

Mohamed A. A. Elrefaiy

Austin, Texas, USA

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Professional Summary

Theoretical chemist and open-source software developer with over five years of multidisciplinary experience in drug design, quantum chemistry, and biophysics.

Education

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| The University of Texas at Austin, Chem. Ph.D. High-throughput Algorithm for understanding excitation energy transport in photosynthetic proteins. | 2023 – Present |
| Southern Methodist University, Ph.D. Graduate Student Completed three years of Ph.D. coursework and research before transferring to UT Austin | 2020 – 2023 |
| Zewail City of Science and Technology, B.S. Major: Drug Design and Development Minor: Nanoscience (Egypt) | 2013 – 2018 |

Research and Professional Experience

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| The University of Texas at Austin / Southern Methodist University Graduate Research Assistant, Mesoscience Lab <ul style="list-style-type: none">* Achieved quantitative prediction of absorption and fluorescence spectra in photosynthetic proteins by pioneering an integrated MCCE/CDC computational pipeline, bridging a critical gap between structural biology and optical spectroscopy.* Demonstrated that non-standard protonation states control spectral shifts in WSCP mutants, revealing a novel mechanism where local electrostatics tune chlorophyll excitation energies.* Created the first structure-based excitonic Hamiltonian for previously uncharacterized photosynthetic complexes (C₂S₂M₂, LHCII/CP47, and IsiA), achieving strong agreement with experimental spectra.* Resolved the IsiA quenching mechanism by proposing a novel two-state protein configuration model that explains the enigmatic red-shifted fluorescence state, advancing the understanding of photoprotection.* Developed and deployed an open-source Python package (MCCE/CDC-TrESP) that automates the complete workflow from PDB files to computed spectra, reducing analysis time from weeks to hours.* Established a predictive framework that quantitatively maps protein environments to electronic properties, enabling the rational engineering of artificial light-harvesting systems with tunable optical characteristics. | August 2023 – Present |
| Southern Methodist University Teaching Assistant, Chemistry Department <ul style="list-style-type: none">* Facilitated lab sessions and guided students in general and organic chemistry courses.* Prepared necessary materials and equipment for laboratory sessions, specifically for CHEM 1301: Chemistry for Liberal Arts. | August 2020 – August 2021 |
| Zewail City of Science and Technology Research Assistant, Center of Drug Design <ul style="list-style-type: none">* Elucidated and validated the binding mode of the natural product Lankacidin C to tubulin, establishing the first structural model for its antitumor activity.* Developed and executed a multi-step computational protocol, integrating ensemble docking, 1.1 μs of molecular dynamics (MD) simulations, and binding free energy calculations.* Applied the validated structural model to perform structure-based design of novel Lankacidin C derivatives optimized for high-affinity binding.* Delivered foundational computational insights that directly guided the successful synthesis of a new class of potent antitumor agents, improving efficacy from micromolar to nanomolar concentrations. | August 2018 – August 2019 |

Selected Open Source Projects

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| AlProtein: Pigment Site Energy Calculator (Alpha Release) Python, BioPython, PyQt5 <ul style="list-style-type: none">* Implemented the Charge Density Coupling (CDC) method for calculating electrostatic interactions in protein systems, enabling computational analysis of photosynthetic complexes. | 2024 |
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- * Built an optimized calculation engine using vectorized NumPy operations, reducing computation time for large protein structures from minutes to seconds.
- * Developed a dual-interface architecture combining a programmatic API for pipeline integration and a PyQt5 GUI with drag-and-drop file loading, background threading, and real-time progress tracking for non-technical users.

Neural Finance: Multi-Modal Stock Prediction Platform | Python, TensorFlow, Flask, React 2025

- * Architected an attention-based LSTM neural network to predict stock prices by unifying market data, news sentiment, and technical indicators into a multi-modal forecasting pipeline.
- * Developed a full-stack platform (Flask/React) featuring interactive Plotly dashboards to visualize real-time predictions, correlation matrices, and portfolio performance.
- * Engineered an asynchronous, real-time prediction engine using WebSockets to stream live forecasts for multiple tickers simultaneously.
- * Built a modular data pipeline with intelligent caching to ingest and preprocess multi-source data, applying robust normalization and missing-value handling to ensure data integrity.
- * Implemented a command-line interface (CLI) to streamline model experimentation, supporting multiple architectures and hyperparameter tuning.

Technical Skills

Scientific Software Development: Built complete Python applications including desktop GUIs (PyQt5) and web interfaces (Flask/React); created open-source packages with comprehensive documentation and testing; experienced with Git version control and collaborative development workflows.

Molecular Dynamics/Quantum Mechanics Simulation: Executed molecular dynamics simulations using GRO-MACS and Amber; performed ensemble docking and MM/PBSA binding energy calculations; analyzed protein structures and predicted binding affinities for drug design applications.

Chemical Informatics: Used RDKit and OpenBabel for molecular descriptor calculation and virtual screening; applied QSAR modeling techniques; processed chemical databases and performed structure-activity relationship analysis.

Machine Learning Implementation: Applied TensorFlow and PyTorch to molecular property prediction and financial forecasting; built Long Short Term Memory (LSTM) networks with attention mechanisms for time-series analysis; handled multi-modal datasets combining numerical and text data sources.

Data Processing & Visualization: Processed large datasets using Pandas and NumPy; created interactive visualizations with Matplotlib and Plotly; handled missing data, normalization, and statistical analysis for both scientific and financial datasets.

High-Performance Computing: Deployed and managed parallel computations on multi-node clusters using the SLURM job scheduler; optimized scientific algorithms for performance and memory efficiency using MPI and OpenMP.

Publications

1. **Elrefaiy, M. A.**, et al. pH-dependent frequency tuning in a model chlorophyll protein: Successes and Challenges of MCCE/CDC Pipeline. *Manuscript under revision*.
2. **Elrefaiy, M. A.**, et al. Quenching of the photosynthetic antenna IsiA subunit is facilitated by its red-emitting states. *Manuscript under submission*.
3. **Elrefaiy, M. A.**, et al. From atomistic structure to light harvesting function of PSII supercomplexes. *Manuscript under submission*.
4. Elkholy, N., Hassan, R., Bedda, L., **Elrefaiy, M. A.**, & Arafa, R. K. (2024). 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. DOI:10.1016/j.aichem.2024.100044
5. Ayoub, A. T., **Elrefaiy, M. A.**, et al. (2022). Bioinspired computational design of lankacidin derivatives for improvement in antitumor activity. *Future Medicinal Chemistry*, 14, 1349–1360. DOI:10.4155/fmc-2022-0134
6. Ayoub, A. T., **Elrefaiy, M. A.**, & Arakawa, K. (2019). Computational prediction of the mode of binding of antitumor lankacidin C to tubulin. *ACS Omega*, 4(2), 4461–4471. DOI:10.1021/acsomega.8b03470

Honors & Awards

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| Poster Prize, Eastern Regional Photosynthesis Conference For "A Structure-Based Approach for Computing Local Transition Energies via MCCE and CDC Calculations" | 2023 |
| Travel Grant (Awarded Twice) Southern Methodist University | 2022 & 2023 |
| Theoretical and Computational Chemistry Research Achievement Award Southern Methodist University | 2022 |

Service & Leadership

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| Technical Reviewer Chemical Science | 2024 |
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Industrial Experience

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| Trainee European Egyptian Pharmaceuticals, Alexandria, Egypt | September 2017 |
| <ul style="list-style-type: none">* Participated in pharmaceutical manufacturing processes and quality control procedures.* Supported the laboratory team in daily operations and learned about pharmaceutical formulations. | |