

# Noah Flynn

APPLIED SCIENTIST @ AWS AGENTIC AI · ADJUNCT FACULTY @ UC BERKELEY · AUTHOR: MACHINE LEARNING FOR DRUG DISCOVERY

Research Interests in Drug Discovery, LLMs, Agentic Systems, Reinforcement Learning, Post-training

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## Education

### Washington University in Saint Louis (WUSTL)

PH.D. DEEP LEARNING, COMPUTATIONAL BIOLOGY

GPA: 3.94/4.00

Aug. 2017 - May 2021

### University of Illinois at Urbana-Champaign (UIUC)

B.S. BIOENGINEERING, MINOR IN COMPUTER SCIENCE

GPA: 3.70/4.00

Aug 2013 - Jun 2017

## Professional Experience

### Amazon - AWS Agentic AI

Santa Clara, CA

APPLIED SCIENTIST II

Sep 2024 - Present

- Accelerated agent development cycles by developing customizable multi-agent primitives, enabling rapid internal deployment of high-value agents for deep research, data science, database analysis, and code transformation
- Co-developed novel agent-as-a-judge evaluation framework in beta with internal AWS teams and enterprise customers, establishing a self-evolving evaluation agent for personalized, custom assessments of deep research agents
- Engineered cost-aware reasoning capabilities for a deep research agent to intelligently query premium data sources, optimizing usage against complex license- and consumption-based pricing models and enabling partnerships with premium data providers (FactSet, IDC, NASDAQ)
- Enhanced model performance and domain adaptability by transforming an 8B parameter internal, hybrid foundation model into a Mixture-of-Experts (MoE) variant, improving knowledge compartmentalization for specialized tasks and future-proofing against copyright concerns
- Mentored applied scientist interns, resulting in 3 publications under review on novel techniques in mixture-of-agents, dynamic context window optimization, and parameter-efficient reinforcement learning

### Amazon - Alexa & AGI

Santa Clara, CA

RESEARCH SCIENTIST II

Jun 2021 - Sep 2024

- Accelerated Alexa's international expansion into 3 new markets (KO, TR, NL) in under 4 months by developing a dynamic data selection strategy that slashed multilingual NLU data requirements by 95%
- Shipped and maintained 20 production releases of conversational AI models, directly serving over 100M monthly active users across 6 international markets (ES, PT, JP, AR, KO, US)
- Improved experimentation velocity, leading to reduction in prematurely halted experiments and inconclusive "No Go" results year-over-year by authoring 70-page manual standardizing Weblab A/B testing across verticals and marketplaces
- Enhanced Amazon Nova foundation model with advanced tool-use capabilities, contributing core API invocation strategies that power Alexa+

### Department of Pathology & Immunology, WUSTL

St. Louis, MO

PHD CANDIDATE

Aug 2017 - Jun 2021

- Secured 1st place and \$20K in pre-seed funding (Boston New Venture Accelerator) by translating research into B2B commercialization proposal
- 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 early-stage drug development, predicting toxicity, reactive species formation, and likelihood of adverse drug reactions
- Developed signal detection approaches for retrospective analysis of electronic health records, guiding clinical decision-making to minimize incidence of drug-drug interactions and drug-induced liver injury

### Earlier Roles

BIO+AI FOCUSED WORK

- Merck (Machine Learning, 2019-2019):** Built generative models for de novo drug design integrated into production docking pipelines, facilitated by reinforcement learning for targeted optimization of binding affinity and properties impacting therapeutic efficacy and safety profiles
- AbbVie Inc. (Software Engineer, 2016-2017):** Developed bioinformatics data visualization suite for analyzing drug-target interactions, protein-protein interactions, and regulatory networks
- National Center Supercomputing Applications (Research Fellow, 2016-2017)** Characterized proteomic and transcriptomic networks via graph theoretical methods to improve genetically modified organisms across functional economy, flexibility, and robustness

## Selected Publications

Noah R. Flynn, **GenCircuit-RL: RL from Hierarchical Verification for Genetic Circuit Design**, *ICML*, 2026

🔗 Reinforcement Learning 🔗 Automated Genetic Circuit Design 🔗 RL Environment Design & Benchmarking

Changhao Li, E B Avraham, et al. (including Noah R. Flynn, **DREAM-Bench: Deep Research Evaluation w/ Agentic Metrics**, *ACL*, 2026

🔗 Agentic AI Evaluation 🔗 Deep Research Systems 🔗 Benchmarking

Noah R. Flynn, **COMPASS: Continual Multilingual PEFT with Adaptive Semantic Sampling**, *TMLR*, 2025

🔗 Continual Learning 🔗 Parameter-Efficient Fine-Tuning 🔗 Data Centric AI

Noah R. Flynn, **Case Study in Kinase Inhibitors for Anti-Cancer Therapies**, *NeurIPS Education Track*, 2025

AI for Science Education

Amazon AGI, et al. (including Noah R. Flynn), **The Amazon Nova family of models: Technical report and model card**, *Amazon Technical Reports*, 2024

Foundation Models Long-Context Reasoning

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

Low-Resource NLP Multimodal Benchmarking

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

Geometric Deep Learning Drug Discovery

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

Model Calibration Uncertainty Estimation

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

Systems Biology Quantitative Pharmacology Cancer Biology

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

Healthcare AI Drug-drug Interactions Causal Inference

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

Cheminformatics Drug Safety, Bioactivation, and Toxicity

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

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

Generative Chemistry Structural Prediction

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

Probabilistic Modeling Network Inference Metabolomics

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, HuggingFace, JavaScript (D3, React), Python (Flask, Numpy, Pandas, Scikit-Learn, PyCUDA), PyTorch, RDKit, SQL, vLLM  
**Have Used** AWS (Bedrock, EC2, Kendra, S3), C++ (CUDA), JAVA, JAX, MatLab, MegatronLM, Neo4j, R, Spark, TensorFlow, Wolfram Language

## Leadership & Recognition

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| 2025 | <b>Technical Advisor</b> , Berkeley SkyDeck Accelerator  | Berkeley, CA  |
| 2022 | <b>1st Place</b> , Boston University New Venture Competition   | Boston, MA    |
| 2017 | <b>Director</b> , Engineering Open House (Educational Non-Profit)  | Champaign, IL |
| 2016 | <b>Most Valuable Intern</b> , Research Park  | Champaign, IL |
| 2015 | <b>Silver Medal</b> , International Genetically Engineered Machines Competition, Biological Computing Division | Boston, MA    |
| 2014 | <b>Scholarship Recipient</b> , Levi, Ray, and Shoup Computer Science Award                                     | Champaign, IL |

## Services

**Reviewer** ACS, AAI, AISTATS, Frontiers, ICLR, ICML, Manning (10+ technical books), NeurIPS, PSB, Springer Nature  
**Course Developer** Algorithms for Computational Bio., Bioinstrumentation, Intro to CS, Intro to Software Engineering