SOUMYA DUTTA

Second year Graduate Student,
Arizona State University

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EDUCATION

8/2022 - Present **Doctor of Philosophy in Chemistry/Biochemistry** — **School of Molecular Sciences, Arizona State University**
Advisor - Dr. Abhishek Singharoy
Research - Computational Biophysics, development and application of Molecular Dynamics simulations and Machine Learning on biomedical and biochemical applications.
GPA - 3.85 of 4.00 (Up until second semester)

7/2020 - 6/2022 **Master of Science in Chemistry** — **Indian Institute of Technology, Guwahati**
Major focus in Physical and Computational Chemistry
CPI - 9.66 of 10.00

7/2017 - 6/2022 **Bachelor of Science in Chemistry** — **University of Calcutta, RKMRC Narendrapur**
With Minors in Physics and Mathematics
CPI - 8.71 of 10.00

PROJECTS

Drug discovery focused:

2/2023 - Present **Investigation of the origins of immunomodulatory drugs-resistance in myeloma patients using Molecular Dynamics simulations**
In collaboration with **Mayo Clinic**
Contributions :
- Developed hypotheses on the potential point of failures of existing drugs due to particular mutations and deletions in substrate receptor of E3-ligase.
- Generated models to accurately depict the deletions in E3-Ligase.
- Identified a conformationally-coupled disassembly pathway of the deformed E3-Ligase system from large-scale MD simulations.

4/2023 - Present **Molecular targeting of Cholangiocarcinoma: Overcoming drug resistive mutations**
In collaboration with **Mayo Clinic**
Contributions :
- Designing models and simulations to investigate the molecular reason for the failure of existing drugs.
- Exploring the molecular characteristics of existing pharmaceuticals through MD simulations and incorporating this insight into the pharmacophore modeling of extensive drug libraries to overcome mutations.

5/2023 - Present **Conducting mechanistic investigations into the polymodal activation of human TRPV1 by heat, protons, and ligands, and elucidating the distinctions in their allosteric pathways**
Contributions :
- Designing coarse-grained simulations and normal mode analysis calculations to determine probable pathways for allosteric changes in the TRPV1 channel.
- Finding suitable small molecules that will potentially be able to activate the proton and heat decoupled allosteric change, to minimize side effects.

12/2021 - 4/2022 **Targeting the SARS-CoV-2 RNA-dependent RNA polymerase (RdRp) with synthetic/designer unnatural nucleoside analogs**
Contributions :
- Designed Molecular docking and pharmacophore modeling of nucleoside analogs.
- Designed MD simulations to investigate the binding kinetics of nucleoside analogs with RdRp of SARS-CoV-2 to test their efficacy.

Biophysics focused:

11/2022 - Present **Investigating the effect of catch-bond formation at the PDZ domain of junctional protein Afadin under mechanical stress.**

Contributions :

- Conducted Steered Molecular Dynamics simulations replicating the stress conditions cell junctions face in biological conditions
- Calculated probable free energy pathways in the event of catch-bond formation.

12/2022 - Present **Investigating how biophysical constraints of foldability shaped the early selection of amino acids in the pre-cellular world.**

Contributions :

- Created a comprehensive dataset of peptide sequences and structures by utilizing the **ESMFold**, AI model from META.
- Created a new dataset of proteins with modifications in the peptide sequences to investigate their effects on folding.

PUBLICATIONS

Published:

2023 **Bag SS, Sinha S, Dutta S, Baishya HJ, Paul S. Targeting the SARS-CoV-2 RNA-dependent RNA polymerase (RdRp) with synthetic/designer unnatural nucleoside analogs: an in silico study. J Mol Model. 2023 Nov 11;29(12):366. doi: 10.1007/s00894-023-05767-2. PMID: 37950101.**

Under Preparation:

2023 - 2024 **catch-bond formation at the PDZ domain of junctional protein Afadin under mechanical stress**

2023 - 2024 **Investigation of the origins of immunomodulatory drugs-resistance in myeloma patients using Molecular Dynamics simulation**

AWARDS AND ACHIEVEMENTS

2017 **INSPIRE Scholarship** **Department of Science and Technology (DST), Govt of India**

2020 **All India Ranking (AIR) 196 in IIT-JAM 2020** **conducted by Indian Institute of Technology, Kanpur**

2021 **All India Ranking (AIR) 41 (JRF Qualified) in CSIR-UGC NET** **Council of Scientific and Industrial Research, India**

2022 **All India Ranking (AIR) 213 in GATE-2022** **conducted by Indian Institute of Technology Kharagpur**

TECHNICAL SKILLS

Molecular Dynamics related
NAMD, GROMACS, MELD (Modeling Employed Limited Data), OpenMM, VMD, Pymol, Discovery Studio, AutoDock

Programming Languages
Python, Pytorch, TCL, BASH, Fortran

IT
Linux, HPC

Supercomputer
Arizona State University - AGAVE, SOL
Oak Ridge National Lab - FRONTIER (ALCC - Oak Ridge Leadership Computing Facility)

TEACHING EXPERIENCE

8/2022 - Present **Mentor at Biosense Network** **Arizona State University**

- Taught high school students and teachers in Biosense network how to use VMD and NAMD to run molecular dynamics simulations.

8/2022 – 4/2023 **Graduate Teaching Assistant** **School of Molecular Sciences**

- Taught general chemistry to undergraduates.

8/2022 – present **Lab Mentor** **School of Molecular Sciences, Singharoy Lab**

- Taught Biophysics to 2 undergraduate students and a high school student, and trained them in molecular dynamics simulations. One of the undergrads and the high school student are in the process of co-publishing with me.

CONFERNCES

2/2024 **Biophysical Society 2024** **Philadelphia, Pennsylvania**
Accepted for poster presentation

EXTRACURRICULAR ACTIVITIES

10/2022 - Present **Member at Biophysical Society Arizona Chapter** **ASU and UA**

REFERENCES

Dr. Abhishek Singharoy (PhD advisor)
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Tempe, Az
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Dr. Mitesh J. Borad, M.D.
Oncology (Medical)
Mayo Clinic Comprehensive Cancer Center
Phoenix, Az
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