NH-dansyl isocolchicine restores the compound's lost biological activity. It inhibits microtubule assembly efficiently with an IC₅₀ of 10 μ M and competes with [³H]colchicine for binding to tubulin. Moreover, though –NH-dansylcol-chicine binding to tubulin involves two steps, the -NH-dansyl isocolchicine-tubulin interact-tion has been found to occur via a one step process. Also, the affinity constant of the -NH -dansyl isocolchicine-tubulin interaction is roughly only 3 times lower than that of the -NH-dansyl colchicinetubulin interaction. These results suggest that the enhanced microtubule inhibitory ability of -NH-dansyl isocolchicine is therefore related to the affinity of the drug-tubulin interaction and not to any other conformational changes upon binding to tubulin. We also observed that the competition of -NH-dansyl isocolchicine with [³H]colchi-cine for binding to tubulin was dependent on tubulin concentration. In conclusion, this report for the first time indicates that a biologically active bifuntional colchicine analog can be designed where the drug binds tubulin through its A and B ring, while the C-ring remains inactive.



-NH-dansyl isocolchicine

Synthesis and structural analysis of different benzylic linked dimers obtained from bis(benzylidene)cyclopentanone using dissolving metal reduction

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Single electron transfer (SET) from the metal surface to carbonyl compounds is a distinctive feature of dissolving metal reductions, which yield a wide variety of monomeric and linked products. This research investigates the reduction of zinc metal to cross-conjugated carbonyl functionalities using proton-free reaction conditions. After treating α, α' -(*E*,*E*)-bis(benzylidene)cyclopentanone with zinc and acetic anhydride under changed circumstances, three dimeric compounds were formed through β,β -benzylic coupling, resulting in unique benzylic carbon coupling patterns.

<u>P-47</u>

Schiff Base: Interfaces between Chemistry and Biology

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Schiff base is prepared from condensation of a carbonyl compound and an amino compound. Schiff base metal complexes¹ have uncommon properties and multipurpose appliances across several fields including industry and biology. These complexes show catalytic activity, biological activities, including antiviral, cytostatic, antibacterial, anticancer, and antifungal properties²⁻³. Few such examples are Fe(III) salEen Schiff base complexes which can be used as MRI contrast agents⁴. These compounds show relaxivities ranging from 0.35 to 0.80 mM⁻¹ s⁻¹ for proton Larmor frequencies from 0.01 to 300 MHz. These compounds exert toxic effects only at concentrations higher than 100 μ M while coincidently reducing colonic epithelial secretory function on colonic epithelial T₈₄ cell monolayers studied. These two features make these complexes to be used as <u>MRI contrast agents</u>.



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Stability of Metal Organic Frameworks: Design Strategies, Recent Advances and Applications

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Metal organic frameworks (MOFs) have gained considerable interest in recent times due to their potential applications in different fields such as gas storage, separation of hydrocarbons and toxic materials, sensing, luminescence, biomedicine, etc. Most popular method for synthesis of MOFs is conventional hydrothermal process. Microwave-assisted synthesis, electrochemical synthesis, mechanochemical synthesis, sonochemical synthetic methods are also reported for the construction of MOFs crystals. Many MOFs are vulnerable to structural destruction in ambient atmospheric environment due to collapse of the bonds between metal and the organic linker. However, in recent times a lot of stable MOFs have been reported. The robust framework can resist the corrosive effects of water molecules on its coordination bonds as well as the MOFs are stable towards acid, alkali, and salt aqueous solutions and water vapor. Several strategies have been for enhancing stability of MOFs. Post-synthetic exchange, post-synthetic modification hydrophobic surface treatment, and composite fabrication approaches are mostly used to form stable MOFs. The chemically stable MOFs have been used in sensing and detection, adsorption and separation, catalysis, biomedical applications and electrochemical storage. This review covers the synthetic strategies and recent advancements in MOF design and synthesis to form stable MOFs with less reactive towards water, acids, bases and suitable usages in a variety of applications.

Microwave-assisted green synthesis of biologically important thiazoles and thiadiazoles: An unconventional activation technique

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Sulfur and nitrogen-containing heterocycles have received a great deal of attention on account of their unique structures and therapeutic relevance. Thiazoles and thiadiazoles are important five-membered heterocycles containing sulfur and nitrogen atoms that draw the special attention of researchers due to their synthetic diversity and potent pharmacological properties. Recent research mainly aims to prepare heterocycles bearing sulfur and nitrogen since compounds having nitrogen is a vital component in proteins and sulfur occurs in all living organisms. Thiazoles and thiadiazoles are used in agrochemicals, liquid crystals, sensors, the cosmetic industry, cyanine dyes, etc. Sometimes organic synthesis including preparation of thiazoles and thiadiazoles with the help of conventional methods is laborious work while synthesis of promising organic molecules under microwave irradiation as a sustainable tool provides better yields, diminishes the reaction time, and reduces unwanted side products. Hence, the present microwave assisted synthesis of thiazoles and thiadiazoles will be presented at the Conference Meeting.

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Progress in recognition of arsenic species using colorimetric and luminescence methods relevant to

biological and environmental sample analysis

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Arsenic and arsenic containing compounds are human carcinogens. Exposure to arsenic occurs occupation ally in several industries, dermal contact and natural sources. Inhalation is the principal route of arsenic ex posure in occupational settings, while ingestion of contaminated drinking water is the predominant source of significant environmental exposure globally. Drinking water contamination by arsenic remains a major public health problem. Arsenic has been found to exist in different forms in natural resources e.g., As(III) a nd As(V), organic arsenic (such as MMA, DMA) and tetra methyl arsonium ion, trimethylarsine oxide (TMA O), and arseno sugars etc. The most available field-test kits for detecting arsenic is based on 'Gutzeit' meth od which is dominated arsenic testing for more than 100 years. This method was first described in 1879¹ a nd used silver nitrate crystals as the detector. Although the silver nitrate crystals were later replaced by a more practical paper strip impregnated with mercuric chloride and subsequently with mercuric bromide. T his method of arsenic detection is still referred to by the name of its original inventor. Gutzeit. It is found t hat the use of organic probes for selective sensing of analytes has suffered several limitations, viz., lower w ater solubility and the potential harm towards living cells. To overcome such problems, biologically relevan t metal complexes² have been used due to their lower toxicity towards living cells. Although several colori metric and luminescence methods relevant to arsenic recognition in biological and environmental sample analysis have been documented, further research is needed to provide a better recognition method and u nderstanding of the arsenic contamination pathways and arsenic-induced diseases in human being.

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Investigating the Photophysical Properties of Cyclometalated Iridium(III) and Rhodium(III) Complexes

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Four mono-nuclear cyclometalated complexes represented as $[M^{III}(ppy)_2(L)]$ (**Ir1** and **Rh1**) and $[M^{III}(bzq)_2(L)]$ (**Ir2** and **Rh2**) [where M = Rh/Ir; L = *N*-(*furan-2-ylmethyl*)-2-pyridinecarboxamide; ppy = 2-phenylpyridine (1); bzq = benzo[h]quinoline (2);] are synthesized and characterized to investigate the significant differences of emission properties between Ir(III) and Rh(III) complexes.¹ Similar kind of metal ion influence in emission behaviors were further reported for other four mono-nuclear cyclometalated Ir(III) and Rh(III) complexes $[M^{III}(C^N)2(4,4'-Cl2bpy)]PF_6$ (M = Rh/Ir; C^N = 2-(*p*-tolyl)pyridinato (**3** and **4**), 2-phenyl-5-chloropyridinato(**5** and **6**); 4,4'-Cl2bpy = 4,4'-dichloro-2,2'-bipyridine).² In both observations^{1 and 2}, it was found that although the structural parameters of iridium(III) and rhodium(III) complexes are similar, considerable differences in emission properties of Ir(III) (5d⁶) and Rh(III) (4d⁶) complexes exist. The complexes were presented with their detailed spectroscopic properties along with the structural studies by single crystal X-ray diffraction.



Synthesis of complexes Ir1-2 and Rh1-2.



Single Crystal structure of complex, Ir1

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Catalysis of Alkene Oxidation by a Dinuclear Cobalt(III) and *in situ* Generated Tetrazole Bridged Dinuclear Cobalt(III)-Schiff Base Complexes

P-52

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Two Schiff bases have been synthesized by condensing diacetylmonoxime with 1,3-diamino-2hydroxy propane (HL¹) and benzilmonoxime with *N*,*N*-dimethylethylenediamine (HL²). The reaction of cobalt perchlorate with HL¹ in presence of sodium azide leads to the formation of a discrete dinuclear complex $[Co^{[II]}(L^1)(N_3)_2]_2$ (**1**). On the other hand, when the same reaction is carried out with HL² leads to the formation of a tetrazolate bridged dinuclear cobalt (III) complex $\{[Co^{[II]}_2(L^2)_2(N_3)_2 (\mu_{1,1}.N_3)(\mu_{N,N}-MTZ)]\}$ (**2**) [MTZ = 5-methylphenyltetrazole]. The ligands and the complexes have been characterized by elemental analysis, UV-Vis, IR spectroscopy. Single crystal structures of both the complexes are also reported. Both the catalysts show the same selectivity for the allylic oxidation of electron-rich olefins, only differing in their relative oxidation rates.



Figure: View of crystal packing of 2 showing dinuclear molecules parallelly packed along the ac plane

Indian Innovations: Name Reactions, Catalysts and Unique Discoveries in Organic Chemistry

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In the vast landscape of organic chemistry, India stands in an important place , with its scientists making groundbreaking steps in the development of name reactions and catalysts. These innovations not only underscore the nation's rich scientific heritage but also play a pivotal role in shaping the global landscape of organic synthesis. In this presentation we specifically focus on name reaction and catalyst that have left an incredible mark on the field. Highlighting the work of the researchers , the poster describes the mechanism and application of key reaction developed by the chemists. The poster aims to celebrate the rich heritage of organic chemistry contributions from the Indian scientific community. By shedding light on these advancements, we seek to inspire further research and collaboration, fostering a deeper understanding of the global impact of Indian chemists on the landscape of organic synthesis.

Effects of positions on the excited-state charge transfer, an insight from quantum dynamics

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Fast charge transfer is of the utmost importance for energy science, photocatalysis, and materials engineer ing. The nonradiative charge separation dynamics of a typical donor-acceptor system have been investigat ed in detail by applying NAMD theory combined with SCC-DFTB methodology. We established that the pos ition of the benzene ring in the composite system greatly influences charge transfer. For the parent system, the simulated lifetime is 104 fs. The rate of quantum transfer becomes faster by a factor of 2 by altering t he position of the auxiliary group. The nonadiabatic coupling, coherence, and involvement of phonon mod es facilitate the quantum transfer. Therefore, our investigation suggests the position of a ring has a positiv e role in determining photovoltaic efficiency and provides important guidelines for further development of solar optoelectronic design.

Monitoring pm2.5 levels in the Rammohan College campus

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Particulate Matter 2.5 (PM2.5) refers to fine particles suspended in the air, with a diameter of 2.5 micrometres or smaller. These particles come from various sources such as vehicle emissions, industrial processes, construction activities, wildfires, and even natural sources like dust and sea spray.

PM2.5 is of particular concern because of its small size, which allows it to penetrate deep into the respiratory system when inhaled. Exposure to PM2.5 has been linked to a range of health problems, including respiratory and cardiovascular diseases, as well as premature death, especially among vulnerable populations such as children, the elderly, and individuals with pre-existing health conditions.

Monitoring and reducing PM2.5 levels are important for protecting public health and improving air quality. A PM2.5 monitor has been installed in the New Science building of Rammohan College in collaboration with Prof. Punyasloke Bhadury, Centre for Climate and Environmental Studies & Department of Biological Sciences, IISER Kolkata to monitor PM2.5 pollution within the campus. The cost-effective sensor development has been validated and through this installation vital data on air quality, in particular for PM2.5, humidity, among others are being generated 24x7. Here we give some data of PM2.5 levels in the past few months to get a clear picture of the air quality in the area. The WHO guideline recommends an annual average concentration of PM2.5 of no more than 10 micrograms per cubic meter (μ g/m³). The college is situated on a very busy road with heavy vehicular traffic, but the air quality is ambient within the campus. The PM2.5 levels show variations with the lowest levels of PM2.5 during the rainy seasons and the highest levels during the winters.

Effect of Salts and Ionic Liquids on the growth and stability of water domains in hydrophobic

environment

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Discrete water domains in hydrophobic environment find relevance in aerosols, oil refinery, the human bo dy, etc. Reverse Micelles (RMs) are self-aggregated system, composed of amphiphilic surfactant molecules dispersed in a hydrophobic continuum. Moreover, since ILs are simple salts of organic cations and organic or inorganic anions, there is always a scope to tune their properties by careful selections of the cations and anions. The interfacial microstructure plays a crucial role in the stability of such water domains. Over the d ecades, the amphiphile-induced electrostatic interaction is considered to be the major stabilizing factor op erating at these interfaces. Here we have taken a case of water/AOT/Dispersed Phase type microemulsion s of varying solvents and seen the effects on water solubilisation of the RM in the hydrophobic environme nt. In our case we have taken a non-protic ionic liquid [1-benzyl-3-methylimidazolium chloride] and seen it s effect on the water intake capacity ω_0 . The effect of differetial salts viz. NaCl, CsCl and RbCl on RM syste ms have also been investigated for comparison. We have carried out Dynamic Light Scattering with sample s having different concentrations of ionic salts as well as ionic liquids to study their effects on the particle s ize. Furthermore, attenuated total reflectance-Fourier Transform Infrared (ATR-FTIR) spectroscopic measu rements were also carried out to unravel the differential H-bonding interaction in confined water and their distribution at the interface.

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Gene silencing and genome editing in controlling plant pathogens and plant growth promotion

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Gene silencing is a negative feedback mechanism that regulates gene expression to define cell fate and also regulates metabolism and gene expression throughout the life of an organism. In plants it can be done either by transcriptional gene silencing (TGS) or by post-transcriptional gene silencing (PTGS). Plant diseases are universal and it severely affect the crop yield and quality, thus pose a great threat to the global food security. So genetic improvement of plant disease resistance is essential for sustainable agriculture. Genome editing is a powerful tool and has been revolutionizing. It provides new methods for genetic improvement of plant disease resistance breeding. In this review work we have tried to summarize the molecular mechanisms of gene silencing, the challenges in developing breeding resistant crops, applications of genome editing technology in generating plants with resistance to bacterial, fungal and viral diseases and also tried to discuss the potential of genome editing for breeding crops that show novel disease resistance in future.

[Key words: Plant diseases, Genome editing, disease resistance]

Synthesis of pyrazole-pyrazolines and their solvent- dependent photophysical property

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2-pyrazoline is an elegant member of heterocyclic compound for its versatile and diverse application in chemistry and biochemistry. Pyrazolines are found to be used as brightening agents in synthetic fibers, papers and textiles, fluorescent probes in some elaborate chemo-sensors, recognition of transition metal ions, hole-transport material, organic electronics, electrophotography and electroluminescence. Many compounds exhibiting anti-bacterial, anti-fungal, anti-viral, anti-parasitic, anti-tubercular, anti-inflammatory, anti-cancer, anesthetic, analgesic and insecticidal properties contain pyrazoline scaffold. The presence of electron donor at N-1 and electron acceptor at C-3 positions of pyrazoline molecule makes it an elegant member of heterocyclic family. Due to presence of donor-π-acceptor (C-3) and the molecule exhibits fluorescence property. This optical property of the compound depends on solvent polarity and substituents present in the ring. In our study, pyrazolines were synthesised from 4-cyanopyrazole-5carbaldehyde via 1,3-dipolar cycloaddition reaction. The presence of cyano group at C-4 of pyrazole increases the conjugation from N-1 to C-3 of pyrazoline derivatives and this affects ICT property which, in turn, exhibits strong fluorescence. The role of solvent polarity with some of the synthesised compounds was also investigated.





Unraveling of the interaction of Heme-protein (Hemoglobin and Myoglobin) with synthesized amino acid based surfactant

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The interaction of heme protein (Haemoglobin and Myoglobin) with synthesized amino acid surfactant (SDMP) which is environment friendly and bio compatible having investigated using various technique like tensiometry, UV-visible spectroscopy, fluorometry and circular dichroism (CD) spectroscopy in a 10 mM phosphate buffer medium(pH=7.4) at 298 K. This synthesize surfactant was characterized by 1H NMR and Mass spectroscopy. The critical micelle concentration (cmc), surface properties which includes Gibbs surface excess (Fmax), the area of exclusion per surfactant monomer (Amin) and surface pressure at cmc (Псmc) were determined. The protein indicates its unique surface-active characteristics, according to surface tension studies. This method implies that the surfactant's monomeric form interacts with the protein to produce tiny induced micelles. The protein is denatured by these micelles' binding to the protein's backbone. More surfactant addition shows the formation of free micelles. A substantial interaction between the protein and the surfactant is revealed by UV-Vis spectroscopy, which causes a red shift for both Mb and Hb. On the other hand, a more pronounced red shift is noted in case of Hb that suggest the formation of a new surfactantprotein complex. Tryptophan is moving away from the heme group residue of Hb and becoming exposed in the external media, as shown by a red shift in fluorometry. CD measurements show a decrease in the negative ellipticity value, suggesting protein denaturation.

Applications of Ruthenium Nanoparticles

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Platinum metal group elements, PGE (Pt, Pd, Rh, Ru, Ir, Os) have almost similar physical and chemical properties. Among all these transition metals, Pt occupied a good position in biological application. Due to similarities in properties, now a days, Ruthenium also attracted a great interest in the field of research. Ru have shown applications as an anticancer, antimicrobial, and antioxidant agents along with wide-ranging catalytic applications. In modern research "small size and more activity" is the main objective and in this way nanomaterials synthesis developed. Various synthesis methods have been suggested to get ruthenium nanoparticles. Ruthenium nanoparticles have broad applications in polymer membranes, plastics, coating, textile and nanowires, synthesis of diesel fuels, methanol fuel cells, azo dye degradation, antibacterial use, organic pollution removal, electronic and, etc. It shows antibacterial performance against gram-negative and gram-positive bacteria. In this poster presentation, various types of applications of RuNPs have been discussed.

Acridone trapped in the biological nanocavity of β -Lactoglobulin: The pivotal role of hydrogen bonding in the hydrophobic pocket

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Spectroscopic exploration divulge that Acridone (AD) penetrates through the complex structure and enters the hydrophobic cavity of the protein β -Lactoglobulin (β LG). AD interacts with only one of the two tryptophan (Trp) residues of β LG, which is validated by the appearance of a single isoemissive point in TRANES, attributed to Trp-19. Modification in the secondary structure of the protein while AD perturbs β LG is understood from circular dichroism spectroscopic study. Steady-state fluorescence study in different temperatures implies the presence of hydrogen bonding in AD- β LG interaction. Furthermore, timeresolved fluorescence anisotropy study indicates the of presence of hydrogen bond in AD- β LG interaction which possibly involves the rotamers of Trp-19. Actually, the involvement of rotamers of Trp-19 is indicated by the increase in fluorescence lifetime of β LG on addition of AD. Docking study substantiates the involvement of hydrogen bonding in AD- β LG interaction. The most prominent evidence of hydrogen bonding between Trp and AD is obtained from the laser flash photolysis studies where the signature of formation of ADH[•] and Trp[•] through hydrogen abstraction between Trp and AD, loosely bound through hydrogen bonding is observed. Thus, binding interaction of AD and β LG involves hydrogen bonding in a hydrophobic pocket of the protein.

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Induction of defense in tea against *Colletotrichum gloeosporioides* using abiotic inducers *Shibu Das*^{1*}, *Aniruddha Saha*² *and Dipanwita Saha*³ ¹Department of Botany, Rammohan College, Kolkata-700009 ²Department of Botany,University of North Bengal, Siliguri-734013 ³Department of Biotechnology,University of North Bengal, Siliguri-734013 ^{*}Email:*shibudas@rammohancollege.ac.in*

Brown blight disease of tea caused by *Colletotrichum gloeosporioides* (*Cg*), is one of the serious diseases of tea plants. The disease severely damage the plants and reduce the production and quality of tea. Application of abiotic inducers induce systemic resistance through various defense enzyems and protect the plants. In the present study, susceptible tea seedlings were treated with two abiotic inducers (BTH and BABA) and inoculated with *Cg* to find out the disease occurrence. Accumulation of defense related enzymes like Phenylalanine ammonia-lyase (PAL) and β -1,3 glucanase were measured in different treatments (treated-inoculated, treated-uninoculated and untreated-uninoculated) to study the effect of inducers in defense induction. From the results, it was found that BTH and BABA both have reduced disease index to 2.80±0.46 and 3.2±0.39 respectively compared with the control (6.72±0.43). The activity of PAL was increased in BTH and BABA treated plants for about 2.3 and 1.8 fold, similarly the β -1,3 glucanase activity was also increased for about 2.2 fold respectively after four days in comparison with control plants. Thus our result showed that both the inducers are effective to induce disease resistance through induction of defense related enzymes.

Keywords: Brown blight, *Colletotrichum gloeosporioides*, abiotic inducer, phenylalanine ammonia-lyase, β-1,3 glucanase

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In silico analysis and molecular docking studies of Moringa oleifera phytochemicals against enzymes of Daboia russelii

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The currently available snake envenomation treatment with antivenom serum is not highly efficient and demonstrates limited effectiveness in reducing snakebite mortality and morbidity. Moringa oleifera is a versatile and nutritionally rich plant which has several phytochemical properties including antivenin activities. This study is designed to identify potent antivenin phytochemicals of Moringa oleifera against the four major Russell viper venom components. The phytochemicals of Moringa oleifera were retrieve and enlisted from various websites, databases, journals, and books. The 3D conformer of these compounds was downloaded from Pubchem (https://pubchem.ncbi.nlm.nih.gov/) and a virtual library was constructed and screened against the four major venom components of Russell viper- phospholipases A_2 (PLA₂), serine proteases (SVSP), snake venom metalloproteases (SVMP), and L-amino oxidase (LAAO). The structure of PLA₂ (PDB ID: 1KPM, resolution: 1.80 Å) of *D. russelii* was downloaded from the Protein Data Bank (https://www.rcsb.org/). As the structures of SVMP, SVSP, and LAAO from D. russelii are not available, homology modelling was used to construct these structures. Their sequences (fasta format) were retrieved from UniProtKB (https://www.uniprot.org/). The Uniprot ID of SVSP, SVMP, LAAO are PODPS3, B8K1W0, G8XQX1 respectively. Proteins were prepared using protein preparation wizard by Schrödinger software and docked using extra precision Glide module. The results of the in silico analysis revealed that a significant number of Moringa oleifera phytochemicals exhibit a strong binding affinity with these key venom components of Russell viper compared to the known standard inhibitors. Given that these components of Moringa oleifera possess inhibitory properties against snake venom components, it may serve as a natural and readily accessible first-aid remedy for snake envenomation. Further in vitro and in vivo studies are warranted to affirm these findings.

Soil-plant interactions in carbon linked fore coming climate predictions.

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Abstract: Greenhouse gases (CO₂: N₂O and CH₄) production can play an impact on global environmental climate change. There are many bio-geochemical cycles like carbon (C), nitrogen (N) and others hydrological cycles are existed. This climatic change and bio-geochemical cycle both are regulated by the soil-plant interaction. For an accurate prediction of the global climate change can predict through the several models. Dynamic global vegetation models are the best fitted prediction models for describing the global climate predictions with the help of terrestrial ecosystem functions and feedbacks. Soil-plant interactions can help the Dynamic global vegetation (DGV) models accurate climatic predictions in a global way. Here, in this very few available resources we can manage to understand the DGV model's structure. The several knowledge gaps are existed for the understanding of soil-plant interactions. To improve the models, we need to understand few parameters meticulously and can modify the simulation processes with the knowledge of 1. Vegetation dynamics, 2. Drought impacts, 3. Soil-carbon and soil-nitrogen dynamics 4. Nitrogen cycles. The main three challenges are globally ongoing can be meetup only collaboration between ecologists and global model making community. We critically incorporate global aspects of soil-plant interactions for simulating the models aptly. The multifold knowledge and meticulous incorporations are crucial. Lastly, we could increase the simulation testing against the large-scale data set and multifactor analysis to predict the accuracy of the models. With this writeup I am trying to depict how the soil-plant interactions helps to build up the simulation modeling accurately. Also, we must understand the detrimental effects of carbon and other molecules for predicting the future climate and understand the use of experimental data generations method to solve the better climate related uncertainty problems.

Key-words: Climate, plant, soil, carbon, DGV models

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Exploring the Potential Interaction Between Snake Venom PLA2 and Human secretary PLA2 Receptors

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Phospholipase A2 (PLA2) enzymes plays crucial roles in numerous physiological processes, including inflammation modulation and immune response regulation. The human secretary PLA2 (hsPLA2) receptor family (C-type Lectin receptors family), specially CD206 and PLA2R, are reported to interact with bee venom PLA2 and result in immunosuppression through Treg induction. A similar immunosuppressive milieu has recently been reported in experimental murine model of Russell's viper snake envenomation. To best of our knowledge, snake venom PLA2 (svPLA2) and hsPLA2 receptor family interaction has not been documented till date. In the present study we tried to explore the possible interaction between svPLA2 and hsPLA2 receptors using protein-protein docking. svPLA2 and hsPLA2 receptor structure were downloaded from Protein Data Bank (https://www.rcsb.org/). For Russell's viper svPLA2 1KPM and for hsPLA2 receptor CTLD containing PLA2 receptor superfamily and domains including C-type lectin domain (PDB id- 6JLI, 5XTS, 6INV, 7L64) and human PLA₂R (PDB id- 7QSR) were selected. Protein-protein docking was conducted using ClusPro webserver (https://cluspro.org/help.php) and the best binding model was selected based on the docking score and visualized by PDBsum (https://www.ebi.ac.uk/thornton-srv/databases/pdbsum/). The findings revealed potential amino acid residues and the bonds responsible for the interaction between Russell's viper svPLA2 and selected receptors. Based on the results of in silico studies, it can be proposed that svPLA2 and hsPLA2 receptor might interact with each other and this may be one of the possible reasons behind immunosuppression after snake envenomation. Furthermore, in detail in vivo and in vitro studies are needed to establish this finding to broaden our understanding of immune regulation and may offer new opportunities for the treatment of snake envenomation and immunosuppressive conditions.

Protein- protein interaction in snake bite envenomation a bio-informatics approach Pratima Maity^{1,2},Roshnara Mishra¹,Raghwendra Mishra² ¹ Department of Physiology, University of Calcutta ²Department of Physiology, Ananda Mohan College

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Venom travels, from the bite site through lymphatic system or directly enter into the blood stream through tissue and circulate throughout the body, leading to systemic effect along its path. Venom toxicity underlying a unclear interplay of protein-protein interactions between venom components and victims tissues, causing physiological effect ranging from local tissue damage to irreversible organ failure. Growing evidence of altered protein profile in snake bite envenomation victim and in experimental model, suggests that the altered protein or group of proteins may play a pivotal role in the venom induced damage and its remodeling .In order to explore these protein and its cluster, we have endeavored to analyse the important protein-protein interaction using published proteomics data with STRING and for better visualization and analysis, we use Cytoscape . The aims of this bio-informatics assisted protein-protein interaction analysis is two- fold i) to gain a deeper understanding of the pathophysiology of this tropical neglected disease. and ii) to perform a predict analysis of regulatory network hubs, that might be interacted with other pathophysiologies that involve various forms of tissue damage (example, various infectious disease and cancer). Our finding supports that , snake venom activate multiples blood and tissue factors that interconnect many biological processes. And through protein-protein interaction analysis, we have pinpointed key molecules indicative of specific cellular pathway. Integrating the analysis of venom induced systemic effects to identify general disease pattern, that pave the way for alternative novel therapeutic development.

Combined Clomiphene-Metformin Regimen Attenuates Erythrocyte Oxidative Stress in Polycystic Ovary Syndrome: a new direction to decode the puzzle

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Abstract: Polycystic ovary syndrome (PCOS) is a major form of dysovulatory infertility, commonly associated with hyperandrogenism, hyperinsulinemia, and/or dyslipidaemia to name a few. Erythrocytes being sensitive to the hyperandrogenic milieu get deformed in response to shear stress by exposure to elevated reactive oxygen species (ROS) resulting oxidative stress. Given the importance of alteration of blood elements in young women with PCOS, limited research has been undertaken to address the issue of hematological parameters from a management perspective.

Twenty (age 22-35 years; BMI 28-32 kg/sqm) women diagnosed with PCOS as per Rotterdam Criteria, 2003 undergone ovulatory treatment/s with clomiphene citrate (CC) 50 mg daily from day 3-7, combined with metformin (500 mg twice daily) for three consecutive ovulatory cycles. Fifteen age-matched women undergoing IVF due to male factor infertility diagnosed as per AUA/ASRM guidelines was treated as control. Markers of membrane damage were evaluated including lipid peroxidation, co-oxidation, carbonylation, ferryl formation in erythrocytes and haemoglobin respectively. Membrane-morphological view by scanning electron-microscopy (SEM) was done to assess cellular injury. Intracellular reactive oxygen species (ROS) has been evaluated by fluorescence-activated-cell-sorting. Osmotic fragility was studied exposing differences of hemolysis to find possible relation with therapeutic functionality. Results were statistically analyzed by student's t-test and ANOVA accordingly.

Lipid peroxidation, co-oxidation, ferryl and carbonyl formation were increased (p<0.04) in PCOS compared to control, cueing to oxidative stress with increased ROS (p<0.05) which significantly (p<0.05) ameliorated by combined metformin-clomiphene regimen. SEM observations indicate presence of stomatocytes, spherocytes and echinocytes in PCOS attributing to alterations in erythrocyte-membrane permeability; clomiphene-metformin dual treatment improving the scenario. Rate of osmotic fragility was lower in PCOS, which was almost reversed back to normal after treatment.

Collectively, we propose erythrocytes as an oxidative- hotspot in PCOS; combined clomiphene-metformin regime possibly playing an ameliorative role in erythrocyte biology to restore intermingled oxidative stress.

A facile approach for selective detection of arsenite ion using plasmonic behaviour of silver nanoparticles

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Abstract:

The millions of people are at high risk due to unsafe levels of arsenite (As(III)) in drinking water and it calls for the development of low-cost simple techniques for rapid on-site monitoring. Herein, for the first time any specific reagent free, aptamer free easy redox strategy is used for selective quantification of arsenite ion using citrate stabilized colloidal silver nanoparticles (AgNP) in bicarbonate medium. The synthesized AgNP were well characterized by UV-Visible spectroscopy, cyclic voltammetry, transmission electron spectroscopy (TEM) and particle size distribution with zeta potential measurement. This colorimetric arsenite ion sensor technique was found to be very selective in the presence of other possible cations and anions as interfering species. The reduction of silver-citrate complex exists in AgNP system by oxidation of arsenite in bicarbonate medium leads to aggregation of nanoparticles which enable naked eye change. We observed that the reported method was quite selective for arsenite particularly in bicarbonate medium. By using the strategy, the nanomolar sensing of arsenite was done with limit of quantification 50 nM (6.45 ppb). The developed sensor was successfully tested for the arsenite in real water samples.

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PALLADIUM COMPLEXES: NEW CANDIDATES AS ANTI -CANCER AGENTS

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Abstract:

The application of transition metals complexes as anti-cancer medicines has increased significantly since the identification and regulatory acceptance of cis-platin in 1978. Various platinum complex analogues were identified and subsequently examined to determine optimal efficacy towards the objective. However, it was quickly discovered that the Pt-complexes were less successful and not the best medication for treating cancer because of their many adverse effects, including neurotoxicity and resistance. As a result, researchers looked into more effective substitutes that may overcome the drawbacks of platinum analogues and demonstrate the capacity to cause cancer cell death. In this poster, the immense bio-activity of Palladium complexes has been discussed and tried to demonstrate that Palladium complexes and its derivatives may function as more effective anti-cancer agents than cis- platin.

Morphology and seasonal occurrence of *Clinostomum phalacrocoracis* (Dubois, 1931) (Trematoda, Clinostomidae) *in Trichogaster fasciata* (Bloch and Schneider, 1801) (Perciformes, Belontidae) from North Bengal, West Bengal

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Abstract:

Fishes are the important source of protein containing food, essential for healthy body growth. But the infection of parasite interferes in the fish production by causing changes in flesh quality, death of fish, and thus hampering the production. This present work deals with the morphological details and seasonal occurrence of trematode, *Clinostomum phalacrocoracis* in freshwater fish *Trichogaster fasciata* from North Bengal, West Bengal. Fishes act as the intermediate host of this parasite but it may infect humans during ingestion of raw or undercooked infected fish, which causes Halzoun syndrome and even cause death. In this present study *Trichogaster fasciata* was found to be infected with *Clinostomum phalacrocoracis*, in anterior part of the body cavity. The parasite was fleshy, stout, and creamy in colour. Morphological characterization under light microscopy reveals that the length of the parasite is 3200μ m - 13500μ m (9800 μ m), breadth 1549.74 μ m - 3200.23μ m (2234μ m), intestinal caeca, anterior, posterior testis, ovary were visible. This work also deals the infestation of this parasite in different seasons. During this study it was observed that this parasite has been found first time from *Trichogaster fasciata*, North Bengal and the prevalence of this parasite was higher during summer season.

Keywords: Trematode, fish parasite, morphology, seasonal occurrence, Trichogaster fasciata, Clinostomum phalacrocoracis

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Role of different biochemical and anthropometric parameters as a predictive marker of PCOS in college going girls of Kolkata

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Introduction: PCOS, one of the most common endocrine disorders in women of reproductive age is affecting a major population of adolescent and young women all over the world. It is associated with menstrual irregularities, obesity, insulin resistance, hypertension, type 2 diabetes, cardiovascular diseases, and infertility. It is basically a metabolic disorder and diagnostic assays of PCOS are very expensive. So, the aim of the present study is to analyse the risk factors for PCOS development in college going girls of Kolkata.

Materials and Methods: The study was carried out in randomly chosen students (age group 18–25 years) of Rammohan College, Kolkata. It was a cross-sectional study, accompanied by biochemical studies of blood samples and few anthropometric studies like measurement of BMI, Waist-hip ratio and body fat percentage.

Results: FSH/LH ratio revealed that approximately 30% of the college students were at high risk of developing PCOS. Many of they were reported to have oligomenorrhea, facial acne, hirsuitism etc. BMI studies revealed that 55% of the students were either overweight or obese. It was found that about 35% students had waist-hip ratio above 0.87 and 40% students had high body fat percentage.

Conclusion: High BMI and waist-hip ratio may act as an indication for PCOS development.

Discussion: The present study is an attempt to understand the risk of development of PCOS by assessment of anthropometric parameters among college going girls of Kolkata. This will create awareness among them and will help them to understand the need of clinical consultation.

Key words: PCOS, BMI, Body fat percentage, FSH/LH ratio, Waist hip ratio.

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Exploring filarial intracellular steroid hormone binding receptor: an in silico study

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Abstract

Lymphatic Filariasis (LF), recognized as a neglected tropical disease, induces significant social stigma in affected individuals. The etiology can be attributed to pathogenic filarial nematodes, specifically *Wuchereria bancrofti, Brugia malayi,* and *B. timori.* Despite governmental efforts through various programs, the efficacy achieved thus far remains suboptimal. Given the current landscape, there is a pressing necessity to investigate novel therapeutic targets. Filarial parasites exhibit prolonged viability within the host by exploiting their endocrine system and nuclear hormones. Existing literature indicates that filarial nuclear hormones engage with intracellular receptors to modulate diverse physiological processes. In the present investigation, a computational methodology was employed to identify intracellular steroid hormone binding receptors (ISHBR) with shared sequence homology across distinct species. Utilizing ClustalW and MEGA XI, sequence alignment was conducted, resulting in the construction of a phylogenetic tree that revealed likeness to the Nuclear hormone receptor family of *Caenorhabditis elegans*. The observed degree of sequence resemblance among diverse taxa hints at their evolutionary interconnectedness and potential functional implications. Given the escalating evolutionary resistance and rising adverse effects due to prolonged use of anti-filarial medications, ISHBR emerges as a paramount preventive intervention against LF.

Cu(II) Metallogel as Nanozyme for Phenoxazinone Synthase-like Activity

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In our present study, we have shown that disodium succinate and hexamethylenetetramine, when allowed to react simultaneously with CuCl₂ in an aqueous medium, instantaneously form a greenish metallogel. The gelation is only attainable in the presence of the two ligands, which ascertains the co-operativity of the ligands to successfully achieve the metallogelation. Physical and structural characterizations of the gel sample were performed using different microanalytical techniques. The gel shows nano dimensional entangled network morphology. The gelation was observed to be highly specific with Cu(II) and the two ligands. The gel also exhibits its stimuli-responsive nature towards different interfering chemical parameters such as pH, selective anions, selective complexing agents, and so forth. Finally, the robust Cu(II) metallogel was deliberately exploited as a heterogeneous catalyst for successful oxidative conversion of 2-aminophenol (OAPH) to phenoxazinone hiring atmospheric oxygen and thereby conferring its role as a biomimetic nanozyme catalyst. The catalytic conversion has been followed spectrophotometrically. The detailed kinetics for the reaction was performed with varied reaction parameters. The Michaelis-Menten model was applied to analyze the results. Finally, recyclability of the catalyst was also verified. This nanozymatic phenoxazinone synthase-like activity of a nanodimensional metallogel is hitherto unknown and thus suggests its enzyme mimicking feature.

Keywords: Copper, Metallogel, Nanozyme, Catalyst, Phenoxazinone Synthase

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Iodine nutritional status among school children in Rampurhat Sub-division of Birbhum district in West Bengal

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lodine is an important micronutrient found in water, soil and plants. Man needs iodine to make thyroid hormones, essential for normal development of the brain and maintenance of the body heat and energy. Lack of iodine in the diet leads to visible and invisible spectrum of health consequences known as iodine deficiency disorders or IDD. The major consequences of iodine deficiency are goitre (enlargement of thyroid gland than normal), mental defect, deaf mutism, stillbirth and miscarriage, weakness and paralysis of muscles as well as lesser degree of physical and mental function. Effects on brain function occur at all stages of life, from foetal damage or hypothyroidism in the neonate, child or adult.

Prevalence of endemic goitre in school children (6-12 years) is the most widely accepted marker to evaluate the severity of IDD in a region. According to WHO/UNICEF/ICCIDD (1994) recommended criteria, a prevalence rate of 5.0-19.9% is considered as mild; 20-29% is considered as moderate and a prevalence rate of above 30 % is considered as a severe public health problem. In all 2712 school children (6-12 years) were clinically examined for goitre from eight C.D. Blocks and two Municipalities of Rampurhat Sub-division of Birbhum district. The overall goitre prevalence was found 13.13 %. Most of the goitre is palpable i.e., grade 1 goitre however visible goitre or grade 2 goitre also exist. Associate iodine deficiency disorders also found from the studied region. From each area 35 salt samples were collected for estimation of iodine. Overall 350 salt samples were collected and iodine content was measured. Observation showed that 18.28 % samples had iodine level less than the recommended value i.e., 15 ppm. Thus about 82% people were consuming adequate level of iodine through edible salt. The mean value of iodine in the drinking water was found 77.9 ± 32.2 μ g/L .lodine content in drinking water. Thus bioavailability of iodine is sufficient in the studied region.

The overall observation suggests that there is a mild degree of goitre endemicity as public health issues though the people consuming adequate iodine through edible salt and they also consume adequate iodine through drinking water. More investigation is essential to find out the exact cause for the persistence of mild degree of goitre endemicity in the studied region.

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Application of Nanofluids: Current and Future (Review article)

Tanu Bagaria. Arup Mandal

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Modern Nanotechnology has enabled the processing and production of Nanomaterials with an average size of the order of 100 nm. Today nanotechnology has a vast application in our daily life. Nanofluids are suspensions of nanoparticles in fluids which shows significant improvement of their properties at optimized nanoparticle concentrations. Many of the publications on nanofluids are about understanding their behavior so that they can be utilized where straight heat transfer enhancement is paramount as in many industrial applications, nuclear reactors, transportation, electronics as well as biomedicine and food. Nanofluid as a smart fluid, where heat transfer can be reduced or enhanced at will, has also been reported. This paper focuses on synthesis, types and properties of nano fluids. This paper reviews on presenting the wide range of recent and future applications that involve nanofluids uses in automobile, biomedical, heat transfer, solar thermal, Detergency, and electronic applications.

Identification of some key genes active during the vegetative growth from the transcriptome analysis from leaf of mango (*Mangifera indica* L. *var* Fazli) from Murshidabad district of West Bengal, India.

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Mangos are a tropical fruit with a rich genetic resource, and their use in breeding programs and related research has become essential. Mango research is making great strides in the fields of breeding and genetic enhancement, which could boost the industry. Mango is also known as the "king of fruits" for its large production volume, rich taste, tremendous variability and presence of bioactive compounds with demonstrated health benefits. Mangos have extensive intra-specific variability, with about 1600 cultivars cultivated worldwide. Traditional breeding methods have limited success in improving the quality of mango due to prolonged time of maturity, self-incompatibility and high degree of heterozygosity in breeding lines. A varied and well-maintained variety of variations and thorough and well-documented information on the genetic material of *Mangifera indica* L. is essential for breeding efforts Recent studies utilizing genomic analysis have identified key genes responsible for economically important characters, suggesting the possibility of Marker Assisted Selection (MAS) in breeding lines through transgenic or specific genotype selection from seedlings. This study is based on the transcriptome analysis of the mango genome (*Mangifera indica* L. var. Fazli) primarily to identify the functions of mango genes during the vegetative growth phase. The major findings include few highly active genes viz. WRKY, NAM, MYB, GoGID1.

Keywords: Mangifera indica L., Transcription analysis. WRKY, MYB, var Fazli,

Exploring the Influence of Micellar Environment on the Dissociation Equilibrium of a Sulfonephthalein pH-indicator Dye via Spectrophotometric Analysis

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The experimental determination of the mono-dianionic dissociation equilibrium constant (pK_{a2}^m) for Bromocresol Green (BCG), a Sulfonephthalein pH-indicator dye, in CTAB micellar media has revealed a departure from its value in pure water (pK_{a2}^w) . This discrepancy suggests that the presence of CTAB micellar media alters the dissociation behavior of BCG compared to its behavior in pure water. Such alterations imply that the micellar environment influences the protonation and deprotonation processes of the dye molecule, likely through interactions between the dye and the micellar environment.

To delve deeper into this phenomenon, theoretical models depicting the dissociation equilibrium of BCG in aqueous micellar solutions were employed. These models utilized Nonlinear Regression analysis methods integrated into Microsoft Excel Solver. The calculations incorporated spectrophotometrically determined binding constants (k_b) and partition coefficients (K_x) of the dye between the micellar pseudo-phase and water.

The obtained pK_{a2}^{m} values for BCG in various pH media were found to exhibit variability. This variability was attributed to the flexible extent of solubilization of the dianionic form of BCG in the CTAB micellar medium, which changes with fluctuations in aqueous pH. Furthermore, the observed relative intensity of absorption bands of mono and dianionic forms of the dye in the micellar medium correlated with these differences in pK_{a2}^{m} magnitudes.

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Phosphorus species as Biosignatures inputs on the NASA-NfoLD Life Detection Knowledge Base (LDKB)

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Chemistry is universal but Earth is the only place yet known in the universe to harbour life as we know it. Life on Earth essentially requires the CHNOPS (Carbon, Hydrogen, Nitrogen, Oxygen, Phosphorus, and Sulphur) elements to sustain itself. The push for the search for life beyond Earth in our solar system and outside it has increased with the discovery of exoplanets. In this context, LDKB (an initiative by the Network for Life Detection- NfoLD, NASA) is a novel attempt to build a one-stop storehouse of information about different biosignatures presenting all sides to arguments supported by evidence from peer-reviewed scientific literature. Here, biosignatures are featured under 3 categories: Chemistry, Structure, and Activity. This Knowledge Base aims to direct future researchers to know what to look out for in their future biosignature studies. The Phosphorus Biosignature inputs at the LDKB serve as good case studies to get a brief overview of the abundance, occurrence, and detection of Phosphorus chemical species beyond Earth and also understand how the biotic and abiotic factors considered for two different molecular species can be different for different environments. We conducted conventional and Technology- enhanced literature reviews (using VOSviewer, v1.6.19) on potential biosignature Phosphorus species. Using the Bibliographic data (2003-2023) from the databases: Scopus, Web of Science, and PubMed, we generated an unbiased visual Bibliometric network amongst relevant keywords (based on their co-occurrence in literature). All three networks generated showed links between Biosignature and Phosphorus with only two Phosphorus species namely, Phosphine and Phosphates. This implied that only these two Phosphorus species have been considered to date as potential biosignatures on different environments in our Solar system like Phosphine in Venusian clouds and Phosphates in sub-surface waters of Enceladus. To sum up, this literature review aimed at listing down the Phosphorus biosignatures studied to date and updating the relevant information on the LDKB to direct future research in the domain with a balanced approach of considering both the biotic and abiotic factors before concluding a chemical species as a 'true biosignature or a false positive'.

The role Heat shock proteins (HSPs) in adaptation of Organisms to Heat stress

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By integrating cell biology into the physiology of whole organisms, researchers can now pursue fundamental questions about how cellular changes affect an organism's ability to adapt. One of these questions is the adaptation of the whole organism to high ambient temperatures and the influence of cellular stress responses on the organism's ability to perform tasks in the heat. Adaptation to heat can be divided into heat tolerance and acclimatization. Thermo-tolerance is a cellular adaptation triggered by a single severe but non-lethal heat exposure that allows an organism to survive subsequent lethal heat stress. In contrast, acclimatization is the ability of an organism to perform more work in the heat through enhanced heat dissipation through repeated small increases in core temperature. In this review, we consider the differences between thermo-tolerance and thermal acclimatization, possible relationships between these forms of thermal adaptation, and possible mechanisms explaining these relationships. Central to understanding the role of cells in thermo-tolerance, and perhaps adaptation, are heat shock proteins (HSPs). In summary, this literature shows that: 1) HSP accumulation attenuates the heat- induced reversible changes of epithelial permeability. 2) The accumulation of HSP70 increases the tolerance of the endotoxin in most of the animal cells. 3) This endotoxin resistance of various cells may trigger a direct effect of endotoxin or may reflect HSP-associated changes to cytokine production and resistance. Although this study used a single relatively intense heat exposure to induce HSP responses, the cellular changes asso ciated with HSP responses do not result in survival of the organism at the lethal heat exposure. They can o nly protect the cells to some extent from intense heat exposure and illustrate the changes of the cellular p hysiology.

Graphene Oxide Quntum Dot Catalysed Green Synthesis of Bio-Active Pyrazolone Derivatives at Room Temperature

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A multicomponent one pot method in an aqueous medium has been established for the synthesis of biologically active 3-methyl-4-substituted benzylidene-pyrazole by the condensation of 3-methyl-pyrazol-5-one with substituted aromatic aldehyde catalyzed by graphene oxide quantum dot (10 mol%) and triethyl amine (2 mol%) at room temperature. With good functional group tolerance, the reactions can be carried out at low catalyst loadings. There final product can be confirmed by comparing melting point reference, IR, NMR and elemental analysis data. Synthesized derivatives are found to have remarkable bioactivities.

Keywords: Bioactive pyrazolone derivatives, Graphene Oxide Quantum Dot, room temp, aqueous medium.

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Green Synthesis Of Bioactive 1,4-Dihydropyridine Derivatives in Aqueous Ethanol Media, Catalyzed By Graphene Oxide Quntum Dot at Room Temperature

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A novel, highly efficient, and eco-friendly one-pot green synthesis has been derived for producing symmetrical and unsymmetrical 1,4-dihydropyridines. This method follows the multi-component Hantzsch synthesis and is conducted in aqueous ethanol media, with catalysis provided by graphene oxide quantum dots (GOQDS) at ambient temperature. The study highlights numerous advantages, including simplicity and environmental friendliness, rendering it highly attractive. Achieving excellent yield within short reaction time with the need of quantum dots catalysts the process and reduces cost.

<u>Keywords</u>: 1,4- dihydropyridines, Hantzsch condensation, multi-component reaction (MCR), GOQDS catalyzed, room temperature.



Mechanistic studies on oxidation of nitrite (NIII) by a mutinuclear {Mn₄O₆}⁴⁺ core in aqueous acidic

media

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In aqueous acidic media complex **1** ($[Mn_4(\mu-O)_6(bipy)_6]^{4+}$, bipy = 2,2'-bipyridine) are reduced to Mn^{II} state b y nitrite $[N(III) = (HNO_2 + NO_2^{-})]$. **1** reacts within pH range 2.0–6.0 to produce nitrate as end oxidation prod uct. **1** undergoes oxo bridge protonation during reaction to produce reactive species **1H** ($[Mn_4(\mu-O)_5(\mu-OH)$ (bipy)_6]^{5+}). As usual protonated metal oxidant **1**H reacts faster than **1**, but an unusual observation of these reaction is kinetic predominancy of HNO₂ over its conjugate base NO_2^{-} . Title complex **1** is stable in aqueous media over a long pH region and shows no ligand dissociative equilibria in presence or absence of reducin g agent. The reaction shows remarkable kinetic isotope effect by increasing the reaction rate in D₂O media. A hydrogen atom transfer (HAT) mechanism (**1**e, **1**H⁺; electroprotic) is appropriate to explain the isotope effect.

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Marine Diversity: source of prospective drugs

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The enormous ecological resources of the sea have been exploited since ancient times and marine animals like fish and preparations from algae are utilized as the sources of medicine. And hence, the drug manufacturers are always on the lookout for new resources to develop effective and safe drugs for the increasing demands of the world population. Seventy-five percentage of earth's surface has been covered by marine water but research about the pharmacology of marine organisms is limited, and most of it still remains unexplored. According to the preliminary reports marine environment represents countless and diverse resources comprising a variety of aquatic plants and animals. These aquatic organisms are screened for antibacterial, immunomodulator, anti-fungal, anti-inflammatory, anticancer, antimicrobial, neuroprotective, analgesic, and antimalarial properties. They are used for new drug developments extensively across the world. Marine pharmacology offers the scope for research on these drugs of marine organisms including bacteria, viruses, animal, algae, fungi and sponges.

Keywords: marine, algae, sponge, antitumor, anticancer, cytotoxic, drugs



Schematic presentation of some prospective drugs from marine resources

Potentials of Nanotechnology in Osteochondral Interfacial Tissue Regeneration

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With successive demographic transpose towards an obese and aging society, a hike in number of patients, suffering from osteochondral diseases are found. Osteoarthritis is a clinical condition caused by cartilage and associated subchondral bone destruction, affecting about 27 million adults in United States and 65 million adults in India. Cartilage is a tissue with low self-repairing potential due to its inherent limited vascularity that results in poor regenerative capacity of chondrocytes, the main cell type present in cartilage. Although limited vascularity is advantageous in graft implantation prospective to promote regeneration as a consequence of lowest immunological responses. Current medical approaches to treat degenerative joint disease (DJD) includes drilling, scaffolds, autologous chondrocyte implantation, and osteochondral transplantation. These options result in the generation of fibrocartilage that contains collagen type I and type II, having decreased strength and resilience as compared to native cartilage. The regenerated tissue degenerates again as coefficient of friction of the fibrocartilage scar tissue is higher than cartilage, that hinder motion compared to the smooth surface of cartilage and results in earlier degeneration. The complex interfacial architecture of articular cartilage and subchondral bone limits the current strategies of tissue regeneration to regenerate the osteochondral tissue effectively. Providentially the nanoparticle/nano-medicine based platform provides a novel strategy for treatment of degenerative joint diseases (DJDs), due to their outstanding biocompatibility effective cellular responses on a nanoscale, high loading capability, targeted capability, increased mechanical properties, enhanced uptake rate and controlled release effect. This promising platform is effective for controlling the symptoms of pain, inflammation and related issues, tissue dysfunction, osteochondral repair and regeneration. This study aims to understand recent advancements of nanoparticle/nanomedicine-based remedies for articular DJDs. Additionally, some prospects are proposed that aim to improve the properties of nanoparticle/nanomedicine-based platforms to insight effective novel ideas for promising and accurate treatment of DJDs.

Keywords: Nanoparticle, Nanomedicine, Osteochondral Tissue, Joint Diseases, Regeneration * Corresponding Author

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Revisiting Luteolin for its efficacy against Metastatic Colon Carcinoma

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Metastatic colorectal carcinoma (mCRC), a multifactorial subtype of human cancers, is rapidly rising in prevalence with time, pertaining to various lifestyle and diet-associated alterations. Wnt- β -catenin or PI3K/AKT/mTOR pathways have exhibited active participation in tumorigenesis and progression into mCRC. Regarding amelioration, phytotherapy is being re-cultivated accounting to the unmanageable and toxic side effects of conventional drugs. In this regard, our study involving the *in silico* screening of 30 phytocompounds based on their anti-inflammatory and anti-mCRC efficacy as well as their molecular docking and binding energy scores with 5 key mediators of mCRC immunopathogenesis, viz. β -catenin, GSK-3- β , PI3K- α , AKT1 and p50 initially rendered luteolin as the superlative choice. Further *in vitro* assays on cell viability, clonogenicity and colospheroids formation post luteolin has demonstrated explicit and exceptional regulatory effects upon the 5 targets, thus intercepting oncogenesis.

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Applications and Future Aspects of Lanthanide-based Nanomaterials

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The application and future aspects of nanomaterials consisting of rare-earth elements continue to make significant progress within biomedical sciences. The rare-earth elements also known as lanthanides, play a crucial role in modern life due to their excellent chemical and photoluminescence stability, narrow emission band, adjustable luminescence color, and longer photoluminescence lifetime (in the range of µs to ms). The diverse applications of nanoparticles with rare-earth elements as the host or doped elements for biomedical applications in the past few years, especially in the area of imaging and disease diagnosis. To enhance biocompatibility, surface modification of lanthanide-based nanoparticles by surfactants or polymers is desirable which has been achieved by researchers. Herein we focus on the latest progress of lanthanide nanomaterials in sensing metal ions, detection of explosives, tumor diagnosis, molecular images by magnetic resonance, and nuclear, optical, or computed tomography imaging. Likewise, photodynamic therapy, targeted radiotherapy, drug delivery guidance, and image-guided tumor therapy are some examples of their potential therapeutic applications.

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Viscometric characterization of sodium alginate in mixed solvent medium at different temperatures:

effect of external electrolyte

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Electrostatic perturbation owing to the conformation and hydrodynamics of sodium alginate was gained through viscometry in different solvent compositions. Both the methanol content and external salt concentration impart the same effect of counterion condensation. At lower salinity, polyion conformation seems to be more alginate concentration dependent. for salt concentration lesser than $0.001 \ mol \cdot L^{-1}$ a reduced polymer concentration of less than 1 is sufficient to make the polyion coil volume half to that at infinite dilution and for the salt-free state, the ratio becomes independent of reduced concentration exceeds the value of 4, this limiting value of concentration is almost half that in the aqueous phase. Alginate chains become more flexible in the mixed solvent phase than in aqueous solution by around 2-3 monomers lesser in each persistence length. Due to the screening of carboxylate ion charges by sodium ions, the radius of gyration decreases to around 20% more during ionic strength increment when compared to aqueous solvation.

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Applications of Förster Resonance Energy Transfer in biological studies

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Förster Resonance Energy Transfer (FRET) is a powerful and versatile tool in both chemical and biological studies. It has been instrumental in characterizing molecular conformational changes and probing solvent environments. Intricate mechanisms involved in innumerable chemical reactions, molecular recognition, and the behavior of supramolecular assemblies has been unraveled with the help of this technique. The integration of FRET into biological studies has revolutionized the understanding of biomolecular interactions and cellular processes. In molecular and cellular biology, FRET has been used to study protein-protein interactions, protein folding dynamics, and conformational changes. It has also enabled the exploration of protein-ligand interactions and facilitated the visualization of molecular signaling events within live cells and tissues. Furthermore, FRET-based biosensors have proven invaluable in studying ion concentrations, pH variations, and enzymatic activities in real-time, thus enabling researchers to gain insights into intricate cellular processes and signaling cascades. Besides, FRET has also found its utility in nanotechnology and materials science, enabling the precise control of energy transfer processes in nanomaterials, optoelectronic devices, and photonic applications.

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Viability of Alkaline Comet Assay As A Measure of Programmed Cell Death By Tea Polyphenols In Human Leukaemia Cells

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Programmed cell death or apoptosis is a physiological process by which genetically damaged cells or undesired cells can be eliminated. Induction of apoptosis is a potential mode as a chemotherapeutic as well as a chemopreventive strategy for cancer control. Apoptosis can be induced by a variety of natural substances of plant origin including polyphenols. Tea is a rich source of polyphenols which preferentially induce apoptosis in cancer cells. Apart from morphological changes, apoptosis is characterized by fragmentation of nuclear DNA. The characteristic DNA ladder formation that is observed on gel electrophoresis does not reflect the DNA breakdown in individual cells. On the other hand, alkaline comet assay as measured by single cell gel electrophoresis accurately measures DNA fragmentation at a single cell level. The comet assay was originally developed as a cytogenetic test to measure the genotoxicity of various chemicals. However, the comet image generated by an apoptotic cell is different from that obtained with a cell treated with a genotoxic agent. The present study deals with the induction of apoptosis by black tea polyphenols EGCG and theaflavin in human leukaemia cells (HL-60 and K-562). Induction of apoptosis by tea polyphenols was evident by typical apoptotic features such as morphological characteristics, FACS analysis, caspase activation and expression of apoptosis related genes bcl-2 and bax. It is apparent from the high degree of correlation observed between the comet tail formation and each parameter of apoptosis that the comet assay can accurately reflect the measure of DNA fragmentation and, hence, can be used to detect a cell undergoing apoptosis.

The selection of chalcogen in C60@exTTF nanohybrids suppresses electron hole recombination: A si mulation using nonadiabatic molecular dynamics

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The efficient and economical conversion of solar energy to electrical power is one of the main problems in s cience and technology. A supramolecular nanohybrids of C60 and extended tetrathiafulvalene (exTTF) are t he promising material for this ultrafast energy conversion, where C60 as electron acceptor hosted by well-k nown sulphur (S) contained electron donor, exTTF. We explored the electron-hole (e-h) recombination dyna mics in C60@exTTF nanohybrids by using time-dependent tight-binding density functional theory with the combination of nonadiabatic molecular dynamics (NAMD). In this study, the role of chalcogen atom in carri er dynamics by comparing with the Selenium (Se) and Tellurium (Te) in the position of Sulphur atom as tetr aselenafulvalene (exTSeF) and tetratellurafulvalene (exTTeF), respectively, has been investigated. The phot o-excitation of fulvalene leads electron transfer to C60, and electron hole recombination occurs from C60 to fulvalene moiety. By using Se atom instead of S, the recombination timescale shows a slower kinetics, whil e for Te, it shows more slow nano-second timescale. The e-h recombination is found in nanosecond regime t o follow the trend C60@exTTF < C60@exTSeF < C60@exTTeF. The decreasing electronegativity with hea vier chalcogen leads low frequency phonons, less orbital overlapping causes small NA coupling values and l arge band gaps in C60@exTTeF nanohybrids followed by slowest recombination timescale. Our investigati on of this atomistic time-domain simulation shows a strong influence of chalcogen atoms in e-h recombinati on dynamics, which may be provide a better knowledge for photovoltaic performance in future.

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Preservation, conservation and Pest controls in 3 College libraries in Kolkata

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We loss huge library documents every year due to the preservation and conservation policies, actions and lack of proper pest control of the libraries. There regular basis pest control is required in libraries. To protect the library from the insects, the application of chemicals is very important. The chemicals Fipronil for ants, termites, fleas, ticks, cockroaches. Hydramethylnon protects ant species. Abamectin protects from mites, aphids and other insects. The chemicals Pyrethrins & pyrethroids prevents library from mosquitoes, flies, ticks, fleas and bed bugs. In pest control the chemicals boric acids, carbamates, Cyfluthrin, Bifenthrin, Deltamethrin, Pyrethrum are also used. High humidity, Poor air circulation, poor housekeeping is also beneficial to insects. Human is also responsible to damage library books. This study will show the preservation, conservation and pest control status and future plans of Rammohan College, City College and Anandamohan College libraries.

Keywords: Preservation, Conservation, Pestcontrol, Insects, Chemicals, Rammohan College library, City College library, Anandamohan College library, Documents preservation.

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Mesoporous Cross-Linked Polymer Supported Silver Nanoparticles Catalyzed Reductive Coupling of Nitrobenzenes and Alcohols using Glycerol as Hydrogen Source Usha Mandi and Sk. Manirul Islam*

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Silver nanoparticle immobilized mesoporous cross-linked polyacrylic acid (Ag-MPAA-1) nanocomposite has been prepared via aqueous-phase polymerization of acrylic acid followed by reaction with silver nanoparticles. The Ag-MPAA-1nanocomposite has been characterized by powder XRD, TEM, SEM, EDX, FT-IR and UV-vis.

Nanocomposites formed by metal nanoparticles (NPs) dispersed in cross-linked polymer, polyacrylic acid, are expected to display several synergistic properties between the polymer and the metal nanoparticles, making them potential candidates for application in several fields such as catalysis [1] and others. Polyacrylic acid (MPAA-1) is a polymer of particular interest, due to its ease of preparation, high catalytic activity and good environmental stability. The choice of Ag in our work is mainly guided by its highest electrical conductivity among all the metals as well as its enhanced catalytic activity [2].

So in our study, we attempt to use Ag-MPAA-1as a potential catalyst in reductive coupling of nitrobenzenes and alcohols using glycerol as hydrogen source. This catalyst can be easily separated by using a simple filtration technique and can be reused five times without significant loss of catalytic activity [3].



Scheme 1. Schematic diagram showing the formation of Ag-MPAA-1 nanocomposite.

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