May **Ahmed**

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Skills

Programming	Python, Bash, R, MATLAB; object-oriented design, Git/GitHub
Cheminformatics	Molecular docking (Glide, GNINA); structural search (Foldseek); RDKit, PDB2PQR, Open Babel; UCSF ChimeraX
Scientific Computing	NumPy, SciPy, pandas, Polars, PyArrow, Biopython, MDAnalysis; Linux/SLURM, HPC
Machine Learning	scikit-learn, PyTorch; supervised learning, feature engineering, Random Forest

Research Experience

Graduate Student Researcher — Dr. Jacob D. Durrant

Department of Biological Sciences, University of Pittsburgh — *Sep 2021 – Present*

- Built **LIGNOVA**, an open-source Python/SLURM pipeline that has generated **232M+ docked protein–ligand poses** (240,124 ligands, 10,851 protein structures, 5.27M pairs) to train structure-based drug-design ML models by integrating PubChem bioactives with GNINA docking on HPC.
- Developed **reqadence**, an open-source, fully-typed async Python package (retries, rate limiting, RFC-9111 caching) powering LIGNOVA's data ingestion from RCSB and PubChem at scale.
- Benchmarked whether **consensus rescoring** can replace explicit-water modeling in docking by recovering pose accuracy while preserving virtual-screening throughput; evaluated three hydration regimes on curated X-ray complexes. Manuscript in prep.
- Led a structure-based discovery pipeline (Foldseek + affinity profiling) that identified candidate arginine-sensing proteins in *S. cerevisiae*; predictions **experimentally validated** to alter arginine-homeostasis phenotypes (O'Donnell lab collaboration).

Undergraduate Student Researcher — Dr. Eman Badr

University of Science and Technology, Zewail City — *Jun 2020 – Apr 2021*

- Trained **Random Forest** models (scikit-learn) to predict drug sensitivity from transcriptomic profiles in AML patients; identified genetic markers correlated with differential drug response.

Education

Department of Biological Sciences, University of Pittsburgh

Ph.D. candidate in Molecular, Cellular, and Developmental Biology, Dr. Jacob Durrant — *Aug 2021 – Expected Apr 2027*

University of Science and Technology, Zewail City

B.S. in Computational Biology and Genomics (Biomedical Science) — *Aug 2017 – Jul 2021*

Publications

Holland, M.*, **Ahmed, M.***; Young, J. M.; Drurey, J. R.; McFadyen, S.; Ostrowski, E. A.; Levin, T. C. Hypermutable hotspot enables the rapid evolution of self/non-self recognition genes in *Dictyostelium*. *PNAS* **2025**, *122*(51). DOI: 10.1073/pnas.2520843122. (*co-first authors)

Kochnev, Y.; **Ahmed, M.**; Maldonado, A. M.; Durrant, J. D. MolModa: Accessible and secure molecular docking in a web browser. *Nucleic Acids Research* **2024**, *52*(W1), W498–W506. DOI: 10.1093/nar/gkae406.

Ahmed, M.; Maldonado, A. M.; Durrant, J. D. From byte to bench to bedside: Molecular dynamics simulations and drug discovery. *BMC Biology* **2023**, *21*(1), 299. DOI: 10.1186/s12915-023-01791-z.

Conferences

2026	**Poster Presenter — LIGNOVA: An Automated Pipeline for Large-Scale Generation of High-Quality Protein–Ligand Complexes**, Computational Medicinal Chemistry School	*Cambridge, MA*
2024	**Poster Presenter — Beyond the Blueprint: A Novel Database for Innovative Drug Design and Discovery**, Gordon Research Conference & Seminar on Computational Chemistry	*Portland, ME*
2023	**Poster Presenter — Augmenting Protein–Ligand Complex Databases with PubChem for Enhanced Drug Discovery**, Gordon Research Conference & Seminar on Computer-Aided Drug Design	*West Dover, VT*

Selected Honors & Awards

2026	NSF ACCESS Allocation (BIO260240), Competitive national computing allocation to scale the LIGNOVA pipeline	*USA*
2021	Provost's Honors Roll, Zewail City of Science and Technology — top 5 students by cumulative GPA	*Giza, Egypt*
2021	Cum Laude, B.S. Computational Biology & Genomics, Zewail City of Science and Technology	*Giza, Egypt*