

DR. ASHLIN JAMES PORUTHOOR



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SUMMARY

Postdoctoral fellow with extensive experience in molecular dynamics, molecular modeling, cheminformatics, and machine learning-based property prediction. Focused on bridging physics-based molecular insights with data-driven ML models to improve predictive performance and decision-making in drug discovery. Experienced in collaborative industry and academic settings, with multiple internships in discovery, medicinal chemistry and modeling teams.

RESEARCH EXPERIENCE

Post Doctoral Fellow

July 2024 - Present

University of Maryland Baltimore, **MacKerell Lab**

Baltimore, MD

- Lead optimization and High Throughput Virtual Screening of SCP2 inhibitors: Using Site Identification by Ligand and Competitive Saturation (**SILCS**) platform, led the fragment-based computational campaign to expand chemical modifications, SAR analysis on targets and off-targets with experimental collaboration¹. **>500 molecules prioritized for synthesis. 10+ congeneric series explored. Improved binding affinities by 10-100x.**
- 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. **Achieved industry standards performance with 10x smaller input vector sizes while enhancing the explainability². Extended the pipeline to out of distribution beyond rule of 5 (bRo5) molecules.**
- Developing an *in-silico* renal proximal tubule model for ADMET prediction with SILCS whole cell simulation. **>10 transporters & enzymes modeled. Training and testing on > 3K small molecule protomers.**
- *In-silico* designing of photoaffinity probes for target characterization and identification for the SCP2 campaign

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** protocols³ ♦ **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 bilayers⁴
- Developed analysis schemes using statistical mechanics 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 AWS⁵ ♦ 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, Maestro ◊ 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 eliminated early runtime termination. Bug fixes, and beta-testing.

URBEST Trainee (2021 - 2024) University of Rochester initiative to **Broaden Experiences in Scientific Training** 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 **Free energy Landscape Of Phase Separating Systems** - to be released soon (**Early version**)

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

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]