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 assesed the their effects on 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[3,4] ⋄ **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
- 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

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]

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]

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.

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

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]