Bodhi P. Vani

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Education

University of Chicago
PhD in Chemistry, M.S. in Chemistry
2015-2021

Indian Institute of Technology, Bombay
M.Sc. in Chemistry, minor in Physics
2010-2015

Research Interests

I apply and develop a combination of machine learning techniques and physics based methods to systems of biological and medical significance. I have a background in stochastic processes and statistical mechanics, enhanced sampling of molecular dynamics simulations of biomolecules, graph neural networks, generative modeling, and equivariance in machine learning models. My goal is to use this skillset to improve human health by attacking the most challenging problems in drug discovery. My current research focuses on intelligently learned manifolds towards generating conformational ensembles and discovering cryptic pockets.

Current Position

Senior Machine Learning Scientist
Prescient Design, Genentech Inc.

Research Experience

Prescient Design, Genentech Inc.
Small Molecule Drug Design team 2021-current
• Leading the effort to build ML-based approaches to assess druggability of targets with covalent and non-covalent small molecule ligands.
• Conceptualized and lead the implementation of a proof-of-principle model to demonstrate conformational sampling for peptides at orders-of-magnitude improvement over current state-of-the-art: Jump Accelerated Molecular Ensembles from Universal Noise (JAMUN)
• Developing a lab-in-the-loop style workflow for pocket ligandability prediction, and cysteine covalent ligandability prediction
• Leading conformational ensemble generation projects for macrocycles and intrinsically disordered peptides
• Conceptualized and executing an annual Dynamics and Novel Conformational Ensembles (DaNCE) workshop.
• Curated a database and metrics for benchmarking cryptic pocket prediction.
• Designing and implementing a workflow for one-shot cryptic pocket structure prediction with Prop-En

University of Maryland, College Park
Primary Investigator: Prof. Pratyush Tiwary 2021-2023
• Developed a computational drug design pipeline based on machine learning algorithms and enhanced sampling methods
• Developed a graph attention network based model to predict ligandability in proteins
• Extending the use of structure prediction algorithms to obtain conformationally diverse structures and guide sampling to obtain relevant states with Boltzmann weights
• Explored native state conformational changes and stabilities to identify druggable pockets for the kinase family of molecules
• Explained and predicting optimal lengths of disordered regions in CAR T-Cell therapies using machine learning models
• Combined equivariant graph neural networks with variational autoencoders to learn bias collective variables without handpicked a priori information

University of Chicago
Advisors: Prof. Aaron R. Dinner, Prof. Jonathan Q. Weare 2016-2021
• Developed an algorithm to accelerate the computation of Feynman-Kac equations using trajectory stratification
• Derived methods to compute Transition path Theory quantities using trajectory stratification
• Studied the folding and unfolding mechanism of the Insulin dimer by deducing key collective variables and residues involved
• Developed a methodology to approach coupled folding-binding problems using a combination of sampling techniques with experimental collaboration

Indian Institute of Technology, Bombay: Master's thesis
Guide: Prof. B. L. Tembe 2014-2015
• Studied the local structures and potential energies of a pair of neopentane molecules in aqueous solutions of taurine, urea, urea-taurine in comparison with pure water using constrained dynamics

Tata Institute of Fundamental Research: Summer internship
Guide: Prof. Ravi Venkataramani Summer 2013
• Studied the aggregation of amino acids in water in collaboration with an experimental group using the transition path sampling algorithm

Indian Institute of Technology, Bombay: Summer Internship
Guide: Prof. Arindam Chowdhury May- July 2012
• Tracked and analyzed the fluorescence spectra of a dye in motion in a polymer layer medium.
• Resolved the single molecule spectra of the polar dye using computational image processing methods to derive the orientation of the molecules in polar coordinates and monitor rotational motion of the molecule in long time scales.

Indian Institute of Technology, Bombay: Summer Internship
Guide: Prof. Y. U. Sasidhar May- July 2011
• Studied the hairpin forming tendencies of a polymer by simulating several mutants and characterizing folding behavior.

Service & Outreach

Mentorship
Mentored 2 summer interns in conformational ensemble generation and covalent druggability prediction respectively - Summer 2024
Mentored a graduate student through multiple projects as a post-doc - 2021-2023

Organizing at Prescient
Leading a collaboration between Dr. Tess Smidt's group at MIT and my group at Prescient.
Organized and lead a Dynamics and Conformational Ensembles (DaNCE) workshop - Mar 2025
Co-organizing women of prescient book club - 2025 Jan - ongoing

Machine learning and pytorch training group
Organized and co-lead a weekly machine learning workshop for graduate students and post-doctoral fellows with a focus on AI for science - 2023

Peer reviewer for publications
Proteins: Structure, Function, and Bioinformatics - 2022
Physical Review Letters - 2023
Journal of Chemical Theory and Computation - 2024

Expanding your Horizons: Science outreach for highschool girls with aptitude in science
Supervised a group of 10 students through all their workshops - 2017
Developed and conducted a workshop on material properties - 2018

Computational Chemistry - University of Chicago Spring 2016
Conducted weekly help sessions, developed, graded, and edited assignments, provided support with final project

General Chemistry & General Chemistry Honors- UChicago Fall 2015, Winter 2016
Conducted weekly discussion sessions and lab sessions

Freshman Quantum Chemistry Course- IIT Bombay Fall 2014
Conducted weekly tutorials for a 45-student class
Single-handedly conducted regular help-sessions for a class of over 200

Publications

JAMUN: Transferable Molecular Conformational Ensemble Generation with Walk-Jump Sampling , A Daigavane, BP Vani, S Saremi, J Kleinhenz, J Rackers
arXiv preprint arXiv:2410.14621
Neurips AIDrugX 2024

Modeling Boltzmann-weighted structural ensembles of proteins using artificial intelligence–based methods
A Aranganathan, X Gu, D Wang, BP Vani, P Tiwary
Current Opinion in Structural Biology 91, 103000

Exploring kinase asp-phe-gly (dfg) loop conformational stability with alphafold2-rave
Bodhi P. Vani, A Aranganathan, P Tiwary
Journal of chemical information and modeling 64 (7), 2789-2797

AlphaFold2-RAVE: From sequence to Boltzmann ensemble
Bodhi P. Vani, Akashnathan Aranganathan, Dedi Wang, Pratyush Tiwary. J. Chem. Theory Comput. 2023; https://doi.org/10.1021/acs.jctc.3c00290

Graph Attention Site Prediction (GASP): Identifying Ligandable Binding Sites with Graph Attention Networks Zachary Smith, Bodhi P. Vani, Michael Strobel, Pratyush Tiwary *Journal of chemical information and modeling 64 (7), 2637-2644*

Hinging on Success: Leveraging the Power of CAR T-Cell Therapy through In-Silico Modeling of Hinge Length and Epitope Location
Justin M. Mirazee, Akashnathan Aranganathan, Bodhi P. Vani, Pratyush Tiwary, Gregoire Altan-Bonnet, Naomi Taylor *In preparation*

Computing transition path theory quantities with trajectory stratification
Bodhi P. Vani, Jonathan Weare, and Aaron R. Dinner. *Journal of Physical Chem.* 157, 034106 (2022)

Molecular dynamics simulations of nucleotide release from the circadian clock protein KaiC reveal atomic-resolution functional insights
Lu Hong, Bodhi P. Vani, Erik H. Thiede, Michael J. Rust, Aaron R. Dinner. *Proceedings of the National Academy of Sciences* Dec 2018, 115 (49)

Insulin Dissociates by Diverse Mechanisms of Coupled Unfolding and Unbinding
Adam Antoszewski, Chi-Jui Feng, Bodhi P. Vani, Erik H. Thiede, Lu Hong, Jonathan Weare, Andrei Tokmakoff, and Aaron R. Dinner. *The Journal of Physical Chemistry B* 2020

Long-timescale predictions from short-trajectory data: benchmark analysis of a miniprotein
John Strahan, Adam Antoszewski, Chatipat Lorpaiboon, Bodhi P. Vani, Jonathan Weare, Aaron R. Dinner. *Journal of Chemical Theory and Computation* 2021, 17, 5, 2948–2963

Accelerating computations of Large Deviation Functions using non-equilibrium stratification
Bodhi P. Vani, Jonathan Weare, and Aaron Dinner *in preparation*

Conferences & Symposia

Neurips, Neurips workshops
Dec 10–Dec 15, 2024
AIDrugX, Structural Biology

MolSSI workshop: Machine Learning and Chemistry: Are We There Yet?
May 31-June 2, 2023

Rare Events Workshop: Analysis, Numerics, and Applications
February 27-March 3, 2023

Protein Dynamics Gordon Research Conference
October 23rd-28th, 2022
Awarded prize for best poster

Protein Dynamics Gordon Research Symposium
October 21st-23rd, 2022

Physical Review Letters Panel Discussion: ***State-of-the-art estimation of protein model accuracy***
December 5, 2022
Invited to moderate panel discussion

Berkeley Statistical Mechanics Meeting
January 11th-14th, 2018

Midwest Theoretical Chemistry Conference
June 21st-23rd, 2018

8th CRSI-RSC joint Symposium in Chemistry
February 6th, 2014

16th CRSI National Symposium in Chemistry
February 7th-9th, 2014

14th CRSI-NCL Theoretical Chemistry Symposium
December 18th-21st, 2014

Scholarships & Awards

The Danute Nitecki graduate fellowship - 2018
University of Chicago

Gordon Research Conference Best Poster
2022 Protein folding and dynamics conference

INSPIRE: Science fellowship 2010-2015
awarded by the Department of Science and Technology, Government of India

References

Dr. Vishnu Sresht, Manager
Director of Small Molecule Drug Discovery, Prescient Design, Genentech
sresht@gene.com

Dr. Joshua Rackers, Former collaborator
Co-Founder and Scientist, Stealth startup
joshrackers@gmail.com

Prof. Pratyush Tiwary, Post-doctoral Advisor
University of Maryland, Institute of Physical Science and Technology
ptiwary@umd.edu.edu

Prof. Aaron R Dinner, Ph.D Advisor
University of Chicago, Department of Chemistry
dinner@uchicago.edu

Prof. Jonathan Weare, Ph.D Co-advisor
Courant Institute of Mathematical Sciences, NYU
weare@cims.nyu.edu

Prof. Suriyanarayan Vaikuntanathan. Ph.D Committee member
University of Chicago, Department of Chemistry
svaikunt@uchicago.edu