

Dr. Edward Ntim GASU



PROFILE

A passionate drug-discovery Chemist and HPC Application Specialist, with 5-years of interfacial research experience in experimental and computational chemistry. I led the in silico discovery of the anti-viral potential of alkaloids from "Nibima," Ghana's first FDA-approved herbal medicine for clinical trials against COVID-19. I designed novel proline-rich antibacterial peptides inspired by marine invertebrate peptides during my Ph.D.

CONTACT DETAILS

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PERSONAL INFORMATION

Citizenship: **Ghana**

Family: **Married**

Languages: **English** (native),
French (B2).

SKILLS

- High Performance Computing,
- C/C++, MPI, CUDA, Fortran,
- Python, MS Office tools,
- Molecular Modeling/Simulations,
- Organic Spectroscopy & Bioassay Development,
- Communication, adaptability and team collaboration

EXPERIENCE

HPC SOFTWARE DEVELOPER at *ICTP (Trieste, Italy)*. **2024.07–pres.**

◇ Optimization of post-processing codes for analyzing Big-Data obtained from Molecular Simulation

SPECTROSCOPIST at *KNUST Central Lab. (Ghana)*. **2017.09–2023.11**

◇ NMR experiment selection, data acquisition and processing, molecular structure verification (Bruker TopSpin) and elucidation; Routine maintenance of liquid nitrogen plant, and instrumental analysis (IR, UV, UV-Florescence Microplate Reader)

RESEARCH ASSISTANT at *KNUST Chemistry (Ghana)*. **2019–2020**

◇ Teaching lab. practicals and providing research assistance (undergraduate mentoring, grant applications, manuscripts writing, presentations, and reports).

EDUCATION

MASTER IN HPC. *ICTP-SISSA, Trieste, Italy*. **2023–2024**

◇ Thesis title: *Optimization of post-processing tools for understanding angular jumps in liquid water*

◇ Molecular dynamics simulation, parallel computing, high-performance python programming and time-series analysis.

PH.D. IN CHEMISTRY. Dept. of Chemistry *KNUST, Ghana*. **2017–2023**

◇ Thesis title: Computer-aided design of proline-rich antimicrobial peptides inspired by peptide from *Olivancillaria hiatala*.

B.Sc. IN CHEMISTRY. Dept. of Chemistry *KNUST, Ghana*. **2012–2016**

◇ Thesis title: Antimicrobial and Antioxidant Activities of Extracts of *Oliva sp.*

PUBLICATIONS

◇ **Gasu E.N.**, Mensah J.K., and Borquaye L.S. Computer-aided design of proline-rich antimicrobial peptides based on the chemophysical properties of a peptide isolated from *Olivancillaria hiatala*. *Journal of Biomolecular Structure and Dynamics*, vol. 41, issue 17, 2023; 8254-8275..

◇ Borquaye L.S., **Gasu E.N.**, Ampomah G.B., *et al.* Alkaloids from *Cryptolepis sanguinolenta* as Potential Inhibitors of SARS-CoV-2 Viral Proteins: An In Silico Study. *Biomed Res Int.*, 2020(Article ID 5324560), 1-14.

◇ **Google Scholar:**  <- Click this Space

◇ Total: 20 Publications, i10-Index: 10

ACADEMIC SERVICES

◇ *Reviewer for: Scientific Reports (and other Springer Nature Journals), Journal of Biomolecular Structure and Dynamics, Journal of Chemistry, Biomed Research International (Wiely)*

AWARDS & HONORS

◇ *ICTP (UNESCO & IAEA), MHPC Fellowship, WARA & MasterCard Foundation Ideas Matter Doctoral Fellowship, First Class Honours, BSc. Chemistry*

HOBBIES

◇ Reading, Scientific conversations, Blogging, Gardening & Fishing.