Mahmoud Ebrahimkhani

Artificial Intelligence Scientist — Drug Discovery — Biotech — Generative Models
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Research & Industry Experience

AI Scientist II, 1910 Genetics – *2023 – Present*

- Lead design of generative AI models (DDPMs, GNNs, Transformers) for molecular generation and property optimization.
- Built E(3)-equivariant autoregressive models and SMILES-based RNNs with RL fine-tuning for CNS-targeted drug discovery.
- Integrated QM-derived features into graph-based models for improved ADMET prediction.
- Benchmarked predictive models with Graphormer, AttentiveFP, and QM cross-attention embeddings.
- Curated datasets (CrossDocked, ChEMBL, MOSES) and deployed pipelines on AzureML.

Lecturer, Northeastern University – *Spring 2025*

- Designed and taught CSYE 7374: *Applied Deep Learning & Generative Models in Healthcare.*
- Topics: diffusion models, transformers, GNNs, protein-ligand modeling, and molecular generation.
- Course website: CSYE7374-2025

Postdoctoral Researcher, Northwestern University – *2022 – 2023*

- Developed deep learning pipelines to estimate aortic blood flow from wearable SCG signals.
- Built CycleGAN + CNN-MLP systems for noninvasive cardiovascular diagnostics.

Ph.D. Research, Stony Brook University – *2017 – 2022*

- Developed signal/image processing and ML models for THz imaging and burn diagnostics.
- Published 8+ first-author papers, co-authored 30+ publications, and presented at major conferences.

Technical Skills

Languages: Python, C++, MATLAB, Bash
AI/ML Frameworks: PyTorch, TensorFlow, Scikit-learn, Optuna, PyCaret
Generative Modeling: Diffusion (DDPM), RNN, Transformer (GPT, T5), VAEs, GANs
Molecular Modeling: RDKit, DeepChem, AutoDock Vina, Open Babel, ESMFold, AlphaFold
Graph ML: Graphormer, GCN, GAT, MPNN, DGL, PyG
Cloud/Deployment: Azure ML, AWS, Docker, SLURM, Git, VSCode
Domains: Drug discovery, ADMET modeling, protein-ligand design, medical imaging, spectroscopy

Education

Ph.D., Biomedical Engineering – Stony Brook University, 2022
Postdoc, AI for Medical Imaging – Northwestern University, 2023
B.Sc., Electrical Engineering – Amirkabir University of Technology, 2016

Select Publications & Patents

- **Multimodal Graph-Attention Networks with QM-Guided Cross-Attention for ADMET Prediction** – First author, submitted to NeurIPS 2025.
- **Deep Learning for Aortic Flow Estimation from SCG** – Annals of Biomedical Engineering, 2023.
- **Published US Patent (2025)** – ML-based system for noninvasive cardiovascular flow mapping using SCG sensors.
- **MolGPT & ImageMol** – github.com/mahmoud-ekhani