

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 Smoothed 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 Smoothed 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 validated gating residues with designed mutations.
- Skills used: **Scientific collaboration**, Biologics Design, Molecular Dynamics Simulations, Statistical Modeling

Cyclopamine Modulates Smoothed 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)

- Colloaborated cross-functionally with wet-lab structural biologists and biochemistry experts to understand design principles for protein-protein interactions.
- Performed Coarse Grained Simuations (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

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| 1. Target Enablement, Preparation, and Validation (Maestro) | Schrodinger, Oct '25 |
| 2. Designing Quality Ligand Libraries (Maestro) | 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 Smoothed Receptor, Biophysical Journal, 2023
- **Bansal, P.**, Kinnebrew, M., Rohatgi, R., Shukla, D. Multiple modes of cholesterol translocation in the human smoothed 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 smoothed 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

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| Perception and translocation of cholesterol in the Human Smoothed Receptor | ACS Spring '25, San Diego |
| Invited talk to ACS's 'Excellence in Pride' symposium. | |
| Class B1 GPCRs show similar active states, but distinct activation mechanisms | BPS Spring '25, Los Angeles |
| Mechanism of activation of the human smoothed receptor | BPS Spring '23, San Diego |

Teaching

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| CHBE594: Computational Methods in Chemical Engineering | Spring 2021 |
| CHBE594: Computational Methods in Chemical Engineering | 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

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

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| 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. | |