ADITHYA POLASA

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Website [Link] | GitHub [Link] | LinkedIn [Link]

Summary

I bring over 7 years of expertise in computational chemistry, specializing in protein research and biotherapeutics development. My research leverages cutting-edge computational tools, including molecular modeling, docking, molecular dynamics simulations, and machine learning, to drive innovation in protein studies and therapeutic antibody discovery.

Insilco Antibody Development | Molecular Dynamics | Docking study | Machine learning

Education

Doctorate in Computational Chemistry, 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]

- **Molecular Modeling:** Homology modeling, protein-ligand docking, structure refinement.
- **Docking software:** Autodock, MOE, Maestro
- **Molecular Dynamics Simulation:** NAMD, VMD, PyMol, Maestro, BioLuminate, MOE
- **Free Energy Calculation:** Umbrella sampling, Alchemical Free Energy Perturbation (FEP), BFEE2, Physics-based binding free energy, Desmond
- **Machine Learning:** TensorFlow, PyTorch, scikit-learn, Keras, Biopython
- **Data Analysis:** NumPy, Pandas, MATLAB, R
- **Bioinformatics:** RDKit, OpenBabel, Biopython
- **Programming Languages:** Python, R, Bash scripting, MATLAB, Linux environment
- **Web Development:** HTML, CSS
- **Data Visualization:** Matplotlib, Seaborn, Gnuplot
- **Supercomputing:** High-Performance Computing (HPC), Parallel Computing, Cluster Computing, Job Scheduling, MPI Programming, Azure, AWS
- **Data Mining and Preprocessing:** Feature engineering, data cleaning, data preprocessing techniques
- **Model Evaluation and Validation:** Cross-validation, ROC curves, precision-recall, evaluation metrics

Experience

Boehringer Ingelheim, Biotherapeutic Development, Ridgefield, CT, USA
Postdoctoral Fellow – Insilco Antibody Development, 11/2023 – Present

- **Led Insilco antibody development projects:** Spearheaded initiatives leveraging computational methods to design and optimize antibodies without relying on traditional laboratory experimentation.
- **Collaborated with cross-functional teams:** Worked closely with experts in diverse fields, including bioinformatics, molecular biology, and immunology, to integrate Insilco strategies seamlessly into antibody discovery workflows.
- **Utilized bioinformatics tools Employed** advanced bioinformatics tools to analyze extensive datasets, extracting valuable insights that informed decision-making in the identification of promising antibody candidates.
- **Implemented machine learning algorithms** Developed and applied machine learning models to enhance predictive modeling for various antibody properties, optimizing the selection of candidates with desired

characteristics.

- **Contributed to the optimization of antibody design processes** Actively participated in refining and streamlining Insilco antibody design processes, leading to increased efficiency and higher success rates in candidate development.
- **Stayed abreast of industry trends** Maintained continuous awareness of the latest developments in Insilco techniques, ensuring the incorporation of cutting-edge methodologies into antibody development practices.
- **Published research findings Shared** insights and advancements through publications in relevant journals, establishing a reputation for thought leadership in the field of Insilco antibody development.

Biomolecular Simulations Group (Moradi Lab), University of Arkansas, [Link] Fayetteville, AR, USA
Postdoctoral Fellow – Computational Chemistry, 12/2022 – 10/2023
Ph.D. Candidate – Computational Chemistry, 01/2018 – 11/2022

- **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]
- **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]
- **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]
- **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]
- **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]
- **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]
- **Predictions of Molecular Descriptors Using QSAR**
  - GitHub: https://github.com/apolasa369/Predictions-of-Molecular-Descriptors-Using-QSAR
  - Developed a machine learning model to predict molecular descriptors using QSAR methodologies.
  - Utilized Python, scikit-learn, and pandas libraries for data preprocessing, feature engineering, and model training.
  - Implemented regression algorithms and QSAR modeling techniques to generate accurate predictions of molecular properties.
  - Conducted extensive data analysis, feature selection, and model evaluation to optimize the performance of the predictive model.
- **Computer-Aided Drug Discovery Using Machine learning.**
  - GitHub: https://github.com/apolasa369/Computer-Aided-Drug-Discovery-
  - Developed a computer-aided drug discovery system to identify potential drug candidates using computational methods.
  - Applied artificial intelligence and machine learning algorithms to enhance information visualization in complex biological systems.
  - Utilized Python, scikit-learn, and pandas libraries for data preprocessing, feature engineering, and

machine learning algorithms.

- Implemented techniques such as virtual screening, pharmacophore modeling, molecular docking, and QSAR analysis to optimize lead selection.
- Conducted extensive data analysis, model training, and validation to identify compounds with high potency, selectivity, and favorable drug-like properties.
- Received positive feedback and achieved promising results in identifying novel drug candidates for further experimental validation.

BINDINSILICO LLC, [Link] Fayetteville, AR, USA
Principal investigator 01/2021 – Present

- A technology start-up for Develop and support to build a physics based binding free energy estimator in combination of computational chemistry and machine learning method and software.
- Led the development of software applications for drug design and clinical development, ensuring efficient and secure data management.
- 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.
- Led a team of researchers in a successful project that received an industry innovation award for its impact on medical research.

Publications/Google Scholar Page: [Link]

- **Polasa, A.,** & Moradi, M. (2023). Towards a purely physics-based computational binding affinity estimation. Nature Computational Science.
- Govind Kumar, V., **Polasa, A.,** Agrawal, S., Kumar, T. K. S., & Moradi, M. (2023). Binding affinity estimation from restrained umbrella sampling simulations. Nature Computational Science, 3(1).
- Sauve, S., Williamson, J., **Polasa, A.,** & Moradi, M. (2023). Ins and Outs of Rocker Switch Mechanism in Major Facilitator Superfamily of Transporters. Membranes, 13(5).
- Benton, M., Furr, M., Govind Kumar, V., **Polasa, A.,** Gao, F., Heyes, C. D., … Moradi, M. (2023). cpSRP43 Is Both Highly Flexible and Stable: Structural Insights Using a Combined Experimental and Computational Approach. Journal of Chemical Information and Modeling.
- **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.
- 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, 20, 2539–2550.
- **Polasa, A.,** Hettige, J. J., Immadisetty, K., & Moradi, M. (2022). An investigation of the YidC-mediated membrane insertion of Pf3 coat protein using molecular dynamics simulations. Frontiers in Molecular Biosciences, 9(2296-889X).
- Govind Kumar, V., Ogden, D. S., Isu, U. H., **Polasa, A.,** Losey, J., & Moradi, M., V. (2022). Prefusion Spike Protein Conformational Changes Are Slower in SARS-CoV-2 than in SARS-CoV-1. Journal of Biological Chemistry.
- **Polasa, A.,** and Moradi, M., Deciphering the Inter-domain Decoupling in the Gram-negative Bacterial Membrane Insertase. bioRxiv 2022.08.09.503346; doi: https://doi.org/10.1101/2022.08.09.503346

Management Skills

- Delegate the project to graduate students (8 Ph.D, 2 Masters & 3 Bachelors) and to be responsible for the delegated work.

Conferences / Presentations

- **Adithya Polasa**, K Immadisetty, R Shelton, M Moradi., 2023 Elucidating the molecular basis of spontaneous activation in an engineered mechanosensitive channel. Biophysical Journal
- **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. Biophysical Journal
- **Adithya Polasa**, Seyed Hamid Tabari, Mahmoud Moradi.,2021. Developing Efficient Transfer Free Energy Calculation Methods for Hydrophobicity Predictions. Biophysical Journal
- **Adithya Polasa**, Dylan S Ogden, Mahmoud Moradi., 2019. Binding Free Energy Calculations of NMDA GlutamateReceptors. Biophysical Journal

Achievements/Awards

- **NSF I-Crops award** of $50,000 for market research and validation of business product.
- **Data science Certification** from University of Arkansas Global Campus
- **Participated in competition on** Kaggle to practice data cleaning, prediction model training and optimization. https://www.kaggle.com/adithyapolasa