Noah **Flynn**

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Education

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

Ph.D. Computational & Systems Biology — *Aug. 2017 - May 2021*

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

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

Professional Experience

Amazon, Alexa AI — *Cambridge, MA*

Research Scientist II — *Jun 2021 - Present*

- Optimized multilingual models with judicious data selection strategies to create a single, unified bundle supporting all i18n locales
- Piloted multilingual language models into production for i18n expansion
- Owned Natural Language Understanding (NLU) model development and production release for Japanese, Portuguese, & Spanish languages
- Tested and deployed new model training and evaluation tooling systems for use by all non-English locale release owners

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

PhD Candidate — *Aug 2017 - Jun 2021*

- Served as core maintainer and developer of *XenoSite* and *XenoNet* prediction web services for small molecule biochemistry
- Modeled 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
- Developed 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

Publications

Noah R. Flynn, S. Joshua Swamidass, **Message Passing Neural Networks Improve Prediction of Metabolite Importance**, *Journal of Chemical Information and Modeling*, 2023

Dakota L Pouncey, Dustyn A Barnette, Riley W Sinnott, Sarah J Phillips, **Noah R Flynn**, Howard P Hendrickson, S J. Swamidass and Grover P. Miller, **Discovery of Novel Reductive Elimination Pathway for 10-Hydroxywarfarin**, *Frontiers in Pharmacology*, 2022

Noah R Flynn, **Computational Approaches for Screening Drugs for Bioactivation, Reactive Metabolite Formation, and Toxicity**, *PhD Thesis*, 2021

Arghya Datta, **Noah R. Flynn**, S. J. Swamidass, **Cal-net: Jointly learning classification and calibration on imbalanced binary classification tasks**, *IJCNN*, 2021

Noah R Flynn, Michael D Ward, Mary A. Schleiff, Corentine M. C. Laurin, Stuart J. J. Conway, Gunnar Boysen, S. Joshua Swamidass, Grover P. Miller, **Bioactivation of isoxazole-containing bromodomain and extra terminal domain (BET) inhibitors**, *Metabolites*, 2021

Arghya Datta*, **Noah R. Flynn***, Na Le Dang, S. Joshua Swamidass, **Machine Learning on Liver-Injuring Drug Interactions with NSAIDs from Hospitalization Data**, *PLOS Computational Biology*, 2021. *Equal contribution as first-authors

Tyler B. Hughes*, **Noah Flynn***, Na Le Dang, S. Joshua Swamidass, **Modeling the Bioactivation and Subsequent Reactivity of Drugs**, *Chemical Research in Toxicology*, 2021. *Equal contribution as first-authors

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*, 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*, 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*, 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*, 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*, 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*, 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*, 2019

Skills

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

Leadership & Recognition

2022	**1st Place,** Boston University New Venture Competition	*Boston, MA*
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*

Services

Main Topic Editor	Frontiers in Pharmacology (Advances in computational studies of drug toxicity)
Conference, Journal Reviewer	AISTATS, ACS, Frontiers in Pharmacology, ICLR, PSB, Springer Nature
Technical Book Reviewer	Engineering Deep Learning Systems, Ensemble Methods for ML, Fast Python for Data Science

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*
2014, 2015	**Course Developer,** Introduction to Computer Science, Honors Section	*UIUC*