

# ASHLIN JAMES PORUTHOOR



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## SUMMARY

Ph.D. candidate in molecular dynamics, modeling, methods development & computer-aided drug design. Experienced in collaborative academic and industry settings, with multiple internships in discovery chemistry and modeling teams.

## EDUCATION

Doctor of Philosophy, Biophysics, University of Rochester	2018 - 2024
Master of Science, Biophysics, University of Rochester	2018 - 2021
Master of Science, Physics, NIT Calicut	2016 - 2018
Bachelor of Science, Physics (Honors), St.Stephen's College, University of Delhi	2013 - 2016

## RESEARCH EXPERIENCE

Graduate Research Student University of Rochester Medical Center, <b>Grossfield Lab</b>	June 2019 - Present Rochester, NY
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- **Developed a computational method** to estimate the free energy landscape of phase separation in the lipid bilayers from molecular dynamics (MD) simulations using **enhanced sampling** protocols ◇ **Analyzed > 100 TB simulation data** ◇ Coarse-Grained MARTINI lipid modeling ◇ GROMACS ◇ **Weighted Ensemble**
- Developed a benchmarking protocol to identify efficient collective variables that simultaneously track phase separating bilayers while driving the enhanced sampling, resulting in faster convergence of free energy landscapes
- Studied the MD finite-box size effects in constructing free energy landscapes of phase separating lipid bilayers
- Developed statistical mechanics-based analysis schemes to track and visualize ultrafast dynamics of Rhodopsin upon light activation to interpret the XFEL experiments ◇ **Analyzed > 10000 short All-Atom simulations** ◇ NAMD ◇ OpenMM ◇ Cross-functional collaboration ◇ **Membrane-GPCR modeling** ◇ Python

Computational Sciences Co-op - Part Time Moderna, <b>Discovery Chemistry</b>	Jun 2023 - Oct 2023 Cambridge, MA
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- Studied the role of ionizable lipids in lipid nanoparticles (**LNPs**) and their preferential interactions with RNA with NAMD3 All-Atom Molecular Dynamics simulations in AWS. **Abstract submitted** to Biophysical Society Meeting 2024, Philadelphia, PA. ◇ RNA-bilayer Modeling ◇ Python suite for end-to-end large-scale data analysis
- Generalized and automated in-house protocol for customized in-silico lipid bilayer model generation

Computational Sciences Co-op - Full Time Moderna, <b>Molecular Engineering and Modeling</b>	January 2022 - June 2022 Cambridge, MA
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- Studied **RNA – lipid bilayer** interactions with NAMD All-Atom Molecular Dynamics simulations
- Studied **RNA - small molecule** interaction via **docking** & Molecular Dynamics. Proposed and implemented a python analysis suite for initial validation of **binding pocket interactions** and ligand conformational dynamics
- Benchmarked different alchemical and geometrical routes for RNA-small molecule **binding free energy calculations**. Implemented a test pipeline molecules that can be extended for an extensive ligand library screening
- Proposed and initiated an internal pilot project that involved cross-functional teams  
◇ Schrödinger Glide, Maestero ◇ BFEE2 ◇ AMBER Antechamber, GAFF2 ◇ Bitbucket ◇ JupyterLab ◇ AWS

Summer Research Fellow JNCASR, Theoretical Sciences Unit	April 2018 - June 2018 Bangalore, India
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- Studied the sensitivity of population dynamics of bacteria towards the nutrient environment using modeling and numerical simulation. Modeled quorum sensing and chemotaxis behaviors and emulated racing conditions

#### Summer Research Fellow

JNCASR, Theoretical Sciences Unit

May 2017 - July 2017

Bangalore, India

- Conducted metabolic network reconstructions and flux balance analyses on constrained-based *in silico* yeast models. Studied the effect of various metabolites on the yeast growth rates upon network perturbations
- Integrated transcriptomic data into *in silico* models of *Plasmodium falciparum* to emulate multiple malaria variants in southeast Asia to understand the rise of drug resistance using cross-functional efforts

### OTHER RELEVANT EXPERIENCE

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#### Moderna – Carnegie Mellon University, Artificial Intelligence (AI) – Academy Certification (2022)

Internal training to educate and empower Moderna employees to integrate AI and ML solutions into their workflow

**Founding Member, Learning Curve Initiative:** A graduate and postdoc trainee-led group to normalize negative data among computational chemistry and biophysics community and share hidden best practices within diverse labs

**Founding President, International Students and Scholars Association (ISSA), University of Rochester (2023 - Present)** Represent the international grad student community in the School of Medicine and Dentistry

**Graduate Student Society, International Student Liaison (2022 - Present)** Formed an internal student committee and conducting focus groups and panel discussions to enhance the international grad student experience

**URBEST Trainee (2021 - Present)** University of Rochester initiative to **B**roaden **E**xperiences in **S**cientific **T**raining for early career scientists. Training on leadership and management skills for scientists via coursework, panel discussions, informational interviews, career stories, mentoring, and other personalized programs

**UR2 Mentorship Program (2020 - 2022):** A program run by graduate students to mentor and train first-generation undergraduates and those from less privileged backgrounds on tools and resources for a research career

**Teaching Assistant, BPH509 - Molecular Biophysics (2020)** Instructed students in theoretical, experimental, and computational methods to study macromolecules. Topics include statistical mechanics, optical melting experiments, dynamic programming algorithms, molecular dynamics, protein folding, and isothermal titration calorimetry

**Open-source Contributions (2020 - 2023)** **LOOS** : A lightweight object-oriented structure analysis library for MD simulations. **WESTPA** : The Weighted Ensemble Simulation Toolkit with Parallelization and Analysis. **FLOPSS 2.0** : pipeline to compute **F**ree energy **L**andscape **O**f **P**hase **S**eparating **S**ystems - to be released soon (**Early version**)

### SCHOLASTIC ACHIEVEMENTS

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**Neuman Travel Award, 2020, 2021, 2023** : To share and present the thesis research at academic conferences

**Biophysics Student Seminar Award, 2021** : For best student seminar based on popular votes

**Graduate Women In Science Mentor-Up Winner, 2021** : University challenge to set and achieve multiple short-term personal and professional goals through mentoring-up and training

**Dr. K. Swaminathan Memorial Award, 2016** : For an excellent academic record and overall achievements in cultural activities during undergrad level, St. Stephen's College, University of Delhi, India

**Top 1%** of all the students who appeared at the state-level Higher Secondary Examination, March **2013**. Nominated by Kerala State Higher Secondary Board for the Central Government Scholarship for higher education

**INSPIRE SHE, 2013 -2018** : Five-year scholarship by the Department of Science and Technology, Government of India, based on an excellent performance at the higher secondary and undergrad level

**INSPIRE AWARD, 2011** : For outstanding academic performance at the high school level, from the Department of Science and Technology, Government of India