Kaustubh Amritkar

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PROFESSIONAL SUMMARY

Analytical PhD candidate in **computational biophysics**, applying molecular modeling and machine learning to ancient protein systems. Experienced in **molecular dynamics** simulations, characterizing **protein-ligand/peptide interactions**, and building reproducible prediction models for data-guided protein engineering. Skilled in presenting computational analysis to interdisciplinary teams translating technical results into actionable biological insights.

SELECT ACHIEVEMENTS

- Designed targeted mutant libraries for inactive ancestral RuBisCOs, with **56% mutants restoring function**, demonstrating data-driven experimental success.
- Identified **4 peptide and 146 small-molecule inhibitor** candidates against 9 viral proteins of Nipah virus, expanding structural coverage by **~90%** and providing a foundation for **rational antiviral drug design**.
- Published peer-reviewed articles in high-impact journals on topics including molecular dynamics, ancestral reconstruction, and protein therapeutics (Google Scholar).

RESEARCH EXPERIENCE

Computational Modeling and Machine Learning for Protein Evolution | *Ph.D. Researcher, UW-Madison*

- Led cross-disciplinary project of high-throughput ancestral RuBisCO activity data, extracting biologically meaningful features and training **machine learning models** on **~3000 variants** to map sequence-function relationships and guide new protein designs.
- Integrated atomistic **molecular dynamics simulations** and **biophysical modeling** to analyze large multimeric protein assemblies, revealing energetic and structural drivers of stability and subunit interaction.
- Engineered novel variants of robust ancient enzymes central to biological functions and coordinated with collaborators to experimentally validate the computational designs.

Computational therapeutics and Peptide Design | *Master's and Undergraduate Researcher, IISER-Pune*

- Worked on therapeutic screening against Nipah virus, by building protein models and scoring protein-ligand interfaces via **Docking** and **MD simulations** to evaluate pose stability and interaction persistence.
- Built a computational framework to predict peptide binders from naturally occurring structural motifs.

Applications of Structural Bioinformatics | *Visiting Researcher (Martin Steinegger Lab), Seoul National University*
Supported by NASA Astrobiology Early Career Collaboration Award & UW-Madison SRGC Award

- Uncovered distant homologs, with **≤ 10% sequence identity**, for ancient proteins using AlphaFold, identifying conserved functional motifs undetectable via sequence homology search.
- Fine-tuned **ESM-2 protein large language model** on RuBisCO dataset to improve the predictive model.

Experimental Engineering of Ancestral Proteins in Cyanobacteria | *Ph.D. Researcher, UW-Madison*

- Validating chaperone-independence of an ancestral RuBisCO variant in *Synechococcus elongatus*.
- Optimized molecular cloning protocol and engineered cyanobacteria with fluorescently tagged ancestral RuBisCO.

SKILLS & EXPERTISE

Languages: Python, R, Bash (Unix shell), MATLAB, SQL, LaTeX

Tools: PyTorch, scikit-learn, AlphaFold, OpenMM, GROMACS, MDAnalysis, ProDy, AutoDock Vina, Schrödinger, Boltz, HuggingFace Transformers, RFDiffusion, ProteinMPNN, PyMOL, UCSF-Chimera, VMD, Git, HTCondor, Slurm, Jupyter

Methods: Machine Learning, Molecular Dynamics, Protein Engineering, protein-protein/ligand interaction analysis, Biomolecular Structure Modeling, Docking, Protein Language Models, Phylogenetics, Dimensionality Reduction, High-throughput Computing, Data Visualization

Wet-lab skills: Cloning, Plasmid Design, Gibson Assembly, PCR, Gel Electrophoresis, Fluorescence Microscopy

EDUCATION

University of Wisconsin-Madison – *Ph.D. Biophysics (Advisor: Dr. Betül Kaçar)* Dec. 2026 (Expected)
Indian Institute of Science Education and Research (IISER), Pune – *BS-MS Dual Degree* Aug. 2020

SCHOLARSHIPS AND AWARDS

- NASA Astrobiology Early Career Collaboration Award, *NASA Astrobiology Program* Nov. 2024
- Best Poster Award, *2025 Protein Society Annual Symposium* Jun. 2025
- Travel Award, *The Protein Society* Apr. 2025
- Student Research Grants Competition (SRGC) – Research Travel Funds, *UW-Madison* Dec. 2024
- Travel Award (South Korea research visit), *UW-Madison Biophysics Program* Nov. 2024
- Travel Award (2023 Biophysical Society Conference), *UW-Madison Biophysics Program* Feb. 2023
- UGC-CSIR Junior Research Fellowship (JRF), *Govt. of India* 2020
- DST INSPIRE Fellowship, *Department of Science & Technology, India* Aug. 2015 to July 2020
  Merit-based fellowship supporting undergraduate and master's education (5 years)

SELECTED PUBLICATIONS

- **Amritkar, K.**, Cuevas-Zuviría, B., Kaçar, B. (2025). Evolutionary Dynamics of RuBisCO: Emergence of the Small Subunit and its Impact Through Time. Molecular Biology and Evolution, 42(1), msae268. https://doi.org/10.1093/molbev/msae268
- Cuevas-Zuviría, B., Detemple, F., **Amritkar, K.**, Garcia, A. K., Seefeldt, L. C., Einsle, O., Kaçar, B. (2025). Nitrogenase structural evolution across Earth's history. eLife, 14. https://doi.org/10.7554/eLife.105613.3
- Sen N., Kanitkar T., Roy A., Soni N., **Amritkar K.**, Supekar S., Nair S., Singh G., Madhusudhan M.S. Predicting and ***designing therapeutics*** against the Nipah virus. PLoS neglected tropical diseases, 13(12). https://doi.org/10.1371/journal.pntd.0007419
- Kanitkar T., Nair S., **Amritkar K.**, Sen N., Soni N., Ramatirtha Y., Madhusudhan M.S. Methods for molecular modelling of protein complexes. In: Owens, R.J. (eds) Structural Proteomics. Methods in Molecular Biology, vol 2305. https://doi.org/10.1007/978-1-0716-1406-8_3 (Book chapter)