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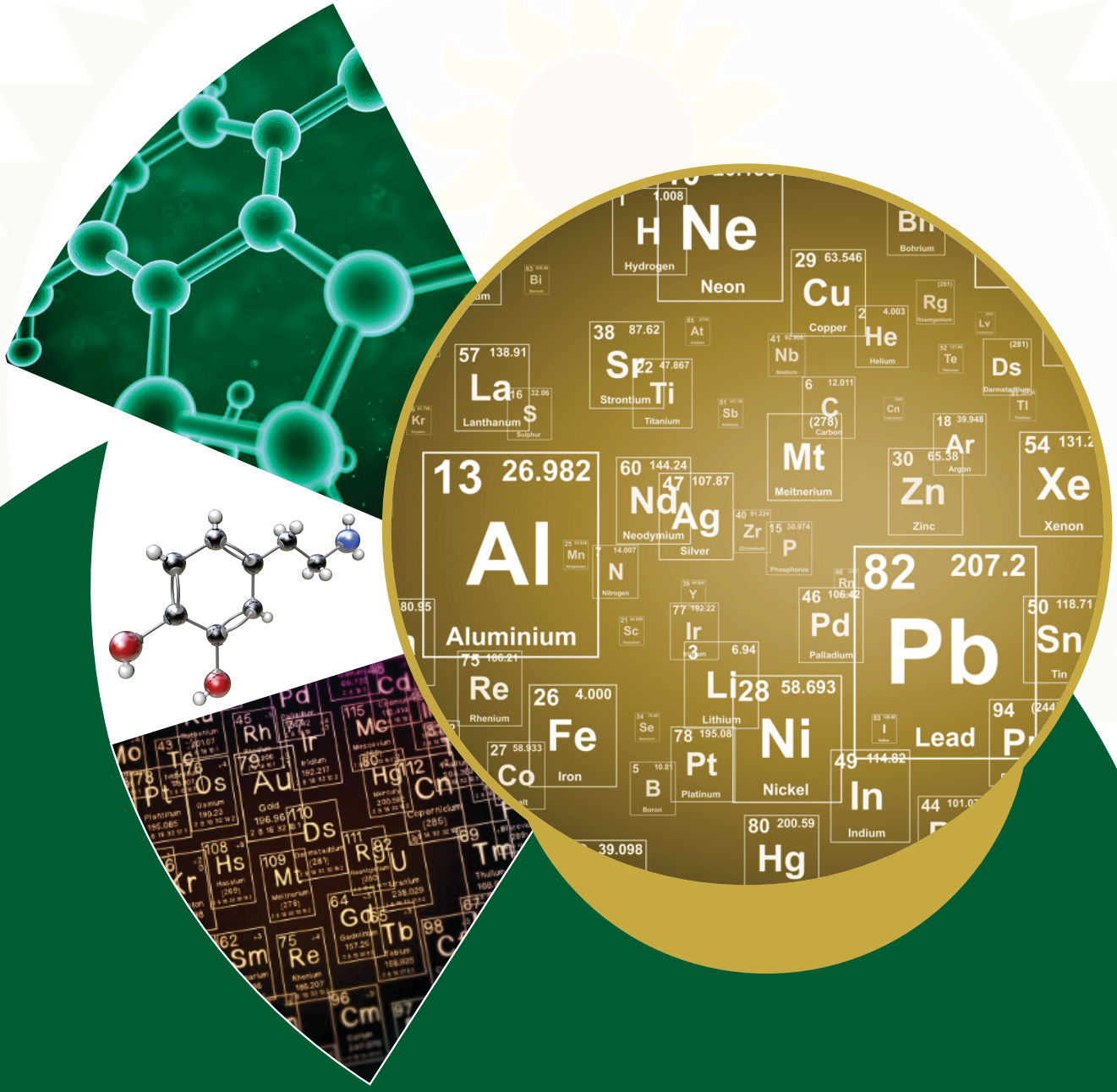

2026 SACI NORTH SECTION
YOUNG CHEMISTS SYMPOSIUM
BOOK OF ABSTRACTS

Dates: Friday, 16 October 2026

The South African Chemical Institute (SACI) North Section

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Doctor NOKUTHULA KHANYILE

CHAIRPERSON
SACI NORTH SECTION

MESSAGE FROM THE CHAIRPERSON OF SACI NORTH SECTION

On behalf of the SACI North Section Executive Committee, it is my great honour and pleasure to welcome you to the 2026 SACI North Section Young Chemists Symposium (YCS). This 9th edition of YCS is hosted by the Department of Chemistry at the University of Limpopo.

This year's theme, "Young Minds Shaping the Future of Chemistry," aligns with the YCS's goal of providing a platform for emerging chemists to share their research, exchange ideas, build scientific networks, and gain confidence as the next generation of leaders in chemistry. The future of our discipline depends not only on the discoveries we make but also on our ability to nurture young scientists who are inquisitive, innovative, collaborative, and prepared to apply chemistry to solve societal problems. Consequently, the YCS is more than just a scientific gathering; it is an investment in the individuals who will shape the future of chemistry in South Africa and beyond.

It is indeed fitting that we meet in Limpopo, a province known for its rich cultural heritage, remarkable biodiversity and abundant natural resources. These attributes serve as a reminder that chemistry is deeply linked to everything, from agriculture and biodiversity to the development of technologies for a sustainable future, and from the minerals beneath our soil to the water that sustains our communities. I urge all our young chemists to take advantage of this opportunity to showcase their work. Build relationships that extend beyond this symposium, ask open questions, receive constructive feedback and criticism, and confidently share your science. Every successful scientist started as an emerging researcher, trying to find their voice and position within the scientific community.

We would like to extend our sincere appreciation to the University of Limpopo, the organizing committee, the participating institutions, the sponsors, the partners, the honoured guests, the adjudicators, and everyone else whose contributions have made this symposium possible. We greatly appreciate your commitment to advancing chemistry and training emerging scientists. I wish all delegates an engaging, inspiring and productive symposium. May the conversations and connections established here contribute to new ideas, collaborations and opportunities.

Welcome to the 2026 SACI North Section YCS. Let us continue to encourage young minds as they shape the future of chemistry. Have a good time!

Yours sincerely

Dr. Nokuthula Khanyile
Chairperson: SACI North Section

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Doctor
R MHLABA
CHAIRPERSON
SACI NORTH SECTION ORGANIZING COMMITTEE

MESSAGE FROM THE SACI NORTH SECTION ORGANIZING COMMITTEE

It gives me a great pleasure to welcome you all to the 9th Young Chemists Symposium (YCS) organized under the banner of the South African Chemical Society (SACI), North Section. This is the third conference hosted by University of Limpopo. The SACI North section is comprised of the following institutions: University of Pretoria (UP), Sefako Makgatho Health Sciences University (SMU), University of Venda (UNIVEN), Tshwane University of Technology (TUT), Council for Scientific and Industrial Research (CSIR), South African Nuclear Energy Corporation Limited (NECSA), University of Mpumalanga (UMP), and University of Limpopo (UL). We feel honored as the University of Limpopo has been granted this great opportunity of hosting YCS 2026.

The theme of this year's event is 'Young Minds Shaping the Future of Chemistry', which celebrates youth as key contributors to advancing chemistry and solving future societal challenges. A total of eleven (11) oral and sixty-five (65) poster presentations will grace this one-day event. Our ambitious and vibrant young chemists from the above institutions, including all invited scientists, will have an opportunity to learn from an invited guest speaker who will hopefully inspire and motivate them in the exciting career of chemistry. Prestigious awards will be given to the top twelve (12) participants from the three categories, i.e., (i) Hons posters presentations (ii) MSc and (iii) PhD oral presentations.

I would like to acknowledge the support of the Acting Executive Dean of the Faculty of Science and Agriculture at UL, the University management and all the support units in their totality. A special word of gratitude goes to our generous sponsors, the School of Physical and Mineral Science (UL), Chemistry Department (UL), Protea Laboratory Solutions, Anton Paar, Wirsam Scientific, Separation Scientific, Mchemlabs suppliers, Metrohm South Africa, Morula services, Royal Society of Chemistry (RSC) and SASOL. Finally, I wish to thank the following people for raising their hands to make success of this great occasion: all our students who will be presenting, together with their supervisors, volunteers, SACI North Section and the Local Organizing Committee (LOC) members.

I wish you all a successful and informative symposium and trust that you will take advantage of this opportunity to establish new friendships, network, and collaborations.

We hope to see you again at our next YCS meeting in a year's time.

Dr. R Mhlaba

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KHANYILE N (Dr)	Chairperson	University of Mpumalanga (UMP)
MOLEFE N (Dr)	Deputy Chairperson	Sefako Makgatho Health Sciences University (SMU)
MAMPA RM (Prof)	Past Chairperson & Scientific Events	University of Limpopo (UL)
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MHLABA R (Dr)	scientific Events	University of Limpopo (UL)
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South African Nuclear Energy Corporation (NECSA)	*Vacant*
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University of Pretoria (UP)	*Vacant*
University of Venda (UNIVEN)	NYEMBE S (Mr)

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1. Dr R Mhlaba
2. Prof RM Mampa
3. Mrs MM Matjena
4. Ms TG Ramakadi
5. Dr NW Masekoameng
6. Dr BP Moloto
7. Dr MV Maphoru
8. Ms J Makgoba

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SACI NORTH SECTION YOUNG CHEMIST SYMPOSIUM

CONFERENCE PROGRAMME

FRIDAY, 16 OCTOBER 2026 VENUE: R40 HALL, UNIVERSITY OF LIMPOPO		
TIME	**PRESENTER**	**ACTIVITY**
8:00 – 9:00	**Arrival, Registration, Coffee & Tea**	
Opening Ceremony Chair: Dr R Mhlaba		
9:00 – 9:15	**Dr R Mhlaba SACI**	**Welcome message and announcements**
9:15 – 9:25	**DVC (UL) Research and Academic**	**Opening Remarks**
9:25 – 9:30	**Prof RM Mampa**	**Introduction of Guest speaker**
9:30 – 10:00	**Dr MW Ngobeni**	**Guest speaker**
SESSION 1	**Dr Makhado Session Chair**	**Presentations by MSc Candidates**
10:00 – 10:15	**UNIVEN T Netshivhazwaulu**	Rational Design and Antiplasmodial Evaluation of Cinnamoyl-Chloroquinoline Hybrids: Exploring Linker and Cinnamoyl Substituents Effects
10:15 – 10:30	**UL TL Mfumadi**	Preferential oxidation of carbon monoxide in hydrogen-rich stream over ceria-manganese-doped Co3O4-based catalysts
10:30 – 10:45	**TUT NP Setlau**	Investigation of the Chemistry-influenced Mechanism Failure Causing Under-deposit Corrosion Leading to Boiler Failures in Matimba Power Station
10:45 – 11:00	**SMU MO Tshamano**	Applications of a Multi-Template Molecularly Imprinted Polymer for Analysis of Selected Antiretroviral Drugs in Wastewater from Gauteng Province, South Africa
11:00 – 11:15	**UL M Kekana**	Engineering the structure of Metal-Cu-MOF (via synthesis) for the efficiency in photocatalytic and photoelectrocatalytic hydrogen generation

11:15 – 11:30	**UNIVEN** KB Moloto	Cinnamoyl Quinoline Hybrids as Corrosion Inhibitors for Zinc and Aluminium in Hydrochloric Acid
SESSION 2	**Session Chair** **Dr M Bvumbi**	**Presentations by PhD Candidates**
11:30 – 11:45	**UNIVEN** S Nyembe	Phytochemicas from african viscum species identified by LC-MS and pearson correlation analysis as anti-corrosive agents for mild steel and aluminum in acidic medium: experimental and theoretical study
11:45 - 12:00	**TUT** NC Qinisa	Development of a Ceria doped ZnO Photocatalyst for phenol degradation in industrial effluent
12:00 – 12:15	**UL** DC Langa	Effect of Plant Extract Concentration on Structural and Photocatalytic Properties of Green Synthesised CuS for Degradation of Dyes in Wastewater
12:15 – 12:30	**TUT** AS Tanko-Djoubi	Deposition of metal nanoparticles on nitrogen-reduced graphene for oxygen reduction reactions
12:30 – 12:45	**UMP** N Madlala	Plant-Extract Composition Influences Nanostructure Formation and Agronomic Performance of a Green Nano-Fertilizer
12:45 – 13:45	**Announcements & Lunch**	
	END OF SESSION 2	
14:00 – 14:45	**POSTER SESSION (coffee and tea available)**	
14:45 – 15:00	**SACI REP**	**PRIZE GIVING SESSION**
15:00 – 15:15	**LOC Rep**	**Vote of thanks and announcement of the host for next Symposium**

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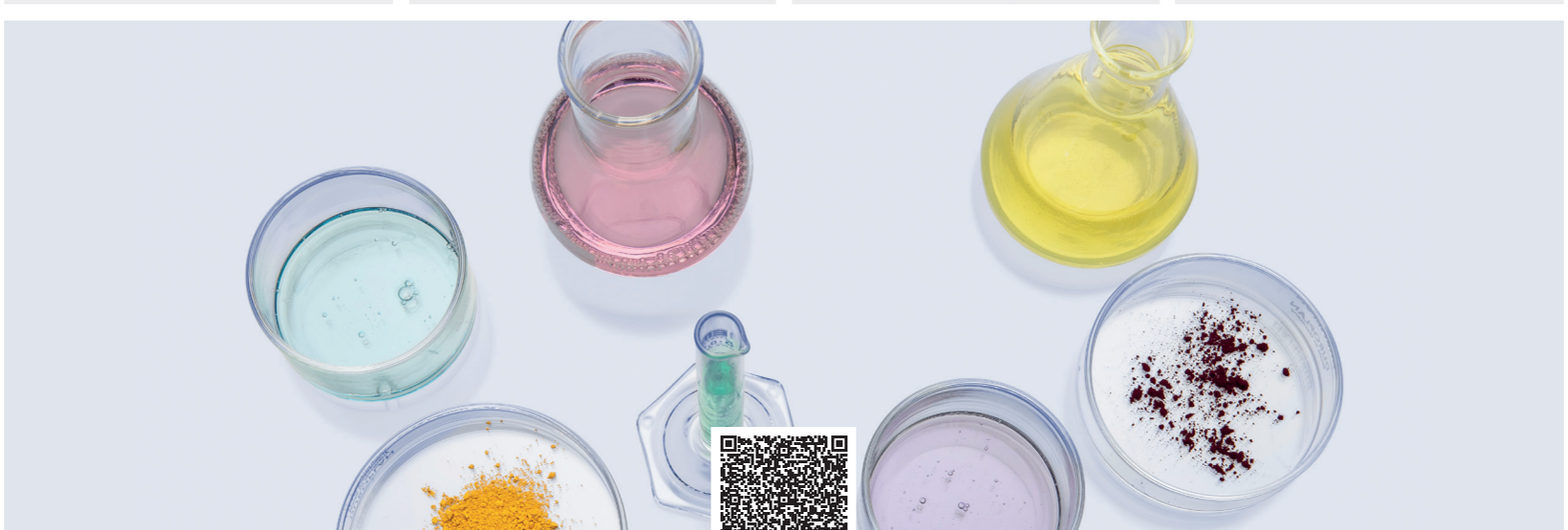

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MASTERS ORAL ABSTRACTS

Investigation of the Chemistry-influenced Mechanism Failure Causing Under-deposit Corrosion Leading to Boiler Failures in Matimba Power Station

[1]NP. Setlau, [2]FA.Melato, [2]SP.Lepule, [3]K. Pule

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[3]Eskom, Germiston, South Africa. Email: Setlaup@eskom.co.za

Under-deposit corrosion (UDC) is a primary deterioration mechanism in once-through subcritical boilers because deposits alter the tube surface chemistry and induce localised corrosion. This study examined chemistry-related UDC mechanisms in an oxygenated treatment (OT) once-through boiler. It examined how pH, ammonia, DO, chloride, sulphate, and specific mass deposit affected boiler tube failures. Under OT, the boiler's pH was steady, indicating bulk cycle-chemistry control. However, ammonia, chloride, and sulphate concentrations fluctuated, and dissolved oxygen levels varied substantially, indicating unstable oxygen regulation. Bulk pH is a good indicator of general chemistry management, although ammonia, DO, chloride, and sulphate can impair oxide stability and create localised chemical conditions beneath deposits.

Low deposit loading was observed, with specific mass deposits < 300 g/cm^2. Deposit loading does not preclude UDC. A deposit's composition, shape, porosity, chemical characteristics, and concentration of aggressive species influence its localised corrosive potential. Hydrogen damage was also found, indicating significant chemistry-related degradation. Other boiler units had corrosion fatigue, indicating that local operating conditions, chemical history, and material susceptibility may cause numerous interacting degradation pathways across the boiler fleet.

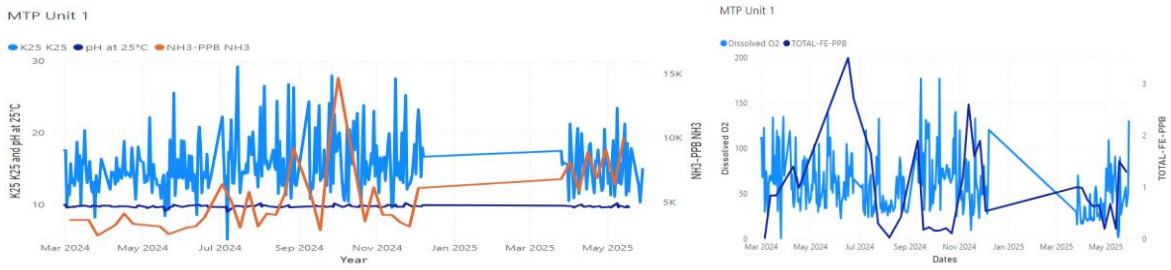

Figure 1: Unit 1 Economiser Inlet pH vs K25 vs NH_3 (March 2024 – June 2025) B) Unit 1 Economiser Inlet Total Particulate Iron and Dissolved Oxygen (March 2024 – June 2025)

References

1. Obot, I. B. (2021). Under-deposit corrosion on steel pipeline surfaces: Mechanisms, mitigation, and current challenges. *Journal of Bio- and Tribo-corrosion*, *7*(2). https://doi.org/10.1007/s40735-021-00485-9

Preferential oxidation of carbon monoxide in hydrogen-rich stream over ceria-manganese-doped Co_3O_4-based catalysts

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Rising carbon emissions have renewed interest in proton exchange membrane fuel cells (PEMFCs) for their high efficiency, power density, and fast start-up. PEMFCs use H_2 and O_2, but reformate H_2 contains 1%CO [1]. Preferential oxidation (PROX) is used to cut CO from 1 vol.% to <10 ppm and prevent Pt-anode poisoning. Noble-metal and metal-oxide catalysts deactivate in moisture and have narrow temperature windows [2]. Metal oxides such as Co_3O_4 and CeO_2 offer oxygen vacancies and redox properties for CO oxidation. MnO_x can promote oxidation of Co^{2+} to Co^{3+} in PROX, while $NaBH_4$ pretreatment tunes surface properties [3]. CeO_2 and MnO_x modified Co_3O_4 catalysts were synthesised by IWI and characterised by XRD, FTIR, BET, and H_2-TPR. FTIR and H_2-TPR confirmed Co^{3+}/Co^{2+} in spinel Co_3O_4, consistent with XRD. PROX tests showed that CeO_2 or MnO_x increased CO oxidation. Bare Co_3O_4 reached 72% CO conversion at 40 °C and achieved complete conversion at 120–200 °C. Optimal binary catalysts were 5wt.% CeO_2/Co_3O_4 (complete conversion at 100–120 °C) and 5wt.% MnO_x/Co_3O_4 (80–200 °C). The ternary 5wt.% CeO_2–5wt.% MnO_x/Co_3O_4 showed 50% CO conversion at 40 °C and complete conversion at 80–200 °C in dry gas. Under moisture, the ternary catalyst improved from 50-60% CO conversion at 40 °C and reached complete conversion from 100–200 °C. Due to high surface area (110.482 m²/g) and abundant Co^{3+}/Mn^{3+} species. The ternary catalyst remained stable, maintaining >90 % CO conversion under dry, wet, CO_2-containing, and H_2O/CO_2 feeds.

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Rational Design and Antiplasmodial Evaluation of Cinnamoyl-Chloroquinoline Hybrids: Exploring Linker and Cinnamoyl Substituents Effects

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Cinnamoyl-chloroquinoline hybrids represent a promising class of compounds for antimalarial drug discovery through the molecular hybridization of two biologically relevant structural scaffolds [1-2]. This study focused on the synthesis and optimization of cinnamoyl-chloroquinoline hybrids and investigated how structural modifications affect their antiplasmodial activity. Computational studies were performed, including molecular docking to investigate ligand-protein interactions and molecular dynamics simulations to assess the stability of selected protein-ligand complexes. A series of cinnamoyl chloroquinoline hybrids with different cinnamoyl substituents and varying linkers was synthesized and characterized using spectroscopic and analytical techniques, including NMR, FTIR, and melting-point. The antiplasmodial activities of the synthesized compounds were evaluated against the *Plasmodium falciparum* NF54 strain to establish structure-activity relationships. Substitution on the cinnamoyl moiety influenced the antiplasmodial activity of the synthesized hybrids, demonstrating the importance of electronic and structural effects in compound optimization.

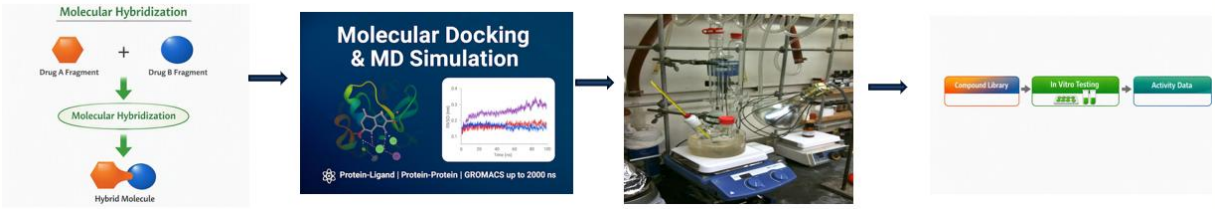

Figure 1: Simple flow diagram of the project

References

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Cinnamoyl Quinoline Hybrids as Corrosion Inhibitors for Zinc and Aluminium in Hydrochloric Acid

K.B. Moloto, G.M. Masuku, M.V. Bvumbi, L.C. Murulana
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Corrosion causes the deterioration of metals, making them unattractive and weaker [1,2]. The current best corrosion mitigation is the use of corrosion inhibitors [3]. This research investigates the potential and effectiveness of cinnamoyl quinoline hybrids as corrosion inhibitors for zinc and aluminium in 1 M hydrochloric acid solution at 30-60 ℃. One of the compounds that was investigated is shown in Figure 1. In this study, Cinnamoyl quinoline hybrids were synthesized and characterized by Nuclear Magnetic Resonance (NMR). Electrochemical impedance spectroscopy (EIS), potentiodynamic polarisation (PDP), and gravimetric analysis were utilized to assess the corrosion inhibition properties of the studied compounds. To learn more about the functional groups that appeared or disappeared during the adsorption/desorption of the inhibitory molecules on the metal, Fourier transform infrared spectroscopy (FTIR) was utilized. The amount of metal content in solutions was determined using atomic absorption spectroscopy (AAS). The surface morphology of the uninhibited and inhibited processes was examined using energy dispersive spectroscopy (EDS) in conjunction with scanning electron microscopy (SEM). Four cinnamoyl quinoline hybrids were successfully synthesised, and all showed promising results, with maximum percentage inhibition efficiencies ranging from 80-99 %. The studied compounds exhibited significantly higher corrosion inhibition efficiency on aluminium than on zinc.

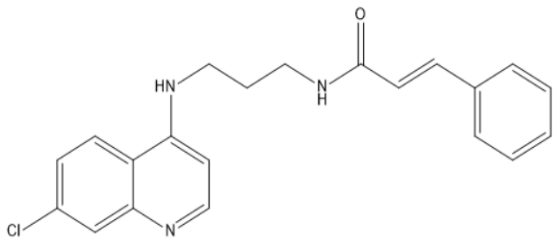

Figure 1: The structure of N-(3-((7-chloroquinoline-4-yl)amino)propyl)cinnamamide utilized as a corrosion inhibitor.

References

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2. V. Kucera, E. Mattsson, Corrosion mechanisms **2020**, *pp. 211-284*.
3. C.M. Hansson, The impact of corrosion on society **2011**, *pp. 2952-2962*.

Applications of a Multi-Template Molecularly Imprinted Polymer for Analysis of Selected Antiretroviral Drugs in Wastewater from Gauteng Province, South Africa

MO., Tshamano[1], S., Ncube[2], N.F.H., Makhubela[1], R.C., Chokwe[3], B.R., Maseko[4]
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Antiretroviral drugs (ARVDs) like efavirenz (EFZ) and nevirapine (NVP) are discharged into aquatic environments, raising ecological and health concerns [1]. This study describes the synthesis and application of a multi-template molecularly imprinted polymer (MIP) for extracting EFZ and NVP from South African wastewater, outperforming a commercial C_{18} sorbent [2]. The MIP, synthesized using EFZ and NVP as templates, displayed superior morphological and thermal properties. It demonstrated effective adsorption following the Freundlich isotherm and pseudo-second-order kinetics, maintaining 64.7% of its binding capacity after ten cycles. Application to real water samples showed improved selectivity, confirming that treatment plants inadequately remove ARVDs, with detected concentrations in effluent and influent suggesting residual contamination in local waters [3].

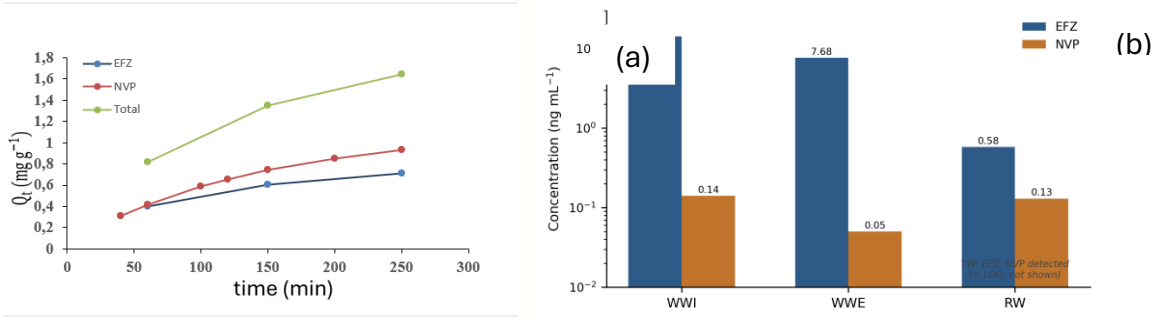

Figure 1. (a) Maximum adsorption capacity (Q_t) of EFZ and NVP, and their total (a). Both compounds were detected in WWI, WWE, and RW, in ng mL^{-1} (b).

References

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[2] Mahlambi, S.P., Mahlambi, P.N., & Madikizela, L.M. (2019). Synthesis and application of a molecularly imprinted polymer in selective solid-phase extraction of efavirenz from water. Water Science and Technology, 79(2), 356–365.

Engineering the structure of Metal-Cu-MOF (via synthesis) for the efficiency in photocatalytic and photoelectrocatalytic hydrogen generation

Mathilda Kekana[1], Daphney Makhafola[1], Daniel Masekela[1], Kwena Modibane[1]
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This study focuses on the influence of synthetic routes on the physicochemical, thermal, morphological, photocatalytical, and photoelectrochemical properties of MOFs for enhanced hydrogen production applications. Furthermore, it also explores the effect of incorporating Ti and Al into the Cu-based framework to form a trimetallic Ti/Al/Cu-MOF and evaluate how the synthesis route affects metal incorporation, structural characteristics, surface properties, charge transfer behaviour, and the efficiency of photocatalytic and photoelectrocatalytic hydrogen generation. Trimetallic Ti/Al/Cu-MOF materials were successfully fabricated using room-temperature stirring and ultrasonic-assisted synthesis as efficient synthetic routes. XRD and FTIR analyses confirmed the successful incorporation of Ti and Al species into the framework, while SEM analysis revealed distinct morphologies depending on the synthetic route. BET analysis demonstrated that Ti/Al/Cu-MOF US possessed a larger surface area (10.202 m^2/g) and pore volume, indicating enhanced porosity and greater accessibility of catalytic active sites. This MOF exhibited highest hydrogen production of 565 µmol within 60 min, outperforming the room-temperature counterpart. Furthermore, photoelectrochemical investigations using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), linear sweep voltammetry (LSV), and Tafel analysis confirmed superior electrochemical behaviour for the Ti/Al/Cu-MOF US. The material demonstrated lower charge transfer resistance (25.6 Ω), higher electrochemical surface area (6.64 cm^2), faster electron diffusion (3.48×10-6 $cm^2 \cdot s^{-1}$).

Keywords: Metal organic framework, photocatalysis, photoelectrocatalysis, hydrogen generation



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BOOK OF ABSTRACTS

DOCTORAL ORAL ABSTRACTS

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Plant-Extract Composition Influences Nanostructure Formation and Agronomic Performance of a Green Nano-Fertilizer

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Plant-derived extracts provide both nutrient elements and phytochemicals for nano-enabled fertilizer development, but their formulation chemistry can influence the physicochemical characteristics of resulting materials. This study, therefore, examined how the composition of banana peel extract (BPE), watermelon rind extract (WRE), and Aloe vera gel extract (ALvE) influenced the properties of green nano-fertilizers and their agronomic performance. BPE and WRE were mixed in proportions (50:50, 75:25, and 25:75), and each mixture was combined with 5, 10, 15 mL ALvE. Formulation composition produced marked differences in the chemical and structural characteristics of the materials. UV-Vis spectra retained the characteristic absorption features of the parent extracts with small spectral shifts, consistent with noncovalent composite formation, while phytochemical screening and SEM-EDS revealed a phytochemical-rich matrix containing multiple mineral elements. TEM showed formulation-dependent changes in particle size, morphology and aggregation, with mean diameters ranging from 4.6 to 540.8 nm. SAED pattern varied from amorphous to polycrystalline and single-crystalline structures. In greenhouse trials, selected formulations containing 5 mL ALvE at lower application doses improved seed emergence and plant height in tomato and bell pepper. Overall, formulation composition strongly influenced material properties and functional performance, demonstrating the feasibility of producing nutrient-bearing nanostructure fertilizer from agricultural residues without inorganic nutrient salt precursors.

Keywords: Green nano-fertilizer, plant-derived extracts, banana peel, watermelon rind, *Aloe vera*, physicochemical properties.

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Phytochemicas from african viscum species identified by LC-MS and pearson correlation analysis as anti-corrosive agents for mild steel and aluminum in acidic medium: experimental and theoretical study

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Corrosion poses a major threat to the durability of metals and structural integrity, with considerable economic and environmental consequences. Conventional corrosion inhibitors, mainly synthetic compounds, are often toxic and hazardous to the environment. This study explores phytochemicals as green corrosion inhibitors, offering a sustainable, affordable, and eco-friendly solution. This study aims to deepen the understanding of the inhibitory mechanisms and effectiveness of African *Viscum* species, which are rich in phytochemicals like alkaloids, flavonoids, and tannins, while also exploring their potential industrial applications [1–4]. Phytochemicals from *Viscum album* and *Viscum combreticola* were identified by LC–MS and FTIR before and after inhibition to monitor functional-group changes associated with adsorption. Their corrosion inhibition performance on mild steel (MS) and aluminium (Al) in 1.0 M HCl was evaluated using gravimetric, electrochemical, DFT, and surface characterization techniques. Gravimetric analysis showed concentration-dependent inhibition, with *Viscum album* achieving the highest efficiency of 98.83% for MS. Adsorption analysis indicated non-ideal adsorption, while the dimensionless separation factor (R_L) confirmed favourable adsorption. Both phytochemical extracts effectively reduced corrosion rates and exhibited mixed-type inhibition for MS and Al. FTIR confirmed adsorbed protective films, while polarization and EIS demonstrated suppression of anodic and cathodic processes and increased charge-transfer resistance. SEM/EDS and contact-angle measurements confirmed hydrophobic protective layers that blocked corrosion sites. DFT calculations demonstrated strong interactions between inhibitor molecules and metal surfaces, supporting the experimental findings.

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Effect of Plant Extract Concentration on Structural and Photocatalytic Properties of Green Synthesised CuS for Degradation of Dyes in Wastewater

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Green synthesis offers an environmentally sustainable route for producing semiconductor photocatalysts for wastewater remediation. In this study, copper sulfide (CuS) nanoparticles were synthesized using *Sutherlandia frutescens* leaf extract at varying concentrations of 5, 10, and 15 g to investigate the influence of phytochemical content on their structural and photocatalytic properties. FTIR analysis confirmed the participation of plant-derived biomolecules in nanoparticle formation and stabilization. XRD analysis revealed hexagonal covellite CuS, with the 10 g sample exhibiting improved phase purity. SEM analysis demonstrated a concentration-dependent reduction in particle size, alongside morphological variations. BET analysis indicated relatively low surface areas, suggesting limited influence in the availability of active surface sites. UV–Vis diffuse reflectance spectroscopy revealed that the 10 g sample possessed the lowest optical band gap of 4.03 eV. Photocatalytic degradation of Congo Red under UV irradiation achieved efficiencies of 75% for the 5 and 10 g samples and 73% for the 15 g sample after 60 min. Despite variations in structural and optical properties, photocatalytic performance remained comparable, indicating that plant extract concentration exerted a modest influence on degradation efficiency. Overall, the 15 g CuS sample demonstrated the most balanced properties, providing a foundation for further optimization of photocatalytic operating conditions.

Deposition of metal nanoparticles on nitrogen-reduced graphene for oxygen reduction reactions

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As demand for renewable energy technology increases, energy conversion devices are being actively studied. Among them, direct alcohol fuel cells (DAFCs) are important candidates owing to their promising nature as energy sources for future technologies. DAFCs have significant advantages over other fuel cells because they use cheaper, liquid-state reductants (like ethanol, ethylene glycol, and glycerol) at room temperature [1]. The oxygen reduction reaction (ORR) is an important reaction that takes place at the cathode of the fuel cell. ORR is a multi-step process and serves as the rate-determining step. For this reason, the use of catalysts is essential to facilitate the reaction in the cells. To date, nitrogen-reduced graphene oxide (NrGO) has been shown to be an effective support for the ORR due to the presence of nitrogen atoms on graphene sheets [2]. Decorating NrGO with low-ratio of 3:1 Ru-M (M = Ce and Sn) nano-catalysts has proven to be an efficient way to enhance DAFCs performance. Herein, the nanocatalysts were prepared by the microwave-assisted hydrothermal. The as-synthesized nano-catalysts were characterized for their morphology and structure using physicochemical techniques, while electrochemical analysis were performed using CV, LSV, K-L plots and CA. Ru-based nano-catalysts on NrGO improve the electrocatalytic properties for AOR/ORR in DAFCs.

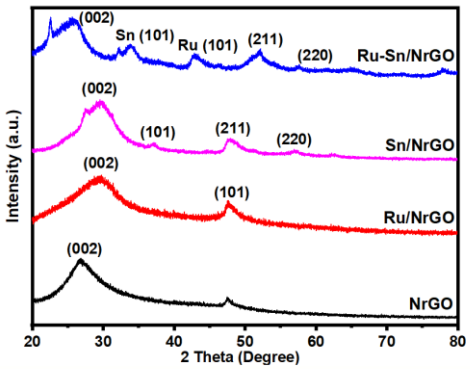

Figure 1: XRD of NrGO, Ru/NrGO, Sn/NrGO and Ru-Sn/NrGO

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Development of a Ceria doped ZnO Photocatalyst for phenol degradation in industrial effluent

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Clean water scarcity is increasingly becoming a global problem, due to the rapid growth in clean water demand caused by a surge in urbanization, agricultural activities and industrial activities [1]. Industries particularly, have become triggers for water pollution risk, because they produce organic compounds such as phenol, which can be threatening to the ecosystem. Phenol is a threat due to its resistance to ecological degradation, toxicity and prolonged persistence within a particular environment [2]. Conventional effluent treatment methods exist but are inadequate and advanced oxidation processes like photocatalysis have become of interest [3].

Recently, zinc oxide semiconductors have gained vast attention [3]. However, they suffer various challenges, which negatively impact their photocatalytic performance during effluent treatment [3]. Therefore mitigation strategies such as doping with CeO_2 are employed to provide alternative pathways for charge carriers and increasing perfomance during effluent treatment. In this study ZnO, CeO_2, CeO_2-ZnO photocatalyst's were synthesised via microwave method and their performance evaluated for phenol degradation in effluent. Characterization via FTIR and XRD (Figure 1a and b) confirmed the successful incorporation of CeO_2 into the ZnO lattice. Photodegradation study (Figure 1c) of phenol at varying rations of CeO_2 showed that, lone ZnO could only achieve 48.2% degradation, which was less, compared to CeO_2 at 76.4% degradation. However, 2% CeO_2 showed slight improved degradation efficiency at 52.5%, while 4% CeO_2 showed the best degradation efficiency at 86.3%. 8% and 10% CeO_2 showed a sudden decrease in degradation and 10% achieved the least degradation at 45.4%.

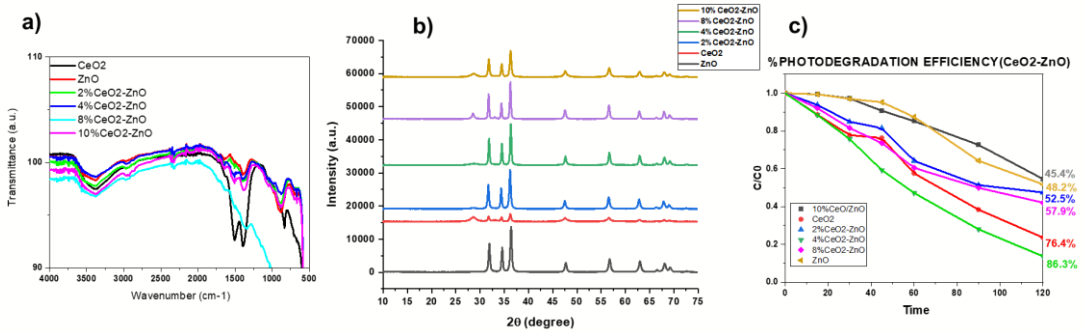

Figure 1: a) FITR Spectrum of ZnO, CeO_2 and CeO_2-ZnO, b) XRD Spectrum of ZnO, CeO_2 and CeO_2-ZnO, c) Photocatalytic degradation of 10ppm phenol using ZnO, CeO_2 and CeO_2-ZnO @ pH≈7

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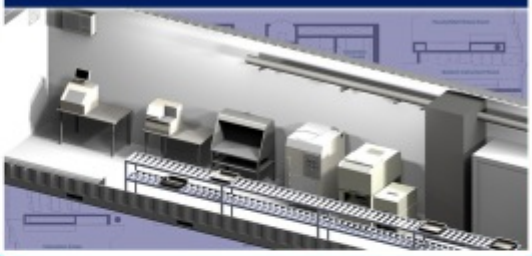

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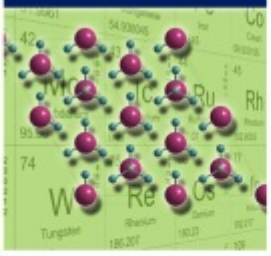

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POSTER ABSTRACTS

P#1–The Synthesis Of 3-Ammino-5-Phenylpyrazole Derivatives As Potential Organic Corrosion Inhibitors Due To Hydrochloric Acid.

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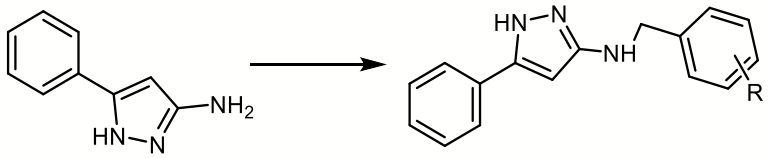
Corrosion is the process of material decay caused by physical or chemical interactions with its environment.[1] This metal corrosion caused by interacting with the surrounding medium will significantly reduce the mechanical properties of the metal, damage the geometric shape of the metal components, shorten the lifespan of the equipment, and even cause catastrophic accidents. Furthermore, metal corrosion has significant economic repercussions, from direct costs like replacing corroded structures and implementing protection measures, to indirect impacts such as industry shutdowns, and environmental costs. Thus, use of corrosion inhibitors is often a good solution to prevent corrosion phenomena and to provide a more acceptable lifetime of metallic structures. Therefore, organic compounds are used as corrosion inhibitors because they contain atoms (nitrogen, oxygen, sulfur and phosphorous), aromatic ring or triple bonds that reduce corrosion attack in aqueous solutions. [1] In this study, 3-amino-5-phenylpyrazole will undergo reductive amination using 3,5-disubstituted salicylaldehyde, followed by acetyl chloride. The synthesized 3-amino-5-phenylpyrazole derivatives will be characterized by ^{1}H and ^{13}C NMR spectroscopy. These compounds will then be experimentally used for gravimetric analysis, potentiodynamic polarization (PDP), and electrochemical impedance spectroscopy (EIS) to investigate their corrosion prevention properties on zinc (Zn) in a 1.0 M hydrochloric acid (HCl) solution. Amsterdam Density Functional (ADF) will be used to corroborate experimental findings.



where R = 5-Br, 3-EtO, H, 5-NO_2

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P#2–METAL DOPED BIOSYNTHESIS OF $CuFe_2O_4$ PHOTOCATALYSTS FOR THE DEGRADATION OF DYES AND PHARMACEUTICALS FROM WASTEWATER.

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Water pollution caused by pollutants such as dyes and pharmaceuticals has led to a major environmental concern due to their persisting effects on human and aquatic life [1]. The Advanced Oxidation Process has emerged as a potential for the degradation of these organic pollutants into harmless products through the photocatalysis method using metal ferrites [2]. In this study, a green-synthesized copper ferrite photocatalyst was synthesized using the *Sutherlandia Frutescens plant*. The FT-IR analysis showed a frequency band around 500cm^{-1} corresponding to the spinel phase recognition of Cu-O and Fe-O. Through SEM analysis, a spherical morphology for all the materials was noted, with particle sizes of 68nm, 83nm and 71nm for 5g, 10g, and 15g respectively. All the materials reported a surface area above 21m^2/g. The high pore size in 15g nanoparticles indicated a potential high photocatalytic activity. The TGA and DTG analysis showed a %weight loss of less than 5%, indicating that the $CuFe_2O_4$ nanoparticles are highly thermally stable. These findings show the capability of the green-synthesized $CuFe_2O_4$ as a photocatalyst for the degradation of dyes and pharmaceuticals.

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P#3–Multi-Scale Evaluation of Advanced Exterior Coatings: Investigating Chemical Stability and Thermal Performance of Reflective Pigments and Flexible Resins in Inland Heat Zones.

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Inland regions experience high temperatures and intense solar radiation, which can accelerate paint degradation and increase heat absorption by building surfaces [1,2,3]. This study evaluates the thermal effectiveness and chemical durability of infrared (IR)-reflective, low-VOC exterior coatings applied to different substrates under conditions representative of inland heat zones. Corrugated iron and aluminium foil substrates were coated with selected paint formulations and exposed to accelerated ultraviolet (UV) exposure for 1000 hours. The different paint formulations were rubber flex, pure acrylic, sheen acrylic, super acrylic and a primer. After every 100 hours of exposure durability test was conducted to check chalking, fading, gloss loss and cracking. FTIR analysis was performed before and after exposure. The degradation test showed fading, gloss loss and chalking after 300-500 hours of exposure and continued to show further degradation, but no cracking was recorded after 1000 hours of exposure. The FTIR results showed that all coatings retained their main spectral framework after UV, but the degree of chemical change differed across formulations. Pure acrylic and rubber flex paints exhibited more pronounced shifts, indicating greater susceptibility to UV induced degradation, while Sheen Acrylic showed moderate modification. Aqua Primer and super acrylic displayed minimal IR changes, with super acrylic proving more stability overall. These results highlighted that primers and high-performance acrylic offer superior molecular durability compared to more flexible or standard acrylic coatings. Future work will include detailed Thermogravimetric analysis (TGA) analysis, scanning electron microscope (SEM) imaging for micro-crack and contact angle for further characterisation.

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P#4–LC-MS-Based Metabolomic Profiling Reveals Tissue-Specific Distribution of Metabolites in Cucumber (*Cucumis sativus*)

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Prostate cancer remains a significant global health challenge, highlighting the need to discover novel therapeutic agents from natural sources [1]. Cucurbitaceae species contain diverse bioactive metabolites, particularly cucurbitacins and other triterpenoids with promising pharmacological activities [2]. The general chemical structure of cucurbitacins is presented in fig 1. This study aimed to investigate the tissue-specific distribution of metabolites in cucumber (*Cucumis sativus*) using LC-MS-based metabolomic profiling. Inner, middle and outer cucumber tissues were analysed to investigate tissue-associated metabolic variation. Principal component analysis (PCA), dendrograms, box plots, volcano plots and PERMANOVA revealed distinct metabolic profiles among the tissues with the outer tissue showing enrichment of several differentially abundant metabolites. Molecular networking enabled metabolite characterisation across the tissues and resulted in the putative annotation of cucurbitacin R in the outer tissue. Targeted LC-qTOF-MS was subsequently applied to selected cucurbitacins, including cucurbitacin A, B, E and cucurbitacin E-2-O-glucoside. The combined metabolomic and molecular networking analyses revealed tissue-associated differences in metabolite distribution and identified cucurbitacin-related metabolites in cucumber tissues.

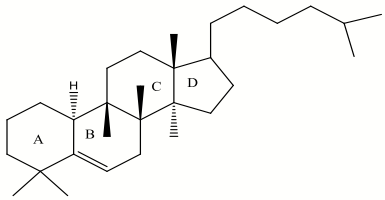

Figure 1: Structure or cucurbitacin

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P#5–Synthesis and Characterization of Cellulose-Iron Oxide nanoparticle composite for removal of Cadmium and Nickel in Acid Mine Drainage

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Acid mine drainage (AMD), an acidic and metal-rich effluent derived from the reaction between pyrite, oxygen, and dihydrogen monoxide, contributes to huge economic and ecosystem loss. This research has synthesized a magnetic bio-adsorbent nanocomposite with a yield of 28.21%. On the other hand, banana peel waste intensifies climate change through enormous methane and soot emissions. This study prepared cellulose nanocrystals (CNC) from banana peels through alkali (NaOH), bleaching (NaOCl), and acid hydrolysis (H_2SO_4) treatments. This prominent renewable, biodegradable, highly flexible resource, with high surface area and abundant functional groups (-OH, -COOH, -NH_2) was mixed with highly magnetic iron-oxide nanoparticles synthesized from ferrous sulphate heptahydrate ($FeSO_4 \cdot 7H_2O$) and ferric chloride hexahydrate ($FeCl_3 \cdot 6H_2O$) through an ex-situ method to produce a nanocomposite of banana peel cellulose nanocrystals-iron oxide nanoparticles (BPNC-IONPs). The materials we characterised using Scanning Electron Microscopy, Transmission Electron Microscopy and Fourier Transform Infrared Microscopy and will be used for recovery of nickel (Ni) and cadmium (Cd) from acid mine drainage These heavy metals are globally associated with environmental and human ill-being through bioaccumulation and biomagnification.

Keywords: acid mine drainage, metal recovery, banana peel cellulose, magnetic iron-oxide nanoparticles, cost-effective adsorbent nanocomposite.

P#6–EXTRACTION, CHARACTERIZATION AND MODIFICATION OF CELLULOSE FROM PEANUT HUSKS.

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BACKGROUND AND OBJECTIVES: The build-up of lignocellulosic agricultural waste, such as peanut husks, puts significant environmental management challenges. Transitioning towards a circular bioeconomy requires us to make use of the local agricultural waste as a primary feedstock for functional biopolymer development. However, raw cellulose extracted from agricultural sources suffers from high hydrophilicity and moderate thermal stability, limiting its industrial applications. This study aims to extract micro-scale cellulose from local peanut husks, modify its surface functional groups through chemical acetylation, and evaluate the resulting structural, thermal, and morphological changes.

METHODS: Raw peanut husks underwent sequential chemical treatments, beginning with alkaline hydrolysis using sodium hydroxide (NaOH) to remove hemicellulose, followed by sodium hypochlorite (NaOCl) as a bleaching agent to remove lignin, followed by acid hydrolysis with sulfuric acid (H2SO4) to expose the hydroxyl groups. The extracted cellulose was surface modified through esterification using glacial acetic acid and acetic anhydride. Structural and chemical functional group changes were characterized using the Fourier Transform Infrared Spectroscopy (FTIR). The crystallinity index was measured through X-Ray Diffraction (XRD), surface morphology was inspected using Scanning Electron Microscopy (SEM), and thermal stability profiles were determined using Thermogravimetric Analysis (TGA).

RESULTS: Spectroscopic analysis will confirm that the non-cellulosic matrix components will be successfully removed and verified by the introduction of acetyl groups (-COCH3) after modification. XRD analysis will show an increase in the Crystallinity Index after the alkaline and bleaching pre-treatments due to the removal of amorphous hemicellulose and lignin, followed by a controlled decrease in Crystallinity Index after acetylation due to the disruption of internal hydrogen bonding. SEM will show a transition from rough raw husk to smooth, clean microfibers after extraction. TGA will show enhanced degradation temperatures and reduced moisture absorption for the acetylated cellulose.

CONCLUSION: It will be concluded that high-purity cellulose micro-fibers will be successfully isolated from peanut husks and surface modified through acetylation. The resulting hydrophobic and thermally stable modified cellulose will show a strong potential as a functional biopolymer for applications in bio-composites, eco-friendly packaging, and environmental remediation.

Keywords: Cellulose, Peanut husks, Acid Hydrolysis, Acetylation, Scanning Electron Microscopy

P#7–Cigarette butt waste as a carbon precursor for high-performance supercapacitor application

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Cigarette butt waste is a globally abundant and environmentally hazardous form of biomass waste that can be valorized into carbon materials for energy storage (Torkashvand et al., 2020; Wang et al., 2017). This study investigated the conversion of discarded cigarette butts into functionalized carbon for supercapacitor electrode applications. Cigarette butt waste was subjected to hydrothermal carbonization to produce hydrochar (HC), followed by nitric acid activation to obtain functionalized hydrochar (FHC). The materials were characterized using Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, Brunauer–Emmett–Teller (BET) analysis, cyclic voltammetry (CV), and galvanostatic charge–discharge (GCD) measurements. FTIR confirmed the introduction of oxygen-containing and nitro functional groups after activation, while Raman spectroscopy showed increased structural disorder, with the D/G ratio increasing from 3.9 for HC to 4.5 for FHC. BET analysis demonstrated an increase in surface area from 120.7 to 167.6 m^2/g and pore volume from 0.15 to 0.18 cm^3/g. Electrochemical measurements (figure 1) showed that FHC exhibited enhanced capacitive behavior compared with HC, attributed to the combined contribution of electric double-layer capacitance and pseudocapacitance. These findings demonstrate the potential of cigarette butt-derived FHC as a sustainable electrode material for supercapacitor applications.

a) b)

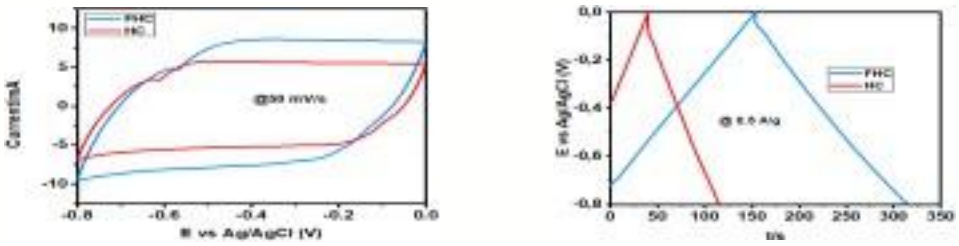

Figure 1: voltammetry(a) and galvanostatic charge–discharge (GCD)(b) profiles of hydrochar (HC) and functionalized hydrochar (FHC) electrodes, showing their electrochemical behavior at a scan rate of 50 mV/s and a current density of 0.5 A/g, respectively

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P#8–Optimized Ultrasound-Assisted NADES Extraction and Bioactivity Evaluation of *Cassia abbreviata* Leaf Metabolites

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Cassia abbreviata is a medicinal plant widely used in African traditional medicine due to its therapeutic properties, which are driven by diverse bioactive metabolites like phenolic compounds [1]. Conventional extraction methods often rely on toxic organic solvents, prolonged processing times, and limited selectivity,compromising both the quality of the extracts and environmental sustainability [2]. This study aimed to develop a green, efficient extraction method combining natural deep eutectic solvents (NADES) with ultrasonic-assisted extraction (UAE). NADES were synthesized using choline chloride as a hydrogen bond acceptor paired with various donors (urea, oxalic acid, citric acid, glycerol, and ascorbic acid), with their formation confirmed through FTIR Spectroscopy. Antioxidant activities were evaluated using TFC, DPPH radical scavenging, and FRAP assays. The NADES-UAE screening yielded lower concentrations of bioactive compounds when compared to the traditional 80% methanol. However, optimization of extraction parameters (ultrasonic temperature, solvent volume, sample mass, extraction time, and sample pH) yielded higher concentrations of bioactive compounds with enhanced antioxidant properties. Ultimately, the optimized NADES achieved a radical scavenging effect of 74%, outperformin the 54.31% achieved by 80% methanol. These results confirm that NADES-UAE is a promising, greener alternative method for extracting bioactive compounds in medicinal plants.

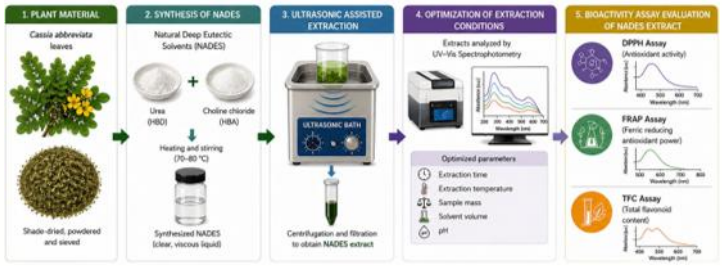

Figure 1: Overview of the NADES-UAE extraction and bioactivity evaluation process.

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P#9–Synthesis of 3-aminoazaindole derivatives and their biological evaluations as possible anticancer agents

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Cancer is a health burden worldwide. The mortality rate from this malignancy continues to rise drastically. Cancer deaths have surpassed all malignancies, including communicable diseases. Global Cancer Observatory (GLOBOCAN) has reported 20.6 million cancer cases and 9.8 million deaths worldwide in 2024, a rise in comparison to the 2023 report, with 18.5 million cases and 9.6 million deaths reported [1]. Azaindole derivatives are very important scaffolds in medicinal and microbial chemistry. Literature has revealed that they possess a wide spectrum of biological and antimicrobial activities [2]. Ten 3-aminoazaindole derivatives have been synthesised and purified using flash chromatography. The structures of the synthesised compounds were confirmed using the spectral methods, F-TIR, ^{1}H-NMR, and ^{13}C-NMR. The activity of the synthesised compounds was tested on T47D breast cancer, HELA cancer cell lines, and normal Hek-293 kidney cells. The mode of cell death induced by the synthesised compounds will be analysed using the Annexin-V-FLUOS staining kit.

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P#10–Experimental And Quantum Chemical Study Of Some Chalcone Derivatives As Possible Corrosion Inhibitors For Mild Steel In Acidic Medium

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Corrosion presents a formidable challenge in industrial applications, significantly compromising the structural integrity and operational efficiency of mild steel components [1]. Organic inhibitors (such as chalcones) serve as critical defence by establishing a protective molecular film on the metallic surface, which acts as a barrier against the aggressive acidic environment [2]. In chalcone derivatives, this process is facilitated by the presence of aromatic rings and heteroatoms such as oxygen or nitrogen, which provide the necessary electron density to form coordinate bonds with the metal surface [1][3]. These compounds allow for electronic modifications that optimize their adsorption strength and inhibition performance [3]. In this work, chalcone derivatives, namely: **1**, **2**, and **3** were investigated as potential corrosion inhibitors for mild steel in a 1M HCl solution using gravimetric measurements and characterised using SEM, EIS, PDP, and modelled through DFT (Density Functional Theory). The inhibition efficiency (%IE) were found to be 68.21%, 90.78%, and 77.01% for **1**, **2**, and **3** respectively. DFT's computations for ΔE (HOMO-LUMO gaps) are 4.751 eV, 3.944 eV, and 4.187 eV for compounds **1**, **2**, and **3** respectively. %IE results concur with the DFT's findings of ΔE.

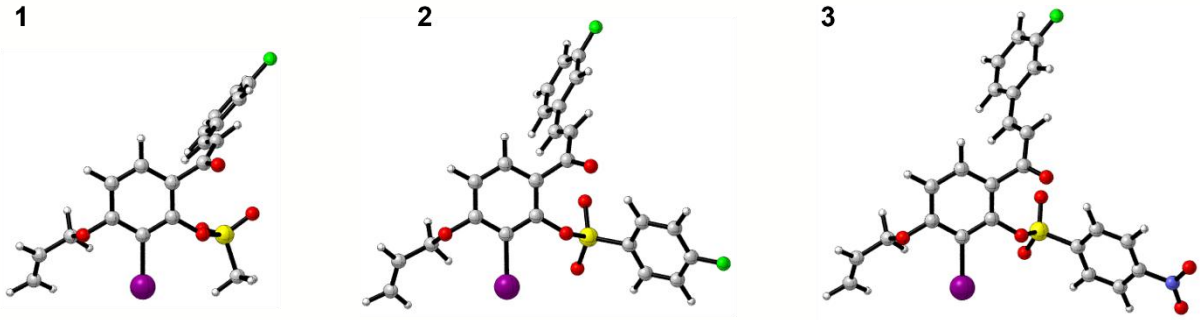

Figure 1: Chalcones used: **1**. M-methanesulfonate **2**. M-4-fluorobenzenesulfonate **3**. M- 4-nitrobenzenesulfonate, where M = (E)-3-(allyloxy)-6-(3-(3-fluorophenyl) acryloyl)-2-iodophenyl.

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P#11–Physico-Chemical Characterisation and Metal Speciation Analysis of Selected Processed Meat Products

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Processed meats are widely consumed in South Africa for convenience and shelf life, yet differences in formulation and processing influence their physico-chemical properties, preservative content and metal composition. Iron and chromium are of interest because toxicity and bioavailability depend on chemical form rather than total concentration [1]. This study characterises selected products and determines iron and chromium speciation.

Smoked and chicken Vienna sausages were purchased from retail outlets and homogenised. Colour was recorded visually, pH determined in triplicate on a 1:10 aqueous homogenate, and moisture by oven-drying at 105 °C, with dry matter by difference. Nitrate and nitrite are being determined by ion chromatography [2], total iron and copper by flame atomic absorption spectrometry after acid digestion, and iron and chromium speciation by a validated method selected for species stability.

Chicken Vienna sausages were more acidic than the smoked product (pH 5.52 ± 0.08 against 6.04 ± 0.04, n = 3) and higher in moisture (68.0 % against 63.8 %), while the smoked product was darker and carried about four percent more dry matter. Nitrate, nitrite and speciation work is ongoing.

The study will provide baseline speciation data for South African processed meats.

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P#12–Synthesis Of Sulfonyl Containing Thiazolidine-2,4-dione (TZD) Derivatives As Potential Anticancer Agents.

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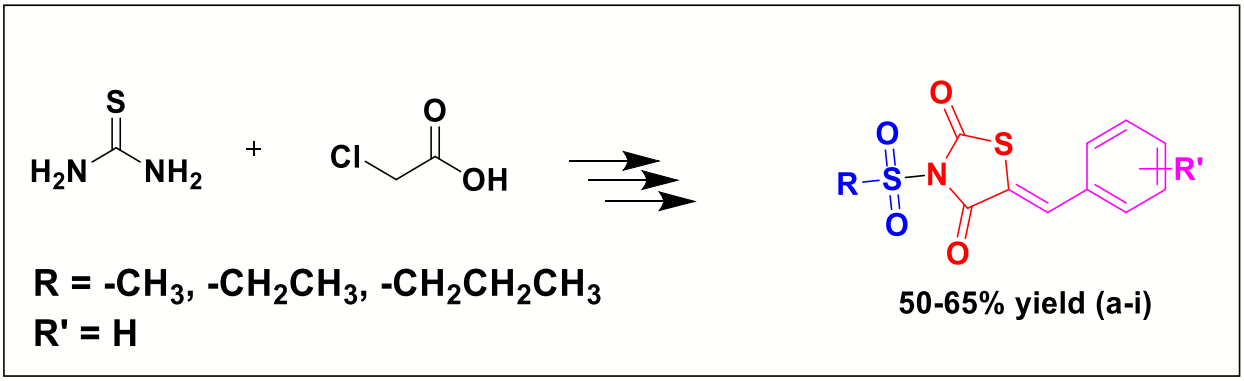
Cancer remains a leading cause of morbidity and mortality worldwide, highlighting the urgent need for the development of new and effective anticancer agents [1]. Organic compounds containing the sulfonyl and thiazolidine-2,4-dione (TZD) frameworks have demonstrated biological potential and structural flexibility suitable for anticancer drug design [2]. This study demonstrates the synthesis and biological evaluation of a series of novel sulfonated thiazolidine-2,4-dione derivatives as potential anticancer agent.



Keywords: Sulfonyl, thiazolidine-2,4-dione, morbidity, mortality.

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P#13–Synthesis, Characterization and Biological Evaluation of Iron(II) and Silver(I) Complexes as Potential Antitubercular Agents

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The increasing prevalence of antimicrobial resistance highlights the need for alternative therapeutic strategies. This study investigated six iron(II) and silver(I) complexes derived from salicylic acid, succinic acid, and mixed salicylate-succinate ligands as potential antimicrobial and antitubercular agents. The complexes were characterized using FTIR, UV-Vis, TGA, PXRD, and XRF, supported by DFT and TD-DFT calculations to investigate their proposed structures and electronic properties.

Antimicrobial activity was evaluated against Staphylococcus aureus, Pseudomonas aeruginosa, and Candida albicans. Silver(I) complexes demonstrated broader antimicrobial activity than the iron(II) complexes, with the mixed-ligand silver(I) complex showing the most consistent activity. Antitubercular activity against Mycobacterium tuberculosis H37Rv was assessed using the Microplate Alamar Blue Assay. All three silver(I) complexes exhibited activity at concentrations of ≤0.125 mg/mL, whereas the iron(II) complexes showed no detectable activity at concentrations up to 2 mg/mL. Silver(I) coordination also enhanced the activity of salicylic acid, which showed an MIC of 0.5 mg/mL. Overall, the findings demonstrate that metal identity and ligand environment influence the biological activity of the complexes and support further investigation of silver(I) coordination compounds as potential antitubercular leads.

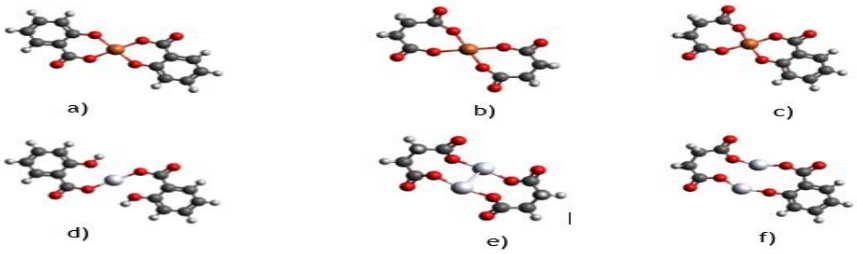

Figure 1: Optimized structures of: a) Iron(II) salicylate, b) Iron(II) succinate, c) Iron(II) salicylate-succinate, d) Silver(I) salicylate, e) Silver(I) succinate, and f) Silver(I) salicylate-succinate

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P#14–SYNTHESIS AND APPLICATION OF MAGNETITE-CELLULOSE-MULTI-WALLED CARBON NANOTUBES FOR THE REMOVAL OF COPPER IONS FROM AQUEOUS SOLUTIONS

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Copper contamination in water from industrial activities poses significant environmental and public-health risks due to its persistence, bioaccumulation potential, and toxicity at elevated concentrations [1,2]. Therefore, this study aimed to synthesise and optimise a magnetite-cellulose-multi-walled carbon nanotube (Fe_3O_4-cellulose-MWCNT) nanocomposite for the removal of Cu^{2+} ions from aqueous solutions. The synthesised materials were characterised using Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDX), thermogravimetric analysis (TGA), X-ray diffraction (XRD) and Brunauer–Emmett–Teller (BET) surface-area analysis. Batch adsorption experiments were conducted, and the optimum adsorption conditions were obtained at pH 6, an adsorbent dosage of 0.8 g/L, an initial Cu^{2+} concentration of 20 mg/L and a contact time of 120 minutes. Among the investigated composites, 10% Fe_3O_4-MWCNT/cellulose-ECH exhibited the highest adsorption performance, achieving more than 95% removal of Cu^{2+} ions from aqueous solutions.

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P#15–Metal-ion selectivity of vanillin and vanillic acid towards M^{n+} cation (M^{n+}=Fe^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+} and Pd^{2+})

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A theoretical investigation was performed with the aim of establishing the relative binding preferences of vanillin (*V*) and vanillic acid (*VA*) ligand (L) species towards biologically relevant free transition metal cations, including Fe^{2+}, Fe^{3+}, Cu^{2+}, Zn^{2+} and Pd^{2+}. The study was performed using the B97-1/def2-TZVP level of theory for Fe^{2+}, Fe^{3+}, Cu^{2+} and Zn^{2+} complexes, and the B97-1/ZORA-def2-TZVP(-f)/SARC-ZORA-TZVP approach for Pd^{2+} complexes. Geometric, thermodynamic, and electronic properties were evaluated across different ligand protonation states, ligand-to-metal cation ratios, and solvation environments. Solvent effects were modelled using the SMD continuum solvation model to represent polar (water) and non-polar (butyl acetate) biological environments. Deprotonated 2:1 ligand-to-metal complexes were consistently identified as the most thermodynamically stable [1], and a comparison of their calculated Gibbs free energies reveals the following order of metal-ion binding affinity: Pd^{2+} > Fe^{3+} > Cu^{2+} > Zn^{2+} > Fe^{2+}. This trend is consistently observed for both *V* and *VA* across all ligand protonation states and solvent environments, although the magnitudes of the binding free energies are greater in butyl acetate than in water. Furthermore, ligand deprotonation substantially strengthens metal coordination, producing more thermodynamically favourable complexes than the corresponding neutral ligands. Overall, the theoretical findings in this study are consistent with previously reported studies, which indicate that Pd^{2+} exhibits a stronger binding affinity than other metal cations utilised in this study [2,3].

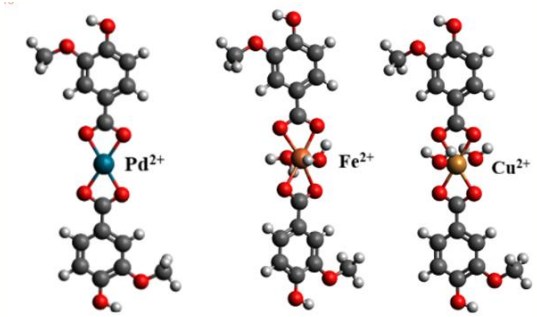

Figure 1: Selected *VA*···M^{n+}···VA complexes with M^{n+} = Fe^{2+}, Cu^{2+} and Pd^{2+} cations.

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P#16–Mixed Ligand Metal–Organic Frameworks containing Naphthalene Diimide ligands: Synthesis and Structural Characterization

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Metal-organic frameworks (MOFs) are highly porous, crystalline materials synthesized from metal-containing nodes linked by organic molecules [1]. The metal ions, sometimes referred to as secondary building units, serve as joints connected by multidentate organic ligands, yielding 1-, 2-, and 3-dimensional networks [1]. MOFs are widely recognized for their properties, such as having high surface area, high porosity, stability, and tunable pore size and shape. They can be synthesized using several methods, such as solvothermal, mechanochemical, and slow-evaporation methods [2]. They can also be used in several applications, including gas storage and separation, drug delivery, catalysis, sensors, and the purification of polluted water [3]. The aim of this study was to synthesize novel MOFs containing diimide ligands for carbon dioxide adsorption studies. Two ligands namely 2,2'-(1,3,6,8-tetraoxo-1,3,6,8tetrahydrobenzo[lmn][3,8] phenanthroline-2,7-diyl)diacetic acid (Lig1) and 2,7-di(pyridin4-yl)benzo[lmn][3,8] phenanthroline-1,3,6,8(2H,7H)-tetraone (Lig2) were successfully synthesized and characterized. Lig1 is a carboxylate O-donor ligand, and Lig2 is a pyridyl N-donor ligand. Two new MOFs were successfully synthesized and characterized using single-crystal X-ray diffraction (SCXRD), thermogravimetric analysis (TGA), powder X-ray diffraction (PXRD), and variable-temperature PXRD. The SCXRD results showed that MMS01 has a one-dimensional structure, while MMS02 has a three-dimensional structure. The PXRD analysis indicated that MMS01 is phase-pure, and the TGA results showed that both MMS01 and MMS02 exhibit similar thermal stability, with a range of 370-385 °C.

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P#17–ATPE-based extraction of organophosphate insecticides from landfill sites

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Organophosphate insecticides are commonly utilized in consumer products, resulting in their ongoing release into the environment following disposal, notably in landfills [1]. Their persistence, mobility, and toxicity pose serious threats to human health and ecosystems. Conventional methods such as solid-phase extraction have been reported to have shortfalls such as matrix interferences and a lack of durability [2]. This study suggests using an aqueous two-phase extraction (ATPE) system to extract organophosphate insecticides from landfill sites. The approach will entail optimizing parameters: pH, salt concentration, and extraction duration, to improve recovery [3]. The optimized approach will be applied to real landfill leachate from Thohoyandou, which will then be analyzed using High-Performance Liquid Chromatography (HPLC). This approach is expected to improve extraction efficiency, reduce environmental effects, and provide valid data for organophosphate pesticide contamination monitoring while supporting sustainable environmental management and green analytical chemistry.

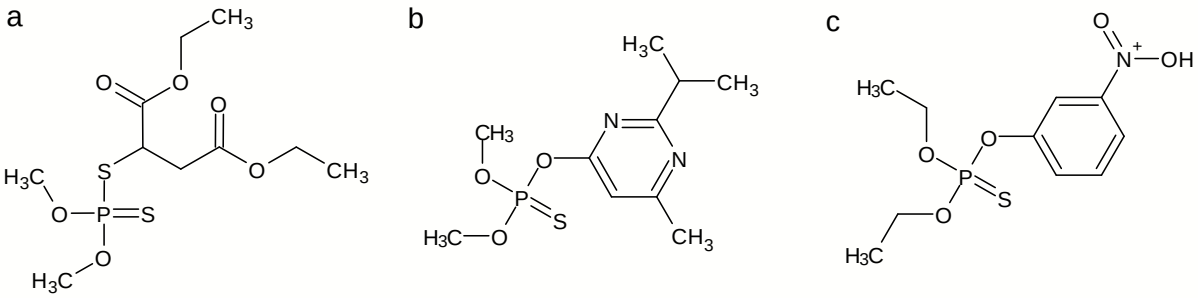

Figure 1: Organophosphate insecticides to be extracted from a landfill site, where (a) Malathion, (b) Diazinon, and (c) Parathion

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P#18–Synthesis of chitosan blended with TiO_2 doped MWCNTs nanocomposite materials for removal of pharmaceuticals from water

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Among varieties of water organic pollutants, pharmaceuticals are the most abundant class of pollutants showing toxic effects on human health [1]. The persistence of diclofenac in aquatic environments and its associated ecotoxicological risks necessitate the development of efficient and reusable adsorbent materials for its removal from water [2]. In this study, chitosan (CTS)-based nanocomposites incorporating titanium dioxide and functionalised and nitrogen-doped multiwalled carbon nanotubes were synthesised and evaluated as adsorbents for DCF removal from aqueous solution. The materials were characterised by FTIR, zeta potential, TGA, SEM-EDS, and BET surface area analysis. Adsorption studies revealed optimal DCF removal within 45 min of the adsorption equilibrium time, with a maximum removal efficiency of 89% at pH 4.5, a dose of 1 g/L, and 25 °C. Adsorption kinetics were best described by the pseudo-second-order model, indicating a chemisorption-dominated mechanism, while thermodynamic analysis confirmed the process was exothermic and spontaneous. Subsequent photocatalytic degradation of the adsorbed and residual DCF further enhanced the removal efficiency to 94%.

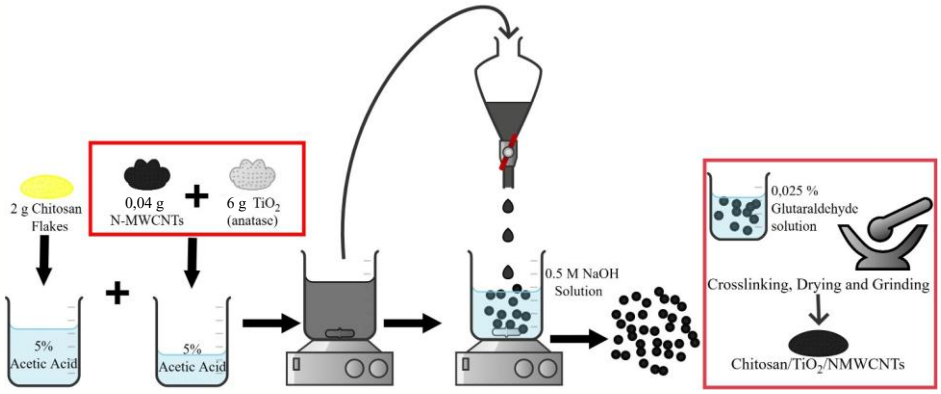

Figure 1: preparation of Preparation of chitosanN-MWCNT/TiO_2.

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P#19–Synthesis and Characterization of Nitrogen-Doped $ZnAl_2O_4$ Nanoparticles for Enhanced Photocatalytic Degradation of Organic Dyes in Wastewater

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Dye-containing industrial effluents pose an environmental risk owing to the persistence and toxicity of synthetic dyes in water systems. Zinc aluminate ($ZnAl_2O_4$) is an attractive photocatalyst owing to its stability and non-toxicity, but its wide band gap (3.8-4.0 eV) and rapid electron-hole recombination limit its activity [1-3]. This study examines the effect of nitrogen doping on the structural, optical and photocatalytic properties of $ZnAl_2O_4$:x % N (x = 0-2.00 %) nanoparticles synthesized by the sol-gel method. XRD confirmed phase-pure cubic spinel $ZnAl_2O_4$ in all samples, with crystallite size peaking at 23.1 nm for 0.50% N. FTIR and EDS verified the expected framework vibrations and elemental composition. UV-Vis showed the narrow gap extending visible-light absorption, while SEM showed more uniform, less agglomerate morphology with increasing nitrogen content. Photocatalytic degradation of methylene blue under UV light rose from 41.4 % (undoped) to 72.2 % at 0.50 % N after 60 min, then declined at higher loadings despite the narrower band gap at 2.00 % N, showing excessive doping promotes recombination. These results identify 0.50 % N as the optimum level, balancing light absorption and charge-carrier separation, and highlight nitrogen-doped $ZnAl_2O_4$ as an effective, low-cost photocatalyst for wastewater treatment.

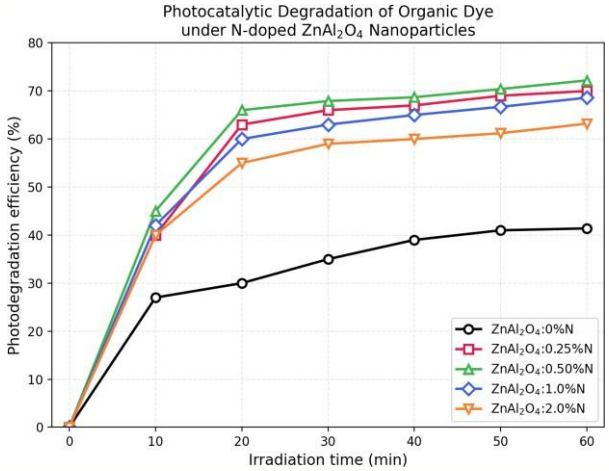

Figure 1 Photodegradation efficiency (%) of $ZnAl_2O_4$:x % N nanoparticles versus irradiation time.

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P#20–Discrimination of isomers using host compounds containing an imide functional group

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Host-guest chemistry is the branch of supramolecular chemistry concerned with the study of non-covalent interactions between a host compound and a guest [1]. The host is defined as a crystalline material capable of accommodating guest species either through cavity-based inclusion or surface binding. Guests are compounds enclosed within or bound to the cavity or binding sites of the host compound [2]. Host compounds can be organic or metal-organic and have numerous applications, one of the most prominent being liquid separation [3]. This application includes the separation of both isomeric and non-isomeric mixtures. This study focuses on the separation of isomeric mixtures, which presents a significant challenge due to the structural similarities among isomers. Existing methods for separating isomers are often energy-intensive, costly, and complex [4].

This study investigates the ability of imide-functionalized host compounds to discriminate picoline isomers. We report the synthesis and characterisation of two organic host molecules: 2-(carboxymethyl)-1,3-dioxoisoindoline-5-carboxylic acid (Host-1) and N-Phthaloylglycine (Host-2). These hosts were exposed to mixtures of picoline and lutidine isomers, and the resulting host–guest complexes were analysed using single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), gas chromatography (GC), and thermogravimetric analysis (TGA). Hirshfeld surface analysis will also be performed to quantify the intermolecular interactions within the complexes. The findings from these techniques are discussed, with a focus on the host compounds' selectivity and preference for specific isomers.

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P#21–Effects of hybridization of sugarcane bagasse cellulose and cotton cellulose on the morphology and thermal properties of LDPE and HDPE nanocomposites

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Low-density polyethylene (LDPE) and high-density polyethylene (HDPE) are widely used thermoplastic polymers owing to their versatility, chemical resistance and ease of processing (Sanjay *et al.*, 2018). However, their extensive use contributes to persistent plastic waste, creating a need for more sustainable approaches to polymer utilization. This study proposes the development of LDPE and HDPE based composites reinforced with sugarcane bagasse and cotton fiber to improve their thermal properties while promoting the use of renewable lignocellulosic resources.

The study will investigate the influence of sugarcane bagasse and cotton fiber incorporation on the thermal behavior of LDPE and HDPE and compare the resulting properties with those of the neat polymer matrices. Attention will be given to thermal stability and melting behavior to establish the extent to which natural-fiber reinforcement can enhance the thermal performance of the polyethylene matrices. Natural fibers are hydrophilic, whereas polyethylene is hydrophobic, resulting in poor interfacial compatibility that can influence the performance of natural-fiber reinforced polyethylene composites (Zulkipli *et al.*, 2022). Therefore, the study will also consider the role of fiber-matrix interaction and, where appropriate, compatibilization in achieving improved composite performance. The expected outcome is a better understanding of how reinforcement type and polymer matrix affect the thermal properties of LDPE and HDPE – based composites. The developed materials may have potential for engineering applications in which improved thermal performance of polyethylene components is required. In addition, the incorporation of sugarcane bagasse and cotton fiber provides an opportunity to valorize natural resources and support the development of more sustainable polymer composite materials (Shan *et al.*, 2022). Overall, the study aims to contribute to the development of natural-fiber reinforced engineering relevance.

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P#22–Photochemical and Conformational Modulation of Cinnamoyl-Chloroquine Hybrids for Targeted Antimalarial Drug Design

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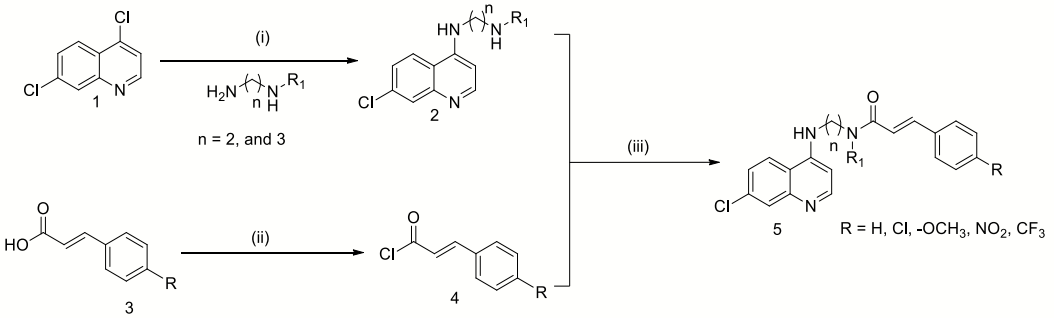
Malaria is a global infectious disease caused by parasites of the Plasmodium genus [1]. Its treatment is difficult due to many factors, including the toxicity of the drugs currently in use and the development of resistance by the parasite [2]. Due to the aforementioned difficulties in treating malaria, the development of new, more effective antimalarial agents is needed. Synthesis of cinnamoyl-chloroquine hybrids was based on the hybridization of cinnamic acid and chloroquinoline pharmacophore, as shown in Scheme **1**. Twenty (20) cinnamoyl-chloroquine Hybrids were successfully synthesized and photoisomerized under UV light irradiation. ^{1}H NMR confirmed that the hybrids co-exist as *anti-* and *syn-rotamers* at room temperature due to their minimal energy difference. ^{1}H NMR confirmed the presence of both trans and cis products after UV irradiation, and Preliminary antiplasmodial activity showed promising results against NF54. Variable-temperature NMR and NOESY will be used to study conformational dynamics. Furthermore, the cytotoxicity and antiplasmodial activities of the synthesized compounds will be evaluated against chloroquine-sensitive and resistant strains of *P. falciparum*.



Scheme 1: (i) Reflux for 18h, (ii) toluene, 3 drops of DMF, RT, 3 h (iii) Dry DCM, TEA, RT, 24h

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P#23–Rational Design and Antiplasmodial Evaluation of Cinnamoyl-Chloroquinoline Hybrids: Exploring Linker and Cinnamoyl Substituents Effects

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Cinnamoyl-chloroquinoline hybrids represent a promising class of compounds for antimalarial drug discovery through the molecular hybridization of two biologically relevant structural scaffolds[1-2]. This study focused on the synthesis and optimization of cinnamoyl-chloroquinoline hybrids and investigated how structural modifications affect their antiplasmodial activity. Computational studies were performed, including molecular docking to investigate ligand-protein interactions and molecular dynamics simulations to assess the stability of selected protein-ligand complexes. A series of cinnamoyl chloroquinoline hybrids with different cinnamoyl substituents and varying linkers was synthesized and characterized using spectroscopic and analytical techniques, including NMR, FTIR, and melting-point. The antiplasmodial activities of the synthesized compounds were evaluated against the *Plasmodium falciparum* NF54 strain to establish structure-activity relationships. Substitution on the cinnamoyl moiety influenced the antiplasmodial activity of the synthesized hybrids, demonstrating the importance of electronic and structural effects in compound optimization.

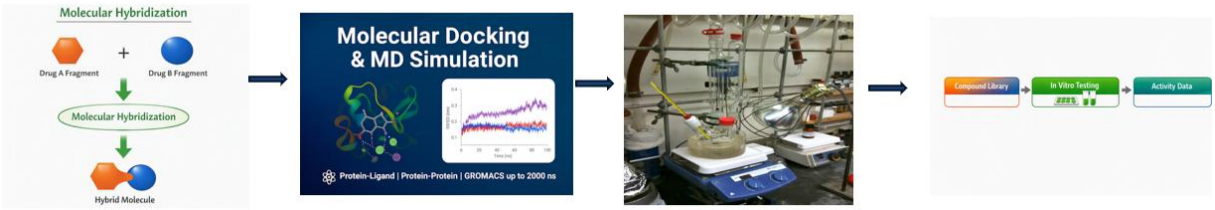

Figure 1: Simple flow diagram of the project

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P#24–Application of Pearson Correlation Bivariate Matrix for Identifying Metabolites in *Tapinanthus Quequensis* Plant Extracts Crude for Corrosion Inhibitory Effects on Aluminum and Mild Steel in an Acidic Medium

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Corrosion is a naturally occurring process in which metals and alloys undergo chemical reactions with their environment, driving them towards a more stable thermodynamic state [1]. Plant extracts used as corrosion inhibitors have the disadvantage that it's not easy to pinpoint the exact metabolites responsible for corrosion inhibition activity [2]. The Pearson correlation bivariate matrix technique can be used to pinpoint the metabolites extracted that are responsible for corrosion inhibition. This study investigates the use of the Pearson bivariate correlation matrix to isolate the active anti-corrosive metabolites in *Tapinanthus quequensis* plant extracts against aluminum and mild steel in acidic environments. This study aims to investigate the potential for inhibition and identify the metabolites in the *T. quequensis* plant extract responsible for corrosion inhibition of aluminum and mild steel in an HCl medium. A range of techniques will be employed to evaluate the inhibition efficiency, corrosion mechanisms, and adsorption behavior of the plant-based inhibitors. Electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) were used to analyze the electrochemical properties, while gravimetric analysis assessed metal loss and inhibitor performance. Fourier-transform infrared spectroscopy (FTIR) will be used to identify the functional groups responsible for metal-inhibitor interactions. Liquid chromatography-mass spectrometry (LC-MS) will be employed to verify the main phytochemical constituents of the *T. quequensis* extract. In addition, scanning electron microscopy (SEM) combined with energy-dispersive spectroscopy (EDS) will be employed to examine the surface morphology of the metals in the presence and absence of the inhibitors. *T. quequensis* reduced the corrosion rates of aluminum and mild steel in 1.0 M HCl.

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P#25–Design, synthesis and *in silico* evaluation of novel A_2B and ABC 1,2,4-triazine based ethionamide hybrids as potential anti-TB agents

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Tuberculosis (TB), caused by *Mycobacterium tuberculosis (Mtb.)*, remains a major global health challenge, particularly in sub-Saharan countries like South Africa.[1] The emergence of drug-resistant strains and the shortcomings of current treatment regimens such as long treatment duration and severe side effects, necessitate the need to develop novel therapeutic agents with high potency and reduced toxicity.[2] In this present study, we have explored 1,2,4-triazine as a scaffold for the design of ethionamide-based hybrid compounds through computational methods. A focused library of 35 ethionamide containing 1,2,4-triazine hybrids were investigated using molecular docking, *in silico* ADME profiling and PkCSM. The library was divided into two structural series (A_2B and ABC) based on the substitution of different functional groups on the 1,2,4-triazine core.

The molecular docking studies were assessed against two selected *Mtb.* protein targets represented by the structures 2BX8 and 4PY8. The compounds were evaluated based on their predicted docking scores and binding interactions within the respective protein binding sites. The docking scores ranging from −4.643 to −8.779 for 4PY8 and from −3.406 to −7.925 for 2BX8. In addition, the SwissADME and PkCSM results revealed favorable pharmacokinetic properties and acceptable toxicity.

As part of our ongoing research towards the synthesis of novel A_2B and ABC 1,2,4-triazine based ethionamide hybrids in Figure 1, we report herein the structurally diverse amines to afford a series of A2B and ABC analogues.

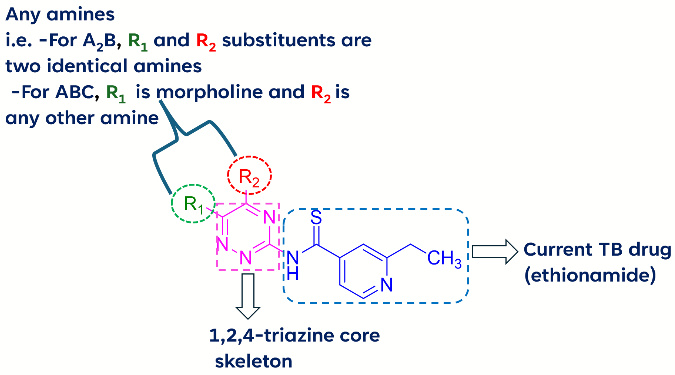

Figure 1: Basic skeleton of hybridisation of 1,2,4-triazine core

P#26–Design, Synthesis and Biological Evaluation of Tetrahydroquinozoline Derivatives as Antimalarial Agents

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Malaria remains one of the world's most significant infectious diseases, particularly in sub-Saharan Africa, where Plasmodium falciparum accounts for a large proportion of malaria-related illness and deaths [1]. The emergence and spread of drug-resistant Plasmodium falciparum strains threaten the effectiveness of current antimalarial therapies [2-3]. This highlights the urgent need to discover new antimalarial agents with improved efficacy and novel mechanisms of action.

This study aims to design, synthesize, and biologically evaluate a series of novel tetrahydroquinozoline derivatives as potential antimalarial agents. The target compounds will be synthesized using standard organic synthesis methods, purified, and characterized by spectroscopic techniques including Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FTIR), and Mass Spectrometry (MS). The synthesized compounds will be evaluated for in vitro antiplasmodial activity against *Plasmodium falciparum* strains and assessed for cytotoxicity using mammalian cell lines to determine their selectivity and metabolic stability. The biological evaluation will be conducted at H3D, University of Cape Town.

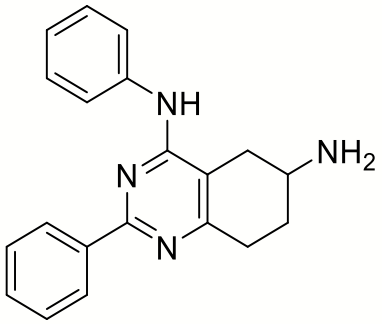

Figure 1: Structure of tetrahydroquinazoline.

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P#27–Eco-Friendly Magnetic Solid Phase Microextraction of Parabens from Water Samples by Biosorbents Synthesized from Avocado Seed.

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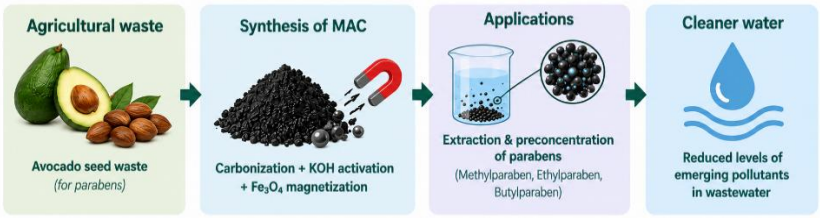
Emerging pollutants such as parabens in water systems pose significant risks to human and ecological health, highlighting the need for effective monitoring and remediation strategies [1]. This study developed a low-cost magnetic activated carbon (MAC) biosorbent from avocado seeds for the simultaneous extraction and preconcentration of methylparaben, ethylparaben, and butylparaben using dispersive magnetic solid-phase microextraction (DMSPME). Experimental parameters were optimized using a fractional factorial design for screening and a central composite design for further optimization. Characterization confirmed successful synthesis of the MAC, with a surface area of approximately 30 m^2/g and a pore volume of 0.1 cm^3/g. SEM, EDS, and FTIR analyses confirmed the porous structure, elemental composition, and functional groups associated with the biosorbent. The 30% KOH-MAC demonstrated the best extraction performance, with optimal conditions of 22.5 mg biosorbent, pH 6.5, and 875 µL of methanol as the elution solvent. Under these conditions, relative recoveries of 80.0–101% were achieved, with LODs of 0.008–0.019 µg/L and LOQs of 0.052–0.090 µg/L. The biosorbent demonstrates its potential as a low-cost, sustainable material for the simultaneous extraction of parabens from wastewater.

Graphical abstract:



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P#28–Synthesis, characterization and *in silico* studies of quinazoline-containing anti-TB drugs with 1,3,5-triazine as a linker

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Tuberculosis (TB) is an infectious disease that mainly affects the lungs and is caused by the bacterium *Mycobacterium tuberculosis*, and it remains a major global health challenge despite being preventable and curable [1,2]. This study aims to synthesize quinazoline-based anti-TB drugs with 1,3,5-triazine as a linker. Molecular hybridization was employed to combine the 4,7-dichloroquinazoline scaffold with the 1,3,5-triazine moiety (**Figure 1**), thereby developing novel hybrid compounds with potentially improved biological activity**.** An in-silico approach involving molecular docking, molecular dynamics simulations, MM/GBSA binding free-energy calculations, DFT, and ADMET was used to investigate the binding potential, stability, binding energies, electronic properties, and drug-likeness of the designed compounds against selected *M. tuberculosis* and human protein targets [3,4]. Compounds with promising computational profiles were selected as hit candidates for chemical synthesis and will be evaluated for their biological activity against *M. tuberculosis* at H3D, University of Cape Town.

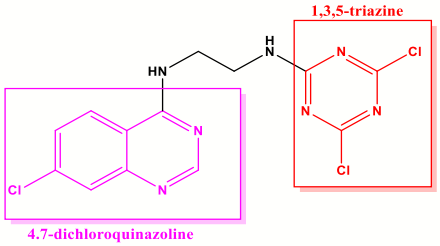

Figure 1: Hybridization of 4,7-dichloroquinazoline and 1,3,5-triazine

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P#29–Crosslinked Chitosan-Glutaraldehyde/ZrO_2 composite for the efficient removal of Ciprofloxacin from aqueous solution.

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Ciprofloxacin (CIP), a broad-spectrum fluoroquinolone antibiotic, is frequently reported due to its high consumption and chemical persistence [1]. Antibiotic existence in aquatic environment causes microorganisms to develop resistance to antimicrobial agents [2]. Glutaraldehyde-crosslinked chitosan-based hybrid nanocomposite was synthesised for the removal of antibiotic Ciprofloxacin and bacteria E. coli from the aqueous solution. The synthesised composites were characterised with Fourier Transform Infrared spectroscopy, Scanning Electron Microscopy, Energy Dispersive X-ray analysis, Thermogravimetric analysis, and BET surface area analysis. Adsorption followed the Langmuir isotherm model and pseudo-second order kinetics, with a maximum adsorption capacity of 36.10 mg g^{-1}. The spontaneous and exothermic nature of adsorption is indicated by negative values of change in Gibbs free energy, enthalpy, and entropy, which also shows decrease in randomness. The systematic examination of photocatalytic degradation of residual CIP in aqueous solution utilising synthesised composites as a photocatalyst activated by UV light was conducted.

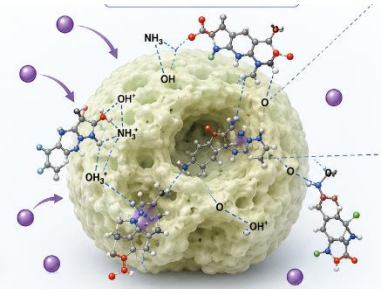

Figure 1: Ciprofloxacin adhesion unto adsorbent composite

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P#30–Characterization of base metals and organics from mine tailings for extraction using ionic liquids

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Gold mine tailings are finely ground residues from mineral processing that can pose environmental risks while also serving as a secondary source of valuable metals and chemical resources [51-2]. This study investigates the extraction of base metals and organic compounds from gold mine tailings using ionic liquids (ILs) to support tailings valorization and reduce the environmental risks of long-term tailings storage. The tailings sample, obtained from the Soweto Cluster tailings dam, was characterized using X-ray fluorescence (XRF), inductively coupled plasma optical emission spectrometry (ICP-OES), inductively coupled plasma mass spectrometry (ICP-MS), Fourier-transform infrared spectroscopy (FT-IR), and gas chromatography-mass spectrometry (GC-MS). Elemental analyses revealed a complex, predominantly aluminosilicate matrix with elevated concentrations of aluminum (30 399mg/kg), iron (21 389 mg/kg), titanium (531 mg/kg), and manganese (208 mg/kg). Potentially hazardous and economically relevant metals, including chromium (144 mg/kg), nickel (109 mg/kg), copper (51.99 mg/kg), zinc (86.29 mg/kg), cobalt (42.95 mg/kg), and vanadium (49.21 mg/kg), were also detected. ICP-MS further revealed a uranium concentration of 78.28 mg/kg, indicating uranium enrichment within the tailings. FT-IR confirmed a predominantly crystalline silicate matrix, while GC-MS screening indicated the presence of trace organic constituents, including 1,2,4-trimethylbenzene and cyclic octaatomic sulfur, with NIST library match scores of 95.5% and 98.0%, respectively. The results demonstrate the polymetallic and organic composition of the tailings and provide a basis for selecting suitable ionic-liquid systems. Future work will focus on optimizing ionic-liquid extraction, recovering and characterizing extracted species, and evaluating ionic-liquid recyclability. The study aims to contribute to the valorization and sustainable management of mine tailings.

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P#31–Fabrication of MoS_2, ZnSe and g-C_3N_4 based heterojunction catalysts and their light driven catalytic degradation of ibuprofen and ciprofloxacin in water

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Pharmaceutical residues, including ibuprofen and ciprofloxacin, can enter aquatic environments through domestic wastewater, healthcare facilities, pharmaceutical manufacturing processes, and agricultural activities. The persistence of these compounds in water highlights the limitations of conventional wastewater treatment processes in achieving their complete removal. Photocatalysis is an advanced oxidation process with considerable potential for the degradation of pharmaceutical contaminants through the generation of reactive oxygen species (ROS), including superoxide radicals ($O_2\bullet^-$) and hydroxyl radicals (•OH), which can promote the mineralization of organic pollutants into relatively harmless products such as CO_2 and H_2O. This study proposes the fabrication of MoS_2/ZnSe, ZnSe/g-C_3N_4, and g-C_3N_4/MoS_2 heterojunction photocatalysts for the visible-light-driven degradation of ibuprofen and ciprofloxacin in aqueous systems. MoS_2 and ZnSe will be synthesized using hydrothermal methods, while g-C_3N_4 will be prepared through thermal polymerization. The structural and chemical properties of the synthesized materials will be evaluated using XRD and FTIR. XRD analysis indicates that MoS_2 exhibits a hexagonal crystal structure, whereas ZnSe adopts a cubic zinc-blende crystal structure. The study aims to establish relationships between heterojunction structure, charge-transfer behaviour, and photocatalytic performance. Ultimately, the research is expected to contribute to the development of reusable, visible-light-responsive photocatalytic materials for the treatment of pharmaceutical-contaminated wastewater and support water recovery in water-stressed environments.

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P#32–Enhanced Base Metal Extraction from South African Coal Fly Ash via Sodium Carbonate Sintering

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The large stockpiles of coal fly ash (CFA) in South Africa present a serious environmental problem; however, the ash is also potentially rich in transition base metals, and could be utilized as an alternative metallurgical raw material [1]. The problem, however, is that of extraction of the metal values from the stable crystalline mullite and quartz phases that enclose the metal values and are not dissolved by acids in conventional extraction procedures [2]. This work investigates the use of thermal activation of the CFA by means of roasting with sodium carbonate (Na_2CO_3) in order to convert the refractory mineral matrices into acid-soluble phases [3]. A selective pre-treatment water wash at 80 °C was used to remove residual, dissolved, alkali and silicate bearing solutions prior to core acid extraction [4]. A series of leaching experiments using 1.5 M HCl at varying liquid-to-solid (L/S) ratios, temperatures and extraction times were conducted on both roasted and unroasted materials [5]. The solid leaching residues were analyzed by X-ray fluorescence (XRF), while the liquid solutions were quantitatively analyzed by ICP-OES at Mintek [6].
The volume contraction was observed for the sintered material with the fixed concentration of Na_2O for the treated matrix at 1.23% as determined by XRF. The water wash acted as a selective pre-leach step to reduce the solid phase impurities of CuO and ZnO to 33.3 ppm and 11.7 ppm respectively from 70.7 ppm and 28.5 ppm for the unroasted material [4]. In contrast the HCl leach of the unroasted material produced a number of heavy mineral cakes that resulted in poor mass dissolution for the unroasted material (13.84%–17.08%) [5]. The roasted material, however, showed excellent dissolution with mass losses of up to 26.48% for the intermediate roasted material with complete dissolution for specific samples. In addition, the absolute amount of metal dissolved increased significantly with iron recovery peaking at 434.25 mg for sample B2 (100 mL) and 428.15 mg for sample C2 (200 mL) as compared with the unroasted control C1 (250 mL) that had a maximum recovery of 156.25 mg [6]. The resulting PLS solutions were found to be stable at room temperature with no sign of silica gel formation. The process of alkaline roasting has therefore effectively disrupted the resistant ash infrastructure and provides a solid basis for the development of downstream sequential precipitation steps to produce high purity fractions of iron, copper and zinc.

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P#33–Synthesis, Characterization and in silico studies of 4- and 5-Oxazolidinedione Derivatives as Potential Antidiabetic Agents

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Type 2 diabetes mellitus (T2DM) remains a major global health challenge, necessitating the discovery of novel therapeutic agents. Oxazolidinediones are heterocyclic compounds with diverse pharmacological activities; however, their antidiabetic potential remains largely unexplored. This study investigates the synthesis and computational evaluation of novel 4- and 5-oxazolidindione derivatives as potential antidiabetic agents. The target compounds are synthesized from commercially available amino acids and substituted benzaldehydes and characterized using FT-IR and NMR spectroscopy. Molecular docking studies against α-amylase and α-glucosidase are performed to investigate binding interactions and inhibitory potential. Molecular dynamics simulations and MM-GBSA calculations are employed to assess the stability and binding affinity of ligand-protein complexes. Furthermore, ADMET predictions and density functional theory (DFT) calculations are used to evaluate pharmacokinetic and electronic properties. The findings of this study are expected to provide insights into the structure-activity relationships of oxazolidinedione derivatives and identify promising lead compounds for the development of new antidiabetic therapies.

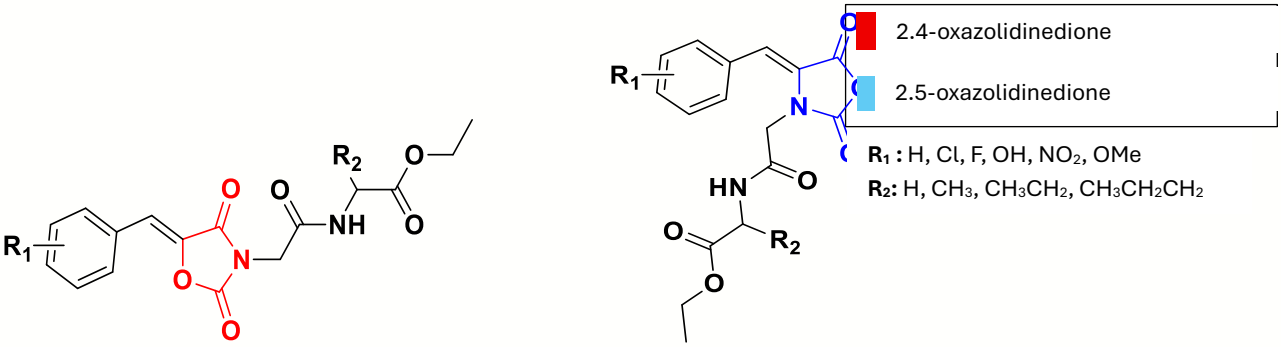

Figure 1: The expected oxazolidinedione final derivatives

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P#34–Synthesis and Properties of Biphenyl-based Electrolyte Additives for Lithium-ion Batteries

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The growing use of electric vehicles and portable electronics has increased the demand for sustainable, clean, and safe energy storage. Lithium-ion batteries (LIBs) are important energy-storage systems with wide industrial applications. However, overcharging can trigger undesirable chemical and electrochemical reactions, rapid temperature increases, thermal runaway, and, in severe cases, fire or explosion. Therefore, this study aimed to address the safety challenges associated with lithium-ion power sources, particularly fire hazards, by synthesizing novel biphenyl-based organic electrolyte additives with potential flame-retardant properties. 1-Amino-2-(4'-methoxyphenyl)-4-methylbenzene was successfully synthesized and characterized as an aromatic amine–type electrolyte additive. Computational chemistry was employed to preliminarily assess the potential of the synthesized compound as an electrolyte additive by evaluating its electronic and molecular properties using density functional theory (DFT). The calculated parameters included the highest occupied molecular orbital energy (HOMO), lowest unoccupied molecular orbital energy (LUMO), energy gap (ΔE), ionization potential (I), electron affinity (A), chemical hardness (η), and dipole moment (μ). These parameters provided insights into the compound's electronic structure, reactivity, polarity, and potential redox behaviour. The compound was further characterized using FTIR, NMR, and flame-retardancy testing to confirm its molecular structure and evaluate its potential contribution to electrolyte safety and thermal stability.

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P#35–Efficacy of synthesized chalcone derivatives as corrosion inhibitors for mild steel in acidic environment

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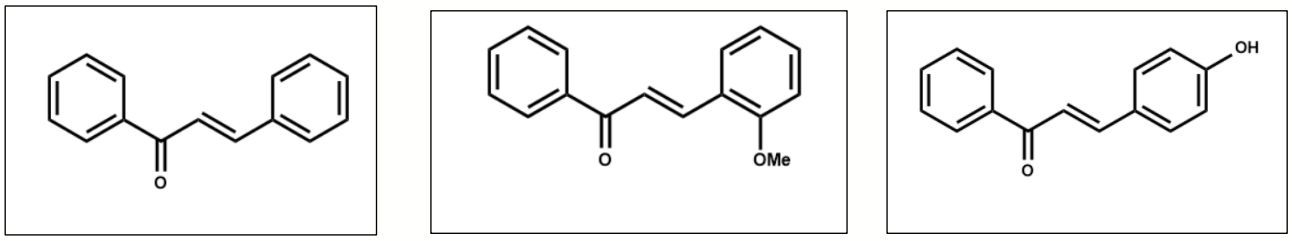
Metals are crucial assets in various industries, but their susceptibility to corrosion are the root cause of many economic, environmental, and well-being calamities [1,2]. Corrosion is a naturally occurring process that affects various industries and infrastructure worldwide costing billions annually in damages and if corrosion is not controlled its effects could be devasting [3,4]. Corrosion cannot be prevented but it can be controlled by utilizing organic corrosion inhibitors that contain heteroatoms and aromatic rings that coordinate to the metal active center. This study utilizes synthesized chalcone derivatives namely; 1,3-diphenylprop-2-en-1-one, 3-(2-methoxyphenyl)-1-phenylprop-2-en-1-one, and 3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one as potential corrosion inhibitors. The synthesized compounds were characterized using spectroscopic techniques such as nuclear magnetic resonance (NMR), and Infrared spectroscopy (IR). The inhibition effects of these compounds were investigated by using gravimetric analysis, potentiodynamic polarization (PDP), electrochemical impedance spectroscopy (EIS), and further calculated the thermodynamic and kinetic parameters. Surface analysis will be done using Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM) and Atomic absorption spectroscopy (AAS) will be utilized to detect the amount of concentration of metals in solutions. The chalcone derivatives were successfully synthesized and characterized using NMR spectroscopy. Weight loss experiments were conducted and the inhibitor compounds showed substantial metal protection with high inhibition efficiency obtained for all three compounds. Based on the observations made 3-(2-methoxyphenyl)-1-phenylprop-2-en-1-one was the best performing inhibitor as compared to the other two inhibitors with its inhibition efficiencies ranging from 70.11% to 99.29% as the concentration and temperature is increased.



(a) (b) (c)

Figure 1: Structures of Inhibitor compounds: (a) 1,3-diphenylprop-2-en-1-one, (b) 3-(2-methoxyphenyl)-1-phenylprop-2-en-1-one, and (c) 3-(4-hydroxyphenyl)-1-phenylprop-2-en-1-one.

P#36–Ag-modified $BiVO_4$ semiconductor for photocatalytic degradation of

Sulfamethoxazole and hydrogen production

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Keywords*: Bismuth-based, sulfamethoxazole, degradation, hydrogen production*. Developing sustainable photocatalysts for wastewater treatment involves achieving a balance between high performance with environmental responsibility [1]. $BiVO_4$, a visible-light response photocatalyst, has considerable attention due to its abundant raw material sources, good stability and low cost however there exist some limitations for further applications due to poor capability to separate electron hole pairs [2-3]. In this work, $BiVO_4$ was synthesised using the hydrothermal route and modified with Ag using the photo-deposition route as an attractive and efficient electron-cocatalyst to reduce the recombination of electron and holes. Analytical techniques such as XRD, SEM, BET, FTIR and UV-DRS were some of the characterization techniques used to confirm the successful synthesis of the materials. Ag modified materials enhanced the optical absorption of $BiVO_4$ in the visible-light region and resulted in a reduced band gap compared with pure $BiVO_4$. This enhancement was associated with the surface plasmon resonance (SPR) of Ag nanoparticles on the $BiVO_4$ surface also promoted charge separation through the formation of a Schottky junction. Consequently, the improved photocatalytic degradation of Sulfamethoxazole (SMX) and hydrogen production performance was mainly attributed to the Ag modification of $BiVO_4$ and its resulting improvement in photogenerated charge separation.

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P#37–Selective extraction of nitroaromatic compounds: Uni- vs multi-templated molecularly imprinted polymers

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Nitroaromatic compounds (NACs) such as 2-nitrotoluene (2-NT) and 2,6-dinitrotoluene (2,6-DNT), are significant environmental pollutants requiring efficient and selective extraction methods for monitoring and remediation. This study details the synthesis and characterization of multi-template molecularly imprinted polymer (MIP) for the simultaneous removal of 2-NT and 2,6-DNT. FTIR analysis confirmed the successful polymerization and verified the incorporation of the templates within the polymer matrix, as well as their subsequent removal after washing. BET analysis revealed a mesoporous structure for the polymers, evidenced by a Type IV isotherm. Crucially, the washed multi-template MIP demonstrated a superior surface area of 43.5 $m^2 g^{-1}$, significantly higher than both the uni-template MIP (31.3 $m^2 g^{-1}$) and the non-imprinted polymer (NIP) control (17.0 $m^2 g^{-1}$). The performance of the MIPs was optimized through batch adsorption experiments. Optimal conditions were determined to be sample pH of 3, which maximized binding interactions, and an adsorbent mass of 15 mg, which yielded the highest imprinting factor of 2.14. Kinetic studies identified an optimal contact time of 30 min, offering an excellent balance of rapid uptake and efficiency by achieving over 91% of the total equilibrium adsorption capacity. Furthermore, adsorption isotherm experiments confirmed that the maximum adsorption capacity (up to 292 µg g^{-1}) was achieved at an initial concentration of 2 mg L^{-1}. These results demonstrate the highly efficient and practical applicability of the synthesized multi-template MIP (1).

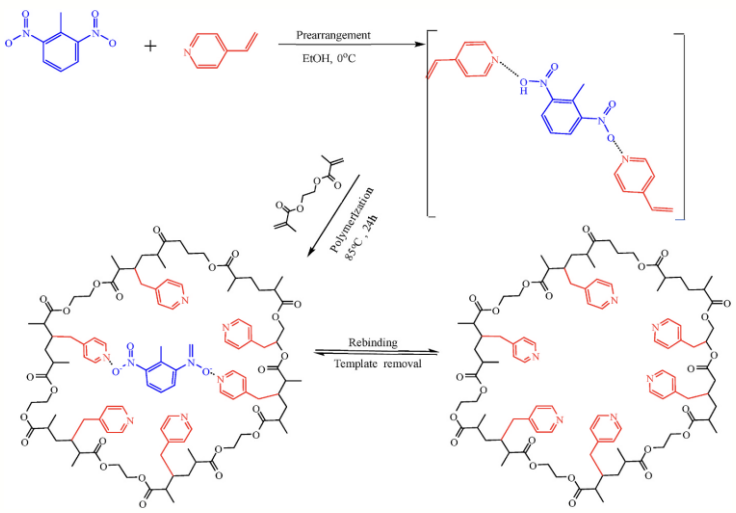

Figure 1:The proposed mechanism for the synthesis of $MIP_{2,6DNT}$

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P#38–Reduced Graphene Oxide-Supported Iron Sulphide Nanocomposites as Advanced Electrochemical Sensors for Detection of Ascorbic and Uric Acids

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Detection of ascorbic and uric acids is important in clinical diagnosis. Various techniques can be used to detect the acids, but they have disadvantages such as the cost, and requiring professionals to operate the instruments [1, 2]. In this study, electrochemical detection was used, using Fe_7S_8/rGO nanocomposite. The iron sulphide (Fe_7S_8) nanoparticles capped with salicylic acid, were used to modify an electrochemical sensor. Various instruments were used to confirm the as-synthesised iron sulphide nanoparticles, such as X-ray diffraction (XRD), which illustrated that Fe_7S_8 nanoparticles have a hexagonal phase. Fourier transform infrared spectroscopy (FTIR) showed the presence of functional groups. Scanning electron microscopy (SEM) displayed that the Fe_7S_8 nanoparticles had a flake-like morphology. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) were used to investigate the electrochemical characteristics of Fe_7S_8 nanoparticles and Fe_7S_8/rGO nanocomposite. The detection of AA and UA took place using Squarewave voltammetry, at the Fe_7S_8/rGO modified electrode, at 0 to 400 µM and 0 to 200 µM, respectively. There was a simultaneous detection of AA and UA, and there was no interference observed.

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P#39–Green Synthesis of NH_2-MIL-53(Al) MOF Using Recycled Aluminum Cans and PET Plastic Waste Bottles Precursors for the Adsorption of NSAIDs from Wastewater

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The widespread occurrence of NSAIDs in aquatic environments poses significant risks to ecosystems and human health, necessitating the development of sustainable and efficient extraction materials for wastewater analysis [1-2]. In this study, a green and cost-effective approach to synthesizing the MOF NH_2-MIL-53 (Al) is presented through the valorization of waste aluminum cans and PET plastics. Aluminum ions were recovered from discarded beverage cans, while PET plastics were depolymerized to obtain the organic linker precursor, 2-aminoterephthalic acid, thereby integrating circular economy principles into advanced material synthesis. The resulting NH_2-MIL-53 (Al) was characterized by PXRD, FTIR, SEM, and BET surface area analysis, confirming the formation of a framework comparable to conventionally synthesized MOFs. The waste-derived MOF was used as an adsorbent to preconcentrate selected NSAIDs from wastewater samples. Influential parameters affecting the extraction efficiency, including pH, adsorbent mass, sample volume, and extraction time, were systematically optimized using FFD and CCD. The synthesized MOF demonstrated high adsorption capacity, good selectivity, and reusability, enabling efficient enrichment of NSAIDs prior to chromatographic analysis. Overall, this work demonstrates that waste-derived NH_2-MIL-53 (Al) can serve as an effective and sustainable sorbent for environmental monitoring applications, offering an environmentally friendly alternative to traditional synthetic routes and reinforcing the potential of waste valorization in analytical chemistry.

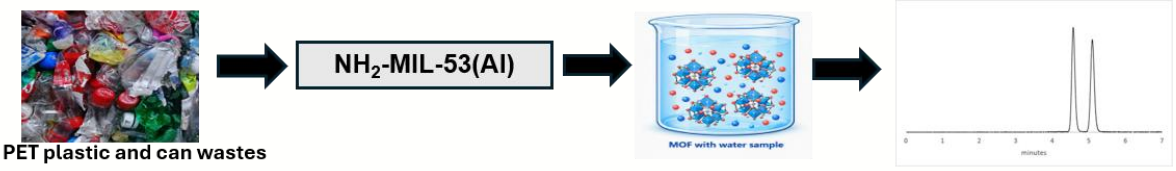

Figure 1: Synthesis-to-analysis workflow for NH_2-MIL-53(Al)-based NSAIDs preconcentration.

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P#40–Synthesis of Fe_3O_4@SiO_2 Derived from Sugar-cane Bagasse for Efficient Adsorptive Removal of Neonicotinoids from Wastewater.

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The presence of pesticide residues in water resources poses significant environmental concerns due to their persistence and potential ecological effects [1]. The removal of imidacloprid (IMD) and thiacloprid (THIA) neonicotinoid insecticides from wastewater was investigated using a magnetic silica nanocomposite synthesized from sugarcane bagasse waste (Fe_3O_4@SiO_2-SBW). Characterization using XRF, FTIR, XRD, TEM and BET confirmed the formation of a porous silica-coated magnetite structure with a surface area of 115.855 m^2/g. Adsorption conditions were optimized using Fractional Factorial Design (FFD) and Central Composite Design (CCD), with contact time and pH identified as the most influential factors. Optimal conditions of 56.21 min and pH 6.5 achieved removal efficiencies above 80% for both analytes. The adsorption data followed the Langmuir isotherm, with maximum capacities of 88.32 mg/g for IMD and 82.30 mg/g for THIA. Kinetic data were best described by the pseudo-second-order model (R^2 > 0.98), while low mean adsorption energies from the Dubinin–Radushkevich model indicated predominantly physical adsorption. Thermodynamic analysis showed that adsorption was spontaneous and endothermic. Application to real wastewater also demonstrated high removal efficiency. These findings demonstrate the potential of Fe_3O_4@SiO_2-SBW as a sustainable, low-cost adsorbent for removing neonicotinoid insecticides from contaminated water.

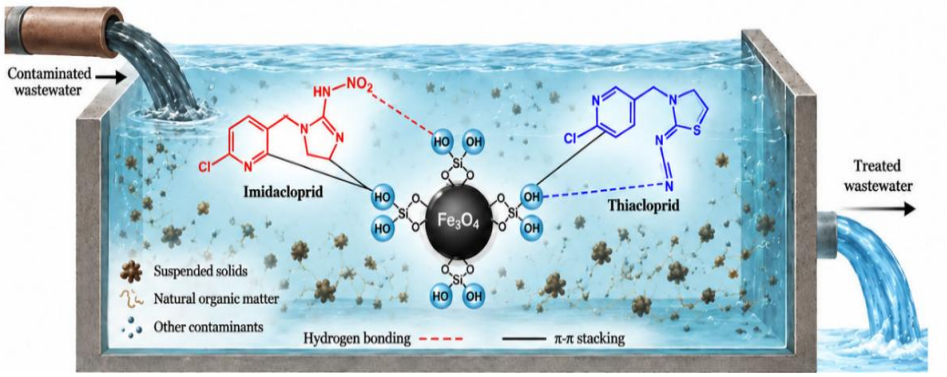

Figure 1: Adsorption mechanism of IMD and THIA onto Fe_3O_4@SiO_2-SBW nanocomposite.

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P#41–Synthesis of Novel Tetrahydroquinazoline Derivatives.

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Tetrahydroquinazolines are nitrogen-containing heterocyclic compounds that serve as important scaffolds in medicinal chemistry due to their structural diversity and ability to interact with a wide range of biological targets.[1] These compounds exhibit a broad spectrum of pharmacological activities, including antimicrobial, antiviral, antimalarial, and antiparasitic effects.[2] In this study, a structure-activity relationship (SAR) approach informed by insights from the Medicines for Malaria Venture (MMV) was employed to guide the optimization of new tetrahydroquinqzoline compounds. Structural modifications were undertaken to enhance antiplasmodial activity, improve aqueous solubility, and increase the selectivity index, thereby minimizing cytotoxicity and improving the overall drug-like properties of the compounds. The synthesized compounds will be characterized by NMR and FTIR spectroscopy.

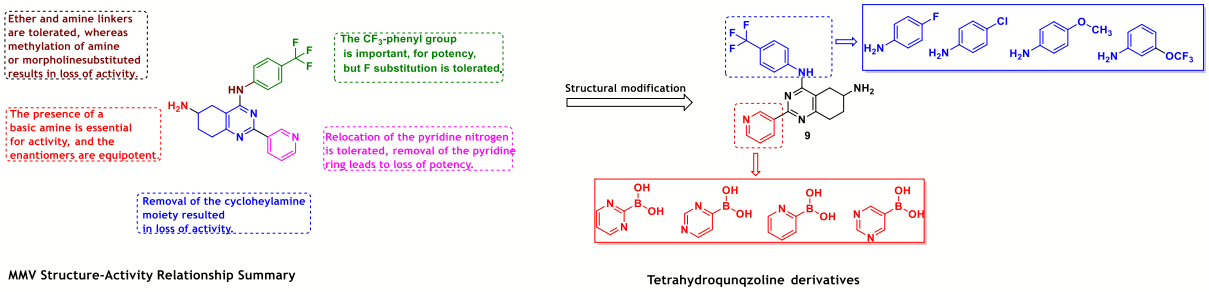

Figure 1: Structure-activity relationship and designed tetrahydroquinazoline derivatives.

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P#42–Improving preferential oxidation of carbon monoxide over Cu-Co_3O_4 based catalysts via cryochemical approach of lanthanum doping.

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Purification of hydrogen (H_2) by preferential oxidation of carbon monoxide (CO-PrOx) is constantly challenged by poor stability of the catalysts in the presence of moisture and or CO_2, as well as selectivity loss at higher temperatures (> 120) [1, 2]. The work explored the role of La (Lanthanum) doped Cu-Co_3O_4 catalysts prepared by co-precipitation/reflux method, evaluating the structural effects of cryochemical quenching in liquid nitrogen ($N_{2(l)}$) on CO-PrOx activity and stability. The Scanning and tunnelling electron microscopy (SEM and TEM), as well as the Brunauer-Emmett-Teller (BET) analysis showed that addition of 0.9 wt.% La on 7Cu-Co_3O_4 catalyst significantly alters the morphology and increase the specific BET surface area (S_{BET}) from 63.9 to 76.8 m^2/g. Cryo-quenching the 0.9La/7Cu-Co_3O_4 catalyst in $N_{2(l)}$ immediately after calcination at 300 °C further increase the S_{BET} to 90.4 m^2/g, due to the smaller crystallite size triggered by rapid cooling in $N_{2(l)}$, as evidenced by the x-ray diffraction (XRD) data. As a result, T_{100} decreased from 120 °C (7Cu-Co_3O_4) to 100 °C (0.9La/7Cu-Co_3O_4($N_{2(l)}$)) in CO-PrOx reaction, and the catalytic performance in moisture environment improved ($T_{(50)}$ = 60 °C). The XRD data further showed that La substitution for tetrahedral $Co^{2+}{}_{(Td)}$ ions distorted the 7Cu-Co_3O_4 crystal structure, enhancing the mobility and availability of active O_{Lat} (lattice oxide) at La^{3+} – O^{2-} – Co^{3+} interfaces, while $N_{2(l)}$ quenching limited excessive Co^{3+} reduction induced by La, as revealed by the X-ray photoelectron spectroscopy (XPS). These La-featured interfacial sites suppressed -OH formation and improves the catalyst stability under moisture, with slight deactivation under CO_2 modified CO-PrOx environment. The study provides significant insight into La doped Cu-Co_3O_4 catalysts and the promotional effect of cryochemical quenching in $N_{2(l)}$ for developments of active CO-PrOx catalysts for proton exchange membrane fuel cell (PEMFC) applications; to resolve climate, pollution and energy crisis.

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P#43–Synthesis of ZIF-8/MWCNTs-Enhanced Polyacrylonitrile Hybrid Nanocomposite Membranes for Brackish Water Desalination

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Brackish water, typically characterised by total dissolved solids (TDS) concentrations ranging from 1,000 to 10,000 mg/L, has become an increasingly important alternative water resource in regions experiencing water stress (1). This trend is driving the development and optimisation of advanced membrane materials aimed at mitigating global freshwater scarcity and enhancing the efficiency and sustainability of desalination processes (2,3). In this work, ZIF-8/MWCNTs-enhanced polyacrylonitrile (PAN) hybrid nanocomposite membranes were fabricated and evaluated to improve brackish water desalination performance. The synthesised materials were characterised using Fourier Transform Infrared (FTIR) spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive spectroscopy (EDS). The morphology and size distribution of the synthesized composites were investigated using Scanning Electron Microscopy. The surface area and pore-size characteristics of the composite membranes were evaluated using the BET method. The membranes were evaluated in terms of their swellability, water content, and porosity. The pristine PAN membrane showed the highest porosity (93.00 ± 1.53%), reflecting a highly porous asymmetric structure typical of PAN ultrafiltration membranes and favouring high water permeability. The membranes containing both ZIF-8 and functionalised MWCNTs showed water contents of 46.00 - 49.33% and porosity of 93.00 ±1.53%, respectively, indicating a high-water permeability and high-water absorption. Incorporation of functionalised MWCNTs reduced water content to 45.00 ± 1.00%, as hydrophilic carboxyl groups are introduced.

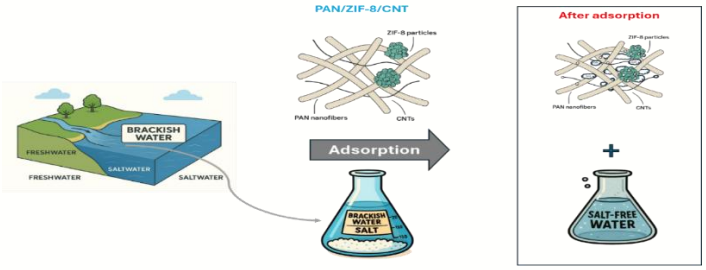

Figure 1: Adsorption mechanism of salts by PAN membrane doped with ZIF-8 MOF and CNT.

P#44–Synthesis of Quinazoline and Quinoline derivatives for biological evaluation against tuberculosis and cancer

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Tuberculosis (TB) and cancer are amongst the important diseases studied around the world [1] [2]. Patients infected with both TB and cancer have been reported, where malignancy of cancer has now become a risk factor in the new diagnosis of TB or the reoccurrence of TB [3]. Previous studies on quinazoline and quinoline moieties as anti-microbial agents [2] led to the synthesis of substituted quinoline and quinazoline derivatives, followed by esterification reaction to form 2-substituted quinazolin-4-yl alkynyl acetate derivatives and ninety-six new candidate compounds were produced as anti-tuberculosis agents. The biological report of the newly synthesized compounds revealed that, the effectiveness of the compounds depends on the type of acetylene used and the phenyl group at the second position of the quinazoline moiety. The most effective compound showed a highly potent activity of 0.12 μM against Mtb H37Rv strain reference to isoniazid and a good selectivity index (SI ≥ 10). The similar compound exhibited to be potent against lung cancer (A459 cell line), with HEK293 cell line used as a positive control. These results will help in the optimisation of the synthesised quinazoline derivatives to get a good candidate pharmacological drug.

Keywords: Tuberculosis, cancer, quinoline, quinazolinone

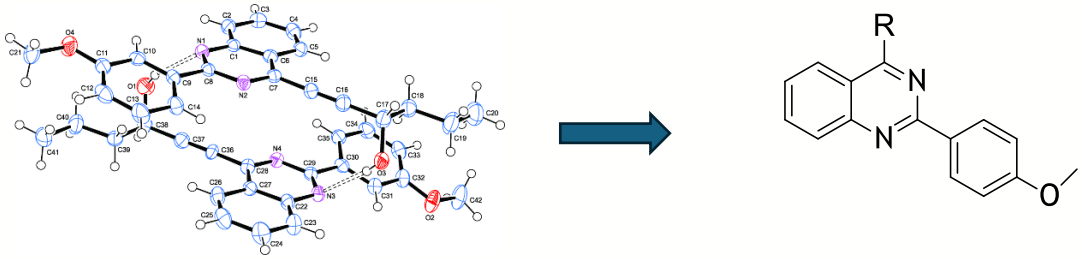

Figure 1: X-ray crystallography of the synthesised 4-acetylenequinazoline

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P#45–Characterisation and bioremediation of microplastics from the Hennops River in South Africa

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Microscopic plastic litter, a persistent (emerging) contaminant found at high concentrations in aquatic and terrestrial environments, is a major problem. Constrained budgets for water supply projects that implement water quality restoration solutions make developing nations like South Africa more vulnerable to water quality issues. Further research is needed on the effects of plastic type, particle size, and shape on microplastic buildup in aquatic habitats and sediments; interactions with other pollutants; toxicity processes; and enzymes in bioremediation. Microplastics were extracted from samples collected using filtration and density separation. Visualisation and identification were conducted using a microscope. Characterisation tools, such as Fourier transform infrared spectroscopy (FTIR), were utilised to identify the primary polymers present in the samples. Inductively coupled plasma optical emission spectroscopy effectively quantified hazardous metals. Gas chromatography-mass spectrometry was utilised to analyse polycyclic aromatic hydrocarbons. Microalgae and enzymes sourced from the surrounding environment were employed to bioremediate microplastics. Every sample contains microplastics; however, the quantity varies by site. Microplastics may combine with other contaminants and human activities to cause variance. As shown in Figure 1, FTIR detected polymers in particles collected from diverse locations, and fingerprinting with standard polymers confirmed the identification.

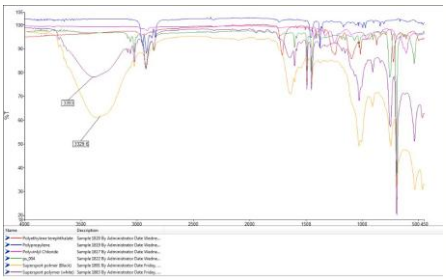

Figure 1: Optimised **Identification of microplastics obtained from the Hennops River using polymer standards.**

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P#46–Development of a Biomass-Based Iron Oxide Nanocomposite through Co-precipitation and Mechanical Modification

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Abstract

Eco-friendly and sustainable nanomaterials from biomass resources have attracted broad interest in research as an alternative to conventional material synthesis. Banana peels contain various oxygen-containing functional groups that enhance their ability to adsorb contaminants from wastewater. Iron oxide nanoparticles (IONPs) exhibit advanced surface and physicochemical properties that enhance their ability to remove pollutants from wastewater. In this study, a biomass-based iron oxide nanocomposite was developed using banana peel powder (BPP) as a host material for IONPs to remove contaminants from wastewater. The BPP, IONPs and the composite material were characterized using scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FTIR) and ultraviolet-visible spectroscopy (UV–Vis). The composite material exhibited properties suitable for removing contaminants from water samples. Future work will focus on evaluating the efficacy of the composite material by optimizing dosage, contact time, pH, and temperature to determine the optimal conditions for removing water contaminants.

Keywords: Iron oxide nanoparticles, Nanocomposite, Banana Peels, Characterization, Co-precipitation.

P#47–Surface-engineered CuO/ZnO heterostructures for light-mediated degradation of tetracycline

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The escalating water contamination by recalcitrant and hazardous agricultural and pharmaceutical pollutants presents a severe threat to ecosystems and human health [1]. These contaminants, particularly antibiotics like tetracycline (TC), contribute extensively to the contamination of surface and groundwater [2]. Conventional treatment methods such as filtration and coagulation fail to remove these low-concentration, highly toxic compounds and thus pose the risk of irrevocable harm to human health as well as aquatic ecosystems [3]. Long-term exposure to antibiotics has been associated with acute renal failure and kidney dysfunction, as well as blood and liver abnormalities [4]. This necessitates the development of efficient and sustainable chemistry technologies. Semiconductor photocatalysis offers an alternative route for complete pollutant breakdown. In this work crystalline monoclinic CuO, hexagonal ZnO, and CuO/ZnO heterostructures were successfully synthesized via a hydrothermal method, as confirmed by XRD and IR spectroscopy **(Figure 1)**. These catalysts will be evaluated to optimize catalyst dosage, pH, and pollutant concentration for TC photodegradation under UV light.

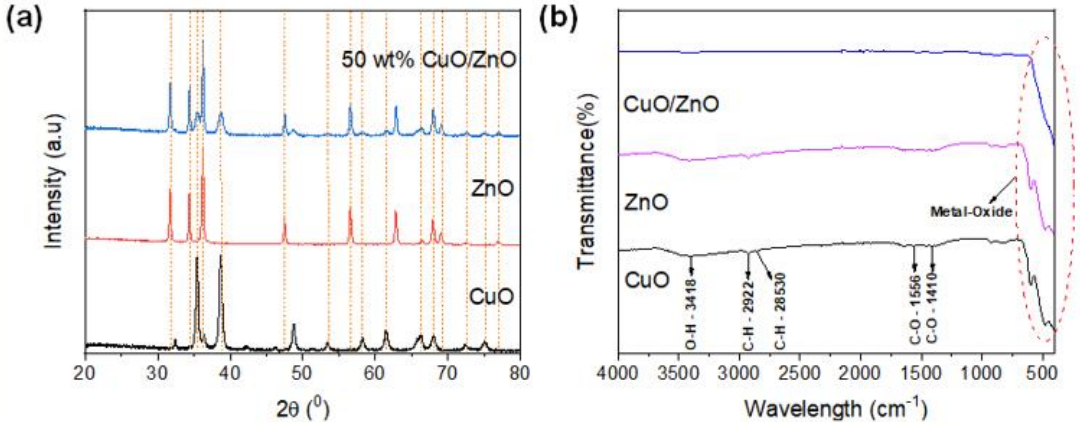

Figure 1: Optimized structures of: a) PAR, b) D1, and c) D2, computed at ZORA-BLYP/TZ2P.

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P#48–Synthesis and Characterization of Zinc Phthalocyanine-Zinc Oxide Composites for Visible Light Photocatalysis Degradation of Rhodamine 6G

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Efficient visible-light-responsive photocatalysts are critical for treating dye-contaminated wastewater because wide bandgap photocatalysts like zinc oxide (ZnO), suffer from rapid electron-hole recombination and inactivity under visible light [1]. In this study, zinc phthalocyanine-zinc oxide (ZnO-ZnPc) nanocomposites were synthesized to evaluate their photocatalytic degradation of Rhodamine 6G (R6G) dye under visible light irradiation [2]. Structural, optical, and morphological characteristics were examined via UV/Vis, FTIR,TEM, XRD and BET analysis. Optical analyses indicated bandgaps of 3.46 eV for pristine ZnO, 3.48 eV (B band) and 1.79 eV (Q band) for ZnPc, and 3.39 eV (B band) and 1.79 eV (Q band) for the ZnO-ZnPc composite. Morphological characterization revealed improved monodispersity and a narrower size distribution in the composite compared to pristine ZnO. Under visible light irradiation with 10 ppm R6G, the ZnO-ZnPc composite achieved a 95% degradation efficiency ($k = -0.02141$ min^{-1}, $t_{1/2} = 32.37$ min), significantly outperforming pristine ZnO (54%, $k = -0.0038$ min^{-1}, $t_{1/2} = 182.40$ min) and ZnPc (44%, $k = -0.00344$ min^{-1}, $t_{1/2} = 201.49$ min). The composite also maintained elevated degradation rates of 82% and 60% at 20 ppm and 30 ppm of R6G, respectively [2,3]. These findings demonstrate that the synergistic interaction between ZnO and ZnPc effectively extends visible-light absorption and enhances charge separation, establishing the composite as an efficient candidate for industrial dye wastewater remediation.

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P#49–Cobalt supported on Carbon Nanohybrids as High Performance, Platinum-Free Electrocatalysts for Acidic PEMFCs.

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Proton Exchange Membrane Fuel Cells (PEMFCs) offer clean energy conversions but are limited by the high cost and low durability of Platinum-based electrocatalysts for the Oxygen Reduction Reaction (ORR) in acidic media [1]. Therefore, the development of durable Platinum group metals-free (PGM-free) electrocatalysts is critical for efficient and sustainable energy conversion in acidic PEMFCs [2]. MOF-derived Metal-Nitrogen-Carbons (M-N-Cs) show great promise but still suffer from poor conductivity and metal sintering [3]. Herein, a carbon supported cobalt catalyst was modified with an amine as a molecular bridge to enhance interfacial contact between carbon black and Cobalt species. This strategy aims to increase conductivity, prevent Co agglomeration, and maximize Co-Nx active site density. The synthesized catalysts exhibited the desired structural and electrochemical characteristics for Oxygen Reduction Reaction (ORR) applications. The incorporation of carbon black enhanced electrical conductivity and facilitated improved catalyst dispersion, while the Co/ZIF-derived support provided a porous framework for nanoparticle anchoring. Although further optimization is required, the results demonstrate that the developed electrocatalyst is a promising candidate for improving ORR performance, and enhancing the durability of PEMFC cathodes. This work contributes to the ongoing development of cost-effective and sustainable electrocatalysts for next-generation fuel cell technologies.

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P#50–Bandgap Engineering of Titanium Loaded Aluminium Based Metal Organic Framework for Enhanced Photocatalytic Hydrogen Evolution

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Photocatalytic water splitting offers a sustainable route for green hydrogen production, yet conventional photocatalysts, including metal-organic frameworks (MOFs) are often limited by wide bandgaps (3.0-3.4 eV), poor visible-light absorption, and rapid chargecarrier recombination [1]. To overcome these challenges, this study proposes a bandgap engineering strategy via titanium (Ti) doping into aluminum-based MOFs (AlMOFs). Incorporating a sustainable waste-to-profit approach, aluminum precursor salts were first extracted from post-consumer waste aluminum cans [2]. The resulting materials were systematically characterized using FTIR, XRD, UV-Vis, SEM, EDS, BET, and TGA to evaluate their functional groups, phase purity, optical band gaps, surface morphology, and thermal stability. Photocatalytic performance was evaluated under visible-light irradiation (>420 nm) in an aqueous reaction vessel. The evolved volume was monitored at intervals, with molar yields calculated via the ideal gas law (PV=nRT). By shifting the valence band edge, narrowing the bandgap (1.23-3.0eV), and suppressing electron-hole recombination, a highly efficient Ti@Al-MOF photocatalyst showed improved photocatalytic hydrogen production compared to the pristine MOF.

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P#51–Synthesis and Photocatalytic Hydrogen Production Performance of Carbon Quantum Dots/Cu-MOF composite

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Due to the depletion of fossil fuels and their negative environmental effects, the conversion of solar energy into green chemical energy is growing in popularity. “Photocatalytic hydrogen generation from water is the direct conversion of solar energy into hydrogen (H_2) fuels”, and it has several advantages and enormous potential [1]. Hydrogen, a promising and eco-friendly energy source with a remarkable energy density, holds a great potential for satisfying increasing energy needs without any negative environmental effects [2]. In this study, a composite containing copper-metal organic framework (Cu-MOF) and carbon quantum dots (CQDs) will be synthesized and characterized via FTIR, SEM, EDX, TGA, and UV-VIS spectroscopy. Thereafter, the photocatalytic hydrogen production performance of the synthesized Cu-MOF/CQDs composite will be evaluated. The Cu-MOF offers a highly porous catalytic structure featuring redox-active copper centers, while the CQDs enhances the absorption of visible light [3]. They enable charge separation and electron transport, thereby boosting the overall photocatalytic hydrogen performance.

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P#52–Effect of Ligand Type on Photocatalytic Hydrogen Evolution of Ni-based Metal Organic Frameworks (MOFs)

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Hydrogen (H_2) is widely recognized as a clean and sustainable energy carrier, offering a promising alternative to fossil fuels in the transition toward carbon-neutral energy systems [1]. Nickel-based metal-organic frameworks (Ni-MOFs) have attracted considerable attention because of their tunable compositions, porous structures, and diverse chemical environments, making them promising candidates for applications such as photocatalysis. This study reports the solvothermal synthesis of three Ni-based MOFs, namely Ni-BDC, Ni-mPDA, and Ni-BDC-mPDA, for visible-light-driven photocatalytic hydrogen evolution. Their photocatalytic performance was evaluated under visible-light irradiation and correlated with their structural and physicochemical properties, which were characterized using Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), and Energy-Dispersive X-ray Spectroscopy (EDAX). Among the synthesized materials, Ni-BDC-mPDA exhibited the highest photocatalytic hydrogen production rate, outperforming both Ni-BDC and Ni-mPDA. Recycling experiments further demonstrated that Ni-BDC-mPDA maintained its photocatalytic activity over multiple reaction cycles, confirming its excellent stability and reusability [2]. The enhanced performance of Ni-BDC-mPDA is attributed to its nitrogen-rich and carboxylate groups from mixed linkers, which increases electron density around the Ni active sites, narrows the band gap, enhances visible-light absorption, and promotes more efficient charge separation and electron transfer during photocatalysis [3]. Overall, these findings demonstrate that Ni-based-mixed linker-MOFs are effective and stable photocatalysts for solar-driven hydrogen production and highlight ligand engineering as a critical strategy for optimizing photocatalytic performance.

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P#53–Surface Doping of Bismuth (Bi) Based Semiconductors for Photocatalytic Wastewater Treatment and Hydrogen Production

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Bi_2WO_6 is a visible-light-responsive photocatalyst that has attracted considerable attention due to its good stability, low cost, and abundant raw materials [1]. However, its practical application is limited by the rapid recombination of photogenerated electron-hole pairs [2]. In this study, Bi_2WO_6 was synthesized using a solvothermal method from bismuth nitrate pentahydrate and sodium tungstate dihydrate, while Ag/Bi_2WO_6 was prepared through a photoreduction process. The structural, morphological, and surface properties of the synthesised materials were characterised using XRD, SEM-EDAX, FTIR, and BET, UV-DRS and EIS. Both Bi_2WO_6 and Ag/Bi_2WO_6 exhibited highly agglomerated, irregular particles with rough surfaces. EDAX confirmed Bi, W, and O in Bi_2WO_6, with Ag additionally detected in Ag/Bi_2WO_6. UV-DRS analysis showed enhanced visible-light absorption after Ag modification, attributed to the surface plasmon resonance of Ag nanoparticles. The band gap decreased from 2.79 eV for Bi_2WO_6 to 2.46 eV for Ag/Bi_2WO_6, indicating improved light utilisation. Under visible-light irradiation, Ag/Bi_2WO_6 showed enhanced methylene blue degradation and hydrogen production compared with pristine Bi_2WO_6. This improved photocatalytic performance was attributed to enhanced surface properties, improved electron transfer, suppressed charge recombination, and efficient electron-hole separation [3]. These results demonstrate that Ag modification effectively improves the photocatalytic activity of Bi_2WO_6 for simultaneous wastewater treatment and hydrogen generation applications.

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P#54–Chemical Treatment of Historical Mining Slag as a Potential Use as Electrocatalyst for Hydrogen Evolution Reaction

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Hydrogen is regarded as a promising clean energy carrier due to its high energy density and environmentally friendly nature. However, the widespread application of hydrogen production through water electrolysis is limited by the high cost of platinum-based electrocatalysts used for the hydrogen evolution reaction (HER) [1,2]. Consequently, there is growing interest in developing low-cost and sustainable electrocatalysts from waste-derived materials [3]. This study investigates the potential use of historical mining slag as an HER electrocatalyst. Historical mining slag was collected from the Valterra Platinum Polokwane Smelters. The slag underwent grinding and ball milling to turn it into fine powder followed by chemical treatment with alkaline, oxidizing and acidic medium. The X-ray fluorescence spectroscopy (XRF) revealed the presence of different metal oxides and base metals at trace level. Furthermore, scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM/EDS) showed that upon chemical treatment of the slag, the morphologies were changing from undetected shapes into more flanky and angular particles. Brunauer-Emmett-Teller (BET) surface area analysis and thermogravimetric analysis (TGA) further confirmed that treatment of slag improves the physicochemical properties (increase in surface area and thermal stability, respectively) which is beneficial for HER studies. The preliminary HER results showed that the chemically treated slags exhibited the exceptional HER properties as they required low overpotential to achieve the current density of 10 $mA.cm^{-2}$. In addition, the kinetics were much improved upon chemical treatment. This was revealed by smaller semi-circle from electrochemical impedance spectroscopy (EIS) and tafel analysis.

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P#55–Synthesis Of Bendamustine Hydrochloride Under Continuous Flow Technology

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Africa does not have a well-established active pharmaceutical ingredients (APIs) manufacturing industry. It currently imports more than 90 % of its APIs which then get formulated into finished-products by local companies such as Aspen. Bendamustine hydrochloride (BMH) is an important anticancer drug for chronic lymphocytic leukemia and multiple myeloma, however, its manufacturing batch process is time consuming with moderate yields, and it involves hazardous and toxic chemicals [1,2]. These drawbacks make the drug expensive, less accessible and hard to produce in large amounts. To address some of these concerns, this study demonstrates novel, efficient, and scalable continuous flow technology (CFT) for synthesizing BMH, leveraging the benefits of flow chemistry for precise control, enhanced safety, and reproducibility [3]. Amidation of 2,4-dinitroaniline was successfully demonstrated under continuous flow conditions, with product formation observed at residence times of 10 and 20 minutes, corresponding to reagent flow rates of 0.85 and 0.425 mL/min, respectively. This work could help lower production costs and make bendamustine hydrochloride more accessible to patients.

Keywords: bendamustine hydrochloride, active pharmaceutical ingredients, continuous flow technology.

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P#56–Synthesis, Structure-Activity Relationship (SAR) and Biological Studies of Sulfonyl Substituted Benzimidazole Derivatives Against TB

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Tuberculosis (TB) remains one of the leading infectious causes of death worldwide [1]. The emergence of multidrug-resistant (MDR-TB) and extensively drug-resistant (XDR-TB) strains, together with the limitations of current therapies, highlights the need for new anti-TB agents [2]. In this study, 10 sulfonyl-substituted benzimidazole derivatives were synthesised via a stepwise approach from *o*-phenylenediamine and 4-chloro-*o*-phenylenediamine [3]. The synthesised compounds were characterised using Fourier-transform infrared (FTIR) spectroscopy, nuclear magnetic resonance (^{1}H and ^{13}C NMR) spectroscopy, and mass spectrometry (MS), confirming their successful synthesis. ADMET predictions indicated that three compounds showed promising drug-like properties. Among these, 2-(4-methoxyphenyl)-1(methylsulfonyl)-1H-benzo[*d*]imidazole showed the most favourable overall profile based on its solubility, lead-likeness, absence of Lipinski violations, and minimal CYP450 inhibition. 2-(4-Chlorophenyl)-1-(methylsulfonyl)-1H-benzo[*d*]imidazole and 5-chloro-2-(4-methoxyphenyl)-1-(methylsulfonyl)-1H-benzo[*d*]imidazole also satisfied lead-likeness criteria and showed no Lipinski violations but exhibited moderate solubility and broader CYP450 inhibition.

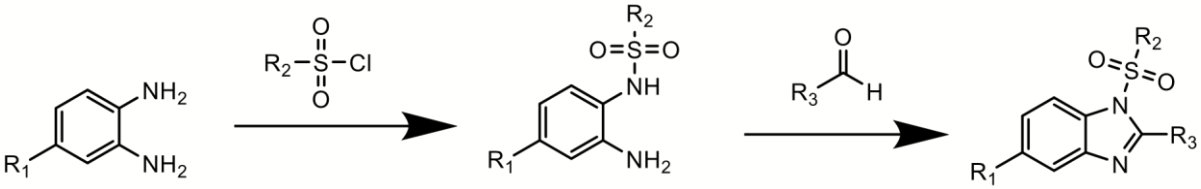

Figure 1: Synthesis of sulfonyl-substituted benzimidazole derivatives

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P#57–Preparation and characterisation of Co-ZIF/GO composite for the removal of palladium from wastewater

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In this study, a cobalt-based zeolitic imidazolate framework/graphene oxide (Co-ZIF/GO) composite was successfully synthesized and evaluated as an effective adsorbent for the removal of palladium Pd (II) from wastewater [1]. FTIR confirmed the presence of characteristic GO and ZIF-67 peaks, verifying successful GO/ZIF-67 synthesis. SEM showed dodecahedral ZIF-67 particles wrapped in pleated GO nanosheets, indicating growth on the GO surface via electrostatic interactions with Co (II) ions. XRD displayed GO's broad peak at 8.35° and ZIF-67's typical diffraction peaks [2], confirming the preserved structure of GO/ZIF-67. Batch adsorption experiments demonstrated that a dosage of 20 mg of the composite achieved a 76% removal efficiency of palladium at an optimal pH of 4. The adsorption equilibrium data fitted well with the Freundlich isotherm model, suggesting multilayer coverage onto heterogeneous active sites. The adsorption process follows a pseudo-second-order kinetic model, while thermodynamic analysis reveals that it is a spontaneous, endothermic process primarily driven by entropy changes. Overall, the synthesized Co-ZIF/GO composite displays high efficiency and potential for the selective recovery of precious metals and remediation of heavy metals from industrial effluents.

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P#58–Synthesis of Bifunctional Nickel-loaded Sulfonated Porous Organic Polymer Catalysts for One-pot Synthesis of 2,5-Dimethylfuran from Biomass-derived Fructose

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The increasing demand for sustainable energy has intensified research into biomass-derived chemicals as a renewable energy substitute to fossil-based resources [1]. Carbohydrates offer a sustainable, abundant, and renewable path to high-energy biofuels, making DMF a viable substitute for gasoline [2]. Nickel nanoparticles are a sustainable substitute for noble metals in biofuel catalysis because they offer good hydrogenolysis at a lower cost and with greater abundance [3]. This study explores the development of a bifunctional nickel-supported sulfonated benzene-based porous organic polymer (BBA) catalyst for the one-pot synthesis of 2,5-Dimethylfuran from fructose. Porous organic polymer (POP) is synthesised via Friedel craft alkylation using benzene benzylamine (BBA) monomer, sulfonated to introduce acidic sites, and subsequently incorporated with nickel nanoparticles using an in-situ method. The influence of temperature, concentration, and time on polymer formation was studied. Preliminary characterization of the POP was conducted using FTIR spectroscopy confirming the characteristic functional groups of the synthesised materials. SEM/EDX was used to evaluate the morphology and elemental composition of the synthesised materials. Further characterization using BET will be conducted to study the porosity of the synthesized materials, and GC-MS and NMR will be used to confirm the identity and structural features of 2,5-DMF, establishing the catalytic efficiency of Ni/BBA-S.

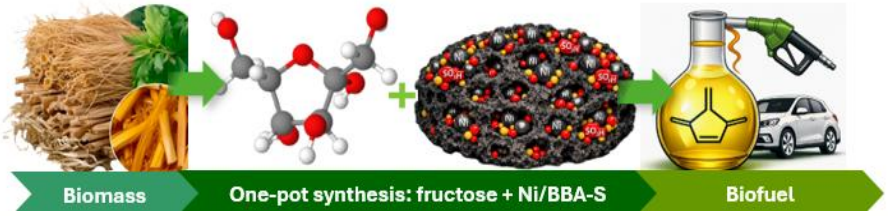

Figure 1: Visual summary of the catalytic pathway from biomass to 2,5-DMF

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P#59–Design, synthesis and anti-tubercular properties of 3-aminoindole derivatives.

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Tuberculosis (TB) is an infectious disease that is transmitted as an airborne and it is usually present in lungs as pulmonary tuberculosis, which is caused by the bacteria called *Mycobacterium tuberculosis (Mtb)* [1]. It is estimated that one third of the world's population is infected with the tuberculosis-causing bacteria. Additionally,10.6 million people became ill with TB in 2021 as compared to 10.1 million in 2020, an increase from the prior year. About 1,6 million people died from TB in 2021, as compared with 1.5 million in 2020 [2]. This study focuses on the synthesis of 3-aminoindole derivatives as potential anti-tubercular drugs with different chemical properties, enhanced efficacy, reduced side effects and reduced disease treatment time. Several 3-aminoindole derivatives were synthesised and purified using flash chromatography. The structures of the synthesised compounds were confirmed using the spectral methods, MS, ^{1}H-NMR, and ^{13}C-NMR. The activity of 20 of the synthesised compounds were tested against mycobacterium TB on human kidney and skin cell lines and only two compounds demonstrated moderate inhibitory with IC_{50} values less than 60 uM.

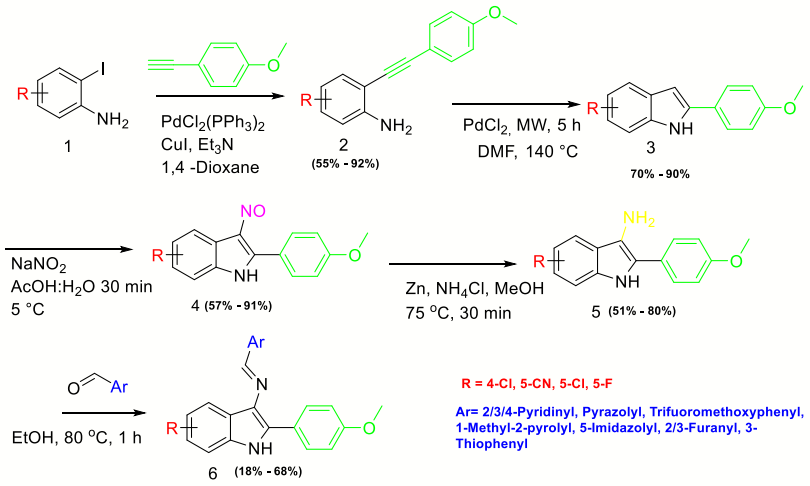

Figure 1: General scheme for the synthesis of 3-aminoindoles

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P#60–Green Synthesis of Cerium-Doped $NiFe_2O_4$ Nanoparticles for the Photodegradation of Methylene Blue Dye

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The increasing discharge of synthetic dyes into aquatic environments poses a significant threat to ecosystems and public health because of their persistence and resistance to conventional wastewater treatment technologies. Methylene blue (MB) is a widely used synthetic dye and a representative organic pollutant requiring effective remediation strategies. Nickel ferrite ($NiFe_2O_4$) is a promising photocatalyst owing to its chemical stability and magnetic properties; however, rapid electron-hole recombination can limit its photocatalytic efficiency. In this study, cerium (Ce)-doped $NiFe_2O_4$ nanoparticles were green-synthesized using *Sutherlandia frutescens* leaf extract. Different Ce concentrations were investigated to determine their influence on the structural, optical, charge-transfer, and photocatalytic properties of $NiFe_2O_4$. XRD confirmed the formation of the spinel $NiFe_2O_4$ phase. Optical analysis revealed a decrease in band-gap energy with Ce incorporation. After 120 min of irradiation, pristine, 1%, 3%, and 5% Ce-$NiFe_2O_4$ achieved approximately 63%, 68%, 72%, and 57% MB degradation, respectively. The 3% Ce-$NiFe_2O_4$ exhibited the highest apparent rate constant of 0.011 min^{-1}, compared with 0.00864 min^{-1} for pristine $NiFe_2O_4$. Electrochemical measurements further indicated improved charge-transfer characteristics for the 3% Ce-doped material. These findings demonstrate that Ce concentration strongly influences the photocatalytic performance of $NiFe_2O_4$ with 3% Ce providing the optimum enhancement for MB removal from water.

Keywords: Green synthesis; $NiFe_2O_4$; cerium doping; photocatalysis; methylene blue; wastewater treatment.

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P#61–Boosting photocatalytic hydrogen production using the natural linker tartaric acid-based metal organic framework: Computational and experimental studies.

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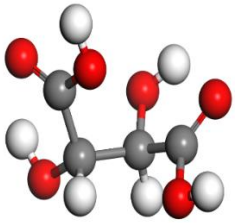
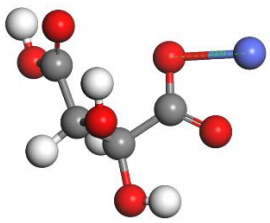
Hydrogen is widely recognized as a promising clean energy carrier with the potential to reduce reliance on fossil fuels and mitigate environmental pollution [1]. In this study, tartaric acid-based metal-organic frameworks (MOFs) incorporating iron (Fe), cobalt (Co), copper (Cu), and nickel (Ni) were designed, synthesized, and evaluated for their potential application in photocatalytic hydrogen production. Density Functional Theory (DFT) calculations were employed to investigate the electronic properties of the proposed MOFs and identify suitable transition metal centres for enhanced photocatalytic performance [2][3]. The materials were synthesized using a solvothermal method and characterized by Fourier Transform Infrared (FTIR) spectroscopy and X-ray diffraction (XRD). Additional characterization using SEM-EDS and BET surface area analysis is planned for future studies. FTIR spectra and XRD patterns of the synthesized MOFs were compared with those of free tartaric acid and the cobalt precursor to confirm successful coordination between the metal ions and the organic linker. Structural and morphological changes observed after synthesis indicated the formation of metal-tartaric acid coordination frameworks. The combined computational and experimental approach provided valuable insights into the structure-property relationships of the materials. Photocatalytic studies demonstrated the potential of these natural linker-based MOFs for hydrogen generation, highlighting their promise for sustainable energy applications.

a) Tartaric acid



b) Monodentate MOF



c) Bidentate MOF (OH-M-

d) Bidentate MOF (COO-M-

P#62–Synthesis Of Zeolite Ferrierite Using Mesoporous Si-MCM-41 As SiO2 Precursor, And Its Investigation In water

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The contamination of water resources by heavy metals poses a critical environmental threat due to its adverse effects on ecosystems and human health. Copper (Cu^{2+}) be toxic at elevated concentrations, highlighting the need for effective and sustainable remediation technologies [1] .This study investigates the synthesis of Zeolite Ferrierite (FER) utilizing mesoporous Si-MCM-41 as a silicon dioxide (SiO_2) precursor and evaluates its potential application in water remediation through the adsorption of Cu^{2+} ions. The zeolite FER was synthesized via the hydrothermal method in order to control the crystallization of its framework. Firstly Si-MCM-41 was synthesized using tetraethyl orthosilicate as the silica source and cetyltrimethylammonium bromide as the structure source. The synthesized Si-MCM-41 was used as the SiO_2 precursor in the preparation of ferrierite. [2]. The XRD, SEM, FTIR and BET confirms that the synthesized zeolite is indeed ferrierite. The zeolite FER was able to remove Cu^{2+} ions from simulated wastewater at concentration of 80 ppm, pH of 8 , absorbent dosage of 0.5 g and contact time of 60 minutes. In conclusion, FER can be used in remediation of Cu ions in wastewater.

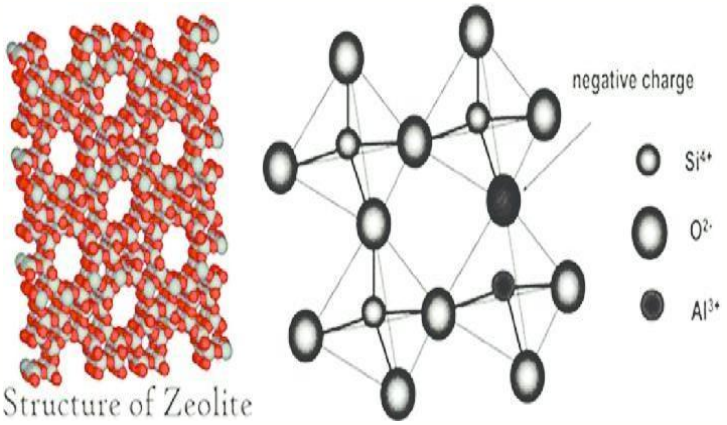

Figure 1 : Structure of Zeolite

P#63–Synthesis-structure/redox/activity relationships in CuO-MnO_x catalysts for preferential CO Oxidation (CO-PrOx)

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Preferential oxidation of carbon monoxide (CO-PROX) is preferred method for reducing carbon monoxide (CO) concentration in hydrogen (H2)-rich gas streams prior to their (hydrogen) use in Proton Exchange Membrane (PEM) fuel cells [1]. The process requires highly active catalysts capable of selectively oxidizing CO with less selectivity to hydrogen. The trace amount of CO 0 ppm) can poison the platinum-based anode catalyst in PEM fuel cells, leading to a substantial decline in their performance and efficiency [2]. In this study, effect of copper (Cu) species load on manganese oxide-based catalysts is investigated for the CO-PROX reaction. Catalysts (MnO_x and CuO-MnO_x) were synthesized via precipitation and co-precipitation method prior to calcination. The synthesized materials were characterized using XRD, BET surface area analysis, FTIR, TGA and their catalytic activity were monitored by Gas Chromatography. These techniques were employed to investigate the catalysts' structural, textural, thermal, and catalytic properties, as well as to assess the synergistic interactions between copper and manganese species. Finally, the catalytic performance and stability of the synthesized catalysts was evaluated through the COPROX reaction to determine the optimum Cu loading for the selective removal of CO from H_2-rich streams.

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P#64–CuNi-BTC Metal Organic Framework for Photodegradation of CIP and Photocatalytic Hydrogen Production in Universal Water Systems

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A multifunctional CuNi-BTC bimetallic metal-organic framework (MOF) was successfully synthesised via a solvothermal route to address the dual challenges of clean energy generation and pharmaceutical pollutant removal. Comprehensive characterisation using XRD, SEM-EDS, FTIR, TGA, and UV-DRS confirmed the successful formation of Cu and Ni into the BTC framework, resulting in enhanced crystallinity, narrowed band gap (3.04 eV), and improved charge separation. Optical studies revealed superior visible-light absorption compared to monometallic analogues, directly contributing to its photocatalytic efficiency. Under visible-light irradiation, CuNi-BTC achieved 79% ciprofloxacin (CIP) degradation within 60 min, outperforming Cu-BTC at 67% and Ni-BTC at 61%. For hydrogen evolution, CuNi-BTC delivered a production rate of 28538.79 μmol g^{-1} h^{-1}, surpassing both monometallic MOFs. Mechanistic investigations identified superoxide radicals ($\bullet O_2^-$) as the dominant reactive species, while synergistic Cu-Ni interactions suppressed electron-hole recombination Crucially, the catalyst was evaluated across diverse real water matrices including rainwater, seawater, and treated wastewater where it retained high activity despite salinity, pH variations, and competing ions, underscoring its robustness beyond idealised laboratory conditions. The catalyst exhibited excellent recyclability, maintaining high activity across multiple cycles in both hydrogen production and CIP degradation. These findings position CuNi-BTC as a robust and versatile photocatalyst, bridging laboratory innovation with real-world applications in sustainable energy conversion and wastewater remediation.

Keywords: Bimetallic MOFs, Photocatalysis, Ciprofloxacin, Hydrogen evolution

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P#65–Organic additive-mediated synthesis of Ce -doped TiO_2 nanostructures for enhanced gas sensing

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Air pollution is a scourge requiring urgent attention, with low levels of good air quality reported globally [1]. Titanium dioxide (TiO_2) is promising for gas sensing applications, however, its performance is often limited by low sensitivity and selectivity [2]. In this work, Ce^{4+}-doped TiO_2 nanomaterials were synthesized with organic additives (*viz.*, glucose, tannic acid, and HDTMA) to investigate additive-assisted surface and defect engineering. Structural and morphological characteristics were investigated using X-ray Diffraction (XRD), Fourier Transform Infrared (FTIR) spectroscopy, Raman spectroscopy, Scanning Electron Microscopy (SEM) coupled with Energy-Dispersive X-ray spectroscopy (EDX), and X-ray photoelectron spectroscopy (XPS). XRD confirmed preservation of the anatase phase, while particle size decreased from 63.33 nm (pure TiO_2) to 38.83 nm at 5% Ce doping. Additives further enhanced size reduction, achieving 24.75 nm (3% Ce, glucose), 29.18 nm (3% Ce, tannic acid), and 20.59 nm (5% Ce, HDTMA), demonstrating suppression of crystal growth through controlled nucleation and surface capping. FTIR indicated Ce–O–Ti bonds in additive-free samples, while organic additives introduced vibrations that masked the metal oxide fingerprint region due to surface modification. Raman spectroscopy verified the anatase structure and revealed CeO_2 segregation in all additive-assisted samples. Morphological analysis showed a transition from agglomerated ellipsoidal structures to more porous and uniformly distributed particles, increasing surface area and active sites. These findings demonstrate that additive-assisted synthesis tunes particle size, porosity, and phase behaviour in Ce–TiO_2, highlighting its potential for gas sensing through Ce^{4+}-induced defect engineering.

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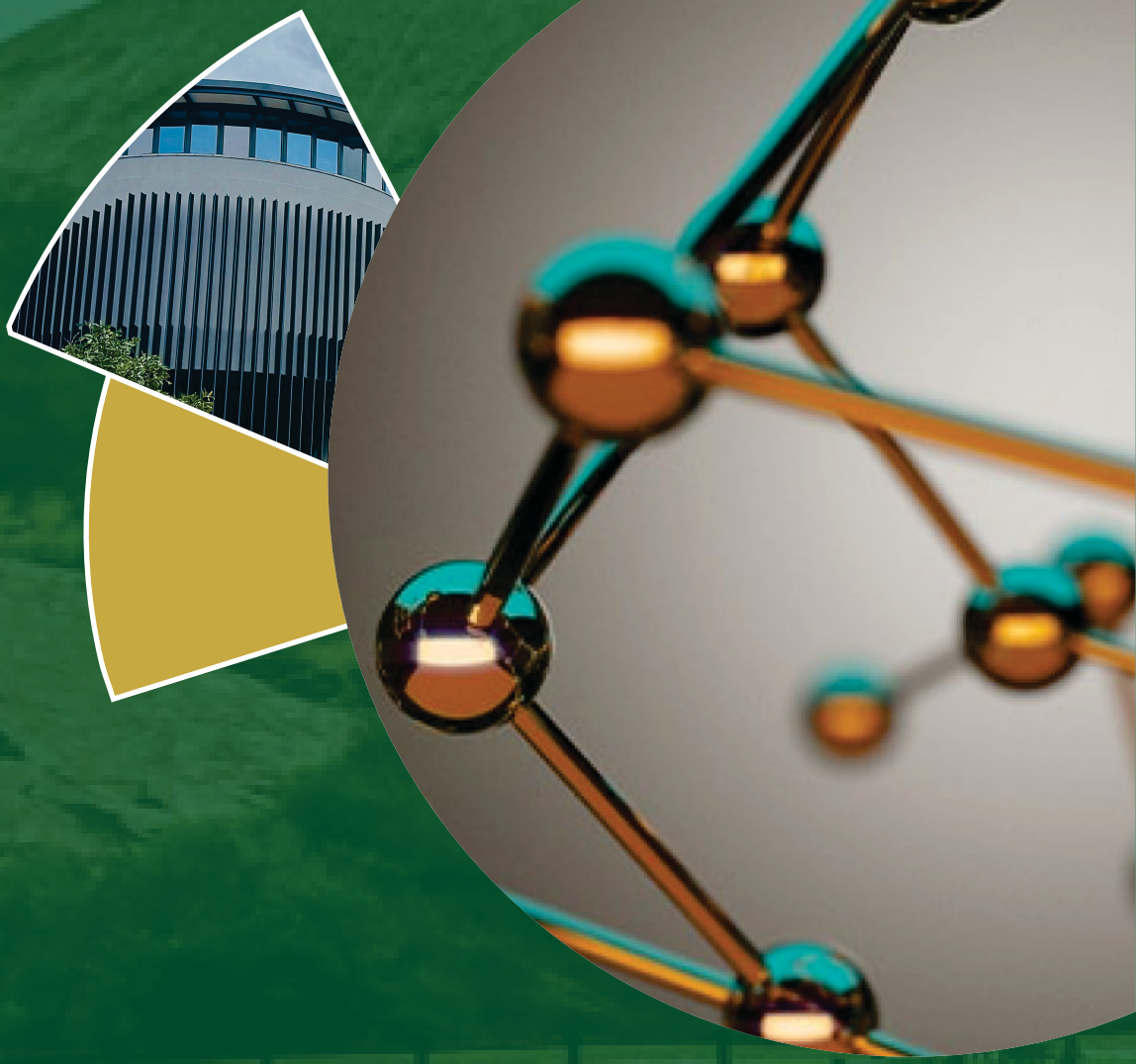

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