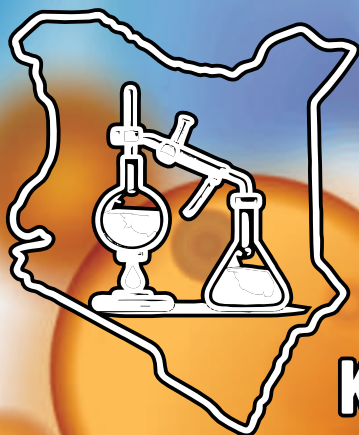




KCS

KENYA CHEMICAL SOCIETY

DELEGATES ABSTRACTS

9th - 11th Sep, 2026

Theme:

"HARNESSING THE POWER OF CHEMISTRY FOR SUSTAINABLE FUTURE"

**The 12th Kenya Chemical Society (KCS) International Conference
and**

The 10th Federation of African Societies of Chemistry (FASC) Congress

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Africa Re-imagined: Opportunities to Advance and Accelerate Cutting-Edge Research in Medicine to Promote and Commercialize Innovation

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Abstract

The ultimate sequencing of the human genome by Francis Collins and Craig Venter was a turning point in the field of drug discovery. Since then, great advances have been made in the field of molecular medicines and related sciences. Research and Development efforts have accelerated the discovery of critical medicines that have been very important in treating or alleviating life-threatening diseases. The advent of molecular biology and the utilization of Artificial Intelligence (AI) and BIG DATA have enhanced the discovery of new modalities in the field; this has led to improved diagnostics and novel approaches to therapies. We are living in the most exciting time, especially in the discovery of new medicines. The future is already here with us when we can have precision medicine and patient-tailored therapies to treat diseases like cancer, diabetes, arthritis, among others.

In this presentation, Dr. George Njoroge a renowned drug-hunter, will discuss opportunities available to African Countries in advancing in this important field of medicine. Africa cannot afford to be left behind in this exciting exercise of saving human lives. Prof. Njoroge will show case his discovery of Victrelis, a Hepatitis C virus (HCV) protease inhibitor drug that was discovered by his team in New Jersey, USA and approved by Food and Drug Administration (FDA) on May 13th 2011 for the treatment of the aforementioned indication. He believes that Africa should not be left behind in game of medical intellect.



Glancing the Kenyan Flora through the Eyes Of NMR: Towards the Discovery of Antimalarial Compounds

Utilizing Mass Spectrometry for addressing problems facing communities in a low resource environment.

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Abstract

Mass spectrometry is a vital analysis technique for all sectors of development including agriculture, health and trade. Good living and economies are highly reliant on analysis for decisions and emerging threats on a daily basis. Instrumentation for mass spectrometry is expensive and not readily available in low resource laboratories particularly in the sub-saharan Africa institutional setup.

We present our experiences in our mass separations laboratory of over 2 decades, with partnership with RSC and PACN which has been a training hub for scientists in mass spectrometry in the region, utilizing equipment which are donated through international partnerships and collaborations including RORO allowing low resource labs to gain MS capacity. The equipment is used for among others tasks to address and community issues. The demand for mass spectrometric analysis has been growing over the years and is yet to peak in Africa. A few key roles the laboratory has achieved in addressing national concerns and pollution disputes will be mentioned.

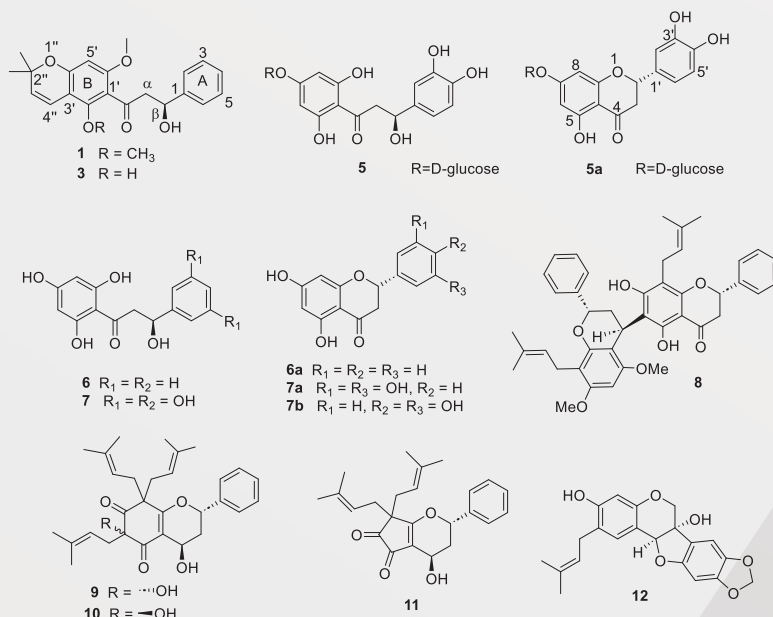
John L. Wilkinson, Ian Thornhill, Rik Oldenkamp, Anthony Gachanja (2023) Pharmaceuticals and personal care products in the aquatic environment: how can regions at risk be identified in the future. Environmental toxicology and chemistry, 43 (4). DOI:10.1002/etc.5763

[https://www.rsc.org/events/find-an-event/lcms-training-a-hands-on-approach-kenya-\(2026\)](https://www.rsc.org/events/find-an-event/lcms-training-a-hands-on-approach-kenya-(2026))

Abstract

Effective utilization of medicinal plants in alleviating infectious diseases requires the combined efforts of scientists in different disciplines. The role of a phytochemist is to isolate and characterize constituents of medicinal plants and make these natural products available to biological scientists to establish the activity of these compounds against different infectious agents. In this regard, our laboratory, at the Department of Chemistry, University of Nairobi, has provided hundreds of compounds for testing. In the process, we can train over a hundred postgraduate students towards MSc and PhD degrees. In this presentation, phytochemical and biological activity results on two *Tephrosia* species will be presented.

In the first example, the CH₂Cl₂/MeOH (1:1) extract of the stems of *Tephrosia uniflora* yielded a new 2'-hydroxydihydrochalcone (S)-elatadihydrochalcone-2'-methyl ether (**1**) along with three known compounds: elongatin (**2**), (S)-elatadihydrochalcone (**3**), and tephrosin (**4**)¹. The structures were elucidated by NMR spectroscopic and mass spectrometric data analyses. Based on the comparison of literature data with that obtained experimentally, and with computationally predicted NMR data, we propose the revision of the structures of three 2'-hydroxydihydrochalcones (**5-7**) to flavanones (**5a-7b**). Five new compounds - , rhodimer (**8**), rhodiflavan A (**9**), rhodiflavan B (**10**), rhodiflavan C (**11**), and rhodacarpin (**12**) - along with 16 known secondary metabolites- were isolated from the roots of *Tephrosia rhodesica*.



Utilizing Mass Spectrometry for addressing problems facing communities in a low resource environment.

They were identified by NMR spectroscopic, mass spectrometric, X-ray crystallographic, and ECD spectroscopic analyses. The crude extract and the isolated compounds showed activity (100% at 10 µg and IC₅₀ = 5–15 µM) against the chloroquine-sensitive (3D7) strain of *Plasmodium falciparum*². The characterization and antiplasmodial activity of some of these compounds will be discussed.

Sustainable preparation of World Health Organisation (WHO) Essential Medicines by Mechanochemistry

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Abstract

Although significant efforts have been made to reduce the environmental impact of active pharmaceutical ingredient (API) production, the use of organic solvents—responsible for about 75% of the total energy consumption—remains a critical step in many processes. Solvent-free synthesis through mechanochemistry aligns with several of the 12 Principles of Green Chemistry, offering a more environmentally responsible alternative for chemical synthesis. This presentation explores the application of mechanochemical methods to the preparation of World Health Organization (WHO) essential medicines at various scales. Using green chemistry metrics, we evaluate the environmental and economic benefits of mechanochemistry, demonstrating its potential to advance greener and more sustainable pharmaceutical manufacturing. Ultimately, these studies highlight mechanochemistry as a key enabler in the transition toward a more sustainable and resilient chemical industry.

Biocatalytic, Phytochemical, and Synthetic Chemistry Approaches to Drug Discovery- Some Examples of our Recent Work

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^bAdvisor ICCBS; International Center for Chemical and Biological Sciences (H. E. J. Research Institute of Chemistry, and Dr. Panjwani Center for Molecular Medicine and Drug Research), University of Karachi, Karachi-75270, Pakistan

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Abstract

As developing world face food security issues, it also confronts the drug insecurity challenges. The current drug development paradigm is cost, time, and labor intensive, which developing nations cannot afford to invest. The UN SDG 3 demands every nation to work towards "Good Health and Wellness" for its people. Therefore, it is important to develop appropriate, efficient, and cost-effective strategies for drug development against prevailing diseases, which must be based on indigenous knowledge resource base, S&T capacity, and patient-friendly approval process.

In the last two decades, we have identified a large number of new and novel chemical substances, through innovative approaches, against various disease-related targets. Our work at the interface of chemistry, biology and ethnomedicine, has been focused on the discovery of chemical constituents from medicinal plants and marine living resources, as well as for designing of new bio-catalytically transformed products with therapeutic potential. This has resulted in the identification of several novel drug leads against various therapeutic targets. Emphasis has been on the discovery of therapeutic agents against infectious diseases, and various chronic disorders, such as cardiovascular disorders, cancers, diabetes, and neurodegenerative disorders.

During this presentation, some recent examples of our studies highlighting the underlying philosophy, and approach of our research on cost-effective discovery of lead molecules will be discussed.

Nanostructured Polymer Membranes for Enhanced Water Filtration in Kenya

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Abstract

Access to safe drinking water remains a critical challenge in Kenya, where the majority of the population relies on unimproved water sources. With rapid urbanization and industrialization, surface water quality has been severely compromised, particularly within the major river basins such as Naivasha, Lake Victoria, Athi, and Nairobi River basins. High levels of microbial pathogens (e.g., E. coli) and Contaminants of Emerging Concern (CECs), such as pharmaceutical residues and personal care products, pose significant public health risks. To address this, water treatment techniques are rapidly evolving from traditional methods toward the advanced use of nanotechnology. Conventional polymeric membranes often suffer from rapid biofouling and low selectivity, limiting their application in decentralized water treatment systems, especially for Kenyan informal settlements and rural communities.

This presentation will explore the transformative potential of nanostructured polymer membranes (NPMs). The significance of these membranes lies in their dual-functional architecture. Unlike conventional filters, nanostructured membranes provide a tunable pore environment that allows for the precise exclusion of ions and viruses. By incorporating nanomaterials, we significantly enhance the hydrophilicity of the polymer, which reduces the adhesion of organic slime and bio-contaminants. This antifouling capability is crucial for Kenyan applications, as it extends the lifespan of the filter and lowers the operational costs for rural communities where chemical cleaning is impractical. Furthermore, the high surface-area-to-volume ratio of the nanostructures facilitates ultra-fast water flux at lower pressures, enabling the use of gravity-fed or solar-powered systems offering a sustainable way to secure potable water for both rural and informal urban settlements in Kenya, which is in line with the United Nations Sustainable Development Goal Number 6.

Keywords: Nanostructured Membranes, Antifouling, Water Purification, Nanoparticles, Sustainable Development Goals.

Machine learning for antimycobacterial drug discovery from African medicinal plants: molecular size confounding inverts the activity ranking of *Zanthoxylum lepreurii* constituents

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Abstract

In 2015, Africa adopted **Agenda 2063**, while the global community embraced the **Sustainable Development Goals (SDGs-2030)** as key development frameworks. More recently, the **Science, Technology and Innovation Strategy for Africa (STISA-2034)** emphasized the role of science and technology in sustainable development. Collectively, these agenda items prioritize universal access to affordable, safe, and sustainable water and sanitation. However, current trends indicate that many of these targets might be missed. Despite progress under **SDG 6**, only approximately 75% water access and 60% sanitation coverage have been realized across the continent, leaving over 400 million out. Achieving these targets requires a critical evaluation of Africa's strengths, constraints, opportunities, and systemic challenges. While the continent faces limitations in scientific infrastructure and capital investment, it possesses significant natural resources and human capacity that can be leveraged for sustainable water management solutions. Notable treatment approaches aligned with locally available resources include: a) **Biomass-based materials**, b) **Earth-based materials**, c) **Synthesized or improvised materials** and increasingly, d) **Digital and computational approaches**.

Computational modelling provides a framework for understanding adsorption mechanisms and predicting material–pollutant interactions, enabling the identification and optimization of effective adsorbents devoid of extensive experimental trials. Complementarily, machine learning and AI techniques facilitate the prediction of key factors governing pollutant removal including, adsorption capacity, selectivity, kinetics, and material performance, hence accelerating the design and screening of treatment systems. As pollutants become increasingly diverse and chemically complex, the integration of resource-based treatment strategies with digital technologies offers promising pathways toward scalable, efficient, and context-appropriate solutions. This work examines the performance of various treatment methods across pollutant classes and discusses strategic directions for enhancing sustainable water treatment innovations in Africa.

Keywords: Water treatment, SDG 6, Agenda 2063, STISA-2034, Biomass, Earth-based materials, Computational modelling, Machine learning

Thiophene and Furan motif compounds designed for Cancer Studies

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Four (4) imino-pyridyl ligands namely; L^1 = (Z)-N-((5-nitrothiophene-2-yl)methylene)-2-(pyridine-2-yl)ethanamine, L^2 = (Z)-N-((5-nitrofuran-2-yl)methylene)-2-(pyridine-2-yl)ethanamine, L^3 = (E)-N-((5'-bromo-[2,2'-bithiophen]-5-yl)methylene)-2-(pyridine-2-yl)ethanamine and L^4 = (N,N'E, N, N'E)-N,N'-(thiophene-2,5-diylbis(methanylydene))bis(2-pyridin-2-yl)ethanamine endowed with a pendant thiophene and furan moieties were synthesized and characterized using standard spectroscopic techniques (¹H and ¹³C NMR). The ligands L^1 and L^2 were unequivocally characterized by single X-ray crystallography.

This drug design interest arose from studying the electronic effects, by varying the fifth position of the thiophene and furan moieties and also the steric hindrance effect by the mono-and-bi-pyridine groups towards the cancer cell lines.

Key Development Milestones in Relation to Water Treatment Methods in Africa

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Abstract

The global increase of multidrug-resistant tuberculosis (MDR-TB) necessitates the rapid identification of novel chemical scaffolds. This study integrates Density Functional Theory (DFT), molecular docking, and Artificial Intelligence (AI) to evaluate the antimycobacterial potential of 18 metabolites isolated from the root and stem bark of *Zanthoxylum leprieurii*, a plant traditionally used in East Africa for respiratory infections. Electronic characterization was performed at the B3LYP/6-31++G** level of theory to calculate reactivity descriptors. Results identified (±)-Savinin as the most reactive candidate, exhibiting the smallest energy gap (3.7862 eV in PCM) and the highest electrophilicity (0.1548 eV), which correlates with its significant experimental potency (MIC 0.98 µg/mL) against the susceptible H37Rv strain. Furthermore, molecular docking revealed that Sesamin (-9.4 kcal/mol) and Hesperidin (-9.1 kcal/mol) possess superior binding affinities to mycobacterial targets compared to the first-line drug Rifampicin (-7.2 kcal/mol). The study highlights the secondary amide linker found in trans-fagaramide (MIC 6 µg/mL) and other active isolates as a critical pharmacophore shared with primary TB drugs like isoniazid and pyrazinamide. To facilitate high-throughput discovery, these quantum mechanical descriptors were further utilized as input features for an AI-driven predictive model. By establishing a quantitative relationship between electronic reactivity fingerprints and mycobacterial cell-wall permeability, this work provides a robust computational pipeline for the virtual screening and design of next-generation antitubercular agents, bypassing traditional trial-and-error isolation methods.

Sub-themes: Health, Computational Chemistry & AI in Chemistry

Thiophene and Furan motif compounds designed for Cancer Studies

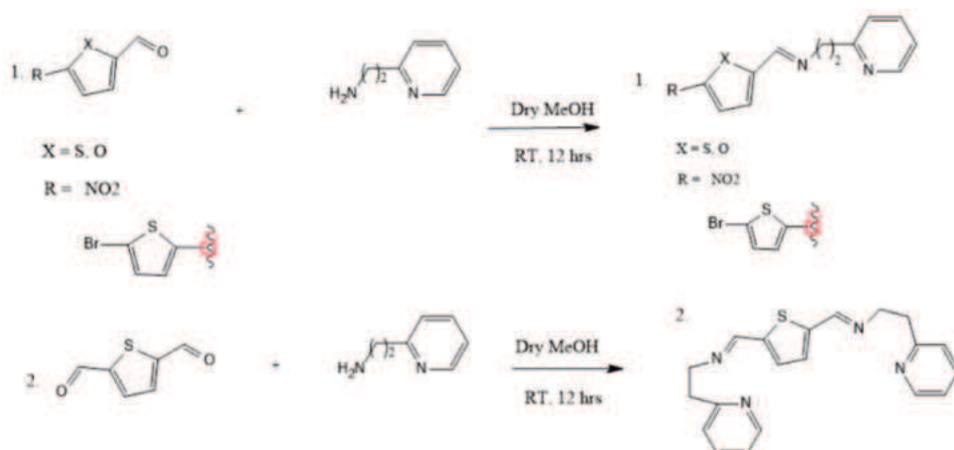
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Four (4) imino-pyridyl ligands namely; **L**¹ = (Z)-N-((5-nitrothiophene-2-yl)methylene)-2-(pyridine-2-yl)ethanamine, **L**² = (Z)-N-((5-nitrofuran-2-yl)methylene)-2-(pyridine-2-yl)ethanamine, **L**³ = (E)-N-((5'-bromo-[2,2'-bithiophen]-5-yl)methylene)-2-(pyridine-2-yl)ethanamine and **L**⁴ = (N,N'E, N, N'E)-N,N'-(thiophene-2,5-diylbis(methanylydene))bis(2-pyridin-2-yl)ethanamine endowed with a pendant thiophene and furan moieties were synthesized and characterized using standard spectroscopic techniques (1H and 13C NMR). The ligands **L**¹ and **L**² were unequivocally characterized by single X-ray crystallography.

This drug design interest arose from studying the electronic effects, by varying the fifth position of the thiophene and furan moieties and also the steric hindrance effect by the mono-and-bi-pyridine groups towards the cancer cell lines.



Design and optimization of laser-induced graphene electrodes for heavy metals ions sensing in water

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Abstract

The use of lasers to carbonize commercial polymers, particularly polyimide, is an emerging strategy for producing functional graphene-like nanocarbons. This approach offers an attractive alternative to conventional screen-printing technologies, with clear advantages in terms of cost, efficiency, and environmental impact. By tuning laser parameters, the morphology of laser-induced graphene electrode (LIGE) can be tailored to yield fibrous architectures, isotropic or anisotropic porous networks, or cellular lattice structures. A broad range of applications has been reported for these electrodes, including sensors for toxic compounds such as nitrite and heavy metal ions and bioactive molecules. In this context, we have developed an unmodified LIGE, following rigorous optimization of laser parameters such as power and spot scanning speed, for the detection of heavy metal ions in rock samples solubilized in acidic media. The laser power and scanning speed were set to 6.4 W and 30 cm·s⁻¹, respectively. The electrode was characterized by electrochemical, optical and Raman spectroscopic techniques which confirmed its 3D porous structure. The LIGE electrode was then employed for the electrochemical detection of Cd²⁺ and Pb²⁺ in 0.1 M acetate buffer at pH 4, using square-wave anodic stripping voltammetry. The sensor exhibited sensitivities of 0.45 and 0.93 μA·ppb⁻¹·cm⁻² for Pb²⁺ and Cd²⁺ with linear detection ranges of 25–1000 ppb (Cd²⁺) and 10–500 ppb (Pb²⁺). The limits of detection were 6.13 ppb for Cd²⁺ and 2.96 ppb for Pb²⁺. The sensor enabled the simultaneous determination of heavy metal ions in tap water and solubilized rock water samples, demonstrating the suitability of optimized LIGEs for monitoring heavy metal ions in complex environmental matrices.

Keywords: Laser-induced graphene, design, sensing, heavy metals, electroanalysis.

Metal Halide Perovskites and their Applications in Solar Cells

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Abstract

The energy sector is a crucial theme and topic in research with current trends involving the reduction of the carbon footprint through renewable energy systems. This has been done through either energy storage or energy conversion mechanisms. Recent studies in energy storage mechanisms have involved studies to substitute lithium in the current state-of-the-art battery with other less toxic cations such as sodium while the energy conversion systems have studied thin film flexible photovoltaics to complement the highly commercialized silicon solar cells (SSCs). This work focuses on metal halide perovskites (MHPs). The appeal of these MHPs is their high efficiencies, tunable bandgaps, high absorption coefficients and their recyclability. This work focuses on making wide band gap perovskite solar cells using green solvent systems such as ethylene carbonate (EC), propylene carbonate (PC) and γ-Valerolactone (GVL); with the aim of replacing the most common hazardous solvent N-N dimethylformamide (DMF). The synthesis of this MHPs involved spin coating, dip coating and inverse temperature crystallization methods (ITCs). The purpose of spin and dip coating was to fabricate thin films while ITCs method was used for single crystal growth (SCs). Here the focus was on FAPbBr₃ and CsPbBr₃ to form stable planar carbon contact devices; carbon was used in the fabrication of thin films due to its corrosion resistance and hygroscopic properties. The talk will examine the benefits of green solvents and show how they can be used to prepare wide bandgap perovskite solar cells with applications for photocatalysis.

Keywords: Anion and cation substitution, power conversion efficiency, perovskites, thin films, single crystals

Carbon-Based Nanocomposites for Fourth-Generation Solar Cells

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Abstract

The increase in global energy demand has led to the extent that conventional energy sources, particularly fossil fuels, are facing a predicament due to their non-renewability. Additionally, they emit greenhouse gases that contribute to undesirable global warming and climate change. Thus, renewable and sustainable energy sources, particularly abundant, clean, and cost-effective solar energy, are sought after. Currently, the first-generation (crystalline silicon) solar cells, which have relatively high-power conversion efficiencies (PCEs), are the most commonly used. However, they are rigid, expensive, and require complex, high-energy fabrication procedures. Subsequently, second-generation (thin-film) solar cells, which are inexpensive and easy to fabricate, emerged; however, they exhibit lower PCEs than their first-generation counterparts.

Thus, the development of third- and fourth-generation solar cells, such as perovskite solar cells, dye-sensitised solar cells, and organic solar cells, has attracted significant research interest owing primarily to their facile fabrication procedures, low cost, lightweight, flexibility, ease of scalability, low environmental impact, and ever-increasing PCE. However, their commercialisation has been set back by their relative instability and relatively lower PCEs. To circumvent these challenges, the recent emergence of novel materials, particularly carbon-based nanomaterials (CNMs), is envisioned to help bridge the gap between fourth-generation and silicon solar cells. CNMs, due to their outstanding optoelectronic properties, excellent stability, non-toxicity, and low cost, have attracted significant research effort. Their incorporation into fourth-generation solar cell components is envisaged to significantly increase the PCE, sustainability, environmental friendliness, and cost-effectiveness of devices.

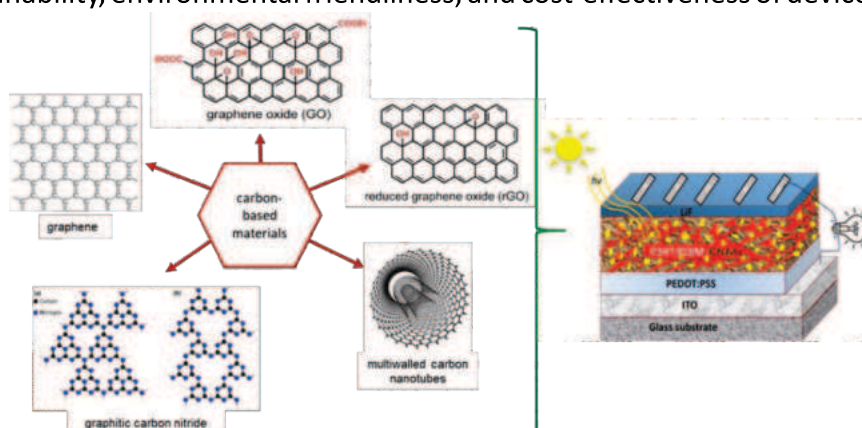


Figure : Carbon-based nanomaterials (CNMs) in fourth-generation solar cell fabrication

Keywords: carbon-based nanomaterials, perovskite solar cells, dye-sensitised solar cells, and organic solar cells.

Reinventing Sample Preparation for a Sustainable Analytical Future

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Abstract

Sample preparation remains a pivotal yet challenging phase in the analytical workflow, traditionally accounting for up to 60% of total analysis time and 30% of chromatographic errors. While the principles of green chemistry advocate for the elimination of solvent-intensive steps, a functional paradox arises as rigorous treatment remains indispensable for achieving high analytical precision. To resolve this, modern research is pivoting toward the integration of sustainable, high-performance materials. This presentation examines the strategic shift toward sustainability through the miniaturization of procedures and the development of advanced functional sorbents, such as biopolymer-based adsorbents and magnetic nanocomposites. By exploring innovative extraction strategies and bio-inspired materials, this session demonstrates how the synergy between material science and green chemistry can optimize analytical performance while adhering to the principles of the circular economy and environmental stewardship.

Design and optimization of laser-induced graphene electrodes for heavy metals ions sensing in water

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Abstract

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Keywords: Laser-induced graphene, design, sensing, heavy metals, electroanalysis.

Metal Halide Perovskites and their Applications in Solar Cells

Mercy N. Nduni*, Petra J. Cameron.

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Abstract

The energy sector is a crucial theme and topic in research with current trends involving the reduction of the carbon footprint through renewable energy systems. This has been done through either energy storage or energy conversion mechanisms. Recent studies in energy storage mechanisms have involved studies to substitute lithium in the current state-of-the-art battery with other less toxic cations such as sodium while the energy conversion systems have studied thin film flexible photovoltaics to complement the highly commercialized silicon solar cells (SSCs). This work focuses on metal halide perovskites (MHPs). The appeal of these MHPs is their high efficiencies, tunable bandgaps, high absorption coefficients and their recyclability. This work focuses on making wide band gap perovskite solar cells using green solvent systems such as ethylene carbonate (EC), propylene carbonate (PC) and γ-Valerolactone (GVL); with the aim of replacing the most common hazardous solvent N,N-dimethylformamide (DMF). The synthesis of this MHPs involved spin coating, dip coating and inverse temperature crystallization methods (ITCs). The purpose of spin and dip coating was to fabricate thin films while ITCs method was used for single crystal growth (SCs). Here the focus was on FAPbBr₃ and CsPbBr₃ to form stable planar carbon contact devices; carbon was used in the fabrication of thin films due to its corrosion resistance and hygroscopic properties. The talk will examine the benefits of green solvents and show how they can be used to prepare wide bandgap perovskite solar cells with applications for photocatalysis.

Keywords: Anion and cation substitution, power conversion efficiency, perovskites, thin films, single crystals

Harnessing Sustainable Chemical Systems: Integrating Green Catalysis and Bio-Based Feedstocks for a Circular Future

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Abstract

Chemistry is at a turning point. Today, we face urgent calls to reduce our impact on the environment, move away from fossil fuels, and support global sustainability efforts. Meeting these challenges means rethinking the way we do things moving from old, linear approaches to new, circular systems. In this keynote, I'll discuss how we can use chemistry's strengths to build a more sustainable future, especially by combining green catalysis with new uses for plant-based materials. From climate change and running out of resources to plastic waste and new types of pollution, our world faces tough environmental problems that need creative solutions—fast. Chemistry sits at the center of both the problems and the answers. By practicing sustainable chemistry, we don't just aim to do less harm; we can actually design processes that help heal and sustain our planet. Guided by the principles of green chemistry, modern approaches emphasize efficiency, safety, and circularity. Innovations such as bio-based materials, biodegradable polymers, and advanced catalytic processes are redefining how we produce and use chemicals, significantly reducing waste, energy consumption, and environmental impact. At the same time, advances in analytical science are improving our ability to detect and address pollutants such as microplastics, strengthening our capacity for environmental stewardship. Yet, the true power of chemistry extends beyond technological breakthroughs. It lies in our ability to rethink systems, transitioning from linear models of production and consumption to circular, sustainable frameworks. While challenges remain in scaling these innovations, aligning economic incentives, and ensuring equitable global adoption, they also present opportunities for collaboration across disciplines, sectors, and borders. By optimizing active-site accessibility and reaction kinetics, these innovative catalytic systems dramatically minimize activation energy barriers, reduce processing temperatures, and eliminate hazardous stoichiometric waste streams at the source. Second, the discussion addresses the atom economy of biomass valorization, evaluating the chemical pathways required to selectively functionalize and transform lignocellulosic agricultural and forestry residues into high-value platform molecules and functional materials. This keynote explores how chemistry can be harnessed not just as a scientific discipline, but as a driving force for sustainable development. It calls for bold thinking, stronger partnerships, and a shared commitment to innovation that prioritizes both people and the planet. Ultimately, the future of sustainability will depend on how effectively we leverage the power of chemistry today to create resilient, inclusive, and environmentally sound solutions for generations to come.

Keywords: Sustainable Chemistry, Green Catalysis, Biomass Valorization, Circular Economy, Life-Cycle Assessment (LCA)

Struvite Precipitation from Wastewater and Hot Spring Water for Fertilizer Use

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Abstract

Struvite, featuring the chemical formula $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$, has attracted growing interest from researchers due to its possible role as a beneficial nutrient for plants within the agriculture industry. The expense of manufacturing this mineral primarily relies on the price of the magnesium source used. This study examined hot spring water as a possibly more cost-effective natural source of magnesium ions, while sewage wastewater served as a provider of phosphate and ammonium ions for struvite synthesis. The synthesized struvite composite was characterized using X-ray fluorescence (XRF), X-ray diffraction (XRD), and scanning electron microscopy (SEM). The precipitate's purity and the recovery of phosphorus were evaluated. XRF results showed that the produced struvite mainly consisted of magnesium oxide and phosphorus oxide. XRD analysis indicated the presence of orthorhombic crystalline phases between 4-9 degrees (2θ), with struvite peaks observed at 2θ values of 15.8, 20.9, and 46.3, aligning with data from the struvite ICDD card. SEM revealed uneven, crystal-like, and rod-shaped morphological forms that align with those recorded in the literature. The produced composite showed a purity level of 68.61% and a phosphorus recovery rate of 76.15%. The addition of phosphorus and nitrogen in the composite, vital macronutrients for plants, makes it a possible inorganic fertilizer for agricultural purposes.

Keywords: Fertilizer, Hot Spring water, Precipitation, Struvite, Wastewater

Abstract

Traditional medicine is a cultural practice with a long history in South Africa, the African continent and the rest of the world. However, there is still a fair amount of scepticism about its use, mostly due to lack of scientific information to support this practice. Presently nearly every “upmarket” mall in RSA's has several, successful herbal shops which are thriving over the idea that “natural is better than synthetic”. Approximately 3000 plants, out of a national biodiversity represented by about 30 000 higher plant species, are used as traditional medicine. Some of these medicinal plants have been investigated in our lab for their phytochemical composition, and this paper seeks to describe some of the contributions based on plant species that have been explored in our laboratories over the years. Selected plant species, which included *Sutherlandia* (*Lessertia*) *frutescens*^{1,2}, *Ecklonia maxima*³, *Protea cynaroides*⁴ some *Searsia*⁵ and *Helichrysum* species⁶ species⁵ among others, were subjected to extraction with organic solvents and water followed by chromatographic fractionation and spectroscopic identification of the isolated compounds. Such isolates included compounds of the flavonoid and terpenoid type as well as their glycosides from organic extracts, while water extracts were rich in pectic polysaccharides for the terrestrial plant species. Assessment of crude extracts and purified compounds for antimicrobial and enzyme inhibition properties revealed some positive results, thus providing some justification for the use of these plants for medicinal purposes.

In-Silico study of New Sulfonyl Urea Analogues as Potential Anti-Diabetic Agents: ADMET, Molecular Docking and Dynamics, MMGBSA and DFT Approach

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Abstract

Type 2 Diabetes Mellitus (T2DM), also known as non-insulin dependent diabetes mellitus, is a high blood glucose metabolic disorder that occurs when the body either rejects or does not respond to the insulin produced by the pancreas. [1] To date, insulin resistance has been identified as a reason why this type of diabetes exists. [2] The current antidiabetic drugs have been associated with fluid retention and increased risk of heart failure, which remains a big challenge when using this medicine to treat type 2 diabetes. Hence, this paves the way for the development of new, affordable anti-diabetic drugs with fewer side effects. In this study, we have designed a new series of glitazone derivatives 1 and 2 (Figure 1) as potential new antidiabetic agents. The in silico approach was carried out to assess drug-likeness properties, antidiabetic activity, binding affinity and interaction and stability of the new Sulfonyl urea analogues 1 and 2 as potential Anti-diabetic agents using ADMET, molecular docking, dynamics, mmgbsa and DFT studies. The results showed that Sulfonylurea 2 have emerged as the most potent inhibitor against SGLT2 with favourable physicochemical, pharmacokinetic properties and more stability confirmed when compared with compound 1. This suggests that compound 2 has drug-likeness characteristics similar to those of SGLT2 and needs further investigation as a next class of new potential anti-diabetic agent.

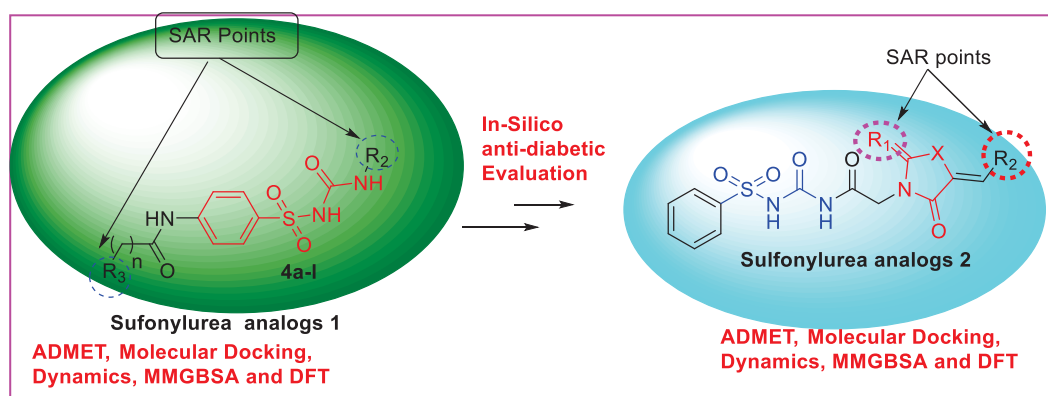


Figure : Design and Synthesis of Sulfonyl Urea Analogues Derivatives 1 and 2

Policy, Legal, and Institutional Frameworks for Safe and Sustainable Chemicals Management in Kenya: Lessons from a Multi-Sectoral Governance Approach

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Abstract

The safe and sustainable management of chemicals is critical to protecting human health, the environment, and achieving sustainable development. Kenya has established comprehensive policy, legal, and institutional frameworks supported by a multi-sectoral governance model that brings together government agencies, industry, academia, civil society, and development partners. This coordination mechanism has helped address overlapping institutional mandates and strengthen implementation of Kenya's commitments under the Global Framework on Chemicals and the Basel, Rotterdam, Stockholm, and Minamata Conventions.

Despite these advances, weak enforcement of environmental legislation, limited capacity for legal interpretation and prosecution of environmental offences, inadequate coordination between national and county governments, and insufficient integration of research into policymaking continue to constrain effective chemicals management. Although the private sector has demonstrated relatively high levels of regulatory compliance, capacity gaps remain across policy, regulatory, judicial, professional, and community levels. These challenges often allow polluters to evade accountability, transferring the environmental and economic costs of pollution to society.

The lessons from Kenya's multi-sectoral governance model are here examined, highlighting the importance of sustained stakeholder engagement, clearly defined roles for National Focal Points and Designated National Authorities, stronger science-policy linkages, and enhanced collaboration between national and county governments. It also emphasizes the need for industry self-regulation, sustainable financing, and continued harmonization of national frameworks with international chemicals governance commitments. In conclusion, an effective multi-sectoral governance, supported by robust enforcement, institutional capacity, and coordinated stakeholder action, is essential for advancing chemical safety and the safe and sustainable management of chemicals in Kenya.

Keywords: Chemical Safety Management; Multi-Sectoral Coordination; Environmental Enforcement; Science-Policy Interface; Policy and Legal Frameworks.

Evaluation of Chemical Composition of Waters and Succulents from Mt. Suswa in Potential Valorization of Cryo-Mesophilic Biogas Systems

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In the volcanic landscape of Mt. Suswa, Kenya, heavy reliance on traditional fuels drives deforestation. This study evaluates the chemical profile of geothermal waters and local succulents to determine their efficacy in optimizing Anaerobic Digestion (AD) biogas systems. Analysis of steam vent waters revealed extreme nitrate levels (8.935 mg/mL) and phosphate levels (0.518 mg/mL), drastically exceeding WHO safety standards. Interestingly, local succulents like the Round Cactus and Sisal were found to bio-accumulate these nutrients, with Round Cactus reaching nitrate concentrations of 265.022 mg/mL. By utilizing these mineral-rich "potency resources" for biogas production, we can transform a significant water-quality risk into a sustainable energy solution for rural communities.

Microplastic contamination in surface waters of the River Nile in Sudan: Physical and chemical characterisation

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Abstract

The rapid increase in plastic production and inadequate waste management have led to widespread microplastic (MP) contamination in aquatic environments. Freshwater systems, particularly in Africa, remain significantly under-researched despite their critical role in sustaining human populations. The River Nile, which supports over 300 million people across eleven countries, is one of the most significant freshwater systems globally; however, no studies to date have investigated MP contamination in its surface waters, with a few studies reporting MPs in Nile. This study aimed to investigate the presence, abundance, and physicochemical characteristics of MPs in surface waters of the River Nile in Khartoum, Sudan, and to identify potential sources of contamination. Forty water samples were collected and subjected to oxidative digestion using Fenton's reagent, followed by density separation with sodium iodide. Potential MPs were isolated via vacuum filtration and analysed under a stereomicroscope to determine their size, shape, and colour. Raman spectroscopy was used to identify polymer composition, while Scanning Electron Microscopy (SEM) was employed to examine surface morphology. Microplastics were detected in all samples, with an average abundance of 1.19 ± 0.44 particles/m³. Fibres and fragments were the predominant shapes, indicating secondary sources. Smaller particles (<1 mm) were the most abundant, suggesting extensive environmental degradation of plastic debris. Coloured MPs, particularly black and brown particles, dominated the samples. Polymer analysis revealed polystyrene (PS) and polypropylene (PP) as the primary polymer types. The observed characteristics point to domestic wastewater discharge, urban runoff, and recreational activities as major sources of contamination. This study provided new evidence and the first data on MP contamination in surface waters of the River Nile and offers insights into their potential sources. It highlights the urgent need for improved waste management strategies and continuous environmental monitoring to mitigate the impacts of MPs.

Photocatalytic Degradation of Pesticides Residue: Case Study of MoO₃ Catalyzed Degradation of Lambda-Cyhalothrin

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Abstract

Although lambda-cyhalothrin (CyH) pesticide is widely applied for the control of food and crop pests, its residues can persist for long periods in plant parts and soil matrices posing environmental pollution and adverse health effects to humans such as cancers. To date, the remediation of CyH pesticide residues and its metabolites and other persistent organic pollutants is still a challenge. The application of metal oxides such as MoO₃ in catalyzing photodegradation of CyH has not been reported in literature. In this study, CyH was exposed to UV irradiation in the absence and in the presence of MnO₂ to investigate the photocatalytic effect of the metal oxide. The photodegradation kinetic profiles were monitored using time-dependent UV-Vis-NIR absorption measurements. The exposure of the CyH pesticide molecules to UV254 nm radiation caused a gradual decrease in absorption bands at 358 nm and at 377 nm for CyH over time indicating a photodegradation reaction. The kinetic experiments also showed that MoO₃ significantly enhanced the photodegradation rate constants when CyH was subjected to UV-irradiation in presence of dosage of MoO₃. In comparison to the UV-induced photodegradation rate constant of CyH, the average pseudo-first-order photodegradation rate constant (k_{av}) increased by a factor of between 2.27 – 2.56 in the presence of both UV radiation and MoO₃. Photocatalytic effect was revealed by the enhanced photodegradation when UV-illumination combined with the MoO₃ exposure, gave a much faster degradation of CyH as opposed to only UV irradiation. These results provide real kinetic models for the photodegradation of CyH that may inform future development of faster and more efficient degradation procedures for applications in the eradication of CyH pesticide residues or possibly others with a view to boosting efforts in environmental remediation of potentially hazardous persistent organic pollutants.

Turning Environmental Research into Actionable Policy in Africa—Lessons from Kenya's "Missing Link" and the Era of Autonomous Science

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Abstract

Sub-Saharan Africa features some of the most progressive environmental legal frameworks globally, yet regional ecosystem degradation continues to accelerate. This institutional paradox highlights a profound disconnect between academic knowledge production and regulatory enforcement—a structural breakdown frequently termed "the missing link." Using Kenya's dual-tier governance system under the Environmental Management and Co-ordination Act (EMCA) as a primary micro-study, this paper diagnoses the systemic bottlenecks preventing empirical environmental data from influencing legislative action, while proposing a forward-looking mitigation framework leveraging autonomous scientific intelligence to accelerate evidence-based policy execution. This paper utilizes a comparative institutional analysis to evaluate the knowledge-policy pipeline across three core dimensions. First, it critiques the political economy of higher education, specifically focusing on the "publish or perish" structural bias that rewards international journal indexing while penalizing local policy outreach. Second, it unpacks the dynamics of foreign donor funding, illustrating how epistemic dependence skews local research agendas away from urgent municipal crises toward global environmental trends. Third, it examines the capacity-mandate asymmetry introduced by the devolution of environmental enforcement to localized county assemblies that lack the technical laboratory or analytical infrastructure required to interpret scientific data. The analysis demonstrates that traditional, manual pathways of knowledge translation are too slow and fragmented to combat rapid environmental degradation or withstand commercial and bureaucratic interference. To repair this broken pipeline, this paper introduces a technological model centered around open-science architectures and autonomous Scientific AI Agents. By augmenting large language models with specialized computational chemistry tools, these agents can instantly synthesize dense, peer-reviewed toxicology and ecological data, cross-reference it with local statutory laws, and generate plain-language, legally sound environmental risk assessments. Ultimately, this study concludes that closing the missing link requires shifting from a model that relies on ad-hoc human translation to a modernized, automated pipeline of scientific data integration. To realize the environmental objectives of the African Union's Agenda 2063, this paper outlines a tripartite action plan: institutionalizing non-technical policy brief mandates within university promotion criteria, deploying shared regional laboratory infrastructure pools, and leveraging open-source scientific AI to democratize elite ecological data directly for frontline enforcement officers.

Keywords: Environmental Management Policy, Knowledge-Policy Pipeline, Devolution, Scientific AI Agents, Sub-Saharan Africa, Institutional Silos.

Developing a New Generation of Non-Heme Iron (II) Complexes as Catalysts for Alkane Oxidation with Machine Learning Techniques and DFT

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Abstract

Catalysis plays a huge role in the chemical industry as almost every chemical process utilized to produce household, industrial and consumer products require the use of a catalyst. Hence the discovery and or development of new catalysts is a very active one with various experimental strategies/techniques employed including synthesis, spectroscopic characterization, and reaction optimization. Although computational chemistry methods allow a speedy implementation of this process, the rise of Chemoinformatics as well as machine learning techniques in chemistry in recent years in addition have created a pathway to accelerate this discovery process even further. Hence in this talk, I will present how a tripartite alliance of these three methods – computational chemistry, chemoinformatics and machine learning can be explored to search for more active catalysts for important chemical processes using non-heme Fe (II) alkane oxidation catalysts as a case study.

Keywords: Alkane oxidation, Machine learning, Cheminformatics, Catalysis

High-resolution characterization of surface water contamination in Kolwezi's mining rivers (DRC): A scientific baseline for sustainable effluent treatment strategies

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Abstract

The Kolwezi region of the Democratic Republic of the Congo (DRC), located in the heart of the Central African Copperbelt, hosts large-scale copper and cobalt mining operations alongside a rapidly expanding artisanal mining sector. These activities discharge largely untreated effluents into rivers, which serve as watersources for local communities for drinking, bathing, agriculture, and fishing. However, comprehensive baseline data required to design targeted remediation strategies. This study aims to provide a high-resolution characterization of surface water contamination in Kolwezi's mining-impacted rivers. Surface water samples were collected along the Luilu, Musonoie, Dilala, and Mpingiri rivers. Samples were analyzed using Inductively Coupled Plasma Mass Spectrometry. The results reveal extreme levels of contamination. Copper concentrations reached up to 5,917 mg/L in mining discharge waters, while cobalt concentrations peaked at 3,164 mg/L. These values far exceed national discharge standards (0.6 mg/L for Cu and 1.0 mg/L for Co). Downstream sampling sites continued to exhibit elevated metal concentrations, with Cu levels of 5.7 and 2.0 mg/L and Co levels of 7.0 and 5.5 mg/L, respectively, indicating persistent contamination along the river continuum. Major elements (Na, Mg, K) aswell as additional trace metals (Mn, Fe, Zn, Pb, As) were also significantly elevated. These findings demonstrate that current effluent management practices in the region are inadequate. The exceptionally high metal loads indicate that natural attenuation processes alone are insufficient. The dataset generated by this study provides a critical baseline for: (1) the design of hybrid treatment systems suitable for high-strength mining effluents; and (2) the calibration of regional water quality models. This study delivers the first comprehensive surface water quality baseline for mining-affected rivers in the Kolwezi region. It provides a scientific foundation to support the transition toward sustainable mining water management in DRC.

Keywords: Green energy, Renewable sources of energy, Biomass, Geothermal, Batteries and Superconductors, Catalysis for Energy, Carbon Capture and Utilization

Characterization and Evaluation of Repellant Effect of Essential Oil of *Mangifera Indica* L. from Kenya

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Abstract

The plant *Mangifera indica* (mango) has long been used in traditional medicine for its therapeutic and insect-repellent properties. With increasing resistance to synthetic repellents and concerns over their safety, there is growing interest in plant-based alternatives for controlling disease vectors such as *Anopheles gambiae*, a primary transmitter of malaria in Africa. This study aimed to characterize the chemical composition of essential oil extracted from *Mangifera indica* leaves collected in Kenya and to evaluate its repellent efficacy against host-seeking female *Anopheles gambiae* mosquitoes. Essential oil was obtained through hydrodistillation of fresh mango leaves. The chemical constituents were identified and quantified using gas chromatography (GC) and gas chromatography–mass spectrometry (GC-MS). Repellent activity was assessed using a human-bait technique designed to simulate natural field conditions, with varying concentrations of the oil applied. A total of 26 compounds were identified, predominantly monoterpene hydrocarbons. The major constituents included α -pinene (33.3%), α - phellandrene (22.6%), and limonene (13.2%). The essential oil demonstrated significant dose-dependent repellency against *Anopheles gambiae*, with higher concentrations providing stronger protection against mosquito bites. The findings indicate that *Mangifera indica* leaf essential oil possesses notable mosquito repellent properties and could serve as a promising natural alternative to synthetic repellents in malaria vector control strategies.

Mechanochemical synthesis of a silylated chitosan hybrid material for sustainable water decontamination

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Abstract

The removal of contaminants from wastewater, can be effectively achieved through adsorption-based processes. Chitosan, a naturally abundant and renewable biopolymer, has attracted considerable interest for this application due to its biodegradability and intrinsic chelating ability of metallic ions. However, the limited adsorption efficiency of raw chitosan necessitates chemical functionalization to improve its performance. Conventional modification strategies largely rely on hazardous organic solvents and generate significant chemical waste. In this context, the present study adopts a green chemistry-driven approach by exploiting mechanochemistry as a solvent-free synthesis route. The objective of this study is to design and synthesize an eco-friendly silylated chitosan derivative using mechanochemistry and to evaluate its effectiveness for metal ion removal from contaminated water, with particular relevance to mining-related effluents. Chitosan was functionalized with 3-(triethoxysilyl)propyl isocyanate via a mechanochemical solid-liquid reaction. This one-step modification process avoids solvent handling, purification steps, and solvent disposal. The resulting hybrid biopolymer was characterized using FTIR, NMR, and elemental microanalysis.

The mechanochemical process successfully yielded a fine silylated chitosan powder without the use of organic solvents, demonstrating the feasibility of greener synthesis routes for advanced functional materials. Spectroscopic and analytical results confirmed the effective grafting of silane functionalities onto the hydroxyl and amine groups of chitosan. Importantly, the functionalized biopolymer can be readily integrated into silica-based matrices, enabling the fabrication of composite materials suitable for robust and scalable metal ion removal. Adsorption experiments revealed efficient uptake of copper ions from simulated wastewater, confirming that performance gains were achieved. Overall, this work validates a novel solvent-free mechanochemical methodology for producing functionalized chitosan-based hybrid materials. By combining renewable raw materials, solvent elimination, process simplification, and effective contaminant removal, this approach offers a sustainable alternative to conventional adsorbent synthesis methods.

Tailoring Electrode Performance with Mil101(Fe)-CQD-TiO₂ ternary composite For Superior Stripping of Toxic Metal ions

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Abstract

Heavy metal pollution in water systems has increased significantly due to large-scale industrialisation worldwide. This study highlights the monitoring and trace detection of heavy metals (Cd²⁺, As⁵⁺, Cu²⁺, As³⁺ and Pb²⁺) in river samples. The ternary composite was synthesized hydrothermally, and the morphological and structural characterisation was examined using physicochemical characterisation techniques to confirm the integration of the ternary composite. The synergy between the Mil101(Fe)-CQD-TiO₂ (metallic organic framework (101)-iron- carbon quantum dot- titanium dioxide) system has rarely been documented in the literature. In this work, it has been shown to enhance the reaction kinetics and electron mobility of the newly developed aptasensor. The improved electron transport, large electroactive surface area, and high conductivity of this ternary composite have significantly increased the electrode's adsorption affinity for heavy metal ions. The new aptasensor platform was examined in both phosphate buffer solutions and water samples using anodic stripping voltammetry (ASV), achieving lower detection limits (LOD) of $1.0 \times 10^{-4} \mu\text{M}$ for Cd²⁺, $1.3 \times 10^{-4} \mu\text{M}$ for As⁵⁺, $3.0 \times 10^{-4} \mu\text{M}$ for Pb²⁺, and $1.0 \times 10^{-4} \mu\text{M}$ for Cu²⁺, and $1.0 \times 10^{-3} \mu\text{M}$ for As³⁺. The aptasensor demonstrated excellent anti-interference capability, high reliability, and impressive performance in water analysis, with recoveries ranging from 88 % to 112 %.

Keywords: Water pollution, heavy metals, LOD, anodic stripping, electrochemical sensors

Toxicity Assessment of *Euphorbia candelabrum* Extracts Against Fall Army Worm (*Spodoptera frugiperda*)

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Abstract

Fall Army Worm (FAW) is believed to have originated in central America and it is an invasive pest affecting production of maize in Sub-Saharan African. The economic losses of FAW on average is 9.4 billion dollars per year. Several methods have been used to control FAW but have challenges like pest developing resistance, environmental pollution and costly. Therefore, a sustainable control strategy of FAW is needed. *Euphorbia candelabrum*, a succulent plant traditionally used in Kilifi County for pest control, presents a promising, eco-friendly alternative. However, scientific information of crude *Euphorbia candelabrum* is unknown. This study sought to test and evaluate the toxicity of sequential extract of *E. candelabrum* latex against FAW in the laboratory to determine the most toxic extract. *Euphorbia candelabrum* branches were randomly collected in Magarini constituency, Kilifi County. Sequential extraction of latex was carried using Hexane, Dichloromethane, Ethyl acetate, Methanol and Water solvent with increasing polarity and 5,15,40,80 and 160mg/mL concentration of each extract was used against FAW compared with chlorpyrifos, as positive test and extracting solvent as negative test. The data obtained was analyzed using One Way ANOVA followed by Student-Newman-Keuls (SNK) test that identified Hexane extract as the most potent solvent extract. Probit analysis with the help of SAS Software was used to determine the LC50 and LC90. The analysis obtained an LC50 of 50.15mg/mL (95% CI 47.10-53.57) and LC90 of 70.01mg/mL (95% CI 64.27-78.74). By validating the effectiveness of this indigenous botanical resource, the study has developed a cost-effective, sustainable pest management strategy, reduce dependence on harmful chemicals, and enhance food security for farmers.

Manganese (II)-Anderson Polyoxometalate Mediated Bioethanol Production from Sugarcane Cake

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Abstract

Biomass remains a critical renewable energy resource globally and is central to sustainable fuel development, particularly in rapidly developing economies such as Kenya, where energy demand continues to rise. Overreliance on fossil fuels has intensified environmental concerns, underscoring the need for efficient biomass utilization within the sugarcane value chain. Sugarcane cake and bagasse, abundant agro-industrial residues, present significant potential for bioethanol and biogas production. However, the recalcitrant lignin matrix that binds cellulose and hemicellulose limits fermentable sugar availability, necessitating robust pretreatment strategies. This study investigates polyoxometalate (POM) salts as alternative, environmentally friendly delignifying agents to conventional sodium hydroxide (NaOH). Unlike NaOH, which requires costly acid neutralization prior to fermentation, POMs—discrete anionic metal oxides (e.g., Keggin, Wells–Dawson, Anderson, and Waugh types)—offer redox-active catalytic properties capable of efficiently oxidizing lignin. Mn (II)-Anderson POM was evaluated alongside NaOH by varying concentration (1–3%), temperature (30–60 °C), and time (2–4 h). Statistical analysis (ANOVA) confirmed significant effects of all parameters on lignin removal and subsequent bioethanol yield.

Results demonstrated that POM pretreatment achieved superior delignification and fermentation performance, with maximum bioethanol quality reaching 46.13% at 3% concentration, 60 °C, and 4 h, compared to 41.3% under equivalent NaOH conditions. Enhanced biomass structural disruption was confirmed via scanning electron microscopy. Biofuel efficiency was assessed through yield quantification and calorific value evaluation. The findings establish polyoxometalate salts as promising green catalysts for improving bioethanol production efficiency and advancing sustainable biofuel development within the sugarcane industry.

Keywords: Bagasse, Cellulose, Hemicellulose, Lignin, Polyoxometalates, Sugarcane Cake

Phytoremediation of Heavy Metals in Aquatic Systems: Harnessing Polar Crude Phytochemicals for Targeted Extraction of Metal Ions

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Abstract

Heavy metal pollution in aquatic environments is a global concern due to its detrimental impacts on both human health such as neurological, liver and kidney damages among other health issues as well as ecosystem damage. The contamination of heavy metals such as iron(III), lead(II), and copper(II) in water bodies is largely attributed to industrialization, urbanization, and agricultural activities, which release untreated or inadequately treated wastewater into aquatic systems. Conventional methods for remediating heavy metals pollution are complex, limiting their practical application. Therefore, there is a growing need for innovative, eco-friendly, and cost-effective solutions to mitigate these pollutions. Phytochemicals offer a promising alternative due to their natural origin and potential for selective metal ion removal. This study extracted polar phytochemicals from South African plants using hot water, followed by precipitation under vacuum. The phytochemicals were dissolved in water-saturated butanol, creating a biphasic system in a vial containing water with a dissolved mixture of ten heavy metals. The biphasic system was shaken on a desktop mechanical shaker for 24 hours. Water samples were collected from the aqueous layer and analysed using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) to assess the removal efficiency of the phytochemicals for metal ions. These phytochemicals demonstrated significant potential in removing heavy metals from aqueous solutions. Specifically, they efficiently extracted iron(III) ions, achieving a removal rate exceeding 80%, while lead(II) and copper(II) ions are removed at rates of over 40% and 20%, respectively. The iron(III) ions are predominantly removed at lower pH levels, followed by lead(II) ions at slightly higher pH values, and copper(II) ions at even higher pH levels. This pH-dependent behaviour highlights the effectiveness of the phytochemicals in selectively removing different metal ions based on the solution's acidity or alkalinity. Iron(III) extraction remains consistent regardless of the concentration of phytochemicals used. However, for lead(II) and copper(II), there is a noticeable increase in extraction efficiency with higher concentrations of the phytochemicals. These phytochemicals demonstrated significant potential in removing heavy metals from aqueous solutions, which positions them as a sustainable and efficient solution for heavy metal decontamination in water treatment applications.

Keywords: Copper(II); flavonoids; green chelators; iron(III); lead(II); phenolics

Mineral composition, phytochemical profile of leaves, bark and roots of *Detarium microcarpum* Guill. & Perr., Fabaceae, harvested in Mali

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Abstract

In a context of valorizing medicinal plants and searching for natural sources of micronutrients and bioactive compounds, the study of mineral composition and phytochemical profile is essential for better assessing their nutritional and therapeutic value. This study aims to determine the mineral element composition and phytochemical profile of *Detarium microcarpum*, a species widely used in West Africa. Leaves, bark and roots were collected from two localities in Mali (Sikasso and Sanankoroba). Mineral elements were determined using Flame Atomic Absorption Spectrophotometry according to standard AOAC methods, while phytochemical screening was carried out using standard qualitative tests. The results show variations depending on plant organs and locations. Calcium content is higher in Sanankoroba (300.6 mg.kg⁻¹ in leaves) than in Sikasso (253.9 mg.kg⁻¹). Potassium reaches 254.2 mg.kg⁻¹ in bark from Sikasso compared to 80.5 mg.kg⁻¹ in Sanankoroba. Iron is highest in roots from Sikasso (23.3 mg.kg⁻¹). Zinc levels range from <LOD to 4.1 mg.kg⁻¹, copper from 0.4 to 1.2 mg.kg⁻¹, chromium from 1.9 to 3.8 mg.kg⁻¹ and nickel from 2.5 to 20.8 mg.kg⁻¹ depending on plant organs and sites. Leaves generally show the highest levels of macroelements. Heavy metals (Pb, Cd) were not detected. Phytochemical revealed the presence of flavonoids, tannins, alkaloids and saponins, among others. The results confirm the nutritional and therapeutic potential of *D. microcarpum*. Further studies on bioavailability and biological activities are needed.

Keywords: Phytochemistry, Minerals elements, SAA, *Detarium microcarpum*

Analysis of the anti- Amyotrophic Lateral Sclerosis Potential of Carica Papaya Phytochemicals by Network Pharmacology

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Abstract

Amyotrophic Lateral Sclerosis (ALS) is a progressive neurodegenerative disorder characterized by misfolding and aggregation of TAR DNA-binding protein 43 (TDP-43) and dysregulation of pro-survival signaling pathways (PI3K/AKT axis). Discovering novel drugs and treatments for ALS is urgently needed. Drugs from natural products have been preferred lately due to their high potential and low toxicity. Carica papaya is a tropical plant with various pharmacological potentials. In this study, the potential of bioactive compounds from Carica papaya as anti-ALS agents was explored using network pharmacology. The compounds were retrieved from PubChem and subsequently, the targets of each corresponding compound were determined with Swiss Target Prediction, while the proteins associated with ALS were identified using GENECard. Furthermore, a protein–protein interaction network and a compound–target interaction network was constructed to identify the most crucial proteins and compounds in the network by employing Cytoscape v3.10.4. The study continued with pathway enrichment analysis using STRING V12, molecular docking with PyRx and Maestro, and molecular dynamics simulation with Gromacs for further confirmation. Docking showed highest binding affinities of beta-carotene 5,6-epoxide (–8.3 kcal/mol) toward TDP-43 and Gibberellin A1 (–9.8 kcal/mol) toward AKT1. C. papaya compounds against TDP-43 and AKT1. MD of TDP-43 with Beta-Carotene 5,6-epoxide and AKT1 with Gibberellin A1 over 100 ns confirmed strong interaction stability with TDP-43 and AKT1, indicating a consistent compact radius of gyration, low RMSD, and minimal RMSF at active site residues. The network pharmacology showed that Phytochemicals regulates several important pathways related to ALS, such as cholinergic synaptic transmission and PI3K2-AKT signaling, and identified their association with key ALS-related pathways, including neuroinflammation, apoptosis, and mitochondrial regulation. Gene Ontology showed the compounds targeted proteins involved in biological processes such as smooth muscle contraction, PI3K2-AKT, reproduction, and nitric oxide synthase activity. These findings suggest that C. papaya phytochemicals are multi-target neuroprotective candidates that have potential in treatment of ALS disease, but these treatments need to be tested experimentally to verify their therapeutic activity.

Keywords: Carica papaya, Amyotrophic Lateral Sclerosis, Molecular Docking, TDP-43, Network Pharmacology, Functional Enrichment.

Evaluation of Microplastic Retention in Nanostructured Polyamic Acid Membrane Cartridges.

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Abstract

Water contamination by microplastics poses significant risks to ecosystems and human health, as smaller particles often escape conventional treatment systems and persist in the environment. This study focuses on developing nanostructured polyamic acid membrane cartridges enhanced with nanoparticles to improve microplastic removal efficiency. The approach offers a scalable, energy-efficient, and sustainable water purification solution, particularly suited for resource-limited settings, while supporting efforts toward cleaner water and healthier ecosystems. To synthesize and optimize nanostructured polyamic acid (PAA) membrane cartridges for microplastic removal. To evaluate microplastic removal efficiency using a cross-flow filtration system across different water sources. To assess the scalability and fabrication feasibility of PAA membranes for practical applications. To investigate the effects of pH and initial concentration on removal efficiency. Nanostructured polyamic acid (PAA) will be synthesized from 4,4'-oxydianiline (ODA) and pyromellitic dianhydride (PMDA), with gold and silver nanoparticles incorporated and confirmed by UV–Vis spectroscopy. Membranes will be fabricated using wet phase inversion. Characterization will include SEM (morphology), FTIR (functional groups), UV–Vis (nanoparticles), contact angle (hydrophilicity), zeta potential (surface charge), and BET analysis (surface area and porosity). Membrane performance will be optimized by controlling phase inversion, incorporating nanoparticles and silanes, and varying thickness, with reusability assessed through repeated filtration cycles. Membranes will be assembled into cartridges and integrated into a portable cross-flow filtration unit. Performance will be evaluated using laboratory and field water samples, while assessing the effects of pH, initial concentration, durability, and cost-effectiveness.

Nanostructured PAA cartridges will efficiently remove microplastics, optimize operating conditions, resist fouling over multiple cycles, and provide scalable, data-driven solutions for sustainable water treatment. This study develops scalable nanostructured PAA membranes for efficient microplastic removal, advancing sustainable water treatment, improving water quality, and supporting global clean water access initiatives.

Ruthenium II Complexes of Thiosemicarbazones: Synthesis, Characterization, Antimicrobial Activity and Molecular Docking Studies

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Abstract

A growing global health crisis, driven by drug resistance and the limitations of current therapies, necessitates the search for novel therapeutic agents. Ruthenium (II) complexes have emerged as promising alternatives to platinum-based anticancer drugs due to their lower toxicity, redox activity and ability to interact with biological targets. Thiosemicarbazone Schiff bases exhibit significant pharmacological properties, including antimicrobial and anticancer activities. This proposal outlines a strategy to synthesize, characterize and biologically evaluate ruthenium- thiosemicarbazone complexes. The project will involve synthesizing two ruthenium complexes with thiosemicarbazone ligands which involves condensation of thiosemicarbazide with pyridine-2-carboxyaldehyde and anisaldehyde and conducting a comprehensive characterization which include elemental analysis, Fourier Transform Infrared Spectroscopy (FTIR), Mass Spectrometry (MS), Ultraviolet Visible Spectroscopy (UV-Vis), Proton Nuclear Magnetic Resonance (¹H NMR), X-ray diffraction (XRD), Scanning Electron Microscope (SEM), conductivity measurements, melting points and thermal analysis (TGA). The central focus will be on a rigorous biological evaluation to determine the complexes' efficacy as anticancer and antibacterial agents. Their cytotoxicity tests will be conducted against selected cancer cell lines such as human prostate cancer cell line (PC-3) and colon cancer cell line (HCT-116) using MTT assay. Their antibacterial activity will be tested against gram-negative bacteria (*Escherichia coli* and *Klebsiella pneumonia*) and gram-positive bacteria (*Staphylococcus aureus* and *Streptococcus mutants*). Additionally, molecular docking studies will be employed to predict and understand the mechanisms of action at a molecular level. This research aims to identify novel compounds with therapeutic properties that could serve as promising alternatives to conventional drugs, addressing critical challenges in cancer and infectious diseases.

Phenolics: Plastic-associated Organic Contaminants

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Abstract

Plastic pollution is an escalating threat to ocean health, with phenolic additives increasingly recognized as emerging contaminants of concern. This study investigated the presence of three phenolic compounds; 4-tert-octylphenol (4-tOP), 4-nonylphenol (4-NP), and bisphenol A (BPA) in water, sediment, and fish species from Lagos Lagoon, Nigeria, a major estuarine system that connects to the Atlantic Ocean. Samples from five locations and eleven fish species were analyzed using validated extraction procedures and GC-MS. Results showed detectable concentrations of BPA and 4-t-OP in water (0.25–0.58 mg/L and ≤0.05 mg/L, respectively) and sediment (0.08–1.90 mg/kg and ≤0.06 mg/kg), while NP was absent. Fish species exhibited significant bioaccumulation, with mean concentrations of 0.99 mg/kg (4-tOP), 2.21 mg/kg (4-NP), and 10.3 mg/kg (BPA), indicating potential for biomagnification across trophic levels. BPA, in particular, occurred at levels substantially higher than those reported in other global estuarine and coastal ecosystems. These findings identify Lagos Lagoon as a hotspot for plastic-derived contaminants, with implications for ecological integrity, fisheries sustainability, and food security in coastal communities. Given its hydrological connection to the Gulf of Guinea, the lagoon may serve as a conduit for contaminant transfer into the wider Atlantic, raising regional and global ocean science concerns. This study provides the first comprehensive evidence of phenolic contamination in Lagos Lagoon and contributes to the broader understanding of plastic-associated pollutants in marine systems. It underscores the urgent need for coordinated monitoring, pollution mitigation, and management strategies to safeguard ocean health under the UN Ocean Decade framework.

Keywords: Plastics pollution, 4-tert-octylphenol, 4-nonylphenol, bisphenol A, water, sediment, fish and Lagos lagoon

Improvement of the oxidative stability and nutritional quality of peanut oil from Senegal by *Moringa Oleifera* L. leaves

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Abstract

Faced with the increasing effects of climate change, the development of resilient oilseed crops, such as peanuts, is a strategic priority to strengthen food and economic security in the Sudan- Sahelian regions. This presentation highlights the increase of stability and nutritional profile of peanut oil enriched with *Moringa* leaves by an ultrasonic assisted method. The study was conducted using peanut oil extracted from peanut samples harvested in the peanut basin of Senegal. The enriched extracts were subsequently irradiated with UV light for eight hours under conditions intended to induce oxidative damage. In order to track oxidative changes over time, oil samples were examined at intervals of two, four, six, and eight hours. Untreated samples were used as controls to establish a baseline for comparison. The free fatty acids, peroxide value, and Rancimat test were examined as well to measure the oxidative properties of the enriched oils. Peanut oil enriched with 0.1% and 0.2% of *Moringa Oleifera* leaves exhibited significantly improved oxidative stability ($p < 0.05$) as compared to the control. On the other hand, both the fatty acid composition and the iodine value remained relatively stable following the addition of *Moringa oleifera* leaves. By significantly improving the oxidation stability of peanut oil, these results help to extend the shelf life of the oil and preserve its aromas, thus strengthening food safety.

Keywords: *Moringa oleifera* leaves, Peanut oil, Rancimat test, Oxidative stability

Principles of Green Chemistry, Biodegradable Polymers, Solvent-Free Reactions, Catalysis for Sustainability, Circular economy in Chemistry, Life Cycle Assessment, Eco-friendly synthesis, Waste-to-resource Conversion

Coriander-Mediated Synthesis of Fe Nanoparticles for Eco-Friendly Dye Removal

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Abstract

This study presents an eco-friendly method for synthesizing iron nanoparticles (Fe NPs) using coriander extract as a natural reducing and stabilizing agent. The green synthesis approach eliminates the need for conventional toxic chemicals such as sodium borohydride, offering a cost-effective and sustainable alternative. The synthesized Fe NPs were thoroughly characterized using FTIR, XRD, SEM-EDX, and UV-Vis analyses, confirming their crystalline structure, nanometric size (≈ 23 nm), and the presence of phytochemicals responsible for particle reduction and stabilization. The catalytic performance of the Fe NPs was evaluated for the removal of Direct Red 80, a persistent anionic textile dye. Key operational parameters—including synthesis ratio, contact time, initial dye concentration, and pH—were optimized. Under optimal conditions (1:1 coriander extract/iron precursor ratio, 60 min contact time, 10 ppm dye concentration, and pH 12), the nanoparticles achieved a high removal efficiency of 92.96%. Adsorption behavior followed nonlinear isotherm models (Redlich–Peterson, Sips, and Toth), and the kinetic study revealed strong agreement with the pseudo-first-order model ($R^2 = 0.97$). Overall, this work demonstrates that coriander-mediated Fe NPs offer a rapid, efficient, and sustainable solution for dye-contaminated wastewater treatment. Their high performance, simple synthesis, and environmental compatibility highlight their potential for future large-scale and industrial applications.

Electrochemical Conversion of CO₂ to Functional Carbon Microspheres in Molten Carbonates for Energy and Materials Applications

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Abstract

The electrochemical conversion of carbon dioxide (CO₂) into value-added materials presents a compelling pathway for simultaneous carbon mitigation and resource generation within emerging energy systems. This study investigates the indirect electrochemical reduction of atmospheric CO₂ in a ternary molten Li–Na–K carbonate electrolyte to produce functional carbon microspheres. The molten salt medium offers distinct advantages over aqueous systems, including enhanced CO₂ solubility, a wide electrochemical window, and simplified product separation, enabling efficient carbon formation under open-air conditions. Electrochemical characterization via cyclic voltammetry identified key reduction processes associated with CO and carbon formation, with deposition occurring at potentials between –2.3 and –2.7 V at 500 °C. Controlled electrolysis yielded carbon microspheres with diameters of 10–30 μm, as confirmed by scanning electron microscopy. Elemental and spectroscopic analyses (EDX and FTIR) revealed oxygenfunctionalized carbon structures, with surface oxygen content of up to ~13%, imparting enhanced physicochemical properties. The morphology and yield of the deposited carbon were strongly dependent on electrochemical parameters, including applied potential and synthesis duration. Microsphere formation was favored under moderate potentials and intermediate electrolysis times, while higher potentials induced structural fragmentation into sheet-like carbon. The formation mechanism is attributed to in situ CO evolution and microbubble templating at the cathode interface. From a materials perspective, the synthesized carbon microspheres exhibit high functional performance, achieving up to ~99% removal of methylene blue under optimized conditions. This performance is linked to oxygen functional groups that enhance adsorption via electrostatic interactions, demonstrating the material's applicability in water treatment and environmental remediation. This work establishes a robust CCU pathway that integrates electrochemical CO₂ conversion with the synthesis of high-value functional carbon materials, positioning molten salt electrolysis as a scalable platform at the intersection of energy systems and processing of functional nanomaterials.

Sub-themes: Energy (Carbon Capture & Utilization), Nanochemistry

Extended Flory-Huggins modelling of endocrine disruptor-alginate interactions

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Abstract

Endocrine-disrupting chemicals (EDCs) pose a threat to aquatic ecosystems, necessitating novel approaches for their removal, yet they are also employed in beneficial pharmaceutical therapies. Accurate prediction of molecular interactions between EDCs and biopolymer-based adsorbents requires detailed knowledge of thermophysical properties; in particular, the free energy landscape of polymer-EDC interactions, mixing energy, and spatial configurations. This study presents systematic investigations into systems comprising water/testosterone/estrogens +poly(mannuronate)/poly(guluronate). Mannuronate and guluronate are key constituents of alginate, a widely used biopolymer. The goal was to determine steric and energetic effects to guide rational polymer design. An extended off-lattice Flory-Huggins approach¹⁻³, coupled with stochastic molecular simulations was used to compute thermophysical properties governing the interaction of water, testosterone, and estrogenic compounds (estradiol, estriol, estrone, ethinylestradiol, diethylstilbestrol, mestranol, and progesterone) with guluronate and mannuronate. Molecular dynamics simulations were used to determine the degree of polymerization needed for Flory-Huggins calculations by examination of the cohesive energy density of the polymers. Potential energy distributions indicated notable differences in polymer chain flexibility, which was higher in the former in aqueous environments. Overall, estrogens were noted to bind more strongly to the former. The results, some of which have been published ahead⁴, indicated pathways towards targeting the binding of several EDCs to alginate, by focussing on enhancing the intermolecular binding onto mannuronate versus guluronate blocks on the polymer chain.

Assessment of Water Quality from Sections of River Chania Adjacent to Leather Industries of Kenya Limited, Kiambu County-Kenya

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Abstract

As River Chania in Kiambu County, Kenya, serves domestic, industrial, and agricultural needs while supporting aquatic life. A section of the river flows near Leather Industries of Kenya Limited (LIK), where tanning activities may contribute to pollutant discharge. Globally, water pollution by industrial effluents, agrichemicals, and domestic waste threatens safe water access. According to the WHO, water quality is assessed using physico-chemical parameters such as pH, electrical conductivity (EC), biochemical oxygen demand (BOD), chemical oxygen demand (COD), total suspended solids (TSS), total phenols, and heavy metals. The study aimed to assess the water quality from sections of the river Chania adjacent to LIK. Water samples ($n=3$) were collected during the wet and dry seasons from the upstream, middle and downstream sections of the river. The physico-chemical parameters were measured using the American Public Health Association standard methods; heavy metals were analyzed by atomic absorption spectroscopy, and total phenols by UV-Vis Spectroscopy. Data was analyzed using the statistical R software, while One-way ANOVA was used to assess parameter variation across the sampling points in both seasons. The levels (mg/l) of TSS (307–1841-wet; 170–884-dry) and BOD (15.40 mg/l- wet; 10.50 mg/l- dry) exceeded the WHO set limits. The levels (mg/l) of Cr (0.119- 0.191), Pb (0.016- 0.025), Cd (0.003-0.004) and total phenols (0.038-0.143)-wet and Cr (0.103- 0.160), Pb (0.013-0.02), Cd (0.002-0.003) and total phenols (0.007-0.116)-dry exceeded the WHO set limits, while Cd remained within the acceptable limits. The findings revealed significant variations ($p<0.05$) in the water quality parameters across the sampling points, with the highest levels at midstream during both seasons, indicating poor water quality in River Chania near LIK. This suggests a possible contamination due to industrial effluents. The findings highlight the need for stricter regulation, active community engagement, and effective wastewater treatment solutions to protect ecosystems and public health.

Quality characteristics of drinking water from selected boreholes in Lodwar Municipality, Turkana County, Kenya

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Abstract

The quality of drinking water from boreholes is of public health importance. The study investigated the quality characteristics of drinking water randomly sampled in triplicates from six boreholes in Lodwar municipality namely: Moi Garden 1D, Moi Garden 1B, Napuu 7, Nabulon 5, Nabulon 6 and Nabulon 8 during the dry season. Physico-chemical parameters were determined in situ using multiparameter electrode (Hann-HI98129). K^+ and Na^+ were determined using flame photometry while Ca^{2+} , Mg^{2+} , Pb^{2+} and Cd^{2+} using Atomic Absorption Spectroscopy (iCE3300 AA System). Cl^- , SO_4^{2-} , CO_3^{2-} and HCO_3^- were determined using titrimetric technique, F^- using HACH ISE fluoride (HQ440dmulti) while NO_3^- analysis used UV/Vis spectrophotometric technique (Vis 130 Spectrophotometer). PH ranged: 7.4 ± 0.00 - 7.933 ± 0.03 , temperature: 33.57 ± 0.03 - 34.8 ± 0.00 °C, turbidity: 0.19 ± 0.00 - 0.73 ± 0.00 NTU, EC: 259.3 ± 0.33 - 688.3 ± 0.33 $\mu S/cm$ and TDS: 130.1 ± 0.06 - 341.1 ± 0.67 ppm and all except EC levels in Napuu 7 and Nabulon 8 fall within WHO limits. F^- ranged: 0.7473 ± 0.00 - 2.087 ± 0.00 mgL⁻¹, Cl^- : 0.6 ± 0.00 - 2.1 ± 0.06 mgL⁻¹, NO_3^- : 0.1033 ± 0.1 - 0.1733 ± 0.00 mgL⁻¹ and HCO_3^- : 2.48 ± 0.00 - 5.440 ± 0.00 mgL⁻¹ with all parameters complying with WHO standard except F^- reading in Napuu 7. SO_4^{2-} ranged: 0.0303 ± 0.00 - 2.081 ± 0.00 mgL⁻¹ and CO_3^{2-} in trace levels with all levels complying with WHO limits. K^+ and Na^+ ranged: 0.633 - 5.117 mgL⁻¹ and 0.0933 - 0.4367 mgL⁻¹, respectively and fall within WHO standards. Ca^{2+} , Mg^{2+} ranged 0.2323 - 0.9133 mgL⁻¹ and 1.083 - 1.423 mgL⁻¹, respectively and complied with WHO limits. Both Pb^{2+} and Cd^{2+} were recorded at trace levels complying with WHO standards. The groundwater quality indices (GWQI) for Moi Garden 1D, Moi Garden 1B, Nabulon 5 and Nabulon 6 fall below 50 confirming the water as safe for consumption. This calls for measures to monitor the elevated F^- and removal in drinking water from Napuu 7. The research findings would also inform evidence-based policy interventions by the government as well as foster research and development of advantage-dominant water purification systems.

Antioxidant Activity, Phytochemical Content and Antibacterial Activity of Extracts of Aloiaampelos Ciliaris

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Abstract

Extensive research on medicinal plants has revealed their antibacterial, antifungal, and antioxidant properties. However, the increasing prevalence of bacterial resistance to conventional antibiotics highlights the need to identify new bioactive compounds from medicinal plants. Currently, natural products account for over 50 % of drugs used in the treatment of different infections. Within this context, the Aloe genus (family Asphodelaceae), comprising approximately 500 Aloe species globally and about 50 species in Kenya, has a long-standing history of medicinal use. Notably, Aloe arborescence, Aloe ferox, and Aloe perryli have been extensively documented for their therapeutic potential. Traditionally, Aloe extracts have been employed for anti-malarial, anti-diabetic, anti-inflammatory, ornamental, and green manure purposes. Despite this established knowledge, inadequate information exists regarding the phytochemical composition, therapeutic evaluation, antioxidant activity, and antibacterial properties of Aloiaampelos ciliaris (A. ciliaris). The present study, therefore, aimed to screen for phytochemicals (tannins, phenols, flavonoids, cardiac glycosides), evaluate antioxidant and antibacterial activities, and determine the total phenolic and flavonoid content of A. ciliaris. Plant samples were collected from Meru County and macerated in 80 % methanol for 48 hours, followed by solvent partitioning (n-hexane, dichloromethane, EtOAc and water). Antioxidant activity was assessed using the 2,2-diphenyl-1-picrylhydrazyl radical (DPPH) radical scavenging assay, with results ranging from 15.67 % (IC₅₀ > 0.0300) to 74.74 % (IC₅₀ > 0.0300) at 0.3mg/mL, using ascorbic acid as a standard reference. Total phenolic content ranged from 105.89 ± 0.07 mg GAE/g in the flower crude extract to 1.46 ± 0.04 mg GAE/g in flower DCM extract, with gallic acid as a reference standard. Similarly, total flavonoid content ranged from 182.69 ± 1.64 mg QE/g in root crude extract to 3.59 ± 0.41 mg QE/g in the flower n-hexane extract, with quercetin as the reference standard. The antibacterial potential of the extracts was tested against pathogenic Gram-positive (E. faecalis, B. subtilis) and Gram-negative bacteria (E. coli, S. typhi) using gentamicin and ciprofloxacin as positive controls and 10 % dimethyl sulfoxide (DMSO) as the negative control. Activity ranged from inhibition of E. coli by the EtOAc extract (12.0 ± 0.500) to inhibition of B. subtilis by the root DCM extract (7.0 ± 0.000). Phytochemical screening revealed the presence of flavonoids, tannins, alkaloids, terpenoids, cardiac glycosides, phenols, and saponins. Furthermore, GC-MS analysis facilitated the separation, identification, and quantification of compounds such as methyl-cyclohexane and dodecane. Overall, the findings demonstrate that A. ciliaris possesses considerable therapeutic potential, attributable to its diverse secondary metabolites, antioxidant activity, antibacterial effects, and total phenolic and flavonoid contents.

Macrophage-capping protein (CapG) nanobody-immunosensor – toward the development of emerging biomarker-based test for hereditary breast and ovarian cancer syndrome (HBOC)

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Abstract

Macrophage-Capping Protein (CapG), Nanobody Macrophage-capping protein (CapG) is a protein which is overexpressed in breast, ovarian and gastric cancers. Thus, the level of CapG in clinical samples can be used as a phenotype test for ascertaining the occurrence of Hereditary Breast and Ovarian Cancer Syndrome (HBOC). This presentation is about our work on a novel sandwich nanobody-based electrochemiluminescent (ECL) immunosensor platform for ultra-sensitive determination of the CapG. The schematic representation of the immunosensor platform is: AuSPE | strep | Nb1 | BSA | biotin | BM | TAG-LiSmZrO₃-Nb2+BSA where AuSPE = gold screen-printed electrode, Nb1 = primary nanobody, Nb2 = secondary nanobody, BSA = bovine serum albumin, BM = CapG, TAG = cysteine. Nb1 and Nb2 are camelid nanobodies for CapG which are fragments of the normal antibodies. For the sensor platform development, Nb2 is covalently attached to cysteine-labelled LiSmZrO₃ perovskite. Electrochemiluminescent (ECL) responses of the immunosensor in buffer and human serum were studied. The work holds great promise for eventually developing nanobody-based immunosensor test for HBOC disease analysis.

Keywords: Electrochemiluminescence (ECL), Hereditary Breast and Ovarian Cancer Syndrome (HBOC)

Silicon Nitride Bioceramic: Synthesis, Characterization and its Adsorptive ability in fixed-bed column treatment of textile dye wastewater

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Abstract

The continued coffee demand in Kenya has amplified the generation of its husk wastes causing disposal problems. This has led to serious pollution to the environment. Therefore, developing a greener and cost-effective ways to handle these wastes is necessary. The current study entailed the use of extracted silica and coffee husk biochar as novel precursor materials for silicon nitride (Si₃N₄) composite synthesis for textile dye wastewater treatment. The silica was extracted from raw sand by alkali fusion route. The biochar was prepared by pyrolytic treatment of raw coffee husk biomass at 300 °C for 5 hours followed by acid leaching. The sand, extracted silica, raw and biochar samples and silicon nitride composites were characterized using XRF, FT-IR, XRD, SEM-EDX and TGA. The results showed that raw sand contain quartz, calcite, microcline and clinocllore. The results for the extracted silica showed a highly amorphous silica containing hydroxyl (-OH) and siloxane (Si-O-Si) functional groups. The characterization of biochar showed an amorphous, porous carbon structure with aromatic carbon bonds (C=C). The characterization of Si₃N₄ bioceramic showed thermally stable and porous composite with α-Si₃N₄ phase and β-Si₃N₄ phase, functional groups of silicon-nitrogen-silicon (Si-N-Si), silanol (Si-OH) and silicon-nitrogen (Si-N) which were hydroxylated in water to give important adsorption sites of silanolate ions (Si-O-) and silazane groups (Si₂=NH₂+) for textile dyes removal. The column sorption studies gave a maximum column capacity of 52.56 ± 0.04 mg/g at optimal column parameters. The column data obtained from the breakthrough curves conformed with Yoon-Nelson and Thomas models (R² > 0.9) in describing fixed-bed operations. The regeneration showed a good reusability of the adsorbent in textile dye wastewater treatment. The research findings report silicon nitride as a potential adsorbent that can be applied in purification of water to safe levels both at household and industrial scale.

Keywords: Extracted silica (ES), Silicon nitride (Si₃N₄), Bamburi Beach Sand (BBS), Coffee husk biochar (CHB), α-Si₃N₄, β-Si₃N₄

Ethnobotanical Knowledge as a Pathway to Antimalarial Drug Discovery: A Case Study of Three Plants Used by Ogiek Community to Treat Malaria in Kenya

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Abstract

The Control of malaria is increasingly a global challenge as more cases of clinical resistance are received from Southeastern Asia and Africa. Our group has joined international efforts to seek for new compounds with novel mechanisms of action. In this study we report in vivo antiplasmodial activity results of three plants *Rhamnus prinoides*, *Rubus keniensis* and *Garcinia buchananii* which are used for malaria treatment by indigenous communities in Kenya. Male and female mice were infected with *Plasmodium berghei* (ANKA) in the Peter's for day suppression test. Five groups of mice; Group 1 (solvent: 5 mL/kg body wt of 1% carboxymethyl cellulose), Group 2 (10 mg/kg body wt chloroquine), Groups 3, 4 and 5 were given 200, 400 and 800 mg/kg body wt of plant extracts. 5% aqueous methanol or 1:1 dichloromethane:methanol extracts were used depending on which exhibited higher activity in preliminary testing. 5% aqueous methanol extracts of *R. prinoides* and *G. buchananii* exhibited higher antiplasmodial activity than the 1:1 dichloromethane: methanol extracts. The doses showing 50% parasite suppression (EC 50) were 139.2 and 169.4 mg/kg body wt for *R. prinoides* and *G. buchananii*, respectively. The 1:1 Dichloromethane:methanol extract of *R. keniensis* showed higher activity than the 5% aqueous methanol extract and 50% parasite suppression (EC50) was 245.1 mg/kg body wt. These findings provide scientific evidence supporting the traditional use of these plants in malaria treatment. Further studies aimed at isolating and characterizing the active compounds are ongoing.

Synthesis of New Salicylaldehyde-based Schiff Base Palladium (II) Complexes and Evaluation of their Antimicrobial/Antioxidant Activities

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Abstract

The rise of drug-resistant microbes poses a significant global healthcare threat, requiring the development of new therapeutic agents. Moreover, oxidative stress is associated with various illnesses and disorders increasing the need for potent antioxidant agents. Schiff base ligands exhibit versatile coordination and biological properties offering a promising framework for drug development. In this study, two new Salicylaldehyde – based palladium (II) Schiff base complexes were synthesized, characterized and their antimicrobial and antioxidant activity investigated. The Schiff base ligands: 2-[[4-fluorophenyl]imino]methyl} phenol, (L1) and 4-Bromo-2-[[4-Fluorophenyl]imino]methyl}phenol, (L2) were prepared and subsequently reacted with dichloro(1,5-cyclooctadiene)palladium(II) in the ratio of 2:1 to yield [Pd(L1)2]2H2O (C1) and [Pd(L2)2]2H2O (C2) respectively. The Schiff base ligands and their respective Pd(II) complexes were characterized using FT-IR, UV-VIS, ¹H NMR, elemental analysis, molar conductance and melting point determination. Spectroscopic data confirmed bidentate coordination of the ligands to the Pd(II) center via the azomethine nitrogen and the phenolic oxygen atoms. FT-IR spectra displayed characteristic shifts of the $\nu(\text{HC}=\text{N})$ and $\nu(\text{C}-\text{O})$ bands to lower frequencies ($1605 \pm 1 \text{ cm}^{-1}$ and $1207 - 1231 \text{ cm}^{-1}$, respectively), while ¹H NMR spectra exhibited an up-field shift of the azomethine proton peak ($0.02 - 0.43 \text{ ppm}$). Molar conductance values ($0.929 - 4.29 \Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$) indicated the non-electrolytic nature of the compounds. Antimicrobial activity was evaluated against four bacterial strains, *B. subtilis*, *S. aureus*, *E. coli*, and *P. aeruginosa*, and one fungal strain, *C. albicans*, using the disc diffusion method. The antioxidant activity was determined using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) scavenging method. Statistical analysis was conducted using one-way ANOVA, followed by Tukey's post hoc test ($p < 0.05$). The Pd(II) complexes exhibited significantly higher antimicrobial and antioxidant activity compared to their free Schiff base ligands, with complex C2 showing the highest overall activity. The antimicrobial activity of Complex C2 was comparable to that of the positive control at higher concentrations; however, its antioxidant activity was lower than that of the positive control.

Keywords: Drug resistance, antimicrobial, Schiff base ligands, and palladium (II) complexes.

Lanthanide-Pillared Ti3C2Tx MXene with Expanded Interlayer Spacing for High-Rate Aqueous Sodium-Ion Batteries

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Abstract

Aqueous sodium-ion batteries (SIBs) involving conversion-type anode materials are promising for large-scale energy storage but are hindered by sluggish charge-transfer kinetics and structural instability during cycling. This study presents a combined experimental and density functional theory (DFT) investigation of Ti3C2Tx MXene as a high-performance anode material. Low-layered 2D Ti3C2Tx was synthesized through a selective etching of the Ti3AlC2 (MAX phase) using an NH4F/HCl acidic system, followed by the hydrothermal incorporation of La³⁺ ions. X-ray diffraction (XRD) confirmed successful MXene conversion and revealed a distinct (002) reflection shift, signifying expanded interlayer spacing due to La³⁺ pillaring. X-ray photoelectron spectroscopy (XPS) verified the presence of La species and strong interactions with surface terminations. DFT calculations indicate that optimal La-doping enhances metallicity by increasing the density of states at the Fermi level and optimizing Na⁺ adsorption energetics. Electrochemical evaluation in 1 M Na2SO4 demonstrates that the La-doped Ti3C2Tx delivers a high specific capacity of 370 mAh g⁻¹ at 100 mA g⁻¹, with 94% capacity retention over extended cycling. These results indicate that lanthanide pillaring effectively mitigates volume fluctuations and accelerates ion transport of Ti3C2Tx MXene through interlayer expansion, improved electronic conductivity, and optimized ion adsorption energetics. This work highlights La³⁺-doping of MXenes as a robust strategy for developing high rate, durable electrodes for next-generation aqueous SIBs.

Keywords: MXene interlayer pillaring, Density functional theory (DFT), La-Ti3C2Tx MXene, Na-ion batteries, Sodiation AI for Drug Discovery, Predictive Analytics, Automation in Labs, Machine Learning

Synthesis and Characterization of Modified Alginate Biopolymer Sorbents for the Removal of Methylene Blue and Cobalt (II) from Aqueous Solution

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Abstract

The discharge of synthetic dyes and heavy metals into aquatic environments poses serious environmental and public health risks, necessitating the development of effective and sustainable treatment technologies. In this study, alginate-based hydrogel sorbents were synthesized and modified to enhance their adsorption performance for MB and Co^{2+} from aqueous solution. Calcium alginate (CA), barium alginate (BA), poly (vinyl alcohol)–reinforced calcium alginate (PVA/CA), and poly (vinyl alcohol)–reinforced barium alginate (PVA/BA) hydrogels were prepared via ionotropic gelation, borate-mediated interpenetrating polymer network formation, and freeze-drying. Structural and compositional characterization using FTIR confirmed successful ionic crosslinking of alginate by Ca^{2+} and Ba^{2+} ions and the formation of borate–PVA networks, evidenced by shifts in hydroxyl and carboxylate vibrational bands. SEM revealed a hierarchical porous morphology with interconnected micro- and nanoscale pores, favorable for mass transfer during adsorption. EDX analysis confirmed the elemental composition, hydrogel purity and homogeneous distribution of crosslinking ions. TGA demonstrated enhanced thermal stability of the modified hydrogels, with PVA/BA samples exhibiting higher residual mass, indicating improved structural rigidity. Batch adsorption experiments were carried out to investigate the effects of pH, contact time, initial MB concentration, adsorbent dosage, and temperature. Adsorption increased with pH, reaching optimum performance at pH 9 due to enhanced deprotonation of alginate carboxylate groups and stronger electrostatic attraction toward cationic MB molecules. Rapid uptake occurred within the first 100 minutes, with equilibrium attained at 140 minutes. Increasing initial MB concentration enhanced adsorption capacity, while higher adsorbent dosages increased removal efficiency but reduced uptake per gram. Adsorption efficiency decreased with increasing temperature, indicating an exothermic adsorption process. Under optimal conditions (pH 9, 180 mg/L MB, 50 mg adsorbent, room temperature), the PVA/BA hydrogel achieved a maximum removal efficiency of 94% and an adsorption capacity of 334– 339 mg/g, outperforming all other sorbents. Therefore, synergistic Ba^{2+} crosslinking and PVA networks enhance alginate sorbents for wastewater treatment.

Keywords: Alginate hydrogel, PVA. Adsorption, Methylene Blue, Cobalt (II) ions, Barium

Redefining Proton Affinity for Heteronuclear Molecular Species: Quantum Chemical Insights

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Abstract

One of the main problems with experimental methods for detecting proton affinity (PA) is that they cannot perform site-specific protonation. For heteronuclear molecular species that have two or more protonation sites, the experimental PA measurement only yields a single PA value for each molecular species, with no information on the protonation site. Using various quantum chemical calculation techniques, various heteronuclear molecular species with two to four protonation sites (with known experimental proton affinity values) were subjected to site-specific protonation in order to characterize the trends of the PA corresponding to the experimentally measured PA values for each heteronuclear molecular species. The results showed additional trends that correspond to the measured PA values, going beyond the widely held belief that the proton moves to the place of the highest electron density during protonation. These tendencies included the proton moving to the site of the lowest electron density. Redefining proton affinity for heteronuclear molecular species is strongly suggested by the many patterns that have been seen. Besides these tendencies, we also found some molecular species that showed significant differences between the actual and computed PA values using various approaches, suggesting that the stated experimental values might be inaccurate. These observations will be presented.

Keywords: Proton affinity, binding sites, heteronuclear species

Abstract

Recent analyses by the Global Research on Antimicrobial Resistance (GRAM) collaboration underscore the urgent need for alternative antimicrobial strategies. In this study, three benzimidazole-based N, N'-bidentate ligands (L1-L3) and their corresponding half-sandwich ruthenium (II) η^6 -p-cymene complexes were successfully synthesized and comprehensively characterized to establish a robust physicochemical foundation for light-activated antimicrobial applications. The ligands were obtained in good yields and coordinated to Ru (II) to afford air-stable piano-stool complexes with systematically tunable electronic properties. FTIR spectra of the free ligands showed characteristic $\nu(\text{N-H})$ bands at 3450–3500 cm^{-1} and strong $\nu(\text{C=N})$ stretching vibrations at 1615–1630 cm^{-1} . Upon coordination, the $\nu(\text{C=N})$ bands shifted to lower wavenumbers by 15–25 cm^{-1} , accompanied by shifts in the $\nu(\text{C-N})$ region and the appearance of new bands at 480–520 cm^{-1} assigned to $\nu(\text{Ru-N})$, confirming N, N'-chelation. ^1H NMR spectra displayed aromatic ligand resonances at δ 7.10–8.75 ppm and benzimidazole N–H signals at δ 12.5–13.2 ppm, which shifted downfield or disappeared upon complexation, while new η^6 -p-cymene resonances appeared at δ 5.30–5.65, 2.60–2.90, and 1.10–1.35 ppm. Corresponding ^{13}C NMR spectra showed C=N carbons at δ 148–154 ppm, shifting downfield by 3–8 ppm in the complexes, with Ru-bound arene carbons observed at δ 82–86 ppm. UV–Vis spectra revealed ligand-centered $\pi \rightarrow \pi^*$ transitions at 250–290 nm and additional metal-to-ligand charge-transfer bands at 400–460 nm upon complexation. The complexes exhibited broad 3MLCT emission between 550 and 625 nm, excited-state lifetimes of 180–610 ns, and singlet oxygen quantum yields ($\Phi\Delta$) of 0.20–0.70, modulated by ligand substituent electronics. Importantly, the complexes retained over 90 % of their absorption intensity under microbiologically relevant irradiation conditions (400–700 nm, 10–50 mW cm^{-2} , up to 100 J cm^{-2}), demonstrating high photostability. These properties indicate that the ligands and their Ru (II) arene complexes are well suited for subsequent antibacterial photodynamic therapy and antifungal investigations.

Keywords: Ruthenium (II) arene complexes, benzimidazole ligands, N, N'-chelation, photophysical properties, singlet oxygen generation.

Green Synthesis of Ag/TiO₂ Nanocomposites Using Watermelon Rind Extract to Enhance Solar Disinfection (SODIS) for Safe Drinking Water in Africa

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Abstract

Safe drinking water remains a critical public health and climate resilience challenge across many African communities, intensified by population growth and weak sanitation systems. Solar Water Disinfection (SODIS) has emerged as a low-cost, accessible household water treatment method, but its efficiency is often limited by weather variability and long exposure times. To significantly enhance SODIS efficacy, this study presents a green synthesis approach for silver/titanium dioxide (Ag/TiO₂) nanocomposites, chosen for their potent antimicrobial and photocatalytic synergy. Watermelon rind extract served as a bio-reducing and stabilizing agent, leveraging readily available agricultural waste to promote circular economy principles, minimize hazardous chemical use, and provide a sustainable innovation for water treatment interventions. Synthesis parameters, including precursor concentration, pH, reaction temperature, and reaction time, were systematically optimized to yield nanocomposites with uniform morphology and high antimicrobial efficacy. Characterization using UV–Vis spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) confirmed successful formation of crystalline Ag/TiO₂ nanocomposites with evenly dispersed silver nanoparticles on the TiO₂ matrix. The nanocomposite-enhanced system achieved complete microbial inactivation within 6 hours under natural sunlight, whereas conventional SODIS showed incomplete inactivation under similar conditions. By applying green chemistry, this method minimizes environmental and human health risks while providing a scalable route for locally sourced functional nanomaterials. The use of agricultural byproducts demonstrates a clear pathway for community-level innovation in sustainable water treatment, directly aligning with the universal priorities for Climate Action, Green Transitions, and Health and Wellbeing for All (SDGs 3, 6, and 12).

Keywords: Green synthesis, Ag/TiO₂ nanocomposites, solar disinfection (SODIS), total coliform, community innovation

Photodynamic Investigation of Nitrogen-Doped Graphene Quantum Dots for Reactive Oxygen Species Generation in Antimicrobial Applications

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Abstract

The growing threat of antimicrobial resistance demands innovative chemistry-based solutions. In line with the theme “Harnessing the Power of Chemistry for a Sustainable Future,” this study explores nitrogen-doped graphene quantum dots (N-GQDs) as metal-free, environmentally benign photosensitizers for antimicrobial photodynamic therapy (aPDT). GQDs and N-GQDs were synthesized via a hydrothermal method and systematically characterized to establish structure–property relationships governing reactive oxygen species (ROS) generation. Raman spectroscopy confirmed graphitic structures with characteristic D ($\sim 1594\text{--}1598\text{ cm}^{-1}$) and G ($\sim 1354\text{--}1357\text{ cm}^{-1}$) bands, with increased defect density upon nitrogen incorporation. FTIR analysis revealed O–H/N–H ($\sim 3400\text{ cm}^{-1}$), C=O ($\sim 1700\text{ cm}^{-1}$), and enhanced C–N/C–O ($1380\text{--}1220\text{ cm}^{-1}$) vibrations, indicating successful doping. XPS analysis showed an increase in nitrogen content from $\sim 4.6\text{ at\%}$ to $\sim 10.4\text{ at\%}$, accompanied by reduced oxygen functionalities and improved carbon matrix homogeneity. Optical studies demonstrated enhanced $\pi\text{--}\pi^*$ transitions ($260\text{--}280\text{ nm}$) and the emergence of nitrogen-induced mid-gap states ($\sim 360\text{--}450\text{ nm}$), resulting in improved visible-light absorption. Fluorescence measurements exhibited excitation-dependent emission with a stable peak at $\sim 490\text{--}500\text{ nm}$, confirming dominant emissive trap states. Photodynamic activity was evaluated using Singlet Oxygen Sensor Green (SOSG), revealing time-dependent singlet oxygen ($^1\text{O}_2$) generation under irradiation. GQDs produced higher ROS levels ($\sim 13.0 \times 10^3\text{ a.u.}$) compared to N-GQDs ($\sim 4.5 \times 10^3\text{ a.u.}$) after 20 minutes, while dark controls remained negligible. Antibacterial assays against *Escherichia coli* and *Staphylococcus aureus* showed significant reductions in viability under light exposure, confirming ROS-mediated bacterial inactivation. This work highlights the potential of N-GQDs as sustainable nanomaterials for antimicrobial applications, contributing to green chemistry approaches for combating resistant infections.

Keywords: Graphene; Doping; ROS; Photodynamic; Oxygen; Antibacterial

Activated carbon from macadamia nutshells for removal of p-Nitrophenol from real wastewater:

Thermodynamic evaluation

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Abstract

Water pollution by organic pollutants remains a matter of significant apprehension since they tend to accumulate in the body to toxic levels and are often resistant to degradation and consequently endure in the surroundings for an extended duration. The targeted p-Nitrophenol (PNP) harmful to ecosystem was to be removed via adsorption. The nutshells were first charred in a muffle furnace at 600°C . The resultant ash was then activated and utilized for the adsorption of PNP from the wastewater. In this study, we utilized macadamia nutshell waste, both in its untreated and activated forms, which had been prepared earlier, to investigate the thermodynamic aspects of adsorbing p-Nitrophenol ions from wastewater. Scanning electron microscopy (SEM) images demonstrated the existence of pores within the adsorbent material, which proved to be advantageous for the adsorption process. Furthermore, the Fourier-transform infrared spectroscopy (FTIR) results indicated the presence of functional groups in both the unaltered and modified resins, highlighting their significance as sites for studying the thermodynamics of adsorbing p-Nitrophenol ions. Thermodynamic analysis revealed that the standard Gibbs' free energy (ΔG°) values for all metals were negative, indicating that the adsorption process was not only feasible but also favorable. Additionally, standard enthalpy change (ΔH°), standard entropy (ΔS°), and activation energy (E_a) were all positive and greater than 50 kJ mol^{-1} . This observation confirmed that the adsorption of p-Nitrophenol ions onto both unaltered and modified adsorbents was primarily governed by chemical interactions between the PNP ions and the active sites of the adsorbent material. This conclusion was further supported by the exceedingly low values of sticking probability (S^*). This investigation did not only show a good performance of the modified macadamia agricultural waste in adsorbing the PNP ions but also provided another way of reducing the negative effects caused by the nutshells disposed in the environment.

Keywords: Macadamia, Thermodynamics, Feasible, Favourable, Activation, Sticking.

Green Synthesis of Iron Oxide Nanoparticles using a Mixture of *Moringa oleifera* and *Hibiscus sabdariffa* Extracts and their Application in Photocatalytic Degradation of Methylene Blue

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Abstract

The development of sustainable nanomaterials using environmentally benign synthesis routes is critical for advancing green technologies in environmental remediation. In this study, iron oxide nanoparticles were synthesized via green approach using a mixed aqueous extract of *Moringa oleifera* leaves and *Hibiscus sabdariffa* calyces as stabilizing agents. The influence of extract ratios (1:1, 1:2, and 2:1) on the structural, optical, morphological, surface, and photocatalytic properties of the nanoparticles was systematically investigated. UV–visible spectroscopy confirmed nanoparticle formation of iron oxide nanocrystalline exhibiting band gaps between 3.0 and 3.6 eV. Fourier Transform Infrared Spectroscopy (FTIR) analysis verified the involvement of plant-derived functional groups in nanoparticle stabilization. Transmission electron microscopy (TEM) analysis showed formation of crystalline quasi-spherical to irregular nanoparticles with sizes in the nano-regime. Powder X-ray diffraction (XRD) patterns of samples confirmed the formation of α -Fe₂O₃ with rhombohedral structure. Surface studies revealed mesoporous characteristics with a surface area of approximately 49.79 m² g⁻¹. The photocatalytic performance of the synthesized nanoparticles was evaluated via degradation of methylene blue under UV irradiation, achieving up to 89% degradation within 120 min at low catalyst dosage (0.2 g L⁻¹). Kinetic studies indicated pseudo-first-order behavior, while adsorption data were best described by the Freundlich isotherm model. These findings highlight the effectiveness of mixed-extract-mediated green synthesis in tailoring iron oxide nanoparticles with enhanced photocatalytic performance for wastewater treatment applications.

Keywords: green synthesis; iron oxide nanoparticles; *Moringa oleifera*; *Hibiscus sabdariffa*; photocatalysis; methylene blue degradation

Synthesis of Nickel-Platinum Bimetallic Nanoparticles on Glassy Carbon Electrode for Enhanced Methanol Electro – Oxidation

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Abstract

Nanoparticle-based electrodes are a promising option to conventional electrodes for portable cells. These electrodes have demonstrated high electrocatalytic efficiency, sensitivity, selectivity, and resistance to fouling. In this study, a nickel-platinum nanoparticle electrode was electrochemically prepared by successive deposition onto GCE. Pt nanoparticles were electrochemically deposited onto a clean GCE from 2 mM hexachloroplatinic acid hydrate (H₂PtCl₆·6H₂O) in 0.5M H₂SO₄ supporting electrolyte solution at a controlled potential of -2V for 60 seconds to form Pt/GCE. Electrodeposition of Ni onto the Pt/GCE was carried out from nickel sulphate solution as the electrolyte and Pt/GCE as the working electrode at a controlled potential of -1V vs Ag/AgCl/NaCl (sat) for 120 seconds. The modified electrode (Ni-Pt/GEC) was conditioned in 0.5 M NaOH for about 40 cycles to obtain a reproducible voltammogram, followed by cyclic voltammetry characterisation. The electro-oxidation of methanol was performed using the Ni-Pt/GCE surface as the working electrode. The results showed that the electrode exhibited good electrocatalytic properties for methanol oxidation, attributable to the combined effect of Pt and Ni. An oxidation peak for 0.3 M methanol in 0.5 M NaOH was observed at about 550 mV vs Ag/AgCl/KCl (3 M). The Ni-Pt/GEC electrode displayed significantly enhanced electrocatalytic activity, excellent stability, and a relatively lower onset potential (0.32 V). The increased efficiency is ascribed to the greater electrochemical surface area afforded by oxygen-rich functional groups in NiOx, the synergistic effects of Pt and Ni, and the excellent utilisation of Pt nanostructures on the glassy carbon support. Thus, this binder-free composite has the potential to be used as an economical, effective, and stable electrocatalyst for methanol oxidation. All experiments were done at room temperature and pressure. The electrode can be employed in methanol fuel cells to boost energy supply.

Keywords: Electro-catalytic, efficiency, sensitivity, selectivity, fouling, electro-chemical cell, nanoparticles, NiOx, synergistic, methanol oxidation, nickel-platinum.

Synthesis of Hybrid Polymeric Nanozyme Membranes for Emerging Contaminant Removal

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Abstract

The increasing occurrence of pharmaceutical contaminants and heavy metals in surface water necessitates the development of advanced treatment technologies with enhanced selectivity, stability, and multifunctionality. This study reports the fabrication and physicochemical characterization of a polymeric nanozyme membrane based on polyamic acid (PAA) embedded with silver (Ag) and gold (Au) nanoparticles for potential application in water treatment. Membranes were fabricated via the non-solvent-induced phase separation (NIPS) technique, with in situ reduction of metal precursors to produce uniformly distributed Ag/Au nanoparticles within the PAA matrix. To address the inherent brittleness of PAA, silane coupling agents were incorporated to improve membrane flexibility and structural integrity. The effects of nanoparticle incorporation on membrane morphology, surface properties, and thermal stability were systematically investigated. Characterization was performed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to evaluate membrane morphology and nanoparticle dispersion. Fourier-transform infrared spectroscopy (FTIR) confirmed chemical interactions within the polymer matrix, X-ray diffraction (XRD) verified the crystalline nature of the embedded nanoparticles, and thermogravimetric analysis (TGA) assessed thermal stability. Contact angle measurements revealed enhanced hydrophilicity in nanozyme-modified membranes. Results demonstrate that in situ nanoparticle synthesis enabled uniform dispersion and strong polymer-nanoparticle interactions, while silane coupling agents improved membrane flexibility without compromising structural integrity. The developed nanozyme membranes exhibit physicochemical properties favourable for the simultaneous removal of organic micropollutants such as levonorgestrel (LNG) and inorganic contaminants, including heavy metals, indicating strong potential for application in advanced water treatment systems.

Keywords: Polyamic acid (PAA); Polymeric nanozyme membrane; Levonorgestrel (LNG); Heavy metals; Water treatment.

Selection of Novel DNA Aptamers against HPV16 Biomarker, E6: An in-silico Approach

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Abstract

Human Papillomavirus type 16 (HPV16) infection, particularly its E6 oncoprotein, is a primary driver of various malignancies, including cervical cancer, highlighting an urgent need for novel therapeutic and diagnostic strategies. Aptamers, with their high affinity, specificity, and structural tunability, represent promising alternatives to antibodies for targeted interventions. This study presents a comprehensive in silico approach for the selection of novel DNA aptamers against the HPV16 E6 biomarker. Initial virtual screening was conducted using AutoDock VinaXB on a proprietary aptamer library to identify high-binding score candidates (cut-off – 9.3 kcal/mol). Following the inclusion of stable structures on both ends of the top 9 candidate aptamers, molecular docking was performed via the HADDOCK web server to assess the binding interactions of the candidate aptamers on the protein surface. To investigate the dynamic stability of these complexes, molecular dynamics (MD) simulations were executed using GROMACS 2019 with the CHARMM36M force field. The structural integrity and binding mechanisms were analyzed via root mean square deviation (RMSD), fluctuation (RMSF), radius of gyration (Rg), solvent accessible surface area (SASA), and hydrogen bond analysis. Finally, molecular mechanics Poisson-Boltzmann surface area (MMPBSA) calculations were performed to comprehensively assess the binding free energies (ΔG_{bind}) and their individual energetic components for the 8 complexes. The analysis revealed a wide range of binding affinities, with Apt1 and Apt8 demonstrating the most favorable values of -138.26 kcal/mol and -136.43 kcal/mol, respectively. These strong interactions were primarily driven by significant van der Waals and electrostatic contributions, synergistically supported by favorable non-polar solvation effects. In contrast, Apt6 exhibited the least favorable binding at -8.36 kcal/mol. These results suggest that Apt1 and Apt8 are highly promising leads for further experimental validation and development as potential therapeutic or diagnostic agents against HPV16.

Keywords: HPV16; E6 oncoprotein; in silico screening; molecular docking; AutoDock VinaXB; HADDOCK; molecular dynamics simulation; GROMACS; MMPBSA; binding free energy; cervical cancer; diagnostic biomarkers.

Optimization of Electricity Production Using a Hybrid System of Solar Photovoltaics, Microbial Fuel Cells, and Anaerobic Digestion for Electricity generation, Biogas production and Biofertilizer Production and Characterization

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Abstract

Unmanaged bovine waste in pastoral communities in Kenya contributes to greenhouse gas emissions, land degradation, water pollution, and limited access to reliable electricity. This study addresses these challenges through a circular economy approach that transforms cattle waste into valuable energy and agricultural resources. The research aims to optimize electricity production using a hybrid system integrating solar photovoltaic (PV), microbial fuel cells (MFCs), and anaerobic digestion (AD), with bovine waste as the primary feedstock. Solar energy is incorporated due to its abundance and ability to provide clean, scalable power, complementing continuous biological processes and enhancing system reliability. The system enables efficient resource recovery, where AD produces biogas and nutrient-rich biofertilizer, while MFCs generate electricity through bioelectrochemical processes. Electroactive bacteria (*Shewanella* and *Geobacter*) are utilized to enhance electron transfer and increase power density. Performance improvements focus on reducing internal resistance and optimizing electrode configurations. Additives such as biochar are introduced to improve microbial activity, substrate degradation, and electron transfer efficiency. Methodologically, the study combines experimental and modeling approaches, applying optimization techniques such as response surface methodology and multi-objective analysis. Key parameters—including pH, temperature, substrate composition, hydraulic retention time, and solar irradiance—are evaluated for their impact on system performance. A life cycle assessment (LCA) is conducted to quantify environmental benefits, including emissions reduction and resource efficiency. Below is a summary of electrochemical reactions in the MFC fuel cell.

Electrochemical Reactions: Anode: $\text{Organic Matter} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H} + +e_-$

Cathode: $\text{O}_2 + 4\text{H} + 4e^- \rightarrow 2\text{H}_2\text{O}$; $\text{O}_2 + 4\text{H} + 4e^- \rightarrow 2\text{H}_2\text{O}$

Results demonstrate improved electricity output, increased biogas yield, enhanced biofertilizer quality, and reduced environmental pollution. Despite limitations such as system complexity and scalability, the approach offers strong potential for decentralized energy production, sustainable waste management, and rural development. The proposed system presents a scalable, low-carbon solution aligned with circular economy principles.

Geochemical Characterization and Safety Assessment of Embolaiy Natural Salt Licks for *Bos taurus* in Narok County, Kenya

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Abstract

Natural mineral licks are widely utilized by livestock in semi-arid rangelands as sources of essential mineral nutrients; however, their geochemical composition, mineralogical characteristics, and associated health risks remain insufficiently characterized. This study evaluated the physicochemical, elemental, mineralogical, and potential toxicological characteristics of Embolaiy natural salt licks used by livestock in Narok County, Kenya. Samples collected from five locations were characterized using inductively coupled plasma optical emission spectroscopy (ICP-OES), X-ray fluorescence (XRF), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR). ICP-OES analysis revealed enrichment of essential macro- and trace elements, particularly calcium (Ca), magnesium (Mg), sodium (Na), potassium (K), iron (Fe), and zinc (Zn), indicating the potential nutritional importance of the salt licks for livestock. However, cadmium (Cd) was identified as the principal element of concern, reaching a maximum concentration of 1.769 mg/kg at Suswa–Mosiro. XRF analysis showed that the samples were dominated by major oxides, including CaO, SiO₂, Fe₂O₃, and Al₂O₃, consistent with silicate–carbonate-rich geological materials. XRD identified mineral phases including calcite, quartz, feldspar, and clay minerals, while FTIR spectra confirmed characteristic carbonate, silicate, hydroxyl, and metal–oxygen functional groups. These mineralogical and spectroscopic characteristics suggest that mineral composition and natural weathering processes may influence elemental occurrence and retention within the salt licks. Risk assessment using contamination factor (CF), estimated daily intake (EDI), hazard quotient (HQ), hazard index (HI), pollution load index (PLI), metal pollution index (MPI), risk quotient (RQ), and risk index (RI) identified Cd as the major contributor to potential health risk. Suswa–Mosiro recorded the highest HI (1.55) and RI (2.179), indicating elevated potential cumulative risk, while Olkinyei also showed comparatively higher risk values. In contrast, Pb, Cr, Ni, and As generally remained within the considered permissible ranges, while PLI values below unity across all sites indicated low overall metal pollution. Overall, the findings demonstrate that Embolaiy salt licks contain nutritionally important mineral elements but exhibit localized Cd enrichment that warrants continued monitoring before extensive use as a livestock mineral supplement. The integration of multi-analytical characterization with quantitative risk assessment provides a comprehensive approach for evaluating the nutritional value and safety of naturally occurring mineral resources used by livestock.

Keywords: Embolaiy; natural mineral licks; ICP-OES; XRF; XRD; FTIR; elemental composition; cadmium; livestock; risk assessment.

Acridone Alkaloids from *Zanthoxylum zanthoxyloides* demonstrate Anti-Candida, Anti-Biofilm and Antifungal-Resistance Modifying Activities against Drug-Resistant *Candida albicans*, *Candida glabrata* and other Non-*albicans* *Candida* Species

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Abstract

Drug-resistant *Candida* infections represent an escalating global health crisis, contributing to high mortality especially in low- and middle-income countries. *Zanthoxylum zanthoxyloides* (Rutaceae) is a West African medicinal plant traditionally used for the management of cutaneous and mucosal infections. This study isolated bioactive alkaloids from its stem bark and evaluated their anti-*Candida*, antibiofilm, and resistance-modifying activities against drug-resistant *Candida* strains and clinical isolates. Phytochemical investigation of the ethyl acetate fraction of the 70% hydroethanolic stem bark extract by column chromatography over silica gel and Sephadex LH-20 yielded three acridone alkaloids, arborinine, fabiocinine, and 1,3-dimethoxy-10-methylacridone and, the coumarin, 6,7,8-trimethoxycoumarin. Anti-*Candida* activity of the compounds was assessed by microbroth dilution following CLSI guidelines against 40 *Candida* strains (5 reference strains, 35 clinical isolates) comprising *C. albicans*, *C. glabrata*, *C. tropicalis*, *C. krusei* and *C. parapsilosis*. The activity of the compounds against biofilm formation and mature biofilms of the *Candida* species was also evaluated. Resistance-modifying effects were then assessed via checkerboard assays with voriconazole, nystatin, and caspofungin. The compounds exhibited strong anti-*Candida* activity. Fabiocinine was the most potent, with MICs of 3.91–31.25 µg/mL against the drug-resistant strains and clinical isolates, comparable to voriconazole. Arborinine and 1,3-dimethoxy-10-methylacridone demonstrated MICs of 15.63–250 µg/mL and 31.25–250 µg/mL, respectively. The acridone alkaloids inhibited biofilm formation (SMIC₅₀ = 45.05–413.48 µg/mL) and disrupted mature biofilms (SMIC₅₀ = 125.25–1224.07 µg/mL). Checkerboard assays revealed strong synergy (FICI ≤ 0.5) between the acridone alkaloids and voriconazole (86.7%) and caspofungin (80%) against the reference strains, suggesting distinct mechanistic profiles from conventional antifungals. These findings demonstrate, for the first time, the anti-*Candida*, antibiofilm, and resistance-modifying activities of acridone alkaloids from *Z. zanthoxyloides*. Fabiocinine, in particular, shows significant promise as a lead compound or adjunct therapy for combating MDR *Candida* infections and warrants further mechanistic and in vivo investigation.

Activated carbon from macadamia nutshells for removal of p-Nitrophenol from real wastewater:

Thermodynamic evaluation

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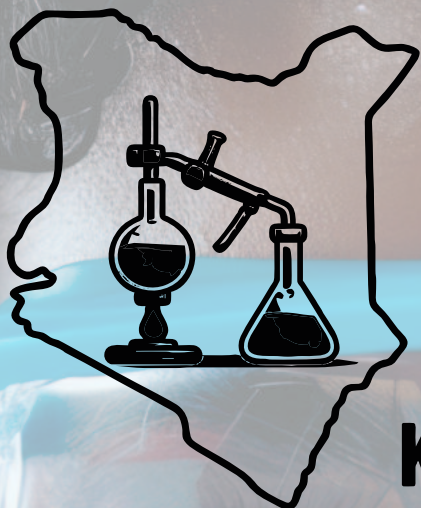
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Abstract

Water pollution by organic pollutants remains a matter of significant apprehension since they tend to accumulate in the body to toxic levels and are often resistant to degradation and consequently endure in the surroundings for an extended duration. The targeted p-Nitrophenol (PNP) harmful to ecosystem was to be removed via adsorption. The nutshells were first charred in a muffle furnace at 600° C. The resultant ash was then activated and utilized for the adsorption of PNP from the wastewater. In this study, we utilized macadamia nutshell waste, both in its untreated and activated forms, which had been prepared earlier, to investigate the thermodynamic aspects of adsorbing p-Nitrophenol ions from wastewater. Scanning electron microscopy (SEM) images demonstrated the existence of pores within the adsorbent material, which proved to be advantageous for the adsorption process. Furthermore, the Fourier-transform infrared spectroscopy (FTIR) results indicated the presence of functional groups in both the unaltered and modified resins, highlighting their significance as sites for studying the thermodynamics of adsorbing p-Nitrophenol ions. Thermodynamic analysis revealed that the standard Gibbs' free energy (ΔG°) values for all metals were negative, indicating that the adsorption process was not only feasible but also favorable. Additionally, standard enthalpy change (ΔH°), standard entropy (ΔS°), and activation energy (E_a) were all positive and greater than 50 kJ mol⁻¹. This observation confirmed that the adsorption of p-Nitrophenol ions onto both unaltered and modified adsorbents was primarily governed by chemical interactions between the PNP ions and the active sites of the adsorbent material. This conclusion was further supported by the exceedingly low values of sticking probability (S^*). This investigation did not only show a good performance of the modified macadamia agricultural waste in adsorbing the PNP ions but also provided another way of reducing the negative effects caused by the nutshells disposed in the environment.

Keywords: Macadamia, Thermodynamics, Feasible, Favourable, Activation, Sticking.



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