Hosein Fooladi

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Professional Summary

Experienced Data Scientist and Machine Learning researcher specializing in drug discovery, computational biology, and causal learning. Proven track record in developing ML tools for drug repositioning and protein degradation, with expertise in deep learning and Bayesian inference.

Education

2022–Present **Ph.D. Student, Pharmaceutical Sciences (Cheminformatics)**, *University of Vienna*, Vienna, Austria.

2015–2017 **M.Sc., Electrical Engineering (Biomedical Engineering)**, *Sharif University of Technology*, Tehran, Iran, *(GPA: 19.35/20)*.

2009–2014 **B.Sc., Mechanical Engineering**, *Amirkabir University of Technology (Tehran Polytechnic)*, Tehran, Iran, *(GPA: 17.26/20 Top 10%)*.

2008 **Diploma in Physics and Mathematics**, *Adib HighSchool* , Tehran, Iran, *(GPA: 19.81/20)*.

Core Competencies

Machine Learning	Deep Learning, Geometric Deep Learning, Reinforcement Learning, Causal Learning, Bayesian Inference
Drug Discovery	Chemoinformatics, Protein Degradation, Drug Repositioning, De Novo Design
Programming	Python, R, TensorFlow, PyTorch, Jax, Rust, C++
Domain Expertise	Computational Chemistry, Computational Biology, Systems Biology, Molecular Modeling

Professional Experience

Job

2021–2022 **Chief Data Scientist (CDS) at Celeris Therapeutics**.

- Led development of ML platform for targeted protein degradation
- Developed novel algorithms for ternary complex prediction, leading to publication
- Managed team of >5 ML engineers and researchers and coordinated with cross-functional teams

2019–2020 **Senior Data Scientist - Chemoinformatics / Machine learning expert at AI VIVO**.

- Worked on machine learning for drug repositioning, drug combination, and de novo drug design
- Developed a software to predict the effect of different perturbations (mostly small molecules) on different cell lines.
- Developed machine learning tools to predict the synergy of drug combinations.

2018–2019 **Chief scientific officer (C.S.O.) at Shenakht Pajouh**.

- Deciphering narrative in short story using NLP, The role of AI in autonomous agency, Reconciling Psychology knowledge with machine learning in order to build automated mental health assistant

2017–2018 **Machine learning researcher at Cambridge system biology centre**, *Deep learning in drug discovery*.

2017–2017 **Researcher at Royan Institute**, *Reconstructing context-specific metabolic networks from gene expression data.*

Project

Winter 2021 **Machine learning for ternary complex prediction**, *CelerisTx.*

Spring 2019 **Recognizing arrow of time in the short stories**, *Shenakht Pajouh.*

Fall 2018 **Genealogy of artificial intelligence paradigms**, *Organizing series of workshop at the department of computer science, Sharif University of Technology.*

Summer 2018 **Deep learning in drug discovery and molecular de novo design**, *Collaboration between University of Cambridge and Sharif University.*

Summer 2017 **Latent space construction of high throughput gene expression profiles**, *Collaboration between University of Cambridge and Sharif University.*

Spring 2017 **Constructing context specific metabolic network**, *Collaboration between Royan Institute and Sharif University.*

Fall 2017 **Mathematical modeling of pattern formation during in-vitro human embryonic cells gastrulation**, *Sharif University of Technology (MSc Thesis).*

Miscellaneous

2010–2011 **Member of Technical and Executive Committee** , *Real Rescue Robot league*, Tehran, Iran.
Khwarizmi and AUTCUP Competitions

Selected Publications

- Fooladi, H., Vu, T. N. L., Mathea, M. and Kirchmair, J.; **Evaluating Machine Learning Models for Molecular Property Prediction: Performance and Robustness on Out-of-Distribution Data**; Journal of Chemical Information and Modeling; 65(19):9871-9891 (2025). DOI: 10.1021/acs.jcim.5c00475
- Vu, T. N. L., Fooladi, H. and Kirchmair, J.; **Integrating Machine Learning-Based Pose Sampling with Established Scoring Functions for Virtual Screening**; Journal of Chemical Information and Modeling; 65(10):4833-4843 (2025). DOI: 10.1021/acs.jcim.5c00380
- Fooladi, H., Hirte, S. and Kirchmair, J.; **Quantifying the hardness of bioactivity prediction tasks for transfer learning**; Journal of Chemical Information and Modeling; 64(10):4031-4046 (2024). DOI: 10.1021/acs.jcim.4c00160
- Mekni, N., Fooladi, H., Perricone, U. and Langer, T.; **Encoding protein-ligand interactions: binding affinity prediction with multigraph-based modeling and graph convolutional network**; ChemRxiv (2023). DOI: 10.26434/chemrxiv-2023-bvps7-v2
- Rao, A., Tunjic, T. M., Brunsteiner, M., Müller, M., Fooladi, H., Gasbarri, C. and Weber, N.; **Bayesian Optimization for Ternary Complex Prediction (BOTCP)**; Artificial Intelligence in the Life Sciences; 3:100072 (2023). DOI: 10.1016/j.ailsci.2023.100072
- Hosseini, F., Fooladi, H. and Samsami, M. R.; **Recognizing Arrow Of Time In The Short Stories**; Proceedings of the 2019 Workshop on Widening NLP; ACL (2019). URL
- Fooladi, H., Moradi, P., Sharifi-Zarchi, A. and Hosein Khalaj, B.; **Enhanced Waddington landscape model with cell–cell communication can explain molecular mechanisms of self-organization**; Bioinformatics; 35(20):4081-4088 (2019). DOI: 10.1093/bioinformatics/btz201

- Sadati, S.M. H., Borgheinejad, M., Fooladi, H., Naraghi, M. and Ohadi, A. R.; **Optimum Design, Manufacturing and Experiment of a Passive Walking Biped: Effects of Structural Parameters on Efficiency, Stability and Robustness on Uneven Trains**; Applied Mechanics and Materials; 307:107-111 (2013). DOI: 10.4028/www.scientific.net/AMM.307.107
- H. Fooladi, P. Gifani; **"Constructing fusion network for drug repositioning: Merging structural, functional and drug target data"**; *In preparation* · May 2020

Teaching Experience

2025 **Diffusion Models Course: Implementation-First Learning**, *Instructor.*

- Developed comprehensive course on score-based and diffusion generative models with emphasis on practical implementation using JAX
- Curriculum covers score matching, denoising score matching, NCSN and DDPM implementations
- Materials available at: hfooladi.github.io/teaching/2025-diffusion-course

2025 **Graph Neural Networks (GNNs) for Chemists**, *Instructor.*

- Created hands-on course implementing various GNN architectures from scratch for molecular property prediction
- Progressive learning approach from basic molecular graph representation to sophisticated models
- Course materials and code: hfooladi.github.io/teaching/2025-gnns-for-chemists

Technical Skills

Machine Learning	TensorFlow, Keras, PyTorch, Jax, Scikit-learn
Computation Chemistry	RDKit, AutoDock Vina, Open Babel, Maestro, Gromacs
Software Dev	Git, Docker, Linux, AWS
Languages	

- **Fluent:** Persian (Native), English (TOEFL: 101)
- **Basic:** German, Japanese, Arabic, French

Reinforcement Learning	OpenAI Gym, Unity, Piston game engine
Mech. Eng.	Solidworks, ADAMS, Ansys, EES
Elect. Eng	MATLAB, HSpice, PSpice
Bioinformatics	Bowtie, Mummer, tophat, velvet, cufflink
General	Office (Word, PowerPoint, Excel), LaTeX, AutoCAD, Adobe Photoshop

Research Interests

Causal learning and inference

Machine Learning in drug discovery

Active causal learning in cognition

Bayesian inference

Cooperation, competition and coordination in social learning

Open domain conversational AI

Computational and system biology

Miscellaneous

Peer Review Service

2025 Journal of Chemical Information and Modeling

2024 Nature Machine Intelligence

2024 Journal of Cheminformatics

2023 Artificial Intelligence in the Life Sciences

Honors and Awards

- Got selected as an exceptional talent by IRAN's Ministry of Science, Research and Technology.
- Ranked top 10% in Mechanical Engineering School and directly accepted to the Mech. Eng. M.Sc. Program at Amirkabir University of Technology. (Rank 8 out of 110)
- First rank among 15 students in Biomedical Engineering, Sharif University of Technology
- Outstanding graduate students reward, Sharif University of Technology, 2017-2018
- Ranked among top 0.1 percent in the Nationwide University Entrance Exam. (Rank 477 out of 500,000)
- Accepted in the first phase of Chemistry Olympiad and ranked in the first 800 students among the country.
- Rank 47th among over 30,000 participants in the nationwide M.Sc. entrance exam in Electrical Engineering Group(Ministry of Science, Research and Technology exam), 2015
- Rank 3rd among over 1000 participants in the nationwide M.Sc. entrance exam in Biomedical Engineering Group(Ministry of Health and Medical Education exam), 2015
- Participated in Real Rescue Robot League of Iran Open 2011 and Khwarizmi 2010 International Robotic Competitions as a member of Pasargad Robotic Team, Iran, 2010, 2011.

Advanced Graduate Course

- Reinforcement Learning, UCL, David Silver (online course)
- Deep Reinforcement Learning, UC Berkeley, Sergey Levine (online course)
- Systems Biology, Fall 2016, Sharif university (Ranked 1st)
- High Throughput Biological Data Analysis, spring 2015, Sharif university (Ranked 1st)
- Medical Image Analysis and Processing, Fall 2016, Sharif university (Ranked 1st)
- Computational Genomics, Fall 2015, Sharif university (Ranked 3rd)
- Probabilistic graphical model, Fall 2017, Sharif university (audit)
- Advanced Dynamics, Winter 2013, Amirkabir university (Ranked 1st)
- Compressed Sensing, Spring 2016, Sharif university (audit)
- Bifurcation and Dynamics of complex systems, Winter 2013, Amirkabir university (audit)
- Neuronal Dynamics, December 2013, edx (part of Massive Online Open Courses)

References

- Univ.-Prof. Dr. Johannes Kirchmair — johannes.kirchmair@univie.ac.at
- Prof. Babak Hossein Khalaj — khalaj@sharif.edu
- Dr. Seyed Abolfazl Motahari — motahari@sharif.edu
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- Dr. Yasaman KalantarMotamedi — ykalantar.cam@gmail.com
- Dr. Peyman Gifani — pg364@cam.ac.uk
- Prof. Abdolreza Ohadi Hamedani — a_r_ohadi@aut.ac.ir