Dakota Folmsbee

Postdoctoral Scholar · University of Pittsburgh
800 Murdoch I Bldg, 3420 Forbes Avenue, Pittsburgh, PA 15260
(+1) 802-683-4502 | dlf57@pitt.edu | dlf57.github.io | dlf57

Experience

T32 Postdoctoral Scholar *March 2022 - Present*
University of Pittsburgh - Koes Group

- Lead a team of 4 undergraduate researchers to investigate the structural basis for potency and efficacy of positive allosteric modulators in ion channels.
- Conducted a comprehensive analysis of existing targets to understand structural properties to aid in identifying potential new targets and ensuring selectivity.
- Developed a computational pipeline for creating, simulating, and analyzing ion channels in a membrane bilayer
- Performed pharmacophore searches to effectively screen known compounds for additional hits, resulting in the identification of promising candidates for further investigation.

Computational/Physical Chemistry Graduate Student Researcher *Jan. 2017 - Feb. 2022*
University of Pittsburgh - Hutchison Group

- Devised a novel approach to generate conformers based on quantum torsional information as an alternative to crystal structure data-based methods.
- Engineered machine learning representations for rapid property prediction of molecules to aid in molecular screening
- Benchmarked state of the art machine learning methods against conventional quantum methods.
- Assisted in the development of a code base utilizing a genetic algorithm for efficient screening of dielectric materials.

General Chemistry Teaching Assistant/Fellow *Aug. 2016 - Dec. 2017*
University of Pittsburgh

- Taught recitation and laboratory sections for multiple general chemistry courses.
- Mentored and supervised new graduate and undergraduate teaching assistants in their teaching duties.

Education

University of Pittsburgh *Aug. 2016 - Feb. 2022*
Ph.D. in Phyiscal Chemistry *Pittsburgh, PA*

Clarkson University *Aug. 2012 - May 2016*
B.S. in Chemistry *Potsdam, NY*

Programming Projects

chemreps *Aug. 2018 - March 2020*
Developer

- https://github.com/chemreps/chemreps
- Directed and developed an open source molecular representation library for machine learning in chemistry

QM/MM Study Group *July 2018 - Dec. 2018*
Instructor & Organizer

- https://github.com/shivupa/QMMM_study_group
- Organized and taught new graduate students various topics pertaining to computational chemistry

Skills

Computational Chemistry	RDKit, Open Babel, Avogadro, Gaussian, ORCA, xTB
Computational Biology	Amber, WESTPA, MDAnalysis, PyMOL, VMD, CHARMM-GUI, AlphaFold
Programming	Python, Scikit-Learn, Tensorflow, Keras, PyTorch, Bash, Git, LaTeX, C++, Julia