ANDREW MCNUTT

@ **E-mail:** and.mcnutt@pitt.edu **Phone:** (317) 509-1583 drewnutt.github.io drewnutt

EDUCATION

Ph.D. Computational Biology
Expected Q1 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

- 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
- Deep Learning, Computer Vision, Scalable Machine Learning, Metric Learning
- Molecular Dynamics, Docking, Pharmacophore Modeling
- Linear Algebra, Vector Calculus, Discrete Math, Probability
- Thermal Physics, Computational Physics, Quantum Mechanics
- Biochemistry, Genomics, Systems Biology

PUBLICATIONS

"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., Gulbronson, 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

"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 & James Faeder

Scalable Machine Learning for Big Data Biology

Jan 2021-May 2021

Graduate Teaching Assistant, University of Pittsburgh Instructors: David Koes & 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