Mohamed A. A. Elrefaiy

Austin, Texas, USA

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Professional Summary

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

Education

The University of Texas at Austin, Theoretical 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 three years of Ph.D. coursework and research before transferring to UT Austin

Zewail 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 / Southern Methodist University **August 2023 – Present**
Graduate Research Assistant, Mesoscience Lab

- 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 ($C_2S_2M_2$, 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.

Southern Methodist University **August 2020 – August 2021**
Teaching Assistant, Chemistry Department

- 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.

Zewail City of Science and Technology **August 2018 – August 2019**
Research Assistant, Center of Drug Design

- 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.

Selected Open Source Projects

AlProtein: Pigment Site Energy Calculator (Alpha Release) | Python, BioPython, PyQt5 **2024**

- Implemented the Charge Density Coupling (CDC) method for calculating electrostatic interactions in protein systems, enabling computational analysis of photosynthetic complexes.
- 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 GROMACS 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

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

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

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

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

Travel Grant (Awarded Twice) **2022 & 2023**
Southern Methodist University

Theoretical and Computational Chemistry Research Achievement Award **2022**
Southern Methodist University

Service & Leadership

Technical Reviewer **2024**
Chemical Science

Industrial Experience

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.