

ACADEMIC STAFF PROFILE

1.1 PERSONAL PROFILE

1.1.1 PERSONAL DETAILS

Name: LUCY W. KIRURI, PH.D., MRSC
DEPARTMENT: CHEMISTRY
DESIGNATION: SENIOR LECTURER
ADDRESS: KENYATTA UNIVERSITY
C/O DEPARTMENT OF CHEMISTRY
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 KU PROFILE

 LINKEDIN



Profile Summary: Accomplished educator and researcher with over 10 years of experience in physical, computational, and inorganic chemistry. Expert in molecular docking, molecular dynamics simulations, quantum chemical (DFT) methods, and AI/ML-driven drug discovery. Strong track record in publications, funding, postgraduate mentorship, and interdisciplinary collaborations in health, energy, and environment.

Area of Specialization: Computational Chemistry & Biophysics: molecular docking, MD, DFT, QSAR, and AI/ML approaches to drug discovery, nanomaterials, and natural product-based therapeutics.

Research Interests:

- AI/ML-based drug discovery for infectious diseases (TB, malaria)
- Molecular docking and molecular dynamics simulations
- Quantum chemical studies of nanoparticles, EPFRs and renewable energy (DSSCs)
- Nanomaterial–biomolecule interactions (encapsulations)

AT A GLANCE

 **Peer-reviewed Publications:** 25

 **Supervised MSc & PhD Students:** (7 completed, 3 ongoing)

 **Grants Secured:** 3 funded (KENET, ICTP)

 **Local & International Collaborations:** ICTP (Italy), NM-AIST (TZ), USIU-A (KE), UDSM (TZ)

 **Specialist Tools:** AI/ML, Gaussian16, Orca, GROMACS, Python, R, L^AT_EX

TEACHING HIGHLIGHTS

- **Courses Taught:** Quantum Chemistry, Coordination Chemistry, Photochemistry
- **Pedagogical Training:** AI in Teaching, Competency-Based Curriculum, Mentoring
- **Student Evaluations:** Consistently rated 85–98% satisfaction

1.1.2 ACADEMIC & PROFESSIONAL QUALIFICATIONS

Louisiana State University, Baton Rouge, LA

Ph.D., Department of Chemistry, August 2013

- Thesis Topic: *Experimental & Computational Studies of Environmentally Persistent Free Radicals (EPFRs) Formation*
- Advisor: Professor Barry H. Dellinger
- Area of Study: Physical & Computational Chemistry

Kenyatta University, Nairobi, KE

M.Sc., Department of Chemistry, July 2009

- Thesis Topic: *Prediction of Reaction Mechanisms & Absolute Rate Constant Using Computer Algorithm: The Bromate Ion in Acidic Media Reaction*
- Supervisor: Professor Gerald K. Muthakia
- Area of Study: Computational Chemistry

B.Sc., Department of Chemistry, December 2004

- Chemistry specialization (Biochemistry - minor)

1.1.3 EMPLOYMENT HISTORY

Senior Lecturer Department of Chemistry, Kenyatta University	Oct. 2025 – To Present Nairobi
Lecturer Department of Chemistry, Kenyatta University	Jan. 2014 – Sep. 2025 Nairobi
Teaching Assistant Louisiana State University	Aug. 2009 – May 2010 Baton Rouge, LA
Assistant Lecturer Mount Kenya University	Jan. 2008 – May 2010 Thika

1.2 PUBLICATIONS

1.2.1 Refereed Journals

1. Abdelrahman Tageldin, Calvin A Omolo, Vincent O Nyandoro, Eman A Ismail, Mohammed A Gafar, Bongani Nkambule, **Lucy Kiruri**, Irene Mackraj, Thirumala Govender. Dual-targeting sepsis-associated inflammation and infection using linoleic acid-based lipid-polymer hybrid nanoparticles. 2026. *Journal of Materials Chemistry B*. doi:10.1039/D6TB00207B)
2. C. N. Ndung'u, **L. W. Kiruri**, M. I. Kaniu, K. A. Kaduki. Interpreting the Raman, IR, and NIR Vibrational Fingerprints of Chlorothalonil Using Anharmonic DFT Analysis. 2026. *Journal of Chemistry*. doi:10.1155/joch/8140242)
3. JM Thuku, MI Kaniu, CN Ndung'u, **LW Kiruri**, KA Kaduki. Rapid trace detection of chlorpyrifos in vegetables using 2D Raman correlation spectroscopy and machine learning. 2025. *LWT*. doi:10.1016/j.lwt.2025.118742
4. Charles N Ndung'u, Kenneth A Kaduki, M Ian Kaniu, **LW Kiruri**. Enhanced Detection of Pesticide Residues Using Two-Dimensional Raman Correlation Spectroscopy and Machine Learning. 2024. *Applied Spectroscopy Practica*. doi:10.1177/27551857241303466

5. Eman Elhassan, Calvin A Omolo, Mohammed Ali Gafar, **LW Kiruri**, Usri H Ibrahim, Eman A Ismail, Nikita Devnarain, Thirumala Govender. Disease-Inspired Design of Biomimetic Tannic Acid–Based Hybrid Nanocarriers for Enhancing the Treatment of Bacterial-Induced Sepsis. 2024. *Molecular Pharmaceutics*. doi:10.1021/acs.molpharmaceut.4c00048
6. CN Ndung'u, MI Kaniu, JM Wanjohi, KO Odongo, **LW Kiruri**, KA Kaduki. Feasibility for rapid on-site screening of pesticide residues in fresh produce using machine learning-assisted diffuse reflectance spectroscopy. 2024. *Food and Humanity*. doi:10.1016/j.foohum.2023.100204
7. Mariana J Shayo, Baraka Samwel, Daniel M Shadrack, Joel Cassel, Joseph M Salvino, Luis J Montaner, Geradius Deogratias, Ian Tietjen, **Lucy W. Kiruri**, Samson Hilonga, Ester Innocent. Drug repositioning identifies salvinorin A and deacetylgedunin (DCG) enriched plant extracts as novel inhibitors of Mpro, RBD–ACE2 and TMPRRS2 proteins. 2024. *RSC advances*. doi:10.1039/D4RA02593H
8. Muhammad Khurram Tufail, Syed Shoaib Ahmad Shah, Salahuddin Khan, Farooq Ahmad, **Lucy W. Kiruri**, Misbah Sehar Abbasi, Ali Ahmad. Designing efficient materials for high-performance organic solar cells: detailed chemical space exploration, machine learning and virtual screening. 2024. *Chemical Physics Letters*. doi:10.1016/j.cplett.2023.140974
9. Nawras Osman, Mahir Mohammed, Calvin A Omolo, Usri H Ibrahim, Mohammed A Gafar, Sanjeev Rambharose, Nikita Devnarain, **Lucy W. Kiruri**, Joshua Nwabuife, & Thirumala Govender. Hyaluronidase inhibitor surface-modified niosomes: An efficient strategy for antibacterial and anti-biofilm drug delivery. 2023. *Materialia*. doi:10.1016/j.mtla.2023.101826
10. Sifiso S Makhathini, Calvin A Omolo, **Lucy W. Kiruri**, Pavan Walvekar, Nikita Devnarain, Chunderika Mocktar, & Thirumala Govender. Synthesis of pH-responsive dimethylglycine surface-modified branched lipids for targeted delivery of antibiotics. 2022. *Chemistry and Physics of Lipids*. doi:10.1016/j.chemphyslip.2022.105241
11. Geradius Deogratias, Daniel M Shadrack, Joan JE Munissi, Grace A Kinunda, Fortunatus R Jacob, Regina P Mtei, Rose J Masalu, Issakwisa Mwakyula, **Lucy W. Kiruri**, & Stephen S Nyandoro. Hydrophobic $\pi - \pi$ stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. 2022. *Journal of Molecular Graphics and Modelling*. doi:10.1016/j.jmngm.2022.108243
12. Victoria O Fasiku, Calvin A Omolo, **Lucy W. Kiruri**, Nikita Devnarain, Mbuso Faya, Chunderika Mocktar, & Thirumala Govender. A hyaluronic acid-based nanogel for the co-delivery of nitric oxide (NO) and a novel antimicrobial peptide (AMP) against bacterial biofilms. 2022. *International Journal of Biological Macromolecules*. doi:10.1016/j.ijbiomac.2022.02.099
13. Peter Kirenga, Stelyus L Mkoma, Sixberth Mlowe, Yohana Msambwa, **Lucy W. Kiruri**, Fortunatus R Jacob, James E Mgaya, Grace A Kinunda, & Geradius Deogratias. Influence of heteroatoms on the optoelectronic properties of triphenylamine-based dyes for DSSCs application: A computational approach. 2022. *Computational and Theoretical Chemistry*. doi:10.1016/j.comptc.2022.113644
14. Said A. H. Vuai, Mtabazi G. Sahini, Isaac Onoka, **Lucy W. Kiruri** and Daniel M. Shadrack. Cation- π interactions drive hydrophobic self-assembly and aggregation of niclosamide in water. 2021. *Journal of RSC Advances*. 11(52): 33136. doi:10.1039/D1RA05358B
15. Stelyus L. Mkoma, Yohana Msambwa, Fortunatus R. Jacob, **Lucy W. Kiruri**, Grace A. Kinunda, Sixberth Mlowe & Geradius Deogratias. Optical and electronic properties of para-functionalized triphenylamine-based dyes: a theoretical study. 2021. *Structural Chemistry*. doi:10.1007/s11224-021-01837-4
16. Shadrack DM, Deogratias G, **Kiruri LW**, Onoka I, Vianney JM, Swai H, Nyandoro SS. Luteolin: a blocker of SARS-CoV-2 cell entry based on relaxed complex scheme, molecular dynamics simulation, and metadynamics. 2021 *Journal of Molecular Modeling*. 27(8):221. doi:10.1007/s00894-021-04833-x

17. Daniel M. Shadrack, Geradius Deogratias, **Lucy W. Kiruri**, Hulda S. Swai, John-Mary Vianney, Stephen S. Nyandoro. Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms, 2021. *Journal of Molecular Graphics and Modelling*. 107871, ISSN 1093-3263. doi:10.1016/j.jmgm.2021.107871
18. Shadrack DM, **Kiruri LW**, Swai H, Nyandoro SS. Solvent effects on host-guest residence time and kinetics: further insights from metadynamics simulation of Toussaintine-A unbinding from chitosan nanoparticle. 2021 *Journal of Molecular Modeling* 27(5):127. doi:10.1007/s00894-021-04735-y
19. Noureen Siraj, Susmita Das, Farhana Hasan, Chengfei Lu, **Lucy W Kiruri**, Karen E Steege Gall, Isiah M Warner. Enhanced S 2 emission in carbazole-based ionic liquids, 2015. *RSC Advances*, 5(13): 9939–9945 doi:10.1039/C4RA12362J
20. James R. Reed, George F. Cawley, Taylor G. Ardoin, Barry Dellinger, Slawomir M. Lomnicki, Farhana Hasan, **Lucy W. Kiruri**, Wayne L. Backes. Environmentally persistent free radicals inhibit cytochrome P450 activity in rat liver microsomes, 2014. *Toxicology and Applied Pharmacology*, 277(2):200–209. doi:10.1016/j.taap.2014.03.021
21. **Lucy W. Kiruri**, Lavrent Khachatryan, Barry Dellinger, and Slawo Lomnicki. Effect of Copper Oxide Concentration on the Formation and Persistency of Environmentally Persistent Free Radicals (EPFRs) in Particulates, 2013. *Environmental Science & Technology*, 48(2):2212–2217. doi:10.1021/es404013g
22. Noureen Siraj, Farhana Hasan, Susmita Das, **Lucy W. Kiruri**, Karen E. Steege Gall, Gary A. Baker, and Isiah M. Warner. Carbazole-Derived Group of Uniform Materials Based on Organic Salts: Solid State Fluorescent Analogues of Ionic Liquids for Potential Applications in Organic-Based Blue Light-Emitting Diodes, 2014. *The Journal of Physical Chemistry C*, 118(5):2312–2320. doi:10.1021/jp410784v
23. Matthew C. Patterson, Nathan D. Keilbart, **Lucy W. Kiruri**, Chad A. Thibodeaux, Slawo Lomnicki, Richard L. Kurtz, E.D. Poliakoff, Barry Dellinger, Phillip T. Sprunger. EPFR formation from phenol adsorption on Al₂O₃ and TiO₂: EPR and EELS studies, 2013. *Journal of Chemical Physics*, 422:277–282, doi:10.1016/j.chemphys.2012.12.003
24. **Lucy W. Kiruri**, Barry Dellinger, and Slawo Lomnicki. Tar Balls from Deep Water Horizon Oil Spill: Environmentally Persistent Free Radicals (EPFR) Formation During Crude Weathering, 2013. *Journal of Environmental Science & Technology*, 47(9):4220–4226, doi:10.1021/es305157w
25. Sarah Mahne, Gin C Chuang, Edward Pankey, **Lucy Kiruri**, Philip J Kadowitz, Barry Dellinger, Kurt J Varner. Environmentally persistent free radicals decrease cardiac function and increase pulmonary artery pressure, 2012. *American Journal of Physiology-Heart and Circulatory Physiology*, 303(9):H1135–H1142, doi:10.1152/ajpheart.00545.2012

1.2.5 Book Chapters

Book Chapter

- **Kiruri LW** (contributing author). In: *Collaborations, Jobs, and Women Leaders in the Global Chemistry Enterprise*. ACS Symposium Series 1195, Chapter 16. ACS Books; 2015. pp. 153–167.

1.2.6. Referred Learning Modules

1. Dr. Lucy Kiruri & Mugambi Gitari; (December, 2020); SCH 408 Quantum Chemistry; Digital School of Virtual and Open Learning in Collaboration with Department of Chemistry; School of Pure and Applied Sciences. VETTED BY: Dr. Macharia Kibe.

2. Dr. Lucy Kiruri; (December, 2020); SCH 309 Introduction to Photochemistry; Digital School of Virtual and Open Learning in Collaboration with Department of Chemistry; School of Pure and Applied Sciences. VETTED BY: Dr. Isaac Mwangi.

1.2.11 Non - Reviewed Conference Papers

1. Lucy W. Kiruri, Gyun-Tack Bae, Barry Dellinger, and Randall Hall. A DFT Study of the Reaction of Chlorinated Phenols with Copper Oxide Clusters. In: *Proceedings of Louisiana EPSCoR RII LA-SiGMA Symposium*, 1-5, 2012.

1.2.15 Scholarly Presentation & Invited Talks at Conferences/Workshops/Seminars

1. Closing Remarks & Vote of Thanks, KENET Research and EdTech Engagement Forum and Launch of KENET GPU Cluster ("Celebrating 20 Years of Research Engagement and Collaboration") — Pullman Upperhill, Nairobi, March 6, 2026 [Invited as Senior Lecturer, Kenyatta University and former KENET Grantee]
2. Selected Participant, *AI2050 AI/ML Tools in Drug Discovery Workshop, organized by the H3D Foundation & Ersilia Open Source Initiative*, Fairview Hotel, Nairobi, Kenya, 8–11 July 2025.
3. Co-Organizer *East-African School for Young Researchers on Advanced Machine Learning Techniques (EASY-ML)*, University of Nairobi (UoN), Nairobi, Kenya, 9 - 22 July 2025.
4. Invited Speaker, *IUPAC Global Women's Breakfast (IUPAC GWB2025) – The Importance and Impact of Quantum Science in All Aspects of Life*, Online, 11 February 2025.
5. Invited Panelist, *Research and EdTech Engagement Forum, Kenya Education Network (KENET)*, Sarova Stanley Hotel, Nairobi, 7 February 2025.
6. Facilitator, *Biophysics School – QM/MM Molecular Dynamics Simulations: Integrated Tools for Life Sciences and Biomedical Application*, Moi University, Eldoret, 22 October – 3 November 2023.
7. Invited Speaker, *KENET Research Outreach Program, Kisumu, Mombasa, Nakuru & Nairobi*, 31 May – 16 June 2023.
8. Invited Speaker, *Targeting COVID-19 Main Pro: A Computational Drug Repurposing Study*, Kenya Chemical Society (KCS) Nairobi Chapter Virtual AGM/Workshop, 11 September 2021.
9. Invited Speaker, *Novel Peptides as Potent Inhibitors of SARS-CoV-2 that work by Two distinct mechanisms: Molecular Docking and Dynamics Approach*. Virtual Conference on 2020 CHPC National Conference held on 30 Nov – 2 Dec 2020.
10. Invited Lecturer, *Summer School – Molecular Dynamics and Related Methods in Biological Applications*, NM-AIST, Arusha, Tanzania, 2–13 November 2020.
11. Invited Speaker, *Molecular Dynamics Study on the Encapsulation of Herbicide Bentazon with Beta-Cyclodextrins and its Derivatives*, Workshop on Scientific Computing and Advancement of Learning, Technical University of Kenya, Nairobi, 21 February 2020.
12. Participant, *Centre for High Performance Computing (CHPC) National Conference*, Birchwood Conference Centre, Johannesburg, South Africa, 1–5 December 2019.
13. Co-Organizer & Invited Lecturer, *School on Biophysical Approaches to Macromolecules and Cells: Integrated Tools for Life Sciences and Medicine*, NM-AIST, Arusha, Tanzania, 9–20 September 2019.

14. Participant, *Pan African Chemistry Network Congress 2018: Managing Resources through Chemistry – Wealth not Waste*, University of Nairobi, Kenya, 6–8 November 2018.
15. Invited Speaker, *Reviving the African Physical Society & Formal Inauguration of the ICTP-East African Institute for Fundamental Research (EAIFR)*, University of Rwanda, Kigali, 17–19 October 2018.
16. Invited Lecturer, *First School on Atomistic Simulation of Biomolecules and Material Science* in Tanzania, NM-AIST, Arusha, Tanzania, 3–23 September 2018.
17. Invited Speaker, *Conference on Atomistic Simulations of Biomolecules: Towards a Quantitative Understanding of Life Machinery (smr 2828)*, ICTP, Trieste, Italy, 6–10 March 2017.
18. Participant, *OpenLab Workshop for Sub-Saharan Africa Scientists – Introduction to Computational Chemistry*, Kenyatta University, Kenya, 7–9 September 2015.
19. Invited Speaker, *Formation and Stabilization of Environmentally Persistent Free Radicals (EPFRs) A DFT study*. February 22nd 2014) *Kenya Chemical Society, AGM/WORKSHOP* in the School of Physical Sciences Boardroom, Chiromo Campus, University of Nairobi.
20. Oral Presentation, Lucy W. Kiruri, Slawo Lomnicki, and Barry Dellinger, (October 15 - 17; 2013). Effects of Metal Concentration on EPFRs Yield, Persistency, and OH Radical Generation. *Superfund Research Program 2013 Annual Meeting* in Hilton Baton Rouge Capitol Center, Baton Rouge, LA (USA).
21. Oral Presentation, Lucy W. Kiruri, Barry Dellinger, and Randall Hall (June 14th, 2013). The Extent of Copper Reduction during Formation of EPFRs: A DFT study. At *Louisiana State University*, Baton Rouge, LA (USA).
22. Poster Presentation, Lucy W. Kiruri, Barry Dellinger, and Randall Hall (June 12 - 13; 2013). A density functional study of the reactions of 2-Chlorophenol, 1; 2-Dichlorobenzene, Chlorobenzene with CuO - Cu₈O₈ clusters. *2nd Annual Annual High Performance Computing User Symposium*, Louisiana State University - Baton Rouge, LA (USA). (Poster)
23. Oral Presentation, Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (May, 14 - 18; 2013). Effect of Cu(II)O concentration in Cu(II)O/Silica particles on the formation of environmentally persistent free radicals (EPFRs) and reactive oxygen species(ROS). *13th International Congress on Combustion By-Products and their Health Effects*, New Orleans, LA (USA).
24. Oral Presentation, Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (October 21 - 24; 2012). Formation And Stabilization Of Combustion-Generated, Environmentally Persistent Radicals On Alumina Surfaces. The *25th Annual Meeting of the Superfund Research Program Marriot City Center* - Raleigh, NC (USA).
25. Poster Presentation, Lucy W. Kiruri, Gyun-Tack Bae, Barry Dellinger, and Randall Hall (July, 2012). Copper Oxide-Cluster Model of Environmentally Persistent Free Radicals Formation. *LA-SiGMA & LA-EPSCoR Annual Symposium*, Baton Rouge, LA (USA).
26. Oral Presentation, Lucy W. Kiruri, Barry Dellinger, and Randall Hall (July, 2012). Global Reaction Route Mapping (GRRM): Study of Al₂O₃ Isomers. Paper presented at the *2nd Annual LA-SiGMA Graduate Students Retreat*, Tulane University, LA (USA).
27. Poster Presentation, Lucy W. Kiruri, Barry Dellinger, and Slawo Lomnicki (June, 2011). Environmentally Persistent Free Radicals in Soot and Bottom Ash from Controlled Wood Burning. *12th International Congress on Combustion By-Products and their Health Effects*, Hangzhou, China.
28. Poster Presentation, Lucy W. Kiruri, Gyun-Tack Bae, Barry Dellinger, and Randall Hall (June, 2011). *Ab initio* Studies of Reactions of Phenol and Chlorinated Phenols with Copper Oxide Clusters. *12th International Congress on Combustion By-Products and their Health Effects*, Hangzhou, China.

29. Participant, *Understanding and meeting information and technology needs to prevent exposures to engineered nanoparticles*. 5 – 7th June, 2013, Southeastern Louisiana University, Hammond, LA (USA).
30. Participant, *LA-SiGMA All-hands Meetings, EPSCoR RII*. 5th August, 2011, Louisiana Board of Regents, Baton Rouge, LA (USA).
31. Participant, *Introduction to Computational Thinking Workshop*. 31st July - 6th August, 2011, Louisiana State University, Baton Rouge, LA (USA).
32. Participant, *Density Functional Theory Workshop*. 23 – 27th July, 2011, Louisiana State University, Baton Rouge, LA, (USA).
33. Participant, *NWChem Workshop*. 8 – 9th June, 2012, Louisiana State University, Baton Rouge, LA (USA).

1.3 QUALITY TEACHING, LEARNING AND MENTORSHIP

1.3.1 Students Evaluations

1. SCH328 - Chemistry of Coordination Compounds– 2024/2025 - Second Semester (87.76% - 92/130 Responses).
2. SCH 207 Introduction to Computational Chemistry – Academic Year; 2020/2021 – Second Semester (72.41%).
3. SCH 207 Introduction to Computational Chemistry – Academic Year; 2019/2020 – Second Semester (98.85%).
4. SCH 309 Introduction to PhotoChemistry – Academic Year; 2019/2020 – First Semester (96.55%).

1.3.2 Training in Higher Education

1. Participant, Workshop on Generative Artificial Intelligence for Teaching, Learning, and Research, Kenyatta University, Nairobi, Kenya, 31 July – 1 August 2025.
2. Participant, Training of Pedagogy Skills' Training (Centre for Teacher Professional Development and Excellence. Zoom (Online) training on Monday 23rd to Thursday 26th October, 2023
3. Participant, SPAS Staff Training on Development and Implementation of the Competency Based Curriculum by Association for Faculty Enrichment in Learning and Teaching (AFELT) in 5 – 6th May, 2021.
4. Participant, Patent Drafting Training, organized by Kenyatta University & Kenya Industrial Property Institute (DAAD Project: Technology Transfer and Commercialization of University Intellectual Property), 22–24 March 2021.
5. Participant, Training of Trainers Workshop for Staff Mentors and Growing Leaders Facilitators at *Kenyatta University Directorate of Career Development and Mentoring Programmes*. February, 2019, BSSC Building room 012
6. Training as a mentor of mentors in *Partnerships for Enhanced Engagement in Research (PEER) & COACH Women in Science Mentoring Program*. 11 – 13 July 2018, Hotel des Mille Collines, Kigali, Rwanda.

1.3.3 Ongoing Supervisions

1. Maubi, Auka Joseph (B. Ed); I56/28856/2019: **Topic** – *In-Silico Evaluation of Selected Natural Products As Potential Duo Inhibitors for Protein Kinases In Mycobacterium Tuberculosis*
2. Samoei Abraham (B. Sc.); I56/38821/2016: **Topic** – *Synthesis, Photo Physical Studies, and Theoretical Computations of Porphyrin Complexes and Their Use in Water Decontamination*
3. Odero, Isaac Odhiambo (B.Ed Sc.); I56/32690/2015: **Topic** – *Synthesis, Characterization, Bioassay and Density functional theory studies on iron half sandwich organometallic complexes of Ethambutol and its structural analogs*

1.3.4 Supervision of Postgraduate Students

1.3.4.1 MSc

1. Maina, Jeremiah Thuku (BSc.); I56/28857/2019: **Topic** – *Rapid Detection of Chlorpyrifos in Kale And Milk Using Machine Learning-Aided Raman*
2. Kiplangat S. Alice (B. Sc. /PGDE); I56/38004/2016: **Topic** – *Determination of Arsenic Concentration and Contamination Factor in Water from Selected Boreholes in Nairobi City, County*
3. Oboiko Prisca Nyanchera (B. Ed. Sc.); I56/CE/22824/2011: **Topic** – *Molecular, Electronic properties, Energies, and Bioactivity scores of Pyrazinamide Analogues of Pyrazinamide Using Density Functional Theory Calculations*
4. Omolloh, George Ochieng B. Sc. (Ind. Chem); I56/27766/2014: **Topic** – *Moving Domain QM/MM Methods for Determination of Interactions Between Human Estrogen Receptor Alpha and Endocrine Disrupters*
5. Kalenda, Rawlings Werunga (B. Sc.); I56/25949/2013: **Topic** – *A Computational Assessment of the Stability of Cocaine and the Effect of Various Functional Groups on the Rate of Cocaine Hydrolysis*

1.3.4.2 PhD

1. Ndegwa Charles Ndung'u (M. Sc.(Physics)); I80/59920/2022: **Thesis Topic** – *Machine Learning Assisted NIR and Raman Spectroscopy and Molecular Modeling for Rapid Screening of Pesticide Residues - A case Study of Chlorothalonil*
2. Katana Chengo,(M. Sc.); I84/32248/2015: **Thesis Topic:** *Synthesis, characterization, bioassay and density Functional theory studies of iron half sandwich complexes of selected heterofunctional active pharmaceutical Agents*

1.4 PROFESSIONAL /CONSULTANCY

1.4.1 Networks/ Collaborations

1. USIU-Africa – Ongoing collaboration with Dr. Calvin A. Omolo on drug delivery and nanocarrier design, resulting in four peer-reviewed publications (2021– 2025).
2. University of Nairobi (Department of Physics) – Co-Principal Investigator in a funded collaborative project, including joint supervision of postgraduate students.
3. NM-AIST, University of Dar es Salaam & St. John's University of Tanzania – Spearheaded a Memorandum of Understanding (MOU) on COVID-19 and related viral infections, leading to five joint publications.

4. Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy – Regular Associate (2018–2024), engaging in collaborative computational chemistry and biophysics research.

1.4.6 Membership to Academic /Prof. Bodies

1. Member, Royal Society of Chemistry (RSC), UK
2. Kenya Chemical Society

1.4.7 Any other (Editorship/Peer review, external examiner, etc)

1.4.7 - Editorship/Peer review

1. **Editorial Board Member**, African Journal of Pure and Applied Sciences (SPAS Journal).
2. **Peer Reviewer**: for international journals, including:
 - New Journal of Chemistry (RSC)
 - Chemosphere (Elsevier)
 - Kenya Chemical Society (KCS)

1.4.7 - External Examiner

1.4.7.1 PhD Theses

1. **Omondi James Oyim** – Indium (III) Porphyrins Immobilized on Carbon-Based Supports for the Remediation of Organic Contaminants and Bactericidal Activity in Water, Rhodes University, South Africa — **Feb, 2025**
2. **F. Kayamba** – A Novel Library of Pyrimidine-Based Hybrids as Potential Antimalarial Agents: Design, Synthesis, Characterization, and in Vitro Biological Evaluation, University of KwaZulu-Natal, Durban, South Africa — **June 2021**.
3. **P. Appiah-Kubi** – Mechanistic Insights and In Silico Studies on Selected G Protein-Coupled Receptors Implicated in HIV and Neurological Disorders, University of KwaZulu-Natal, Durban, South Africa — **April 2021**.

1.4.7.1 MSc Theses

1. **Awaatif Patel** – QSAR Studies of Non-Heme Iron(II) Complexes as Catalysts for Selective Oxidation of C–H Bonds, University of Johannesburg, South Africa — **Oct., 2024**

1.5 ADMINISTRATIVE RESPONSIBILITY

1.5.1 Recognized University Administrative Positions

1. Examination Coordinator, Department of Chemistry, Kenyatta University (Sep. 2025 - To present).
2. Coordinator, Departmental Research, Innovation and Outreach Board, Kenyatta University (Jan. 2024 – Sep. 2025).
3. Staff Mentor, Supporting student academic and personal growth through the University's Mentorship Programme (2017 - present)
4. Coordinator / Organizer, 2 International Summer Schools on Molecular Modelling and Machine Learning in East Africa (2020 – 2025).

5. Warden, Aberdares Hostels, Kenyatta University (2019 – 2023).
6. Member, School Committee on Collaboration with Industry and Government, School of Pure & Applied Sciences, Kenyatta University (2019).
7. Team Leader, Fourth Year Academic Advisor, Department of Chemistry (2019/2020 Academic Year).

1.5.2 Other Responsibility in the University

1. Member, Curriculum Review Committee, Department of Chemistry (2024/2025 Academic Year).
2. Departmental Timetabler, Department of Chemistry (2018 - present).
3. Team Leader, Research & Collaboration Committee (2020/2021 Academic Year).
4. Team Leader, ICT and Library Services Committee (2020/2021 Academic Year).
5. Team Leader, Service Delivery Evaluation Committee (2020/2021 – present).

1.6 COMMUNITY ENGAGEMENTS AND OTHER CONTRIBUTIONS

1.6.1 Research Funding (Grants)

1. **Principal Investigator**, “Binding of Heavy Metals Cations – Ethylenediamine Cellulose Complexes: Insights from Density Functional Theory – Molecular Dynamics (DFT-MD)”, KENET Mini-Grant (USD 15,000), May 2019 – May 2020. (Research concluded).
2. **Co-Principal Investigator**, “Machine Learning Assisted Diffuse Reflectance Spectroscopy and Molecular Modelling for Rapid Screening of Pesticide Residues – A Case Study of Chlorothalonil”, KENET Research and Innovation Grant (USD 15,000), July 2022 – June 2023.(Research concluded).
3. **Co-Principal Investigator**, “School on Biophysical Approaches to Macromolecules and Cells: Integrated Tools for Life Sciences and Medicine (SMR 3323)”, Euro 20,000, 9 – 20 September 2019.
4. **Co-Principal Investigator**, NRF Multidisciplinary Project: “In silico and biological potency evaluation of anticancer molecules from East African medicinal plants”. (Unsuccessful application).
5. **Principal Investigator**, Bill & Melinda Gates Foundation – Grand Challenges: “Innovative Data and Modeling Approaches to Measure Women’s Health” (2025). (Unsuccessful application, highly competitive — over 1300 proposals submitted).

1.6.2 Fellowships, Awards, and Scholarships

1. Advancing Science Award, NOBCCChE, USA (2013).
2. Graduate Award, Louisiana Alliance for Simulation Guided Materials Application (LA-SiGMA), USA (2013).
3. PhD Chemistry Fellowship, Louisiana State University, Baton Rouge, LA, USA (2009). Full fellowship including stipend.
4. Graduate Scholarship, Kenyatta University (2006)

1.6.2 Community outreach

1. Academic Committee and member of Board of Management – Ng’araria Girls Secondary School, P. O. Box 1500 – 01000 Thika, Kenya from June, 2019 - June, 2021
2. Academic Committee and member of Board of Management – St. Mathew Kianyingi Secondary School, P. O. Box 1006 – 01000 Thika, Kenya from June, 2019 - present

1.6.5 Any other sub-category

Expertise, Programming & Technical Skills

Quantum Chem: Gaussian16, NWChem, ORCA, GAMESS-US; DFT, QSAR, pharmacophore modelling ...

Biophysics: GROMACS, AutoDock Vina, metadynamics, free energy calculations, QM/MM simulations ...

Visualization: GaussView, VMD, PyMOL, Chimera, Avogadro, Jmol, Molden ...

Data Science: Machine Learning, Python (scikit-learn, RDKit, Pandas, NumPy), R/RStudio, chemometrics

Spectroscopy: EPR spectroscopy, GC-MS, FTIR, UV-Vis, NIR and Raman (ML-assisted)

HPC: CHPC South Africa (CHEM1032), Linux/Ubuntu, bash scripting, L^AT_EX, Vim

Soft Skills: Teaching & curriculum development, postgraduate supervision, project management, international collaboration, leadership ...



REFEREES

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