PRANAV M. KHADE

Ph.D. Bioinformatics / Computational Biology

pranav.m.khade@gmail.com +1 515-708-2019 San Francisco Bay Area, CA pranavkhade.github.io
pranavkhade github.com/Pranavkhade 0000-0002-0756-9828

JOB EXPERIENCE

Scientist I

Research Data Sciences | Gilead Sciences

April 2025- Present Foster City, CA

- Participate in cutting-edge development of AI/ML models for drug discovery and scientific applications.
- Development and optimize exploratory analysis tools for interpreting multi-dimension dataset generated during biologics discovery workflow.
- Apply and advance artificial intelligence and machine learning (AI/ML) approaches, particular generative AI models, across stages of large molecule workflows, including molecular property predictions, AI-guided candidate selection and engineering.
- Work closely with data engineers to manage and preprocess large datasets, ensuring data quality and pipeline scalability.
- Communicate findings and insights to stakeholders through reports, presentations, and visualizations.
- Engage actively in the evaluation and coordination of collaborations with academic institutions, startups, and outsourcing partners.
- Stay updated on the latest advancements in AI/ML and computational biology and apply new techniques to improve existing workflows.
- Mentor and provide guidance to junior data scientists and research associates.

Postdoctoral Fellow

Prescient Design | Genentech | Roche

May 2022- April 2025 South San Francisco, CA

- Built a novel Graph Neural Network to predict develop-ability
- Work on Ab and TCR binding prediction with AI ML and Novel Coarse-grained MD
- Work on investigating geometric patterns responsible for molecular interactions.
- Work on embedding extraction from the protein-protein interfaces with custom architectures for UMAP analysis and various applications in the therapeutics space.

EDUCATION

Ph.D Bioinformatics

Iowa State University

August 2017 – April 2022 Ames, IA

- Aided in research input into four grants from which $1M NSF (1856477) was awarded in 2019
- Served on Bioinformatics and Computational Biology Graduate Student Organization Committee (2019)

M.Sc. Bioinformatics

Savitribai Phule Pune University, India

2014 – 2016 Pune, India

- GPA: 5.34 out of 6
- Thesis Project: Systematic Conformer Generation (Cheminformatics)

HONORS AND AWARDS

Research Excellence Award
University President and Graduate College Dean of Iowa State University

- The intent of this program is to recognize "the best of the best" graduating students who have submitted theses and dissertations.

IGIB-GNR Scholarship
Institute of Genomics and Integrative Biology, Delhi, India

- Issued for Excellent performance in the entrance and academics at the Bioinformatics Centre, University of Pune.

DBT Fellowship
DBT, Government of India

- For each semester of M. Sc., top-performing students are awarded a monthly fellowship.

NSF Travel Grant
National Science Foundation, United States Government

- Support to attend “International Conference on Mathematical Multiscale Modeling in Biology”-Guanacaste, Costa Rica.

BCB Travel Fund
BCB Program, Iowa State University

- Based on my performance and work presentation

STRENGTHS

Innovative | Quick Learner | Versatile | Persistent

Antibody | TCR Design | GNNs | GenAI

PROGRAMMING

Python	●●●●●
PyTorch +Lightning	●●●●●
AWS Infrastructure	●●●●◐
R	●●●●○
C++	●●●◐○

- Training: Cell Biology, Immunology, Structural Biology, Genetics, Omics, Evolution, Cheminformatics, and Data Mining.

B.Sc. Biotechnology

Savitribai Phule Pune University, India

2011 – 2014 Pune, India

- Grade: First-Class
- Training: Several wet-lab techniques and experiment formulation.

COMPLETED PROJECTS

PACKMAN API

github.com/Pranavkhade/PACKMAN

70000+ Downloads Featured on PDB website.

BRIDGE

https://github.com/prescient-design/BRIDGE

Antibody Engineering Foundational AI Model

Delaunay Graph Neural Network

https://github.com/prescient-design/D-GNN

Antibody Developability Meaninful Biological Priors for XAI

GOThresher

https://github.com/FriedbergLab/GOThresher

Information Theory

clinical_SVs

github.com/collaborativebioinformatics/clinical_SVs

Structural Variants Hackathon

PUBLICATIONS

Book Chapters

- Jernigan, R. L. [Robert L.], Khade, P. M., Kumar, A., & Kloczkowski, A. (2021). *Using surface hydrophobicity together with empirical potentials to identify protein-protein binding sites. application to the interactions of e-cadherins*. Computer Simulations of Aggregation of Proteins and Peptides, Springer US.

Journal Articles

- Khade, P. M. [Pranav M.], & Watkins, A. M. (2025). Bridge: A coarse-grained architecture to embed protein-protein interactions for therapeutic applications. *bioRxiv*. doi:10.1101/2025.04.11.648307. eprint: https://www.biorxiv.org/content/early/2025/04/17/2025.04.11.648307.full.pdf
- Joshi, P., Banerjee, S., Hu, X., Khade, P. M., & Friedberg, I. (2023). GOThresher: a program to remove annotation biases from protein function annotation datasets. *Bioinformatics*, *39*(1). btad048. doi:10.1093/bioinformatics/btad048

CONFERENCES & TALKS

- PEGS 2024 (Boston), **Speaker** (AI-Guided Optimization & Rules for Developability)
- BPS Annual Meeting (2020/21/22/23) (**Platform Speaker** in 2022)
- The Society of Mathematical Biology (eSMB) 2020 (https://smb2020.org/Pranav-Khade/)
- Intelligent Systems for Molecular Biology (2020)
- International Conference on Mathematical Multiscale Modeling in Biology 2019, Guanacaste, Costa Rica
- Conference on Modeling of Protein Interactions 2018, KS
- 102nd Indian Science Congress, Mumbai

REFEREES

Dr. Andrew Watkins (Postdoc advisor)
Director, Genentech Inc.
watkins.andrew_@gene.com

Dr. Robert L. Jernigan (Ph.D. advisor)
Charles F. Curtiss Distinguished Professor, Iowa State University
jernigan@iastate.edu

Dr. Vladimir Gligorijevic (Mentor)
Senior Director, Genentech Inc.
gligorijevic.vladimir@gene.com

- Khade, P. M. [Pranav M], Maser, M., Gligorijevic, V., & Watkins, A. M. (2023a). Mixed structure- and sequence-based approach for protein graph neural networks with application to antibody developability prediction. *bioRxiv*. doi:10.1101/2023.06.26.546331
- Khade, P. M. [Pranav M], & Jernigan, R. L. [Robert L]. (2022a). PACKMAN-Molecule: Python Toolbox for Structural Bioinformatics. *Bioinformatics Advances*. vbac007. doi:10.1093/bioadv/vbac007
- Khade, P. M. [Pranav M.], & Jernigan, R. L. [Robert L.]. (2022b). Entropies derived from the packing geometries within a single protein structure. *ACS Omega*. doi:10.1021/acsomega.2c00999
- Kumar, A., Khade, P., Dorman, K., & Jernigan, R. L. (2022). Coarse-Graining Protein Structures into Their Dynamic Communities with DCI, A Dynamic Community Identifier. *Bioinformatics*. btac159. doi:10.1093/bioinformatics/btac159
- Scaramozzino, D., Khade, P. M., & Jernigan, R. L. (2022). Protein fluctuations in response to random external forces. *Applied Sciences*, *12*. doi:10.3390/app12052344
- Khade, P. M. [Pranav M.], Scaramozzino, D., Kumar, A., Lacidogna, G., Carpinteri, A., & Jernigan, R. L. (2021). Hdanm: A new comprehensive dynamics model for protein hinges. *Biophysical Journal*. doi:https://doi.org/10.1016/j.bpj.2021.10.017
- Scaramozzino, D., Khade, P. M., Jernigan, R. L., Lacidogna, G., & Carpinteri, A. (2020). Structural Compliance - A New Metric for Protein Flexibility. *Proteins*. doi:10.1002/prot.25968
- Khade, P. M. [Pranav M], Kumar, A., & Jernigan, R. L. (2019). Characterizing and Predicting Protein Hinges for Mechanistic Insight. *Journal of molecular biology*. doi:10.1016/j.jmb.2019.11.018