

INTERNATIONAL CONFERENCE & 22ND ANNUAL GENERAL MEETING

THEME

Chemistry for a Healthier Planet: Leveraging Smart Materials,
AI, and Partnerships for Climate Resilience and Well-being.



DATE
TUESDAY 13-
THURSDAY 15
OCTOBER, 2026

VENUE
ISSER, UNIVERSITY
OF GHANA, LEGON,
ACCRA

TIME
8:00AM
PROMPT
EACH DAY

HOST INSTITUTION



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ABOUT GHANA CHEMICAL SOCIETY

The Ghana Chemical Society (GCS) is the professional society for practitioners of the chemical sciences in Ghana. Founded in 1981 and incorporated in 1995, the Society brings together professionals from academia, industry, research institutions, government agencies, and related fields to promote the advancement and application of chemistry for national and global development.

GCS provides a platform for the dissemination of scientific knowledge, professional development, research collaboration, and advocacy in the chemical sciences. Through its annual conferences, seminars, workshops, schools, and community outreach programmes, the Society promotes scientific excellence while supporting the development of young scientists and innovators through mentorship, training, and professional engagement.

The Society is committed to professionalism, integrity, creativity and innovation, accountability, critical thinking, passion for chemistry, community building, and partnership. Its mission is to advance chemical education, research, and innovation through collaboration with professional bodies, allied chemical institutions, government agencies, industry, and other stakeholders for the development and well-being of society.

The current national leadership of the Ghana Chemical Society comprises Prof. Akwasi Acheampong (Kwame Nkrumah University of Science and Technology, KNUST), President; Dr. Michael Baah Mensah (KNUST), Secretary; and Mrs. Janet Atebiya (Ghana Water Limited), Treasurer. The leadership, elected in 2024, represents a significant collaboration between academia and industry and includes the Society's first woman (from industry) to serve in an executive position. The GCS Secretariat is hosted at the Department of Chemistry, KNUST, and being supported by National Service Personnels: Mr. Abdul Rasheed Mohammed and Mr. Michael Fiifi Essien.

Today, GCS continues to strengthen the chemistry community in Ghana by fostering research excellence, innovation, professional networks, industry–academia collaboration, and the responsible application of chemistry to address national and global challenges. More information about GCS can be found from the Society's website: <https://www.ghchemsoc.org>.



Prof. Akwasi Acheampong
President, GCS
(KNUST)



Dr. Michael Baah Mensah
Secretary, GCS
(KNUST)



Mrs. Janet Atebiya
Treasurer, GCS
(GWL)



Mr. Abdul Rasheed Mohammed
National Service Personnel
(KNUST)



Mr. Michael Fiifi Essien
National Service Personnel
(KNUST)

WHY JOIN THE GHANA CHEMICAL SOCIETY?

Membership of the GCS provides opportunities to:

- Network with professionals in academia, industry, research, and government.
- Grow professionally through conferences, workshops, seminars, training, and access to professional resources.
- Advance research through collaboration, knowledge sharing, publications, and research networks.
- Enhance your career through professional connections, mentorship, career guidance, and exposure to opportunities.
- Develop leadership skills by participating in Society activities, committees, and initiatives.
- Contribute to the advancement of chemistry through advocacy, outreach, and engagement with industry and policymakers.

HOW TO BECOME A MEMBER

Membership is open to individuals and organisations involved in the chemical sciences.

Prospective members can:

1. Choose the appropriate membership category (e.g., student, professional, or corporate).
2. Complete the online membership application, providing the required personal, professional, and institutional information.
3. Submit the application for verification by the GCS Secretariat.
4. Pay the applicable annual membership dues after approval.
5. Receive confirmation of membership and gain access to GCS programmes, events, publications, and professional networks.

Join the GCS and become part of Ghana's growing community of chemistry professionals.

PAYMENT DETAILS



Ghana Chemical Society (GCS)

REGISTRATION OF MEMBERSHIP STEPS

1. Visit bit.ly/GCS_Gh to access form
2. Fill form to register
3. Pay amount to GCS MoMo Merchant ID 818136 /
4. MTN MoMo Number 0530446824
7. Send a screenshot of payment to membership.gcs@gmail.com to confirm payment

You can now also pay via bank

Account Number: 6271180003048

Account Name: Ghana Chemical Society

Bank: GCB Bank PLC

Branch Name: Bantama

Swift Code: GHCBGHAC

Bank Code: 040

MEMBERSHIP TYPES

MEMBERSHIP TYPE

1. Regular Member
2. Student Member
3. Diaspora Member

PAYMENT

250 cedis
100 cedis
20 dollars



**Register your
membership today**

bit.ly/GCS_Gh

Visit the link above or scan the QR code
to access form to register



GCS INTERNATIONAL CONFERENCE AND 22ND ANNUAL GENERAL MEETING

Ghana faces escalating environmental challenges, including poor waste management, plastic pollution, galamsey-related water contamination, and declining air quality, all of which threaten public health, ecosystems, and economic growth. Pollution of major rivers such as the Pra River, Ankobra River, and Birim River, together with climate change impacts, has increased pressure on water resources and livelihoods.

Addressing these issues requires innovative, science-driven solutions and strong collaboration. The GCS International Conference aims to bring together key stakeholders to advance practical solutions for environmental sustainability and public health.

This conference aligns with Ghana's national priorities on environmental sustainability, climate resilience, and industrial transformation, as well as global frameworks such as the Sustainable Development Goals (SDGs)—particularly SDGs 3 (Good Health), 6 (Clean Water), 9 (Industry & Innovation), 11 (Sustainable Cities), 12 (Responsible Consumption), 13 (Climate Action), and 17 (Partnerships for the goals).

Notably, the conference will also host the Commonwealth Chemistry Executives Board Meeting, marking a significant milestone for GCS and providing an exceptional opportunity for international engagement, visibility, and partnership development.

CONFERENCE GOAL

To advance the role of chemical sciences in delivering innovative, technology-driven, and partnership-based solutions for environmental sustainability and climate resilience in Ghana and beyond.

Specific Objectives

- Promote the application of smart and functional materials for environmental remediation and health.
- Explore the integration of AI and data-driven approaches in chemical research and environmental management.
- Strengthen waste management and circular economy strategies, including waste-to-resource innovations.
- Foster partnerships between academia, industry, and policymakers to enhance research uptake and implementation.
- Build capacity of early-career scientists and students in emerging areas of chemistry and sustainability.
- Generate policy-relevant recommendations to support national and regional environmental governance.

CONFERENCE LOCAL ORGANIZING COMMITTEE



Prof. Collins Obuah
LOC Chair
(UG, Legon)



Dr. Anita Oppong
LOC Secretary
(UG, Legon)



Prof. Dorcas Osei- Safo
Scientific Committee Chair
(UG, Legon)



Dr. Louis Hamenu
Sponsorship Chair
(UG, Legon)



Dr. Michael Baah Mensah
Publicity Chair
(KNUST)



Dr. Dr. Bozumeh Som
Registration and Souvenir Chair
(UG, Legon)



Dr Aaron Aryee
Tourism, Chair
(UG, Legon)

Full list of Committee Members

#	Name	Affiliation	Role
1	Prof. Collins Obuah	University of Ghana	Chairman
2	Dr. Anita Oppong	University of Ghana	Secretary
3	Dr. Irene Agbo	University of Health and Allied Sciences	Member, Academia
4	Dr. Bozumah Som	University of Ghana	Member, Academia
5	Dr. Aaron Aryee	University of Ghana	Member, Academia
6	Prof. Dorcas Osei-Safo	University of Ghana	Member, Academia
7	Dr. Louis Hamenu	University of Ghana	Member, Academia
8	Prof. Albert Aniagyei	University of Health and Allied Sciences	Member, Academia
9	Dr. Cedric Dzidzor Amengor	University of Health and Allied Sciences	Member, Academia
10	Dr. Benjamin Kinsley Harley	University of Health and Allied Sciences	Member, Academia
11	Dr. Martin Owusu-Asante	Ghana Atomic Energy Commission	Member, Research
12	Ing. Dr. Latifatu Mohammed	Council for Scientific and Industrial Research - Institute for Industrial Research	Member, Research
13	Mrs. Gifty Kyei Baffour	Kasapreko Company Limited	Member, Industry
14	Mr. Moses Paintsil	Ghana Water Company Limited	Member, Industry
15	Dr. David Adu-Poku	University of Energy and Natural Resources	Member, Academia
16	Dr. Mary-Magdalene Padevoah	University of Technology and Applied Sciences	Member, Academia
17	Prof. Lawrence S. Borquaye	Kwame Nkrumah University of Science and Technology	Member, Academia
18	Dr. Genevieve Adukpo	University of Cape Coast	Member, Commonwealth Chemistry and Academia
19	Prof. Mercy Badu	Kwame Nkrumah University of Science and Technology	Member, Academia
20	Dr. Gershon Amenuvor	Kwame Nkrumah University of Science and Technology	Member, Academia
21	Prof. Isaac Asiamah	University of Cape Coast	Member, Academia
22	Mrs. Judith Odei Owusu-Asante	Council for Scientific and Industrial Research	Member, Research
23	GCS President	Kwame Nkrumah University of Science and Technology	Member, Student
24	Dr. Emmanuel Ramsey Buabeng	Georgia State University, USA	Member, Diaspora
25	Dr. Lilian Sarpong	Kwame Nkrumah University of Science and Technology	Member, Academia

MESSAGE FROM THE CHAIRMAN OF THE LOCAL ORGANISING COMMITTEE

It is with great pleasure and a deep sense of responsibility that I welcome you to the 22nd Ghana Chemical Society International Conference and Annual General Meeting, being held from 13th to 15th October 2026 at the Institute of Statistical, Social and Economic Research (ISSER), University of Ghana, Legon, Accra. The conference, themed “Chemistry for a Healthier Planet: Leveraging Smart Materials, AI, and Partnerships for Climate Resilience and Well-being,” brings together scientists, researchers, industry professionals, policymakers, educators, and students from Ghana and beyond to explore innovative chemical solutions to some of the world's most pressing challenges.

The theme of this year's conference reflects the growing importance of chemistry as a driver of sustainable development, environmental stewardship, human health, and technological advancement. As climate change, environmental degradation, and public health concerns continue to affect societies globally, the role of chemistry in developing smart materials, advancing artificial intelligence-driven discoveries, and fostering collaborative partnerships has never been more critical. This conference provides a unique platform for exchanging knowledge, sharing research findings, and building networks that can drive impactful solutions for a healthier and more resilient future.

On behalf of the Local Organising Committee, I extend our heartfelt appreciation to the Ghana Chemical Society, the University of Ghana, Commonwealth Chemistry, our distinguished speakers, sponsors, participating institutions, exhibitors, and all delegates whose contributions have made this event possible. We are particularly honoured to host renowned experts from academia, industry, and research institutions who will share valuable insights and experiences that will enrich our discussions and inspire future collaborations.

The success of an event of this magnitude depends on the dedication and commitment of a capable team. I am therefore deeply grateful to the members of the Local Organising Committee who have worked tirelessly to make this conference a reality. I would like to acknowledge the invaluable contributions of Dr. Anita Oppong (Secretary), Dr. Irene Agbo, Dr. Bozumeh Som, Dr. Aaron Aryee, Prof. Dorcas Osei-Safo, Dr. Louis Hamenu, Prof. Albert Aniagyei, Dr. Cedric Dzidzor Amengor, Dr. Benjamin Kinsley Harley, Dr. Martin Owusu-Asante, Ing. Dr. Latifatu Mohammed, Mrs. Gifty Kyei Baffour, Mr. Moses Paintsil, Prof. David Adu-Poku, Dr. Mary-Magdalene Padevoah, Prof. Lawrence S. Borquaye, Dr. Genevieve Adukpo, Prof. Mercy Badu, Dr. Gershon Amenuvor, Prof. Isaac Asiamah, Mrs. Judith Odei Owusu-Asante, the Ghana Chemical Society Student Representative, Dr. Emmanuel Ramsey Buabeng, and Dr. Lilian Sarpong as well as the support of our partners and volunteers, who have ensured that we provide an engaging and memorable experience for all participants. I am sincerely appreciative of their efforts and sacrifices.

As we gather over the next few days, I encourage each participant to take full advantage of the scientific sessions, keynote lectures, poster presentations, exhibitions, and networking opportunities. Let us engage in meaningful discussions, forge new partnerships, and explore innovative ideas that will strengthen the role of chemistry in addressing societal needs and advancing sustainable development.

I wish you a productive, inspiring, and enjoyable conference, and I look forward to the valuable outcomes that will emerge from our interactions during this important gathering.

Thank you and welcome to the 22nd Ghana Chemical Society International Conference and Annual General Meeting.

Prof. Collins Obuah

Chairman, Local Organising Committee

22nd Ghana Chemical Society International Conference & AGM

University of Ghana, Legon, Accra

CONFERENCE SPONSORS

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CONFERENCE PROGRAMME

Day 1: Tuesday 13 th October 2026		
Time	Activity	Facilitator
8:00	Registration	
8:30	Opening Prayer	Moderator
8:35	Welcome Address/Opening Remarks	President (<i>Ghana Chemical Society</i>)
8:45	Introduction of Chair	Moderator
8:50	Chair's response	Prof. Nana Aba Appiah Amfo (<i>Vice-Chancellor, University of Ghana, UG</i>)
9:10	Introduction of Guest Speaker	Moderator
9:15	Guest Speaker	Prof. Nana Ama Browne Klutse (<i>CEO, Environmental Protection Agency, EPA</i>)
9:45	Keynote Address	Dr. Joseph Siaw Agyepong (<i>CEO, Zoomlion Gh Ltd</i>)
10:10	Message from Sponsors	Moderator
10:25	Chair's Closing Remarks	Prof. Nana Aba Appiah Amfo (<i>VC, UG</i>)
10:30	Snack break & Networking	
10:45	Parallel sessions I 1. <i>Smart and Sustainable Materials for a Low-Carbon Future and Digital Chemistry and AI-Driven Innovations</i> 2. <i>How to Publish (Workshop)</i> 3. <i>Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development</i>	Main Auditorium & Syndicate Room 1 Dr. Andrew Shore (Commonwealth Chemistry/RSC)
13:00	Lunch & Poster Session	
14:00	Parallel sessions II 1. <i>Green Chemistry for Climate Resilience and Environmental Sustainability</i> 2. <i>Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development</i>	Main Auditorium & Syndicate Room 1
15:30	Introduction of Speaker	Moderator
15:35	Scientific Presentation 1: <i>Bimetallic Nanoparticles for sustainable chemical production from bio-derived furfural, levulinic acid and glycerol</i>	Prof. Michael Forde (<i>University of West Indies, Trinidad and Tobago</i>)
16:05	Q&A	Moderator
16:10	Break	
16:25	Introduction of Speaker	Moderator
16:30	Scientific Presentation 2: <i>Electronic structure and mechanistic pathways of N₂ reduction on 1,3,5,7-tetra-bora adamantane</i>	Prof. Sarah Masters (<i>Commonwealth Chemistry</i>)
16:50	Q&A	Moderator
17:00	Scientific Presentation 3: <i>Creative Designs and Chemistries for Advanced Technologies and the Advancement of Sustainability</i>	Dr. Silas Owusu-Nkwantabisah, (<i>PPG Automotive Coatings, USA</i>)
17:20	Q&A	Moderator

17:30	Special Talk 1: <i>Innovating Chemistry: Designing Labs for Disability Inclusion</i>	Dr. Alejandra Palermo (Commonwealth Chemistry/RSC)
17:50	Q&A	Moderator
18:00	Poster Session & Networking	
19:00	Closing	
Day 2: Wednesday 14th October 2026		
8:00	Registration	
8:30	Welcome & Acknowledgement of Dignitaries	Moderator
8:35	Introduction of Speaker	Moderator
8:40	Scientific Presentation 4: <i>Fischer-Tropsch catalysts supported on carbon</i>	Emeritus Prof. Neil Coville (University of Witwatersrand, South Africa)
9:10	Q&A	Moderator
9:20	Scientific Presentation 5: <i>Digital Chemistry and AI-Driven Innovations in Addressing Healthcare Challenges</i>	Dr. Yaw Osafo (CEO, Medicas Hospital, Ghana)
9:40	Q&A	Moderator
9:50	Scientific Presentation 6: <i>Are soils amended with antiretroviral drug-contaminated biosolids safe?</i>	Prof. Bice S. Martincigh (Commonwealth Chemistry)
10:10	Q&A	Moderator
10:20	Snack break & Networking	
10:40	Parallel sessions III 1. <i>Green Chemistry for Climate Resilience and Environmental Sustainability</i> 2. <i>Human Health Strengthening Cross-Sector Partnerships for Sustainable Development</i>	Main Auditorium & Syndicate Room 1
13:00	Lunch & Poster Session	
14:00	Parallel sessions IV 1. <i>Green Chemistry for Climate Resilience and Environmental Sustainability.</i> 2. <i>Human Health Strengthening Cross-Sector Partnerships for Sustainable Development</i>	Main Auditorium & Syndicate Room 1
15:30	Scientific Presentation 7: <i>The Azobispyrrole Framework</i>	Prof. Alison Thompson (Commonwealth Chemistry)
15:50	Q&A	
16:00	Scientific Presentation 8: Progress in Accelerating Drug Discovery in Africa	Prof. Richard K. Amewu (University of Ghana)
16:20	Q&A	
16:30	Panel Discussion: <i>Industry-Academia Networking Forum</i>	Mr. Moses Abeiku Paintsil (Ghana Water Company), Prof. David Adu-Poku (University of Energy and Natural Resources), Prof. Samson Abah Abagale (University of Technology and Applied Science), Dr. Edward Akwetey (Fumman Ghana Limited)
17:15	Poster Session & Networking	
18:30	Closing	

Day 3: Thursday 15 th October 2026		
8:00	Registration	
8:30	Welcome & Acknowledgement of Dignitaries	Moderator
8:35	Introduction of Speaker	Moderator
8:40	Scientific Presentation 9: <i>Boron in Sustainability and Catalysis: A Computational Molecular Perspective</i>	Dr. Felipe Fantuzzi (<i>University of Kent, UK</i>)
9:00	Q&A	Moderator
9:10	Special Talk 2: <i>Communicating Research Findings – Science and Social Media</i>	Giovanni Ortolani (<i>UNESCO-TWAS</i>)
9:30	Q&A	Moderator
9:40	Scientific Presentation 10: <i>In pursuit of new vulnerabilities in HIV-1 replication for drug discovery: Structural characterization of HIV-1 Pol Polyprotein using single particle cryo-EM</i>	Dr. Jerry Joe Harrison (<i>University of Ghana</i>)
10:00	Q&A	Moderator
10:10	Snack break & Networking	
10:30	Keynote: <i>Milestones to an Academic Career-Requirements, Issues, Potential Challenges and Outcomes</i>	Prof. Emeritus Ivan Addae-Mensah (<i>Former Vice-Chancellor, University of Ghana</i>)
11:00	Q & A	Moderator
11:10	Scientific Presentation 11: <i>Integration of pretreatment processes with smart membranes for complex wastewater remediation</i>	Prof. Richard Moutloali (<i>University of South Africa</i>)
11:30	Q & A	Moderator
11:40	Special Talk 3: <i>Pathways and Skills for the Next Generation Chemists: The Role of Networking, Mentorship and Capacity Building Platforms</i>	Prof. Marian Asantewah Nkansah (<i>Kwame Nkrumah University of Science and Technology, Ghana</i>)
12:00	Q & A	Moderator
12:10	Special Talk 4: <i>Collaboration in Research: Lessons from My Independent Research Career</i>	Prof. James Darkwa (<i>Center for Innovation and Entrepreneurship, CSIR College of Science and Technology, Ghana</i>)
12:30	Q&A	Moderator
12:40	Scientific Presentation 12: <i>Waste valorisation for product development: A sustainable approach</i>	Prof. Fidelis Kpodo (<i>University of Health and Allied Sciences, Ghana</i>)
13:00	Q&A	Moderator
13:10	Lunch Break	
14:00	Scientific Presentation 13: <i>In-Silico study of new Sulfonyl urea Analogues as Potential Anti-Diabetic Agents: ADMET, Molecular Docking and Dynamics, MMGBSA and DFT Studies</i>	Dr. Ndivhuwo Tshiluka (<i>University of Johannesburg, South Africa</i>)
14:20	Q&A	Moderator
14:30	Scientific Presentation 14: <i>Advancing Natural Products Towards Antimalarial Hit-to-Lead Development: The Salacia debilis Story</i>	Prof. Lawrence S. Borquaye (<i>Kwame Nkrumah University of Science and Technology, Ghana</i>)
14:50	Q&A	Moderator
15:00	Ghana Chemical Society General Meeting	GCS Executives
18:00	Dinner and Awards	
20:00	Closing	

PROFILE OF MAIN SPEAKERS

PROFESSOR NANA ABA APPIAH AMFO (Conference Chair)

Professor Nana Aba Appiah Amfo is a trailblazing Ghanaian academic, an internationally renowned Professor of Linguistics, and the current Vice-Chancellor of the University of Ghana, Legon. She is making institutional history as the first female Vice-Chancellor of Ghana's premier and largest university and stands out as a visionary institutional leader whose administrative, scholarly, and transformative impact spans more than two decades. Professor Amfo's academic journey is rooted in a rich foundation of global higher education. She began her tertiary studies at the University of Ghana, where she earned her Bachelor of Arts degree in French and Linguistics. Recognizing the power of language in human development, she proceeded to the Norwegian University of Science and Technology (NTNU) in Trondheim, Norway, where she successfully completed both her Master of Philosophy (MPhil) and Doctor of Philosophy (PhD) degrees in Linguistics. While she presides over an annual conference dedicated to the advancement of the chemical sciences, Professor Amfo beautifully embodies the intersection of interdisciplinary academic mastery. Her primary research domain lies within the intricate structures of Pragmatics and Semantics focusing heavily on how context shapes meaning in human communication. Her extensive research portfolio includes: Sociolinguistics and African Languages and Specialized Communication Domains. The Ghana Chemical Society (GCS) is deeply honored and privileged to have her serve as the Conference Chair for this year's Annual Conference, where her dedication to cross-disciplinary innovation will guide our academic deliberations.

PROF. NANA AMA BROWNE KLUTSE

Prof. Nana Ama Browne Klutse is a Physicist and Professor at the University of Ghana. Appointed as EPA CEO in January 2025, she also serves internationally as Vice-Chair of IPCC Working Group I. She earned her BSc from the University of Cape Coast and PhD from the University of Cape Town. Past leadership includes heading the Physics Department and managing the Climate Centre at the Ghana Space Science Institute. Her expertise spans atmospheric physics, regional climate modeling, and West African monsoon dynamics. She contributed to the CORDEX experiment and served as an IPCC Sixth Assessment Lead Author. She is a UNESCO IBSP board member and mentors young women in STEM.

His broader research interests include chemical bond theory, astrochemistry and the origins of life, and the computational design of functional molecules and materials. Boron chemistry remains a recurring theme, with applications spanning catalysis, optoelectronics, sensing, molecular materials, and health-related technologies.

DR. JOSEPH SIAW AGYEPONG

Dr. Joseph Siaw Agyepong is a Ghanaian entrepreneur, business leader, and environmental advocate known for his contributions to waste management, sanitation, and sustainable enterprise development. He is the Founder and Executive Chairman of the Jospong Group of Companies, one of Ghana's largest diversified business groups, with interests spanning environmental services, finance, ICT, manufacturing, logistics, agriculture, and construction.

A key part of his entrepreneurial journey is Zoomlion Ghana Limited, established in 2006 to deliver integrated waste management solutions. Under his leadership, the company has become a major player in Ghana's environmental sanitation sector, with operations in waste collection, recycling, composting, sewerage treatment, medical waste management, and related services.

Dr. Agyepong has championed innovative and locally relevant approaches to environmental and sanitation challenges, promoting waste as a resource while supporting cleaner communities and sustainable livelihoods. He also emphasises collaboration among government, industry, local authorities, and communities in advancing sustainable waste management.

His contributions to industry and national development have earned him several honours, including the Order of the Volta, an honorary doctorate from Kwame Nkrumah University of Science and Technology, and the Ghana Business Awards' Entrepreneur of the Decade award in 2020.

His experience across entrepreneurship, environmental management, innovation, and sustainable development offers valuable industry perspectives on how science, technology, and partnerships can contribute to healthier and more resilient communities.

PROF. MICHAEL FORDE

Prof. Michael Forde is President of Commonwealth Chemistry, making history as the first Caribbean leader to head the federation of 56 national chemical societies worldwide. He is also a Senior Lecturer in Chemistry at The University of the West Indies (The UWI), St. Augustine Campus, Trinidad and Tobago, and Secretary of the Trinidad and Tobago Chemical Society (TTCS).

Prof. Forde is committed to strengthening scientific capacity and fostering mentorship for the next generation of chemists by bridging the gap between senior practitioners and early-career scientists across Commonwealth nations. He holds an MChem from The UWI and a PhD in Heterogeneous Catalysis from Cardiff University, awarded in 2012.

Beyond academia, Prof. Forde is an entrepreneur in cosmetic manufacturing and an active community leader. His interests include local environmental initiatives such as end-of-life tire recycling and greenhouse crop cultivation, reflecting his broader commitment to science, innovation, sustainability, and community development.

PROF. EMERITUS NEIL COVILLE

Prof. Emeritus Neil Coville is a distinguished inorganic and materials chemist whose research spans carbon chemistry, organometallic chemistry, and heterogeneous catalysis, with applications in catalysis, materials science, sensors, and renewable energy.

He obtained his BSc (Hons) and MSc from the University of the Witwatersrand (Wits), Johannesburg, and his PhD from McGill University, Montreal, in 1973. Following postdoctoral research at Harvard University, he returned to Wits in 1976, progressing to Chair of Inorganic Chemistry before becoming Professor Emeritus. He has also contributed to the DSI-NRF Centres of Excellence in Catalysis and Strong Materials and held research sabbaticals at leading universities in the United States.

His research focuses on the synthesis, shaping, and doping of carbon materials, with applications including Fischer-Tropsch catalysis, sensors, and solar cells.

Prof. Coville served as President of Commonwealth Chemistry from 2022 to 2024, following his term as President-Elect and later serving as Past-President. His leadership focused on strengthening collaboration among Commonwealth chemical societies, scientific capacity building, international research, and opportunities for early-career scientists.

Through his research and international leadership, Prof. Coville has contributed significantly to the advancement of chemistry and scientific collaboration across Africa and the wider Commonwealth.

DR. YAW OSAFO

Dr. Yaw Osafo is a Medical Doctor, Specialist Chemical Pathologist, and Chief Executive Officer and Chief of Medical Staff at Medicas Hospital, Ghana. He obtained his MBChB from the University of Ghana Medical School and his postgraduate qualification in Laboratory Medicine, specializing in Chemical Pathology, from the Ghana College of Physicians and Surgeons. He also holds an MBA in Health Services Administration from the University of Ghana Business School.

His clinical expertise spans Clinical Biochemistry, Metabolic Medicine, and Medical Toxicology. He previously served as a Chemical Pathologist at Korle-Bu Teaching Hospital, where he provided clinical care at the Endocrine Metabolic Clinic and contributed to the training of medical students and residents.

Dr. Osafo contributes to medical literature and has co-authored notable publications, including *Principles of Medicine in Africa*. He also serves on the Clinical Experts Committee of the National Health Insurance Authority (NHIA), contributing technical expertise to clinical governance and the advancement of standards in toxicology and clinical biochemistry.

DR. FELIPE FANTUZZI

Dr. Felipe Fantuzzi is a Lecturer in Chemistry at the University of Kent, United Kingdom, where he serves as Director of the Supramolecular, Interfacial and Synthetic Chemistry (SISC) research group and Co-Director of the Kent Astrochemistry, Irradiation, Origins and Space (KAIIROS) initiative. His research spans theoretical chemistry, astrochemistry, radiation science, and functional materials within an interdisciplinary framework.

He obtained his BSc, MSc, and PhD in Chemistry from the Federal University of Rio de Janeiro, Brazil, followed by postdoctoral research in Brazil, the United States, and Germany. His career has been supported by fellowships from CAPES, CNPq, the Alexander von Humboldt Foundation, and ASF-PNNL. He received the Octávio Augusto Ceva Antunes Medal for the best PhD thesis.

Dr. Fantuzzi combines quantum chemical methods and multiscale modelling to investigate electronic structure, chemical bonding, and molecular reactivity. His work explores unconventional main-group chemistry, including radical and biradical systems and low-valent compounds of boron, aluminum, and beryllium, alongside theoretical approaches to bonding in complex molecular systems. His research also encompasses astrochemistry, combining

computational chemistry with irradiation and spectroscopy to explore molecular processes under extreme conditions. His work on complex organic molecules, polycyclic aromatic hydrocarbons, fullerenes, and astrophysical ice analogues provides insights into molecular transformation and reactivity in space.

PROF. RICHARD KWAMLA AMEWU

Prof. Richard Kwamla Amewu is an Associate Professor of Organic and Medicinal Chemistry and Leader of the Drug Innovation Group in the Department of Chemistry at the University of Ghana, Legon. He holds an MSc and PhD in Medicinal and Organic Chemistry from the University of Liverpool, United Kingdom, where he pursued his academic and research career for over a decade.

He joined the University of Ghana in 2013, where his research focuses on drug discovery for communicable and non-communicable diseases, particularly malaria, tuberculosis, and cancer. His work integrates organic and medicinal chemistry to support the development of new therapeutic candidates and strengthen drug discovery capacity in Africa.

Prof. Amewu contributes to international research networks, including the Malaria Drug Accelerator (MalDA) consortium and the Africa-Europe Horizon Europe RAFIKI consortium, which aims to advance early-stage drug discovery and infectious disease research in sub-Saharan Africa.

His research and collaborations reflect a commitment to translating medicinal chemistry into impactful drug discovery while building sustainable research capacity and strengthening Africa's contribution to global health innovation.

MR. MOSES ABEIKU PAINTSIL

Mr. Moses Abeiku Paintsil is the Chief Manager for Water Resources and Water Quality Assurance at Ghana Water Limited (GWCL). With extensive experience in industrial water chemistry and utility management, he oversees the strategic framework for protecting raw water resources and ensuring the quality and safety of treated municipal water systems. He has built his career within GWCL, previously serving as a Regional Water Quality Assurance Manager.

Mr. Paintsil is a strong advocate for water security and resource protection in Ghana. His work has contributed to research and public sector interventions addressing the growing chemical and financial challenges posed to municipal water treatment by illegal mining and environmental pollution.

His expertise lies at the intersection of environmental chemistry, process engineering, and public health, with a focus on protecting water resources and supporting sustainable access to safe water across Ghana.

DR. SILAS OWUSU-NKWANTABISAH

Dr. Silas Owusu-Nkwantabisah is a chemical scientist, materials engineering leader, and Science & Technology Manager for Automotive Refinish at PPG Industries, USA, a global leader in paints and coatings. He holds a BSc in Chemistry from Kwame Nkrumah University

of Science and Technology (KNUST), followed by an MS and PhD in Chemistry from the University of Maryland, College Park, and the University of Maine, respectively. He also holds an MBA from the University of Illinois Urbana-Champaign.

His career spans R&D and engineering roles across major technology and materials science companies, including Engineering Manager at Intel Corporation and Research Scientist positions at Cabot Microelectronics and Eastman Kodak Company. His expertise encompasses polymer chemistry, advanced automotive coatings, and structural hydrogels.

Dr. Owusu-Nkwantabisah brings together fundamental chemistry, materials science, and engineering to develop technologies with practical industrial applications. His work reflects the translation of chemical research into high-value materials and manufacturing solutions, bridging academic innovation with global industry.

ABSTRACTS FOR THE 22nd INTERNATIONAL CONFERENCE

MAIN (PLENARY) SESSION

Chemistry in the Circular Economy: Converting Waste into Valuable Resources for Climate Resilience, Public Health and Sustainable Cities

Dr. Joseph Siaw Agyepong; Rev. Ing. Dr. Glenn Kwabena Gyimah; Dr. Mrs. Gloria Boamah Kusi. Zoomlion Ghana Limited, Accra

The convergence of escalating waste generation, climate vulnerability, and public health crises, particularly across rapidly urbanising regions of the Global South, demands a fundamental rethinking of how societies value and manage waste. This paper examines the pivotal role of chemistry in transitioning from linear waste disposal to circular resource valorisation, positioning chemical science not merely as a technical enabler but as the foundational discipline through which waste streams become feedstocks for climate adaptation, health protection, and urban sustainability. Drawing on peer-reviewed literature, development agency reports, and documented field interventions, the paper explores three critical waste streams: organic waste (through composting and anaerobic digestion), plastics (through chemical recycling and mechanochemical depolymerisation), and electronic waste (through hydrometallurgical and pyrometallurgical recovery). It then connects these chemical pathways to three operational imperatives: climate resilience through emissions reduction and renewable energy generation, public health protection through the elimination of open burning and toxic exposure, and sustainable urbanism through the formalisation of waste value chains and the creation of green livelihoods. The paper argues that chemistry's contribution to the circular economy is most impactful when embedded within integrated systems that combine technological innovation with policy reform, infrastructure investment, and community-level economic participation. A framework is proposed for operations seeking to translate chemical valorisation principles into practice, emphasising context-appropriate technology selection, extended producer responsibility, and the strategic formalisation of informal sector actors. The conclusion asserts that chemistry provides the essential molecular toolkit for circularity, but that its transformative potential is realised only when coupled with deliberate operational design that centres equity, resilience, and long-term sustainability.

Keywords: circular economy, waste valorisation, green chemistry, climate resilience, public health, sustainable cities, chemical recycling, anaerobic digestion

Bimetallic Nanoparticles for sustainable chemical production from bio-derived furfural, levulinic acid and glycerol

Nakisha P Mark,¹ Freida V Kauffmann² and Michael M Forde^{2*}

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Keywords: sustainable catalysis; supported nanoparticles, sustainable chemicals, hydrogenation, materials characterisation

Chemical production from biomass derived feedstocks supports the introduction of sustainable chemicals that replace fossil-fuel derived feedstocks but with the same functionality. One approach to selective and high yield transformation of bio-derived platform chemicals is the use of bimetallic supported nanoparticles where one metal species modified the activity or selectivity of the other metal species, or to couple two different but complimentary reactions to increase sustainability. This talk will explore these two approaches using low loading bimetallic catalysts for furfural hydrogenation and levulinic acid hydrogenation with glycerol as a green hydrogen donor. In the furfural reaction, careful characterization of the catalysts using XAS reveal that the two metal species are not alloying during catalyst preparation, though routine HR-TEM-EDS analysis would suggest alloying. The introduction of a third, non-catalytically alkaline metal, stabilizes the catalyst from loss of the highly disperses nanoparticles while maintaining its high activity. In the levulinic acid system, an antagonistic effect of coupling two metals on the same catalyst surface is observed and Pt based materials are shown to be highly active in the hydrogenation reaction using a green liquid hydrogen donor. The talk highlights the need for complementary materials characterization techniques in catalyst development.

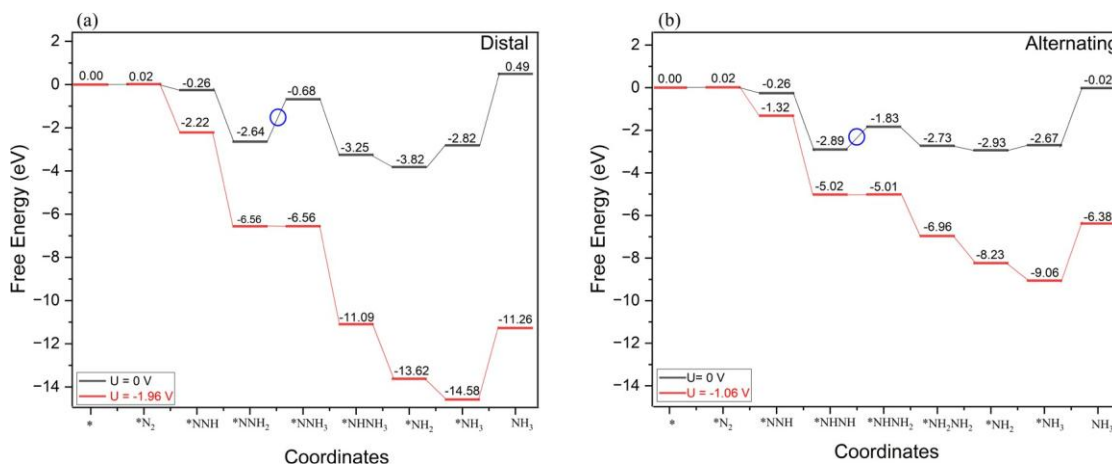
Electronic structure and mechanistic pathways of N₂ reduction on 1,3,5,7-tetra-bora adamantane

Aminu H. Yusuf, Vladimir B. Golovko, Sarah L. Masters*

School of Physical and Chemical Sciences, University of Canterbury, Christchurch, New Zealand, 8140; MacDiarmid Institute for Advanced Materials and Nanotechnology; E-mail: sarah.masters@canterbury.ac.nz

The development of efficient and sustainable methods for ammonia synthesis remains a challenge in addressing global agriculture and energy needs.¹ This study investigates the electrochemical nitrogen reduction reaction (NRR) on a metal-free catalyst, 1,3,5,7-tetra-bora adamantane (4TBA) using density functional theory.^{2,3} The 4TBA catalyst demonstrates effective N₂ activation evidenced by a moderate adsorption energy (-0.44 eV) that enables effective catalysis without surface poisoning, a red shift in the N≡N vibrational frequency (149 cm⁻¹), and bond elongation. Mechanistic analysis reveals that the alternating pathway¹ has a lower theoretical overpotential (0.90 V), however the kinetic barrier is high ($\Delta G^\ddagger = 1.06$ eV). In contrast, the distal pathway, characterized by a higher overpotential (1.80 V), has an undetectable kinetic barrier for the hydrogenation steps (See Figure). This evidence suggests that the distal pathway is preferred for the NRR using 4TBA. These findings contribute to the

fundamental understanding of 4TBA as a metal-free catalyst for the NRR and provides valuable insight to the importance of kinetic analysis over purely thermodynamic assessments in mechanistic studies.⁴



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Innovating Chemistry: Designing Labs for Disability Inclusion

Alejandra Palermo*

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Disability inclusion is essential to creating a chemistry community in which everyone can thrive. Yet disabled chemists continue to face barriers affecting their experiences, career progression and retention. Drawing on data and research into the experiences of disabled chemists in laboratories, this talk will explore the current landscape of disability inclusion and the practical changes needed to create more accessible laboratory environments.

Our research highlights gaps between organisational commitments and lived experiences, including limited awareness of barriers, difficulties accessing adjustments and communication challenges. It also emphasises the need for anticipatory inclusion, where accessibility is considered from the outset rather than relying on individuals to advocate for their needs.

The talk will showcase practical solutions from a growing library of laboratory case studies, demonstrating how simple and cost-effective changes can improve accessibility and the experience of all laboratory users.

Ultimately, creating inclusive laboratories requires collective action. By removing barriers rather than expecting individuals to adapt, we can ensure disabled talent is supported, retained and able to reach its full potential in chemistry.

Keywords: inclusion, diversity, accessibility, disability inclusion, sustainable workforce

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Fischer-Tropsch catalysts supported on carbon.

Neil Coville

University of the Witwatersrand (Wits), Johannesburg, South Africa

The Fischer-Tropsch (FT) reaction is a process to make chemicals and fuels from numerous carbon sources including biomass/coal/gas/oil. The FT reaction produces a wide range of products with the recent focus being to make sustainable aviation fuels (SAFs) in the range C8 to C16 hydrocarbons. The active catalyst (Co or Fe) in FT is supported on a wide variety of supports, including carbons. One of these, the hollow carbon sphere (HCS) has a core-shell structure in which the core is empty. This allows for metals to be placed both inside and outside the shell. The HCSs have a high surface area, excellent electronic conductivity, low weight, are mesoporous and are relatively chemically inert. The encapsulation of active metal nanoparticles allows the HCSs to be used as nanoreactors for the active metal encapsulated by the carbon structure. The relative chemical inertness of HCSs also reduces the Co-carbon interaction and enables simpler reducibility and enhanced metal catalytic activity. In this talk an introduction to the FT process will be given and the influence of catalyst promoters on the reaction using HCSs will be given. The role of AI in a recent study will also be given

Digital Chemistry and AI-Driven Innovations in Addressing Healthcare Challenges

Dr. Yaw Osafo (*CEO, Medicas Hospital, Ghana*)

The state of the earth's climate is inextricably linked with the well-being of mankind. Faced with unprecedented adverse climatic events, severe environmental degradation from illegal mining, and uncomfortable national healthcare statistics, there is an urgent need to renew commitments to ensure healthy lives and well-being for all. This keynote address explores how two key concepts—Digital Chemistry and Artificial Intelligence (AI)-Driven Innovation—can serve as the essential keys to unlock Ghana's full development potential in the health sector in a sustainable and climate-friendly manner. Historically, Chemistry intervened to transform medical diagnostics, shifting medicine away from archaic and hazardous practices. Today, digital chemistry treats chemical discovery as a programmable, computable workflow. This interdisciplinary domain leverages advanced computation, machine learning, and automation to dramatically compress drug development timelines, optimize clinical success rates, and eliminate physical resource waste. Furthermore, AI-driven diagnostic innovations, such as machine learning algorithms applied to routine full blood counts, offer low-middle-income countries a high-accuracy, cost-effective alternative to expensive, outsourced molecular tests. Beyond diagnostics, the address highlights the integration of smart materials and AI building management systems to transform carbon-intensive hospitals into sustainable, green healthcare centres. Looking to the future, embedding digital chemistry into the healthcare fabric of Africa will democratize vital medical disciplines, power decentralized Lab-on-a-Chip diagnostics, and

enable predictive, patient-centred care. Realizing this vision requires a robust call to action for transdisciplinary integration, strategic cross-sectoral partnerships, substantial government financing for research institutions, and pragmatic mentorship programs for the next generation of scientists.

Are soils amended with antiretroviral drug-contaminated biosolids safe?

Bice S. Martincigh

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Biosolids are treated solid products from wastewater treatment plants that are nutrient-rich and beneficial for soil enhancement. They serve as a sink for emerging pollutants, such as antiretroviral drugs (ARVDs), which can be toxic and persistent in the environment. The application of biosolids can introduce ARVDs into terrestrial environments, leading to potential uptake by plants. In this study, the uptake and bioconcentration of twelve ARVDs by four cultivars grown in biosolid-amended soils were investigated. Bioconcentration of the ARVDs in the plants ranged from low to high, with didanosine showing the greatest tendency to accumulate. The soil type and the nature of the plant cultivar played significant roles in ARVD uptake. However, the concentrations of ARVDs in the plant samples were below the maximum permissible residue limits for similar pharmaceuticals in food. The estimated daily intake of ARVDs from consuming these crops was low for all population groups studied. The findings collectively show that the interplay among soil type, drug physicochemical properties, and amendment method controls the transfer of ARVDs from soil to crops, with polar ARVDs having a greater potential to enter edible tissues. These results offer significant empirical support for the environmental risk assessment of ARVDs in agroecosystems altered with biosolids.

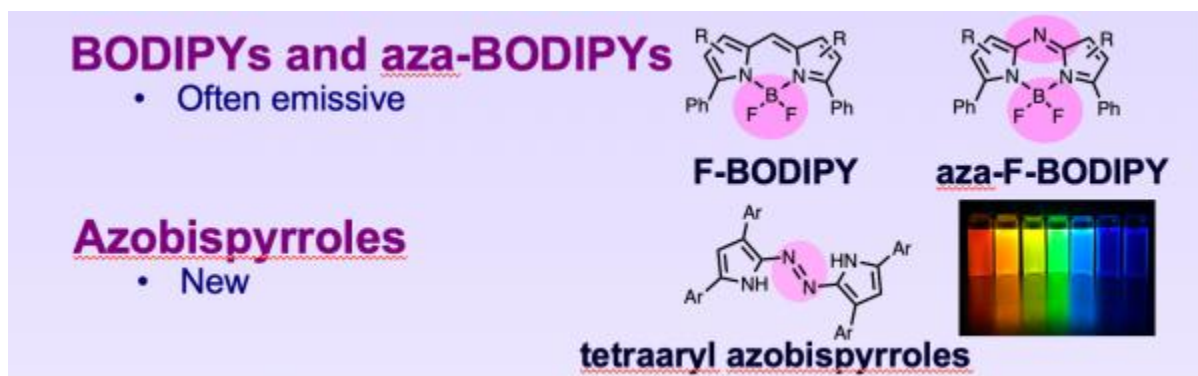
Keywords: antiretroviral drugs, biosolid-amended soil, plant uptake, dietary exposure, sludge reuse.

The Azobispyrrole Framework

Dr. Alison Thompson

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Synthetic chemistry involving pyrroles is challenging courtesy of electron-rich aromaticity and the propensity to oxidise or polymerise. BODIPYs and azobispyrroles incorporate two pyrrole units – double the fun, and double the challenge! Harnessing the chemistry of the pyrrolic motif leads to dipyrrolic structures that exhibit desirable properties as ligands and as photoactive species useful in chemical biology sensing/staining, photodynamic therapy and energy harvesting. Azobispyrroles will be described, alongside strategies for their synthesis over the well-established aza-dipyrin framework.



Keywords: pyrrole, azo dye, synthesis, absorption, emission

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Progress in Accelerating Drug Discovery in Africa

Prof. Richard Kwamla Amewu

Department of Chemistry, University of Ghana, Legon

Africa disproportionately has one of the highest burdens of infectious and non-infectious diseases, yet the contributions of Africans to finding solutions to these health challenges are limited. The people of Africa will benefit significantly if African scientists, through innovations, participate in the global efforts to tackle the continent's heavy disease burden with localised, effective, and independent medical solutions.

Drug discovery in Africa is heavily constrained by severe financial underinvestment, inadequate laboratory infrastructure, and a reliance on external donor funding. In collaboration with several international partners, efforts such as the Grand Challenges Africa Drug Discovery Accelerator (GCADDA), H3D Foundation, Global Health Mentorship Programs, and the EU-Africa Research Infrastructure Alliance to Foster Infectious Disease Research, Knowledge Sharing and Innovation (RAFIKI) are accelerating drug discovery in Africa. This presentation discusses these efforts and progress from selected groups in drug discovery on the continent.

Computational Chemistry for a Healthier Planet: From Molecular Design to Sustainable Materials

Felipe Fantuzzi^{1*}, Caroline R. Kwawu^{1,2}

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Keywords: Computational chemistry; Boron chemistry; Functional materials; Photo-assisted chemical vapour deposition; Medicinal chemistry.

Computational chemistry provides a powerful framework for connecting fundamental electronic structure with the design of molecules and materials relevant to sustainability, energy and human health. In this contribution, we present examples from our research showing how quantum-chemical calculations, combined with experiment, can clarify chemical bonding, predict molecular properties and guide functional molecular design. Particular attention will be given to boron chemistry,^{1,2} where electron deficiency and unusual bonding patterns enable distinctive reactivity and opportunities for new main-group compounds and materials. We also discuss photo-assisted chemical vapour deposition (PACVD) precursors,³ where excited-state calculations and analysis of selective ligand dissociation help rationalise precursor activation and the formation of functional thin films. Further examples involve quinone-based systems, ranging from redox-active organic molecules for aqueous energy storage to functionalised naphthoquinones with potential applications against neglected tropical diseases.⁴ Across these areas, electronic-structure calculations provide a common platform for understanding structure, reactivity, stability and mechanism, while integration with experiment and international partnerships supports the development of smarter chemical solutions for a healthier and more sustainable planet.

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From Evidence to Impact: Storytelling and Communication Skills for Scientists

Mr. Giovanni Ortolani

UNESCO-TWAS

If facts alone changed minds, communicating science would be easy. Yet people connect with stories, images, and messages that resonate with their values and experiences. This talk examines how scientists can use storytelling, audience awareness, and media engagement to communicate research findings beyond academic circles, making complex evidence accessible, relevant, and memorable without compromising scientific accuracy.

In pursuit of new vulnerabilities in HIV-1 replication for drug discovery: Structural characterization of HIV-1 Pol Polyprotein using single particle cryo-EM

Jerry Joe Harrison, Eddy Arnold

University of Ghana, Legon, Accra

To eradicate HIV, new therapeutic interventions are needed for the close to 40 million people living with the disease. In retroviruses including HIV, Gag is the principal agent that drives virus particle formation while protease (PR) encoded at the downstream end of Gag in Gag-Pol orchestrates virus maturation, an obligate step for infectivity. Gag-Pol polyprotein which also contains the enzymes reverse transcriptase (RT) and integrase (IN) is produced through a programmed -1 frameshift caused by a slippery sequence at the 3'-end of the *gag* mRNA and constitutes ~5% of the viral proteins. To understand how maturation is orchestrated by PR while still embedded in Gag-Pol, we solved the structure of HIV-1 Pol polyprotein, a key intermediate produced very early during maturation, using single particle cryo-EM. The structure of the RT in Pol was found to have a similar arrangement as the mature RT heterodimer, and its dimerization likely draws together two PR monomers to activate proteolytic processing. HIV-1 thus may leverage the dimerization interfaces in Pol to regulate assembly and maturation of polyprotein precursors.

Milestones to an Academic Career- Requirements, Issues, Potential Challenges and Outcomes

Prof. Emeritus Ivan Addae-Mensah

University of Ghana

The road to an academic or professional career in the sciences, and indeed in all disciplines, is marked by several milestones. These include the teaching and learning, research and the career phases. Each phase is characterised by various requirements, challenges, issues and possible outcomes. This plenary lecture will select some of these milestones and address the critical issues that will confront any potential academic or professional, including ethical issues, practice, communication with and to peers, subordinates, the general public, governance and policy matters. The lecture will seek to assist participants to discover and address any positive outcomes as well as shortcomings in their various current stages of the selected milestones, help them to appreciate the causes and consequences of their scientific and professional direction, and effectively develop strategies to achieve competence and guide them to future career success.

Graphene oxide modifications with metal organic frameworks: Exploring selective interaction and membrane performance in wastewater treatment

Richard M. Moutloali

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The decrease in the quality and quantity of potable water resources is a growing challenge facing humanity in this century. The physical limit of less than 1% freshwater available to humanity is exacerbated not only by increasing human population but by the rapidly increasing freshwater pollution by industry and other human activities. This calls for increasing wastewater reuse as a potential solution towards this increasing limited clean water for human consumption and use. A variety of technologies are utilized to achieve wastewater reuse, amongst these, mixed matrix membrane technology is gaining increasing attention to its better performance in solute selectivity and overall performance.

The full potential of membranes is hindered by the two challenges: (i) the flux and selectivity trade-off and (ii) membrane fouling. Several approaches are utilized to address these two challenges, the first is tackled by using nanoporous fillers based as actuators that not only promote flux but also increase membrane selectivity if judiciously chosen. The second challenges are generally addressed by increasing membrane surface hydrophilicity, which can also aid in increasing water flux.

Our research has utilized both approaches to fabricate membranes with increasingly improving performances when measured against these two performance indicators. The presentation will detail work done within the past eight years and highlight major milestones achieved in that period. Specifically, the work on utilizing metal organic framework-graphene oxide (MOF@GO) composites as fillers to increase membrane solute rejection and selectivity and the grafting of hydrophilic brushes on the main polymer component will be presented. Potentials and challenges experienced throughout this period will also be outlined briefly.

Keywords: *blending; fouling; grafting; hydrophilic, metal organic framework, selectivity*

Pathways and Skills for the Next Generation Chemists: The Role of Networking, Mentorship and Capacity Building Platforms

Prof. Marian Asantewah Nkansah

Department of Chemistry, Kwame Nkrumah University of Science and Technology (KNUST), Kumasi, Ghana; Founder & Convener, Women in Chemistry Network (WICN)

As a central science driving a **\$5.7 trillion global industry**, chemistry underpins 96% of all manufactured goods and powers critical global solutions across medicine, clean energy, and sustainable agriculture. However, navigating a modern career in the chemical sciences requires the next generation of scientists to strategically balance traditional academic foundations with rapidly evolving industrial demands.

This presentation outlines the multi-tiered career pathways available to chemistry graduates, bridging the gap between academia and vital roles in manufacturing, biomedical health, sustainability, and government policy. It addresses systemic challenges within the competitive academic pipeline, funding gaps, and the intensive demands of modern research environments. To successfully navigate this landscape, emerging chemists must cultivate a diverse toolkit. This includes mastering core technical capabilities alongside emerging interdisciplinary skills—such as AI, data science, and green chemistry—while simultaneously developing essential human skills like cross-disciplinary communication.

Crucially, the presentation highlights that technical aptitude alone is insufficient; networking, intentional mentorship, and capacity-building platforms are non-negotiable for career

longevity. By examining the structure and strategic initiatives of platforms like the Women in Chemistry Network (WICN), we demonstrate how structured mentorship (e.g., WICSMEP) and early capacity-building programs can empower emerging scientists. Ultimately, utilizing these cross-border networks enables the next generation to embrace agile, non-linear career trajectories that actively drive global industrial growth and sustainable development.

Keywords: Career Pathways, Chemistry Education, Interdisciplinary Skills, Mentorship, Capacity Building, WICN

Collaboration in Research: Lessons from My Independent Research Career

James Darkwa

Centre for Innovation and Entrepreneurship, CSIR College of Science and Technology, Accra, Ghana

Although independent research can often be viewed by some early career chemists as a solitary pursuit, collaboration was central to my early research career because of the limited resources at institutions where I started my independent research. As a result, I had no choice but to find collaborators I could work with to enhance the impact of my research outputs. In this talk, I reflect on the lessons learned from building productive collaborations across disciplines, institutions, and countries. Through examples from my own experience, I will show how collaboration can enhance research quality, create new opportunities, and broaden impact; but also highlight instances where there have been challenges around challenges on managing authorship expectations and IP issues. This presentation will offer insights for researchers at all career stages seeking to develop strong and sustainable collaborative relationships.

Waste valorization for product development: A sustainable approach

Prof. Fidelis Kpodo

University of Health and Allied Sciences, Ghana

The agricultural sector, and fruit/ vegetable processing industries significantly contribute to fruit waste in the form of pulps, peels, seeds and kernels. About one-third of food produced globally is wasted, from processing by-products to unsold retail products. Globally fruits and vegetables account for the highest amount (45%) of food wastes. Improper management of fruit wastes and increased disposal of these wastes result in environmental pollution. Cucurbita pepo L., Citrullus lanatus T. and Cucumis melo L. belong to the family Cucurbitaceae and are cultivated for their seeds which find limited utilization in stew/soups as protein supplements. After seed removal from the fruits, the peel and pulp which become agricultural by-products are either discarded or left on the farm for microbial decomposition. The biomass is known to comprise 90% of the fresh fruit. The discarded fruit pulp however potential source of bioactive compounds and functional polysaccharides. Plant polysaccharide comprises of varied sugars and has found useful applications as functional ingredients in both food and pharmaceutical products. The bioactive activities of polysaccharides which include anti-oxidative, anti-diabetic, anti-glycation, anti-tumor, anti-coagulant, anti-proliferative and immunomodulatory properties is of current interest. The lecture will discuss the concept of waste valorisation and describe how agricultural and food processing by-products and food-waste can be transformed into value-added ingredients and products. The effective management of agro-waste and its subsequent utilization would reduce environmental pollution, build a circular economy and provide new sources of cheaper functional ingredients for the food and non-food industries.

***In-Silico* Study of New Sulfonylurea Analogues as Potential Anti-Diabetic Agents: ADMET, Molecular Docking and Dynamics, MMGBSA and DFT Approach**

Ndivhuwo. R. Tshiluka*, Kabelo P Mokgopa and Simon S Mnyakeni-Moleele

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

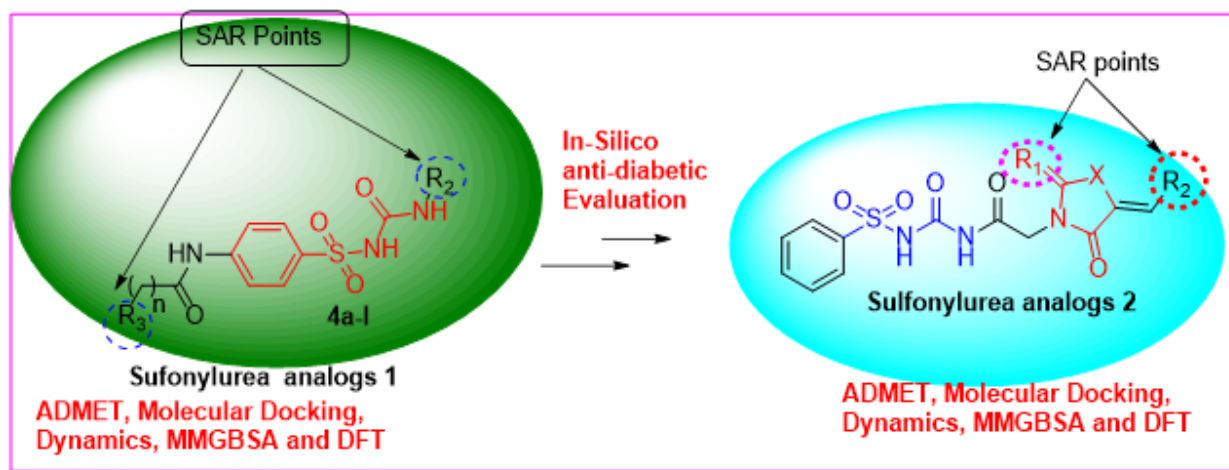


Figure 1: Design and Synthesis of Sulfonyl Urea Analogues Derivatives **1** and **2**

Keywords: Sulfonylureas, *In Silico* Approach, Type 2 Diabetes Mellitus, Treatment

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Advancing Natural Products Towards Antimalarial Hit-to-Lead Development: The *Salacia debilis* Story

Lawrence Sheringham Borquaye

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Kwame Nkrumah University of Science and Technology, Kumasi – Ghana;
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Salacia debilis (G. Don) Walp. (Celastraceae) is a tropical plant traditionally used in Ghana and other parts of Africa for the treatment of malaria and related ailments. Our work on the plant began with the isolation and structural characterization of three compounds and has developed into a multidisciplinary investigation of their antimalarial potential. The compounds have been evaluated through *in vitro* and *in vivo* antimalarial studies, DMPK and solubility investigations, and computational studies of potential molecular targets and ligand–protein interactions. These studies have guided the redesign of the natural-product scaffold and the synthesis of a series of derivatives, which are being evaluated for their solubility and antimalarial activity. The presentation will trace the progression of the *S. debilis* programme from natural-product isolation and biological validation, through DMPK and computational investigation, to synthetic exploration for early hit-to-lead development, and will discuss the emerging relationships between structure, physicochemical properties and antimalarial activity.

ABSTRACTS FOR PARRALLEL SESSIONS

Day 1: Tuesday 13th October 2026 (10:45 to 13:00) (Main Auditorium)

Abstracts for Parallel sessions I: *Smart and Sustainable Materials for a Low-Carbon Future, and Digital Chemistry and AI-Driven Innovations*

Moderator: Dr B. Som

Computational Evaluation of the Performance of C₂₄N₂₄ Single Atom Catalysts for Methane Oxidation: A Combined QTAIM, IBO and DIAS Analysis

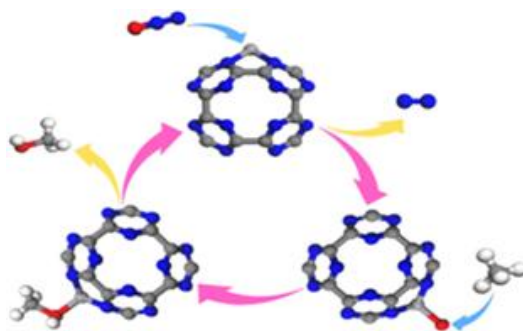
KC Ngubane^a, Mafereka FT Mosoabisane^b and AS Adeyinka

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The development of efficient and selective catalysts for the direct oxidation of methane to methanol remains a major challenge due to the strength of the methane C-H bond and methanol's propensity to undergo overoxidation. In this study, the catalytic performance of first-row (Mn, Fe, Co, Ni, and Cu) and second-row (Ru, Rh, and Pd) transition metal single-atom catalysts (SACs) supported on N-doped fullerene (C₂₄N₂₄) was investigated using density functional theory (DFT) calculations. Reaction energy profiles and activation barriers were computed with ORCA 6.0.0, while the Distortion-Interaction Activation Strain (DIAS) model, Quantum Theory of Atoms in Molecules (QTAIM), and Intrinsic Bond Orbital (IBO) analyses were employed to elucidate the factors governing methane activation. The results show that Ni- and Cu-based SACs exhibit the lowest activation barriers, arising from minimal structural distortion and stronger stabilizing interactions at the transition state. QTAIM analysis revealed distinct variations in bonding characteristics across the metal centres, whereas IBO analysis demonstrated that highly active catalysts facilitate more delocalized electron redistribution during C-H bond activation. In contrast, Ru- and Mn-based SACs exhibit greater structural reorganization and electron localisation, leading to higher activation barriers.

These findings highlight the critical roles of geometric, electronic, and orbital effects in controlling SAC activity for methane oxidation. The study provides mechanistic insights and design principles for developing highly efficient catalysts for methane valorisation through targeted atomic-level modifications.



Keywords: Methane Oxidation, Transition metal, Single-atom catalyst, Fullerene, Activation Energy

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Photocatalytic Pathways to Carbon Valorization: From CO₂ Activation to Hydrocarbon Transformation

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The photocatalytic utilization of carbon dioxide has emerged as a promising strategy for mitigating greenhouse gas emissions while simultaneously producing value-added chemicals through solar-driven catalytic processes. Recent advances in molecular photocatalysis have demonstrated that integrating efficient light-harvesting systems with robust catalytic centres provides an effective route for enhancing CO₂ activation and selective carbon-carbon bond formation.¹ Herein, we report the rational design of molecular and hybrid photocatalysts for sustainable CO₂ valorization *via* the photocatalytic carboxylation of hydrocarbons under mild reaction conditions. A series of nickel(II)- and ruthenium(II)- BODIPY complexes were developed to integrate visible-light absorption with catalytic activity, while α -Fe₂O₃-based hybrid nanocomposites were engineered to promote efficient charge separation, interfacial electron transfer, and enhanced catalyst stability. The influence of catalyst architecture, reaction parameters, substrate scope, and catalyst recyclability was systematically investigated to establish structure-activity relationships governing photocatalytic performance.

The molecular-semiconductor hybrid strategy significantly improves photocatalytic efficiency by combining the high selectivity of molecular catalysts with the durability and charge-transport characteristics of semiconductor materials.² These findings highlight the critical role of interfacial electronic communication in facilitating efficient CO₂ activation and carbon fixation, providing important design principles for next generation photocatalysts capable of converting greenhouse gases into value-added chemicals using solar energy. Overall, this work advances the development of sustainable photocatalytic systems for carbon valorization and demonstrates that hybrid molecular-semiconductor catalyst engineering represents a versatile

platform for efficient solar-driven CO₂ utilization. The insights gained contribute to the broader objective of designing high-performance photocatalytic materials that support the transition towards a circular carbon economy and net-zero chemical manufacturing.

Keywords: Carbon dioxide valorization; photocatalysis; CO₂ fixation; molecular photocatalysts; hybrid nanocomposites; BODIPY; Nickel complexes; Ruthenium complexes; Sustainable catalysis

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Machine Learning- and Molecular Dynamics-Guided Mining of the Human Gut Microbiome for Antimicrobial Peptides

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The human gut microbiome represents a vast and underexplored reservoir of bioactive peptides with potential applications in addressing the growing challenge of antimicrobial resistance (AMR). This study developed a machine learning-guided computational pipeline to mine the human gut microbiome for candidate antimicrobial peptides (AMPs) and investigate their molecular interactions with biological membranes and nucleic acids. More than 680,000 peptide sequences were systematically screened using predictive models for antimicrobial activity, membrane-disruptive potential, toxicity, hemolytic activity, and cell-penetrating properties. High-confidence candidates were subsequently subjected to structural prediction using AlphaFold 3 and characterized through coarse-grained molecular dynamics (MD) simulations to investigate their interactions with biological membranes and DNA. The identified candidate peptides showed high predicted antimicrobial activity, with AMP probabilities of ≥ 0.97 , together with predicted membrane-disruptive and DNA-binding properties. MD simulations revealed peptide-induced membrane perturbation involving lipid displacement, membrane insertion, pore formation, membrane curvature, and loss of membrane integrity. These interactions were consistent with distinct membrane-disruption modes, including barrel-stave, toroidal-pore, and carpet-detergent mechanisms. The peptides also interacted with DNA in the simulations, suggesting a potential complementary intracellular mechanism involving cellular entry followed by nucleic-acid binding. The integration of machine learning, structural prediction, and molecular dynamics enabled systematic prioritization of microbiome-derived peptide sequences and provided mechanistic insights into their predicted membrane and DNA interactions. The findings highlight the human

gut microbiome as a source of candidate antimicrobial peptides and provide a computational framework for prioritizing sequences for experimental validation and further peptide development.

Keywords: Antimicrobial peptides; human gut microbiome; machine learning; molecular dynamics simulations; membrane disruption; DNA binding; AlphaFold 3; antimicrobial resistance.

DFT Insights into CO₂ Reduction on Transition-Metal-Doped NiP(100) Surfaces

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Density functional theory calculations were used to investigate CO₂ electroreduction on pristine and transition-metal-doped orthorhombic NiP(100) surfaces, with Cr, V, Hf, Ti, Zr, and Ta as substitutional dopants. Substitution energies, electronic properties, CO₂ and H adsorption, and free-energy profiles for CO and HCOOH formation were evaluated within the computational hydrogen electrode framework. All dopants showed negative substitution energies at the selected Ni site and modified the surface electronic structure. Doping generally strengthened CO₂ adsorption relative to pristine NiP. Initial protonation favored COOH* formation on pristine NiP and Zr–NiP, whereas Cr–NiP, V–NiP, Hf–NiP, and Ti–NiP favored OCHO* formation. Cr–NiP showed a favorable balance between OCHO* stabilization and HCOOH release, with OCHO* formation at –0.79 eV and HCOOH desorption at 0.03 eV, while V–NiP exhibited a slightly lower uphill OCHO*→HCOOH* step of 1.21 eV. Ti–NiP and Zr–NiP showed strong product-binding limitations, while Ta–NiP was excluded after hydrogen adsorption screening. Overall, the results show that dopant selection must balance CO₂ activation, intermediate stabilization, product release, and hydrogen competition.

Keywords: CO₂ electroreduction; NiP; transition-metal doping; density functional theory; formic acid

Zinc Oxide/Activated Carbon Nanocomposites for Amoxicillin Removal: Precursor-Mediated Solventless Synthesis and Characterization

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The growing demand for functional and sustainable materials is critical to advancing technologies in environmental remediation. Zinc oxide-based nanomaterials with their tunable surface chemistry encoded during synthesis offer considerable potential for water treatment applications. A zinc oleate single-source precursor was synthesized in this work. FTIR probed functional groups, while NMR confirmed oleate coordination to Zn²⁺ via carboxylate groups. TGA revealed the decomposition pathways to efficient conversion into zinc oxide. Nanoparticles were synthesized via solventless thermolysis (melt) of the metal oleate complex,

a low-cost, rapid, scalable, sustainable technique. XRD confirmed the presence of crystalline zincite with an average crystallite size of 11.23 ± 4.36 nm, indicating phase-pure nanoparticles. Zeta potential measurements revealed strongly negative surface charges of -61.2 mV, indicating stable colloidal dispersions. Incorporating the oleate-derived oxide nanoparticles into activated carbon yielded ZnO/activated carbon nanocomposites. After optimization, a 30 wt% metal oxide loading removed 72.99% of amoxicillin from aqueous solution, the best performance achieved. Equilibrium data fitted the Temkin model, indicating a heterogeneous surface energy distribution, and thermodynamic analysis showed a low heat of adsorption value of -0.41 kJ/mol, confirming exothermic, physisorption-governed uptake through synergistic electrostatic attraction, π - π stacking, hydrogen bonding, and pore filling. Solventless thermal decomposition is therefore a viable, eco-friendly route to efficient adsorbents for pharmaceutical wastewater treatment.

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How to Publish (Workshop) - Dr. Andrew Shore (Commonwealth Chemistry/RSC)

Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development (Day 1: Tuesday 13th October 2026 (10:45 to 13:00, Syndicate room 1))

Moderator: Dr L. Hamenu

Scaffold Hopping – Driven Design of Novel Chemical Frameworks for Anthelmintic Drug Development

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The emergence of resistance to benzimidazole anthelmintics in *Haemonchus contortus* poses a significant challenge to parasite control and livestock health. This study explores a computational drug discovery approach to identify novel chemical scaffolds that overcome β -tubulin-mediated resistance. In the absence of an experimentally resolved structure, *H.*

contortus β -tubulin was modelled using homology techniques, followed by the generation of resistance-associated mutants (Q134H, F167Y, E198A, and F200Y). Rigorous structural validation confirmed the reliability of the generated models. Molecular docking of standard benzimidazole drugs revealed reduced binding affinity and deviations in ligand-binding poses within the binding pockets of the mutants compared with the ligand bound to the wild-type protein, particularly in the Q134H and E198A mutants. Molecular dynamics (MD) simulations of these drugs showed clear displacement of ligands from the binding pockets of Q134H and E198A mutants. These observations support their role in conferring resistance. To overcome challenges posed by these mutations, a scaffold-hopping strategy was employed using 9 reference benzimidazole drugs, generating a diverse library of 72,004 novel compounds. Virtual screening against the Q134H mutant, which was used as a stringent resistance model, identified over 5,000 high-affinity candidates (≤ -8.5 kcal/mol), representing 7.34% of the library. Subsequent filtering excluded compounds retaining the benzimidazole core to prioritise structurally novel candidates with reduced susceptibility to cross-resistance. Ongoing molecular docking and MD simulations of β -tubulin–ligand complexes aim to predict the mechanisms of action of selected scaffolds. Overall, this work integrates homology modelling, docking, scaffold hopping, and virtual screening to systematically identify novel anti-parasitic candidates. The findings provide a foundation for developing next-generation anthelmintics with improved efficacy against resistant *H. contortus* strains.

Keywords: Benzimidazole resistance, protein mutations, single-nucleotide polymorphism, in silico studies, and beta-tubulin.

Computational Mining of Ghanaian Plant Natural Products for Rice Weevil (*Sitophilus oryzae*) Acetylcholinesterase Inhibitors

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The rice weevil (*Sitophilus oryzae*) is a major storage pest responsible for significant post-harvest grain losses worldwide. The extensive use of synthetic insecticides, including phosphine and pirimiphos-methyl, raises concerns about environmental contamination and ecotoxicological effects, highlighting the need to explore alternative pest-control agents. This study employed a structure-based computational workflow to identify natural products from Ghanaian medicinal plants with potential inhibitory activity against *S. oryzae* acetylcholinesterase (AChE). Because an experimental three-dimensional structure of *S. oryzae* AChE was unavailable, a homology model was constructed using *Anopheles gambiae* AChE as the template, with 67.96% sequence identity. The resulting model showed 94.58% of residues in the Ramachandran favored regions, supporting its use for structure-based screening. A library of 467 natural products isolated from the volatile oil fractions of Ghanaian medicinal plants was screened against the modeled enzyme. Compounds with binding affinities comparable to or stronger than that of the reference pesticide derivative, pirimiphos-methyl-

oxon, were subsequently evaluated for selectivity against human AChE and subjected to ADMET and physicochemical property filtering. The workflow yielded 136 initial hits, which were refined to 14 candidates following selectivity and pharmacokinetic filtering. Ethyl cinnamate, olivetol, methyl anthranilate, and thymol showed favorable predicted binding energies and interactions with key residues within the catalytic site, together with suitable predicted pharmacokinetic properties. These compounds emerged as candidates for further evaluation as potential inhibitors of *S. oryzae* AChE. Molecular dynamics simulations and experimental bioassays are underway to assess complex stability and determine whether the computationally predicted interactions translate into insecticidal activity. The study provides a structure-based framework for prioritizing Ghanaian plant natural products for further investigation as potential alternatives to conventional insecticides.

Keywords: *Sitophilus oryzae*; rice weevil; acetylcholinesterase; natural products; molecular docking; ADMET; Ghanaian medicinal plants; computational screening.

IMPACT OF GC-MS ANALYTICAL CONDITIONS ON THE CHEMICAL STABILITY AND BIOACTIVITY INTERPRETATION OF ACTIVE COMPOUNDS: A REVIEW

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Gas chromatography–mass spectrometry (GC–MS) is a widely applied analytical technique for identifying and characterizing bioactive compounds in natural products. However, analytical conditions such as elevated injector and column temperatures, derivatization procedures, ionization modes, and matrix effects can compromise chemical stability and distort bioactivity interpretation. This can be seen in vinblastine which degrades into anhydrovinblastine and other fragments. This review was conducted through systematic searches of Google Scholar, Web of Science, Science Direct, PubMed, and Research Gate using relevant keywords. Identified studies were screened for relevance, duplication, and adequacy of methodological detail before inclusion. Articles published before 2010 were excluded, while those from 2010 onward were incorporated. The review critically examined how GC–MS parameters influence thermal degradation, fragmentation, artefact formation, and misidentification of bioactive compounds, with implications for bioactivity profiling. For instance, resveratrol is prone to GC-MS analytical degradation, and derivatization artefacts formation affect interpretations of antioxidative properties if not validated with other methods. Similarly, artemisinin have fragile bonds under GC-MS conditions due to the peroxide bridge. These artefacts and fragments affect interpretations of GC-MS analysis without orthogonal validation. Also, GC–MS analytical conditions, including inherent instrument properties, temperature settings, matrix effects, and functional group degradation substantially affect the detection and identification of bioactive compounds. Thus, serine and threonine can undergo oxime isomerization producing multiple GC-MS peaks that can complicate identification and interpretation. Also,

γ -butyrolactone degrades under severe high GC-MS analytical condition which generates misleading peaks linking to wrong bioactivity profiling. Similarly, scopolamine degrades into apoa tropine-like structures and other rearranged fragments. These evidences demonstrate the risks of erroneous bioactive attribution arising from analytical-induced degradations. The findings highlight the necessity of optimizing GC-MS parameters and employing complementary techniques to ensure accurate chemical elucidation and reliable interpretation of biological activities in natural product research.

Keywords: Bioactive compounds, GC-MS, analytical conditions, chemical stability, artefact formation, matrix interferences,

Ethnobotanical Documentation and In-Silico Polypharmacological Evaluation of Phytochemicals from Medicinal Plants Used for Schistosomiasis Management in Mankessim, Ghana.

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Schistosomiasis remains a major neglected tropical disease in endemic regions such as Ghana, with continued reliance on praziquantel and limited alternative therapeutics. This study aimed to identify potential multi-target antischistosomal agents from medicinal plants used in Mankessim, Ghana. An ethnobotanical survey documented medicinal plants used by local herbal practitioners, and a phytochemical library was curated for in silico screening. Selected compounds were evaluated against *Schistosoma mansoni* targets—thioredoxin glutathione reductase (SmTGR), histone deacetylase 8 (SmHDAC8), and methylthioadenosine phosphorylase (SmMTAP)—using molecular docking and Prime MM-GBSA. Pharmacokinetic and toxicity profiles were assessed using ADMET predictions. Several compounds demonstrated strong binding affinities exceeding those of co-crystallized ligands, with key interactions at Asp230 (SmMTAP), the SmTGR allosteric pocket, and Asp100/Tyr341 in SmHDAC8. ADMET analysis indicated favorable drug-like properties for most compounds, with minimal predicted toxicity. Three hit compounds—CMP1 (1-O-caffeoylglucose), CMP2 (1-O-p-coumaroyl- β -D-glucose) from *Securidaca longepedunculata*, and CMP4 (luteolin-7-Oglucoside) from *Vernonia amygdalina*—exhibited balanced multi-target activity and pharmacokinetic profiles. Notably, several high-performing compounds were derived from plants reported by a single experienced practitioner. This study demonstrates that integrating ethnobotanical knowledge with computational polypharmacology is an effective strategy for identifying multi-target antischistosomal agents. The identified hit compounds exhibited strong binding to key parasite proteins and favorable pharmacokinetic profiles, supporting their potential as promising candidates for therapeutic development. These findings provide a robust

scientific basis for the traditional use of these plants and justify further in vitro and in vivo validation toward the development of novel antischistosomal therapies.

Keywords: Neglected tropical diseases, Schistosomiasis, Mankessim, Ethnobotanical, Polypharmacology.

Maternal Hepatitis B Status and Infant Vaccine Seroconversion: A Cross-Sectional Study from Bolgatanga Municipality in the Upper East Region of Ghana

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Background: Hepatitis B virus (HBV) infection is a major public health concern globally, with 296 million chronically infected individuals. Mother-to-child transmission (MTCT) drives chronic HBV in high-prevalence regions like sub-Saharan Africa. This study evaluated the impact of maternal HBV status on infant seroconversion following the pentavalent HBV vaccine in Bolgatanga Municipality, Ghana.

Methods: A cross-sectional study was conducted among 224 mother-infant pairs attending postnatal clinics. Mothers were screened for HBsAg and other HBV markers, and infants were tested for HBsAg and anti-HBs antibodies using ELISA after completing the three-dose vaccine series. Infant and maternal demographics, vaccination history, and HBV knowledge were collected via questionnaires. Seroconversion was defined as anti-HBs ≥ 1 mIU/mL, and seroprotection as ≥ 10 mIU/mL. Antibody responses in infants and mothers were summarised using geometric mean titres (GMTs), and the association between maternal HBV status and infant antibody response was assessed by comparing mean log-transformed infant antibody titres between maternal HBV groups using two-sample t-tests.

Results: Mothers had a mean age of 27.9 ± 4.9 years, with the majority married (92.0%), self-employed (72.3%), and educated to the Senior High School level (60.3%). Infants were predominantly delivered through spontaneous vaginal delivery (82.1%), with a median gestational age of 38 weeks (IQR: 36-40), median birth weight of 3.0 kg (IQR: 2.7-3.2), and exclusive breastfeeding (63.4%) predominated. Among mothers, 52 (23.2%) were HBsAg-positive; all infants tested negative for HBsAg, indicating 0% MTCT. Infant vaccine coverage was 100%, with 98.7% achieving seroconversion and 90.8% reaching protective anti-HBs levels, with an overall geometric mean titer of 14.2 mIU/mL (95% CI: 12.8-15.7). All HBsAg-positive mothers were HBeAg-negative, reflecting low viral replication. Infant seroconversion did not differ by maternal vaccination or HBV status.

Conclusion: The HBV immunization program in the Bolgatanga Municipality, Upper East Region, Ghana, demonstrated a protective effect on infant seroconversion and prevented perinatal transmission, even among infants of HBsAg-positive mothers. The vaccine's effectiveness has been affirmed. To maximize public health impact, routine maternal HBV screening, post-vaccination testing for high-risk infants, booster doses when needed, and strengthened maternal education are recommended. Ongoing surveillance and long-term follow-up will ensure sustained immunity and further reduce MTCT in high-prevalence regions.

Keywords: Hepatitis B Immunoglobulin, Mother-to-Child Transmission, Post-Vaccination Serological Testing, Hepatitis B Surface Antigen (HbsAg), Antibodies

Day 1: Tuesday 13th October 2026 (14:00 to 15:30)

Parallel sessions II: *Green Chemistry for Climate Resilience, Environmental Sustainability and Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development*

Green Chemistry for Climate Resilience, Environmental Sustainability (Main Auditorium)

Moderator: Dr G. Amenuvor

Tuning the structure-activity relationship in vanadia-catalysed waste cooking oil transesterification

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Biodiesel production via transesterification or esterification to produce fatty acid methyl esters is sustainably beneficial, offering renewable, non-toxic, sulfur-free, and economically favorable energy solutions.[1] In particular, waste biomass as the feedstock evades the food vs fuel conflict and reduces feedstock cost.[2] This study aims to optimize the tandem transesterification-esterification of waste cooking oil (WCO) to fatty acid methyl esters (FAMEs, biodiesel) using bifunctional vanadia-derived heterogeneous catalysts, alongside mechanistic investigations to correlate active site functionality with catalytic activity and selectivity. While numerous studies have examined the influence of waste cooking oil quality and catalyst type on biodiesel production,[3–5] systematic investigations correlating acid-base tuning of heterogeneous catalysts with reaction pathways and product selectivity across variable feedstocks remain limited. This is important in improving conversion of waste and inedible oils which typically contain >0.5 wt.% free fatty acids, compromising selectivity and leading to soap formation.[6] Tailoring catalyst acid-base properties minimizes pre-treatment steps while enhancing FAME yield. This investigation provides insight into how catalyst design influences biodiesel production, supporting more adaptable tandem transesterification–esterification of waste biomass processes.

Keywords: Waste cooking oil; Transesterification; Biodiesel; Metal oxides; Vanadia.

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Valorization and Thermodynamic Study of *Clarias gariepinus* Oil for the Synthesis of Environmentally Friendly Surfactants

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This study investigated the synthesis and characterization of surfactants derived from the oil of *Clarias gariepinus* (African catfish). The oil was extracted using the Soxhlet method and characterized by determining its acid value, free fatty acid (%FFA), refractive index, density, and viscosity. The oil had a lipid content of 18.57% and an acid value of 12.29 mg KOH g⁻¹. Fourier Transform Infrared Spectroscopy (FTIR) confirmed the presence of carboxylic acids, esters, and alkyl functional groups, while Gas Chromatography–Mass Spectrometry (GC–MS) revealed that the oil is rich in long-chain fatty acids, with oleic acid (27.49%), n-hexadecanoic acid (21.48%), hexadecanoic acid methyl ester (10.87%), and octadecanoic acid (7.75%) as the major constituents. Three surfactants were synthesized by sulphonation at 25, 30, and 45 °C. Their surface-active properties were evaluated using surface tension, critical micelle concentration (CMC), foam stability, and wetting tests. The surfactants exhibited CMC values of approximately 2.0, 2.5, and 2.2, with corresponding γ_{CMC} values of 30, 40, and 50 mN m⁻¹, respectively. Foam stability ranged from 90–92%, while wetting times were 6.8–7.2 s. These results demonstrate that *Clarias gariepinus* oil is a promising renewable feedstock for environmentally friendly surfactants for soap and detergent applications.

Keywords: Valorization, *clarias gariepinus*, surface tension, sulphonation, environmentally friendly

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A promising type-II GaAs/BiSI van der Waals heterostructure photocatalyst for overall water-splitting with high solar hydrogen production efficiency

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Photocatalytic water splitting continues to depend on finding semiconductor systems that absorb sunlight efficiently while keeping photogenerated electrons and holes apart long enough to perform reactions. This study employed first-principles density functional theory calculations to design and validate a GaAs/BiSI van der Waals heterostructure (vdWH) as a potential solar-driven photocatalyst for hydrogen production. The AB1 configuration was the most stable among eight stacking configurations examined, with a binding energy of -21.413 meV/Å² and a lattice mismatch of only 2.12% between the GaAs and BiSI layers. Ab initio molecular dynamics and phonon dispersion studies demonstrate that this arrangement is thermally and dynamically stable, and its elastic constants indicate strong mechanical stability as well. The heterostructure has a direct bandgap of 1.64 eV, which is less than either monolayer alone, due to the type-II band alignment that places the valence band maximum on the GaAs side and the conduction band minimum on the BiSI side. Charge density difference plots and Bader charge analysis demonstrate that 0.0035 |e| travels from GaAs to BiSI per unit cell, creating a built-in electric field that prevents photoexcited carriers from mixing. The heterostructure's band edges straddle the water redox potentials throughout pH ranges of 0 to 3. Biaxial strain of up to ±8% adjusts the bandgap and interfacial charge transfer without disrupting the type-II alignment. Enhanced visible light absorption ($10.19 \times 10^5 \text{ cm}^{-1}$) and a high solar to hydrogen efficiency of 20.34% further demonstrate its strong solar energy conversion capability. These findings suggest that the GaAs/BiSI vdWH photocatalyst is stable, strain-responsive, and visible-light active, making it worth investigating experimentally for solar hydrogen generation.

Keyword: Strain, 2D van der Waals heterostructures, photocatalytic water splitting, type II band alignment, Density Functional Theory

SUSTAINABLE GREEN ENERGY IN THE 21ST CENTURY: STRENGTHS, CHALLENGES AND SOLUTION

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Green energy has emerged as a central pillar of sustainable development in the 21st century, offering a viable alternative to fossil-fuel-based energy systems. This paper examines the strengths, challenges, and solutions associated with green energy adoption. Its key strengths include reduced greenhouse gas emissions, improved energy security, declining technology costs, job creation, and enhanced public health. Nevertheless, the transition to green energy faces persistent challenges: intermittency of renewable sources, limited energy storage capacity, inadequate grid infrastructure, high upfront costs, policy instability, supply chain constraints for critical minerals, land-use conflicts, and unequal access to clean energy, especially in developing countries. To address these challenges, the paper proposes solutions including advanced battery storage, smart grid development, green hydrogen, demand-side management, carbon pricing, renewable energy subsidies, public-private partnerships, international technology transfer, circular economy practices, and community-based energy initiatives. It concludes that while a green energy transition is technically feasible and economically beneficial, its success depends on sustained investment, supportive policies, technological innovation, and inclusive governance. Coordinated action among governments, industries, researchers, and civil society is essential to achieve a low-carbon, equitable, and sustainable energy future.

Keywords: Circular economy, Green energy, Sustainable development, Climate change, Energy transition

Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development (Day 1: Tuesday 13th October 2026 (14:00 to 15:30 Syndicate room 1))

Moderator: Prof A. Aniagyei

Integrated Virtual Screening and Molecular Dynamics for the Identification of Potential *Plasmodium falciparum* D-Enoyl-ACP Reductase Inhibitors

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The emergence and spread of drug-resistant *Plasmodium falciparum* strains underscore the need for new antimalarial agents that target essential parasite-specific pathways. *P. falciparum* D-enoyl-acyl carrier protein reductase (PfENR), an essential enzyme involved in fatty acid

biosynthesis, represents a potential target for antimalarial drug discovery. This study employed an integrated virtual screening and molecular dynamics (MD) simulation workflow to identify and prioritize potential PfENR inhibitors. A library of 78,000 compounds with reported antimalarial properties was retrieved from the ChEMBL database in SMILES format and filtered by molecular weight and structural redundancy, yielding 71,200 unique compounds for screening. The compounds were subjected to three independent molecular docking runs against PfENR to assess the consistency of predicted binding interactions. Compounds with mean docking scores of ≤ -8.5 kcal/mol were shortlisted, with further prioritization based on the occurrence of more than five predicted binding poses within the PfENR active site. Selected candidates were subsequently subjected to MD simulations to evaluate the stability and conformational behaviour of the protein-ligand complexes. Trajectory analyses included protein and ligand root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (Rg), ligand RMSF, free energy landscape (FEL), and principal component analysis (PCA). Among the screened compounds, ChEMBL4127624 and ChEMBL120484 exhibited favourable predicted interaction profiles and maintained stable associations with PfENR throughout the simulations, with complex behaviour comparable to or more favourable than that of the co-crystallized reference ligand under the simulated conditions. These compounds were prioritized as potential PfENR inhibitors for further investigation. Experimental biochemical and antimalarial assays will be required to determine their inhibitory activity and validate the computational predictions. The study demonstrates an integrated computational workflow for prioritizing small molecules targeting PfENR and provides candidates for subsequent experimental evaluation against *P. falciparum*.

Keywords: *Plasmodium falciparum*; D-enoyl-ACP reductase; PfENR; ChEMBL; virtual screening; molecular docking; molecular dynamics; antimalarial drug discovery.

Computationally Guided Design and Synthesis of Triazolium Salts for Antimalarial Drug Discovery

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The continuing emergence of *Plasmodium falciparum* resistance to established antimalarial drugs highlights the need for new chemical scaffolds and more efficient target-guided discovery strategies. This study employed molecular docking to guide the design, prioritisation and synthesis of triazolium salts as potential antimalarial agents. A virtual library of derivatives was generated by varying aromatic and *N*-alkyl substituents and screened against two *P. falciparum* targets: the formate-nitrite transporter PfFNT (PDB ID: 6VQQ) and plasmepsin IV (PDB ID: 1LS5). An MMV reference compound was included for comparative docking. Compounds were prioritised on the basis of predicted binding profiles and key interactions within the target binding sites. Selected candidates were subsequently prepared through organic azide synthesis, copper-catalysed azide-alkyne cycloaddition to afford 1,2,3-triazoles, followed by *N*-alkylation to generate the corresponding triazolium salts. Computational screening

informed the synthesis of a 91-member triazolium library incorporating diverse aromatic and alkyl substituents. Docking identified predicted interactions for several candidates at both protein targets, providing a rational basis for prioritising structural features and supporting subsequent structure-activity relationship studies. Spectroscopic characterisation and biological evaluation are ongoing to confirm compound structures and determine antiparasitic activity, cytotoxicity and selectivity. Overall, integrating digital molecular modelling with synthetic chemistry enabled a focused and rational approach to triazolium-based antimalarial discovery. Further molecular dynamics simulations, ADMET profiling and in vitro assays will establish the potential of the prioritised compounds as leads for future antimalarial development.

Keywords: triazolium salts; antimalarial drug discovery; molecular docking; PfFNT; plasmepsin IV

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Stigmasterol from *Rhodognaphalon brevicuspe* Stem Bark: Antimicrobial and Antibiofilm Activity

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The increasing prevalence of antimicrobial resistance and biofilm-associated infections underscores the need to identify bioactive compounds from medicinal plants. This study investigated the phytochemical composition, antimicrobial and antibiofilm activities of *Rhodognaphalon brevicuspe* stem bark, with emphasis on an isolated sterol constituent. The stem bark was extracted with ethanol and partitioned by liquid-liquid extraction to obtain petroleum ether and ethyl acetate fractions. Qualitative phytochemical screening revealed the presence of alkaloids, tannins, saponins, glycosides, and terpenoids/steroids, while flavonoids and coumarins were not detected. Chromatographic separation of the ethyl acetate fraction yielded RB06, which was characterized by Fourier-transform infrared (FT-IR) and nuclear magnetic resonance (NMR) spectroscopy and identified as stigmasterol. The antimicrobial activities of the crude extract, fractions, and isolated compound were evaluated against selected

Gram-positive and Gram-negative bacteria and *Candida albicans* using the broth microdilution method. Antibiofilm activity was assessed using microtiter plate assays and microscopic visualization. The ethyl acetate fraction exhibited antimicrobial activity against *Pseudomonas aeruginosa* and *Staphylococcus aureus*, with minimum inhibitory concentrations (MICs) of 1.56 mg/mL, and against *C. albicans* with an MIC of 0.75 mg/mL. RB06 demonstrated antimicrobial activity against *S. aureus* and *C. albicans*, with MICs of 500 µg/mL, whereas inhibition against *P. aeruginosa*, *Escherichia coli*, and *Enterococcus faecalis* occurred at concentrations above 500 µg/mL. The isolated stigmasterol also reduced biofilm formation in the tested bacterial and fungal organisms in a concentration-dependent manner, although its activity was lower than that of the reference antimicrobial agents. Microscopic examination showed alterations in biofilm architecture and reduced biofilm cohesion following treatment. These findings establish the presence of stigmasterol in *R. brevicuspe* stem bark and demonstrate antimicrobial and antibiofilm activity associated with the isolated compound. The study provides further chemical and biological characterization of *R. brevicuspe* and supports continued investigation of its bioactive constituents.

Keywords: *Rhodognaphalon brevicuspe*; stigmasterol; antimicrobial activity; antibiofilm activity; phytochemicals; natural products; minimum inhibitory concentration

Ghanaian Medicinal Plant Phytochemicals as Inhibitors of Alpha-Glucosidase, Alpha-Amylase, and VEGFR-2 for Antidiabetic Therapy: Molecular Docking, Molecular Dynamics, and Mechanistic Insights

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Diabetes mellitus is a multifactorial disease involving persistent postprandial hyperglycemia and vascular complications. Although alpha-glucosidase and alpha-amylase inhibition remains an important strategy for controlling postprandial glucose elevation, this approach does not directly address complication-related pathways such as abnormal angiogenic signaling mediated by VEGFR-2. Therefore, there is a need to identify candidate compounds that can support a combined antidiabetic strategy targeting both glycemic control and diabetes-associated vascular complications.

This study computationally evaluated 855 phytochemicals from Ghanaian medicinal plants against alpha-glucosidase, alpha-amylase, and VEGFR-2. The workflow involved molecular docking, Prime MM-GBSA, a 200 ns molecular dynamics simulation, post-MD stability analysis, MM/GBSA and residue decomposition analysis, and ADME/toxicity prediction. Docking and Prime MM-GBSA did not identify a single compound with consistent activity across all three targets. Instead, the results revealed overlapping enzyme-targeting candidates for alpha-glucosidase and alpha-amylase, and a separate VEGFR-2 candidate group. MD

stability analysis showed that the retained complexes maintained overall protein stability, compactness, and ligand-dependent hydrogen-bond interactions during simulation.

After MD simulation, 1,3,6 tri-O-galloyl glucoside showed the strongest dual enzyme profile, with post-MD MM/GBSA binding free energies of -28.40 kcal/mol against α -glucosidase and -33.99 kcal/mol against α -amylase. It performed better than acarbose and voglibose for α -glucosidase and better than acarbose for α -amylase. Penta-O-galloyl-glucose showed the strongest α -amylase binding energy at -34.95 kcal/mol. For VEGFR-2, sorafenib remained the strongest reference inhibitor at -47.93 kcal/mol. However, the prioritized VEGFR-2 phytochemicals, including gingerenone-A, 1,7-bis-(4-hydroxy-3-methoxyphenyl), 10-gingerdione, hydroxytetrahydrocurcumin, and hexahydrocurcumin, all performed better than sunitinib, with gingerenone-A showing the strongest phytochemical binding energy at -39.04 kcal/mol.

Residue decomposition supported binding contributions from catalytic residues in the enzyme targets and ATP-binding-site residues in VEGFR-2. ADME/toxicity prediction further supported candidate prioritization based on drug-likeness, absorption, and safety-related properties. Overall, this study identifies 1,3,6 tri-O-galloyl glucoside as a promising dual enzyme inhibitor scaffold and highlights prioritized VEGFR-2 phytochemicals as complementary candidates for a combined antidiabetic strategy.

Comparative Phytochemical Analysis and Behavioral Responses of *Cosmopolites sordidus* to Synthetic and Natural Theaspirane Matrices

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The banana weevil, *Cosmopolite sordidus* is a severe pest that attacks all kinds of bananas and plantains (*Musa spp.*) worldwide. Semiochemicals occurring as volatile organic compounds (VOCs) have often been reported as attractants of the weevil. (2*R*,5*S*)-theaspirane, a component of senesced banana leaves, was previously identified as active attractant to the weevil. *Vitis vinifera* (red grapes), *Camellia sinensis* (fresh tea) leaves, processed green tea, Gingseng-flavoured processed green tea, fresh tobacco *Nicotiana tabacum* (tobacco) leaves, and senesced banana leaves have all been previously reported to contain theaspirane. In the current laboratory studies, olfactory responses of the weevil, and phytochemical screening of the natural theaspirane containing materials were evaluated. All the test materials were significantly ($P < 0.05$) attractive to the weevil compared to clean air. Also, there was no significant difference in attraction between *Vitis vinifera* leaves and Gingseng-flavoured processed green tea ($P > 0.05$). Fresh tea (*Vitis vinifera*) leaf was the most attractive (mean of $7.70 \pm 0.423 \approx 8$) sample, and ahead of the fresh tobacco leaf (mean of $7.30 \pm 0.60 \approx 7$), attracting approximately 8.0 and 7.0 weevils respectively. Banana leaf was the least attractive, with a mean of $4.90 \pm 0.379 (\approx 5)$ weevils attracted. There was a significant difference ($P > 0.05$) between attraction of the weevils by the two top attractive samples and senesced banana leaf.

Phytochemical analysis found saponins, tannins, phenols, reducing sugars, flavonoids, anthraquinones, terpenoids, and alkaloids in the most attractive sample, fresh *Vitis vinifera* leaf. Most of these metabolites were also found in the fresh tobacco leaves. Fresh tea leaves and fresh tobacco leaves were recommended for further investigation in laboratory and field studies. These studies for characterisation/isolation are required along with field evaluation of the capacity of the test materials in push-pull strategies to manage the weevil.

Keywords: *Cosmopolite sordidus* (Banana weevil), (2*R*,5*S*)-theaspirane, attractants, olfactory studies, push-pull

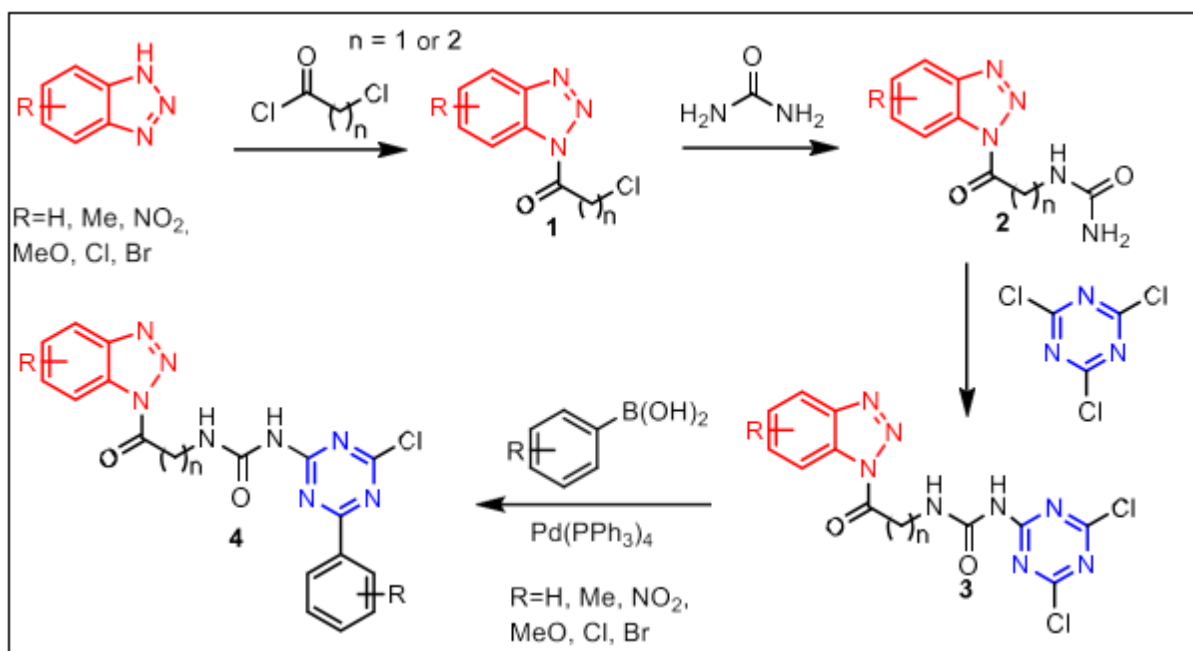
Molecular hybridization of Benzotriazole-Triazine Derivatives as potential UV absorbers for Sunscreen Applications

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Ultraviolet (UV) radiation (100-400 nm) poses significant risks to human health, including skin cancer¹, necessitating the development of effective UV-absorbing agents for sunscreen formulations. While commercial organic UV-absorbing agents such as triazine, benzotriazole, benzophenone, and salicylate derivatives are widely used²³, there is a growing demand for the development of new UV absorbers with improved efficacy. This research aims to synthesise novel molecular hybrids integrating triazine and benzotriazole moieties to explore their potential as alternative UV-absorbing compounds, as outlined in **Scheme 1**. All target compounds **4** will be characterised using a combination of NMR, IR and HRMS spectroscopies. The UV-absorption and thermal stability properties of the hybrids will be evaluated via a UV-vis spectrophotometer and Thermogravimetric analysis (TGA), respectively, to assess the suitability for sunscreen applications.



Scheme 1: Triazine-Benzotriazole hybrids **4** synthesis scheme

Keywords: Benzotriazole-Triazine, Synthesis, UV absorbers, Sunscreen Applications

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Day 2: Wednesday 14th October 2026 (10:45 to 13:00)

Parallel sessions III: *Green Chemistry for Climate Resilience, Environmental Sustainability, Human Health Strengthening Cross-Sector Partnerships for Sustainable Development*

Green Chemistry for Climate Resilience, Environmental Sustainability (Main Auditorium)

Moderator: Prof Lawrence S. Borquaye

Solvent- Assisted Dye Removal and Depolymerization of Waste Polyester Textiles via Hydrolysis Using HZSM-5 as Catalyst

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The increasing consumption and disposal of polyester/ poly(ethylene) terephthalate (PET) textile waste pose significant environmental challenges globally and especially in Ghana,

where large volumes of second-hand clothing waste are poorly managed. PET recycling can be achieved via mechanical recycling and chemical recycling[1]. Chemical recycling is the most suitable and efficient approach for PET textile recycling due to its ability to convert the wastes into high value products via depolymerization[1]. However, the presence of dyes prior to depolymerization hinder the activity of catalyst used, contaminate the monomer stream and deteriorate the overall purity of the final product[2]. Hydrolysis which is one of the less employed chemical recycling methods represents an environmentally benign and efficient approach to depolymerize PET into its monomers terephthalic acid (TPA) and ethylene glycol (EG)[1]. However, due to its slow kinetics, catalysts systems are required to increase the rate of the reaction and reduce the overall cost of the process. Previously used catalyst systems are mostly homogeneous, hazardous and difficult to recover after the reaction. In this study propylene carbonate is investigated as a green solvent for the efficient extraction of disperse dyes from polyester textiles. To enhance the kinetics of the reaction, HZSM-5 zeolite is proposed as a heterogeneous catalyst. Other advantages of using HZSM-5 zeolite is its easy recoverability and reusability [3]. The outcomes of this study are expected to support waste management strategies, reduce the reliance on fossil fuels for virgin polyester production, and contribute to Sustainable Development Goals 12 (Responsible Consumption and Production) and 13 (Climate Action).

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Green Synthesis of Magnetic Fe₃O₄/CuS Nanocomposite for Selective Adsorption of Mercury From Water

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The contamination of water resources by toxic mercury (Hg(II)) ions poses a serious threat to ecosystems and human health, necessitating efficient and sustainable remediation strategies. In this study, magnetic Fe₃O₄/CuS nanocomposites were synthesized via a green route using castor oil as a renewable solvent and stabilizer. The composites were designed to exploit the strong thiophilic affinity of copper sulfide (CuS) for mercury binding and the magnetic properties of iron oxide (Fe₃O₄) for easy separation. Fe₃O₄ nanoparticles were prepared by coprecipitation, followed by solvothermal decomposition of a copper diethyldithiocarbamate precursor in castor oil to form CuS and Fe₃O₄/CuS nanocomposites with mass ratios of 1:1, 1:4, and 1:8. Structural and physicochemical characterization (FT-IR, XRD, SEM/EDX, TGA, NMR) confirmed the formation of crystalline nanocomposites with the intended core-shell

morphology. SEM analysis revealed that CuS formed spherical nanoparticles, while Fe₃O₄ appeared as spherical particles with noticeable aggregation, leading to a composite structure with good surface interaction. Batch adsorption experiments revealed that the Fe₃O₄/CuS (1:8) composite achieved a high performance, with a maximum adsorption capacity of 295 mg g⁻¹ at pH 8, 20 mg dosage, and 200 min contact time. Kinetic and isotherm modeling indicated that Hg(II) uptake followed a pseudo-second-order model and fit the Langmuir isotherm, suggesting chemisorption on a homogeneous surface. The nanocomposite also exhibited outstanding selectivity, removing Hg(II) quantitatively even in the presence of excess competing ions (Cd²⁺, Pb²⁺, Zn²⁺), and retained ~80 % efficiency after four regeneration cycles. These findings demonstrate that castor oil-mediated synthesis offers a sustainable pathway to highly efficient, selective, and magnetically recoverable Fe₃O₄/CuS nanocomposites, highlighting their promise as a scalable, engineering innovation for practical mercury remediation.

Keywords: Mercury removal, Adsorption, Copper sulfide, Iron oxide, Green synthesis, Castor oil

Thiol-Functionalized Magnetic Iron Oxide Nanocomposite for the Adsorptive Removal of Diclofenac Sodium

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The increasing consumption of pharmaceuticals, particularly nonsteroidal anti-inflammatory drugs (NSAIDs), has contributed to their occurrence in pharmaceutical and other wastewater streams, raising environmental concerns. This study investigated the development of a functionalized magnetic nanocomposite for the adsorptive removal of diclofenac sodium from aqueous solution. Magnetite nanoparticles (Fe₃O₄) were synthesized by co-precipitation, followed by silica coating using the Stöber method to produce Fe₃O₄@SiO₂. The silica-coated nanoparticles were subsequently functionalized with thiol groups using 3-mercaptopropyltriethoxysilane (MPTES). The materials were characterized by Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), zeta-potential analysis, and UV-visible spectroscopy. FT-IR confirmed the functional groups associated with the successive modification steps, while XRD confirmed the crystalline nature of the materials and gave an average crystallite size of 14.7 nm. Zeta-potential measurements provided information on surface charge and colloidal stability, while changes in the UV-visible absorption spectra reflected the progressive modification of the nanoparticles. The effects of contact time, adsorbent dosage, pH, and initial diclofenac sodium concentration on adsorption performance were investigated. At an initial diclofenac sodium concentration of 20 mg/L, removal efficiencies of 30–90% were observed across the investigated pH range, with maximum

removal achieved at an adsorbent dosage of 1.0 g/L. The results demonstrate the potential of the synthesized functionalized magnetic nanocomposite for the removal of diclofenac sodium from aqueous systems.

Keywords: Diclofenac sodium; magnetic nanocomposite; adsorption; Fe₃O₄@SiO₂; water remediation.

Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development (Day 2: Wednesday 14th October 2026 (10:45 to 13:00 Syndicate room 1))

Moderator: Prof. Isaac Asiamah

Hit to Lead Optimization and Repurposing of MMV084978 as Antileishmanial Agents

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Leishmaniasis is a neglected tropical disease with limited treatment options, high costs of treatment, significant drug-associated toxicity, and emerging drug resistance. This study explored the antileishmanial potential of MMV084978, a diacylhydrazide-based hit compound from the Medicines for Malaria Venture (MMV) Pathogen Box, through drug repurposing and medicinal-chemistry optimisation.

A focused series of structural analogues (SC008, SC011, SC014, SC017, and SC555) were designed, synthesised, and structurally characterised using FTIR spectroscopy, LC/ESI-MS, and ¹H and ¹³C NMR analyses. The in-vitro activity was evaluated against *Leishmania aethiopica* promastigotes. All compounds demonstrated concentration-dependent growth inhibition, with SC011 and SC014 showing the highest potency (IC₅₀ = 1.745 and 1.825 µM, respectively), surpassing the parent compound (MMV084978; IC₅₀ = 4.924 µM) and identifying benzoyl-ring dichlorination as the most productive structural modification. Multi-target molecular docking revealed CYP51 as the strongest single-target hypothesis, with SC014 uniquely outperforming both the native ligand and the reference drugs pentamidine and miltefosine. Additional predicted interactions with APRT, PTR1, and biotin protein ligase supported a potential multi-target profile for the analogue series. In silico ADMET predictions supported generally favourable drug-like properties. Collectively, these findings identify MMV084978 as a chemically tractable and promising antileishmanial scaffold, and highlight SC011 and SC014 as priority analogues for further investigation.

Key words: MMV084978, Leishmaniasis, Drug repurposing, Diacylhydrazide, Structure-Activity Relationship

Isolation, In Vitro, and In Silico Anthelmintic Evaluation of Compounds from *Alstonia Boonei*

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Alstonia boonei stem bark is used across West Africa to treat intestinal worm infections, yet the responsible compounds remain largely unidentified, and no new anthelmintic drug class has emerged in over three decades amid growing benzimidazole and ivermectin resistance. This study aimed to isolate active anthelmintic constituents of *A. boonei* stem bark and propose their likely molecular target. A 70% ethanolic extract was partitioned into petroleum ether, ethyl acetate, and aqueous fractions and screened against *Eudrilus eugeniae* using time of paralysis (TOP) and time of death (TOD), with albendazole as reference. The ethyl acetate fraction, the most active overall, yielded two triterpenoids: β -amyrin and methyl commate A, the latter reported for the first time from this species. At 25 mg/mL, methyl commate A produced a TOP (32.39 ± 1.06 min) statistically indistinguishable from albendazole (31.34 ± 1.07 min, $p > 0.05$), an equivalence retained at 10 mg/mL, while β -amyrin was consistently less potent. Molecular docking against Glu-C1 and β -tubulin reproduced this ranking, with methyl commate A showing the stronger binding energy at Glu-C1 (-51.58 vs. -39.32 kcal/mol), forming a hydrogen bond within ivermectin's subpocket. These findings validate the ethnomedicinal use of *A. boonei* and identify methyl commate A as a promising anthelmintic lead.

Keywords: *Alstonia boonei*; anthelmintic; methyl commate A; β -amyrin; molecular docking

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SYNTHESIS, CHARACTERIZATION, AND ANTI-MICROBIAL PROPERTIES OF COPPER SULFIDE NANOPARTICLES FROM DIETHYLDITHIOCARBAMATE COMPLEXES

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Antimicrobial resistance (AMR) is a growing global health challenge that compromises the effectiveness of conventional antimicrobial agents and necessitates the exploration of alternative therapeutic materials. This study investigated the synthesis, characterization, and antimicrobial activity of copper sulfide (CuS) nanoparticles. Copper diethyldithiocarbamate complexes were synthesized via a precipitation method and characterized using UV–visible, nuclear magnetic resonance (NMR), and Fourier-transform infrared (FTIR) spectroscopy. The resulting complexes were subsequently decomposed using a melt method to produce CuS nanoparticles, which were characterized by zeta potential analysis and X-ray diffraction (XRD). XRD analysis confirmed the formation of covellite-phase CuS with a hexagonal crystal structure and an average crystallite size of 34.73 nm. The antimicrobial activity of the CuS nanoparticles was evaluated against three bacterial strains, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Enterococcus faecalis*, and the fungal strain *Candida albicans* using the broth serial dilution method. The nanoparticles exhibited notable antifungal activity against *C. albicans*, as indicated by a low minimum inhibitory concentration (MIC), but showed no significant inhibitory activity against the tested bacterial strains. These findings demonstrate the potential of CuS nanoparticles as antifungal agents and provide a basis for further investigation of their antimicrobial properties and possible applications in addressing emerging challenges associated with antimicrobial resistance.

Keywords: Antimicrobial, antifungal, nanoparticle, precipitation, diethyldithiocarbamate.

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Anthelmintic Constituents of *Holoptelea grandis* Stem Bark: Bioassay-Guided Fractionation and Isolation

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Helminthiases, particularly soil-transmitted helminth infections, remain an important public health concern in tropical and subtropical regions, including Ghana. The increasing prevalence of anthelmintic resistance and limitations associated with existing treatments have stimulated interest in medicinal plants as sources of bioactive natural products. *Holoptelea grandis* is traditionally used as a vermifuge in Ghana, although its anthelmintic activity and chemical constituents have received limited scientific investigation. This study evaluated the anthelmintic activity of *H. grandis* stem bark and employed bioassay-guided fractionation to isolate and characterize its chemical constituents. The stem bark was extracted with ethanol and subsequently fractionated using petroleum ether and ethyl acetate. Anthelmintic activity was evaluated in vitro using paralysis and death time assays against *Pheretima posthuma*. The active ethyl acetate fraction was subjected to chromatographic separation, and isolated constituents were characterized using gas chromatography-mass spectrometry (GC-MS), nuclear magnetic resonance (NMR) spectroscopy, and infrared (IR) spectroscopy. Phytochemical screening revealed the presence of tannins, saponins, alkaloids, and terpenoids. The ethyl acetate fraction exhibited greater anthelmintic activity than the crude extract and petroleum ether fraction, producing shorter paralysis and death times against *P. posthuma*. Two isolates, designated HGS01 and HGS02, were obtained from the active fraction. HGS01 was characterized as a complex mixture dominated by alkanes, alkenes, and alcohols, while HGS02 was conclusively identified as the pentacyclic triterpenoid friedelan-3-one (friedelin) based on NMR and MS data. The findings demonstrate anthelmintic activity in the stem bark extract and its ethyl acetate fraction and establish the presence of friedelin among the isolated constituents. Further evaluation of the isolated constituents is required to determine their individual contributions to the observed anthelmintic activity and their potential as sources of anthelmintic agents.

Keywords: *Holoptelea grandis*; anthelmintic activity; friedelin; friedelan-3-one; bioassay-guided fractionation; *Pheretima posthuma*; natural products

Nodule-Specific Cysteine-Rich Peptides as Potential FtsZ Inhibitors: Molecular Docking Insights into a Broad-Spectrum Antimicrobial Strategy

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Antimicrobial resistance (AMR) poses a major global health challenge within the One Health framework, creating a need for antimicrobial strategies that target essential bacterial processes through mechanisms distinct from those of conventional antibiotics. Bacterial cell division is an attractive target because proliferation depends on the assembly and function of the FtsZ protein, a highly conserved GTPase-like protein that polymerizes to form the Z-ring and coordinate cytokinesis. FtsZ shares limited sequence similarity with human tubulin, providing a basis for investigating it as a potential antimicrobial target. Most reported FtsZ inhibitors interact with the protein at sites associated with GTP binding or polymerization. The antimicrobial peptide MciZ provides an alternative mechanism, binding to the C-terminal region of FtsZ in *Bacillus subtilis* and interfering with Z-ring formation and cell division. Nodule-specific cysteine-rich (NCR) peptides produced by legumes have also been reported to affect bacterial cell division in rhizobia, suggesting a possible connection between NCR peptide activity and FtsZ function. This study investigated the potential of NCR peptides as FtsZ inhibitors across selected microbial species using molecular docking. Docking analyses showed that the evaluated NCR peptides associated with the C-terminal region of FtsZ across multiple microbial species, with binding patterns that showed similarities to the reported interaction of MciZ with FtsZ. These results suggest that NCR peptides may interact with a conserved region of FtsZ beyond their established biological context in rhizobial systems. Molecular dynamics simulations are ongoing to assess the stability and persistence of the predicted NCR-FtsZ interactions and to further characterize the molecular basis of peptide binding. The study provides a computational basis for investigating NCR peptides as potential modulators of bacterial cell division and supports further evaluation of their antimicrobial activity against diverse bacterial pathogens.

Keywords: NCR peptides; FtsZ; antimicrobial peptides; bacterial cell division; molecular docking; molecular dynamics; antimicrobial resistance; One Health.

Day 2: Wednesday 14th October 2026 14:00 to 15:30

Parallel sessions IV: *Green Chemistry for Climate Resilience, Environmental Sustainability, Human Health Strengthening Cross-Sector Partnerships for Sustainable Development*

Green Chemistry for Climate Resilience, Environmental Sustainability (Main Auditorium)

Moderator: Dr. Irene Agbo

Evaluation of Human Health Risk Associated with Heavy Metals in Drinking Water Contaminated by Illegal Mining Activities in Tetrem Bontefufuor, Amansie West District, Ashanti Region, Ghana

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Water is essential to life, and its quality determines suitability for human use. Heavy metals, even at low concentrations, can be toxic and enter the environment through various pathways. This study investigated heavy metal contamination and the effects of physicochemical parameters on drinking water quality in a small-scale illegal mining (galamsey) village. Two water samples were collected from a river (upstream and downstream) and three samples from boreholes. The samples were preserved in an ice chest to maintain temperature. Physicochemical parameters were determined in the laboratory and compared with WHO guidelines for drinking water. The samples were digested with 1 M nitric acid, with distilled water used as a blank. Concentrations of heavy metals specifically lead (Pb), arsenic (As), cadmium (Cd), copper (Cu), and iron (Fe) were measured using atomic absorption spectroscopy (AAS). Results showed that surface water recorded the highest copper concentration, while arsenic was the lowest relative to groundwater sources. Despite lower concentrations, heavy metals remain toxic and pose significant health risks due to their persistence and potential for bioaccumulation. The hazard index for non-carcinogenic health risk was higher in children than in adults. Based on the water quality index computed from physicochemical parameters, groundwater sources (G.1, G.2, and G.3) were the most suitable for consumption compared to surface water sources (S.1 and S.2). This study underscores the importance of monitoring and regulating water quality in areas affected by illegal mining to protect public health.

KEYWORDS: Water pollution, illegal mining, heavy metals, physicochemical parameters, health risk assessment

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Castor Oil-Mediated Green Synthesis of Lead Sulfide and Tin Sulfide Nanoparticles from Ethyl Xanthate and Dithiocarbamate Single-Source Precursors

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Lead sulfide (PbS) and tin sulfide (SnS and SnS₂) nanoparticles were synthesized via a green solvothermal approach using castor oil as a sustainable reaction medium and capping agent. Lead(II) and tin(II) ethyl xanthate and diethyldithiocarbamate complexes were prepared as single-source precursors and thermally decomposed based on their decomposition profiles. The products were characterized using TGA, XRD, SEM-EDS, FTIR, and UV-Vis spectroscopy. XRD confirmed phase-pure cubic PbS from both precursor systems, while tin precursors yielded orthorhombic SnS from the ethyl xanthate and SnS₂ from the diethyldithiocarbamate. Average crystallite sizes were 24.04 ± 4.47 nm (PbS) and 39.60 ± 10.24 nm (SnS) for xanthate-derived products, and 32.00 ± 6.63 nm (PbS) and 8.61 ± 4.49 nm (SnS₂) for dithiocarbamate-derived products. SEM revealed precursor-dependent morphologies, ranging from faceted and dendritic structures to compact granular assemblies. FTIR confirmed metal sulfide formation and castor oil capping. UV-Vis spectroscopy showed strong UV absorption and direct optical band gaps of 4.02–4.32 eV, indicating quantum confinement. Overall, precursor selection strongly influenced phase, crystallite size, morphology, and optical properties, while castor oil provided an environmentally friendly synthesis medium.

Keywords: Castor oil, single – source precursor, tin sulfide, lead sulfide, green solvothermal approach.

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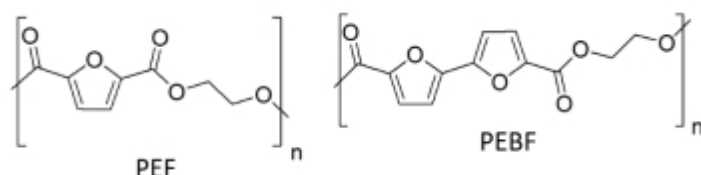
Investigating The Effect of Gamma Irradiation on Furan-Based Plastics (Biopolyesters)

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The environmental persistence of petroleum-derived plastics such as PET has intensified interest in sustainable alternatives. Furan-based polyesters, including polyethylene furanoate (PEF) and polyethylene bifuranoate (PEBF), are promising bio-derived materials synthesized from renewable lignocellulosic biomass and exhibit favourable thermal, mechanical, and barrier properties^{1,2}. This study aimed to synthesize and characterize PEF and PEBF as a foundation for future investigations into the effects of gamma irradiation on these materials.



PEF and PEBF were synthesized through two-stage melt polycondensation using dimethyl 2,5-furandicarboxylate and dimethyl 2,2'-bifuran-5,5'-dicarboxylate, respectively. The polymers were purified and characterized using Fourier-transform infrared (FTIR) spectroscopy, UV–Visible spectroscopy, and melting-point analysis. FTIR spectra confirmed successful polyester formation, while UV–Visible analysis revealed λ_{max} values of 268 nm for PEF and 322 nm for PEBF, reflecting the greater conjugation present in PEBF. Thermal analysis showed melting ranges of 205–220 °C for PEF and 215–270 °C for PEBF.

Although gamma irradiation experiments were not completed within the project period, the successful synthesis and characterization of PEF and PEBF establish a platform for future studies on radiation-induced crosslinking and degradation. These findings further support the potential of furan-based polyesters as sustainable alternatives to conventional plastics.

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Human Health and Strengthening Cross-Sector Partnerships for Sustainable Development (Day 2: Wednesday 14th October 2026 (14:00 to 15:30 Syndicate room 1))

Moderator: Dr. Gershon Amenuvor

Phytochemical Composition and Antimicrobial Potential of *Xylopia villosa* Stem Bark

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Antimicrobial resistance is a major global health challenge, creating a need for new sources of antimicrobial agents. Medicinal plants are important sources of chemically diverse natural products with potential biological activities. *Xylopia villosa* is a Ghanaian medicinal plant traditionally used in the management of infectious diseases, but its phytochemical composition and antimicrobial properties remain insufficiently characterized. This study investigated the phytochemical composition and antimicrobial potential of the stem bark of *X. villosa*, with preliminary isolation and characterization of a constituent. The stem bark was extracted with ethanol, and the crude extract was subjected to phytochemical screening and antimicrobial evaluation using the broth microdilution method. Bioassay-guided chromatographic separation involving repeated column chromatography, thin-layer chromatography, and recrystallization yielded a pure compound designated XV01. Spectroscopic characterization using infrared and nuclear magnetic resonance spectroscopy indicated the presence of carboxylic acid, carbonyl, and aliphatic functional groups. Phytochemical screening of the crude extract revealed the presence of alkaloids, triterpenoids, glycosides, phytosteroids, tannins, saponins, flavonoids, and anthraquinones. The crude ethanolic extract exhibited minimum inhibitory concentrations (MICs) of 6.25 mg/mL against *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Escherichia coli*, and *Enterococcus faecalis*, and 25 mg/mL against *Candida albicans*. The isolation of XV01 provides a basis for further structural elucidation and biological evaluation. Further antimicrobial testing of XV01 and the purified fractions is required to determine their individual contributions to the observed activity. This study contributes to the phytochemical characterization of *X. villosa* stem bark and provides a basis for further investigation of its chemical constituents and biological activities.

Keywords: *Xylopia villosa*; phytochemical composition; antimicrobial activity; minimum inhibitory concentration; natural products; bioassay-guided fractionation

Targeting Angiogenesis in Diabetes: In Silico Evaluation of Phytochemicals from Ghanaian Medicinal Plants as VEGFR-2 Inhibitors.

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Diabetes mellitus is a multifactorial metabolic disorder that remains a leading cause of morbidity and mortality worldwide. A major contributor to disease progression is the development of vascular complications, including diabetic retinopathy, which are largely driven by dysregulated angiogenesis. The vascular endothelial growth factor receptor-2 (VEGFR-2), a key tyrosine kinase receptor, plays a central role in mediating angiogenic signaling and pathological neovascularization. Although current therapeutic strategies target specific pathways, they often inadequately address angiogenesis-driven complications, highlighting the need for novel therapeutic strategies targeting vascular pathways. Medicinal plants widely used in Ghana for diabetes management represent a rich source of bioactive phytochemicals; however, their molecular mechanisms of action, especially in relation to angiogenic targets such as VEGFR-2, remain poorly understood. In this study, an integrative computational approach was used to investigate the potential of selected phytochemicals from Ghanaian medicinal plants as VEGFR-2 inhibitors. Molecular docking studies were conducted using the crystal structure of VEGFR-2 (PDB ID: 4ASD) to evaluate binding affinities, interaction profiles, and the ability of the compounds to occupy the active site of the receptor. Several phytochemicals exhibited strong binding scores and favorable interaction patterns, including hydrogen bonding and hydrophobic contacts with key amino acid residues critical for receptor activity, suggesting significant inhibitory potential. To further validate these findings, the most promising candidates will be subjected to molecular dynamics simulations to evaluate stability of ligand–receptor complexes over time, as well as ADMET analyses to provide insights into pharmacokinetic properties and safety profiles. Overall, this study provides molecular-level insights into the anti-angiogenic potential of phytochemicals from Ghanaian medicinal plants and identifies promising hit compounds that could serve as new scaffolds for further optimization into therapeutics for managing angiogenesis-related diabetic complications.

Keywords: Neglected tropical disease, Diabetes, Angiogenesis, Tyrosine kinase receptor, VEGFR-2.

Pharmacological Evaluation of the Ethanolic Extract of the Stem Bark of *Daniellia ogea* and Characterization of its Isolated Phytochemical(s)

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Medicinal plants are an important source of natural product discovery with potential applications in the management of infection, inflammatory, and parasitic diseases. *Daniellia ogea* (Fabaceae) is a medicinal plant whose stem bark is traditionally used in Ghana for managing conditions such as malaria, infections, gonorrhea, cough, asthma, pain, and wounds. Despite these uses, there is limited research on it. This study therefore investigated the phytochemical composition, pharmacological activities, and chemical constituents of the stem bark of *D. ogea*.

The stem bark of *D. ogea* was extracted with ethanol using Soxhlet extraction. The crude extract was subjected directly to silica gel column chromatography using ethyl acetate: petroleum ether. Phytochemical screening was performed on the pulverized stem bark and crude extract. The extract was evaluated for antioxidant, anti-inflammatory, anthelmintic, and antimicrobial activities, while isolated compounds were characterized using spectroscopic techniques.

Total antioxidant capacity increased with extract concentration, with calculated values of 6.02, 10.50, 13.00 and 22.69 mg AAE at 100, 200, 250 and 300 mg/mL, respectively, based on the ascorbic acid calibration curve ($R^2 = 0.999$). The extract demonstrated concentration-dependent anti-inflammatory activity. In the Anthelmintic assay, extract concentrations of 10, 7.5, 5 and 1 mg/ml produced paralysis at 21.00 ± 0.89 , 28 ± 0.98 , 47.00 ± 1.09 and 66.17 ± 1.17 min respectively and death at 45.40 ± 1.14 , 46.83 ± 1.32 , 55.16 ± 1.47 and 76.00 ± 1.67 min respectively. Antimicrobial testing exhibited MIC values of 3.125 μ g/mL against *Staphylococcus aureus*, MRSA, *Escherichia coli*, resistant *E. coli*, and *Candida albicans*. Spectroscopic characterization has led to the isolation of β -sitosterol as one of the identified constituents.

The findings demonstrate that the stem bark of *D. ogea* contains secondary metabolites and exhibits pharmacological activities. The isolation of β -sitosterol provides chemical evidence for the presence of pharmacologically relevant phytosterols in the species and supports further investigation of *D. ogea* as a potential source of bioactive natural products.

Keywords: *Daniellia ogea*, antimicrobial activity, anti-inflammatory activity, anthelmintic activity, column chromatography

Biofilm and Efflux Modulation by Constituents of *Salacia debilis*

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The rise of antimicrobial resistance (AMR) poses a major challenge to the treatment of bacterial infections, particularly those caused by multidrug-resistant pathogens. Conventional antibiotics exert strong selective pressure by targeting bacterial viability, creating a need for complementary strategies that interfere with virulence-associated processes. Antivirulence approaches targeting processes such as quorum sensing, biofilm formation, and efflux-mediated resistance offer an alternative strategy for attenuating bacterial pathogenicity. *Salacia debilis*, a medicinal shrub traditionally used in Ghanaian medicine, contains bioactive constituents with reported antimicrobial activity, although its effects on bacterial virulence-associated processes remain insufficiently explored. This study investigated the antivirulence activities of compounds isolated from *S. debilis*. The crude and ethyl acetate extracts exhibited antimicrobial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, with minimum inhibitory concentrations (MICs) ranging from 6.25 to 25.0 mg/mL. Bioassay-guided fractionation yielded two compounds, SD-03 (benzyl 2-methoxybenzoate) and SD-04 (1,10-dihydroxy-6H-benzo[c]chromen-6-one), which were isolated and characterized. At MIC and sub-MIC concentrations, neither compound inhibited bacterial growth; however, both reduced biofilm formation and disrupted preformed biofilms in *S. aureus* and *P. aeruginosa*. Efflux pump inhibition, evaluated using the ethidium bromide accumulation assay, showed concentration-dependent activity for both compounds. SD-03 recorded maximum specific activities of approximately 295 RFI/μmol against *P. aeruginosa* and 90 RFI/μmol against *S. aureus*, while SD-04 showed activities of approximately 150 RFI/μmol against both bacterial species. Molecular docking predicted favorable interactions of SD-03 and SD-04 with the quorum sensing regulators LasR, RhIR, and PqsR, as well as the NorA efflux pump protein. SD-03 and SD-04 showed predicted binding energies of −9.8 and −10.4 kcal/mol, respectively, against LasR. These computational results provide mechanistic hypotheses for the observed antivirulence effects and warrant further experimental investigation of the compounds' interactions with quorum sensing pathways. The findings demonstrate that constituents of *S. debilis* can modulate biofilm formation and efflux-associated phenotypes without directly inhibiting bacterial growth.

Keywords: *Salacia debilis*; antimicrobial resistance; antivirulence; biofilm; efflux pump; quorum sensing; molecular docking; natural product.

POSTER SESSION PRESENTATIONS

P1

Green chemistry for climate resilience, environmental sustainability and human health.

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Lead (Pb(II)) contamination of water is a persistent environmental and public health concern due to its toxicity, persistence, and bioaccumulation. Sustainable and environmentally benign approaches to heavy-metal pollution are therefore essential for protecting water resources, promoting human health, and strengthening climate resilience. This study investigates a computational-experimental approach for identifying and validating DNA aptamers capable of selectively recognizing Pb(II) in aqueous environments. The study aims to identify Pb(II)-binding aptamers from a fully randomized single-stranded DNA library and determine whether Pb(II) recognition is associated with thymine-thymine (T-T) mismatch motifs or alternative sequence and structural motifs. Computational screening will employ Python/Bio-Python, mFold, 3DNA, Oligo-Analyzer, molecular docking, and molecular dynamics simulations using GROMACS, AMBER, and VMD to evaluate candidate sequences, Pb(II)-DNA interactions, binding stability, and structural behavior. BLASTn will assess sequence similarity and conserved motifs. Selected aptamers will be experimentally validated using UV-Visible spectrophotometry, fluorescence assays, and agarose gel electrophoresis. The study is expected to identify stable and selective Pb(II)-binding aptamers and elucidate their molecular recognition mechanisms. By integrating computational screening with experimental validation, the research supports green chemistry through reduced resource-intensive screening and advances sustainable, low-cost approaches for Pb(II) monitoring, safer water management, and human health protection.

Keywords: DNA aptamer; computational screening; molecular dynamics; water contamination; heavy-metal detection.

P2

Rational Design of Novel Anthelmintic Chemical Frameworks Through Scaffold Hopping

Philip Teye Thompson, Mercy Badu, Michael Konney Laryea, Elliot Sarpong Menkah, and Lawrence Sheringham Borquaye

The widespread emergence of benzimidazole resistance in *Haemonchus contortus* has become a major obstacle to effective parasite control and sustainable livestock production. This study employed an integrated computational drug discovery strategy to identify novel chemical scaffolds capable of overcoming β -tubulin-mediated resistance. In the absence of an experimentally resolved β -tubulin structure, a high-quality homology model of *H. contortus* β -tubulin was constructed, followed by the generation of four resistance-associated mutants (Q134H, F167Y, E198A, and F200Y). Comprehensive structural validation confirmed the accuracy and reliability of the generated models. Molecular docking of clinically relevant benzimidazole anthelmintics demonstrated reduced binding affinities and altered ligand-

binding orientations in the mutant proteins relative to the wild-type, with the Q134H and E198A variants exhibiting the greatest perturbations. These findings were further supported by molecular dynamics (MD) simulations, which revealed pronounced ligand displacement from the binding pockets of the Q134H and E198A mutants, providing mechanistic evidence for their role in drug resistance. To identify alternative chemotypes capable of circumventing resistance, a scaffold-hopping approach was applied using 9 reference benzimidazole drugs, generating a virtual library of 72,004 structurally diverse compounds. Virtual screening against the Q134H mutant, selected as a stringent resistance model, identified more than 5,000 compounds with high predicted binding affinities (≤ -8.5 kcal/mol), representing 7.34% of the screened library. To maximize structural novelty and minimize the likelihood of cross-resistance, compounds retaining the benzimidazole pharmacophore were excluded from further consideration. Ongoing molecular docking and MD simulations of selected β -tubulin–ligand complexes are being used to elucidate their binding mechanisms and evaluate their potential as next-generation anthelmintic leads. Collectively, this study integrates homology modelling, molecular docking, scaffold hopping, virtual screening, and molecular dynamics simulations to facilitate the rational discovery of novel antinematodal chemotypes. The findings establish a strong computational framework for the development of effective anthelmintic agents against drug-resistant *H. contortus*.

Keywords: Benzimidazole resistance, protein mutations, single-nucleotide polymorphism, in silico studies, and beta-tubulin.

P3

SYNTHESIS OF FeS-MgAl LAYERED DOUBLE HYDROXIDE NANOCOMPOSITE FOR ADSORPTION OF MERCURY FROM WATER

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Mercury contamination of water is a major environmental and public health concern because of its persistence, toxicity, and bioaccumulative nature. Conventional adsorbents often show limited selectivity and stability for Hg^{2+} removal. This study reports the synthesis of an iron sulfide–magnesium aluminum layered double hydroxide (FeS–MgAl LDH) nanocomposite using iron(III) tris(diethyldithiocarbamate) as a single-source precursor through a solventless method. The solventless approach provides a greener and more sustainable route by minimizing solvent use and reducing chemical waste. FTIR analysis confirmed the characteristic hydroxyl, carbonate, and metal–oxygen functional groups of MgAl LDH, while XRD revealed a well-crystallized hydrotalcite-like structure. Characterization of the nanocomposite further verified the successful incorporation of FeS within the LDH matrix. The composite exhibited structural stability between pH 4 and 8, with no measurable dissolution under the tested conditions. Batch adsorption experiments conducted at an initial mercury concentration of 20 ppb and an adsorbent dosage of 20 mg showed nearly complete Hg^{2+} removal at pH 7 and 8. The enhanced performance is attributed to the synergistic combination of the high surface area of MgAl LDH and the sulfur-rich active sites of FeS, enabling strong Hg–S chemisorption.

Keywords: Layered double hydroxide, FeS – MgAl LDH, Solventless method, single-source precursor, Adsorption.

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P4

Castor Oil-Mediated Green Synthesis of Lead Sulfide and Tin Sulfide Nanoparticles from Ethyl Xanthate and Dithiocarbamate Single-Source Precursors

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Lead sulfide (PbS) and tin sulfide (SnS and SnS₂) nanoparticles were synthesized via a green solvothermal approach using castor oil as a sustainable reaction medium and capping agent. Lead(II) and tin(II) ethyl xanthate and diethyldithiocarbamate complexes were prepared as single-source precursors and thermally decomposed based on their decomposition profiles. The products were characterized using TGA, XRD, SEM-EDS, FTIR, and UV-Vis spectroscopy. XRD confirmed phase-pure cubic PbS from both precursor systems, while tin precursors yielded orthorhombic SnS from the ethyl xanthate and SnS₂ from the diethyldithiocarbamate. Average crystallite sizes were 24.04 ± 4.47 nm (PbS) and 39.60 ± 10.24 nm (SnS) for xanthate-derived products, and 32.00 ± 6.63 nm (PbS) and 8.61 ± 4.49 nm (SnS₂) for dithiocarbamate-derived products. SEM revealed precursor-dependent morphologies, ranging from faceted and dendritic structures to compact granular assemblies. FTIR confirmed metal sulfide formation and castor oil capping. UV-Vis spectroscopy showed strong UV absorption and direct optical band gaps of 4.02–4.32 eV, indicating quantum confinement. Overall, precursor selection strongly influenced phase, crystallite size, morphology, and optical properties, while castor oil provided an environmentally friendly synthesis medium.

Keywords: Castor oil, single – source precursor, tin sulfide, lead sulfide, green solvothermal approach.

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P5

Synthesis of Copper Sulfide–Magnesium Aluminium Layered Double Hydroxides Nanocomposite for Selective Adsorption of Mercury from Water

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Mercury contamination of aquatic ecosystems is a major environmental and public health challenge, particularly in Ghana's mining-impacted communities, where artisanal and small-scale gold mining (ASGM) is widespread. However, its remediation at trace (ppb) levels is challenging. This study reports the fabrication and evaluation of a copper sulfide-magnesium aluminium layered double hydroxide (CuS@MgAl-LDH) nanocomposite as an adsorbent for Hg²⁺ removal from contaminated water. MgAl-LDH was prepared by a hydrothermal method, and the CuS@MgAl-LDH nanocomposite (CuS: MgAl-LDH mass ratio of 1:1) was then synthesised via a solventless thermal process, in which the CuS phase was generated in situ from a CuS single-source precursor, copper diethyldithiocarbamate (CuDDTC) in the presence of MgAl-LDH. FTIR and XRD confirmed the characteristic peaks corresponding to CuS incorporation on the LDH framework, demonstrating successful composite fabrication. Batch adsorption experiments conducted at an initial Hg²⁺ concentration of 20 ppb with a 20 mg adsorbent dosage, showed that CuS@MgAl-LDH removed nearly all Hg²⁺ ($\geq 99.7\%$) within 120 mins across a pH range of 4- 8, with the most precise and reproducible result obtained at pH 7, corresponding to an adsorption capacity of $50 \mu\text{g g}^{-1}$. These results demonstrate the significant potential of CuS@MgAl-LDH as a structurally stable, highly efficient, and pH-tolerant adsorbent for trace-level Hg²⁺ removal from wastewater treatment impacted by ASGM. Further work will examine the effect of initial Hg²⁺ concentration, adsorbent dose, contact time and temperature on adsorption performance, and determine the equilibrium adsorption capacity, kinetics and thermodynamic behaviour of the CuS@MgAl-LDH nanocomposite.

Keywords: Layered double hydroxide, CuS nanocomposite, Mercury adsorption, Green synthesis, Water treatment.

P6

PROXIMATE COMPOSITION, FUNCTIONAL PROPERTIES, AND MINERAL CONTENT OF COMPOSITE FLOUR PRODUCED FROM CEREAL-LEGUME BLENDS

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Cereals and legumes have found utmost acceptance by many people across the globe due to their great contribution to health and the economy. This study was conducted to determine the proximate and mineral compositions as well as the functional properties of composite flours from cereal-legume blends in order to evaluate their nutritional potential and promote public awareness of the health benefits of cereal-legume composites. The samples of cereals and legumes were obtained from Kotokuraba Market, a suburb of Cape Coast, processed and analyzed for proximate composition, functional properties, and mineral content. Five samples were subjected to treatment. Three out of the total (5) were formulations of wheat, maize, soybean, and oats flours made by mixing the flours (wheat, maize, soybean, and oats) in the ratios (composite 1=25:25:25:25, composite 2=50:20:20:10, and composite 3=20:20:50:10), respectively. The remaining two samples were set as controls (100% Soybean and 100% wheat). The results showed that moisture, protein, fat, ash, and soluble carbohydrate contents ranged from 1.93-5.41%, 16.17-40.45%, 4.88-10.38%, 2.05-3.57%, and 38.39-60.59%, respectively. Bulk density, water absorption capacity, oil absorption capacity, swelling capacity, emulsion activity, and emulsion stability ranged from 0.67-0.77g/mL, 253.33-273.33%, 200.00-206.67%, 35.33-42.00%, 3.85-16.03%, and 5.13-9.62%, respectively. Also, phosphorus, iron, copper, sodium, potassium, zinc, calcium and magnesium contents ranged from 3493-6216µg/g, 141-274µg/g, 169-294µg/g, 2196-5920µg/g, 5238-12625µg/g, 170-227µg/g, 0.711-1.11% and 0.080-0.143% respectively. It was concluded that supplementing cereal diets with legumes boosts mineral and protein levels that may be absent or deficient. Hence, a formulation made from cereals and legumes would contain a better nutritional profile than a single cereal diet consumed alone for proper growth and development.

Keywords: Cereals, legumes, composite flour, formulation, nutrient profiling

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P7

Solvent- Assisted Dye Removal and Depolymerization of Waste Polyester Textiles via Hydrolysis Using HZSM-5 as Catalyst

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The increasing consumption and disposal of polyester/ poly(ethylene) terephthalate (PET) textile waste pose significant environmental challenges globally and especially in Ghana, where large volumes of second-hand clothing waste are poorly managed. PET recycling can be achieved via mechanical recycling and chemical recycling[1]. Chemical recycling is the most suitable and efficient approach for PET textile recycling due to its ability to convert the wastes into high value products via depolymerization[1]. However, the presence of dyes prior to depolymerization hinder the activity of catalyst used, contaminate the monomer stream and deteriorate the overall purity of the final product[2]. Hydrolysis which is one of the less employed chemical recycling methods represents an environmentally benign and efficient approach to depolymerize PET into its monomers terephthalic acid (TPA) and ethylene glycol (EG)[1]. However, due to its slow kinetics, catalysts systems are required to increase the rate of the reaction and reduce the overall cost of the process. Previously used catalyst systems are mostly homogeneous, hazardous and difficult to recover after the reaction. In this study propylene carbonate is investigated as a green solvent for the efficient extraction of disperse dyes from polyester textiles. To enhance the kinetics of the reaction, HZSM-5 zeolite is proposed as a heterogeneous catalyst. Other advantages of using HZSM-5 zeolite is its easy recoverability and reusability[3]. The outcomes of this study are expected to support waste management strategies, reduce the reliance on fossil fuels for virgin polyester production, and contribute to Sustainable Development Goals 12 (Responsible Consumption and Production) and 13 (Climate Action).

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Green Synthesis of Magnetic Fe₃O₄/CuS Nanocomposite for Selective Adsorption of Mercury From Water

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The contamination of water resources by toxic mercury (Hg(II)) ions poses a serious threat to ecosystems and human health, necessitating efficient and sustainable remediation strategies. In this study, magnetic Fe₃O₄/CuS nanocomposites were synthesized via a green route using castor oil as a renewable solvent and stabilizer. The composites were designed to exploit the strong thiophilic affinity of copper sulfide (CuS) for mercury binding and the magnetic properties of iron oxide (Fe₃O₄) for easy separation. Fe₃O₄ nanoparticles were prepared by co-precipitation, followed by solvothermal decomposition of a copper diethyldithiocarbamate precursor in castor oil to form CuS and Fe₃O₄/CuS nanocomposites with mass ratios of 1:1, 1:4, and 1:8. Structural and physicochemical characterization (FT-IR, XRD, SEM/EDX, TGA, NMR) confirmed the formation of crystalline nanocomposites with the intended core-shell morphology. SEM analysis revealed that CuS formed spherical nanoparticles, while Fe₃O₄ appeared as spherical particles with noticeable aggregation, leading to a composite structure with good surface interaction. Batch adsorption experiments revealed that the Fe₃O₄/CuS (1:8) composite achieved a high performance, with a maximum adsorption capacity of 295 mg g⁻¹ at pH 8, 20 mg dosage, and 200 min contact time. Kinetic and isotherm modeling indicated that Hg(II) uptake followed a pseudo-second-order model and fit the Langmuir isotherm, suggesting chemisorption on a homogeneous surface. The nanocomposite also exhibited outstanding selectivity, removing Hg(II) quantitatively even in the presence of excess competing ions (Cd²⁺, Pb²⁺, Zn²⁺), and retained ~80 % efficiency after four regeneration cycles. These findings demonstrate that castor oil-mediated synthesis offers a sustainable pathway to highly efficient, selective, and magnetically recoverable Fe₃O₄/CuS nanocomposites, highlighting their promise as a scalable, engineering innovation for practical mercury remediation.

Keywords: Mercury removal, Adsorption, Copper sulfide, Iron oxide, Green synthesis, Castor oil

Synthesis and Characterization of Novel 1,2,3-Triazole Derivatives and Phosphonium Salts as potential antimalarials

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Objective

To synthesize and characterize novel 1,2,3-Triazole (“clicked”) derivatives and their corresponding phosphonium salts as potential candidates for subsequent biological evaluation

Method

A series of novel compounds comprising 17 1,2,3-triazole derivatives and 21 phosphonium salts was synthesized, giving a total of 38 compounds. The synthesized compounds were characterized using infrared (IR) spectroscopy, high-resolution mass spectrometry (HRMS), nuclear magnetic resonance (NMR) spectroscopy, including ¹H, ¹³C, DEPT-135, and ³¹P NMR, as well as melting-point determination.

Results

A total of 38 novel compounds were successfully synthesized, comprising 17 1,2,3-triazole derivatives and 21 phosphonium salts. Spectroscopic and analytical characterization provided structural information consistent with the formation of the target compounds. The combined IR, HRMS, NMR, and melting-point data supported the successful synthesis and characterization of the compound series.

Conclusion

The study successfully generated and characterized a library of 38 novel 1,2,3-triazole derivatives and phosphonium salts. These compounds provide a basis for further investigations into their biological properties, including planned in vitro antimalarial and cytotoxicity evaluations against *Plasmodium falciparum*.

Keywords: Synthesis, Characterization, 1,2,3-Triazole, Phosphonium salts, antimalarial

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SYNTHESIS, CHARACTERIZATION, AND ANTI-MICROBIAL PROPERTIES OF COPPER SULFIDE NANOPARTICLES FROM DIETHYLDITHIOCARBAMATE COMPLEXES

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Antimicrobial resistance (AMR) is a growing global health challenge that compromises the effectiveness of conventional antimicrobial agents and necessitates the exploration of alternative therapeutic materials. This study investigated the synthesis, characterization, and antimicrobial activity of copper sulfide (CuS) nanoparticles. Copper diethyldithiocarbamate complexes were synthesized via a precipitation method and characterized using UV–visible, nuclear magnetic resonance (NMR), and Fourier-transform infrared (FTIR) spectroscopy. The resulting complexes were subsequently decomposed using a melt method to produce CuS nanoparticles, which were characterized by zeta potential analysis and X-ray diffraction (XRD). XRD analysis confirmed the formation of covellite-phase CuS with a hexagonal crystal structure and an average crystallite size of 34.73 nm. The antimicrobial activity of the CuS nanoparticles was evaluated against three bacterial strains, *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Enterococcus faecalis*, and the fungal strain *Candida albicans* using the broth serial dilution method. The nanoparticles exhibited notable antifungal activity against *C. albicans*, as indicated by a low minimum inhibitory concentration (MIC), but showed no significant inhibitory activity against the tested bacterial strains. These findings demonstrate the potential of CuS nanoparticles as antifungal agents and provide a basis for further investigation of their antimicrobial properties and possible applications in addressing emerging challenges associated with antimicrobial resistance.

Keywords: Antimicrobial, antifungal, nanoparticle, precipitation, diethyldithiocarbamate.

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Anthelmintic Constituents of *Holoptelea grandis* Stem Bark: Bioassay-Guided Fractionation and Isolation

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Helminthiases, particularly soil-transmitted helminth infections, remain an important public health concern in tropical and subtropical regions, including Ghana. The increasing prevalence of anthelmintic resistance and limitations associated with existing treatments have stimulated interest in medicinal plants as sources of bioactive natural products. *Holoptelea grandis* is traditionally used as a vermifuge in Ghana, although its anthelmintic activity and chemical constituents have received limited scientific investigation. This study evaluated the anthelmintic activity of *H. grandis* stem bark and employed bioassay-guided fractionation to isolate and characterize its chemical constituents. The stem bark was extracted with ethanol and subsequently fractionated using petroleum ether and ethyl acetate. Anthelmintic activity was evaluated in vitro using paralysis and death time assays against *Pheretima posthuma*. The active ethyl acetate fraction was subjected to chromatographic separation, and isolated constituents were characterized using gas chromatography-mass spectrometry (GC-MS), nuclear magnetic resonance (NMR) spectroscopy, and infrared (IR) spectroscopy. Phytochemical screening revealed the presence of tannins, saponins, alkaloids, and terpenoids. The ethyl acetate fraction exhibited greater anthelmintic activity than the crude extract and petroleum ether fraction, producing shorter paralysis and death times against *P. posthuma*. Two isolates, designated HGS01 and HGS02, were obtained from the active fraction. HGS01 was characterized as a complex mixture dominated by alkanes, alkenes, and alcohols, while HGS02 was conclusively identified as the pentacyclic triterpenoid friedelan-3-one (friedelin) based on NMR and MS data. The findings demonstrate anthelmintic activity in the stem bark extract and its ethyl acetate fraction and establish the presence of friedelin among the isolated constituents. Further evaluation of the isolated constituents is required to determine their individual contributions to the observed anthelmintic activity and their potential as sources of anthelmintic agents.

Keywords: *Holoptelea grandis*; anthelmintic activity; friedelin; friedelan-3-one; bioassay-guided fractionation; *Pheretima posthuma*; natural products

Nodule-Specific Cysteine-Rich Peptides as Potential FtsZ Inhibitors: Molecular Docking Insights into a Broad-Spectrum Antimicrobial Strategy

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Antimicrobial resistance (AMR) poses a major global health challenge within the One Health framework, creating a need for antimicrobial strategies that target essential bacterial processes through mechanisms distinct from those of conventional antibiotics. Bacterial cell division is an attractive target because proliferation depends on the assembly and function of the FtsZ protein, a highly conserved GTPase-like protein that polymerizes to form the Z-ring and coordinate cytokinesis. FtsZ shares limited sequence similarity with human tubulin, providing a basis for investigating it as a potential antimicrobial target. Most reported FtsZ inhibitors interact with the protein at sites associated with GTP binding or polymerization. The antimicrobial peptide MciZ provides an alternative mechanism, binding to the C-terminal region of FtsZ in *Bacillus subtilis* and interfering with Z-ring formation and cell division. Nodule-specific cysteine-rich (NCR) peptides produced by legumes have also been reported to affect bacterial cell division in rhizobia, suggesting a possible connection between NCR peptide activity and FtsZ function. This study investigated the potential of NCR peptides as FtsZ inhibitors across selected microbial species using molecular docking. Docking analyses showed that the evaluated NCR peptides associated with the C-terminal region of FtsZ across multiple microbial species, with binding patterns that showed similarities to the reported interaction of MciZ with FtsZ. These results suggest that NCR peptides may interact with a conserved region of FtsZ beyond their established biological context in rhizobial systems. Molecular dynamics simulations are ongoing to assess the stability and persistence of the predicted NCR-FtsZ interactions and to further characterize the molecular basis of peptide binding. The study provides a computational basis for investigating NCR peptides as potential modulators of bacterial cell division and supports further evaluation of their antimicrobial activity against diverse bacterial pathogens.

Keywords: NCR peptides; FtsZ; antimicrobial peptides; bacterial cell division; molecular docking; molecular dynamics; antimicrobial resistance; One Health.

Thiol-Functionalized Magnetic Iron Oxide Nanocomposite for the Adsorptive Removal of Diclofenac Sodium

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The increasing consumption of pharmaceuticals, particularly nonsteroidal anti-inflammatory drugs (NSAIDs), has contributed to their occurrence in pharmaceutical and other wastewater streams, raising environmental concerns. This study investigated the development of a functionalized magnetic nanocomposite for the adsorptive removal of diclofenac sodium from aqueous solution. Magnetite nanoparticles (Fe_3O_4) were synthesized by co-precipitation, followed by silica coating using the Stöber method to produce $\text{Fe}_3\text{O}_4@\text{SiO}_2$. The silica-coated nanoparticles were subsequently functionalized with thiol groups using 3-mercaptopropyltriethoxysilane (MPTES). The materials were characterized by Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), zeta-potential analysis, and UV-visible spectroscopy. FT-IR confirmed the functional groups associated with the successive modification steps, while XRD confirmed the crystalline nature of the materials and gave an average crystallite size of 14.7 nm. Zeta-potential measurements provided information on surface charge and colloidal stability, while changes in the UV-visible absorption spectra reflected the progressive modification of the nanoparticles. The effects of contact time, adsorbent dosage, pH, and initial diclofenac sodium concentration on adsorption performance were investigated. At an initial diclofenac sodium concentration of 20 mg/L, removal efficiencies of 30–90% were observed across the investigated pH range, with maximum removal achieved at an adsorbent dosage of 1.0 g/L. The results demonstrate the potential of the synthesized functionalized magnetic nanocomposite for the removal of diclofenac sodium from aqueous systems.

Keywords: Diclofenac sodium; magnetic nanocomposite; adsorption; $\text{Fe}_3\text{O}_4@\text{SiO}_2$; water remediation.

Biofilm and Efflux Modulation by Constituents of *Salacia debilis*

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The rise of antimicrobial resistance (AMR) poses a major challenge to the treatment of bacterial infections, particularly those caused by multidrug-resistant pathogens. Conventional antibiotics exert strong selective pressure by targeting bacterial viability, creating a need for complementary strategies that interfere with virulence-associated processes. Antivirulence approaches targeting processes such as quorum sensing, biofilm formation, and efflux-mediated resistance offer an alternative strategy for attenuating bacterial pathogenicity. *Salacia debilis*, a medicinal shrub traditionally used in Ghanaian medicine, contains bioactive constituents with reported antimicrobial activity, although its effects on bacterial virulence-associated processes remain insufficiently explored. This study investigated the antivirulence activities of compounds isolated from *S. debilis*. The crude and ethyl acetate extracts exhibited antimicrobial activity against *Staphylococcus aureus* and *Pseudomonas aeruginosa*, with minimum inhibitory concentrations (MICs) ranging from 6.25 to 25.0 mg/mL. Bioassay-guided fractionation yielded two compounds, SD-03 (benzyl 2-methoxybenzoate) and SD-04 (1,10-dihydroxy-6H-benzo[c]chromen-6-one), which were isolated and characterized. At MIC and sub-MIC concentrations, neither compound inhibited bacterial growth; however, both reduced biofilm formation and disrupted preformed biofilms in *S. aureus* and *P. aeruginosa*. Efflux pump inhibition, evaluated using the ethidium bromide accumulation assay, showed concentration-dependent activity for both compounds. SD-03 recorded maximum specific activities of approximately 295 RFI/μmol against *P. aeruginosa* and 90 RFI/μmol against *S. aureus*, while SD-04 showed activities of approximately 150 RFI/μmol against both bacterial species. Molecular docking predicted favorable interactions of SD-03 and SD-04 with the quorum sensing regulators LasR, RhIR, and PqsR, as well as the NorA efflux pump protein. SD-03 and SD-04 showed predicted binding energies of −9.8 and −10.4 kcal/mol, respectively, against LasR. These computational results provide mechanistic hypotheses for the observed antivirulence effects and warrant further experimental investigation of the compounds' interactions with quorum sensing pathways. The findings demonstrate that constituents of *S. debilis* can modulate biofilm formation and efflux-associated phenotypes without directly inhibiting bacterial growth.

Keywords: *Salacia debilis*; antimicrobial resistance; antivirulence; biofilm; efflux pump; quorum sensing; molecular docking; natural products

Phytochemical Composition and Antimicrobial Potential of *Xylopia villosa* Stem Bark

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Antimicrobial resistance is a major global health challenge, creating a need for new sources of antimicrobial agents. Medicinal plants are important sources of chemically diverse natural products with potential biological activities. *Xylopia villosa* is a Ghanaian medicinal plant traditionally used in the management of infectious diseases, but its phytochemical composition and antimicrobial properties remain insufficiently characterized. This study investigated the phytochemical composition and antimicrobial potential of the stem bark of *X. villosa*, with preliminary isolation and characterization of a constituent. The stem bark was extracted with ethanol, and the crude extract was subjected to phytochemical screening and antimicrobial evaluation using the broth microdilution method. Bioassay-guided chromatographic separation involving repeated column chromatography, thin-layer chromatography, and recrystallization yielded a pure compound designated XV01. Spectroscopic characterization using infrared and nuclear magnetic resonance spectroscopy indicated the presence of carboxylic acid, carbonyl, and aliphatic functional groups. Phytochemical screening of the crude extract revealed the presence of alkaloids, triterpenoids, glycosides, phytosteroids, tannins, saponins, flavonoids, and anthraquinones. The crude ethanolic extract exhibited minimum inhibitory concentrations (MICs) of 6.25 mg/mL against *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Escherichia coli*, and *Enterococcus faecalis*, and 25 mg/mL against *Candida albicans*. The isolation of XV01 provides a basis for further structural elucidation and biological evaluation. Further antimicrobial testing of XV01 and the purified fractions is required to determine their individual contributions to the observed activity. This study contributes to the phytochemical characterization of *X. villosa* stem bark and provides a basis for further investigation of its chemical constituents and biological activities.

Keywords: *Xylopia villosa*; phytochemical composition; antimicrobial activity; minimum inhibitory concentration; natural products; bioassay-guided fractionation

Integrated Virtual Screening and Molecular Dynamics for the Identification of Potential *Plasmodium falciparum* D-Enoyl-ACP Reductase Inhibitors

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The emergence and spread of drug-resistant *Plasmodium falciparum* strains underscore the need for new antimalarial agents that target essential parasite-specific pathways. *P. falciparum* D-enoyl-acyl carrier protein reductase (PfENR), an essential enzyme involved in fatty acid biosynthesis, represents a potential target for antimalarial drug discovery. This study employed an integrated virtual screening and molecular dynamics (MD) simulation workflow to identify and prioritize potential PfENR inhibitors. A library of 78,000 compounds with reported antimalarial properties was retrieved from the ChEMBL database in SMILES format and filtered by molecular weight and structural redundancy, yielding 71,200 unique compounds for screening. The compounds were subjected to three independent molecular docking runs against PfENR to assess the consistency of predicted binding interactions. Compounds with mean docking scores of ≤ -8.5 kcal/mol were shortlisted, with further prioritization based on the occurrence of more than five predicted binding poses within the PfENR active site. Selected candidates were subsequently subjected to MD simulations to evaluate the stability and conformational behaviour of the protein-ligand complexes. Trajectory analyses included protein and ligand root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (Rg), ligand RMSF, free energy landscape (FEL), and principal component analysis (PCA). Among the screened compounds, ChEMBL4127624 and ChEMBL120484 exhibited favourable predicted interaction profiles and maintained stable associations with PfENR throughout the simulations, with complex behaviour comparable to or more favourable than that of the co-crystallized reference ligand under the simulated conditions. These compounds were prioritized as potential PfENR inhibitors for further investigation. Experimental biochemical and antimalarial assays will be required to determine their inhibitory activity and validate the computational predictions. The study demonstrates an integrated computational workflow for prioritizing small molecules targeting PfENR and provides candidates for subsequent experimental evaluation against *P. falciparum*.

Keywords: *Plasmodium falciparum*; D-enoyl-ACP reductase; PfENR; ChEMBL; virtual screening; molecular docking; molecular dynamics; antimalarial drug discovery.

Stigmasterol from *Rhodognaphalon brevicuspe* Stem Bark: Antimicrobial and Antibiofilm Activity

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The increasing prevalence of antimicrobial resistance and biofilm-associated infections underscores the need to identify bioactive compounds from medicinal plants. This study investigated the phytochemical composition, antimicrobial and antibiofilm activities of *Rhodognaphalon brevicuspe* stem bark, with emphasis on an isolated sterol constituent. The stem bark was extracted with ethanol and partitioned by liquid-liquid extraction to obtain petroleum ether and ethyl acetate fractions. Qualitative phytochemical screening revealed the presence of alkaloids, tannins, saponins, glycosides, and terpenoids/steroids, while flavonoids and coumarins were not detected. Chromatographic separation of the ethyl acetate fraction yielded RB06, which was characterized by Fourier-transform infrared (FT-IR) and nuclear magnetic resonance (NMR) spectroscopy and identified as stigmasterol. The antimicrobial activities of the crude extract, fractions, and isolated compound were evaluated against selected Gram-positive and Gram-negative bacteria and *Candida albicans* using the broth microdilution method. Antibiofilm activity was assessed using microtiter plate assays and microscopic visualization. The ethyl acetate fraction exhibited antimicrobial activity against *Pseudomonas aeruginosa* and *Staphylococcus aureus*, with minimum inhibitory concentrations (MICs) of 1.56 mg/mL, and against *C. albicans* with an MIC of 0.75 mg/mL. RB06 demonstrated antimicrobial activity against *S. aureus* and *C. albicans*, with MICs of 500 µg/mL, whereas inhibition against *P. aeruginosa*, *Escherichia coli*, and *Enterococcus faecalis* occurred at concentrations above 500 µg/mL. The isolated stigmasterol also reduced biofilm formation in the tested bacterial and fungal organisms in a concentration-dependent manner, although its activity was lower than that of the reference antimicrobial agents. Microscopic examination showed alterations in biofilm architecture and reduced biofilm cohesion following treatment. These findings establish the presence of stigmasterol in *R. brevicuspe* stem bark and demonstrate antimicrobial and antibiofilm activity associated with the isolated compound. The study provides further chemical and biological characterization of *R. brevicuspe* and supports continued investigation of its bioactive constituents.

Keywords: *Rhodognaphalon brevicuspe*; stigmasterol; antimicrobial activity; antibiofilm activity; phytochemicals; natural products; minimum inhibitory concentration

Scaffold Hopping – Driven Design of Novel Chemical Frameworks for Anthelmintic Drug Development

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The emergence of resistance to benzimidazole anthelmintics in *Haemonchus contortus* poses a significant challenge to parasite control and livestock health. This study explores a computational drug discovery approach to identify novel chemical scaffolds that overcome β -tubulin-mediated resistance. In the absence of an experimentally resolved structure, *H. contortus* β -tubulin was modelled using homology techniques, followed by the generation of resistance-associated mutants (Q134H, F167Y, E198A, and F200Y). Rigorous structural validation confirmed the reliability of the generated models. Molecular docking of standard benzimidazole drugs revealed reduced binding affinity and deviations in ligand-binding poses within the binding pockets of the mutants compared with the ligand bound to the wild-type protein, particularly in the Q134H and E198A mutants. Molecular dynamics (MD) simulations of these drugs showed clear displacement of ligands from the binding pockets of Q134H and E198A mutants. These observations support their role in conferring resistance. To overcome challenges posed by these mutations, a scaffold-hopping strategy was employed using 9 reference benzimidazole drugs, generating a diverse library of 72,004 novel compounds. Virtual screening against the Q134H mutant, which was used as a stringent resistance model, identified over 5,000 high-affinity candidates (≤ -8.5 kcal/mol), representing 7.34% of the library. Subsequent filtering excluded compounds retaining the benzimidazole core to prioritise structurally novel candidates with reduced susceptibility to cross-resistance. Ongoing molecular docking and MD simulations of β -tubulin–ligand complexes aim to predict the mechanisms of action of selected scaffolds. Overall, this work integrates homology modelling, docking, scaffold hopping, and virtual screening to systematically identify novel anti-parasitic candidates. The findings provide a foundation for developing next-generation anthelmintics with improved efficacy against resistant *H. contortus* strains.

Keywords: Benzimidazole resistance, protein mutations, single-nucleotide polymorphism, in silico studies, and beta-tubulin.

Computational Mining of Ghanaian Plant Natural Products for Rice Weevil (*Sitophilus oryzae*) Acetylcholinesterase Inhibitors

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The rice weevil (*Sitophilus oryzae*) is a major storage pest responsible for significant post-harvest grain losses worldwide. The extensive use of synthetic insecticides, including phosphine and pirimiphos-methyl, raises concerns about environmental contamination and ecotoxicological effects, highlighting the need to explore alternative pest-control agents. This study employed a structure-based computational workflow to identify natural products from Ghanaian medicinal plants with potential inhibitory activity against *S. oryzae* acetylcholinesterase (AChE). Because an experimental three-dimensional structure of *S. oryzae* AChE was unavailable, a homology model was constructed using *Anopheles gambiae* AChE as the template, with 67.96% sequence identity. The resulting model showed 94.58% of residues in the Ramachandran favored regions, supporting its use for structure-based screening. A library of 467 natural products isolated from the volatile oil fractions of Ghanaian medicinal plants was screened against the modeled enzyme. Compounds with binding affinities comparable to or stronger than that of the reference pesticide derivative, pirimiphos-methyl-oxon, were subsequently evaluated for selectivity against human AChE and subjected to ADMET and physicochemical property filtering. The workflow yielded 136 initial hits, which were refined to 14 candidates following selectivity and pharmacokinetic filtering. Ethyl cinnamate, olivetol, methyl anthranilate, and thymol showed favorable predicted binding energies and interactions with key residues within the catalytic site, together with suitable predicted pharmacokinetic properties. These compounds emerged as candidates for further evaluation as potential inhibitors of *S. oryzae* AChE. Molecular dynamics simulations and experimental bioassays are underway to assess complex stability and determine whether the computationally predicted interactions translate into insecticidal activity. The study provides a structure-based framework for prioritizing Ghanaian plant natural products for further investigation as potential alternatives to conventional insecticides.

Keywords: *Sitophilus oryzae*; rice weevil; acetylcholinesterase; natural products; molecular docking; ADMET; Ghanaian medicinal plants; computational screening

Membrane Engagement and Stereochemical Dependence of a Minimal Thrombin-Derived Antimicrobial Peptide (Mandy-1)

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The rational reduction of antimicrobial peptides (AMPs) can generate compact sequences while retaining structural features associated with membrane interaction. Building on the previously characterized thrombin-derived peptide FRL16 (FRLKKWIKVIDQFGE), this study investigated Mandy-I (FLWIVIF), a seven-residue derivative designed to retain key hydrophobic and aromatic determinants of membrane interaction. Molecular dynamics simulations were employed to characterize peptide-membrane association, membrane penetration, structural behaviour, and bilayer perturbation, while the influence of stereochemistry was examined by comparing the L- and D-enantiomers. Mandy-I showed strong membrane association and penetration, with interactions at the membrane interface dominated by its hydrophobic and aromatic residues. The simulations revealed localized bilayer perturbation accompanied by membrane deformation, changes in lipid organization, and curvature induction, indicating substantial interaction between the shortened peptide and the membrane environment. Time-resolved structural analyses further showed persistent peptide-membrane association throughout the simulated trajectories. Comparison of the L- and D-enantiomers indicated that stereochemical configuration influences peptide behaviour at the membrane interface, providing insight into structural factors that may govern the activity of this minimal peptide. The study was informed by previously established membrane-active behaviour of FRL16, including interactions with bacterial outer membranes, translocation through lipopolysaccharide-rich environments, and disruption of the inner membrane. In silico prediction further indicated high probabilities of antibacterial, antiviral, and antifungal activity for Mandy-I, with predicted probabilities of 0.988, 0.95, and 0.96, respectively, while the peptide was predicted to have low activity against human erythrocytes. The findings indicate that substantial membrane engagement can be retained following marked peptide truncation and highlight the influence of hydrophobic composition and stereochemical configuration on the membrane behaviour of short thrombin-derived peptides. Mandy-I provides a compact framework for further mechanistic investigation, peptide optimization, and experimental validation of short membrane-active antimicrobial peptides.

Keywords: antimicrobial peptides; peptide design; Mandy-I; molecular dynamics simulation; membrane interaction; membrane disruption; stereochemistry; thrombin-derived peptides

α -Amylase and α -Glucosidase Inhibitory Activity of *Salacia debilis* Stem Bark

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Diabetes mellitus is a chronic metabolic disorder characterized by persistent hyperglycaemia and remains a major global health challenge. Despite the availability of several antidiabetic therapies, limitations associated with long-term treatment have stimulated the search for alternative sources of bioactive compounds. Medicinal plants continue to provide important sources of chemical diversity for drug discovery. Although several *Salacia* species have demonstrated antihyperglycaemic activity, the antidiabetic potential of the West African species *Salacia debilis* remains relatively unexplored. This study evaluated the *in vitro* antidiabetic activity of *S. debilis* and investigated the activity of its solvent fractions. Powdered stem bark of *S. debilis* was extracted with ethanol and fractionated by solvent partitioning to obtain three fractions. The crude extract and solvent fractions were evaluated for α -amylase and α -glucosidase inhibitory activities using concentration-dependent enzyme inhibition assays, and inhibitory potency was determined from IC₅₀ values. Phytochemical screening was also performed using standard procedures. The crude extract and solvent fractions exhibited concentration-dependent inhibition of both enzymes. The ethyl acetate fraction showed the greatest inhibitory activity, with IC₅₀ values of 169.2 μ g/mL against α -amylase and 18.38 μ g/mL against α -glucosidase, compared with 16.8 μ g/mL and 7.21 μ g/mL, respectively, for acarbose. Percentage inhibition ranged from 39.13–70.53% for α -amylase and 24.55–77.12% for α -glucosidase across the tested concentrations. Phytochemical screening revealed the presence of tannins, saponins, alkaloids, flavonoids, and glycosides, which may contribute to the observed enzyme-inhibitory activity. The ethyl acetate fraction is currently undergoing chromatographic purification and spectroscopic characterization to identify the constituents associated with the observed activity. These findings provide preliminary evidence for the *in vitro* antidiabetic potential of *S. debilis* and support further investigation of its bioactive constituents.

Keywords: *Salacia debilis*; α -amylase; α -glucosidase; antidiabetic activity; enzyme inhibition; phytochemicals; IC₅₀.

Stereochemical Engineering of a Thrombin-Derived Antimicrobial Peptide: Molecular Dynamics Insights into D-Amino Acid Effects on FRL16 Structure and Membrane Activity

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FRL16, a thrombin-derived antimicrobial peptide previously shown to exhibit selective dual-state membrane engagement in Gram-negative bacterial membranes, represents a promising scaffold for peptide-based therapeutics. However, its native L-amino acid composition renders it susceptible to proteolytic degradation, limiting its stability in biological environments. This study investigates the effect of stereochemical modification through D-amino acid substitutions on the structural dynamics and membrane activity of FRL16, with emphasis on preserving its antimicrobial function while enhancing resistance to enzymatic degradation. All-atom molecular dynamics simulations were performed to compare the native peptide with stereochemically modified variants in model lipid bilayers representative of bacterial inner membranes. Consistent with earlier observations, the L-form FRL16 exhibits dynamic insertion, conformational adaptability, and pronounced membrane perturbation. Introduction of D-amino acids results in altered backbone geometry and reduced α -helical stability, reflecting the sensitivity of peptide secondary structure to stereochemical inversion. Despite these structural changes, membrane-binding affinity and insertion depth remain largely preserved across several modified variants. Notably, substitutions at key functional residues; KK and WI motifs, retain membrane insertion profiles and disruption capacity comparable to the native peptide. These residues appear to play a dominant role in governing peptide–membrane interactions, enabling maintenance of amphipathic balance and lipid engagement even under stereochemical perturbation. Analyses of bilayer properties, including membrane thinning, lipid disorder, and water permeation, demonstrate that both native and D-substituted peptides induce similar levels of membrane destabilization. Transient pore formation and water channeling events are consistently observed, indicating preservation of the peptide’s core membrane-disruptive mechanism. These findings establish that stereochemical modification can decouple peptide helicity from functional activity in FRL16 while maintaining critical residue-driven interactions. The retention of membrane disruption following targeted D-amino acid substitution highlights a viable strategy for improving proteolytic stability without compromising antimicrobial efficacy. This work provides mechanistic insight into the structure–function relationships of thrombin-derived peptides and supports the rational design of stereochemically optimized antimicrobial agents.

Keywords

Antimicrobial peptides; FRL16; D-amino acid substitution; molecular dynamics simulation; membrane disruption; pore formation; proteolytic stability

QSAR-Guided Design and Computational Evaluation of Small-Molecule GLP-1 Receptor Agonist Candidates

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The glucagon-like peptide-1 receptor (GLP-1R) is an important therapeutic target for type 2 diabetes mellitus and obesity, with small-molecule agonists offering a potential route to orally active therapies. This study employed an integrated computational workflow combining quantitative structure-activity relationship (QSAR) modelling, molecular docking, molecular dynamics (MD) simulations, and molecular mechanics/generalized Born surface area (MM/GBSA) analysis to design and evaluate small-molecule GLP-1R agonist candidates. A dataset of 113 experimentally validated danuglipron-chemotype GLP-1R agonists was used to develop QSAR models. The descriptors nLevel6, nHAcc, C-026, and P_VSA_ppp_hal were identified as important predictors of activity, with the multilayer perceptron model achieving R^2 values of 0.65 and 0.80 for the training and test sets, respectively. Ten designed compounds (EAFS_1–EAFS_10) were subsequently evaluated against the active-state human GLP-1R structure (PDB ID: 6X18). Docking scores ranged from –2.60 to –8.02 kcal/mol, compared with –9.61 kcal/mol for danuglipron. MD simulations identified EAFS_2, EAFS_8, and EAFS_9 as showing relatively stable ligand trajectories. EAFS_3, EAFS_8, EAFS_9, and EAFS_6 also exhibited favourable predicted MM/GBSA binding free energies of –28.87, –23.23, –28.15, and –20.75 kcal/mol, respectively, compared with –33.32 kcal/mol for danuglipron. The results indicate that hydrophobic and electrostatic interactions contribute to the predicted stability of the designed ligands. The identified compounds provide candidates for further optimization and experimental evaluation of GLP-1R agonist activity.

Keywords: GLP-1 receptor; QSAR; molecular docking; molecular dynamics; MM/GBSA; small-molecule agonists.

Bioassay-Guided Exploration of Anthelmintic Alkaloids from *Desmodium adscendens*

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Helminthiasis remains a major global health challenge, affecting more than 1.5 billion people, particularly in low- and middle-income countries. The increasing prevalence of resistance to conventional anthelmintics has intensified the search for alternative sources of bioactive

compounds. *Desmodium adscendens*, widely used in Ghanaian ethnomedicine for the management of helminth infections, represents a promising but underexplored source of potential anthelmintic agents. This study explored the contribution of alkaloids to the anthelmintic activity of *D. adscendens* using a bioassay-guided fractionation approach. Preliminary phytochemical screening of the crude extract revealed the presence of alkaloids, flavonoids, saponins, tannins, phenols, and sterols, while triterpenoids were not detected. In vitro anthelmintic activity was evaluated against *Pheretima posthuma*. At 20 mg/mL, the crude extract induced paralysis and death after 13.95 ± 0.81 and 51.30 ± 0.85 min, respectively. Enrichment of the alkaloid fraction resulted in improved activity, with paralysis and death occurring after 10.70 ± 0.80 and 42.60 ± 1.10 min, respectively, at the same concentration. Although levamisole exhibited greater activity, the enhanced activity of the alkaloid-rich fraction relative to the crude extract suggests that alkaloids contribute substantially to the observed anthelmintic activity. To identify the constituents associated with this activity, 42.78 g of the crude alkaloid fraction was subjected to silica gel column chromatography using petroleum ether:ethyl acetate (8:2, v/v), yielding ten fractions. Fraction 1 was further separated using petroleum ether:ethyl acetate (9:1, v/v) to afford three sub-fractions, which are currently being investigated for the isolation and structural characterization of individual alkaloidal constituents. The isolated compounds will subsequently be evaluated for in vitro anthelmintic activity, while molecular docking and molecular dynamics simulations will be used to investigate potential molecular targets and mechanisms of action. This integrated approach is expected to identify alkaloidal constituents associated with the anthelmintic activity of *D. adscendens* and provide a basis for further investigation of plant-derived anthelmintic candidates.

Keywords: *Desmodium adscendens*; alkaloids; anthelmintic activity; bioassay-guided fractionation; molecular docking.

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Antimicrobial Activity and Fractionation of Bioactive Constituents from *Microglossa afzelii*

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Antimicrobial resistance (AMR) is a major global health challenge that threatens the effectiveness of existing antimicrobial therapies and increases the burden of infectious diseases. This has intensified the search for new antimicrobial agents, including those from medicinal plants. *Microglossa afzelii* (Pofiri), an indigenous medicinal plant used in African traditional medicine for the management of skin infections, otitis, sore throat, gonorrhoea, respiratory disorders, and arthritis, remains relatively underexplored. This study investigated the antimicrobial potential of *M. afzelii* and initiated the isolation of its bioactive constituents. Plant material was collected, authenticated, air-dried, milled, and extracted with 96% ethanol using a Soxhlet apparatus, yielding 14.45% crude extract. Preliminary phytochemical screening indicated the presence of alkaloids, triterpenoids, flavonoids, tannins, and saponins.

The crude extract was successively partitioned into petroleum ether and ethyl acetate fractions, and the antimicrobial activities of the crude extract and fractions were evaluated using the broth microdilution method against *Pseudomonas aeruginosa*, *Escherichia coli*, *Enterococcus faecalis*, *Staphylococcus aureus*, and *Candida albicans*. The crude extract exhibited minimum inhibitory concentrations (MICs) of 25 mg/mL against *P. aeruginosa*, *E. coli*, *E. faecalis*, and *S. aureus*, and 50 mg/mL against *C. albicans*. The ethyl acetate fraction showed the highest activity, with an MIC of 6.25 mg/mL against all five test microorganisms. The petroleum ether fraction exhibited MICs of 25 mg/mL against *P. aeruginosa*, *E. coli*, and *C. albicans*, and 50 mg/mL against *E. faecalis* and *S. aureus*. Based on its enhanced antimicrobial activity, 45 g of the ethyl acetate fraction was subjected to silica gel column chromatography using petroleum ether:ethyl acetate (5.5:4.5, v/v), yielding seven fractions. These fractions are being further investigated using chromatographic techniques to isolate and purify the constituents associated with the observed antimicrobial activity. The isolated compounds will be structurally characterized using spectroscopic techniques and evaluated for antimicrobial activity through *in vitro* assays. The study provides a basis for the phytochemical exploration of *M. afzelii* and the identification of compounds associated with its reported traditional medicinal applications.

Keywords: *Microglossa afzelii*; antimicrobial activity; antimicrobial resistance; minimum inhibitory concentration; bioactive constituents; fractionation.

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Acute Oral Toxicity and Biochemical Assessment of *Xylopia villosa* and *Desmodium adscendens* Extracts in Wistar Rats

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Medicinal plants continue to play an important role in primary healthcare across many African communities, where they are widely used in the management of various diseases. Despite their extensive ethnomedicinal use, the safety profiles of many medicinal plants remain inadequately characterized. This study evaluated the acute oral toxicity of ethanolic extracts of *Xylopia villosa* (XV) and *Desmodium adscendens* (DA) in female Wistar rats and assessed selected biochemical markers of liver and kidney function. Preliminary phytochemical screening was also performed to identify major classes of secondary metabolites present in the extracts. The acute oral toxicity study was conducted in accordance with Organisation for Economic Co-operation and Development (OECD) Guideline 423. Female Wistar rats received single oral doses of 50, 300, and 2000 mg/kg body weight of each extract and were monitored for 14 days for mortality, clinical signs of toxicity, behavioural changes, and changes in body weight. Liver and kidney function parameters were assessed at the end of the observation period. Qualitative phytochemical screening revealed the presence of alkaloids, flavonoids, glycosides, saponins, and tannins in the extracts. No mortality or major clinical signs of toxicity were observed in any treatment group throughout the 14-day observation period. Changes in body weight did not exhibit a consistent dose-dependent pattern. Based on the absence of mortality at the highest

administered dose, the median lethal dose (LD₅₀) of both extracts was estimated to be greater than 2000 mg/kg body weight under the conditions of the study. Biochemical analysis showed variations in total protein, albumin, urea, total bilirubin, direct bilirubin, and creatinine levels across the treatment groups, although these changes did not display a consistent dose-dependent pattern. The findings indicate low acute oral toxicity for the ethanolic extracts of *X. villosa* and *D. adscendens* at the doses investigated. The observed biochemical variations highlight the need for further subacute and chronic toxicity studies, including histopathological assessment, to establish the longer-term safety profiles of the extracts.

Keywords: *Xylopi* *villosa*; *Desmodium adscendens*; acute oral toxicity; Wistar rats; LD₅₀; biochemical assessment; liver and kidney function; phytochemical screening; medicinal plants.

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Mapping the Antimicrobial and Anti-inflammatory Bioactivities of Three Ghanaian Medicinal Plants: *Rhodognaphalon brevisuspe*, *Xylopi* *villosa*, and *Microglossa afzelii*

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The increasing prevalence of antimicrobial resistance and limitations associated with conventional anti-inflammatory drugs have intensified the search for bioactive compounds from medicinal plants. This study evaluated the antimicrobial and anti-inflammatory activities of ethanolic extracts of *Rhodognaphalon brevisuspe*, *Xylopi* *villosa*, and *Microglossa afzelii*. Plant materials were extracted with ethanol using Soxhlet extraction and subjected to qualitative phytochemical screening. Anti-inflammatory activity was evaluated using the carrageenan-induced paw oedema model in chicks, while antimicrobial activity was assessed against *Staphylococcus aureus*, *Escherichia coli*, *Pseudomonas aeruginosa*, *Enterococcus faecalis*, and *Candida albicans* using the broth microdilution method. Phytochemical screening revealed the presence of alkaloids, terpenoids, saponins, flavonoids, and phytosterols, with profiles varying among the three species. All extracts reduced carrageenan-induced paw oedema and showed lower area under the curve values relative to the negative control. Antimicrobial activity was observed across the tested organisms, with minimum inhibitory concentrations ranging from 3.125 to 25.0 mg/mL. *Xylopi* *villosa* showed the strongest antimicrobial activity, particularly against *P. aeruginosa*, *E. coli*, and *E. faecalis*, with MICs as low as 3.125 mg/mL. The findings demonstrate antimicrobial and anti-inflammatory activities in extracts of the three medicinal plants and support further investigation of their chemical constituents and mechanisms of action.

Keywords: *Rhodognaphalon brevisuspe*; *Xylopi* *villosa*; *Microglossa afzelii*; antimicrobial activity; anti-inflammatory activity; phytochemicals.

Chemical Profiling and Computational Evaluation of Bioactive Constituents from Selected Ghanaian Medicinal Plants

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Ghana possesses a rich diversity of medicinal plants that have long been used in traditional healthcare, yet the chemical composition and biological potential of many species remain insufficiently characterized. This study integrated phytochemical profiling and computational approaches to investigate five Ghanaian medicinal plants, *Xylopi villosa*, *Holoptelea grandis*, *Rhodognaphalon brevicuspe*, *Microglossa afzelii*, and *Desmodium adscendens*, as sources of bioactive natural products. Plant materials were authenticated, air-dried, and extracted with ethanol using Soxhlet extraction. Preliminary phytochemical screening revealed alkaloids, flavonoids, tannins, saponins, terpenoids, and glycosides, with their distribution varying among the species. High-performance liquid chromatography (HPLC) generated characteristic chromatographic fingerprints for comparative phytochemical profiling. Gas chromatography-mass spectrometry (GC-MS) coupled with the National Institute of Standards and Technology (NIST) spectral library was used to identify volatile and semi-volatile constituents. The identified compounds were subsequently evaluated against selected biological targets using molecular docking, followed by molecular dynamics simulations to investigate the stability and persistence of protein-ligand interactions. Several identified constituents showed favourable predicted interactions with the selected targets and maintained stable associations during the simulations. The integration of chromatographic profiling with molecular docking and molecular dynamics provided a systematic approach for characterizing plant-derived constituents and prioritizing compounds for further biological investigation. The study establishes a computationally informed framework for the exploration of Ghanaian medicinal plants as sources of bioactive natural products.

Keywords: Ghanaian medicinal plants; phytochemical profiling; HPLC; GC-MS; natural products; molecular docking; molecular dynamics; computational drug discovery.

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Nanoemulsification Enhances the Antioxidant and Antimicrobial Activities of Volatile Oils from *Cananga odorata*

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Antimicrobial resistance remains a major global public health challenge, creating interest in plant-derived volatile oils as sources of bioactive compounds. Despite their antimicrobial and antioxidant properties, the application of essential oils is limited by poor aqueous solubility, volatility, and limited stability. This study investigated whether nanoemulsification could improve the biological activity and stability of volatile oil from *Cananga odorata* (ylang-ylang). Volatile oil was extracted from the leaves and flowers by steam distillation and formulated into nanoemulsions using Tween 80 at surfactant-to-oil ratios of 7:3, 8:2, and 9:1. The antioxidant and antimicrobial activities of the formulations were evaluated and compared with those of the non-formulated oil. All formulations exhibited antioxidant activity, while the 9:1 formulation showed the greatest physical stability and enhanced antimicrobial activity. The 9:1 nanoemulsion exhibited a minimum inhibitory concentration (MIC) of 25 mg/mL compared with 50 mg/mL for the volatile oil. These findings indicate that nanoemulsification can improve the physical stability and antimicrobial activity of *C. odorata* volatile oil and provides a formulation strategy for further investigation of its biological applications.

Keywords: *Cananga odorata*; volatile oil; nanoemulsion; antimicrobial activity; antioxidant activity; minimum inhibitory concentration; formulation.

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Acute Oral Toxicity and Isolation of Bioactive Constituents from *Rhodognaphalon brevicuspe*

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Medicinal plants are important sources of bioactive compounds, but their complex chemical composition necessitates systematic evaluation of their safety and chemical constituents. *Rhodognaphalon brevicuspe* is traditionally used in Ghanaian medicine for the management of conditions including arthritis and venereal diseases, although its toxicological profile and chemical constituents remain insufficiently characterized. This study evaluated the acute oral toxicity of the crude ethanolic extract of *R. brevicuspe* and isolated selected chemical constituents from the plant. Stem bark material was extracted with ethanol, and the crude extract was subjected to chromatographic separation and repeated recrystallization, yielding

four isolates designated RB01, RB02, RB03, and RB04. Acute oral toxicity was evaluated in rats according to Organisation for Economic Co-operation and Development (OECD) Guideline 423. Animals were monitored for 14 days for mortality and clinical signs of toxicity, while selected biochemical parameters were assessed at the end of the observation period to evaluate potential effects on liver and kidney function. No mortality or major clinical signs of toxicity were observed during the 14-day observation period. Biochemical analysis showed no significant differences between the control and extract-treated groups in the assessed liver and kidney biomarkers. The approximate median lethal dose (LD₅₀) was greater than 2000 mg/kg body weight under the conditions of the study. The results indicate low acute oral toxicity of the crude ethanolic extract at the doses investigated and establish a basis for further structural characterization and biological evaluation of the isolated constituents.

Keywords: *Rhodognaphalon brevicuspe*; acute oral toxicity; LD₅₀; Wistar rats; biochemical assessment; liver function; kidney function; isolation; natural products.

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Comparative Anthelmintic Activity of *Microglossa afzelii* and *Xylopi* *villosa* against *Pheretima posthuma*

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Helminthiasis remains an important public health concern, particularly in tropical and subtropical regions, while the increasing use of anthelmintic drugs has contributed to growing concern about resistance and treatment limitations. These challenges have stimulated interest in medicinal plants as sources of potentially bioactive anthelmintic compounds. *Microglossa afzelii* and *Xylopi villosa* are medicinal plants used traditionally for the management of various ailments, including gastrointestinal conditions, although their anthelmintic activities remain insufficiently characterized. This study evaluated the anthelmintic activity of ethanolic extracts and solvent fractions of *M. afzelii* and *X. villosa* against *Pheretima posthuma*. Powdered whole plant material of *M. afzelii* and stem bark of *X. villosa* were extracted with ethanol by Soxhlet extraction, yielding 10.08% and 4.80% extracts, respectively. Phytochemical screening revealed the presence of several secondary metabolite classes, with alkaloids being prominent in both plant extracts. The crude ethanolic extracts were subsequently fractionated using petroleum ether, ethyl acetate, and water. Anthelmintic activity was assessed at different concentrations using paralysis and death times, with levamisole serving as the reference drug. At 100 mg/mL, the crude ethanolic extract of *M. afzelii* produced paralysis and death times of 4.33 and 6.00 min, respectively, whereas *X. villosa* produced corresponding times of 4.67 and 21.67 min. Among the fractions evaluated, the ethyl acetate fraction of *M. afzelii* exhibited the strongest anthelmintic activity. The results demonstrate concentration-dependent anthelmintic activity in extracts and fractions of both medicinal plants against *P. posthuma*, with *M. afzelii* showing greater activity under the conditions evaluated. These findings provide experimental evidence supporting further investigation of *M. afzelii* and *X. villosa* as sources of anthelmintic constituents.

Keywords: *Microglossa afzelii*; *Xylopi villosa*; anthelmintic activity; *Pheretima posthuma*; medicinal plants; phytochemicals; natural products.

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Bioactive Compounds from *Salacia debilis* Stems: Isolation, Antiplasmodial Evaluation and Cytotoxicity

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Salacia debilis stem decoctions are used in Ghanaian traditional medicine to treat malaria, yet few of the plant's constituents have been isolated and tested, and its cytotoxicity is unknown. This study isolated and characterized its antiplasmodial compounds and evaluated their efficacy and safety. Dried stems were Soxhlet-extracted with ethanol, and chromatographic purification yielded friedelin (SDS-01) and stigmasteryl palmitate (SDS-02), reported here from this species for the first time. Structures were elucidated by 1D/2D NMR and IR spectroscopy. Antiplasmodial activity against chloroquine-sensitive 3D7 and chloroquine-resistant Dd2 strains was determined by SYBR Green I assay. Cytotoxicity against HepG2 cells was assessed by MTT assay. Combinations with chloroquine were evaluated for interaction effects. Friedelin was most active against 3D7 ($IC_{50} = 1.886 \pm 0.062 \mu M$), followed by stigmasteryl palmitate ($4.588 \pm 0.023 \mu M$) and the crude extract ($2.75 \mu g/mL$). Against Dd2, friedelin activity declined markedly ($11.640 \pm 0.148 \mu M$), whereas stigmasteryl palmitate declined less ($5.359 \pm 0.075 \mu M$); the extract had an IC_{50} of $6.75 \mu g/mL$. All resistance indices exceeded 1. Selectivity indices were above 10 for both strains. Chloroquine combinations markedly improved Dd2 activity but were not synergistic ($\Sigma FIC_{50} > 1$). These findings support the traditional use of *S. debilis* and identify friedelin and stigmasteryl palmitate as promising, low-toxicity antiplasmodial leads warranting further optimization.

Keywords: *Salacia debilis*; antiplasmodial activity; friedelin; *Plasmodium falciparum*; natural products

Integrating LC-MS Metabolomics with Antioxidant and Anti-Inflammatory Activity to Unveil the Therapeutic Potential of Banana and Pineapple Peel Extracts

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Keywords: LC-MS, banana peel, pineapple peel, DPPH, antioxidant, anti-inflammatory, phenolic compounds, valorization, apigenin-C-diglucoside.

Abstract

Background: The disposal of fruit peels from banana (*Musa acuminata*) and pineapple (*Ananas comosus*) represents a significant environmental burden despite these by-products being rich repositories of bioactive phenolic compounds.

Objective: This study aimed to characterize the phytochemical profiles of banana and pineapple peel extracts using LC-MS, correlate their HPLC-UV chromatographic fingerprints with mass spectrometric data, and evaluate their *in-vitro* antioxidant and anti-inflammatory activities.

Methods: Peel samples were subjected to methanolic extraction followed by LC-MS analysis in both positive and negative ionization modes. Chromatographic separation was achieved with UV detection across 210-400 nm. Antioxidant activity was assessed *via* DPPH radical scavenging assay, while anti-inflammatory potential was evaluated through bovine serum albumin (BSA) denaturation inhibition assay. IC₅₀ values were calculated by non-linear regression analysis.

Results: LC-MS analysis revealed distinct bioactive profiles from both extracts. Banana peel exhibited predominant peaks at *m/z* 285.385, 281.985, and 284.802 [M+H]⁺, corresponding to flavonoid glycosides and phenolic acids. Pineapple peel demonstrated characteristic ions at *m/z* 179.223, 415.239, and 825.922 in negative mode, indicative of gallic acid derivatives and flavonoid-C-glycosides. UV spectrophotometry showed maximum absorbance at 248.5 nm for major peaks in both extracts. Pineapple peel extract demonstrated superior DPPH scavenging activity (IC₅₀ = 62.7 ± 1.9 µg/mL) compared to banana peel extract (IC₅₀ = 95.8 ± 2.1 µg/mL). Both extracts exhibited potent anti-inflammatory activity with IC₅₀ values of 35.2 ± 1.2 µg/mL and 38.5 ± 1.4 µg/mL for banana and pineapple peels, respectively.

Conclusion: Banana and pineapple peels represent valuable sources of natural antioxidants and anti-inflammatory agents. Pineapple peel shows superior radical scavenging capacity, while both peels demonstrate comparable protein denaturation inhibition. LC-MS fingerprinting provides a reliable method for quality control of these bioactive extracts.

Comparative Synthesis and Characterization of Coconut-Shell Activated Carbon Using H_3PO_4 , NaOH , and CaCl_2

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This study investigated the production and characterization of activated carbon from coconut shell (CoS) waste using phosphoric acid (H_3PO_4), sodium hydroxide (NaOH), and calcium chloride (CaCl_2) as chemical activating agents. Process parameters were optimized, including carbonization temperature (400–700 °C), carbonization time (1.0–2.5 h), and impregnation ratio (IR) (0.6–1.2), based on recovered carbon yield. The highest recovered masses were obtained at 400 °C, 1 h, and an IR of 1.2, producing 22.9 g and 17.3 g for CoS- H_3PO_4 and CoS- NaOH , respectively. Increasing temperature and carbonization time generally reduced yield, whereas increasing IR improved mass recovery under the investigated conditions. Characterization showed that CoS-AC (H_3PO_4) achieved the highest iodine value (743.02 mg/g), while CoS-AC (CaCl_2) exhibited the highest measured apparent pore volume (0.65 mL/g). CoS-AC (NaOH) recorded the highest carbon content (57.78%), together with moisture content of 3.40% and volatile matter of 30.82%. SEM revealed marked changes in surface morphology after activation, while FTIR and TGA indicated changes in functional groups and thermal behaviour. Activating agent selection influenced the measured physicochemical properties of the carbons. Overall, the findings demonstrate the potential of coconut-shell waste as a feedstock for producing activated carbon with varied physicochemical properties for potential environmental and industrial applications.

Keywords: Activated carbon; Coconut Shell; Chemical activation agents; Surface characterization; Sustainable Materials

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Toxicological Profile and Isolation of Compounds from *Rhodognaphalon brevicuspe*

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Medicinal plants have long served as sources of therapeutic agents for various human ailments. However, their complex chemical compositions may also present toxic effects, underscoring the need for scientific evaluation to ensure safety. *Rhodognaphalon brevicuspe*, traditionally used in the treatment of arthritis and certain venereal diseases, has not been scientifically assessed for its toxicity. This study evaluated the acute oral toxicity of the crude ethanolic extract of *R. brevicuspe*. Plant material was extracted with ethanol, and column chromatography combined with repeated recrystallization yielded four isolates: RB01, RB02, RB03 and RB04. Acute oral toxicity testing of the crude extract was performed in rats according to OECD guideline 423. Over a 14-day observation period, no mortality or significant signs of toxicity were recorded. Clinical biochemistry of blood samples after 14 days of treatment with extract showed no significant differences between control and extract treatment groups for liver and kidney biomarkers. The extract's approximate median lethal dose (LD₅₀) was > 2000mg/kg. These findings suggest that the crude extract of *R. brevicuspe* is relatively safe under the conditions tested, supporting its continued investigation as a potential source of therapeutic agents.

Keywords: *Rhodognaphalon brevicuspe*, acute oral toxicity, median lethal dose (LD₅₀)

Isolation of bioactive compounds from *Ageratum conyzoides* for antidiabetic activity

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Keywords: *Ageratum conyzoides*, α -Amylase, Antidiabetic, Phytochemical screening, Extraction.

Diabetes mellitus presents a major global health challenge, driving the need for accessible therapeutic alternatives. This study investigated the *in vitro* antidiabetic potential and phytochemical profile of *Ageratum conyzoides* L. (Asteraceae), a plant traditionally used in Ghana for managing hyperglycemia. Cold maceration of 5 kg of plant material yielded 121.5 g of crude extract, which was partitioned into petroleum ether, ethyl acetate, ethanol, and aqueous fractions. Phytochemical screening confirmed the presence of tannins, alkaloids, triterpenoids, flavonoids, phenolics, and glycosides in both raw and crude extract forms. In α -amylase inhibition assays (0.0625–2 mg/mL), the ethyl acetate fraction demonstrated the highest potency among the tested plant samples ($IC_{50} = 0.3645$ mg/mL), outperforming the crude extract ($IC_{50} = 0.5573$ mg/mL) and petroleum ether fraction ($IC_{50} = 0.768$ mg/mL). These results support the ethnomedicinal use of *A. conyzoides* and highlight the ethyl acetate fraction as a candidate for downstream isolation and structural elucidation of bioactive antidiabetic compounds.

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Screening and preliminary characterisation of amylase and cellulase producing microorganisms associated with decomposing mango-processing waste

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Mango-waste residues contain a heterogeneous matrix of polysaccharides and other biopolymers that require multiple glycosidases for efficient degradation. Microorganisms capable of producing cellulases and amylases therefore represent promising candidates for agro-waste bioprocessing. This study aimed to isolate and screen microorganisms from decomposing mango waste for amylase and cellulase production. Bacterial and fungal isolates were obtained from mango-waste samples and screened for enzyme activity using standard plate and submerged fermentation methods. Selected isolates exhibited amylolytic, cellulolytic or dual enzyme activities. Based on enzyme activity, *Bacillus subtilis* and *B. amyloliquefaciens* were identified as promising amylase producers, while *B. licheniformis* exhibited both cellulolytic and amylolytic activity. *Aspergillus foetidus* and *A. tubingensis* were identified as effective cellulase-producing isolates. Medium formulation, particularly carbon and nitrogen sources, influenced glycosidase production, while temperature and pH affected enzyme activity. Maximum amylase activity for *B. subtilis* and *B. amyloliquefaciens* was obtained at 40 °C and pH 7.0, while *B. licheniformis* showed cellulase activity at relatively higher temperatures. The *Aspergillus* isolates achieved optimal cellulase activity at 50°C and pH 5.0. These findings demonstrate the potential of mango-waste associated microorganisms as sources of hydrolytic enzymes and provide a basis for subsequent process optimization and application in fruit-waste bioconversion.

Keywords: Mango waste; glycosidases; cellulase; amylase; microbial screening

Valorization of Post-Consumer PET Textile Waste: Chemical Recycling and matter® Technology Transfer

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Rapid population growth globally, coupled with improvements in living standards and fast fashion have collectively set up substantial increase in textile production and consumption. Consequently, textile solid waste has emerged as a challenge for waste management authorities across both developed and developing nations. Plastic wastes impose substantial environmental, economic and public health burden on both local and central governmental bodies in developing nations. In Ghana and throughout Sub-Saharan Africa, although marginal advances have been made in the recycling of plastic materials utilized in water and beverage packaging, the area of textile waste recycling remains comparatively underdeveloped. The present study seeks to address this critical gap through the application of chemical recycling approaches for the valorization of polyethylene terephthalate (PET) textile waste, alongside the technology transfer of the matter® depolymerization process from Germany to Ghana, positioning the country as a pioneer in textile waste recycling within the region.

Keywords: Valorization, PET, Decolorization, Recycling

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Sustainable Dye Removal using Plantain Peel Starch-Crosslinked Chitosan/Rice Husk Composite: Characterization, Kinetics, and Isotherms

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A biodegradable, low-cost composite was developed from plantain peel starch, chitosan, and rice husk agro-waste for dye removal. The composite was characterized by FTIR, XRD, Zeta potential, Raman, and SEM. FTIR and Raman confirmed the hydroxyl, amine, and Si-O-Si groups. XRD revealed a semi-crystalline and amorphous structure. Zeta potential was positive (~ 7.8 mV), favoring anionic dye adsorption. Maximum removal (99.6%) occurred near pH of 7. Increased dosage raised adsorption efficiency. Equilibrium was reached within 150-180min. adsorption followed pseudo second order kinetics ($R^2=1.0$; $q_e=24.99$ mg/g) indicating chemisorption. Freundlich ($R^2=0.9919$; $n=1.53$) and Temkin ($R^2= 0.9860$) isotherms best described the data. Van't Hoff analysis gave $\Delta H^\circ = -62.75$ kJ/mol, $\Delta S^\circ = -165.20$ J/molK, and ΔG° values ranging from -13.52 to -8.56 kJ/mol, confirming a spontaneous and exothermic adsorption. The composite retained high efficiency after four regeneration cycles, losing only 1.4%. This sustainable agro-waste adsorbent is promising for dye contaminated wastewater treatment.

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Evaluation of Human Health Risk Associated with Heavy Metals in Drinking Water Contaminated by Illegal Mining Activities in Tetrem Bontefufuor, Amansie West District, Ashanti Region, Ghana

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Water is essential to life, and its quality determines suitability for human use. Heavy metals, even at low concentrations, can be toxic and enter the environment through various pathways. This study investigated heavy metal contamination and the effects of physicochemical parameters on drinking water quality in a small-scale illegal mining (galamsey) village. Two water samples were collected from a river (upstream and downstream) and three samples from boreholes. The samples were preserved in an ice chest to maintain temperature. Physicochemical parameters were determined in the laboratory and compared with WHO guidelines for drinking water. The samples were digested with 1 M nitric acid, with distilled water used as a blank. Concentrations of heavy metals specifically lead (Pb), arsenic (As), cadmium (Cd), copper (Cu), and iron (Fe) were measured using atomic absorption spectroscopy (AAS). Results showed that surface water recorded the highest copper concentration, while arsenic was the lowest relative to groundwater sources. Despite lower concentrations, heavy metals remain toxic and pose significant health risks due to their persistence and potential for bioaccumulation. The hazard index for non-carcinogenic health risk was higher in children than in adults. Based on the water quality index computed from physicochemical parameters, groundwater sources (G.1, G.2, and G.3) were the most suitable for consumption compared to surface water sources (S.1 and S.2). This study underscores the importance of monitoring and regulating water quality in areas affected by illegal mining to protect public health.

KEYWORDS: Water pollution, illegal mining, heavy metals, physicochemical parameters, health risk assessment

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Green chemistry for climate resilience, environmental sustainability and human health.

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Lead (Pb(II)) contamination of water is a persistent environmental and public health concern due to its toxicity, persistence, and bioaccumulation. Sustainable and environmentally benign approaches to heavy-metal pollution are therefore essential for protecting water resources, promoting human health, and strengthening climate resilience. This study investigates a computational-experimental approach for identifying and validating DNA aptamers capable of selectively recognizing Pb(II) in aqueous environments. The study aims to identify Pb(II)-binding aptamers from a fully randomized single-stranded DNA library and determine whether Pb(II) recognition is associated with thymine-thymine (T–T) mismatch motifs or alternative sequence and structural motifs. Computational screening will employ Python/Bio-Python, mFold, 3DNA, Oligo-Analyzer, molecular docking, and molecular dynamics simulations using GROMACS, AMBER, and VMD to evaluate candidate sequences, Pb(II)–DNA interactions, binding stability, and structural behavior. BLASTn will assess sequence similarity and conserved motifs. Selected aptamers will be experimentally validated using UV–Visible spectrophotometry, fluorescence assays, and agarose gel electrophoresis. The study is expected to identify stable and selective Pb(II)-binding aptamers and elucidate their molecular recognition mechanisms. By integrating computational screening with experimental validation, the research supports green chemistry through reduced resource-intensive screening and advances sustainable, low-cost approaches for Pb(II) monitoring, safer water management, and human health protection.

Keywords: DNA aptamer; computational screening; molecular dynamics; water contamination; heavy-metal detection.

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Solvothermal synthesis of silver sulfide nanomaterials in castor oil using single source precursor

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Silver sulfide (Ag₂S) nanoparticles have attracted considerable interest due to their direct band gap, photostability, and potential applications in photovoltaics, infrared detectors, and biomedical imaging. However, conventional synthesis methods often involve toxic solvents and complex procedures. This study investigated the green solvothermal synthesis of Ag₂S nanoparticles using silver ethyl xanthate and silver diethyldithiocarbamate as single-source precursors and castor oil as a renewable solvent. The precursors were synthesized and characterized using FTIR, melting point, TGA-DTA, and DSC analyses. The synthesized Ag₂S nanoparticles were characterized using XRD, SEM, and UV-Vis spectroscopy. TGA-DTA

showed that both precursors underwent single-step decomposition. XRD analysis revealed average crystallite sizes of 14.57 nm and 19.50 nm for nanoparticles derived from silver ethyl xanthate and silver diethyldithiocarbamate, respectively. The precursor type influenced the structural properties, with the former producing smaller cubic particles and the latter larger monoclinic particles. The study demonstrates the potential of castor oil as a renewable, biodegradable, and non-toxic solvent for cleaner Ag₂S nanoparticle synthesis.

Keywords: Silver sulfide nanoparticles, green synthesis, Solvothermal synthesis, Single source precursor, Nanomaterials

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Migration of Per- and Polyfluoroalkyl Substances from Food-Contact Materials and Non-Stick Cookware: Chemistry, Analytical Limits, and Research Priorities for Ghana

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Per- and polyfluoroalkyl substances (PFAS) are persistent, bioaccumulative, and linked to immune, hepatic and developmental effects. Diet is the dominant exposure route. They are used in grease-resistant paper packaging and non-stick cookware, creating a dietary exposure pathway distinct from environmental contamination of raw commodities. This review synthesizes evidence on where PFAS occur in food-contact materials, how they migrate into food, and how well current methods can trace that migration. PFAS have been found in paper, board, plastic and non-stick cookware, though levels vary widely by product. Migration depends on temperature, contact duration, food-matrix composition, recycled material and worn-out surfaces. It proceeds through three concurrent mechanisms: chemicals moving out of the material, precursor compounds breaking down into stable acids, and flakes shedding from damaged coatings. Targeted LC-MS/MS remains the dominant technique but accounts for only a small fraction of extractable organic fluorine. Therefore, non-detection on a targeted panel cannot establish absence. Broader screening is needed. Evidence on cookware is sparse, and data from Ghanaian migration studies are limited. Yet local practices of repeated frying in vegetable oil, fish smoking and long hot-holding in grease-proof wrappers remain untested. Migration trials under Ghanaian conditions are a priority to determine their occurrence and distribution.

Keywords: PFAS; food-contact materials; migration; organic fluorine; Ghana

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Strain-Engineered Type II SiC/Al₂OS van der Waals Heterostructure with Efficient Charge Separation for Photocatalytic Water Splitting

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The search for efficient semiconductor photocatalysts has become increasingly important in efforts to address both energy demand and environmental concerns. In this study, a SiC/Al₂OS van der Waals heterostructure (vdWH) was proposed and examined its geometric and electronic properties, in addition to its suitability for photocatalytic water splitting. The results suggest that SiC/Al₂OS vdWH remains stable from thermodynamic, mechanical and thermal perspectives. The calculated electronic structure reveals a type II band alignment with a band gap energy of 1.91 eV. This configuration supports efficient separation of charge carriers. In addition, the internal electric field helps suppress recombination of charge carriers, which can enhance the overall photocatalytic performance. The SiC/Al₂OS vdWH shows strong red shift absorption compared with the monolayer. The band edge positions of SiC/Al₂OS vdWH are well aligned for overall water splitting, allowing both hydrogen and oxygen evolution reactions across a pH range from 0 to 6. As the applied strain increases, the band gap energy decreases in a nearly linear manner and eventually closes when the strain reaches –8%. Importantly, photocatalytic activity is preserved within the strain range from –2% to +8%, since the band edge positions continue to satisfy the required oxidation and reduction potentials. Overall, this study offers understanding into the water splitting capability of SiC/Al₂OS vdWH and highlights practical strategies for enhancing oxygen and hydrogen evolution reactions in photocatalytic systems.

Keyword: Strain, 2D van der Waals heterostructures, photocatalytic water splitting, type II band alignment, Density Functional Theory

Synthesis and anti-inflammatory evaluation of tertiary alcohols derived from mannich bases

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Keywords: Mannich bases; Tertiary alcohols; Grignard reaction; Anti-inflammatory activity; Cyclohexanone.

Although non-steroidal anti-inflammatory drugs (NSAIDs) have the capacity to control pain and inflammation, they can cause adverse side effects such as gastrointestinal bleeding (Tawfik et al., 2026). This constraint makes it necessary to explore new compounds that could have anti-inflammatory actions. Derivatives of Mannich bases are structurally diverse and biologically active; therefore, they constitute good candidates for research. The purpose of the present study was to synthesize Mannich bases and their tertiary alcohol derivatives, characterize the synthesized products through FT-IR spectroscopy, follow the course of the reactions using TLC, and evaluate their anti-inflammatory actions. The Mannich bases, 2-((N, N-dimethylamino)methyl)cyclohexanone and 2-((N, N-diethylamino)methyl)cyclohexanone were synthesized through the Mannich reaction followed by synthesis of tertiary alcohols via the Grignard reaction. The anti-inflammatory actions of tertiary alcohols were assessed by using the egg albumin denaturation test. The synthesized tertiary alcohols showed different inhibitions on the egg albumin denaturation. This study demonstrated the potential of synthesized tertiary alcohols to be anti-inflammatory agents.

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Waste-Derived γ -Boehmite for Adsorptive Fluoride Removal: A Sustainable Approach to Water Treatment

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Groundwater fluoride contamination is a significant public health concern in several regions of Ghana, particularly the Upper East and Northern regions. Chronic exposure to elevated fluoride levels can cause dental and skeletal fluorosis. This study investigated γ -boehmite synthesized from post-consumer aluminum cans as a sustainable and low-cost adsorbent for fluoride removal from water. The γ -boehmite was characterized using powder X-ray diffraction, Fourier-transform infrared spectroscopy, zeta potential analysis, and point of zero charge determination. Batch adsorption experiments were performed at $\text{pH } 5.5 \pm 0.3$. The effects of initial fluoride concentration, adsorbent dosage, and contact time were assessed. An adsorbent dosage of 1.0 g/L and a contact time of 2 h were used as baseline conditions. The γ -boehmite achieved a maximum fluoride removal efficiency of 88.2%, and an adsorption capacity of 5.50 mg/g. Nonlinear isotherm analysis showed that the Langmuir model best described the equilibrium data, suggesting adsorption onto relatively homogeneous surface sites. The kinetic data were best fitted by the pseudo-second-order model, indicating a dominant contribution from surface interactions during fluoride uptake. Overall, the waste-derived γ -boehmite showed strong potential for fluoride removal while supporting the conversion of aluminum waste into a useful water-treatment material.

Keywords: Aluminum waste valorization; spectrophotometric color-quenching; Surface Chemistry.

Poor Quality Nifedipine Extended-Release Tablets in Accra, Ghana

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Keywords: Nifedipine; Extended-release tablets; Pharmaceutical quality; RP-HPLC; Post-market surveillance.

Background

Quality antihypertensive medicines are essential for blood pressure control. Nifedipine is a first-line antihypertensive in Ghana. Its demand and proliferation of generic products increase the risk of substandard medicines. Limited post-market surveillance data exist on nifedipine ER tablets in Ghana. This study evaluated quality of nifedipine ER tablets marketed in Accra.

Methods

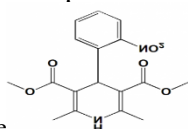
Fifteen brands of nifedipine ER tablets (20 mg and 30 mg) were purchased from pharmacies and distributors in Accra. Weight uniformity was assessed according to United States Pharmacopeia (USP) specifications. An RP-HPLC method using a C18 column, acetonitrile:0.05 M potassium phosphate buffer (60:40, v/v), and UV detection at 240 nm was used to assay nifedipine content.

Results

The method demonstrated linearity ($r^2 \geq 0.9925$), accuracy (99.31–102.05%), and precision (%RSD <2%). All brands complied with USP weight uniformity requirements. Nifedipine content ranged from 56.3% to 108.0% of the labelled claim. Using USP 2024 assay criteria (98.0–102.0%), 14 of 15 brands (93.3%) failed; 12 (80.0%) contained less than labelled claim, whilst two (13.3%) exceeded it. Only one brand (6.7%) met the USP specification.

Conclusion

The prevalence (93.3%) of poor-quality nifedipine ER tablets highlights the need for strengthened post-market surveillance and stricter regulatory enforcement to remove substandard products from Ghana.



Nifedipine

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CITRIC ACID FUNCTIONALIZED CALABASH SHELL BIOMASS AS A LOW-CARBON GREEN ADSORBENT FOR THE REMOVAL OF LEAD, MERCURY, TURBIDITY AND MICROBIAL LOAD FROM WATER

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Water contamination by heavy metals such as Lead (Pb) and Mercury (Hg), along with turbidity and microbial load from anthropogenic activities including illegal mining, remains a critical environmental and public health challenge in Ghana. Conventional treatment materials are expensive and associated with high carbon emissions.

This study presents a green chemistry approach for developing a low-cost, biodegradable biosorbent from calabash fruit shell waste (*Crescentia cujete*). Calabash shells were washed, sun-dried and milled into powder. The biomass was pretreated with 0.2M NaOH for delignification, dewaxing and hemicellulose removal to expose cellulose and reactive hydroxyl groups. The pretreated biomass was functionalized with 0.8M citric acid and thermally cured at 120°C to induce esterification, introducing free carboxyl (-COOH) groups to enhance chelation capacity.

The raw, pretreated and functionalized biomass will be characterized using FTIR for functional group confirmation, pH point of zero charge (pHpzc), Boehm titration for quantification of acidic groups, and SEM for surface morphology. Batch adsorption performance will be evaluated at pH 6.72 for Pb(II), Hg(II), turbidity and microbial load. Adsorption data will be fitted to isotherm and kinetic models.

This work exemplifies green chemistry and circular economy by valorizing local agro-waste using a food-grade reagent (citric acid) via a low-energy, water-based process. It provides a low-carbon, climate-resilient and locally adaptable solution that promotes environmental sustainability and safeguards human health from heavy metal toxicity.

P49

Development of a BTBAB-Catalysed Hybrid Glycolysis-Alkaline Hydrolysis Process for the Selective Recycling of Polycotton Textile Waste

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Polyester and cotton make up 75 % of the global fiber production. However, the blended (polycotton) waste of these materials is difficult to recycle due to the material heterogeneity, limiting the conventional mechanical recycling. Some existing chemical processes like glycolysis and alkaline hydrolysis can depolymerize PET and cotton cellulose simultaneously,

but often require long reaction times and severe conditions. In this work, we developed a BTBAB-catalysed hybrid glycolysis-alkaline hydrolysis process for selective polycotton recycling, where the phase transfer catalyst accelerates the transfer of hydroxide ions to the PET surface so that depolymerization can occur under milder conditions. Bench-scale experiments optimized reaction temperature and alkaline dosage, with and without catalyst. The optimized process was applied to two polycotton blends (85:15 and 50:50 polyester cotton), successfully recovering terephthalic acid and intact cotton fibers. SEM confirmed distinct fiber morphologies smooth cylindrical polyester versus flat, twisted cotton ribbons validating effective component separation. Results demonstrate that BTBAB-catalysed hybrid processing offers a promising, catalyst-assisted route for closed-loop recycling of heterogeneous textile blends, overcoming key limitations of current recycling strategies. NMR, TGA, FTIR confirmed product purity and structural integrity.

P50

Quality Assessment of Amlodipine Immediate Release and Nifedipine Extended-Release Tablets in Accra, a RP-HPLC Method

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Background: Amlodipine and nifedipine are dihydropyridine calcium channel blockers used to manage hypertension and angina. Reports of variability in marketed medicine quality necessitate regular evaluation. This study assessed the quality of amlodipine immediate-release and nifedipine extended-release tablets available in Accra.

Objective: To assess the quality of different brands based on weight uniformity, disintegration, dissolution, and active pharmaceutical ingredient content.

Methods: Ten brands of amlodipine and five brands of nifedipine extended-release tablets were obtained from pharmacies across Accra. Samples were evaluated for weight uniformity, disintegration, and dissolution. Drug content was quantified using a validated reverse-phase high-performance liquid chromatography method.

Results: Nine of 15 samples (60%), comprising seven amlodipine and two nifedipine brands, complied with the British Pharmacopoeia assay specification of 95–105% of the labelled amount. Six samples (40%) failed; two exceeded and four fell below their label claims. All samples complied with weight uniformity requirements. Ten samples (66.7%) passed dissolution testing, while five (33.3%) failed.

Conclusion: Variability was observed in assay and dissolution performance among amlodipine and nifedipine tablets, although all products complied with weight uniformity requirements. Strengthened regulatory oversight, GMP compliance, and routine post-market surveillance are recommended to ensure consistent medicine quality and protect patients from substandard or inconsistent medicines.

**SYNTHESIS, ANTHELMINTIC AND ANTI-INFLAMMATORY
ACTIVITIES OF 2-((N, N) DIMETHYLAMINO) METHYL
CYCLOHEXANONE (MANNICH BASE) AND ITS DERIVATIVES**

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Keyword: Mannich base, anthelmintics, anti-inflammatory, derivatives, and Mannich reaction

Drug resistance continues to threaten the effectiveness of modern therapeutics, often arising from the overuse of drugs and incomplete treatment regimens. These resistance mechanisms alter drug targets and reduce drug target interactions, emphasizing the need for novel bioactive agents. Mannich bases, synthesized via the Mannich reaction, are known for their broad pharmacological properties, including anti-inflammatory, anticancer, antibacterial, and antiviral activities. In this study, Mannich base amides, cyclohexylamines, cyclohexylamides, and Mannich base amines were synthesized, characterized using FT-IR and evaluated for their anti-inflammatory and anthelmintic properties. The compounds demonstrated measurable anti-inflammatory activity, though not superior to standard drugs such as diclofenac and aspirin. Notably, all synthesized compounds demonstrated potent anthelmintic activity, exceeding the efficacy of the reference drugs levamisole and albendazole. These findings highlight the potential of Mannich base derivatives as promising candidates for developing new anthelmintic therapies.

Quality Assessment Of Different Brands Of Atorvastatin Tablets In Accra by RP-HPLC

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Keywords: Atorvastatin, reverse-phase liquid chromatography, validated, quality.

Background: Atorvastatin is a widely prescribed lipid-lowering medicine whose therapeutic effectiveness depends on the quality and amount of its active pharmaceutical ingredient. This study assessed the quality of different brands of atorvastatin tablets marketed in Accra.

Methodology: A reverse-phase high-performance liquid chromatography (RP-HPLC) method was developed and validated according to International Council for Harmonisation (ICH) guidelines. Validation assessed linearity, precision, accuracy, robustness, limit of detection (LOD), and limit of quantification (LOQ). The validated method was used to assay ten commercial brands. Weight uniformity and dissolution tests were also performed according to British Pharmacopoeia (BP) specifications.

Results: The method showed excellent linearity ($R^2 = 0.998$), high precision ($\%RSD \leq 0.40\%$), acceptable accuracy (98.3–102% recovery), and good robustness ($\%RSD < 2\%$). The LOD and LOQ were 0.001346% w/v and 0.004079% w/v, respectively. Six of the ten brands complied with BP content specifications, while four failed. All brands passed the weight uniformity test, and nine met the dissolution requirement of releasing at least 80% of the drug within 30 minutes.

Conclusion: The validated RP-HPLC method was suitable for routine quality assessment. The findings highlight the need for continuous post-market surveillance, adherence to Good Manufacturing Practices, and strengthened regulatory oversight to ensure medicine quality and patient safety.

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Quality Assessment of Metformin Tablets in Accra, Ghana

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Keywords: Metformin; Immediate-release tablets; Accra; RP-HPLC; .

Background: Metformin, an anti-diabetic agent, is the first-line therapy for type 2 diabetes due to its efficacy and safety. Ensuring that the quality of marketed metformin tablets are consistent is critical, as substandard formulations can cause detrimental therapeutic outcomes. Post-marketing quality assessment using pharmacopeial standards and validated analytical methods is therefore essential to protect the health of patients.

Methods: Ten brands of immediate-release metformin tablets marketed in Accra, were randomly sampled from registered pharmacies. Tablets were subjected to pharmacopeial quality control tests including uniformity of weight, disintegration, and assay of active pharmaceutical ingredient (API) content using a validated reverse phase high-performance liquid chromatography (RP-HPLC) method. Diazepam served as the internal standard, with detection at 220 nm. The RP-HPLC method was validated according to ICH guidelines for linearity, precision, accuracy, robustness, specificity, and sensitivity.

Results: The RP-HPLC method demonstrated excellent linearity ($r^2 = 0.9997$), precision (%RSD < 2%), and recovery within 98–102%, confirming its reliability. All ten brands complied with pharmacopeial requirements for API content (95–105% of label claim) and disintegration times. Nine brands passed the uniformity of weight test, while one brand (MB) failed, showing deviations beyond the $\pm 5\%$ British Pharmacopoeia limit.

Conclusion: Most metformin tablets marketed in Accra meet established pharmacopeial quality standards, reflecting satisfactory manufacturing practices. However, the failure of one brand in the uniformity of weight test highlights the need for continuous surveillance to ensure consistency. Continuous quality monitoring is important to maintain patient confidence in anti-diabetic therapy.

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Antibiotic Modulation by Plant Alkaloids: Experimental Evidence for Dose-Sparing and Enhanced Bactericidal Activity.

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Antimicrobial resistance (AMR) causes approximately 1.27 million deaths annually and may reach 10 million deaths per year by 2050 without effective intervention. This urgency has refocused attention on bioactive natural products, not only as alternative antimicrobials but also as antibiotic adjuvants capable of restoring or enhancing the efficacy of existing drugs whose clinical usefulness is declining. This study examined total alkaloid extracts from *Zanthoxylum zanthoxyloides* (ZZ-TA, 1.40% w/w) and *Ocimum gratissimum* (OG-TA, 1.18% w/w) against Gram-positive and Gram-negative pathogens. Both extracts showed strain dependent bacteriostatic effects, with stronger suppression of Gram-positive strains in time kill assays. Checkerboard testing showed OG-TA enhanced tetracycline activity against *Salmonella poona*, yielding additive interactions at 1MIC:1MIC (125 µg/mL OG-TA:15.6 µg/mL tetracycline, FIC=2) and 2MIC:½MIC (250 µg/mL OG-TA:7.8 µg/mL tetracycline, FIC=2.5), indicating dose-sparing potential. Time-kill assays confirmed these combinations were bactericidal, outperforming individual agents by 5–9.5-fold and matching ciprofloxacin's suppression over 24 hours. LC-MS (ESI+) analysis identified key bioactive alkaloids, including Zanthoamide I, Nor-chelerythrine, 8-acetonyldihydrochelerythrine, Skimmianine, and Benzimidazol-5-amine, providing a chemical rationale for the observed antibacterial effects. Collectively, these findings demonstrate that plant-derived alkaloid extracts, even at low abundance, are potent antibacterial agents and can serve as effective modulators of conventional antibiotics, supporting strategies aimed at reducing antibiotic doses while maintaining or enhancing therapeutic efficacy, a promising approach in addressing antimicrobial resistance.

Keywords: Antimicrobial resistance, Antibiotic modulation, *Zanthoxylum zanthoxyloides*, *Ocimum gratissimum*, Alkaloidal extract

Assessing Machine learning models for predicting CO₂ binding energies on transition-metal-doped Iron surfaces for high-throughput screening of CO₂RR catalysts.

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Keywords: CO₂ Reduction, Electrocatalysis, Machine Learning,

The electrochemical reduction of carbon dioxide (CO₂RR) is a way of converting CO₂ into value-added chemicals and fuels, reducing atmospheric emissions of CO₂. Reported spontaneous CO₂ activation (a critical first step in CO₂RR) on Iron surfaces makes it a promising catalyst for CO₂RR. However, observed extremely strong CO₂ binding leads to catalyst surface poisoning and renders the catalyst ineffective. Surface modification through doping aids in tuning the adsorption properties of catalysts and identifying improved catalyst candidates. However, exploring the vast compositional space of doped iron surfaces using experiments or density functional theory (DFT) is computationally expensive and time-consuming. In this work, we investigate the potential of machine learning (ML) models for predicting CO₂ adsorption energies on transition-metal-doped iron surfaces using DFT-generated data. Various regression algorithms were developed and evaluated using standard statistical metrics, including the coefficient of determination (R²) and root mean square error (RMSE). Among the models examined, the best-performing models achieved R² values above 0.8 (80% accuracy), demonstrating excellent agreement with DFT-calculated adsorption energies. While no high-throughput screening of catalyst candidates was conducted in this study, the strong predictive accuracy obtained highlights the capability of ML approaches to predict CO₂ adsorption energies at near-DFT accuracy at a fraction of the computational cost.

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Tunable Sulphur-doped Graphitic Carbon Nitride (S-g-C₃N₄) for the Photocatalytic Degradation of Chlorpyrifos in Water.

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Pesticide contamination of water resources poses significant environmental and public-health concerns, particularly for persistent organophosphorus compounds such as chlorpyrifos. This study focuses on developing tunable sulphur-doped graphitic carbon nitride (S-g-C₃N₄) as a visible-light-responsive photocatalyst for chlorpyrifos degradation. S-g-C₃N₄ materials will be synthesized through controlled sulphur incorporation and hydrothermal–thermal polymerisation, with sulphur loading tailored to modify structural, optical, surface, and charge-carrier properties. The photocatalysts will be comprehensively characterized and evaluated for chlorpyrifos degradation under visible-light irradiation. The influence of sulphur loading and key operational parameters will be established using kinetic analysis. The study aims to elucidate structure–property–activity relationships and advance efficient photocatalytic treatment of pesticide-contaminated water.

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Engineering Magnetic Biochar–Alginate Composites for Enhanced Ciprofloxacin Adsorption: Synthesis, Characterization and Adsorption Mechanisms.

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The persistence of antibiotic residues in aquatic environments presents growing ecological and public-health concerns, particularly because of their potential contribution to antimicrobial resistance. This study developed and evaluated magnetic biochar–alginate composites with varying iron-oxide contents for the removal of ciprofloxacin from aqueous media, alongside raw and magnetic biochar as comparative adsorbents. The materials were characterized using Fourier-Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Dynamic Light Scattering (DLS), and X-ray diffraction (XRD) to elucidate their surface chemistry, morphology, particle characteristics, and crystallinity. Batch adsorption experiments were conducted over 6 h to assess ciprofloxacin removal and adsorption kinetics. Marked differences in adsorption performance were observed among the three adsorbent classes, with magnetic biochar exhibiting rapid equilibration and superior ciprofloxacin uptake. Consequently, magnetic biochar composites were further evaluated under varying operational conditions. Kinetic and diffusion analyses indicated a multistep adsorption mechanism involving external mass transfer followed by intraparticle diffusion. Iron-oxide incorporation enhanced magnetic responsiveness and facilitated adsorbent recovery, while alginate

functionalization increased the availability of adsorption-active sites. The composites also maintained appreciable adsorption performance across successive regeneration cycles. Overall, the findings demonstrate the potential of magnetic biochar–alginate materials as recoverable adsorbents for ciprofloxacin-contaminated water and provide a promising platform for application in pharmaceutical- and hospital-effluent treatment.

P58

Ecotoxicological Evaluation of Microplastics in Sediment, Water and Fish in the Owabi River Basin, Ashanti.

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Microplastic pollution is an emerging environmental concern due to its persistence, widespread occurrence and potential adverse effects on aquatic and terrestrial ecosystems, as well as potential risks to human health. This study investigated the occurrence, distribution, physicochemical characteristics, and ecotoxicological risks of microplastics in surface water, sediments, and fish from the Owabi River Basin, Ashanti Region, Ghana. Samples collected across multiple sites were analysed using stereomicroscope, Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscopy-Energy Dispersive X-ray Spectroscopy (SEM-EDX). Ecological risks were evaluated using contamination factors, polymer hazard indices, and ecological risk models. Microplastic abundance differed between sampling periods, with strong positive correlations between June and November concentrations in surface water ($r = 0.815$, $p = 0.001$) and sediments ($r = 0.983$, $p < 0.001$). Mean concentrations in June were 31.818 ± 11.400 MPs/L in water, 215.555 ± 96.839 MPs/kg in sediments, and 5 ± 2.366 MPs/fish, compared with 16 ± 6.030 MPs/L, 173.33 ± 90.554 MPs/kg, and 4 ± 1.095 MPs/fish, respectively, in November. Fibres and foams predominated, while polypropylene and polyethylene terephthalate were the major polymers. SEM revealed weathered surfaces with cracks and pits, whereas EDX showed declining carbon and increasing oxygen contents, indicating oxidative degradation, together with adsorbed zinc, barium, and titanium. Ecological risk assessment revealed low to high risk levels depending on site characteristics and polymer composition. These findings demonstrate widespread microplastic pollution across in the Owabi River Basin and to mitigate these impacts, the study recommends enhanced monitoring programs, improved waste and management strategies.

Mapping Documented Traditional and Indigenous Agro-Ecological Knowledge in Ghana: Evidence and Opportunities for AI-Enabled Climate Services

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Traditional and indigenous agro-ecological knowledge (TAEK) provides locally grounded information for agricultural decision-making and climate adaptation. However, this knowledge remains scattered across different sources, limiting its potential integration into digital and artificial intelligence-driven climate services. This systematic review mapped documented TAEK practices in Ghana, examined their geographical distribution and identified knowledge gaps. Following searches and screening conducted in accordance with PRISMA guidelines, 43 studies met the inclusion criteria. The studies documented practices relating to climate forecasting, soil fertility, crop management, pest and disease control, water management, biodiversity and livestock production. Climate-forecasting practices included observing tree flowering, bird behaviour, cloud patterns and other environmental indicators. Farmers also used fallowing, organic manure, crop diversification and mixed cropping to support agricultural production. Research was concentrated mainly in the Guinea Savannah and Forest–Savannah Transition zones, with limited coverage of other agro-ecological zones. Pollination and ecosystem services, agroforestry, biodiversity and water management were also insufficiently studied. These findings provide an evidence base for identifying, digitising and validating locally relevant indicators that could be integrated with meteorological data using machine learning. Such integration could support more accessible and context-specific climate information services for smallholder farmers in Ghana. Keywords: Indigenous knowledge; Machine learning; Climate information services; Climate resilience; Ghana

Physicochemical Properties, Carbon Stability and Aromaticity of Corn Cob Biochar for Sustainable Construction Applications

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The conversion of agricultural residues into biochar has gained considerable attention as a sustainable strategy for waste valorization, carbon sequestration and the development of environmentally friendly construction materials. Among the numerous agricultural by-products generated worldwide, corn cob represents an abundant lignocellulosic biomass with significant potential for producing high-quality biochar through thermochemical conversion. This study evaluated the effect of pyrolysis temperature on the physicochemical properties, aromaticity, polarity and carbon stability of corn cob biochar produced at 500, 600 and 700°C.

The corn cob feedstock was first characterized and found to contain Neutral Detergent Fiber (66.75%), Acid Detergent Fiber (50.69%), cellulose (34.49%), hemicellulose (16.06%) and lignin (16.20%), confirming its suitability as a lignocellulosic precursor for biochar production. The produced biochar was analyzed for pH, electrical conductivity, elemental composition, moisture, ash, volatile matter, fixed carbon and atomic H/C and O/C ratios.

Increasing pyrolysis temperature from 500 to 700°C resulted in progressive carbon enrichment, with carbon concentration increasing from 68.32% to 78.23% and fixed carbon from 63.12% to 77.38%. Similarly, pH increased from 8.86 to 9.34, electrical conductivity from 1,398 to 1,820 $\mu\text{S cm}^{-1}$, and ash content from 3.78% to 5.83%. Conversely, hydrogen, oxygen, moisture and volatile matter contents declined with increasing temperature. FTIR analysis revealed a progressive reduction in distinctly resolved organic-associated absorption bands, consistent with the observed elemental transformations.

Among the investigated treatments, biochar produced at 700°C exhibited the highest carbon concentration and fixed carbon content. Nevertheless, determining overall carbon retention and long-term environmental persistence requires additional assessment of biochar yield, carbon recovery and direct stability measurements.

These findings provide baseline evidence of temperature-dependent transformations in corn cob-derived biochar and support further investigations into agricultural waste valorization and potential environmental and engineering applications.

Keywords: Corn cob biochar; Pyrolysis temperature; Aromaticity; Carbon stability; Agricultural waste valorization; Carbon sequestration; Sustainable construction

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BIOLOGICAL ACTIVITIES OF METHANOL STEM BARK EXTRACT OF *AGANOPE LEUCOBOTRYA*

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The stem bark of *Aganope leucobotrya* has traditionally been used in the management of diarrhoea, as a blood tonic, to promote bone healing, and to control nose bleeding. This study aimed to investigate the phytochemical constituents and determine the antimicrobial, anti-helminthic, and antioxidant activities of the methanolic extract of *Aganope leucobotrya* stem bark. Phytochemical constituents were identified using standard screening procedures. The antimicrobial activity of the extract was evaluated using the broth dilution method, while its antioxidant potential was assessed using the 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical-scavenging and hydrogen peroxide-scavenging assays. The anti-helminthic activity was investigated in vitro using *Eudrilus eugeniae* earthworms. Phytochemical screening revealed the presence of phenols, tannins, saponins, quinones, and polyphenolic compounds in the methanolic extract. The extract demonstrated notable antimicrobial activity, with a minimum inhibitory concentration (MIC) of 12.5 ± 0.01 mg/mL against *Streptococcus pyogenes* and *Candida albicans*. In the DPPH radical-scavenging assay, the half-maximal inhibitory concentration (IC₅₀) values for the methanolic extract and reference drug were 49.96 ± 0.10 µg/mL and 32.35 ± 0.05 µg/mL, respectively. At a concentration of 20 mg/mL, the methanolic extract produced paralysis and death of the earthworms at 15 and 36 minutes, respectively, whereas the corresponding times for mebendazole were 29 and 50 minutes. In the hydrogen

peroxide-scavenging assay, the extract exhibited an IC_{50} value of $185.63 \pm 0.152 \mu\text{g/mL}$, compared with $151.80 \pm 0.094 \mu\text{g/mL}$ for gallic acid. Overall, the findings indicate that the methanolic stem-bark extract of *Aganope leucobotrya* possesses appreciable antioxidant, antimicrobial, and anti-helminthic properties. These activities may be associated with the bioactive phytochemical constituents identified in the extract and provide scientific support for some of the plant's traditional medicinal applications.

Keywords: *Aganope leucobotrya*; anti-helminthic activity; antimicrobial activity; antioxidant activity; minimum inhibitory concentration (MIC); minimum bactericidal concentration (MBC).

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Cu/Al Layered Double Hydroxide for the Removal of Mercury from Water; an Adsorption Study

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Mercury (Hg) contamination in aquatic systems poses severe ecological and health risks, particularly in regions impacted by artisanal gold mining such as Ghana, where concentrations of $0.145\text{--}1.078 \mu\text{g/L}$ have been reported in the Ankobra basin. Conventional removal methods (coagulation, membrane filtration, electrochemical treatment) are often costly and ineffective at trace levels, making adsorption a more viable alternative. In this study, Cu/Al Layered Double Hydroxides (LDHs) were synthesized and evaluated as adsorbents for mercury removal from water. Characterisation confirmed successful LDH formation: XRD revealed strong basal reflections with a crystalline size of 16.7 nm , while FTIR spectra showed characteristic OH^- and CO_3^{2-} vibrations. Adsorption experiments demonstrated that removal efficiency increased from 49% at 20 mg dosage to 72% at 160 mg, with maximum uptake of 0.19 mg/g at 210 min before plateauing. Kinetic modelling yielded R^2 values of 0.971 (PFO) and 0.969 (PSO), indicating contributions from both physisorption and chemisorption. Isotherm analysis further supported dual interaction mechanisms, with Freundlich ($R^2 = 0.973$) and Langmuir ($R^2 = 0.978$) fits. The strong binding affinity of Cu/Al LDHs for Hg(II) is explained by Pearson's Hard-Soft Acid-Base principle, highlighting their potential as scalable, cost-effective adsorbents. Regeneration strategies such as thermal treatment and solidification, reported in recent literature, suggest pathways to enhance stability and reusability. Overall, Cu/Al LDHs present a promising solution for mercury remediation in contaminated waters, combining tuneable chemistry, high surface area, and environmental compatibility.

Keywords: Cu/Al layered double hydroxides; mercury removal; adsorption kinetics; isotherm models; water treatment

Catalytic transfer hydrogenation of furfural to furfuryl alcohol over ruthenium-based catalysts

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The increasing need for sustainable chemical feedstocks has prompted extensive research on the catalytic transformation of biomass-derived platform molecules as substitutes for petroleum-based resources. Furfural, produced through the acid-catalyzed dehydration of hemicellulose, is a versatile C5 intermediate that can undergo selective hydrogenation to form furfuryl alcohol, a key precursor used in resins, solvents, foundry binders, and fine chemicals.

In this study, two half-sandwich ruthenium(II) complexes containing a chelating 2-(diphenylphosphino)benzoate ($P^{\wedge}O$) ligand were synthesized and characterized using FT-IR and ^1H NMR spectroscopy. The monometallic complex C1, $[RuCl(\eta^6\text{-}p\text{-cymene})(\kappa^2\text{-}P,O\text{-}Ph_2PC_6H_4CO_2)]$, along with its bimetallic trichlorostannyl counterpart C2, $[Ru(SnCl_3)(\eta^6\text{-}p\text{-cymene})(\kappa^2\text{-}P,O\text{-}Ph_2PC_6H_4CO_2)]$, was investigated as a homogeneous catalyst for the selective transfer hydrogenation of furfural into furfuryl alcohol. Formic acid functioned as the hydrogen donor in the presence of triethylamine under mild conditions.

Catalyst C1 converted approximately 98% of the furfural to furfuryl alcohol, whereas C2 produced approximately 89% conversion under the same conditions. Formation of the desired product was verified by the emergence of the characteristic hydroxymethyl singlet at ~ 4.45 ppm in the ^1H NMR spectra of the crude reaction mixtures. The observed high chemoselectivity is ascribed to the electronic and steric characteristics of the mixed-donor $P^{\wedge}O$ ligand, which promotes effective hydride transfer to the aldehyde carbonyl while inhibiting over-reduction of the furan ring.

Overall, these findings establish that well-defined, readily accessible $P^{\wedge}O$ -chelated ruthenium(II) arene complexes are effective catalysts for the sustainable valorization of biomass-derived furfural.

Keywords: Furfural, Furfuryl alcohol, Ruthenium(II) complexes, Catalytic transfer hydrogenation, Biomass valorization, Mixed-donor ligands.