

AYOBAMI HASSAN DIYAOLU

(Profile page: <https://ayodiyaolu23.github.io/>)

Ph.D. Candidate (2021- present)
Modeling and Simulation Lab
College of Pharmacy and Pharmaceutical Sciences
Washington State University.
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EDUCATION

Washington State University, Ph.D.

Pharmaceutical Sciences and Molecular Medicine

2021 - Present

(Specialization in computer-aided drug design)

Thesis: Allosteric Modulation and Gating Mechanisms of GABA_A Receptors

Advisor: Senthil Natesan

GPA: 3.79/4.0

University of Ilorin, Nigeria, BPharm

2012 - 2017

Bachelor of Pharmacy

GPA: 4.6/5.0

EXPERIENCE

Washington State University

2021 - Present

Graduate Teaching and Research Assistant, Modeling and Simulation Lab | Advisor: Senthil Natesan |

Allosteric modulation and Gating mechanism of GABA_A receptors.

Unraveling the gating mechanisms of GABA_A receptor using classical and enhanced sampling simulations. Delineate ion transport and conductance using Umbrella sampling, and Computational electrophysiology. Discovery of allosteric modulators for the GABA_A receptor using deep learning models.

MicrobicPro, Nigeria

2019 - 2021

Co-Founder, | Advisors: Orange Corners Nigeria |

Development of a novel mobile phone application for antimicrobial stewardship in clinical settings.

Commonwealth Pharmacist Association, United Kingdom

2020 - 2021

Technical advisor, | Advisors: Diane Ashiru-Oredope |

Development of a CWPAMS app for 12 commonwealth countries

National Institute for Pharmaceutical Research, Nigeria

2017 - 2018

Research Scientist Intern, Phytochemistry team | Advisor: Yetunde Isimi

Isolation and GC/MS characterization of components from plant essential oils

University of Ilorin, Nigeria

2016 - 2017

Undergraduate Researcher | Advisor: Haishat Olufadi-Ahmed

Monitored antimicrobial sensitivity patterns of pathogens isolated from UTI patients.

AWARDS AND HONORS

Travel Awards

- **ASWUHS Travel Award**, Washington State University April 2023
- **James and Diann Robbers Student Research Award**, Washington State University April 2023
- **Biophysical Society Travel Award**, Biophysical International Scientific Society Feb 2024

Entrepreneurial Awards

- **Orange Corners Innovation Fund Award**, Kingdom of Netherland Government 2020

Academic Excellence Awards

- **1st Position, People's Choice**, 3-minute thesis competition, CPPS, Washington State University 2024
- **Best Graduating Student in Pharmaceutical Chemistry**, Bioraj Pharmaceuticals 2017
- **TOTAL/NNPC National Undergraduate Scholarship Award**, Nigeria 2015-17
- **Murli Chelleram Foundation Scholarship**, University of Ilorin 2015
- **University Scholar Award for Top Student in Pharmacy**, University of Ilorin 2014-17
- **1st Position, Undergraduate Essay competition**, Pharmaceutical Society of Nigeria 2016
- **Finalist, National Centenary Quiz Competition**, Federal Government of Nigeria 2014
- **Abayomi Jiboku Foundation Scholarship**, University entrance award 2012

LEADERSHIP EXPERIENCE

- **PhD. Senator-at-large**

Associated Students of Washington State University

Uphold the student government constitution and bylaws. Sponsor bills on behalf of Ph.D. students at senate meetings Actively solicit student opinions, concerns, and welfare.

PUBLICATIONS

In Press

Obi P, GC J, Mariasoosai C, **Diyaolu A**, Natesan S. (2024). Application of generative artificial intelligence to predicting membrane partitioning of drugs: Combining denoising diffusion probabilistic models and MD simulations reduces the computational cost to one-third. *J Chem Theory Comput.* 20(14):5866-5881.

GC J, Szlenk CT, **Diyaolu A**, Obi P, Wei H, Shi X, Gibson KM, Natesan S, Rouillet JB. (2023). Allosteric modulation of $\alpha 1\beta 3\gamma 2$ GABA_A receptors by farnesol through the neurosteroid sites. *Biophys J.* 122(5):849-867.

Kamere, N., Garwe, S.T., Akinwotu. O.O., Tuck, C., Krockow, E.M., Yadav, S., Olawale, A.G, **Diyaolu AH**, Munkombwe, D., *et al.* (2022). Scoping Review of National Antimicrobial Stewardship Activities in Eight African Countries and Adaptable Recommendations. *Antibiotics.* 11(9):1149. <https://doi.org/10.3390/antibiotics11091149>

Fatokun, O.T., **Diyaolu, A.H.**, Esievo, K.B., Adamu, A., Aboh, M.O., Okhale, S.E. (2019). Chemical Composition and Antibacterial Activity of the Essential oil of *Dysphania ambrosioides* (L.) Mosyakin & Clemants from Northcentral Nigeria. *JOPAT* Vol., 18(2) 304-31

Under preparation

Diyaolu, A, Obi, P, Balijepalli, P, Meier, K, and Natesan, S. Structural basis for the differential activation of lysophosphatidic acid receptor 1 (LPAR1) by 18:0 and 18:1 LPAs. (*Under review: Journal of chemical information and modelling*)

Diyaolu, A.H. and Natesan, S. (2022). Structural determinants and energetics of GABA binding to GABA_A receptor. (*Planned Submission: Spring 2025*)

Diyaolu, A.H., and Natesan, S. Deep learning-based screening of ultra large chemical libraries for new non-steroidal neurosteroid site modulators of GABA_A receptors. (*Planned Submission: Spring 2025*)

CONFERENCE PRESENTATIONS/POSTERS

- **Diyaolu, A.H.**, Obi, P., Payghan, P., and Natesan, S. (2023). Structural basis for the allosteric modulation of GABA_A receptors by neurosteroids, 67th annual meeting of the Biophysical Society, San Diego, CA, **February 19 -23, 2023**.
- **Diyaolu, A.H.**, and Natesan, S. (2024). Mechanism of activation and allosteric modulation of the GABAA receptor, Globalization of Pharmaceuticals Education Network, Copenhagen, Denmark, **July 13 -17, 2024**
- **Diyaolu, A.H.**, Obi, P., Ramya Chandar, M., and Natesan, S. (2024). Structural determinants, pathways and energetics of GABA binding and unbinding to the GABAA receptor, 68th annual meeting of the Biophysical Society, Philadelphia, PA, **February 10 -14, 2024**.
- **Diyaolu, A.H.**, Obi, P., Balijepalli, P., Meier, K., and Natesan, S. (2022). Molecular basis for the differential activation of lysophosphatidic acid receptor 1 (LPAR1) by 18:0 and 18:1 LPAs. *Poster presented at the Inland Northwest Research Symposium. March 2022*

TEACHING EXPERIENCE

- **Teaching Assistant, Washington State University** Aug. 2021-May 2023
Pharmaceutics Laboratory, (Spring 2022)
Pharmaceutics I (Fall 2022)
PharmD Exams Proctoring (Fall 2021 and Spring 2023)

CERTIFICATIONS

- **IBM Data Science Professional certificate** Aug. 2024
Coursera
- **Machine Learning Specialization** July. 2024
Coursera

TECHNICAL SKILLS

- **Scientific Programming:** Python, TCL.
- **Python Tools & Modules:** Pandas, Numpy, Sklearn, Seaborn, Matplotlib, SciPy
- **Structure-Based Drug Design:** Binding site characterization, Protein preparation, Virtual screening from chemical libraries,
- **Cheminformatics:** Preparation of small libraries, SMARTS, SMILES, Morgan fingerprints
- **Ligand-Based Drug Design:** Development of small molecule database, generating conformations and pharmacophore. Tools: MOE software, PLUMED, and CHARMM-GUI.
- **MD Simulation expertise:** Classical MD simulations, Well-tempered metadynamics, Steered MD, Umbrella sampling, Computational electrophysiology simulations, FEP.
- **MD Simulation Suites:** GROMACS, NAMD, AMBER
- **Visualization/ Analysis software:** VMD, Pymol, UCSF Chimera, HOLE, Wordom, CHAP, mdtraj, MDanalyses, Hydrascreen.
- **Machine Learning:** Regression, Classification models, Recommender systems, Anomaly detection.
- **Deep Learning:** Deep neural networks, Neural relation inference, Diffusion models.