OLABUNTU, BABATUNDE AFEEZ

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RESEARCH INTEREST: Molecular Genetics & Bio-informatics **|** Artificial Intelligence (AI) in healthcare **|** Drug Discovery

EDUCATION

Bachelor of Science (B.Sc. Hons.) in Biochemistry **2018-2024**
University of Ibadan, Ibadan, Oyo, Nigeria
Thesis: *Evaluation of the inhibitory effects of the methanol extract of Waltheria indica L. on alpha-amylase using in vitro, machine learning, and molecular docking techniques*

RESEARCH EXPERIENCE

Graduate Research Intern **2025-till date**
The International Institute of Tropical Agriculture (IITA), Ibadan, Nigeria. **Yam Breeding Unit**
Supervisor: Dr. Agre Paterne

- Performed GWAS on 1,470 yam accessions, identifying SNP markers and candidate genes linked to yield traits (yield and stress tolerance) in yam using GAPIT (R), PLINK, and TASSEL 5.
- Designed and implemented custom RNA-seq pipelines by scripting in Bash and R, automating QC, trimming, alignment and differential gene expression analysis for stalked vs. unstalked yam leaf and stem samples, using FastQC, Fastp, HISAT2, FeatureCount, SAMtools, DESEQ2, and edgeR.
- Conducted genomic selection on MET data from 1,400 yam accessions, applying deep learning, machine learning, GBLUP, and other models to predict GEBVs and compared results to choose best model to accelerate the breeding program.
- Built a genomic database for genomic markers (SNP) data storage, conversion, and management using SQL, Python, batch scripting, and CSS to improve data efficiency and accessibility.
- Assisted in DNA separation and quantification of over 20 yam samples using gel electrophoresis and Nanodrop spectrophotometry, prepared sequencing samples, and amplified target DNA via PCR.
- Analyzed crop and nematode diversity across 14 plantain plots using Shannon indices; applied linear, beta, and binomial GLM regressions to assess links between crop diversity, phytophagous nematode reduction, and parasitic nematode abundance.
- Taught students in the unit programming languages such as Python and R, and provided training on data analysis, visualization, and interpretation to enhance research and analytical skills.
- Performed data cleaning and analysis on phenotypic and genotypic datasets (50+ accessions) and automated workflows in Python, reducing processing time by 95%.

Graduate Research Intern **2023- till date**
Nutrition and Industry Lab Department of Biochemistry, University of Ibadan, Oyo State, Nigeria
Supervisors: Professor C.O.O Olaiya & Dr. M.O Ogunyemi

- Prepared methanol extracts of *Waltheria indica L.* and conducted in vitro assays (α-amylase inhibition, FRAP, total phenolic content). Built and optimized ML models to predict pIC_{50}/IC_{50} values, and performed molecular docking to assess inhibitory activity and binding affinities. Identified 3 potential α-amylase inhibitors for type 2 diabetes treatment by integrating computational and experimental findings.
- Built a Multiple Parameter Optimization (MPO) web tool for efficient drug candidate screening, allowing parameter selection (IC_{50}, ADMET) for ranking. Developed with Python, Streamlit, and CSS to ensure usability and time savings.
- Performed RNA-Seq and Ribo-Seq analyses in R to identify differentially expressed genes between AUX- treated and control samples; conducted gene ontology annotation and enrichment analysis to characterize associated biological functions and pathways.

- Developed and optimized machine learning and deep learning (feedforward) models to predict the bioactivity of phytochemicals against key malaria proteins (Plasmodium falciparum farnesyl transferase and Falcipain-2); integrated molecular docking and predictive modeling to identify African plant-derived phytochemicals as potential low-toxicity antimalarial drug candidates.
- Assisted undergraduate research projects by analyzing experimental results and creating data visualizations, leveraging digital skills to support laboratory research and presentations.
- Built ML/DL models for therapeutic targets linked to major diseases, HMG-CoA reductase (cardiovascular), aldose reductase (diabetic complications), and β-secretase and GSK-3β (Alzheimer's), using Binding DB and ChEMBL data; validated hits through molecular docking and dynamics simulations to assess binding stability and interactions.

Graduate Research Intern **2023**

Drosophila Research and Training Center, Ibadan, Nigeria.

Supervisors: Professor Abolaji & Dr. MO Ogunyemi

- Maintained *Drosophila* cultures by feeding, sorting, changing vials, and preparing fly feed for both normal and transgenic lines. Conducted research on *Drosophila* larvae models of colon cancer, testing potential treatments through controlled experimental procedures.
- Investigated the therapeutic potential of naringenin against Parkinson's disease through gene enrichment, KEGG pathway mapping, and gene–gene interaction analysis. Identified target genes via PharmMapper and NCBI, visualized interaction networks in Cytoscape, performed KEGG analysis in ShinyGO, and validated targets through molecular docking with Parkinson's-related proteins.

TEACHING EXPERIENCE

Programming and Bio-informatics Tutor **2025**

The International Institute of Tropical Agriculture (IITA), Ibadan, Nigeria.

- Taught students how to perform data manipulation, visualization, and interpretation, and guided research students in analyzing and presenting their experimental results.
- Taught fellow students, IT staff, and interns programming skills, primarily in R and Python, and provided training in Excel, enhancing their technical proficiency and improving practical data analysis capabilities.

Academic Tutor **2023**

Department of Biochemistry, University of Ibadan, Oyo, Nigeria

- Coached and mentored prospective undergraduates, achieving over a 70% average success rate in admissions and academic advancement.
- Served on the Academic Committee, organizing and leading study sessions that improved students' understanding of complex biochemical concepts and boosted exam performance.

Python Programming and Bio-informatics Tutor **2024**

Nutrition and Industry Lab Department of Biochemistry

- Provided hands-on tutorials in Python programming for data analysis, machine learning, deep learning, and bioinformatics techniques such as molecular docking, guiding students through practical, project- based learning.
- Coached students in data science and bioinformatics projects, achieving over 80% proficiency in Python- based analysis, modeling, and applications, and contributed to curriculum development and ongoing academic support.

VOLUNTEERING & LEADERSHIP EXPERIENCE

- Led a committee that taught programming with a focus on data analysis, equipping students with skills to interpret and analyse data across diverse domains. **2025**
- Served in the Community Development Service – Education (NYSC) Medical Unit, educating the community on health implications and disease prevention and organizing free medical check-ups for community members. **2025**

- Designed and developed a voting website for faculty and departmental elections (Basic Medical Science C Biochemistry) and conducted data analysis on the election results to ensure accuracy and transparency. **2024**
- Served on the Biochemistry Academic Committee, providing academic support and delivering lessons to enhance students' understanding and performance. **2023**

SKILLS AND COMPETENCES

Personal Strengths: Outstanding communication and interpersonal skills **|** Leadership and effective teamwork capabilities | Strong organizational skills | Proficient in time and project management | Excellent problem-solving ability
Digital Skills: Python | Machine Learning | Deep Learning | R programming | Data analysis | Batch Scripting | HTML | CSS | Automation | SQL | Web scraping |Molecular Docking|Linux and Windows Operating System **Analysis**: RNA-Seq and Ribo-Seq Analysis | Gene ontology and Enrichment **|** Network Pharmacology (Protein- to-Protein interaction) | ANOVA | Principal component analysis | K-Mean Analysis | Hierarchical Clustering
Python, R packages and Batch tools: scikit-learn **|** Pytorch **|** Hugging Face **|** PEFT **|** BitsAndBytes **|** NLTK **|** pandas **|** tidy verse **|** selenium **|** flask **|** beautifulsoup4 **|** Pyautogui **|** Bioconductor **|** DESeq2 **|** edgeR **|** RDKit **|** clusterProfiler **|** Biopython **|** bwa **|** Bowtie **|**Trimmomatic **|** FastQC **|** SAM tools **|** plink
Software: PyRx | Discovery studio | Visual studio | Schrodinger | ChemDraw | FunRich | Tassel5
Laboratoryskills:DNA extraction,Antioxidant Assays(such as FRAP,total phenolic, and total flavonoids)
Equipment: PCR machine, gel electrophoresis, spectrophotometer

PUBLICATIONS

Oludare M Ogunyemi, Esther O Adeyeye, Oladimeji S Macaulay, **Babatunde A Olabuntu**, J Achem, Gideon A Gyebi, Charles O Olaiya, Saheed Sabiu (2025). **Machine learning-based QSAR and molecular modeling identify promising PTP1B modulators from Ocimum gratissimum for type 2 diabetes therapy**. [Molecular Diversity] DOI (10.1007/s11030-025-11255-x) **LINK**

Clive Okonta, Oludare Michael Ogunyemi, **Babatunde Olabuntu**, Amos Olalekan Abolaji (2025). **Ameliorative role of naringenin in MPTP-induced Parkinsonism: Insights from Drosophila melanogaster experimental model combined with computational biology**. [Toxicology Reports] **DOI** (doi.org/10.1016/j.toxrep.2025.102004) **LINK**

Fidelix, A., Akingbade, T., Jatin, J., **Babatunde Olabuntu**, Olutola, A., and Juwon Akingbade (2025). **In silico study and validation of natural compounds derived from *Macleaya cordata* as a potent inhibitor for BTK**. [Medinformatics] **DOI** (10.47852/bonviewMEDIN52024239) **LINK**

PRESENTATIONS

9TH UNIBADAN CONFERENCE OF BIOMEDICAL RESEARCH **2025**
AfriNutraX: An AI-driven platform for machine learning predictions and multi-parameter optimization of African plant-derived nutraceutical and drug leads

INDUSTRIAL TRAINING PRESENTATION **2023**
Presented Molecular Docking as a tool in Drug Discovery, University of Ibadan, Nigeria

PROFESSIONAL MEMBERSHIPS

- **American Chemical Society (Member)** **2025**
- **Nigerian Bioinformatics and Genomics Network (Member)** **2025**

CONFERENCE AND WORKSHOPS

INTERNATIONAL INSTITUTE OF TROPICAL AGRICULTURE-BIOSCIENCE CENTER **2025**

Workshop: Hands-on Training in Molecular Biology Techniques

9TH UNIBADAN CONFERENCE OF BIOMEDICAL RESEARCH **2025**

Theme: AI in Translational Biomedical Research

8TH UNIBADAN CONFERENCE OF BIOMEDICAL RESEARCH **2023**

Theme: Global Trends of Biomedical Translation Research

PROJECTS AND CODES

- Developed a Python script implementing a CNN (Convolutional Neural Network) to classify brain MRI scans for tumor presence, handling image preprocessing, modeltraining, and evaluation. **|** **LINK**
- Developed a complete pipeline for RNA-seq processing for Quality, Trimming, Alignment and Feature count using FastQC, Fastp, HISAT2, FeatureCount, samtool **|** **LINK**
- Developed an end-to-end LLM fine-tuning pipeline with advanced parameter-efficient techniques, reducing training costs by 75% and deployment time by 60%. | **LINK**
- Developed a Python script using a feed-forward neural network in PyTorch to classify breast tumors as malignant or benign, including data preprocessing, model training, and performance evaluation. **|** **LINK**
- Developed an R script utilizing DESeq2 for differential gene expression analysis, including data normalization, statistical testing, and visualization of significantly expressed genes. **|** **LINK**
- Developed a Python script implementing a deep learning CNN architecture to predict DNA sequence motifs and identify transcription factor binding sites, including data preprocessing, model training, and validation. **|** **LINK**
- Developed an R script to perform gene ontology enrichment analysis, identifying overrepresented biological processes, molecular functions, and cellular components from gene lists. **|** **LINK**
- Developed a Python-based classification model to predict diabetes status from clinical features, including data preprocessing, feature selection, model training, and performance evaluation. **|** **LINK**
- Developed an R script utilizing edgeR and limma for differential gene expression analysis, including data normalization, statistical testing, and identification of significantly expressed genes. **|** **LINK**
- Developed a Python-based Random Forest Regression model to predict the bioactivity (IC_{50}) of drugs against the Cyclooxygenase-2 (COX-2) enzyme, a key target in inflammation, leveraging machine learning techniques for training, validation, and performance evaluation. **|** **LINK**

CERTIFICATION AND COURSES

- Hands-on Training in Molecular Biology Techniques | **Certificate** **2025**
- 9th UnIbadan Conference of Biomedical Research | Certificate **2025**
- DataCamp RNA-Seq with Bioconductor **|** **Certificate** **2025**
- Python Cheminformatics-Driven Molecular Docking **|** **Certificate** **2025**
- DataCamp Introduction to Bioconductor **|** **Certificate** **2025**
- DataCamp Intermediate R **|** **Certificate** **2025**
- Mentorness Machine Learning Internship **|** **Certificate** **2024**
- DataCamp Introduction to Python **|** **Certificate** **2023**
- DataCamp Intermediate Python **|** **Certificate** **2023**

LANGUAGE

ENGLISH: Distinguished levels of Listening, Speaking, Reading, and Writing