CURRICULUM VITAE

Payam Kelich

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EDUCATION

[01/2020-12/2023] **The University of Texas at El Paso, El Paso, TX**
Ph.D. Chemistry
Dissertation: "Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"
Supervisor: Dr. Lela Vuković

[09/2013-06/2016] **The Isfahan University of Technology, Isfahan, Iran**
Master's Degree, Polymer Engineering- Polymer Industry
Dissertation: "Molecular Dynamics Simulation of Poly (ethylene succinate) Crystallization Induced by Carbon Nanotubes and Graphene Nanosheets"
Supervisor: Dr. Ahmad Asadinezhad

[09/2008-09/2013] **The Isfahan University of Technology, Isfahan, Iran**
Bachelor's Degree. Chemical Engineering

WORK EXPERIENCES

[2024 - Present] **Postdoctoral Research Associate**
University of Illinois Urbana-Champaign, IL, USA
Supervisor: Dr. Emad Tajkhorshid
Experiences:

- Developed and applied machine learning models using Chemprop for predictive analytics and REINVENT4's generative AI to design novel molecules, utilizing datasets retrieved from ChEMBL 34 to efficiently screen extensive chemical libraries and identify potential ligands for specific protein targets. Employed Diffdock for docking, enhancing the accuracy and efficiency of target-ligand interactions. Designed NLP models to map functional descriptions to cellular function labels, enabling precise classification of ligands based on target location and tissue specificity.
- Utilized DiffLinker, a diffusion generative model, to design linkers between chemical fragments to create new Metal-Organic Frameworks (MOFs) aimed at CO_2 adsorption. Responsible for retraining DiffLinker using COMPAS, CoREMOF, and hMOF databases to generate novel MOFs.
- Modeled and simulated a novel stomatin structure using AlphaFold 3, MOE, and NAMD—the first simulation of its kind—to assist experimentalists in observing cholesterol behavior within lipid rafts near stomatin.
- Utilized DiffDock to identify the binding site of chloroquine on P. falciparum CQ-resistance transporter (PfCRT), revealing structural insights into drug resistance mechanisms. Performed Molecular Dynamics simulations with NAMD on PfCRT variants 7G8 and HB3, uncovering conformational differences contributing to resistance—findings that aided in developing potential therapeutic strategies.
- Developed a VMD (Visual Molecular Dynamics) plugin for antibody annotation using the KABAT algorithm based on the antibody sequence alone, enhancing the structural analysis of antibodies. Investigated antibody interactions with polymeric interfaces as

part of a collaborative project with Merck KGaA, contributing to advancements in biocompatible material design.

- Leveraged the DeepChem cheminformatics library, utilizing Graph Convolutional Neural Networks (GCNNs), to train models on DNA Encoded Libraries represented in SMILES format. Aimed to predict novel binders to target proteins.
- Administered Linux systems to establish and maintain computational environments for running deep-learning Python libraries and molecular dynamics simulations on local clusters and high-performance computing (HPC) resources. Installed and configured deep learning frameworks (TensorFlow, PyTorch) and molecular dynamics software (NAMD, GROMACS), managing software dependencies and environment modules.

[2020 - 2023] **Ph.D. Research Associate**
University of Texas at El Paso, TX, USA
Supervisor: Dr. Lela Vuković
Experiences:

- Conducted a cheminformatics study utilizing machine learning classification models to predict the subcellular localization of small molecules using a retrieved dataset of SMILE representation of chemical compounds from ChEMBL, Pharos, and Drug Central databases. Trained models on RDKit molecular fingerprints, combinations of molecular descriptors, and DeepChem GCNNs models.
- Developed deep learning models, including convolutional neural networks (CNNs), artificial neural networks (ANNs), and variational autoencoders (VAEs), to predict and generate DNA sequences that enhance the optical response of DNA-wrapped single-walled carbon nanotube (DNA–SWNT) sensors for neurotransmitter detection. Utilized Keras with TensorFlow backend to implement these models, employing long short-term memory (LSTM) and CNN architectures to classify DNA ligands based on near-infrared fluorescence responses and to train VAEs for generating novel DNA sequences.
- Developed BinderSpace, an open-source Python package, by designing and implementing advanced features for bioinformatics analysis of large datasets of target-binding molecules such as aptamers and peptides, led the creation of modules for motif analysis, sequence space visualization, clustering analyses, and sequence extraction from clusters of interest.
- Installed and maintained Elasticsearch and Kibana on AWS and Google Cloud platforms. Collaborated with teams to support data visualization and search functionalities as part of a project at the University of North Texas.

[2016 - 2019] **Python Programmer and DevOps Engineer**
Fanava IDC, Tehran, Iran
Experiences:

- Developed and implemented efficient Python scripts to streamline business processes and optimize data operations.
- Managed Linux servers as a System Administrator, ensuring optimal performance, security, and high uptime.
- Engineered, deployed, and maintained Python web applications using Django and Flask frameworks on Linux servers, enhancing system efficiency and functionality.
- Served as a Junior MLOps Engineer, integrating machine learning models into production and managing their lifecycle to ensure continuous effectiveness.

OTHER EXPERIENCES

[2020-2023] **Ph.D. Teaching Assistant**
University of Texas at El Paso, TX, USA

- Assisted in delivering course materials for General Chemistry and Organic Chemistry labs.

[Jul 2024] **Advanced Python Instructor**
University of Maryland Institute for Health Computing, MD, USA
- Serving as an instructor for a summer school program on Pandas, a Python library for data manipulation and analysis.

PUBLICATIONS

Published Papers:

1. "Fluorescence changes in carbon nanotube sensors correlate with THz absorption of hydration". S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vuković, S. Kruss, M. Havenith. *Nature Communication* 15,1 (2024).
DOI: https://doi.org/10.1038/s41467-024-50968-9

2. "Predicting Serotonin Detection with DNA-Carbon Nanotube Sensors Across Multiple Spectral Wavelengths." **P Kelich**, J Adams, S Jeong, N Navarro, MP Landry, L Vukovic. *Journal of Chemical Information and Modeling*. 64, 10, 3992–4001(2024)
DOI: https://doi.org/10.1021/acs.jcim.4c00021

3. "Directed Evolution of Near-Infrared Serotonin Nanosensors with Machine Learning-Based Screening."S An, Y Suh, **P Kelich**, D Lee, L Vukovic, S Jeong. *Nanomaterials* 14,3 (2024).
DOI: https://doi.org/10.3390/nano14030247

4. "Genetically-Encoded Discovery of Perfluoroaryl-Macrocycles that Bind to Albumin and Exhibit Extended Circulation in-vivo." J.YK. Wong, A.I. Ekanayake, S. Kharchenko, S.E. Kirberger, R. Qiu, **P. Kelich**, S. Sarkar, E.R. Alvizo-Paez, J. Miao, S. Kalhor-Monfared, J.J. Dwyer, J.M. Nuss, Y.S. Lin, M.S. Macauley, L. Vuković, W.CK. Pomerantz, R. Derda. *Nature Communication* 14,1 (2023).
DOI: https://doi.org/10.1038/s41467-023-41427-y

5. "BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules" **P. Kelich**, H. Zhao, L. Vuković. *Journal of Computational Chemistry* (2023).
DOI: https://doi.org/10.1002/jcc.27130

6. "Characterizing the Interactions of Cell Membrane-Disrupting Peptides with Lipid-Functionalized Single-Walled Carbon Nanotube Systems for Antimicrobial Discovery" A. Yadav, **P. Kelich***, N.E. Kallmyer, N.F. Reuel, L. Vuković. *ACS Applied Materials & Interfaces,* 15, 24084–24096 (2023). (***** co-first author)
DOI: https://doi.org/10.1021/acsami.3c01217

7. "Machine learning enables discovery of DNA-carbon nanotube sensors for serotonin." **P. Kelich**, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković. *ACS Nano*, 16, 736–745 (2021).
DOI: https://doi.org/10.1021/acsnano.1c08271

8. "Computational Modeling of the Virucidal Inhibition Mechanism for Broad-Spectrum Antiviral Nanoparticles and HPV16 Capsid Segments". P. Chaturvedi, **P. Kelich**, T.A. Nikita, L. Vuković. *The Journal of Physical Chemistry B 125, 48, 13122–13131*(2021).
DOI: https://doi.org/10.1021/acs.jpcb.1c07436

9. "Genetically Encoded Fragment-Based Discovery from Phage-Displayed Macrocyclic Libraries with Genetically Encoded Unnatural Pharmacophores." A.I. Ekanayake, L. Sobze, **P. Kelich**, J. Youk, N.J. Bennett, R. Mukherjee, A. Bhardwaj, F. Wuest, L. Vuković, R. Derda. *Journal of the American Chemical Society,* 143, 5497–5507 (2021).
DOI: https://doi.org/10.1021/jacs.1c01186

10. "Molecular simulation study on brushes of poly (2-ethyl-2-oxazoline)", **P. Kelich**, A. Asadinezhad. *Materials Today Communications.* 21,100681(2019).
DOI: https://doi.org/10.1016/j.mtcomm.2019.100681

11. "Effects of carbon nanofiller characteristics on PTT chain conformation and dynamics: A computational study A. Asadinezhad, **P. Kelich**. *Applied Surface Science,* 392,981-990(2017).
DOI: https://doi.org/10.1016/j.apsusc.2016.09.137

12. "Adsorption of poly(ethylene succinate) chain onto graphene nanosheets: A molecular simulation" **P. Kelich**, A. Asadinezhad. *Journal of Molecular Graphics and Modelling,*69,26-38 (2016).
DOI: https://doi.org/10.1016/j.jmgm.2016.08.003

13. "Molecular Dynamics Insights into Behavior of Poly(ethylene succinate) Single Chain on Carbon Nanotube Surface" **P. Kelich**, A. Asadinezhad. *The Journal of Physical Chemistry C*, 119,26143-26153 (2015).
DOI: https://doi.org/10.1021/acs.jpcc.5b07844

Accepted:

14. "β -Cyclodextrin Derivatives Bind Aromatic Side Chains of the Cyclic Peptide Lanreotide." N. Jafari, J. Douglas, S. Neuenswander, **P. Kelich**, M. Hageman. *Journal of Pharmaceutical Sciences.*

In Preparation:

15. "Discovery of DNA-Carbon Nanotube Sensors for Oxytocin Detection Through Machine Learning, Generative Models, and Near-Infrared Fluorescence Spectroscopy." **P. Kelich**, J. Adams, M.P. Landry, L. Vuković.

16. "Machine Learning Models for Predicting the Subcellular Localization of Small Molecules." **P. Kelich**, A. Yadav, Md Nurunnabi, L. Vuković.

SKILLS

- **Major skills:** Machine learning, Data science, Cheminformatics, Molecular dynamics simulation, Molecular docking, Data mining, Database management, Generative AI.
- **Programming Languages:** Python, C, Bash Script, TCL
- **Python Machine Learning Libraries:** NumPy, Pandas, PyTorch, TensorFlow, Scikit-Learn, Deepchem, Matplotlib
- **Python Cheminformatics Libraries:** Chemprop, REINVENT4, Biopython, RDKit
- **Computational Chemistry Software:** NAMD, AutoDock, VMD, MOE, Schrodinger Maestro, MDAnalysis
- **Operating Systems:** Linux, Unix-based operating systems, Docker

PRESENTATIONS

[2021] Selected as a Texas Researcher to Present at TACC Symposium
P. Kelich, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković, "Learning and Predicting DNA Sequences in DNA-nanotube Conjugates with High Response to Serotonin". *TACCSTER 2021 Proceedings,* Virtual meeting, 2021. (Presentation).

[2022] Presented at ACS Fall 2022 conference.
P. Kelich, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vuković, "Machine learning and near-infrared fluorescence spectroscopy for discovery of DNA-carbon nanotube sensors of serotonin". *American Chemical Society Meeting*, Chicago, Illinois, August 21 - 25, 2022. (Presentation).

[2023] Presented at Annual Biochemistry and Chemistry Day at University of Texas at El Paso.
P. Kelich, What ChatGPT means for chemistry? concerns and ethical usage. (Presentation)

[2023] Presenting at ACS Fall 2023 conference.

P. Kelich, H. Zhao, L. Vuković, "BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules". *American Chemical Society Meeting*, San Francisco, California, August 13-17, 2023. (Poster).

[2023] Presenting at Theoretical and Computational Biophysics Group at UIUC.
P. Kelich.
"Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"

[2023] Presenting at Ding Group at Tufts UTufts University.
P. Kelich.
"Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding"

MEDIA COVERAGE

[2021] Texas Advanced Computing Center highlighted our research. News Link
[2021] UTEP NewsFeed highlighted our NSF grant. News Link

LANGUAGE SKILLS

- **English**: Fluent
- **French:** Basic

SERVICE

American Chemical Society (Since 2022)

Biophysical society (Since 2024)

Dr Vuković lab system admin (Since 2020)

REFERENCES

Dr. Lela Vuković, Associate Professor of Chemistry
Department of Chemistry and Biochemistry, The University of Texas at El Paso, El Paso, TX, USA.
Email: lVuković@utep.edu

Dr. Markita Landry, Associate Professor of Chemical and Biomolecular Engineering
Department of Chemical Engineering, the University of California, Berkeley, Berkeley, CA, USA.
Email: landry@berkeley.edu

Dr. Ratmir Derda, Professor of Chemistry
Department of Chemistry, the University of Alberta, Edmonton, AB, Canada.
Email: ratmir@ualberta.ca