

PRANAV M. KHADE

Ph.D. Bioinformatics

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pranavkhade

JOB EXPERIENCE

Postdoctoral Fellow

Prescient Design | Genentech | Roche

May 2022 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.

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 and several others under review
- 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)
- 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

60000+ Downloads Featured on PDB website.

Delaunay Graph Neural Network

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

Antibody Developability AI ML

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

Graph Neural Networks

API Development

Molecular Models

PROGRAMMING

Python

Perl

R

C++



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

- 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
- 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

CONFERENCES & TALKS

- PEGS 2024 (Boston), Speaker (AI-Guided Optimization & Rules for Developability)
- Biophysical Society 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

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Dr. Robert L. Jernigan (Charles F. Curtiss Distinguished Professor)

@ Iowa State University

✉ jernigan@iastate.edu

Dr. Vladimir Gligorijevic

@ Senior Director, Genentech Inc.

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Dr. Michael Maser

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