

Oluwatosin Abideen Saibu

CONTACT INFORMATION

Department of Chemistry and Biochemistry
New Mexico State University, USA
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Google Scholar:
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EDUCATION

New Mexico State University, USA
Ph.D. in Chemistry and Biochemistry
Research Focus: Computational biophysics, membrane protein dynamics, molecular simulations, drug discovery, and multiscale method development.
Advisor: Dr. Marat Talipov
Aug 2023 – Dec 2027 (expected)

New Mexico State University, USA
Master of Science in Chemistry
Aug 2023 – May 2026

Ladoke Akintola University of Technology, Ogbomoso, Nigeria
Bachelor of Technology in Biochemistry
Thesis: Protective effect of Hesperidin and related bioactive compounds against Aluminum Phosphide induced hepatotoxicity (Mouse Model)
2012 – 2018

RESEARCH EXPERIENCE

PhD Student, New Mexico State University Aug 2023 – present
USA

- Conducted experimental research on cancer cell lines (MCF7 and MDA-MB-231), performing protein extraction, Western blotting, PCR, and molecular characterization of signaling pathways.
- Collaborated on computational drug discovery projects investigating phytoene as a tyrosinase inhibitor and identifying potential inhibitors of the NEK4 protein using molecular modeling and cell-based validation.
- Lead computational studies of HER2 receptor and Piezo ion channels using all-atom and coarse-grained molecular dynamics simulations, bioinformatics, and enhanced sampling to investigate protein dynamics, mutations, and therapeutic targets.
- Developed mixed-resolution molecular simulation methodologies and performed membrane protein modeling, molecular docking, and trajectory analysis using GROMACS, CHARMM-GUI, and MARTINI.
- Performed Density Functional Theory (DFT) calculations using Gaussian and ORCA to study molecular properties, reaction mechanisms, and support molecular modeling and force-field development.
- Utilized Linux-based high-performance computing (HPC) systems to automate workflows and execute large-scale molecular simulations.

**Research Assistant, Central Research Laboratory, Adekunle
Ajasin University**

May 2020 – Apr 2023
Nigeria

Phytomedicine & Computational Biology Laboratory

- Therapeutic target and novel biomarker discovery, target validation, and lead compound identification and optimization.
- Screening and testing of biologically active compounds on animal and cell culture models for drug discovery.
- In vitro/in vivo toxicity assays, enzyme activity assays, and gene expression analysis.
- Designed novel enzyme inhibitors/receptor modulators against cancer, SARS-CoV-2, and neurodegenerative diseases through computer-aided drug design.
- Performed homology/pharmacophore modeling, molecular docking, virtual high-throughput screening, QSAR, MM-GBSA/MM-PBSA, molecular dynamics simulations, and PK/PD studies.
- Phylogenetic analysis, multiple sequence alignment, in silico cloning, in silico primer design, and density functional theory analysis.

**Research Assistant, Toxicology Laboratory, Vrije Universiteit
(VU) Amsterdam**

Oct 2021 – Feb 2022
Netherlands

- Evaluation of the pharmacological and toxicological effects of pesticides on invertebrates.

**Research Intern, Dept. of Molecular Genetics, University of
Duisburg-Essen**

May 2020 – Sep 2021
Germany

- Elucidated chromosomal aberrations and DNA damage resulting from toxicant exposure in cultured fibroblasts and mammalian cell lines, including Chinese Hamster Ovary (CHO) cells, via designed genotoxicity experiments.

Research Assistant, College of Medicine, University of Lagos

Mar 2018 – Oct 2019
Nigeria

- Extraction, purification, and qualitative/quantitative assay of phytochemicals, including enzymatic and toxicological profiling.

**Research Assistant, Nigerian Institute of Medical Research,
Yaba, Lagos**

Feb 2017 – Nov 2017
Nigeria

- Genomic DNA/RNA extraction, DNA Sanger sequencing, gel electrophoresis, PCR, in vitro culture, and ELISA.

PUBLICATIONS

Saibu, O. A., Hammed, S. O., Oladipo, O. O., Odunitan, T. T., Ajayi, T. M., Adejuyigbe, A. J., ... Omoboyowa, D. A. (2023). "Protein-protein interaction and interference of carcinogenesis by supramolecular modifications." *Bioorganic & Medicinal Chemistry*, 81, 117211.

Saibu, O. A., Ajayi, T. M., Omoboyowa, D. A., Oladipo, O. O., Hammed, S. O., Odunitan, T. T., ... Bodun, D. S. (2023). "Molecular mechanics and dynamics simulation of CD-47/SIRP α blockade study: a computational study on overcoming immunotherapeutic resistance in pancreatic ductal adenocarcinoma." *Arabian Journal of Chemistry*, 16(11), 105265.

Saibu, O. A., Singh, G., Omoboyowa, D. A., Oyejoke, A. K., Olugbodi, S. A., Bamisaye, A., ... Francis, A. C. (2023). "Discovery of putative natural compounds inhibitor of the germinant spore receptor CspC in *Clostridioides difficile* infection: gaining insights via in silico and bioinformatics approach." *Informatics in Medicine Unlocked*, 42, 101339.

Saibu, O. A., Singh, G., Olugbodi, S. A., Oluwafemi, A. T., Ajayi, T. M., Hammed, S. O., ... Omoboyowa, D. A. (2023). "Identification of HER2 inhibitors from curcumin derivatives using combination of in silico screening and molecular dynamics simulation." *Journal of Biomolecular Structure and Dynamics*.

Odunitan, T. T., **Saibu, O. A.**, Apanisile, B. T., Omoboyowa, D. A., Balogun, T. A., Awe, A. V., ... Abdulazeez, W. O. (2023). "Integrating biocomputational techniques for breast cancer drug discovery via the HER-2, BCRA, VEGF, and ER protein targets." *Computers in Biology and Medicine*.

Balogun, T. A., Nureni, I., Olayemi, T. A., Oluwasegun, M. I., Omoboyowa, D. A., Akinwumi, C. J., **Saibu, O. A.**, Wumi, F. A., Ebenezer, A. O. (2021). "Computational evaluation of bioactive compounds from *Colocasia affinis* Schott as a novel EGFR inhibitor for cancer treatment." *Cancer Informatics*, 20, 1–12.

Balogun, T. A., Muhammad, N. I., **Saibu, O. A.**, Michael, O. A., Olubodun, M. L., Uche, C. N., Olayemi, T. A., Omoboyowa, D. A. (2021). "Discovery of potential HER2 inhibitors from *Mangifera indica* for the treatment of HER2-positive breast cancer: an integrated computational approach." *Journal of Biomolecular Structure and Dynamics*, 39, 1–13.

Balogun, T. A., Oluwasegun, M. I., Alausa, A., Chijioke, O. O., Tiamiyu, Z. A., Omoboyowa, D. A., **Saibu, O. A.**, Olayemi, T. A. (2021). "Receptor tyrosine kinases as a therapeutic target by natural compounds for cancer treatment." *Future Journal of Pharmaceutical Sciences*, 7, 197–212.

Omoboyowa, D. A., Balogun, T. A., Omomule, O. M., **Saibu, O. A.** (2021). "Identification of terpenoids from *Abrus precatorius* against Parkinson's disease proteins using in silico approach." *Bioinformatics and Biology Insights*, 15, 1–8.

Omoboyowa, D. A., Balogun, T. A., Chukwudozie, O. S., Nweze, V., **Saibu, O. A.**, Alausa, A. (2021). "SARS-CoV-2 spike glycoprotein as inhibitory target for in silico screening of natural compounds." *Biointerface Research in Applied Chemistry*, 11(6), 14974–14985.

Omoboyowa, D. A., Joshua, P. E., Nwodo, O. C., **Saibu, O. A.**, Aribigbola, T. C., Akinnubi, C. O., Olatunji, D. I. (2021). "*Tithonia diversifolia* (Hemsl.) A. Gray fractions enhanced anti-plasmodial efficacy of chloroquine in resistant *Plasmodium yoelii* infected mice." *EC Pharmacology and Toxicology*, 9(1), 18–32.

Omoboyowa, D. A., Omomule, O. M., Balogun, T. A., **Saibu, O. A.**, Matibemu, D. S. (2021). "Protective potential of ethylacetate extract of *Abrus precatorius* (Linn) seeds against HCl/EtOH-induced gastric ulcer via proinflammatory regulation: in vivo and in silico study." *Phytomedicine Plus*.

Omoboyowa, D. A., Balogun, T. A., **Saibu, O. A.** (2020). "Inhibitory potential of phyto-constituents from sorghum stem on neuro-modulatory enzymes: a computational approach." *J. Comput Sci Syst Biol.*, 13, 326.

Balogun, T. A., Omoboyowa, D. A., **Saibu, O. A.**, Chukwudozie, O. S., Alausa, A., Samuel, O. O., Olayemi, T. A. "Structure-based discovery of selective CYP17A1 lyase inhibitors for prostate cancer treatment." *Biology, Methods and Protocols*.

SOFTWARE DEVELOPMENT	Founder and Lead Developer, SimLab Science	2026 – present USA
	simlabscience.com • Founded and built a browser-based computational science platform for molecular docking, system building, molecular dynamics, DFT, and trajectory analysis, allowing researchers and students to run these workflows without local installation. • Developed integrated tools for protein–ligand, protein–protein, and protein–peptide docking, MD system preparation, trajectory analysis (RMSD, RMSF, PCA), 3D structure and trajectory viewing, and molecule search and drawing. • Launched SimLab Academy, a cohort-based training program with hands-on GPU labs, enrolling 163 students across 5 cohorts (as of September 2026). • Platform usage to date: 1,724 ligands docked across 96 docking runs, 43 systems built, and 46 molecular dynamics simulations run (as of September 2026). • Designed and implemented the full stack using Next.js, TypeScript, Prisma, and Python microservices for ADMET and molecular property prediction.	
TEACHING EXPERIENCE	Founder and Lead Instructor, SimLab Academy	2026 – present USA
	• Design and teach cohort-based courses in computational chemistry, molecular docking, and molecular dynamics for students and early-career researchers, including hands-on GPU labs.	
	Graduate Teaching Assistant, New Mexico State University	Aug 2023 – present USA
	• Instructed undergraduate laboratory sections for General Chemistry I and II, guiding students through experimental technique, data analysis, and laboratory safety practices.	
	Tutor, Nigerian Society of Biochemistry Students, Ladoke Akintola University of Technology	Feb 2014 – Jul 2016 Nigeria
	• Taught pre-clinical and paraclinical students biochemistry, pharmacology, molecular biology, protein chemistry, enzymology, genomics, and bioinformatics.	
	Tutor, School of Nursing, Federal Medical Center, Abeokuta	Mar 2018 – Feb 2019 Nigeria
	• Taught nursing students pharmacology and microbiology.	
AWARDS AND HONORS	Winner , Biochemistry InterVarsity Competition, Ilorin (2016)	
TALKS AND WORKSHOPS	“Computational investigation of HER2 V659E mutation and clinical applications,” <i>Talk</i>, PACES Computational Training, Albuquerque, NM (2025) <i>PACES Computational Training Workshop</i>, Albuquerque, NM (2025) <i>Poster Presentation</i>, Society of General Physiologists Annual Meeting (2024) “Computational investigation of HER2 V659E mutation and clinical applications,” <i>Poster Presentation</i>, Research and Creativity Week and Graduate Research and Arts Symposium, New Mexico State University (2024) “Medicinal plants and their therapeutic efficacies on allergic reactions,” <i>Seminar Presentation</i>, Department of Biochemistry, Ladoke Akintola University of Technology, Nigeria (2017)	

Introduction to Genome Wide Association Studies and Polygenic Risk Scoring, Pre-Conference Workshop, Nigerian Bioinformatics and Genomics Network (NBGN)

SKILLS

Computational Chemistry & Drug Discovery: Computer-aided drug design (CADD), molecular dynamics simulations, molecular docking, bioinformatics, mixed-resolution modeling, Density Functional Theory (DFT), Gaussian, ORCA

Laboratory Techniques: Cell culture, protein extraction, Western blotting, PCR, column chromatography, HPLC, GC-MS, atomic absorption spectroscopy (AAS)

Software & Programming: GROMACS, CHARMM-GUI, GraphPad Prism, R, Python, Linux/Unix, High-Performance Computing (HPC)

Web & Platform Development: Next.js, TypeScript, React, Prisma, Python microservices, full-stack scientific web application design and deployment

CERTIFICATIONS

Drug Discovery, University of California, San Diego (Coursera, 2022)

Introduction to the Biology of Cancer, Johns Hopkins University (Coursera, 2022)

ICH Good Clinical Practice (2022)

PROFESSIONAL AFFILIATIONS

Member, American Chemical Society (2023)

Member, Society for Experimental Biology of Nigeria (2021)

Member, Nigerian Bioinformatics and Genomics Network (2020 – present)

Member, Nigerian Society of Biochemistry and Molecular Biology Students (2016 – 2020)

Member, Nigerian Society of Biochemistry Students (2016 – 2020)

Member, Society of General Physiologists (2024 – present)