Payam Kelich

Visa Status: Green Card Holder

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Qualification Summary

Analytical and results-driven computational chemist with advanced expertise in machine learning, molecular dynamics (MD) simulations, and innovative docking techniques to accelerate drug discovery and elucidate complex biomolecular interactions. Highly skilled computational chemist specializing in machine learning and MD simulations applied to DNA and small molecules for biomedical applications. Proven ability to accelerate drug discovery by integrating advanced MD techniques and AI-driven molecular design to study DNA and protein dynamics, conformational changes, and small molecule interactions with DNA and proteins. Proficient in Python and Bash scripting, with expertise in NAMD, VMD, RDKit, DeepChem, and Chemprop. Published in high-impact journals such as *ACS Nano*, *JACS*, and *Nature Communications*.

Technical Proficiencies

Major Skills: Machine learning, Data science, Cheminformatics, Molecular dynamics simulation, Molecular docking, Data mining, Database management, Generative AI.

Programming Languages: Python, Bash Scripting, TCL

Python ML Libraries: NumPy, Pandas, PyTorch, TensorFlow, scikit-learn, DeepChem, Matplotlib

Python Cheminformatics Libraries: RDKit, Chemprop, REINVENT4

Computational Chemistry Software: NAMD, AutoDock, VMD, MOE, MDAnalysis

Operating Systems: Unix-based systems, Docker

Professional Experience

Postdoctoral Research Associate Jan 2024 – Present
University of Illinois Urbana-Champaign, IL, USA

- Developed a computational pipeline integrating AlphaFold3, MOE, CHARMM-GUI, NAMD3, and MDAnalysis to model and simulate a stomatin structure from cryo-EM data.
- Engineered a cheminformatics framework combining a local ChEMBL instance, REINVENT4, Chemprop, DeepChem, and RDKit to predict small molecule subcellular localization.
- Applied DiffDock and MD simulations to identify binding sites on the *P. falciparum* CQ-resistance transporter, revealing insights into drug resistance mechanisms.
- Created a VMD plugin for antibody annotation using the KABAT algorithm in collaboration with Merck KGaA.
- Utilized the DiffLinker generative model to design linkers for novel metal–organic frameworks (MOFs) targeting CO_2 adsorption.

Ph.D. Research Associate Jan 2020 – Dec 2023
University of Texas at El Paso, TX, USA

- Developed deep learning models (CNNs, MLPs, VAEs) to optimize DNA sequences for enhanced optical response of DNA-SWNT sensors.
- Led the development of BinderSpace, an open-source Python package for motif analysis, clustering, and visualization of affinity-selected oligonucleotides and peptides.
- Constructed MD simulation pipelines to study ligand binding (e.g., dopamine, riboflavin) and the impact of antimicrobial peptides on DNA-SWNT conjugates.
- Automated docking studies via Linux shell scripting and AutoDock Vina for evaluating HPV capsid surface interactions.
- Oversaw deployments of Elasticsearch and Kibana on AWS and Google Cloud for advanced data visualization.

Python Programmer and DevOps Engineer Oct 2016 – Dec 2019
Fanava IDC, Tehran, Iran

- Developed Python scripts to optimize business processes and data operations.
- Managed server performance, security, and uptime.

- Deployed and maintained Python web applications using Django.
- Integrated machine learning models into production environments, managing their lifecycle for continuous effectiveness.

Additional Experience

Ph.D. Teaching Assistant Jan 2020 – Dec 2023
University of Texas at El Paso, TX, USA

Advanced Python Instructor Jul 2024
University of Maryland Institute for Health Computing, MD, USA

Education

Ph.D. in Chemistry Jan 2020 – Dec 2023
University of Texas at El Paso, El Paso, TX, USA
Coursework (Computer Science Department): Machine Learning, Data Mining, Database Management, Artificial Intelligence, Computer Vision

Master's Degree in Polymer Engineering Sep 2013 – Jun 2016
Isfahan University of Technology, Isfahan, Iran

Bachelor's Degree in Chemical Engineering Sep 2008 – Sep 2013
Isfahan University of Technology, Isfahan, Iran

Selected Publications

1. **P. Kelich**, J. Adams, S. Jeong, N. Navarro, M.P. Landry, L. Vukovic.
Predicting Serotonin Detection with DNA-Carbon Nanotube Sensors Across Multiple Spectral Wavelengths.
Journal of Chemical Information and Modeling. (link)

2. **P. Kelich**, H. Zhao, J.R. Orona, L. Vukovic.
BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules.
Journal of Computational Chemistry. (link)

3. **P. Kelich**, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vukovic.
Discovery of DNA–Carbon Nanotube Sensors for Serotonin with Machine Learning and Near-infrared Fluorescence Spectroscopy.
ACS Nano. (link)

4. A. Yadav, **P. Kelich**, N.E. Kallmyer, N.F. Reuel, L. Vukovic.
Characterizing the Interactions of Cell Membrane-Disrupting Peptides with Lipid-Functionalized Single-Walled Carbon Nanotube Systems for Antimicrobial Discovery.
ACS Applied Materials & Interfaces. (link)

5. S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vukovic, S. Kruss, M. Havenith.
Fluorescence Changes in Carbon Nanotube Sensors Correlate with THz Absorption of Hydration.
Nature Communications. (link)

6. A.I. Ekanayake, L. Sobze, **P. Kelich**, J. Youk, N.J. Bennett, R. Mukherjee, A. Bhardwaj, F. Wuest, L. Vukovic, R. Derda.
Genetically Encoded Fragment-Based Discovery from Phage-Displayed Macrocyclic Libraries with Genetically Encoded Unnatural Pharmacophores.
Journal of the American Chemical Society. (link)