

# ANDREW MCNUTT

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🔗 [drewnutt.github.io](https://drewnutt.github.io)🌐 [drewnutt](https://drewnutt.github.io)

## EDUCATION

Ph.D. Computational Biology

📅 Jan 2025

Carnegie Mellon University- University of Pittsburgh

B.S. Physics and B.S. Mathematics, Minor: Chemistry

📅 May 2019

Purdue University

## RESEARCH EXPERIENCE

Graduate Student Researcher

University of Pittsburgh

Advisor: David Koes

📍 Pittsburgh, PA

📅 Aug 2019 – Current

- Engineered a novel, structure-aware virtual screening method, enabling the efficient screening of billion-molecule libraries
- Analyzed convolutional neural network (CNN) scoring functions within molecular docking pipeline
- Developed Siamese CNN network to predict relative binding free energy of congeneric series ligands
- Open-sourced a docking pipeline to use pairwise statistics for improved docking performance

Student Intern at Regenstrief Institute

Center for Biomedical Informatics

Mentor: Shaun Grannis

📍 Indianapolis, IN

📅 May 2019 – Aug 2019

- Engineered several machine learning approaches for record-linkage, identifying records that are from the same patient
- Analyzed and compared the performance of record-linkage techniques

Undergraduate Research Assistant at Purdue University

Department of MCMP

Advisor: Markus Lill

📍 West Lafayette, IN

📅 Jan 2017 – December 2018

- Analyzed a novel coarse-grained approach for modeling protein-ligand interaction
- Customized a random forest scoring function for coarse grained modeling of protein-ligand binding
- Enhanced a convolutional neural network with the ability to use probe-protein interaction data to better classify ligand binding poses

Student Intern at Indiana University-Purdue University Indianapolis

Division of Nephrology

Advisor: Tarek M. Ashkar

📍 Indianapolis, IN

📅 May 2018 – Aug 2018

- Researched and determined the strengths and weaknesses of various approaches for clustering and dimensionality reduction
- Collaborated on the development of a full release version of a volumetric cell cytometry software for use on tissue images
- Expanded the capability of the cell cytometry software to include clustering and dimensionality reduction on the data created with the software

Indiana University O'Brien Student Intern

Division of Nephrology

Advisor: Bruce A. Molitoris

📍 Indianapolis, IN

📅 May 2017 – Aug 2017

- Prototyped the merging of a 3D visualization software with an application developed for cell cytometry in tissue images
- Developed procedures for integrating native code into Java applications

## SKILLS AND CLASSES

- Python, PyTorch, Pandas, NumPy, RDKit, Java, Bash, Git
- Molecular Dynamics, Docking, Pharmacophore Modeling
- Thermal Physics, Computational Physics, Quantum Mechanics
- Deep Learning, Computer Vision, Scalable Machine Learning, Metric Learning
- Linear Algebra, Vector Calculus, Discrete Math, Probability
- Biochemistry, Genomics, Systems Biology

## PUBLICATIONS

### “Interpretable adenylation domain specificity prediction using protein language models”

Adduri, A.K., McNutt, A.T., Ellington, C.N., Suraparaju, K., Fang, N., Yan, D., Krummenacher, B., Li, S., Bodden, C., Xing, E.P., Behsaz, B., Koes, D., Mohimani, H.  
 bioRxiv (2025) DOI:10.1101/2025.01.13.632878

### “Scaling Structure Aware Virtual Screening to Billions of Molecules with SPRINT”

McNutt, A.T., Adduri, A.K., Ellington, C.E., Dayao M.T., Xing, E.P., Mohimani, H., Koes, D.R.  
 arXiv (2025) DOI:10.48550/arXiv.2411.15418

### “Duvelisib is a novel NFAT inhibitor that mitigates adalimumab-induced immunogenicity”

Bhingarkar, A., Wang, Y., Hoshitsuki, K., Eichinger, K.M., Rathod, S., Zhu, Y., Lyu, H., McNutt, A.T., Moreland, L.W., Mcdermott, L., Koes, D.R., Fernandez, C.  
 Frontiers in Pharmacology (2025) DOI:10.3389/fphar.2024.1397995

### “Condensing Molecular Docking CNNs via Knowledge Distillation”

McNutt, A.T., Li, Y., Francoeur, P., and Koes, D.R.  
 ChemRxiv (2024) DOI:10.26434/chemrxiv-2024-0jh8g

### “Open-ComBind: Harnessing unlabeled data for improved binding pose prediction”

McNutt, A.T. and Koes, D.R.  
 Journal of Computer-Aided Molecular Design (2024) DOI:10.1016/j.bpj.2023.11.1206

### “Conformer Generation for Structure Based Drug Design: How Many and How Good?”

McNutt, A.T., Bisiriyu, F., Song, S., Vyas, A., Hutchison, G. and Koes, D.R.  
 Journal of Chemical Information and Modeling (2023) DOI:10.1021/acs.jcim.3c01245

### “Improving $\Delta\Delta G$ predictions with a multi-task convolutional Siamese Network”

McNutt, A.T. and Koes, D.R.  
 Journal of Chemical and Information Modeling (2022) DOI:10.1021/acs.jcim.1c01497

### “GNINA 1.0: molecular docking with deep learning”

McNutt, A.T., Francoeur, P., Aggarwal, R., Masuda, T., Meli, R., Ragoza, M., Sunseri, J. and Koes, D.R.  
 Journal of Cheminformatics (2021) DOI:10.1186/s13321-021-00522-2

### “Integrated cytometry with machine learning applied to high-content imaging of human kidney tissue for in-situ cell classification and neighborhood analysis”

Winfree, S., McNutt, A.T., Khochare, S., Borgard, T.J., Barwinska, D., Sabo, A.R., Ferkowicz, M.J., Williams, J.C., Lingeman, J.E., Gulbranson, C.J. and Kelly, K.J.,  
 Laboratory Investigation (2023) DOI:10.1016/j.labinv.2023.100104

### “In situ classification of cell types in human kidney tissue using 3D nuclear staining”

Woloshuk, A., Khochare, S., Almulhim, A.F., McNutt, A.T., Dean, D., Barwinska, D., Ferkowicz, M.J., Eadon, M.T., Kelly, K.J., Dunn, K.W. and Hasan, M.A.  
 Cytometry Part A (2021) DOI:10.1002/cyto.a.24274

## PRESENTATIONS

### “SPRINT Enables Interpretable and Ultra-Fast Virtual Screening against Thousands of Proteomes”

Machine Learning for Structural Biology Workshop, NeurIPS 2024 (Poster) Dec 2024

### “Enhancing ultra-large library virtual screening with SPRINT”

5<sup>th</sup> Molecular Machine Learning Conference (Poster) Nov 2024

### “Ultra-High-Throughput Virtual Screening for Antimicrobials”

Machine Learning in Computational Biology (Poster) Sept 2024

### “Is the future of molecular docking really here?”

Invited Talk: Genesis Therapeutics July 2023

### “Open-ComBind: An open-source docking pipeline harnessing pairwise pose statistics”

ACS Spring 2023 Mar 2023

### “GNINA 1.0: molecular docking with deep learning”

Broad Institute: Machine Learning in Drug Discovery (Poster) Oct 2022

Molecular Machine Learning Conference (Poster) Oct 2022

ACS Spring 2021 April 2021

### “Exploring $\Delta\Delta G$ prediction with Siamese Networks”

Machine Learning for Structural Biology (MLSB) Workshop at NeurIPS (Poster)

Dec 2021

"Comparison of Supervised Machine Learning and Probabilistic Approaches for Record Linkage"

AMIA Summit 2020 (Accepted, but conference cancelled due to COVID-19)

March 2020

## MENTORING

Summer Research Mentor

📅 Summer 2024

University of Pittsburgh, TECBio Research Experience for Undergraduates

Student: Matthew Joyson

- Acted as primary research mentor for an undergraduate student completing graduate-level research to improve a neural network scoring function; final work presented at university student research symposium

Neural Network Knowledge Distillation

📅 May 2022-Aug 2023

University of Pittsburgh

Student: Yanjing Li

- Advised a Master's student project to distill ensembles of CNN molecular docking scoring functions
- Guided the development of a poster for the PhD program orientation and ACS Spring 2023; work culminated in manuscript

First Year PhD Student Book Club Mentor

📅 Aug-Oct 2022

University of Pittsburgh

- Facilitated conversations around assigned readings on various topics related to PhD studies, such as research methods, stress management, and mentorship

Summer Research Mentor

📅 Summer 2021

University of Pittsburgh, TECBio Research Experience for Undergraduates

Student: Maddie Bonanno

- Acted as primary research mentor for an undergraduate student completing graduate-level research in drug discovery
- Advised project to completion; final work presented at university student research symposium

## LEADERSHIP

Treasurer

📅 2021-2023

Carnegie Mellon-University of Pittsburgh Computational Biology Graduate Student Association

- Managed a budget of \$10,000 for the graduate student association
- Recorded and handled reimbursements for all purchases made by the graduate student association
- Developed a website to disseminate information created by the graduate student association

Admissions Committee Member

📅 2021, 2022

Carnegie Mellon-University of Pittsburgh Computational Biology PhD Program

- Assessed PhD program applicant's academic backgrounds, research experiences, and fit with the program's focus areas
- Collaborated with faculty members to identify top candidates for the PhD program

Senator

📅 2020-2021

Carnegie Mellon-University of Pittsburgh Computational Biology Graduate Student Association

- Organized several in-person and online events for the PhD program
- Assisted in transitioning our PhD program to virtual events during the COVID-19 pandemic

## TEACHING

Intro to Computational Structural Biology

📅 Aug 2022-Dec 2022

Graduate Teaching Assistant, University of Pittsburgh

Instructors: David Koes &amp; James Faeder

Scalable Machine Learning for Big Data Biology

📅 Jan 2021-May 2021

Graduate Teaching Assistant, University of Pittsburgh

Instructors: David Koes &amp; Maria Chikina

Modern Mechanics

📅 Jan 2019-May 2019

Undergraduate Teaching Assistant, Purdue University

Electric And Magnetic Interactions

📅 Aug 2016-Nov 2018

Undergraduate Teaching Assistant, Purdue University