# Abhinav K. Adduri, aadduri@andrew.cmu.edu

About Me

My research interest is in applied deep learning and building and using foundation models to accelerate natural product discovery and drug discovery. I am currently a 5th year Ph.D. student in the Computational Biology Department at CMU. I have been advised by Dr. Hosein Mohimani for the past two years.

EDUCATION

# Carnegie Mellon University

Expected January 2025

Ph.D. Computer Science / Computational Biology, GPA: 4.0

Ph.D. Minor Machine Learning (formerly secondary masters), GPA: 3.94

Teaching Assistant: 10-701 Machine Learning, 02-613 Algorithms and Advanced Data Structures

# University of California, Berkeley

May 2019

B.A. Computer Science, GPA 3.8

B.A. Biochemistry and Molecular Biology, GPA 3.7

Programming

Rust, Python, C++, Typescript, HTML, CSS, C, Java

TECHNOLOGIES

Linux, PyTorch, Git, React, Docker

Publications

Yan, D.\*, Zhou, M.\*, **Adduri, A.**\*, Guler, M., Liu, S., Shin, H., Kovach, T., Oh, G., Liu, X., Deng, Y., Cao, L., Behsaz, B., Mohimani, H. (Expected 2024). Seq2PKS: Discovering modular type I cis-AT polyketide natural products by integrating computational mass spectrometry and genome mining. *Manuscript awaiting final decision in Nature Communications*.

**Adduri, A.**, Kim, S. (Expected 2024). Ornaments for accurate and efficient allele-specific expression estimation with bias correction. *Manuscript awaiting final decision in The American Journal of Human Genetics*. [ArXiv]

Mongia, M., Baral, R., **Adduri, A**., Yan, D., Liu, Y., Bian, Y., Kim, P., Behsaz, B., Mohimani, H. (2023). AdenPredictor: Accurate prediction of the adenylation domain specificity of nonribosomal peptide biosynthetic gene clusters in microbial genomes. Bioinformatics, 39(Supplement 1), i40-i46.

**Adduri, A**. (2019). IoT integration in manufacturing processes. In Simulation for Industry 4.0: Past, Present, and Future (pp. 129-139).

**Adduri, A.**, Schruben, L. (2017). The Tao of simulation. In 2017 Winter Simulation Conference (WSC) (pp. 607-616). IEEE.

PENDING PUBLICATIONS Behsaz, B.\*, Adduri, A.\*, Guler, M.\*, Mohamed, O. G., Caraballo-Rodríguez, A. M., Duggan, B., Chaudhary, N., Miller, C., Liu, S., Krummenacher, B., Broders, K., Zamith-Miranda, D., Schultz, P. J., Sherman, D. H., Clement, J., Nakayasu, E., Nosanchuk, J., Dorrestein, P. C., Tripathi, A., Mohimani, H. (Expected 2024). Pathogen-oriented platform for large-scale natural product discovery identifies novel antifungal targeting drug-resistant candidiasis. *Manuscript in preparation for submission to Nature*.

Adduri, A., Donghui Y., McNutt, A., Mustafa, G, Chaitanya, S., Nan, F., Koes, D., Ashootosh, T., Hosein, M. (Expected 2024). Using protein language models for interpretable adenylation domain specificity prediction to discover novel type I polyketide and non-ribosomal peptide hybrids. *Manuscript in preparation for submission to Nature Methods*.

\*Equal contribution.

Ongoing Research

# NPDiscover

January 2022 - Present

- Developed algorithms and used protein language models to predict natural product structures with drug-like properties from microbial genomes
- Discovered a novel antifungal which displays promising mice model results against the multidrug-resistant fungal pathogen *Candida Auris* (deemed an urgent threat by the CDC)
- Developed molecular structure clustering schemes to reduce the number of predicted drug candidates by 100x while retaining prediction quality

### PLMs for interpretable A-domain specificity prediction

August 2023 – Present

- Used protein language models to improve small molecule binding prediction for adenylation (A-) domains, which recruit monomers into mature natural products
- Achieved state of the art performance and over 20% improvement in out-of-distribution generalization benchmark

Seq2Hybrid March 2023 – Present

• Generalized previous approaches to predict hybrid natural product structures (e.g. non-ribosomal peptide and polyketide hybrid structures)

• Linked a microbial genome to the production of the immunosuppressants SW-163A and B

### **Ornaments**

May 2021 - August 2023

• Developed *Ornaments*, a graph-based alignment tool for unbiased allele-specific read mapping. Improved runtime and accuracy over state of the art by 11.6x / 2x respectively

### Coursework

### Relevant Graduate Coursework

10-701 Machine Learning, A
10-708 Probabilistic Graphical Models, A
02-730 Cellular & Systems Modeling, A
10-725 Convex Optimization, A
10-707 Advanced Deep Learning, A
36-705 Intermediate Statistics, A02-710 Computational Genomics, A+
PT-2030 Intro to Computational Structural Biology, A+

# Relevant Undergraduate Coursework

CS 170 Efficient Algorithms, ACS 186 Database Systems, A
EE 120 Signals and Systems, A
CS 189 Machine Learning, A
CS 294 Machine Learning in Biology, ACS 170 Efficient Algorithms, ACS 162 Operating Systems, AMath 110 Linear Algebra, A
EE 123 Digital Signal Processing, A
EE 126 Probability and Random Processes, A
CS 176 Algorithms in Computational Biology, A

# Previous Experience

### Square / Caviar, San Francisco, CA

Data Science Engineer Intern

May 2019 - August 2019

- Improved recall / precision of chargeback fraud-detection models by 3.5x / 2.5x respectively
- Improved pre-checkout food delivery ETA predictions for restaurants

### Rubrik, Palo Alto, CA

Software Developer Intern

May 2018 – August 2018

- Designed and implemented distributed cache system for filesystems team
- Designed RPCs to expose node cache space to other nodes in the same cluster

### Mozilla, Portland, OR

Software Developer Intern

May 2017 - August 2017

- Designed and implemented Firefox Send, a tool for private, end-to-end encrypted file transfer
- Firefox Send was used globally and was covered by news outlets such as Forbes and TechRepublic

#### PATENTS

Automated Review of Source Code for Style Issues, Rubrik 2018

### Honors and Awards

CMU-Pitt Ph.D. in Computational Biology: Diversity, Equity and Inclusion Award CMU SCS Graduate Student Service Award Winner

### Past Projects

Seqtools with Nir Yosef - A pipeline for processing ATAC-Seq and RNA-Seq data, 2018 Homolog Identification with Jennifer Doudna - Test and discern evolutionary origin for specific

CRISPR mutations, 2017