Mohamed Ali Ahmed Elrefaiy

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Professional Summary

- 7+ years of expertise in scientific modeling for biological systems
- Experienced in translating theoretical concepts into practical computational solutions using Python-based frameworks

Education

The University of Texas at Austin, Chemistry Ph.D. 2020 - present
Thesis: High-throughput Algorithm for building Structure-based Hamiltonian in the Pigment Protein complex

Southern Methodist University, Ph.D. Graduate Student 2020 - 2023
Completed 3 years of Ph.D. coursework and research before transferring to UT Austin

Zewial City of Science and Technology, B.S. 2013 - 2018
Major: Drug Design and Development - Minor: NanoScience *Egypt*

Research and Professional Experience

The University of Texas at Austin August 2023 - Present
Graduate Research Assistant, Mesoscience Lab, Chemistry Department

- Applied and extended a computational pipeline for constructing Hamiltonians across multiple photosynthetic systems (PSII, WSCP, IsiA), utilizing electrostatic models to accurately calculate site energies for various chlorophyll chromophores (Chl a/b)
- Demonstrated that non-standard protonation states significantly impact protein behavior in hydrophobic microenvironments, revealing limitations in conventional protonation state calculations
- Validated that optimized electrostatic models achieve comparable results to QM calculations while requiring substantially fewer computational resources

Southern Methodist University August 2021 - August 2023
Graduate Research Assistant, Mesoscience Lab, Chemistry Department

- Developed and extended open-source software tools for modeling and analyzing light harvesting processes in photosynthetic systems
- Implemented computational methods for calculating excitation energies in pigment-protein complexes
- Created documentation and validation protocols to ensure software reliability and accessibility
- Applied computational tools to establish structure-function relationships in photosynthetic light-harvesting complexes

Southern Methodist University August 2020 - August 2021
Teaching Assistant, Chemistry Department

- Facilitated lab sessions and guided students in general and organic chemistry courses.
- Graded assignments and exams, upholding high academic standards.
- Prepared necessary materials and equipment for laboratory sessions, specifically for CHEM 1301 - Chemistry for Liberal Arts.

Center of Drug Design, Zewail City, Egypt August 2018 - August 2019
Research Assistant

- Performed computational drug design research using molecular dynamics simulations and binding free energy calculations to evaluate potential therapeutic compounds
- Established and maintained high-performance computing resources to support laboratory research activities
- Developed and delivered training materials on computational chemistry methods for graduate students and research staff

Technical Skills

Programming Languages: Advanced Python development (NumPy, Pandas, scientific computing libraries), with strong command of Bash scripting and Linux/Unix environments

Version Control: Git, GitHub

High-Performance Computing (HPC): SLURM, Google Colab

Machine Learning: Foundational experience with TensorFlow, Keras, and PyTorch

Data Visualization: Experience with data visualization tools such as ChimeraX, Pymol, VMD, Matplotlib

Cloud Technologies: Basic understanding of cloud infrastructure and distributed system design

Molecular Dynamics and Quantum Chemistry: Gromacs, Amber, Gaussian

Chemical Informatics: RDKit, OpenBabel

Publications

Elkholy, N., Hassan, R., Bedda, L., **Elrefaiy, M. A.**, Arafa, R. K. Exploration of SAM-I riboswitch inhibitors: In-Silico discovery of ligands to a new target employing multistage CADD approaches. *Artificial Intelligence Chemistry*, 2(1), 100044 (**2024**). DOI:10.1016/j.aichem.2024.100044

Ayoub, A. T., **Elrefaiy, M.A.**, et al. Bioinspired computational design of lankacidin derivatives for improvement in antitumor activity. *Future Med Chem* 14, 1349–1360 (**2022**).DOI:10.4155/fmc-2022-0134

Ayoub, A. T., **Elrefaiy, M. A.,** and K. Arakawa. Computational prediction of the mode of binding of antitumor lankacidin C to tubulin. *ACS Omega*, 4(2), 4461–4471 (**2019**). DOI:10.1021/acsomega.8b03470

Honors & Awards

Poster Prize - Eastern Regional Photosynthesis Conference 2023
A Structure-Based Approach for Computing Local Transition Energies via MCCE and CDC Calculations

Travel grant [twice] 2022 - 2023
Southern Methodist University

Theoretical and Computational Chemistry Research Achievement Award 2022
Southern Methodist University

Service & Leadership

Technical Reviewer
Chemical Science *2024*

Industrial Experience

Trainee March 2018
Advanced Clinical and Experimental Immunology Department, 57357, Cairo, Egypt
- Gained hands-on experience in clinical and experimental immunology practices and techniques.

Trainee September 2017
European Egyptian Pharmaceuticals, Alexandria, Egypt

– Participated in pharmaceutical manufacturing processes and quality control procedures.
– Supported the laboratory team in daily operations and learned about pharmaceutical formulations.