CURRICULUM VITAE

Payam Kelich

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Education

Ph.D. in Chemistry Jan 2020 – Dec 2023
University of Texas at El Paso, El Paso, TX

Dissertation: *Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High Affinity Target Binding*
Supervisor: Dr. Lela Vukovic

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

Dissertation: *Molecular Dynamics Simulation of Poly (ethylene succinate) Crystallization Induced by Carbon Nanotubes and Graphene Nanosheets*
Supervisor: Dr. Ahmad Asadinezhad

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

Experience

Postdoctoral Research Associate Jan 2024 – present
University of Illinois Urbana-Champaign, IL, USA
Supervisor: Dr. Emad Tajkhorshid

- Developed a computational pipeline to model and simulate a stomatin structure by integrating diverse techniques. Employed AlphaFold3 to add missing residues based on cryo-EM data and used MOE for small-gap modeling and protonation state determination. Constructed the membrane environment with CHARMM-GUI and ran molecular dynamics (MD)/steered molecular dynamics (SMD) simulations using NAMD3, with trajectory analysis performed via MDAnalysis and an in-house Visual Molecular Dynamics (VMD) script.
- Engineered an integrated cheminformatics framework to predict the subcellular localization of small molecules. Managed a local ChEMBL35 instance with custom SQL queries to extract SMILES and protein targets, applying REINVENT4 for data augmentation in sparse regions. Designed a Python API to retrieve protein family data from the Pharos database, and integrated Chemprop's message passing neural network and DeepChem's graph convolutional network for deep model training, while employing RDKit fingerprints for generating feature vectors in traditional machine learning. Containerized the workflow to streamline deployment and enable scalable predictions.
- Utilized DiffDock, MOE to identify the binding site of chloroquine on *P. falciparum* CQ-resistance transporter (PfCRT), revealing structural insights into drug resistance mechanisms. Performed MD 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 plugin for antibody annotation using the KABAT algorithm based solely on the antibody sequence and PDB file in a collaborative project with Merck KGaA.
- Utilized DiffLinker, a diffusion generative model, to design linkers between chemical fragments for new Metal-Organic Frameworks (MOFs) aimed at CO_2 adsorption. Retrained DiffLinker using COMPAS, CoREMOF, and hMOF databases to generate novel MOFs.

Ph.D. Research Associate Jan 2020 – Dec 2023
University of Texas at El Paso, TX, USA
Supervisor: Dr. Lela Vukovic

- Developed deep learning models—including convolutional neural networks (CNNs), multi-layer perceptron neural networks, 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.

- Developed BinderSpace, an open-source Python package for bioinformatics analysis of large datasets of affinity-selected molecules such as oligonucleotides and peptides. Led the creation of modules for motif analysis, sequence space visualization, clustering, and sequence extraction, applying unsupervised learning techniques and dimensionality reduction methods to uncover hidden patterns in high-dimensional data.
- Engineered a workflow to investigate how dopamine and riboflavin bind to DNA-SWCNT conjugates and influence water distribution at the CNT surface. First, employed NAMD with SMD to pack DNA onto the SWCNT, generating the initial conformations. Then, ran MD simulations to analyze ligand binding events, and used an in-house Python script to quantify changes in water coverage.
- Established a pipeline to investigate how antimicrobial peptides affect membrane distribution using SWNT sensor-based MD simulations.Developed an automated script to generate initial POPC-SWNT conformations and proceeded with simulations using various peptides to evaluate their impact on membrane behavior.
- Developed a general-purpose Linux shell script that integrates with AutoDock Vina to automate docking for any ligand–protein pair, outputting binding sites based on the best docking scores. This tool streamlines the docking process and was applied to HPV capsid surfaces to guide sulfonated NP placements on L1 protein segments.
- Installed and maintained Elasticsearch and Kibana on AWS and Google Cloud platforms, collaborating with teams to support data visualization and search functionalities.

Python Programmer and DevOps Engineer Oct 2016 – Dec 2019

Fanava IDC, Tehran, Iran

- Developed 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 frameworks on Linux servers.
- Served as a Junior MLOps Engineer, integrating machine learning models into production and managing their lifecycle.

Other Experiences

Ph.D. Teaching Assistant Jan 2020 – Dec 2023

University of Texas at El Paso, TX, USA

- Assisted in delivering course materials for general chemistry and organic chemistry labs.

Advanced Python Instructor Jul 2024

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 paper:

1. **β-Cyclodextrin Derivatives Bind Aromatic Side Chains of the Cyclic Peptide Lanreotide** 2024
   N. Jafari, J. Douglas, S. Neuenswander, **P. Kelich**, M. Hageman.
   Journal of Pharmaceutical Sciences, 114, 878–886.
   DOI: https://doi.org/10.1016/j.xphs.2024.10.042

2. **Fluorescence Changes in Carbon Nanotube Sensors Correlate with THz Absorption of Hydration** 2024
   S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vukovic, S. Kruss, M. Havenith.
   Nature Communications 15, 1.
   DOI: https://doi.org/10.1038/s41467-024-50968-9

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

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

5. **Genetically-Encoded Discovery of Perfluoroaryl-Macrocycles that Bind to Albumin and Exhibit Extended Circulation in-vivo** 2023
J.Y.K. 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. Vukovic, W.CK. Pomerantz, R. Derda.
Nature Communications 14, 1.
DOI: https://doi.org/10.1038/s41467-023-41427-y

6. ***BinderSpace*: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules** 2023
P. Kelich, H. Zhao, J.R. Orona, L. Vukovic.
Journal of Computational Chemistry 44(22), 1836–1844.
DOI: https://doi.org/10.1002/jcc.27130

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

8. **Discovery of DNA–Carbon Nanotube Sensors for Serotonin with Machine Learning and Near-infrared Fluorescence Spectroscopy** 2021
P. Kelich, S. Jeong, N. Navarro, J. Adams, X. Sun, H. Zhao, M.P. Landry, L. Vukovic.
ACS Nano, 16, 736–745.
DOI: https://doi.org/10.1021/acsnano.1c08271

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

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

11. **Molecular Simulation Study on Brushes of Poly (2-ethyl-2-oxazoline)** 2019
P. Kelich, A. Asadinezhad.
Materials Today Communications, 21, 100681.
DOI: https://doi.org/10.1016/j.mtcomm.2019.100681

12. **Effects of Carbon Nanofiller Characteristics on PTT Chain Conformation and Dynamics: A Computational Study** 2017
A. Asadinezhad, **P. Kelich**.
Applied Surface Science, 392, 981–990.
DOI: https://doi.org/10.1016/j.apsusc.2016.09.137

13. **Adsorption of Poly(ethylene succinate) Chain onto Graphene Nanosheets: A Molecular Simulation** 2016
P. Kelich, A. Asadinezhad.
Journal of Molecular Graphics and Modelling, 69, 26–38.
DOI: https://doi.org/10.1016/j.jmgm.2016.08.003

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

To be submitted:

- 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. Vukovic.
- Machine Learning Models for Predicting the Subcellular Localization of Small Molecules. **P. Kelich**, A. Yadav, S. Sirimulla, L. Vukovic.
- An Integrative Experimental–Computational Study of Stomatin: Merging Cryo-EM Data and Computational Modeling to Explore Structure and Dynamics. F. Vallese, **P. Kelich**, E. Tajkhorshid, O.B. Clarke.

Presentations

- **Presented at the Biophysical Society 2025 Conference** (Poster) 2025
AVANA: an Open-Source VMD Plugin for Kabat Antibody Annotation and Visualization.

- **Presented at Scientific Review Meetings 2025 at Merck KGaA** (Presentation) 2024
Molecular Dynamics Simulation of Antibody Interactions with Material Surfaces in Drug Product Development.

- **Presented at Annual Biochemistry and Chemistry Day at University of Texas at El Paso** (Presentation) 2023
What ChatGPT Means for Chemistry? Concerns and Ethical Usage.

- **Presented at ACS Fall 2023 conference** (Poster) 2023
BinderSpace: A Package for Sequence Space Analyses for Datasets of Affinity-Selected Oligonucleotides and Peptide-Based Molecules.

- **Presented at Theoretical and Computational Biophysics Group at UIUC** (Presentation) 2023
Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High-Affinity Target Binding.

- **Presented at Ding Group at Tufts University** (Presentation) 2023
Computation-Assisted Molecular Discovery for Biomedical Applications: Seeking Small Molecules and DNA Sequences with High-Affinity Target Binding.

- **Presented at ACS Fall 2022 conference** (Presentation) 2022
Machine learning and near-infrared fluorescence spectroscopy for discovery of DNA-carbon nanotube sensors of serotonin.

- **Presented as a Texas Researcher at TACC Symposium (TACCSTER 2021 Proceedings)** (Presentation) 2021
Learning and Predicting DNA Sequences in DNA-nanotube Conjugates with High Response to Serotonin.

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. Vukovic lab system admin (Since 2020)
- Dr. Tajkhorshid lab system admin (Since 2024)

References

- **Dr. Lela Vukovic**
  Associate Professor of Chemistry and Biochemistry
  The University of Texas at El Paso, El Paso, TX, USA
  Email: lvukovic@utep.edu
- **Dr. Markita Landry**
  Associate Professor of Chemical and Biomolecular Engineering
  University of California, Berkeley, CA, USA
  Email: landry@berkeley.edu
- **Dr. Ratmir Derda**
  Professor of Chemistry
  The University of Alberta, Edmonton, AB, Canada
  Email: ratmir@ualberta.ca