Cyril Tsopmedjio Namba Nzanguim

Qualifications Summary

I am a computational chemistry researcher with a Master's degree in Chemistry and currently pursuing a PhD. I have strong expertise in Python and Bash scripting, as well as Computer-Aided Drug Design (CADD), including molecular docking, QSAR modelling, molecular dynamics, and binding free energy calculations, alongside experience in natural product database construction for virtual screening. I combine computational approaches with practical laboratory skills in organic synthesis and compound characterization, enabling effective translation from *in-silico* design to experimental validation. I am a collaborative and detail-oriented scientist with strong communication skills and a solid record of peer-reviewed publications, committed to delivering high-quality research in multidisciplinary environments.

Professional Experience

- ***UNIVERSITY OF TRIESTE***– TRIESTE, ITALY

PhD Student in Chemistry, Research Assistant – 01/11/2024 – Current

- Recruited as a PhD researcher and research assistant to conduct advanced studies, develop in silico protocols, and provide technical support across diverse areas of Computer-Aided Drug Design (CADD).
- Focused on hit and lead identification and optimization, with active involvement in data analysis, workflow development, and the preparation of scientific manuscripts for publication.

- ***UNIVERSITY OF TRIESTE*** – TRIESTE, Italy

Graduate Teaching Assistant (GTA) – 21/03/2025 – 16/05/2025

- Preparing the laboratory for the students
- Assisting, guiding, and tutoring the students in the laboratory

- ***LANDMARK METROPOLITAN UNIVERSITY*** – BUEA, CAMEROON

Chemistry Lecturer (Part-time) – 01/03/2024 – 01/06/2024

- Give chemistry classes to second-year students in Civil Engineering (04 hours/week)

- ***UNIVERSITY OF BUEA CENTRE FOR DRUG DISCOVERY (UB-CeDD)*** – BUEA, Cameroon

Research Assistant – 01/06/2021 – 01/12/2023

- Among others, I was recruited to provide relevant support for the project "Nature-inspired Discovery of Novel Antivirals with Distinctive Mechanisms of Action: Focus on HIV and SARS-CoV-2" funded by the Bill and Melinda Gates Foundation via the Calistous Juma Science Leadership for African Grand Challenges Initiative.
- To be involved in staff training and maintaining the computer network of CBIC/UBCeDD, as well as participate in writing grants and scientific publications for the centre.

Education and Training

- ***UNIVERSITY OF TRIESTE***– TRIESTE, ITALY

PhD in Chemistry (01/11/2024 – Current)

PhD Thesis: *My research focuses on leveraging Computer-Aided Drug Design (CADD) alongside artificial intelligence and machine learning to identify and optimize bioactive compounds targeting key biological systems.*

I am actively involved in multiple drug discovery projects, applying a wide range of in-silico tools and methodologies for molecular modelling, structural optimization, and physiologically based pharmacokinetic (PBPK) simulations. My work integrates platforms/tools such as ChemDraw, MOE, Modeller, LigandScout, GOLD, AMBER, KNIME, R, FLAP, BioGPS, and GRID, alongside AI- and ML-driven approaches, including REINVENT and in-house developed models. Key project areas include:

- Virtual screening for Blood-brain barrier-penetrant Estrogen Receptor radiotracers
- Beyond Traditional CADD: Unravelling the Transformative Role of AI and Machine Learning in Drug Design and Development

For the majority of my projects, I work within a Linux-based environment, through which I have developed advanced programming skills. This includes writing and optimizing Python and Bash scripts for computational workflows, as well as executing automated scripts for molecular simulations, data processing, and analysis.

- ***UNIVERSITY OF DUNDEE – Wellcome Centre Anti-Infectives Research (WCAIR)***

Certification: Drug metabolism and pharmacokinetics (DMPK) – (01/06/2023 – 24/08/2023)

- This course revolved around the Determination of the ADMET and (Pharmacokinetics) PK properties of drugs. It also had workshops on in vitro DMPK, PK profiling and scaling. This course elaborated on topics like absorption and permeability; Metabolic processes in drug discovery; the Relationship between physicochemical properties of drugs and DMPK; 3R's and animal testing in drug discovery; Pharmacokinetics; Free drug hypothesis and Drug-drug interactions and reactive species.
- This course provided me with a good insight into DMPK properties and better know-how in analysing computational results.

- ***UNIVERSITY OF BUEA – BUEA, CAMEROON***

Master of Science in Chemistry – (01/11/2020 – 01/07/2023)

Master's Thesis: *De novo Design, Synthesis and Biological Evaluation of SARS-CoV-2 Spike/ACE2 Binders.*

- I took courses in Organic Chemistry, Physical Chemistry, Inorganic Chemistry, Analytical Chemistry, Pharmaceutical Chemistry, and Computational Chemistry.
- I built computational skills by learning Computer Aided Drug Design (CADD) (especially in Homology Modelling, Molecular Docking, Quantitative Structure-Activity Relationship (QSAR) Modelling and prediction, Molecular
- Dynamics (MD), Binding Free Energy (BFE) Calculations, and natural product (small drug-like molecule) database construction for applications in CADD.
- My research project revolved around building a database of synthetic compounds capable of inhibiting the Spike/ACE2 complex protein formation from literature, carrying out virtual screening on this database to have hits, and confirming the results through an in vitro approach. Applying de novo design to optimize an inactive compound from the database gave birth to a scaffold and led to the synthesis and characterization of two novel spiro compounds and their binding affinity and desired activity were evaluated using in-silico and in vitro approaches,

respectively. The bioassay was done in partnership with the Wistar Institute in Philadelphia, USA.

Bachelor of Science in Chemistry with Minor in Pharmaceutical Chemistry – (01/09/2015 – 01/08/2019)

Thesis: Moringa oleifera as a medicinal plant.

- I have completed courses in various branches of Chemistry, including Organic, Inorganic, Analytical, Pharmaceutical, Quantum and Physical Chemistry, and University Requirements like French, Civics and Ethics, Sports, and English. During my studies, I gained ample experience in laboratory work through practical sessions that were designed by the Department of Chemistry. Apart from Chemistry, I also enrolled in mathematics and physics courses from different departments to expand my knowledge in other areas of science.

OF NOTE

CADD Tools/Languages: MOE, Schrödinger packages, Gold, ChemDraw, Python, Amber, OpenBabel, KNIME, Gaussian, PyMol, GRID, FLAP, BioGPS, HPCs, and Bash Script.

Communication skills: Good communication skills gained through my experiences in conferences and active participation in writing articles.

LANGUAGES

English: Native **French:** Native **Yemba:** Native **Pidgin English**: Very good **Italian**: Fairly

Organizational/managerial skills:

- Leadership (Head of the simulation laboratory of the University of Buea Centre for Drug Discovery (UB-CeDD) 01/06/2021 – 01/12/2023)
- Conference Organization Committee Member for the Hybrid Drug Discovery Workshop, University of Buea Centre for Drug Discovery, University of Buea, Cameroon, 01/09/2023 – 09/2023
- Leadership (President of the school Cooperative at Government High School Buea (GHS Buea)) for the 2014/2015 Academic Year)

Job-related skills:

- Good mastery of some Chemoinformatic/*in silico* software such as: Molecular Operating Environment (MOE), Schrodinger (Maestro, canvas, Phase), Gold, Amber, Modeller, ChemDraw, AutoDock, Knime FLAP GRID, BioGPS, etc.
- Able to independently generate and interpret results from the above-mentioned software.
- Good mastery of general chemistry gained during my undergraduate studies.
- Has been involved in organizing tutorials for undergraduate courses in physical/organic chemistry.
- Cumulative years of internship and experience in cheminformatics-related projects with a small-sized company.

Computer skills:

- Good command of Microsoft Windows, Microsoft Office™, and Microsoft WorkTM tools, and some other software compatible with Microsoft Windows.
- Good command of Linux and some Linux software.
- Basic knowledge of computer hardware and software maintenance.
- Good knowledge of coding/programming.

Other skills: ▪ Organic Synthesis, Chemical Databases Development, Drug Discovery, Molecular Structure, Organic Chemistry, Chemoinformatics and Computational Chemistry, Molecular Simulation, Phytochemistry, Physical Organic Chemistry, Drug Design, Theoretical Chemistry, Molecular Modelling, Computational Drug Designing, Molecular Dynamics Simulation.

ADDITIONAL INFORMATION

Honours and awards

1. **Italian Ministry of University and Research (MUR) PhD Scholarship:** Fellowship award for long research stays for doctoral candidates (Full PhD research in Italy, November 01, **2024**)
2. **Award:** Best Poster Presentation Award at the Hybrid Workshop, University of Buea Center For Drug Discovery (UBCeDD) – 29/09/2023
3. **Award:** Academic year Presidential Excellence Award by the Cameroon Government for the academic year – 2021/2022
4. **Travel Grants:** For attending and presenting a poster at Drug Discovery Africa (DDA), travel and accommodation funding at Afe Babalola University, Ado-Ekiti State, Nigeria – 01/08/2022
5. **Award:** Academic year Presidential Excellence Award by the Cameroon Government for the academic year – 2022/2023
6. **Travel Grants:** Travel and accommodation funding for the Biophysics school on integrated machine learning and QM/MM molecular dynamics simulations in understanding biological systems & cell machinery at the University of Dodoma, Dodoma, Tanzania– 01/08/2021

Publication List

1. Betow JY; Qaseem A; Bekono BD; Feng Y; Moumbock AF; Simoben CV; Babiaka SB; Tanyi SA; Shu VA; Ndi AT; Onguéné PA; Clovis SM; Simeon A; Donatus BE; **Namba-Nzanguim CT**; Mathieu J MT et al. African Natural Products Database (ANPDB): A resource for exploring the therapeutic potential of natural compounds from Africa. Nucleic Acids Research. **2026** Jan 6;54(D1):D1336-44. https://doi.org/10.1093/nar/gkaf1186

2. Babiaka, S.B., Ekayen, D.E., Simoben, C.V., **Namba-Nzanguim, C.T**., Chi, G.F., Monah, N.L., Nubed, L.N., Njimoh, D.L., Nziko, V.D.P.N., Singla, R.K. and Ebot-Arrey, C.A., **2025**. Natural Products in Cyperus Species (Cyperaceae): Phytochemistry, Pharmacological Activities, and Biosynthesis. Chemistry & Biodiversity, 22(8), p.e202403352. https://doi.org/10.1002/cbdv.202403352

3. **Namba-Nzanguim, C.T**., Simoben, C.V., Bekono, B.D., Tietjen, I., Cassel, J., Salvino, J.M., Montaner, L.J., Davis, R.A. and Ntie-Kang, F., **2024**. Investigation of some plant stilbenoids and their fragments for the identification of inhibitors of SARS-CoV-2 viral spike/ACE2 protein binding. The Microbe, 3, p.100059. https://doi.org/10.1016/j.microb.2024.100059

4. Eni, D.B., Cassel, J., **Namba-Nzanguim, C.T**., Simoben, C.V., Tietjen, I., Akunuri, R., Salvino, J.M. and Ntie-Kang, F., **2024**. Design, synthesis, and biochemical and computational screening of novel oxindole derivatives as inhibitors of Aurora A kinase and SARS-CoV-2 spike/host ACE2 interaction. Medicinal Chemistry Research, 33(4), pp.620-634. https://doi.org/10.1007/s00044-024-03201-7

5. Paul, L., **Namba-Nzanguim, C.T**., Telesphory, A., Mensah, J.O., Mteremko, D., Costa, R., Katundu, S.M., Kwiyukwa, L.P., Kambaine, N.D., Juvenary, J. and Mlowe, S., **2023**. Investigation of the structure, stability, and relative solubility of psilocybin in water and pure organic solvents: A molecular simulation study. *Journal of Molecular Liquids*, p.123479.doi.org/10.1016/j.molliq.2023.123479

6. Simoben, C.V., Babiaka, S.B., Moumbock, A.F., **Namba-Nzanguim, C.T**., Eni, D.B., Medina-Franco, J.L., Günther, S., Ntie-Kang, F. and Sippl, W., 2023. Challenges in natural product-based drug discovery assisted with in silico-based methods. *RSC advances*, *13*(45), pp.31578-31594.. doi:10.1039/D3RA06831E

7. Majoumo-Mbe, F., Sangbong, N.A., Tcho, A.T., **Namba-Nzanguim, C.T**., Simoben, C.V., Eni, D.B., Isa, M.A., Cassel, J., Salvino, J.M., Montaner, L.J. and Tietjen, I., **2023**. 5-chloro-3-(2-(2, 4-dinitrophenyl) hydrazono) indolin-2-one: synthesis, characterization, and biochemical and computational screening against SARS-CoV- 2. https://doi.org/10.1007/s11696-023-03274-5

8. **Namba-Nzanguim, C.T**., Turon, G., Simoben, C.V., Tietjen, I., Montaner, L.J., Efange, S., Duran-Frigola, M. and Ntie-Kang, F., **2022**. Artificial intelligence for antiviral drug discovery in low resourced settings: A perspective. *Frontiers in Drug Discovery*, *2*, p.1013285. doi.org/10.3389/fddsv.2022.1013285

Previous and Current Funded Research Projects I have participated in.

- **2021-2026:** Nature-Inspired Antivirals with Distinctive Mechanisms of Action: Focus on HIV and SARS-CoV-2 (A Calistous Juma Science Leadership Fellowship funded by Bill & Melinda Gates Foundation, USA). Funding amount: USD 941,429; Duration: 60 months. PI: Dr. Fidele Ntie-Kang

Memberships

1. International Younger Chemistry Network (IYCN) since, 2022
2. International Natural Scientist Product Taskforce (INSPT) since, 2022
3. Digital Health and Safety Platform (DHSPT) since, 2022