Nikša Praljak

Ph.D. Candidate in Biophysics at the University of Chicago

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Professional Summary

PhD candidate in Biophysics developing deep generative models and multimodal approaches for protein design, focused on bridging the gap between *in silico* performance and wet-lab success in Al-driven drug discovery.

Education

Note: Words highlighted in blue are clickable links.

University of Chicago Autumn 2020 - Present

Chicago, Illinois

PhD Student: Biophysical Sciences Graduate Program (NSF Graduate Research Fellow) *Thesis:* Molecular Dialogues: Guiding Protein Design through Natural Language Prompts

PhD co-advisors: Professors Rama Ranganathan and Andrew Ferguson

- 1. Developed **BioM3**, a multimodal protein language model, enabling novel protein sequence generation directly from natural language prompts.
 - o Implemented a multi-GPU pretraining workflow (PyTorch, DeepSpeed) aligning protein and biomedical language models via contrastive learning.
 - Created a conditional diffusion model for text-prompted protein design; experimentally confirmed model-generated proteins were functional *in vivo* and *in vitro*.
 - Deployed an interactive demo on Hugging Face Spaces.
- 2. Developed and applied novel Variational Autoencoder (VAE) architectures for generative protein design:
 - Engineered synthetic SH3 signaling domain orthologs using an information-maximizing VAE; experimentally validated designs and analyzed novelty. (Co-first author publication featured in *Patterns*).
 - O Created ProtWave-VAE, integrating autoregressive sampling with VAE latent inference for alignment-free design, enabling property guidance via latent conditioning. (Work featured in ACS Synthetic Biology special issue).
- Actively developing novel deep learning methods for protein prediction and design, focusing on large-scale model
 post-training (DPO for mutation effects, scaling laws) and improved text-to-protein generation (discrete flow matching,
 frontier model integration).

Case Western Reserve University

Autumn 2018 - Summer 2020

Autumn 2016 - Spring 2020

Cleveland, Ohio

Department of Physics: Visiting Student and Researcher

GPA: 4.0

Research: Integrating computer vision with protein adhesion-based microfluidic assays for sickle cell patient diagnostics Advisors: Drs. Michael Hinczewski (Theoretical Biophysics Research Group) and Umut Gurkan (CASE Biomanufacturing and Microfabrication Laboratory)

Cleveland State University

Cleveland, Ohio

Undergraduate Majors: Honors Mathematics and Honors Physics

Summa Cum Laude (COSHP Valedictorian)

Undergraduate Honors Thesis: Pulsatile Flow Through Idealized Renal Tubules

Publications

These are selected publications. For a complete list, please see my Google Scholar profile. * Denotes co-first authors

- 1. N Praljak, H Yeh, M Moore, M Socolich, R Ranganathan, A L Ferguson (2024). Natural Language Prompts Guide the Design of Novel Functional Protein Sequences. bioRxiv, doi:10.1101/2024.11.11.622734.
 - Presented in AlDrugX workshop at NeurIPS 2024.
 - BioM3-app: Deployed text-to-protein generation demo.
- 2. X Lian*, N Praljak*, SK Subramanian*, S Wasinger, R Ranganathan, ... (2024). Deep-learning-based design of synthetic orthologs of SH3 signaling domains. Cell Systems, 15(8), 725-737.
 - Featured in: Fu X. How deep can we decipher protein evolution with deep learning models. Patterns, Volume 5, Issue 8, 9 August 2024, 101043. This preview highlights our work on applying deep learning to protein evolution and design.
- 3. N Praljak, X Lian, R Ranganathan, AL Ferguson. (2023). ProtWave-VAE: Integrating autoregressive sampling with latent-based inference for data-driven protein design. ACS Synthetic Biology, 12(12), 3544-3561.
 - Featured in: Martín García H, Mazurenko S, Zhao H. Special Issue on Artificial Intelligence for Synthetic Biology. ACS Synth. Biol. 2024, 13, 2, 408–410. This special issue highlights and features our work on integrating Al with synthetic biology.

Patents

- Techniques for Artificial Intelligence (AI) Based Protein Engineering Using Natural Language Prompting.
 Inventors: A. Ferguson, N. Praljak, R. Ranganathan. (Application Submitted)
- Classification of Blood Cells. Inventors: N. Praljak, I. Shamreen, U. Goreke, M. Hinczewski, et al. US App. No. 17/928,976.
- Additional patents (link).

Talks & Presentations

- 1. **Praljak N**. "Natural language prompts guide the design of novel functional protein sequences" Invited/Nominated talk, PhD Student Research Day, Data Science Institute, Univ. of Chicago, Dec 2024. (Link)
- 2. **Praljak N.**, "A multimodal generative model with natural language for protein design" Oral presentation, Multimodal Al Workshop, Toyota Tech Institute at Chicago (TTIC), Jan 2024. (Link)

Honors & Awards

- 2023 UChicago DSI AI+Science Grant (\$10k) for project: "Discovering Design Rules..."
- 2021 Finalist, Grier Prize for Innovative Research in Biophysics; UChicago Duchossois Family Institute Fellow
- 2020 NSF Graduate Research Fellowship; COSHP Valedictorian

Technical Skills

Programming Python, C++, R, MATLAB

ML Software PyTorch, DeepSpeed, HuggingFace, Jax, TensorFlow, Scikit-learn

Data Science NumPy, Pandas, Matplotlib, Seaborn, SciPy, Dask, TensorBoard, HDF5

Tools Git, Linux, HPC Environments, PBS, SLURM, bash