

BAKARY N'TJI DIALLO, PHD

Computational Biologist - Bioinformatician, Computational Chemist - Cheminformatics

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SUMMARY

Experienced bioinformatics and computational biologist with academic and industrial backgrounds in drug discovery and general molecular modeling. Expertise in computer-aided drug design, with a Ph.D. and Master's degree from Rhodes University. Experienced in building virtual screening, binding energy, molecular dynamics, protein mutations effect evaluation, and large-scale quantum chemistry calculations pipelines. Skilled in Python, Bash and high-performance computing on premise cluster and in the cloud. Tech enthusiast to drive innovation in healthcare and pharmaceutical research.

SKILLS

Bioinformatics and Computational Biology:

Small molecule drug discovery, Protein design, Drug discovery, Cheminformatics, Quantum Chemistry, Molecular modelling, Molecular biology (lab experiments), Microbiology (Thesis paper + lab experience), In-silico Drug Design

Programming:

Python (Intermediate), Bash (Intermediate), R (Intermediate), SQL (Intermediate), Java (beginner), PHP-HTML/CSS (beginner), Matlab (Beginner), C++(elementary)

Machine Learning - Artificial intelligence - Statistics:

Molecular QSAR – RDkit Model building with sklearn (Basics), and pytorch and Matlab (Basics).

DevOps / IT:

High-performance and Cloud Computing: GCP, AWS (basics), Docker (intermediate). Distributed Computing (Python Multiprocessing, Ray, Dask, GNU parallel) PBS pro (Linux Clusters) GNU Parallel fd ripgrep awk. VCS: Git, Gitlab ; Editors: Jupyter Notebooks, VScode, PyCharm, Databases SQL, Communications and Networking

PROFESSIONAL EXPERIENCE

University of Science Techniques and Technologies of Bamako (USTTB) – PostDoctoral Researcher April 2024 - Present

- Working on the virtual Screening of natural products on antimalarials drug targets for antimalarials.

InstaDeep – Computational Biologist Consultant Remote May 2021 Mar 2024

- Contributed to the <https://deepchain.bio/> product: molecular simulation workflows using Gromacs, OpenMM, Martini, CP2K...
- Contributed to the development of mutation effect evaluation benchmarking and modular pipelines for protein-protein binding energy and protein stability (Rosetta, Osprey, OpenMM, Gromacs-PMX and ML models...)
- Contributed to the development of machine learning force field using EGNN architecture and large scale DFT data generation on protein fragments: Psi4, Rdkit, OpenBabel, Scine, Pytorch, Jax

PhD research fellow at CMCDD (Computational Mechanistic Chemistry And Drug Discovery Research Unit) and RUBI: (Research Unit in Bioinformatics)

2018 - 2021

- Development of ligands and structure based virtual screening approaches.

Centre Charles Merieux - Pharmacy Intern

February 2015 - April 2016

- Pharmacy thesis: evolution of staphylococcus aureus resistance to antibiotics at the center of infectious diseases Charles Merieux between 2006 and 2015
- Daily medical laboratory diagnostics

EDUCATION

Rhodes University

PhD in Bioinformatics and Computational Biology

2018 - 2021

Thesis: [Application of computer-aided drug design for identification of P. falciparum inhibitors.](#)

Rhodes University	Master's in bioinformatics and computational Biology	2017 - 2018
	Thesis: In silico study of Plasmodium 1-deoxy-d- xylulose 5-phosphate reductoisomerase (DXR) for identification of novel inhibitors from SANCDB	
University of the People	Computer Science, Associate Degree in Computer Science	2013 - 2016
University of Bamako	Doctor of Pharmacy (Pharm.D.)	2007 - 2016
	Thesis: Evolution of <i>Staphylococcus aureus</i> antibiotics resistance at the centre of infectiology Charles Merieux from 2006 to 2015	
Prytanée Militaire Saint-Louis	Baccalaureate, High School/Secondary Diplomas and Certificates	2000 - 2007

PUBLICATIONS – POSTERS - HONORS – AWARDS - COMMUNITIES - VOLUNTEER EXPERIENCES

- **Publications:**

1. Diallo BN, Swart T, Hoppe HC, Tastan Bishop Ö, Lobb K. **Potential repurposing of four FDA approved compounds with antiplasmodial activity identified through proteome scale computational drug discovery and in vitro assay.** Scientific Reports [Internet]. 2021 Dec 14 [cited 2021 Jan 27];11(1):1413. Available from: <https://www.nature.com/articles/s41598-020-80722-2>, Featured in [Top 2022 100 papers in Chemistry](#)
2. Diallo, B.N., Glenister, M., Musyoka, T.M. et al. **SANCDB: an update on South African natural compounds and their readily available analogs.** J Cheminform 13, 37 (2021); <https://doi.org/10.1186/s13321-021-00514-2>
3. The Atomwise AIMS Program. **AI is a viable alternative to high throughput screening: a 318-target study.** Scientific Reports. volume 14, Article number: 7526 (2024). Available from: <https://www.nature.com/articles/s41598-024-54655-z>
4. Subramaniam S, Yang S, Diallo BN, Fanshu X, Lei L, Li C, et al. **Oral Phyto-thymol ameliorates the stress induced IBS symptoms.** Scientific Reports [Internet]. 2020 Dec 17 [cited 2021 Jan 25];10(1):13900. <https://doi.org/10.1038/s41598-020-70420-4>
5. Diallo BN, Tastan Bishop Ö, Lobb K. Novel potential antimalarials through drug repurposing and multitargeting: a computational approach. F1000Research. 2019; <https://doi.org/10.7490/f1000research.1117266.1>

- **Posters | Conferences Workshops:**

1. [Machine learning of force fields towards molecular dynamics simulations of proteins at DFT accuracy](#) GEM workshop, ICLR 2024
2. [Protein binding affinity prediction under multiple substitutions applying eGNNs on residue and atomic graphs combined with language model information: eGRAL](#) GEM workshop, ICLR 2024
3. [In silico study of Plasmodium 1-deoxy-d-xylulose 5-phosphate reductoisomerase \(DXR\) for identification of novel inhibitors from SANCDB](#)
4. [Novel potential antimalarials through drug repurposing and multitargeting: a computational approach](#)

- **Communities:**

[Github](#) – [Stackoverflow](#) - [ChemistryStackexchange](#) - [ResearchGate](#) - [University of the People Alumni](#) - [Biostars](#) - [Focusmate](#)

- **Awards:**

1. Master Thesis graduation with Distinction
2. [Atomwise AIMS Award](#)

- **Volunteering:**

Ebola Vaccine Testing Center for Vaccine Development (CVD) -Mali

ADDITIONAL INFORMATION

Languages: Bamanan/Bambara (Native), Arabic (Reading), French (Closed to native) English (Professional capability), Spanish (Reading)

Interests: Hiking, Cycling, [Couchsurfing](#), Travelling, Coffee/Tea