Hossam M. Ashtawy

Curriculum Vitae

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About Me

Over 15 years of experience in machine learning research and its applications in life sciences. Serving as Sr. Director of AI/ML at Ensem Therapeutics, where I lead predictive and generative modeling efforts as well as physics-based simulations.

Work Experience

2024–present **Sr. Director of AI/ML**, *Ensem Therapeutics*, Waltham, MA

- Leading the development of physics-informed AI/ML platform for drug discovery and optimization.
- Contributing to the development of generative models for molecular design and protein metastable-state sampling, leveraging diffusion, autoregressive models, and reinforcement learning.
- Training and evaluating deep learning models for structure and pose prediction, binding affinity, and molecular design.
- Assisting in the design and implementation of an automated pipeline using LLMs, VLMs, and OCSR models to extract biochemical data from patents and scientific literature.

2022–2024 **Director of AI/ML**, *1859 Inc.*, San Diego, CA

- Led a team of AI/ML scientists to build deep-learning models for drug discovery and optimization.
- Built a scalable compute infrastructure for training and inference, enabling high-throughput screening of billions of compounds.
- Developed graph neural networks and SE(3) Transformer models for structure and ligand-based drug design.
- Implemented generative models to design molecules optimized for potency, selectivity, ADMET, and drug-likeness.
- Communicated technical insights and research outcomes to senior leadership and external stakeholders.

2019–2022 **Staff Machine Learning Scientist**, *Atomwise*, San Francisco, CA

- Designed and implemented Atomwise's ligand-based drug discovery platform that integrated domain-specific constraints and rigorous validation protocols.
- Built pipelines for data ingestion, curation, training, and inference at scale.
- Implemented sample-efficient 3D graph neural networks to model over 30 potency and ADMET properties simultaneously.
- Developed a continual learning framework that incorporated weekly experimental data updates, effectively mitigating model drift.
- Built efficient (docking-free) sequence-based models to predict protein-ligand interactions across billion-scale chemical libraries.
- Implemented and applied generative models for de novo molecular design and multi-objective optimization.

2016–2019 **Automated Driving Tech Lead**, *Ford Motor Co.*, Dearborn, MI

- Contributed to the development and enhancement of Path Planning algorithms for Ford's Level 2 autonomous driving system (BlueCruise).
- Assisted in the implementation and evaluation of sensor fusion algorithms for integrating camera and radar inputs.
- Designed and refined real-time models to handle complex road and lane configurations under noisy sensor conditions.
- Researched ML-based trajectory prediction and path-planning algorithms.

Education

2016 **Ph.D. in Electrical and Computer Engineering**, *Michigan State University*, East Lansing, MI
GPA: 3.94
Conducted research in machine learning and its application in drug discovery.

2011 **M.S. in Electrical and Computer Engineering**, *Michigan State University*, East Lansing, MI
GPA: 4.00
Full scholarship recipient. Conducted research in ML & computational drug discovery.

Skills

P. Languages: Python, C/C++, CUDA, Java, HTML, SQL, R

Libraries & Frameworks: PyTorch, TensorFlow/Keras, Pandas, NumPy, SciPy, Matplotlib, Scikit-learn, FastAPI, RDKit, OpenBabel, AlphaFold, HuggingFace Transformers, PyTorch Lightning, DeepSpeed, Horovod, LLM Fine-tuning, Prompt Engineering

Dev/ML Ops: Docker, Kubernetes, AWS, GCP, Git, CI/CD, MLFlow, Argo, Apache Airflow

Professional Society Affiliations

IEEE Member of the Institute of Electrical and Electronics Engineers

ACS Member of the American Chemical Society

Awards

- Recipient of $4,200 AWS Cloud Credit for Research in 2015
- Ph.D. Dissertation Fellowship from Michigan State University in 2015

Patents

- H. Ashtawy, et al., "Systems and Methods for Evaluating Absorption, Distribution, Metabolism, Excretion, Toxicity, and Potency of a Compound". 63/492,184. March 24, 2023.
- H. Ashtawy, et al., "Methods and Systems for In-Silico and Empirical Screening". WO2024097863A1. May 10, 2024.

Select Publications

A. Pedawi, H. Ashtawy, and B. Anderson, "Uncertainty quantification for neural network based molecular property prediction," in *ACS Spring 2022 Meeting*,

2022. http://tinyurl.com/bb8x6p3y.

H. Ashtawy, B. Anderson, J. Sorenson, and I. Wallach, "Pretraining graph neural networks on ultra large chemical libraries to learn generalizable ADMET predictors," in *ACS Fall 2021 Meeting*, 2021. http://tinyurl.com/mr3kh633.

H. M. Ashtawy and N. R. Mahapatra, "Task-specific scoring functions for predicting ligand binding poses and affinity and for screening enrichment," *Journal of chemical information and modeling*, vol. 58, no. 1, pp. 119–133, 2018.

H. M. Ashtawy and N. R. Mahapatra, "Descriptor data bank (ddb): A cloud platform for multiperspective modeling of protein–ligand interactions," *Journal of chemical information and modeling*, vol. 58, no. 1, pp. 134–147, 2018.

H. M. Ashtawy and N. R. Mahapatra, "Boosted neural networks scoring functions for accurate ligand docking and ranking," *Journal of bioinformatics and computational biology*, vol. 16, no. 2, p. 1850004, 2018.

H. M. Ashtawy and N. R. Mahapatra, "Machine-learning scoring functions for identifying native poses of ligands docked to known and novel proteins," *BMC Bioinformatics*, vol. 16, no. Suppl 6, p. S3, 2015.

H. M. Ashtawy and N. R. Mahapatra, "A comparative assessment of predictive accuracies of conventional and machine learning scoring functions for protein-ligand binding affinity prediction," *Computational Biology and Bioinformatics, IEEE/ACM Transactions on*, vol. PP, no. 99, pp. 1–1, 2014.

H. M. Ashtawy and N. R. Mahapatra, "Molecular docking for drug discovery: Machine-learning approaches for native pose prediction of protein-ligand complexes," in *Computational Intelligence Methods for Bioinformatics and Biostatistics*, pp. 15–32, Springer, 2014.

H. M. Ashtawy and N. R. Mahapatra, "Enn-score: An ensemble neural networks scoring function for accurate binding affinity prediction of protein-ligand complexes," in *Proc. 9th International Symposium on Bioinformatics Research and Applications (ISBRA 2013)*, pp. 54–61, 2013.