Prateek Bansal

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EDUCATION

PhD Candidate, Chemical and Biomolecular Engineering — Expected Spring 2025.
University of Illinois, Urbana-Champaign (UIUC), Urbana, Illinois — CGPA: 3.7/4.00

Bachelor of Engineering, Chemical Engineering — 2015-19
Institute of Chemical Technology, Mumbai, India — CGPA 9.23/10

PHD RESEARCH

Activation studies of **non-Class A G Protein-Coupled Receptors** — Aug 2019-Present

- Implemented extensive millisecond scale atomistic Molecular Dynamics, Mutual Information and Markov Models to uncover the conformational dynamics of Class F GPCR activation. Lead to discovery a novel molecular motif and intermediate states.
- Implemented Free Energy Perturbations and Deep Learning to explore the differential binding of a drug molecule to a membrane protein.
- Developed an in-house pipeline to compute absolute free energy computations.
- Used Umbrella Sampling and Steered MD to compute the binding free energy of a protein - protein complex
- Implemented extensive millisecond scale atomistic Molecular Dynamics, mutagenesis and adaptive-biasing force based simulations to sample the transport of cholesterol via the human Smoothened receptor
- Implementing Deep Learning based Neural Relational Inference Graph Neural Network Model to compute a sequence-to-allostery model for G-Protein Coupled Receptors

PUBLICATIONS

1. Jacobs, M., **Bansal, P.** , Shukla, D. , Schroeder, C.; Understanding Supramolecular Assembly of Supercharged Proteins *ACS Central Science*, 2022, 8(9), 1350-1361. Link
2. **Bansal, P.**, Dutta, S. , Shukla, D., **Activation Mechanism of the Human Smoothened Receptor**, *Biophysical Journal*, 2023. Link
3. Kihong, K., **Bansal, P.**, Shukla, D., Binding position dependent modulation of smoothened activity by cyclopamine. 2024. *Accepted in Communications Biology.* Link
4. **Bansal, P.**, Kinnebrew, M., Rohatgi, R., Shukla, D. A mechanism for the transport of cholesterol in the human Smoothened Receptor, 2024, *Biorxiv* Link
5. **Bansal, P.**, Dutta, S., Paul, R., Shukla, D.; Markov State Models of Biomolecular Dynamics (book) under review at *ACS in Focus.*

COMPUTATIONAL SKILLS

- **Programming:** Python (Expert), Machine-Learning (scikit-learn, **pytorch**) (Intermediate), Command Line Interface, Use of Git and Github, Large Language Models, Autoencoders
- **Molecular Modeling:**
  1. Docking: Autodock, RosettaDock (Intermediate)
  2. Free Energy Perturbations
  3. Simulations: Amber, OpenMM, GROMACS, NAMD, VMD, PyMOL, Chimera, Membrane Protein Simulations (Expert)
  4. Modeling: Packmol, Modeller, Rosetta (Expert)
  5. Statistics: Markov State Models, Mutual Information, Shannon Entropy, Bayesian Modeling (Expert)
  6. Techniques: All-atom Simulations, Coarse Graining, Unbiased/biased simulations, Umbrella Sampling, Metadynamics, Free Energy Landscapes, Estimating Rate Constants
  7. Analysis: cpptraj, MDAnalysis, mdtraj, RDKit

HONORS AND AWARDS

- **Awardee - A.T. Widiger Fellowship** **Fall 2023-Spring 2024**
- **Winner - SCS Image Challenge** **Fall 2022**
  Won the competition for the best Journal Cover - xSchool of Chemical Sciences, UIUC
- **List of Teaching Assistants ranked as excellent** **Fall 2021**
  Department of Chemical and Biomolecular Engineering, UIUC
- **University Fellowship** **Aug 2019 - May 2020**
  Department of Chemical and Biomolecular Engineering, UIUC
- **National Winner - Design is in my DNA** **Oct 2018**
  Undergraduate Review Paper Presentation competition, Asian Paints Limited, India

CONFERENCE PRESENTATIONS

- **3rd Annual ECI GPCR Symposium for Early Career Investigators** **Fall 2023**
  Activation mechanisms of non-Class A GPCRs
  Bansal, P.; Shukla, D.
- **American Chemical Society Spring Meeting, Indianapolis** **Spring 2023**
  Universality in activation mechanisms of Class B GPCRs
  Bansal, P.; Shukla, D.
  Presented talk under **Early Career Investigators** in Biological Chemistry section.
- **Annual Biophysical Society Meeting, San Diego** **Spring 2023**
  Cholesterol transport mechanism of the Human Smoothened Receptor
  Bansal, P.; Shukla, D.

OUTREACH ACTIVITIES

- **Head Lab Assistant, CURIE Summer Camp, UIUC** **Summer 2022, Summer 2023**
  Organized and Mentored multiple lab assistants for engineering outreach camp. Taught high school students concepts in chemical engineering.
- **Lab Assistant, CURIE/WYSE Summer Camp, UIUC** **Summer 2020, Summer 2021**
  Introduced chemical engineering to high school students.