

RESEARCH INTERESTS

Computational Chemistry; Drug Discovery; Metabolic Disorders; Cancer Biology; Pharmacokinetics.

EDUCATION

Bachelor of Science, Biochemistry (GPA: 3.54/ 5.0; 3.22/4.0)

May 2024

Adekunle Ajasin University, Akungba-Akoko, Ondo State, Nigeria.

Research-Thesis: Antidiabetic Mechanism of N-Butanol Extract of *Parquentina Nigrescens* via Alpha Amylase Inhibition.

Advisor: Dr Damilola Alex Omoboyowa Grade: (A)

PROFESSIONAL AND RESEARCH EXPERIENCE

Graduate Assistant (National Youth Service Corps)

Nov 2024 – Nov 2025

Faculty of Clinical Science, College of Health Sciences, Obafemi Awolowo University Ile-Ife, Osun State.

- Provided comprehensive administrative support to the dean's office, managing correspondence and documentation for faculty operations.
- Prepared and drafted official letters and documents for medical students, processing an average of 15 student requests daily with accuracy and adherence to university protocols.
- Supported medical students with academic and administrative needs, facilitating their educational experiences.
- Managed day-to-day administrative duties, including filing, scheduling, and interdepartmental communication.

Research Assistant

March 2024 – Sept 2024

Computational and Phytomedicine Laboratory, Akungba Akoko, Ondo State.

Research Advisor: Dr. Damilola Alex Omoboyowa

- Conducted virtual screening with Maestro Schrödinger Software to identify novel Fibroblast Growth Factor receptor 2 (FGFR2) inhibitors, prioritizing Gefitinib-like compounds, including Derazantinib as a potential therapeutic candidate.
- Curated and processed protein structures from the Research Collaboratory for Structural Bioinformatics Protein Data Bank database and 3D phytochemical structures from PubChem for molecular docking studies of ligand-protein interactions.
- Mentored seven undergraduate research interns, guiding them through basic wet-laboratory procedures such as gel electrophoresis, and trained them in the use of Schrödinger's Maestro software to analyze molecular interactions.
- Prepared 156 phytochemical structures from *Aframomum melegueta* using Marvin Sketch software for use in virtual screening studies targeting kidney cancer-related proteins.
- Performed QSAR (Quantitative Structure–Activity Relationship) modeling on 46 phytochemicals to identify key structural features and improve the efficacy of drug candidates.

Undergraduate Research Assistant

April - August 2023

Central Laboratory, Adekunle Ajasin University.

Research Advisor: Dr. Jamiyu A. Saliu

- Investigated the impact of oxidative stress and hyperglycemia using the (*Drosophila melanogaster*).
- Administered *Parquentina nigrescens* n-butanol plant extracts and hydrogen peroxide orally to induce stress responses.
- Incorporated geotaxis methods to elevate gravity locomotion and natural vertical movement behavior.
- Dissected flies and prepared homogenates for biochemical assays targeting oxidative stress markers such as Malondialdehyde, Glutathione-s-transferase, Nitric oxide level, Glutathione peroxidase, and Total thiol content.
- Maintained fly stocks, ensured aseptic lab conditions, and accurately recorded treatment regimens and results.

Teady Bioscience Research Laboratory, Plural Garden Estate, Akure, Ondo State.*Research Advisor: Dr O.O. Elekofehinti*

- Investigated the therapeutic effects of *Cissus populnea* in a rat model of erectile dysfunction induced via oral administration of paroxetine and confirmed via behavioral assays with estrogenized female rats.
- Retrieved and prepared the crystal structure of phosphodiesterase-5 from the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB) for docking analysis.
- Amplified and visualized gene targets using PCR and agarose gel electrophoresis.
- Performed molecular docking using Schrödinger Maestro to identify putative ligands with strong binding affinities against cancer-related proteins such as Survivin and mTOR.
- Evaluated pharmacokinetics of putative 15 small molecule inhibitors using SwissADME applying Lipinski's Rule of Five, P-gp substrate, and CYP450 metabolism filters.

PUBLICATIONS

1. Elekofehinti, O. O., **Ajiboro, P. A.**, Akinjiyan, M. O., Saliu, T. P., Ayodeji, F. O., Ojo, F. M., & Oluwamodupe, C. (2023). Identification of natural inhibitors from *Aframomum melegueta* targeting survivin and mammalian rapamycin signaling pathway in Kidney Cancer. *Informatics in Medicine Unlocked*, 41, 101320 doi: <https://doi.org/10.1016/j.imu.2023.101320>.
2. Sofela, S. O., Bodun, D. S., Omoboyowa, D. A., **Ajiboro, P. A.**, Nwankwo, D. O., Ashimiyu-Abdusalam, Z., & Ajayi, I. H. (2023). Virtual screening for novel FGFR2 inhibitors: Exploring Gefitinib-like compounds as promising therapeutic candidates. *Informatics in Medicine Unlocked*, 42, 101368 doi: [10.1016/j.imu.2023.101368](https://doi.org/10.1016/j.imu.2023.101368).
3. Akinjiyan, Moses Orimoloye, Olusola Olalekan Elekofehinti, **Ayomide Precious Ajiboro**, and Elizabeth Foluke Awodire, et al. "Involvement of *Cissus populnea* Derived Compounds in Phosphodiesterase Pathway in Erectile Dysfunction: In Silico Study." *J Comput Sci Syst Bio* 15 (2022):432 doi: [10.37421/0974-7230.2022.15.432](https://doi.org/10.37421/0974-7230.2022.15.432).
4. Omoboyowa, D. A., **Ajiboro, P. A.**, Aribigbola, T. C., Oni, A. E., Bodun, D. S., & Akinsulure, S. T. (2025). Exploration of *Bauhinia variegata* compounds as STK-16 antagonists via molecular docking and dynamic simulation for oncogenic pathway targeting. *The Nucleus*, 1-12. doi: <https://doi.org/10.1007/s13237-025-00564-z>.
5. Oluyele, O., Owolade, A. J. J., **Ajiboro, A. P.**, Unuaru, V. O., Adegbenro, T. I., Esther, A. B., ... & Bodun, D. S. (2025). HPLC characterization, molecular docking, QSAR, and molecular dynamics simulation of *Alstonia boonei* phytochemical analogs as potent 5-alpha reductase inhibitors. *Discover Chemistry*, 2(1), 1-24. doi: <https://doi.org/10.1007/s44371-025-00209-9>.
6. Bodun, D. S., **Ajiboro, A. P.**, Kareem, J. A., Adaramola, I. M., Sofela, S. O., Ashimiyu-Abdusalam, Z., & Iwuji, C. B. (2025). Exploring Inhibition of ASK1 by Phytochemicals from *Momordica charantia* (Linn.) for Pancreatic Cancer: An *in silico* Investigation. doi: <https://doi.org/10.33263/LIANBS143.129>

CONFERENCE PRESENTATIONS AND WORKSHOPS**Conference Presentation**

- Identification of natural inhibitors from *Aframomum melegueta* targeting survivin and mTOR in Kidney Cancer, presented at the Nigeria Institute of Medical Research (NIMR), Nov 2024.
- Biochemistry of Autism, Seminar Presentation, Adekunle Ajasin University, May 2023.

Workshops and Training

- Free Biomolecular Workshop: RNA extraction, Reverse Transcription, and Bioinformatics, Teady Bioscience Laboratory, Ondo State, May 2022.
- Chemoinformatic Academy Workshop on Computer-Aided Drug Design (CADD), Ondo State, Feb 2022.
- Computational Drug Discovery Workshop (Molecular Docking, Pharmacophore Modeling, PK Analysis), Institute of Bioinformatics & Molecular Therapeutics, Osun State, Mar 2022.

VOLUNTARY EXPERIENCE AND COMMUNITY SERVICE

Academic Tutor

2021 -2024

Faculty of Science, Adekunle Ajasin University, Ondo State, Nigeria

- Tutored and supported junior colleagues in Biochemistry I and II and Biostatistics, enhancing their exam preparations and understanding of key concepts.
- Guided peers in experimental design, in vivo and in vitro techniques, and data analysis for final year projects.

Community Sensitization Volunteer

2024 - 2025

National Youth Service Corps (NYSC), NDLEA CDS Group, Treasurer

- Collaborated with the National Drug Law Enforcement Agency (NDLEA) CDS group to organize and lead a community sensitization campaign on drug abuse prevention.
- Educated community members (Students and market women) on the dangers of drug misuse and practical steps towards addiction recovery and drug-free living.
- Managed group finances and maintained accurate records of all income expenditures.
- Budgeted and allocated funds for community projects and group activities.
- Ensured financial transparency and accountability through detailed record-keeping.

PROFESSIONAL AFFILIATION

Nigeria Society of Biochemistry students (NSBS)

2019 - present

National Association of Science Students (NASS)

2019- present

HONOURS AND AWARDS

Ondo State Government Scholarship Undergraduate Award (NGN50, 000)

April 2021

Honorable Adeogun Bursary Award for Undergraduate Students (NGN20, 000)

August 2022

SKILLS

- Laboratory: PCR, Gel Electrophoresis, Enzyme Assays, Pharmacokinetics Profiling, RNA extraction, Tissue sample preparation, spectrophotometric quantification, cDNA synthesis.
- Computational: Schrödinger Maestro, PyRx, PyMOL, SwissADME, Marvin Sketch, and ImageJ.
- Data Tools: PubMed, RCSB PDB, SWISS-MODEL.