

# Hunter Nisonoff — Curriculum Vitae

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## Education

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- **University of California, Berkeley** **Berkeley, CA**  
*PhD Computational Biology* *2019–2024 (Expected)*
- **Duke University** **Durham, NC**  
*B.S. Mathematics with a Minor in Chemistry, Magna Cum Laude* *2011–2015*

## Experience

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- **University of California, Berkeley** **Berkeley, CA**  
*Graduate Student Researcher* *August 2019 – Present*  
Machine learning researcher advised by Jennifer Listgarten and member of the Berkeley Artificial Intelligence Research Lab (BAIR). I develop machine learning models and algorithms for problems in protein engineering. My interests lean towards (1) collaborating closely with experimentalists to understand experimental constraints and opportunities for ML-enabled protein engineering (2) structure-based approaches to protein engineering and (3) Bayesian methods that enable uncertainty quantification for improved experimental design.
- **Octant Bio** **Emeryville, CA**  
*Graduate Student Intern* *May 2022–August 2022*  
Worked on the medicinal chemistry team building computational models of ligand-protein interactions as well as machine learning models of small-molecule properties. I remain a part-time consultant, working with chemists across three programs and I have been listed as an inventor on one patent application.
- **D. E. Shaw Research** **New York, NY**  
*Scientific Associate* *August 2016–August 2019*  
Conducted computational chemistry research spanning cheminformatics and biomolecular simulation. Developed a novel deep learning framework for inverting QSAR models, enabling efficient small-molecule design for drug discovery applications. This work resulted in a first-author publication. Additionally, spearheaded structure-based drug discovery projects targeting two therapeutic proteins, developing specialized computational methods for analyzing molecular dynamics simulations. One of these projects successfully advanced a therapeutic candidate into clinical trials.
- **Donald Lab, Duke University Department of Computer Science** **Durham, NC**  
*Research Associate* *August 2015–August 2016*  
Conducted research in the area of physics-based computational protein design on the development of novel algorithm for computing the partition function under the rigid-rotamer model.

## Awards and Honors

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- **ACS Editors' Choice**  
Designation given to feature scientific articles of broad public interest. Awarded to our paper "Coherent Blending of Biophysics-Based Knowledge with Bayesian Neural Networks for Robust Protein Property Prediction"
- **Newton Fellowship Recipient for 2021-2022**  
Provided partial tuition and stipend support for a graduate students working in the area of synthetic biology
- **2019 Hertz Fellowship Finalist**  
Selected as one of 41 finalists from a pool of 800 applicants
- **Graduation with High Distinction in Mathematics**  
Thesis: 'Efficient Partition Function Estimation in Computational Protein Design: Probabilistic Guarantees and Characterization of a Novel Algorithm'
- **Phi Beta Kappa National Honor Society**

## Outreach

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- **Be a Scientist Program** **Berkeley, CA**  
*Volunteer* *August 2019–May 2022*  
I mentored middle school students in the Berkeley Unified School District by helping them design, implement, and analyze their own science experiment.

## Publications

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**Hunter Nisonoff\***, Junhao Xiong\*, Stephan Allenspach\*, and Jennifer Listgarten. Unlocking Guidance for Discrete State-Space Diffusion and Flow Models. *arXiv preprint arXiv:2406.01572*, 2024.

Yekaterina Shulgina\*, Marena I Trinidad\*, Conner J Langeberg\*, **Hunter Nisonoff\***, Seyone Chithrananda\*, Petr Skopintsev\*, Amos J Nissley\*, Jaymin Patel, Ron S Boger, Honglue Shi, et al. RNA Language Models Predict Mutations that Improve RNA Function. *Nature Communications (In press)*, 2024.

Noam Prywes, Naiya R Philips, Luke M Oltrogge, Sebastian Lindner, Yi-Chin Candace Tsai, Benoit de Pins, Aidan E Cowan, Leah J Taylor-Kearney, Hana A Chang, Laina N Hall, . . . , **Hunter Nisonoff**, . . . , and David F Savage. A Map of the Rubisco Biochemical Landscape. *Nature (In press)*, 2024.

Jose Manuel Martí, Chloe Hsu, Charlotte Rochereau, Chenling Xu, Tomasz Blazejewski, **Hunter Nisonoff**, Sean P Leonard, Christina S Kang-Yun, Jennifer Chlebek, Dante P Ricci, et al. Gentangle: Integrated Computational Design of Gene Entanglements. *Bioinformatics*, 40(7):btac380, 2024.

**Hunter Nisonoff**, Yixin Wang, and Jennifer Listgarten. Coherent Blending of Biophysics-Based Knowledge with Bayesian Neural Networks for Robust Protein Property Prediction. *ACS Synthetic Biology*, 12(11):3242–3251, 2023.

Peter H Yoon, Petr Skopintsev, Honglue Shi, Lin-Xing Chen, Benjamin A Adler, Muntathar Al-Shimary, Rory J Craig, Zheng Li, Jasmine Amerasekera, Marena Trinidad, **Hunter Nisonoff**, . . . , and Doudna, Jennifer. Eukaryotic RNA-guided Endonucleases Evolved From a Unique Clade of Bacterial Enzymes. *Nucleic Acids Research*, 51(22):12414–12427, 2023.

Alexander M Taylor, Bret R Williams, Fabrizio Giordanetto, Elizabeth H Kelley, André Lescarbeau, Kelley Shortsleeves, Yong Tang, W Patrick Walters, Alfonso Arrazate, Christine Bowman, . . . , **Hunter Nisonoff**, . . . , and Lindsay Willmore. Identification of GDC-1971 (RLY-1971), a SHP2 Inhibitor Designed for the Treatment of Solid Tumors. *Journal of Medicinal Chemistry*, 66(19):13384–13399, 2023.

Jack B Greisman, Lindsay Willmore, Christine Y Yeh, Fabrizio Giordanetto, Sahar Shahamadtar, **Hunter Nisonoff**, Paul Maragakis, and David E Shaw. Discovery and Validation of the Binding Poses of Allosteric Fragment Hits to Protein Tyrosine Phosphatase 1B: From Molecular Dynamics Simulations to X-ray Crystallography. *Journal of Chemical Information and Modeling*, 63(9):2644–2650, 2023.

Chloe Hsu, **Hunter Nisonoff**, Clara Fannjiang, and Jennifer Listgarten. Learning Protein Fitness Models from Evolutionary and Assay-Labeled Data. *Nature Biotechnology*, pages 1–9, 2022.

Amirali Aghazadeh, **Hunter Nisonoff**, Orhan Ocal, David H Brookes, Yijie Huang, O Ozan Koyluoglu, Jennifer Listgarten, and Kannan Ramchandran. Epistatic Net Allows the Sparse Spectral Regularization of Deep Neural Networks for Inferring Fitness Functions. *Nature Communications*, 12(1):1–10, 2021.

Youjin Lee, Derek Bogdanoff, Yutong Wang, George C Hartoularos, Jonathan M Woo, Cody T Mowery, **Hunter Nisonoff**, David S Lee, Yang Sun, James Lee, et al. XYZeq: Spatially Resolved Single-Cell RNA Sequencing Reveals Expression Heterogeneity in the Tumor Microenvironment. *Science Advances*, 7(17):eabg4755, 2021.

Paul Maragakis\*, **Hunter Nisonoff\***, Brian Cole, and David E. Shaw. A Deep-Learning View of Chemical Space Designed to Facilitate Drug Discovery. *Journal of Chemical Information and Modeling*, 60(10):4487–4496, 2020. PMID: 32697578.

Pablo Gainza, **Hunter Nisonoff**, and Bruce R Donald. Algorithms for Protein Design. *Current Opinion in Structural Biology*, 39:16–26, 2016.

\* Co-first author