Jonathan Evan Ash

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LinkedIn | GitHub | Personal Website

I am a **computational chemist** and **machine learning scientist** specializing in developing deep learning models for **protein interaction prediction**, **therapeutic screening**, and **drug discovery**. I develop predictive and design-oriented ML workflows to support **variant effect forecasting**, **functional sequence space exploration**, and **binder optimization** across therapeutically relevant protein systems. My work emphasizes generalizability, scale, and integration with **HPC-enabled drug discovery pipelines.**

Education

2021 - 2026: Ph.D. Candidate in Quantitative Biomedicine - Rutgers University
- Advisor: Sagar Khare
- GPA: 3.864
- Thesis: Deep Learning Approaches for Protein Binding Prediction and Design

2017 - 2021: Bachelor of Science - Rutgers University
- School of Environmental and Biological Sciences, Honors Program
- Majors: Biotechnology (Bioinformatics track), Biomathematics
- Minor: Mathematics
- GPA: 3.67; Graduated *cum laude*; Ranked within Top 5 of Biotechnology Major

Skills

Machine Learning and Numerical Computing: PyTorch · PyTorch-Geometric · Scikit-Learn · Graph Neural Networks · Attention-based Models · Contrastive Learning · NumPy · Pandas
Computational Biology: AlphaFold · PyRosetta · Modeller · ProteinMPNN · RFDiffusion · ESM suite (ESM2, ESM-IF, ESMFold) · FoldSeek · MMseqs2
Programming: Python (Primary) · R · Matlab · Java
Infrastructure: Linux · SLURM · Git · Shell Scripting · RADICAL Toolkit (CyberTools, Pilot, ENTK)

Research Experience

Rutgers University, Khare Lab - Senior Computational Researcher (2021 - Present)

Lead computational researcher on several projects, developing HPC-coupled ML and DL networks to enable distal functional sequence space exploration and *in silico* therapeutic design.

- **Adaptive Protein Design with HPC-Enabled Dynamic Workflows**
  - Developed a scalable protein binder design pipeline coupling ML model inference and dynamic HPC resource utilization
  - Pipelines are modular with customizable scoring and generation tasks, and can be scaled to large batches of input protein complexes
  - Designs optimized with my protocol exhibited enhanced AlphaFold-predicted quality over baseline metrics (pLDDT +32.8%, pAE -1.3% from control run)
  - Paper published in IPDPS workshop HPAI4S 2025
- **Variant Effect Forecasting of SARS-CoV-2 RBD Using Deep Learning**
  - Built highly accurate and generalizable deep learning models for RBD binding prediction across 43,000 unique sequences
  - Discovered ~2000 diverse and functional mutants highly distant from the WT while still retaining binding to ACE2

    - Highlighted limited epistasis in the RBD by using logistic regression to interrogate contribution of pairwise and triplet interactions to variant fitness
    - Manuscript in review at Cell Systems
- **Predicting Protein Binding Specificity Using Sequence-Based Contrastive Learning**
    - Built structure-aware graph classifier and sequence-based contrastive learning network to recapitulate PDZ-peptide interactions across 64,000 experimentally derived samples
    - Applied contrastive learning framework to 10 other therapeutically relevant systems (MHC, SH2, WH1, etc)
    - Generated both peptide and PDZ *de novo* sequence designs using ESM2
    - ~10000 designs were screened with the model, then filtered and validated experimentally using yeast surface display (YSD)
    - Publication currently being written

Publications

- **Ash, J. E.,** Hadisadegh, N., Khare, S. D. (2026). Prediction and design of protein-peptide binding specificity using deep learning. *Manuscript in preparation*
- **Ash, J. E.***, Francino-Urdaniz*, I. M., Kells, S. P., Davis, C. N., Whitehead, T. A., Khare, S. D. **Co-first authors* (2025). Graph attention with structural features improves the generalizability of identifying functional sequences at a protein interface. bioRxiv, DOI (In review at Cell Systems)
- Alsaadi, A.*, **Ash, J. E.***, Titov, M., Turilli, M., Merzky, A., Jha, S. & Khare, S. **Co-first authors* (2025). Adaptive protein design protocols and middleware. IPDPS HPAI4S, 2025 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW) pp. 1011-1015, DOI
- Hackl, M., Contrada, E. V., **Ash, J. E.**, Kulkarni, A., Yoon, J., Cho, H.-Y., Lee, K.-B., Yarbrough, J. M., López, C. A., Gnanakaran, S. & Chundawat, P. S. S. (2022). Acoustic force spectroscopy reveals subtle differences in cellulose unbinding behavior of carbohydrate-binding modules. Proceedings of the National Academy of Sciences, 119(42), e2117467119. DOI

Conferences

RosettaCommons - Panel Chair and Organizer at Summer RosettaCon (2025)

- Proposed panel topic on machine-learning approaches for protein-protein interaction prediction and design
- Wrote panel abstract, organized speaker slide decks, and delivered panel introduction to audience of ~150 conference attendees and industry professionals
- Delivered a talk on sequence-based contrastive learning for protein binding prediction

Academic Experience

Academic Journal Peer Reviewer (2021 - Present)

- Served as peer reviewer for several machine-learning manuscripts submitted to Proteins and Nature Communications

Rutgers University - TA for General Biology (2024 - 2025)

- Taught core concepts in Biology and lead supplementary office hours as supporting instructor in a course with ~2000 students enrolled

Honors and Awards

Robert M. Rauch Award (2021) - Exemplifying leadership and service within Biotechnology
Richard W. Herbert Memorial Scholarship (2020) - Superior academic performance
Outstanding Research Writing Project in Rutgers SEBS (2018) - Most extensive SEBS research paper presented at Undergraduate Research Writing Conference
Rutgers SEBS Honors Program (2017 - 2021) - Offered to ~50 top undergraduates upon entry