

CURRICULUM VITAE

Payam Kelich

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EDUCATION

- [01/2020 - Present] **The University of Texas at El Paso, El Paso, TX**
Ph.D. Chemistry (expected graduation date: December 2023)
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, 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, Isfahan, Iran**
Bachelor’s Degree. Chemical Engineering

WORK EXPERIENCES

- [2020 - Present] **PhD Research Associate**
University of Texas at El Paso, TX, USA
Supervisor: Dr. Lela Vuković
Responsibilities:
- Played an instrumental role in groundbreaking research concerning the binding and sensing of molecular analytes in DNA-CNT conjugates, driving forward the scientific understanding in this field.
 - Facilitated future research proposals by creating comprehensive preliminary data reports and project specifications, thereby improving team efficiency.
 - Participated in critical research of peptidomimetics, derived from genetically encoded libraries, for high-affinity binding to protein targets, contributing to advancements in drug design and biotechnology.
 - Collaborated with international researchers to perform advanced computational modeling of nanoscale systems, promoting interdisciplinary knowledge exchange and expediting progress in nanotechnology research.
 - Developed the Linux infrastructure necessary for running molecular dynamics (MD) simulations and machine learning projects, enhancing research capabilities and outcomes.
- [2020-Present] **PhD Teaching Assistant**
University of Texas at El Paso, TX, USA
- Assisted in delivering course materials for General Chemistry and Organic Chemistry labs, enriching the students' learning experience.

[2016 - 2019]

Python Programmer and DevOps Engineer

Fanava IDC, Tehran, Tehran, Iran

Responsibilities:

- Developed and implemented efficient Python scripts, streamlining business processes and data operations.
- Operated as a System Administrator for Linux servers, ensuring optimal performance, security, and maintaining high uptime.
- Engineered, deployed, and maintained Python applications on Linux servers to enhance system efficiency and functionality.
- Worked as a Junior MLOps engineer, integrating Machine Learning models into production and managing the lifecycle of these models to ensure their effectiveness.

PUBLICATIONS

Published Papers:

1. “Genetically-Encoded Discovery of Perfluoroaryl-Macrocycles that Bind to Albumin and Exhibit Extended Circulation in-vivo”. 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. Vuković, W.C.K. Pomerantz, R. Derda. *Nature Communication* 14,1 (2023).
DOI: <https://doi.org/10.1038/s41467-023-41427-y>
2. “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>
3. “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>
4. “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>
5. “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.jpcc.1c07436>
6. “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>
7. “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>
8. “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>
9. “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>

10. "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>

Papers in preparation:

11. "Local Solvation of DNA Functionalized Carbon Nanotube Biosensors Probed with THz Spectroscopy". S.S. Nalige, P. Galonska, **P. Kelich**, S. Ramos, L. Sistemich, C. Herrmann, L. Vuković, S. Kruss, M. Havenith.
12. "Predicting New DNA-Nanotube Sensors of Serotonin from Extended nIR Emission Spectra". **P. Kelich**, L. Vuković.
13. "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.
14. "Machine Learning Models for Predicting the Subcellular Localization of Small Molecules". **P. Kelich**, A. Yadav, Md Nurunnabi, L. Vuković.

SKILLS

Programming Languages: Python, C, Bash Script

Python Cheminformatics Libraries: Biopython, RDKit, DeepChem

Python Scientific Libraries: NumPy, Pandas, PyTorch, TensorFlow, Scikit-Learn

Computational Chemistry Software: GROMACS, NAMD, AutoDock, VMD

Operating Systems: Linux and Unix-based Operating Systems, Windows

Other Software: Microsoft Office, Mendeley, Zotero

CERTIFICATES

- [2023] [Coursera: Machine Learning Specialization](#)
- [2023] [Coursera: Deep Learning Specialization](#)
- [2023] [Coursera: Generative Adversarial Networks \(GANs\) Specialization](#)

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*, Chicago, Illinois, August 13-17, 2023. (Poster).

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
- **Farsi (Persian):** Native

SERVICE

American Chemical Society (Since 2022)

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: lvukovic@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.
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