# ASHLIN JAMES PORUTHOOR

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## SUMMARY

Post-doctoral fellow 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

**Post Doctoral Fellow** July 2024 - Present
University of Maryland Baltimore, **MacKerell Lab** Baltimore, MD

- Developed ensemble learning and deep learning models to predict small molecule membrane permeability using physics-based SILCS continuum models with fragment-based 3D mapping of membranes of varying complexity. Feature engineered multiple novel molecular descriptors and assessed their effects on the explainability of models[1]
- Lead optimization and High Throughput Virtual Screening of SCP2 inhibitors: Using Site Identification by Ligand Competitive Saturation (SILCS) platform, I led the fragment-based computational campaign to expand chemical modifications, corresponding SAR analysis on targets and off-targets with experimental collaboration[2]
- In-silico designing of photoaffinity probes for target characterization and identification for the SCP2 campaign
- Developing an *in silico* renal proximal tubule model for ADMET prediction with SILCS whole cell simulation

**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[3] ⋄ **Analyzed > 100 TB simulation data** ⋄ Unsupervised Learning ⋄ Coarse Grained MD ⋄ **Weighted Ensemble** ⋄ GROMACS
- Studied the MD finite-box size effects in constructing free energy landscapes of phase separating lipid bilayers[4]
- 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[5] ⋄ RNA-bilayer Modeling
- 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 module 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 constraint-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

**Software Contributions (2024 - Present)** SILCS: Created protocols for handling complex user-input custom membranes for SILCS-Membrane tool that elimiated early runtime termination. Bug fixes, and beta-testing.

**URBEST Trainee (2021 - 2024)** **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

**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)

## RELEVANT PUBLICATIONS

1. Elizabeth S. Liedhegner, Caitlin Bauer, Nathalia Rocha Lainetti, **Ashlin Poruthoor**, Alexander MacKerell, Christopher Cunningham, Cecilia Hillard. Sterol Carrier Protein 2 (SCP-2), trafficker of endocannabinoids, interacts with the phytocannabinoids, cannabidiol (CBD) and cannabigerol (CBG). GRC Cannabinoid Function in the CNS, New Hampshire, August 2025 [Poster]

2. **Ashlin Poruhtoor**, Alexander MacKerell Jr. Lessons learned from predicting drug permeability by bridging physics and machine learning using the SILCS methodology. ACS Fall Meeting 2025, Washington, D.C. [Poster]

3. **Ashlin Poruhtoor**, Akshara Sharma, Alan Grossfield. (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.

4. **Ashlin Poruhtoor**, Jack Stallone, Megan Miaro, Akshara Sharma, Alan Grossfield (2024). System size effects on the free energy landscapes from molecular dynamics of phase-separating bilayers. J. Chem. Phys. 161, 145101

5. **Ashlin Poruthoor**, Sepehr Dehghanighahnaviyeh, Semiha Bali, Mehtap Isik, Sreyoshi Sur. (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. [Poster]