Noah **Flynn**

PhD Candidate · Machine Learning for Drug Discovery

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Education

Washington University in Saint Louis (WUSTL) — *GPA: 3.94/4.00*

Ph.D. Computational Biology — *Aug. 2017 - Present*

University of Illinois at Urbana-Champaign (UIUC) — *GPA: 3.70/4.00*

B.S. Bioengineering — *Aug. 2013 - May 2017*

- Minor in Computer Science

Publications

Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam — *Toxicology*

Dustyn A. Barnette, Mary A. Schleiff, Laura R. Osborn, **Noah Flynn**, Matthew Matlock, S. Joshua Swamidass, and Grover P. Miller — *May 2020*

Vol. 440 — *Online Link*

Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation — *Biochemical Pharmacology*

Dustyn A. Barnette, Mary A. Davis, **Noah Flynn**, Anirudh S. Pidugu, S. Joshua Swamidass, and Grover P. Miller — *Dec 2019*

Vol. 170 — *Online Link*

CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches — *Chemical Research in Toxicology*

Mary A. Davis, Dustyn A. Barnette, **Noah R. Flynn**, Anirudh S. Pidugu, S. Joshua Swamidass, Gunnar Boysen, and Grover P. Miller — *Mar 2019*

Vol. 32 — *Online Link*

Skills

Proficient	Docker, Neo4j, Python (Flask, Numpy, Pandas, Scikit-Learn), PyTorch, TensorFlow 2.0
Comfortable	C++ (CUDA), JavaScript (D3, React), Hadoop, Jekyll, MatLab, Spark, SQL
Have Used	JAVA, R, WolfRam Language

Experience

Department of Pathology & Immunology, WUSTL — *St. Louis, MO*

PhD Candidate — *Mar 2018 - Present*

- Serving as a core maintainer of *XenoSite*, a prediction web service for small molecule biochemistry that hosts several of our labs published models
- Modeling drug metabolism networks via deep learning methods, e.g. graph neural networks, to guide drug development in early stage prediction of drug toxicity, formation of reactive chemical species, and likelihood of adverse drug reactions
- Developing ML models for predicting incidence of drug-induced liver injury given a molecular compound

Merck (MSD) — *West Point, PA*

Modeling & Informatics Machine Learning Intern — *May 2019 - Aug 2019*

- Implemented deep generative models for the purpose of de novo molecular generation and design
- Tuned libraries of generated molecules to desired chemical properties via reinforcement learning
- Applied novel chemical libraries of generated molecules for use in molecular dynamics simulations and to generate new structures for use in ongoing Merck chemistry projects
- Documented and launched an initial release of the tool for use by employees in Merck's Research Labs

AbbVie Inc. *Champaign, IL*

Software Engineer Intern *Jan 2016 - May 2017*

- Created a suite of reusable, web-based data visualization elements and deployed those elements in applications across the pharmaceutical research space to reveal novel views of data
- Programmed and launched a web application for managing all bioinformatics tools, either open-source or developed in-house, that AbbVie R&D uses for drug development and testing
- Managed Oracle database system of relations between researchers and drugs within the company's research space

National Center for Supercomputing Applications *Urbana, IL*

Research Fellow *Aug. 2014 - Apr. 2016*

- Conducted analysis of biomolecular networks to differentiate between organisms of differing economy, flexibility, and robustness and subsequently classify modified organisms within such predefined classes
- Constructed and characterized protein-protein interaction networks, transcription factor networks, and regulatory networks, based off centrality measures, node connectivity, node degree distributions, path detection, and k-core decomposition
- Applied preliminary framework to genetically modified organisms within the context of synthetic biology

Leadership & Recognition

2017	**Director**, Engineering Open House (Educational Non-Profit)	*Champaign, IL*
2016	**Most Valuable Intern**, Research Park	*Champaign, IL*
2015	**Semifinalist**, International Genetically Engineered Machines Competition, Biological Computing Division	*Boston, MA*
2014	**Presenter on Youth STEM Initiatives**, U.S. House of Representatives	*Washington, D.C.*
2014	**Scholarship Recipient**, Levi, Ray, and Shoup Computer Science Award	*Champaign, IL*

Teaching Experience

2018	**Teaching Assistant**, Algorithms for Computational Biology	*WUSTL*
2016	**Teaching Assistant**, Bioinstrumentation Lab	*UIUC*
2015	**Resident Project Advisor (RA)**, Illinois Engineering First-Year Experience, Summer Scholars Program	*UIUC*
2015	**Teaching Assistant**, Engineering Professional Development	*UIUC*
2015	**Course Assistant**, Introduction to Computer Science, Honors Section	*UIUC*
2014	**Course Developer**, Introduction to Computer Science, Honors Section	*UIUC*