ADITHYA POLASA
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Website [Link] | GitHub [Link] | LinkedIn [Link]

Summary

Highly skilled computational chemist with experience in drug discovery and a strong background in MD simulations and machine learning. Adept at developing and applying computational methods in biophysics, chemistry, and other computationally intensive fields. Proven track record of optimizing and parallelizing scientific programs for accelerated computers, supercomputers, and conventional clusters. Passionate about solving challenging problems in the field of computational chemistry.

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

Education

Doctorate in Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR; GPA: 3.6/4.0 (2018-2022).
Master's in Biomedical 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 [Link]

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: NAMD, GROMACS

Free Energy Calculation (FEP): Free energy calculations along the refined transition path (Umbrella sampling), Ligandprotein binding free energy calculations, and Alchemical Free Energy Perturbation Calculations.

- FEP Software: ParseFEP tools, BFEE2, Physics-based binding free energy calculations

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, MOE, MODELLER, Swiss-DOCK, QSAR

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

- Software: Phenix, VMD, MDFF

Computer-Aided Drug Design: Pharmacophore Modelling, QSAR analysis, Similarity search/clustering, R-group decomposition, Matched pair analysis, Docking, Active site/ Pocket identification, ADMET modeling, [Link]

Programming: Python, R, High Performance Computing (HPC) Cluster, Linux, Bash scripting, MATLAB.

Experience

Biomolecular Simulations Group (Moradi Lab), University of Arkansas, [Link] — Fayetteville, AR, USA
Postdoctoral Fellow – Chemistry and Biochemistry Dept., 12/2022 – Present
Ph.D. Candidate – Chemistry and Biochemistry Dept., 01/2018 – 11/2022

- Project 1: Develop and support to build a physics based binding free energy estimator method and software.

With the proposed approach, binding affinities are calculated using an orientation quaternion formalism instead of the conventional three Euler angles, enhanced sampling derived from biased computer simulations, and a theoretical foundation based on Riemannian geometry.[Link]

- Project 2: Recombinant fusion protein effects on peptide-directed nanoparticles. This work discusses at the molecular level the influence of amino acid sequence on peptide binding affinity to palladium particles and the GFPuv protein's capacity to manage free energies regardless of peptide sequence. This research will help create free and protein-attached peptides that allow well-regulated nanoparticle production.[Link]
- Project 3: 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]
- Project 4: Elucidating the molecular basis of activation of an engineered mechanosensitive channel. The 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 free energy of activation processes.[Link]
- Project 5: Computational characterization of SARS Coronavirus One and Two's. Our simulations show clearly justhow active these proteins become. We distinguish the structural and conformational difference between SARS CoVone and two.[Link]
- Project 6: pH-dependent conformational dynamics of influenza hemagglutinin and the associated membrane-fusion process. All-atom microsecond-level MD simulations have been used to study the effects of protonating asingle conserved histidine on HA conformational dynamics.[Link]
- Project 7: Generated a machine learning algorithm for CADD structural-based drug discovery for drug lead optimization using the Python libraries NumPy, Pandas, Seaborn, SciPy, and Scikit-Learn in combination with Molecular Docking.[Link]

BINDINSILICO LLC, [Link] Fayetteville, AR, USA
Entrepreneurial Lead 01/2021 – Present

- A technology start-up for 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.
- 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 andchemical 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.
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Graduate Coursework

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

Management Skills

- Delegate the project to graduate students (6 Ph.D, 2 Masters & 3 Bachelors) and to be responsible for the delegated work.

Publications/Google Scholar Page: [Link]

- **Polasa, A.**, V. Govind Kumar, S. Agrawal, T. K. S. Kumar, and M. Moradi. (2022). Binding Affinity Estimation from Restrained Umbrella Sampling Simulations. Nature Computational Science.[Link]
- **Polasa, A.,** Jeevapani Hettige, Kalyan Immadisetty and Mahmoud Moradi. (2022). An Investigation of the YidC-Mediated Membrane Insertion of Pf3 Coat Protein Using Molecular Dynamics Simulations. Front. Mol. Biosci.Sec. Biological Modeling and Simulation.[Link] (Impact Factor: 6.113)
- **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: 5.598)
- 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 YidCMediated 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]
- **Adithya Polasa**, Dylan S Ogden, Mahmoud Moradi., 2019. Binding Free Energy Calculations of NMDA GlutamateReceptors. [Link]