

Prateek Bansal

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Education

University of Illinois Urbana Champaign, PhD and MS in Chemical Engineering

Aug 2019 – July 2025

GPA: 3.7/4.0

Institute of Chemical Technology, BS in Chemical Engineering

Aug 2015 – May 2019

GPA: 9.23/10

Research Experience

Conformational Sampling for activation Mechanism of the Human Smoothened Receptor (Biophysical Journal, 2023)

- Simulated 300 μ s GPU-accelerated molecular dynamics for a human receptor protein and learned state pathways, revealing a conserved molecular switch.
- Performed protein-ligand bound simulations and linked ligand binding to tunnel opening/closing via Markov Models through PyEMMA, guiding **structure-based drug design** for healthcare applications.
- Skills used: Molecular Dynamics Simulations, Statistical Modeling, Probability and Information Theory

Multiple Modes of Cholesterol Translocation in the Human Smoothened Receptor for Protein Design (eLife, 2025)

- Lead model development for quantification of cholesterol-entry energetics with ms-scale simulations and free-energy profiles, showing a lower-barrier outer-leaflet path while confirming both routes.
- Collaborated cross-functionally with experimentalists to validate gating residues with designed mutations.
- Skills used: **Scientific collaboration**, Biologics Design, Molecular Dynamics Simulations, Statistical Modeling

Cyclopamine Modulates Smoothened Receptor Activity in a Binding Position-Dependent Manner (Communications Biology, 2024)

- Mentored an undergraduate student to independent research practices by holding weekly one-on-one discussions, delegating responsibilities, leading to first author paper written under my mentorship.
- Performed alchemical free-energy perturbation calculations (thermodynamic integration) for **small molecules** using GROMACS for testing binding of a ligand to two distinct sites, resulting in insights useful for inhibitor design.
- Skills used: Mentorship, Team Collaboration, Scientific Publishing, **Oral and Written Communication Skills**, GROMACS, **Free Energy Perturbations (FEP)**, Project Management

Coarse Grained and biased simulations for understanding Supramolecular Assembly of Supercharged Proteins (ACS Cent. Sci., 2022)

- Collaborated cross-functionally with wet-lab structural biologists and biochemistry experts to understand design principles for protein-protein interactions.
- Performed Coarse Grained Simulations (using MARTINI3 on GROMACS) to probe interface interactions for self-association, analyzed data using MDAnalysis.
- Computed binding-energy landscapes via enhanced sampling using NAMD, linking net charge to interaction fate and surface patterns to assembly architecture.
- Skills used: NAMD, Collaboration, Scientific Publishing, Oral and Written Communication Skills, Biased Molecular Dynamics, **using Coarse-Grained forcefields**

Sequence-based predictive modeling of allosteric interactions in GPCRs using deep learning (In preparation, 2025)

- Built a sequence-only transformer/GNN to predict allosteric residue pairs, enabling rapid AI driven mutagenesis prioritization.
- Scaled training across GPCR families with automated pipelines and hyperparameter sweeps (~5,200 models), improving property prediction and reducing turnaround.
- Skills used: Deep Learning, Data Science, Graph Neural Networks, Large-scale data analysis, software pipeline generation, feature engineering

Computational Skills

Computational Chemistry and Molecular Modeling: Structural modeling, cheminformatics (RDKit), Molecular dynamics simulations (GROMACS, OpenMM, Schrodinger), PyEMMA, MDAnalysis, mdtraj, parameterization, quantum mechanics calculations (ORCA), docking, free energy calculations, bioinformatics, biophysics, **thermodynamics**

Machine Learning (ML), Scientific Computing, Data Analysis & Artificial Intelligence: Python, PyTorch, pandas, scikit-learn, Scipy, Numpy, Graph Neural Networks (GNNs), Transformers (LLMs), LSTMs, Variational Auto-encoders,

Applied Mathematics & Statistical Expertise: Markov State Models, Dimensionality Reduction (t-SNE, UMAP), Time-Series Analysis, Feature Engineering

Tooling and Development: C++ (Intermediate), Cython, Linux environment, Bash scripting, **HPC clusters, GPU acceleration (CUDA - Intermediate)**, Git, version control, cloud platforms

Certifications

1. Target Enablement, Preparation, and Validation (Maestro)
2. Designing Quality Ligand Libraries (Maestro)

Schrodinger, Oct '25
Schrodinger, Nov '25

Publications

In preparation:

- **Bansal, P.**, Kleiman, D., Shukla, D. Sequence based prediction of allosteric interactions in G-Protein Coupled Receptors using deep learning, In Preparation, 2025

Published/Under Review:

- **Bansal, P.**, Dutta, S. , Shukla, D., Activation Mechanism of the Human Smoothened Receptor, Biophysical Journal, 2023
- **Bansal, P.**, Kinnebrew, M., Rohatgi, R., Shukla, D. Multiple modes of cholesterol translocation in the human smoothened receptor, eLife, Aug 2025.
- **Bansal, P.**, Shukla, D. All roads lead to Rome: Class B1 GPCRs show similar activation states but distinct activation states, bioRxiv, 2025
- **Bansal, P.**, Shukla, D. Sequence constraints predispose Class D receptor STE2 to follow a non-canonical activation mechanism, bioRxiv, 2025
- Kihong, K., **Bansal, P.**, Shukla, D., Binding position dependent modulation of smoothened activity by cyclopamine. Communications Biology, 2024
- Jacobs, M., **Bansal, P.** , Shukla, D. , Schroeder, C.; Understanding Supramolecular Assembly of Supercharged Proteins ACS Central Science, 2022

Conference Proceedings/Invited Talks

Perception and translocation of cholesterol in the Human Smoothened Receptor
Invited talk to ACS's 'Excellence in Pride' symposium.

ACS Spring '25, San Diego

Class B1 GPCRs show similar active states, but distinct activation mechanisms
Mechanism of activation of the human smoothened receptor

BPS Spring '25, Los Angeles
BPS Spring '23, San Diego

Teaching

CHBE594: Computational Methods in Chemical Engineering
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Spring 2021
Fall 2021

TA for an introductory python course undergrad students. Graded, held office hours and answered questions.
Made it to list of TA's ranked as excellent

Honors and Awards

Spring 2025 Graduate College Conference Presentation award
Travel award sponsored by the department awarded to promising students.

Spring 2025

ACS PRIDE Merck Graduate Research Award

Spring 2025

American Chemical Society award for excellent queer graduate students in the chemical sciences.

A.T. Widiger Fellowship

Fall 2023

Departmental fellowship to students with exceptional performance.

Outreach

Outreach Camp Coordinator, CURIE Summer Camp, UIUC

Summers 2022–2023

Organized and mentored a team of lab assistants for an engineering outreach camp; taught 150+ high school students core concepts in chemical engineering through hands-on activities.

Lab Assistant, CURIE/WYSE Summer Camp, UIUC

Summers 2020–2021

Introduced high school students to chemical engineering; demonstrated a distillation experiment and shared insights on the engineering career path.