# ASHLIN JAMES PORUTHOOR

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## SUMMARY

Ph.D. candidate skilled in molecular dynamics, modeling, methods development, and computer-aided drug design. Experienced in collaborative 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** June 2019 - Present
University of Rochester Medical Center, **Grossfield Lab** Rochester, NY

- **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** ⋄ Unsupervised Learning ⋄ Coarse Grained MD ⋄ **Weighted Ensemble** ⋄ GROMACS
- 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

**Discovery Chemistry Co-op** - Part Time Jun 2023 - Oct 2023
**Moderna, Computational Sciences** Cambridge, MA

- 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 & GRC Biotherapeutics and Vaccines Development 2024. ⋄ 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

**Molecular Engineering and Modeling Co-op** - Full Time January 2022 - June 2022
**Moderna, Computational Sciences** Cambridge, MA

- 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
- Studied **RNA - lipid bilayer** interactions with NAMD All-Atom Molecular Dynamics simulations
- 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** April 2018 - June 2018
**JNCASR**, Theoretical Sciences Unit Bangalore, India

- 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** May 2017 - July 2017
**JNCASR**, Theoretical Sciences Unit 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

**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)** **U**niversity of **R**ochester 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

**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

## PUBLICATIONS

**Poruthoor, Ashlin** & Sharma, Akshara & Grossfield, Alan. (2023). Understanding the Free Energy Landscape of Phase Separation in Lipid Bilayers using Molecular Dynamics. Biophysical Journal. 122. 10.1016/j.bpj.2023.09.012.

**Poruthoor, Ashlin** & Stallone, Jack & Miaro, Megan & Sharma, Akshara & Grossfield, Alan. (2024). Finite-size effect on the free energy landscape of phase separation in lipid bilayers estimated using molecular dynamics. (In preparation)

**Poruthoor, Ashlin** & Dehghanighahnaviyeh, Sepehr & Bali, Semiha & Isik, Mehtap & Sur, Sreyoshi. (2024). Interactions between ionizable amino lipids and a short RNA hairpin: Insights from molecular dynamics simulations for lipid nanoparticle optimization. (In preparation)

## CONFERENCE PRESENTATIONS

Poruthoor, Ashlin & Sharma, Akshara & Stallone, Jack & Miaro, Megan & Grossfield, Alan. (2024). Finite-size effect on the free energy landscape of phase separation in lipid bilayers estimated using molecular dynamics. Biophysical Journal. 123. 94a. 10.1016/j.bpj.2023.11.688.

Poruthoor, Ashlin & Dehghanighahnaviyeh, Sepehr & Bali, Semiha & Isik, Mehtap & Sur, Sreyoshi. (2024). Interactions between ionizable amino lipids and a short RNA hairpin: Insights from molecular dynamics simulations for lipid nanoparticle optimization. Biophysical Journal. 123. 97a. 10.1016/j.bpj.2023.11.699.

Poruthoor, Ashlin & Grossfield, Alan. (2023). Accurate estimation of free energy landscape of phase separation in lipid bilayers. Biophysical Journal. 122. 85a-86a. 10.1016/j.bpj.2022.11.665.

Poruthoor, Ashlin & Grossfield, Alan. (2022). Modeling the free energy landscape of phase separation in lipid bilayers. Biophysical Journal. 121. 368a. 10.1016/j.bpj.2021.11.928.