May **Ahmed**

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Education

Department of Biological Sciences, University of Pittsburgh — *Pittsburgh, PA, USA*

Ph.D. Candidate in Molecular, Cellular, and Developmental Biology — *Aug 2021 – Expected Apr 2027*

- Advisor: **Dr. Jacob Durrant**
- Research focus: cheminformatics, structure-based drug design, and scientific software development.

University of Science and Technology, Zewail City — *Giza, Egypt*

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

- Advisor: **Dr. Eman Badr**
- Graduated *cum laude*; awarded a **90% merit-based scholarship** throughout all four years of study.

Research Experience

Graduate Student Researcher — *Pittsburgh, PA, USA*

Department of Biological Sciences, University of Pittsburgh — *Sep 2021 – Apr 2027*

- **LIGNOVA: large-scale protein–ligand complex generation pipeline**: Designed and built a fully automated, open-source pipeline that docks bioactive compounds against experimentally determined protein structures, yielding over **232 million docked poses** (240,124 ligands across 10,851 protein structures; 5.27M protein–ligand pairs) to date — assembling large-scale receptor-bound structural data for structure-based drug design and ML training.
- **reqadence: open-source async API-client library**: Developed an open-source, fully-typed asynchronous Python package (automatic retries, rate limiting, RFC-9111 response caching) that powers LIGNOVA's large-scale data ingestion from RCSB and PubChem.
- **Water modeling in protein–ligand docking**: Investigating whether **consensus-based rescoring** can substitute for explicit water modeling in docking by recovering the pose-prediction accuracy that ordered water provides while preserving the throughput required for large-scale virtual screening. Benchmarking curated high-quality X-ray complexes across multiple hydration conditions to characterize when consensus scoring can recover near-native poses in the absence of water. **Manuscript in preparation.**
- **Structure-based discovery of arginine sensors in yeast** (collaboration with the O'Donnell Lab): Identified **4 candidate arginine-sensing proteins** in *S. cerevisiae* invisible to sequence-homology approaches, combining Foldseek structural search against 5 human CASTOR1 structures with MolModa docking. Experimental validation confirmed altered arginine-homeostasis phenotypes in the identified candidates.
- Developed and maintained Python pipelines with **HPC automation** for large-scale structural and molecular data processing across all projects.

Undergraduate Student Researcher — *Giza, Egypt*

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

- Trained Random Forest regression models (scikit-learn) to predict **drug sensitivity from transcriptomic profiles** in acute myeloid leukemia patients, identifying genetic markers correlated with differential drug response.

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.

Honors & Awards

2026	**NSF ACCESS Allocation (BIO260240)**, Competitive national allocation on the Purdue Anvil and TAMU ACES clusters to scale the LIGNOVA pipeline	*USA*
2026	**GPSG Travel Grant**, Graduate & Professional Student Government, University of Pittsburgh	*Pittsburgh, PA*
2024 & 2026	**Elizabeth Baranger Excellence in Teaching Award (Nominated)**, A&S Graduate Student Organization, University of Pittsburgh; nominated by undergraduate students for teaching Biochemistry	*Pittsburgh, PA*
2021	**Provost's Honors Roll**, Zewail City of Science and Technology; awarded to the top 5 students by cumulative GPA	*Giza, Egypt*
2021	**Cum Laude**, B.S. Computational Biology & Genomics, Zewail City of Science and Technology	*Giza, Egypt*
2017–2021	**Merit-Based Scholarship (90%)**, Full merit scholarship for undergraduate studies, Zewail City of Science and Technology	*Giza, Egypt*

Conferences & Talks

2026	**Poster Presenter** — LIGNOVA: An Automated Pipeline for Large-Scale Generation of High-Quality Protein–Ligand Complexes, Computational Medicinal Chemistry School	*Cambridge, MA*
2026	**Speaker** — Putting the Pieces Together *in silico* to Build Drugs from Fragments, MCDB Noon Seminar Series, University of Pittsburgh	*Pittsburgh, PA*
2024	**Speaker** — DeepFrag Meets LIGNOVA: Transforming Drug Design with Fragment-Based Lead Optimization, MCDB Noon Seminar Series, University of Pittsburgh	*Pittsburgh, PA*
2024	**Poster Presenter** — Beyond the Blueprint: A Novel Database for Innovative Drug Design and Discovery, Gordon Research Conference & Seminar on Computational Chemistry	*Portland, ME*
2024	**Speaker** — Beyond the Blueprint: A Novel Database for Innovative Drug Design and Discovery, MCDB Noon Seminar Series, University of Pittsburgh	*Pittsburgh, PA*
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, VA*
2022	**Speaker** — Testing the Impact of a Newly Built Receptor–Ligand Dataset on DeepFrag Accuracy, MCDB Noon Seminar Series, University of Pittsburgh	*Pittsburgh, PA*

Skills

Programming	Python, Bash, R, MATLAB; object-oriented design
Computational Tools	Git, GitHub, Linux/SLURM, HPC cluster management
Machine Learning	Supervised Learning, Feature Engineering, Model Evaluation, Graph Neural Networks, Random Forest
Data Analysis	Statistical Modeling, Data Visualization (Matplotlib, Seaborn)
Packages	PyTorch, scikit-learn, NumPy, pandas, Polars, SciPy, RDKit, Biopython, MDAnalysis, PyArrow
Molecular Modeling	Docking (Glide, GNINA), Structural Search (Foldseek), Preparation (PDB2PQR, Gypsum-DL, Open Babel), Visualization (UCSF ChimeraX)
Languages	English (Fluent), Arabic (Native)

Teaching & Mentorship Experience

Undergraduate Research Mentor — *Pittsburgh, PA, USA*

TECBIO REU, Department of Computational & Systems Biology, University of Pittsburgh — *May 2024 – Jul 2024*

- Co-mentored an undergraduate student on a 10-week project applying AlphaFold2 to explore HIV protease conformations for drug design.
- Supervised development of a research poster, presented at the Research Symposium at Duquesne University.

Graduate Teaching Assistant & Fellow (Biochemistry) — *Pittsburgh, PA, USA*

Department of Biological Sciences, University of Pittsburgh — *Spring 2024, Fall 2025*

- Conducted recitation sections and held weekly office hours for ~200 students; mentored 15 undergraduate teaching assistants.
- Nominated for the **Elizabeth Baranger Excellence in Teaching Award** based on outstanding student evaluations.

Undergraduate Teaching Assistant (Python) — *Giza, Egypt*

University of Science and Technology, Zewail City — *Sep 2020 – Jan 2021*

- Guided students in writing and debugging Python code; held weekly office hours.

Leadership & Service

Pitt Biological Sciences Graduate Student Organization — *Pittsburgh, PA, USA*

Arts & Sciences Graduate Student Organization Representative — *Aug 2024 – Sep 2026*

- Represent Biological Sciences at school-wide GSO meetings, addressing department concerns.
- Coordinate with the GSO executive board on event planning, policy discussions, and decision-making processes.
- **Served on the Summer Research Grant panel**, evaluating graduate student research proposals across different A&S departments.

Pitt Biological Sciences Graduate Student Organization — *Pittsburgh, PA, USA*

Graduate Diversity, Inclusion, and Belonging (DIB) Committee Member — *Sep 2023 – Dec 2024*

- DIB works on fostering an inclusive environment for underrepresented students in the department.
- Organize intercultural celebrations and distribute informational resources highlighting the diverse cultural traditions within the department.

Zewail City Opencourseware — *Giza, Egypt*

Vice President — *Jan 2018 – Mar 2020*

- Led a team making university course materials (lecture notes, videos, assignments) freely available online for Egyptian students.
- Selected courses to document each semester, coordinated sub-teams, and contributed LaTeX-typeset lecture notes and solutions.

Bio Team Egypt *Egypt*

Head of Strategy Committee *Jan 2017 – Sep 2017*

- Managed 3 subcommittees (Events, Awareness Campaigns, Charities) and organized 3 biotechnology seminars.
- Coordinated 4 public awareness campaigns introducing biotechnology to high school students across Egypt.