Noah **Flynn**

noahrflynn@gmail.com | www.noahrflynn.com | nrflynn2 | noahflynn | Noah Flynn | Book: Machine Learning for Drug Discovery

Education

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

Ph.D. Computational Biology & Deep Learning — *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 (Current: AWS AI Labs; Former: Alexa, AGI) — *Santa Clara, CA*

Applied Scientist II — *Jun 2021 - Present*

- Researching large language models (LLMs) regarding (1) novel reward modeling and preference optimization strategies for multilingual LLMs and (2) enabling LLMs to use tools and automate routines by invoking APIs
- Developed dynamic data selection strategy for multilingual natural language understanding, reducing data overhead by 95% and increasing ease of model expansion to support new international markets (e.g., KO, TR, NL)
- Owned 18 production release cycles for conversational agents and NLP models across 6 markets and 4 languages (ES, PT, JP, AR), including data ingestion and processing and model development, training, evaluation, deployment, monitoring, maintenance, and patching
- Developed calibration methods to improve NLU robustness to uncertainty introduced by upstream automatic speech recognition (ASR) models

University of California, Berkeley — *Berkeley, CA*

Adjunct Instructor & Course Developer — *Jun 2024 - Present*

- Redesigning "Software Engineering Fundamentals for Molecular Sciences" to teach software development, data structures, and algorithms through project-based curriculum of increasingly complex software packages for molecular science applications
- Responsible for teaching graduate-level courses in machine learning, cheminformatics, and computational chemistry

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), Modeling & Informatics — *West Point, PA*

Machine Learning Intern (Generative AI) — *May 2019 - Aug 2019*

- Implemented and launched 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

AbbVie Inc. — *Champaign, IL*

Software Engineer — *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 web application for managing all bioinformatics tools that AbbVie R&D uses for drug development
- 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, Genomics & Proteomics — *Aug. 2016 - May 2017*

- 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
- Conducted analysis of biomolecular networks to differentiate between organisms of differing economy, flexibility, and robustness
- Applied preliminary framework to genetically modified organisms within the context of synthetic biology

Publications

Noah R. Flynn, **Machine Learning for Drug Discovery**, *Manning Publications*, 2024

Holy Lovenia, et al. (including **Noah R. Flynn**), **SEACrowd: A Multilingual Multimodal Data Hub and Benchmark Suite for Southeast Asian Languages**, *EMNLP*, 2024

Noah R. Flynn, **Target Greedy Sampling for Multilingual NLU**, *Under Review*, 2024

Noah R. Flynn, Grover P. Miller and S. Joshua Swamidass, **Editorial: Advancements in Computational Studies of Drug Toxicity**, *Frontiers in Pharmacology*, 2023

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**, et al., **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**, et al., **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**, et al., **CYP2C19 and 3A4 Dominate Metabolic Clearance and Bioactivation of Terbinafine Based on Computational and Experimental Approaches**, *Chemical Research in Toxicology*, 2019

Skills

Proficient	Docker, Git, JavaScript (D3, React), Python (Flask, Numpy, Pandas, Scikit-Learn, PyCUDA), PyTorch, RDKit, SQL
Have Used	AWS, C++ (CUDA), JAVA, JAX, MatLab, Neo4j, 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

Conference, Journal Reviewer	ACS, AAAI, AISTATS, Frontiers in Pharmacology, ICLR, PSB, Springer Nature
Technical Book Reviewer	Engineering Deep Learning Systems, Ensemble Methods for ML, Fast Python for Data Science
Course Developer, Instructor	Algorithms for Computational Biology, Bioinstrumentation Lab, Intro to Computer Science (Honors)
Resident Project Advisor (RA)	Illinois Engineering First-Year Experience @ UIUC Summer Scholars Program