ANDREW MCNUTT

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EDUCATION

Ph.D. Computational Biology
Jan 2025

Thesis: *"Efficiency through Abstraction: Representation Learning for Cost-Effective Drug Discovery"*

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 Medicinal Chemistry and Molecular Pharmacology — **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, scikit-learn, Java, Bash, Git
- Deep Learning, Computer Vision, Metric Learning, Representation Learning, Transformers
- Molecular Dynamics, Docking, Pharmacophore Modeling, Virtual Screening
- Linear Algebra, Vector Calculus, Discrete Math, Probability
- Thermal Physics, Computational Physics, Quantum Mechanics
- Biochemistry, Genomics, Systems Biology, Structural Biology

PUBLICATIONS

GNINA 1.3: the next increment in molecular docking with deep learning

McNutt, A.T., Li, Y., Meli, R., Aggarwal, R., Koes, D.R.
Journal of Cheminformatics (2025) **DOI:**10.1186/s13321-025-00973-x

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., 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

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
5th 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 & 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