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

- Developing better machine learning models to predict membrane permeability using feature engineering from continuum models depicting chemical environments and curation of datasets with high-quality metadata.
- High Throughput Virtual Screening of potential SCP2 inhibitors: Using Site Identification by Ligand Competitive Saturation (SILCS) platform to screen for potential candidates and their effect on targets and off-targets.
- In-silico designing of photoaffinity probes for target characterization and identifications
- Developing a renal *in silico* continuum model for ADMET prediction using SILCS

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.
  Poster presented at Biophysical Society Meeting 2024, Philadelphia, PA & GRC Biotherapeutics and Vaccines Development Meeting 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

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

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)

RELEVANT 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). System size effects on the free energy landscapes from molecular dynamics of phase-separating bilayers. J. Chem. Phys. 161, 145101

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)