AMIR HOSSEIN AMANZADI

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RESEARCH

Clinical Data Scientist

Karolinska University Hospital

March 2022 – Present Stockholm, Sweden

- Worked with **Jesper Tegnér** and **Pierre-Emmanuel Rautou** on **DECISION EU Project**, analyzing 2500+ decompensated cirrhosis patients and identified three optimal combinatorial treatments. Candidates are currently under animal model studies by **Novartis**.
- Under the supervision of **Narsis Kiani**, I established a Systems Medicine pipeline to determine synergistic mechanisms of action (MoA) of the candidate drug combinations.
- Facilitated **David Gomez-Cabrero** by developing a multimodal ML model for prognosis of Chronic Liver Failure from the multi-omics data.

Master Thesis Intern

Center for Molecular Medicine

January 2021 – June 2021 Stockholm, Sweden

- Under the supervision of **Ola Spjuth** & **Narsis Kiani**, I established a chemistry-informed and interpretable Graph Convolutional Network (GCN) model that predicts polypharmacy side effects of drug combinations based on their SMILES.

Machine Learning Researcher

Karolinska Institute

August 2020 – January 2021 Stockholm, Sweden

- Collaborated with **Hassan Abolhassani** on developing a robust few-shot learning method for early detection of Ataxia-Telangiectasia disorder in children based on their genetic profiles.

Summer Research Intern

Algorithmic Dynamics Lab

June 2020 – August 2020 Solna, Sweden

- Assisted **Hector Zenil** in investigating the applicability of Algorithmic Information Dynamics in the causal discovery of synergistic mechanisms behind drug combinations. Project was part of the **AstraZeneca-Sanger Drug Combination DREAM Consortium**.

Graduate Research Assistant

Karolinska Institute

November 2019 – June 2020 Stockholm, Sweden

- Aided **Narsis Kiani** during the pandemic, by developing a variety of graph representation learning models to identify clinically viable drug combinations for diabetic patients suffering from COVID-19 comorbidity. Project was funded by the **Novo Nordisk Foundation**.

Research Assistant

Sharif University of Technology

October 2016 – September 2018 Tehran, Iran

- Designed a multifunctional peptides for Alzheimer's disease. Led by **Amir Shamloo**.
- Synthesised a green bio-compatible hydrogel under the supervision of **Ali Pourjavadi**, for rapid wound healing.

RESEARCH INTERESTS

Drug Discovery and Development • Toxicology • Graph Neural Networks • Computational & Structural Biology • Drug Combination • Computational Chemistry • Medical Machine Learning • Personalized Medicine • Systems Medicine • Bioinformatics • Complex diseases

EDUCATION

M.Sc. in Pharmaceutical Science

Uppsala University

Sep 2019 – Jul 2021 GPA: 3.88/4.0

B.Sc. in Chemistry & Mechanical Engineering *(Minor)*

Sharif University of Technology

Sep 2013 – Jul 2018 GPA: 3.11/4

WORK EXPERIENCE

AI/ML Lead

Celeris Therapeutics

Apr 2021 – Mar 2022 Menlo Park, CA, USA

- Led a team of three computational chemists and established **Xanthos**, an active learning PROTAC and Molecular Glue design engine.
- Developed a Geometric deep learning method for predicting Protein–Protein Interaction susceptible to **Targeted Protein Degradation**.
- Have identified and patented hits via in silico screening against alpha-synuclein (Parkinson's disease) that is currently in **Lead optimization**.
- Contributed directly to the advancement of key partnership projects with **Merck kGaA**, **Boehringer Ingelheim**, and **IRBM**.

Co-founder & ML Engineer

Shenakht Pajouh (Cognition Research)

Jan 2017 – May 2019 Tehran, Iran

- Contributed to the development of various generative models used to establish a conversational AI agent for people in mental health crises (Available on **GitHub**).
- Worked with **Reza Lashgari** on designing an AI-based EEG interface for binary communication with Coma patients.

LANGUAGES

- Persian: Native
- English: Fluent **(TOEFL: 107)**
- Swedish, German: Elementary Proficiency

TEACHING

Artificial Intelligence in Drug Discovery

Uppsala University

October 2022 — Uppsala, Sweden

- Guest lecturer, reviewed the applications of Graph Neural Networks (GNN) in Biomedical research.

Biomedical Engineering

Sharif University of Technology

September 2017 – January 2018 — Tehran, Iran

- Teaching assistant, evaluating course projects in molecular dynamics simulation.

Chemistry

Amir High School

August 2013 – April 2016 — Tehran, Iran

- Taught and nurtured more than 250 talented students in grade 9, 10 and 11.

PUBLICATIONS

[1] Orasch, O., Weber, N., Müller, M., **Amanzadi, A.**, Gasbarri, C., & Trummer, C. (2022). Protein–protein interaction prediction for targeted protein degradation. *International Journal of Molecular Sciences*, *23(13)*, 7033. doi:10.3390/ijms23137033

[2] **Amanzadi, A.** (2021). Predicting safe drug combinations with Graph Neural Networks (GNN) (Dissertation). *Uppsala University*. http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-446691

[3] **Amanzadi, A.**, & Kiani, N. (2021). Explainable polypharmacy side effect prediction with Siamese graph convolutional neural networks. *4th RSC-BMCS Conference, Royal Society of Chemistry*.

[4] Pourjavadi, A., Mazaheri Tehrani, Z., Salami, H., Seidi, F., Motamedi, A., **Amanzadi, A.**, Zayerzadeh, E., & Shabanian, M. (2020). Both tough and soft double network hydrogel nanocomposite based on o-carboxymethyl chitosan/poly(vinyl alcohol) and graphene oxide: A promising alternative for tissue engineering. *Polymer Engineering & Science*, 60(5), 889–899. https://doi.org/10.1002/pen.25297

[5] Shamloo, A., Asadbegi, M., Khandan, V., & **Amanzadi, A.** (2018). Designing a new multifunctional peptide for metal chelation and A inhibition. *Archives of Biochemistry and Biophysics*, 653, 1–9. https://doi.org/10.1016/j.abb.2018.06.004

TECHNICAL SKILLS

- **Programming:** Python, R, Julia, Mathematica, MATLAB and bash.
- **ML and Data Analytics:** PyTorch, Keras, TensorFlow, PyG, DGL, Scikit-learn, Numpy, Pandas, Spark, RAPIDS and SQL.
- **DevOps:** AWS, Azure, GCP, Git, Docker, Singularity and tmux.
- **Cheminformatics:** RDKit, Schrödinger, GROMACS, Gaussian, gnina, AutoDock, Open Babel, OpenMM and OpenEYE.
- **Bioinformatics:** Bowtie, Mummer, tophat, velvet and cufflink.
- **PK/PD:** NONMEM, PKSIM, GastroPlus, TDMx and SIMCA.
- **Visualization:** Matplotlib, Seaborn, plotly, ggplot2, Blender, Unreal Engine and Adobe Photoshop.
- **Wetlab Techniques:** HPLC, NMR, IR, Mass Spectrometry (MS) and LC-MS.
- **IDE and Editors:** LaTeX, Office, Jupyter, Vim, VSCode, and RStudio.

SELECTED COURSEWORK

Deep Learning Specializations (Coursera) • Machine Learning with Graphs (Stanford) • Reinforcement Learning, David Silver (UCL) • Artificial Intelligence in Drug Discovery • Advanced Molecular Modelling • Drug discovery and Development • Computational Medicinal Chemistry • Pharmaceutical Bioinformatics • Preclinical and Clinical Data Analysis • Clinical Pharmacokinetics and Pharmacodynamics • Medical Neuroscience (Coursera) • Molecular Dynamics Simulation • Systems Medicine (Karolinska Institute)

HONORS & AWARDS

- Granted full research sponsorship by the European Foundation for the study of chronic liver failure (EF Clif).
- Ranked first in the Pharmaceutical Science master's program at Uppsala University.
- Ranked among the top 0.1% in Iran's Nationwide University Entrance Exam.
- Accepted in the first phase of the Physics Olympiad and ranked among the first 200 students in the country.

VOLUNTEERING

- First aid volunteer - Swedish Red Cross.
- Co-Founder and Event Manager - Sharif Cognitive Sciences Community (Shenasa).
- Conference Organizer - Institute for Research in Fundamental Sciences (IPM).
- Event Coordinator for freshmen camp - Sharif University of Technology.
- Teacher - Yarigaran Sharif Student Club.

SOFT SKILLS

Leadership | Communication | Teamwork | Interdisciplinary Research | Self-learning | Adaptibility | Problem-solving

REFERENCES

Dr. Narsis A. Kiani
@ Karolinska Institute
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Prof. Jesper Tegnér
@ King Abdullah University of Science and Technology (KAUST)
jesper.tegner@kaust.edu.sa

Prof. Ola Spjuth
@ Uppsala University
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