## 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

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**

♀ 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 (SciLifeLab)

Movember 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**

- 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

GPA: 3.88/4.0

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

**Sharif University of Technology** 

GPA: 3.11/4.0

## **WORK EXPERIENCE**

#### AI/ML Lead

#### **Celeris Therapeutics**

max 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)

▼ Tehran, Iran

- Facilitated the development of various NLP models for the end goal of building a conversational AI agent to aid people in mental health crisis (Available on GitHub).
- Worked with Reza Lashgari on designing an Al-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**

Ctober 2022

**Q** Uppsala, Sweden

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

## **Biomedical Engineering**

#### **Sharif University of Technology**

• 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 I C-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 Interdisciplinary Research

Self-learning

Teamwork

Adaptibility Problem-solving

## REFERENCES

#### Dr. Narsis A. Kiani

- ✓ narsis.kiani@ki.se

#### Prof. Jesper Tegnér

- @ King Abdullah University of Science and Technology (KAUST)
- jesper.tegner@kaust.edu.sa

#### Prof. Ola Spjuth

- @ Uppsala University
- ✓ ola.spjuth@farmbio.uu.se