ADITHYA POLASA

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Summary

Develop and apply computational methods in biophysics, chemistry, and other computationally intensive fields. Optimize and parallel scientific programs for accelerated computers, supercomputers, and conventional clusters. Solve challenging problems in the field of computational chemistry,

Molecular Modeling | Molecular Dynamics | Drug Design | Structural Mechanics | Docking study | Free Energy Calculation

Education

Doctorate in Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR; GPA: 3.6/4.0 (2018- present).
Master's in Bio-medical Science (MS), Long Island University, Greenvale, NY; GPA: 3.8/4.0 (2015 - 2017).
Bachelor's in Pharmacy (BS), Anurag group of Institutions, Hyderabad, India; GPA: 3.8/4.0 (2011 - 2015).

Technical Skills

Atomistic Simulations of *Protein:* Molecular dynamics (MD) of proteins and nanoparticles, Steered molecular dynamics (SMD), Exploring Complex Conformational Transition Pathways, and Refining the transition pathway (String Method with Swarms of Trajectories).

- MD Software: VMD, Charmm-gui, NAMD, Phenix,

Programming: Python, R, High Performance Computing (HPC) Cluster, Linux TCL/TK scripting, MATLAB.
Free Energy Calculation (FEP): Free energy calculations along the refined transition path (Umbrella sampling), Ligand protein binding free energy calculations, and Alchemical Free Energy Perturbation Calculations.

- FEP Software: Chimera, ParseFEP tools,

Molecular Modeling and Drug Design: Homology modeling of proteins, Construction of protein drug docking models, Investigated the structure, dynamics, surface properties, and thermodynamics of inorganic, biological, and polymeric systems using MD.

- Software: Auto dock vina, MODELLER, PyMoL, UCSF Chimera, Swiss-model

Molecular Dynamics Flexible Fitting: Structural refining of low-resolution x-ray and cryo-EM crystallographic diffraction data.

- Software: Phenix, VMD

Research Experience

University of Arkansas, [Link] *Fayetteville, AR, USA*
Senior Research Assistant – Chemistry and Biochemistry Dept., 01/2018 – Present

- *Project 1:* Computational characterization of SARS Coronavirus One and Two's. Our simulations show clearly just how active these proteins become. We distinguish the structural and conformational difference between SARS CoV one and two. [Link]
- *Project 2:* pH-dependent conformational dynamics of influenza hemagglutinin and the associated membrane-fusion process. All-atom microsecond-level equilibrium MD simulations have been used to study the effects of protonating a single conserved histidine on HA conformational dynamics. [Link]
- *Project 3:* Elucidating the molecular basis of pH activation of an engineered mechanosensitive channel. The orientation-based method in this work for generating and optimizing an open model of engineered MscL is a promising method for generating unknown states of proteins and for studying the activation processes in ion channels. This work facilitates the studies aimed at designing pH-triggered drug delivery liposomes (DDL), which embed MscL as a nanovalve. [Link]
- *Project 4:* Computational elucidation of recombinant fusion protein effect on peptide-directed nanoparticles. This study describes, at the molecular level, the role of the amino acid sequence on binding affinity of the peptide to the surface of the palladium particles, and the functional ability of the GFPuv protein controlling these free energies irrespective of peptide sequence. This study will provide a framework for designing free and protein attached peptides that facilitate peptide-mediated nanoparticle formation with well-regulated properties. [Link]
- *Project 5:* An investigation of the YidC-mediated membrane insertion of a pf3 coat protein using MD simulations. This study provides a complete conformational transition involved in the mechanism of protein insertion into membrane by Yidc independently. [Link]

Experience

Affinitator, [Link] *Fayetteville, AR, USA*
Entrepreneurial Lead 01/2021 – Present

- Develop and support to build a physics based binding free energy estimator method and software.
- Co-authored a grant winning NSF proposal for Industrial Innovation and Partnerships.
- Conducted over 100 customer discovery interviews in pharmaceutical and antibody development industries.
- Cohort member of NSF I-Crops 2021-a program for learning entrepreneurial skills necessary to identify valuable market opportunities for our product.

Long Island University, *Long Island, NY, USA*
Chemistry Lab assistant 12/2015 – 12/2017

- Performed sample characterization of experiment products by HPLC, FTIR and GC techniques.
- Used cell disruption centrifuge in cell separation and filtration processes.
- Performed routine maintenance of laboratory balances, pH meters, and organized reagent solutions in lab.
- Calibrated and troubleshot laboratory instruments like GC and IR spectroscopy
- Drafted standards and specifications for processes, facilities, products, and tests.
- Handled lab safety assurance officer responsibilities and harmonized laboratory safety standards across the department.
- Maintained laboratory chemical inventory as well optimized reagent and buffer solution preparation.
- Supervised and evaluated student's laboratory work like synthesis of drugs, Qualitative analysis experiments and chemical testing experiments.

Pharmadeep ltd, *Hyderabad, India*
Quality Control Intern 05/ 2014 - 12/2014

- Assist in the evaluation of new techniques and procedures in product development lab.
- Evaluated therapeutic efficacy of anti-depressants, anti-hypertensive drug substances on simulated animal tissues in lab.
- Perform calculations, draft experimental procedures, and maintain accurate lab records.
- Executed quality control experiments, interpreted results, and summarized data in reports.

Graduate Coursework

- Computational Statistics | Statistical Thermodynamics | Biomedical Statistics | Applied molecular biology | Advanced Genome testing and analysis | Tissue culture | Biochemistry | Physical Biochemistry | Medicinal chemistry

Management Skills

- Delegate the project to graduate students (2 Ph.D, 2 Masters & 3 Bachelors) and to be responsible for the delegated work.

Publications/

Google Scholar Page: [Link]

- Polasa, A., Mosleh, I., Losey, J., Abbaspourrad, A., Beitle, R., & Moradi, M. (2022). Developing a Rational Approach to Designing Recombinant Proteins for Peptide-Directed Nanoparticle Synthesis. *Nanoscale Adv*. [Link] (Impact Factor: 4.553)
- Immadisetty, K., Polasa, A., Shelton, R., & Moradi, M. (2022). Elucidating the Molecular Basis of Spontaneous Activation in an Engineered Mechanosensitive Channel. *Computational and Structural Biotechnology Journal*. [Link] (Impact Factor: 7.271)
- Govind Kumar, V., Ogden, D. S., Isu, U. H., Polasa, A., Losey, J., & Moradi, M. (2022). Prefusion Spike Protein Conformational Changes Are Slower in SARS-CoV-2 than in SARS-CoV-1. *Journal of Biological Chemistry*. [Link] (Impact Factor = 5.157)

Conferences / Presentations

- **Adithya Polasa**, Jeevapani J Hettige, Kalyan Immadisetty, Mahmoud Moradi., 2022. An Investigation of the YidC Mediated Membrane Insertion of a Pf3 Coat Protein Using MD Simulations. [Link]
- **Adithya Polasa**, Seyed Hamid Tabari, Mahmoud Moradi.,2021. Developing Efficient Transfer Free Energy Calculation Methods for Hydrophobicity Predictions. [Link]
- Vivek Govind Kumar, Dylan S Ogden, **Adithya Polasa**, Mahmoud Moradi., 2020. An Investigation of the Influenza Hemagglutinin Membrane Fusion Process using Microsecond-Level MD Simulations. [Link]
- **Adithya Polasa**, Dylan S Ogden, Mahmoud Moradi., 2019. Binding Free Energy Calculations of NMDA Glutamate Receptors. [Link]