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 ◇ Enhanced sampling ◇ 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

Computational Sciences Co-op - Part Time Jun 2023 - Oct 2023
Moderna, Discovery Chemistry 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. ◇ 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

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

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

Please refer to https://orcid.org/0000-0003-3952-8884