

Jordan Epstein

PRODUCT · CHEMISTRY · SOFTWARE

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Education

New York University

New York, NY

B.S. IN CHEMISTRY

May 2017

- Graduated High Honors, Major GPA 3.83/4.00
- Focused coursework in Quantum Mechanics along with computer science and molecular biology

Undergraduate Thesis

Femtosecond Dynamics of the Plant Phytochrome Cph1

- Generated mutations in the Cph1 apoprotein to compare with wildtype
- Used spectroscopic techniques (2D/3D Electronic Spectroscopy, Transient Absorption) to elucidate the femtosecond dynamics following photoexcitation of the Cph1 holoprotein
- Constructed models to explain observed kinetics by describing the excited-state potential energy surface - including a possible conical intersection in the E → Z isomerization
- Designed active-learning optimization algorithm for optical pulse shaper

Work Experience

Product Manager (Large Scale Applications)

May 2023 - May 2025

SCHRÖDINGER

- Took FEP+ Protocol Builder, an automated workflow for model optimization, from a closed-beta to a full release
 - FEP+ is Schrödingers proprietary, physics-based free energy perturbation technology for predicting protein-ligand binding affinities
- Led the development of FEP+ in LiveDesign and FEP+ Pose Builder, a browser-based platform for running pose generation and FEP+ calculations at scale, leading to accelerated Hit to Lead and Lead Optimization time frames
- Performed research on FEP+ best practices, enabling automation and usage of FEP+ in drug discovery at large scale

Senior Software Developer (Desmond)

January 2022 - May 2023

SCHRÖDINGER

- Drove development of new feature requests and new workflows using the Pythonic API for the FEP+ and Desmond (Schrödinger's Molecular Dynamics software) products
- Implemented FEP+ groups, a framework to analyze ensemble averaged affinity predictions over enumerated microstates (protonation, tautomeric, conformational)
- Collaborated on scientific projects, leading to a publication which benchmarked the usage of protein FEP+ and the effect of using the aforementioned FEP+ groups framework

Software Developer II (Desmond)

March 2020 - January 2022

SCHRÖDINGER

- Developed the command line interfaces for running Schrödinger's FEP+ and Molecular Dynamics-based tools
- Created Python APIs for usage by front-end team
- Refactored legacy code, setting the foundation to accelerate future feature development
- Addressed usability of Schrödinger's FEP-based technologies through improvements to command line interfaces, documentation, and code quality

Software Developer I (Python Front-end Development)

June 2017 - March 2020

SCHRÖDINGER

- Worked alongside scientists and UX designers to implement a PyQt based front-ends for chemical modeling software spanning a range of scientific domains
- Wrote javascript (React, Redux) web tools for integration with Schrödinger's LiveDesign
- Developed bespoke Python scripts requested by customers to complement their use of Schrödinger software in their scientific workflows

Research Experience

Turner Lab

January 2016 - June 2017

NEW YORK UNIVERSITY, DEPARTMENT OF CHEMISTRY

- Completed senior honors thesis and performed research leading to three publications
- Used femtosecond spectroscopy to study nonadiabatic dynamics in phytochrome Cph1
- Generated point mutations in Cph1, optimized recombinant protein expression protocol, wrote MATLAB software for data acquisition

Mazzoni Lab

February 2015 - December 2015

NEW YORK UNIVERSITY, DEPARTMENT OF BIOLOGY

- Used molecular neurobiology techniques to study embryonic stem cell development and differentiation
- Generated multiple cell lines for use in transfection, imaged cells in various stages of development using confocal microscopy

Restrepo Lab

May 2015 - September 2015

UNIVERSITY OF COLORADO - ANSCHUTZ

- Used electrophysiological and genetic techniques to study sensory signal processing in the olfactory system of mice
- Developed software for data acquisition and processing, performed immunohistochemistry to analyze proliferation of neurons

Publications

- Sampson JM, Cannon DA, Duan J, **Epstein JCK**, Sergeeva AP, Katsamba PS, Mannepalli SM, Bahna FA, Adihou H, Guéret SM, Gopalakrishnan R, Geschwindner S, Rees DG, Sigurdardottir A, Wilkinson T, Dodd RB, De Maria L, Mobarec JC, Shapiro L, Honig B, Buchanan A, Friesner RA, Wang L. Robust Prediction of Relative Binding Energies for Protein-Protein Complex Mutations Using Free Energy Perturbation Calculations. *J Mol Biol.* 2024 Aug 15;436(16):168640.
- Bizimana LA, **Epstein J**, Turner DB. Inertial water response dominates protein solvation dynamics. *Chem Phys Lett.* 2019 Aug;728:1-5.
- Farfan CA, **Epstein J**, Turner DB. Femtosecond pulse compression using a neural-network algorithm. *Opt Lett.* 2018 Oct 15;43(20):5166.
- Bizimana LA, **Epstein J**, Brazard J, Turner DB. Conformational homogeneity in the Pr isomer of phytochrome Cph1. *J Phys Chem B.* 2017 Mar 16;121(12):2622-30.

Achievements

- 2017 **Phi Lambda Upsilon**, Chemistry Honor's Society
- 2017 **Undergraduate Research Conference Presenter**, NYU
- 2017 **Dean's List**, College of Arts and Science
- 2016 **Dean's List**, College of Arts and Science
- 2014 **Dean's List**, College of Arts and Science

Awards

- 2016 **DURF Recipient - Fall**, Dean's Undergraduate Research Fund
- 2016 **DURF Recipient - Spring**, Dean's Undergraduate Research Fund
- 2016 **DURF Recipient - Winter**, Dean's Undergraduate Research Fund

Skills

- **Programming Languages:** Professional experience in Python (including Qt framework,) Javascript (React, Redux). Additional proficiency in Java, MATLAB, TeX
- **Product:** Greenfield to full product release, JIRA, project management, presentations
- **Software Development:** Object-Oriented Programming, GUI Design Implementation, Git, Code Review, Scientific Software Design, Data Structures
- **Laboratory:** Designing and executing research projects independently, spectroscopic data analysis, protocol optimization, software development, molecular biology (PCR, cloning, gel electrophoresis, protein expression and purification).
- **Other:** Easily adapts to learning new subjects, always looking for new ways to improve performance.