

# Pradyumn Sharma

PhD Student, Chemical Engineering, Indian Institute of Science (IISc)

## Contact

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## Summary

PhD student trained in computational biophysics with strong communication skills and ability to work independently or as part of a team.

- Special expertise in molecular simulations, enhanced sampling methods and data analysis.
- Experience of working in collaboration with industry in a team of experimental and theoretical collaborators from interdisciplinary backgrounds.
- Worked on projects with a team of post-doc, PhD and masters students which in turn helped in nourishing time and project management skills.

## Education

### Int. PhD in Chemical Engineering

Indian Institute of Science (IISc), Bangalore  
2016-2021 (anticipated)

Advisor – Prof. K. Ganapathy Ayappa

### Bachelor's in Chemical Engineering

Meerut Institute of Engineering and Technology (MIET), Meerut  
2011-2015

## Accomplishments

**2019:** Student President of Departmental Society CEA (Chemical Engineering, IISc)

**2019:** Organised the first Student Biomembrane Symposium (IISc)

**2014:** President of Departmental Society ACES (Chemical Engineering, MIET)

## Experience

Worked as a consultant for Unilever funded project in IISc to study bacterial membranes, which involved teamwork with multidisciplinary experts from academia and industry.

- Developed protocols to observe the barriers properties of bacterial membranes for drug permeation, using in-silico models.
- Developed a MARTINI model for bacterial cell wall.
- Gleaned insights into interactions of surfactants with bacterial membranes.

Performed phase transition study of the MARTINI lipid membranes and benchmarked their ability to capture the ripple phase.

## Conference Presentation

Feb 2020	Poster	Biophysical Society Meeting	San Diego, USA
Dec 2019	Invited Talk	ESKAPE Pathogens Symposium	Bangalore, India
Mar 2019	Poster	Indian Biophysical Society Meeting	Kolkata, India

## Publications

- Pradyumn Sharma**, Srividhya Parthasarathi, Nivedita Patil, Morris Waskar, Janhavi S. Raut, Mrinalini Puranik, K. Ganapathy Ayappa, Jaydeep Kumar Basu. *Assessing Barriers for Antimicrobial Penetration in Complex Asymmetric Bacterial Membranes: A Case Study with Thymol*, **Langmuir** 2020, 36, 30, 8800–8814
- Rakesh Vaiwala, **Pradyumn Sharma**, Mrinalini Puranik, K. Ganapathy Ayappa. *Developing a Coarse-Grained Model for Bacterial Cell Walls: Evaluating Mechanical Properties and Free Energy Barriers*, **J. Chem. Theory Comput.** 2020, 16, 8, 5369–5384

## Skills

### Programming

Python C & C++ Shell scripting LaTeX JAVA SQL

### Software/Packages

GROMACS PLUMED VMD Quantum ESPRESSO MS Office

### Technical

Molecular dynamics simulations Atomistic and mesoscale modelling Enhanced sampling methods

Drug discovery Membrane biophysics Protein-Membrane interactions Force field development

Monte Carlo simulations Quantum mechanical calculations

## References

### **K. Ganapathy Ayappa**

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