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 & Systems Biology — *Aug. 2017 - Present*

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

B.S. Bioengineering, Minor in Computer Science — *Aug. 2013 - May 2017*

Relevant Courses: Machine Learning, Cloud Computing with Big Data, Bioinformatics, Genomics, Parallel Programming, Numerical Analysis, Database Systems, Control Systems, Natural Language Processing, Algorithms for Computational Biology, Linear Algebra

Publications

Tyler B. Hughes*, **Noah Flynn***, Na Le Dang, S. Joshua Swamidass, **Modeling the Bioactivation and Subsequent Reactivity of Drugs**, *Chemical Research in Toxicology*, Jan 2021

Mary A. Schleiff, **Noah R Flynn**, Sasin Payakachat, Benjamin Schleiff, Anna Pinson, Dennis Province, S. Joshua Swamidass, Gunnar Boysen, Grover Miller, **Significance of Multiple Bioactivation Pathways for Meclofenamate as Revealed through Modeling and Reaction Kinetics**, *Drug Metabolism and Disposition*, Nov 2020

Dustyn A. Barnette, Mary A. Schleiff, Arghya Datta, **Noah Flynn**, S. Joshua Swamidass, Grover P. Miller, **Meloxicam methyl group determines enzyme specificity for thiazole bioactivation compared to sudoxicam**, *Toxicology Letters*, Nov 2020

Tyler Hughes, Na Le Dang, Ayush Kumar, **Noah R Flynn**, S. Joshua Swamidass, **The Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites**, *Journal of Chemical Information and Modeling*, Sep 2020

Noah R Flynn, Na Le Dang, Michael D. Ward, S. Joshua Swamidass, **XenoNet: Inference and Likelihood of Intermediate Metabolite Formation**, *Journal of Chemical Information and Modeling*, Jun 2020

Dustyn A. Barnette, Mary A. Schleiff, Laura R. Osborn, **Noah Flynn**, Matthew Matlock, S. Joshua Swamidass, and Grover P. Miller, **Dual mechanisms suppress meloxicam bioactivation relative to sudoxicam**, *Toxicology*, May 2020

Dustyn A. Barnette, Mary A. Davis, **Noah Flynn**, Anirudh S. Pidugu, S. Joshua Swamidass, and Grover P. Miller, **Comprehensive kinetic and modeling analyses revealed CYP2C9 and 3A4 determine terbinafine metabolic clearance and bioactivation**, *Biochemical Pharmacology*, Dec 2019

Mary A. Davis, Dustyn A. Barnette, **Noah R. Flynn**, Anirudh S. Pidugu, S. Joshua Swamidass, Gunnar Boysen, and Grover P. Miller, **CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches**, *Chemical Research in Toxicology*, Mar 2019

*Equal contribution as first-authors

Skills

Proficient Docker, Neo4j, RDKit, Python (Flask, Numpy, Pandas, Scikit-Learn), PyTorch, TensorFlow

Comfortable C++ (CUDA), JavaScript (D3, React), Hadoop, MatLab, SQL

Have Used AWS, JAVA, R, Spark, WolfRam Language

Selected Projects

XenoNet Web Server — *Link*

Primary Contributor & Developer

Develop and maintain network-level models for analyzing the metabolism, reactivity, and bioactivation of drugs

XenoSite Web Server — *Link*

Current Maintainer

Host and maintain several previously published, site of metabolism models for metabolism and reactivity

Carbohydrate Counting Mobile Application for Diabetic Patients

Core Contributor

Worked with a team to develop a mobile application to classify images containing food and assess nutritional content that the user can track

Experience

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

PhD Candidate *Aug 2017 - Present*

- Serving as a core maintainer and developer of *XenoSite* and *XenoNet* prediction web services for small molecule biochemistry
- 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 machine learning approaches for predicting incidence of drug-induced liver injury given electronic health records

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 and integration of QSAR models
- Applied novel chemical libraries of generated molecules for use in docking and molecular dynamics simulations and to generate new structures for use in ongoing Merck chemistry projects and virtual screening
- 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. 2016 - May 2017*

- 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	**Silver Medal**, 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*

Reviewer Activity

Conferences

AISTATS 2021, Pacific Symposium on Biocomputing (PSB) 2021

Technical Books

Ensemble Methods for Machine Learning (Manning Publications)