Dr. Anup K. Prasad

Postdoctoral Research Associate
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Education

IIT Bombay and Monash University   Mumbai (India), Clayton (Australia)
(Ph.D., Biophysics)   Jan-2019-Feb2024
IITB-Monash Research Academy
(Joint PhD programme at IIT Bombay and Monash University)   Supervisors: Prof. Ajay S. Panwar
Thesis: *Amyloid formation in antimicrobial peptides: exploring*   (IIT Bombay), Prof. Lisandra L
the role of helical intermediates   Martin (Monash University)

National Institute of Technology Allahabad   Allahabad, India 2016-2018
(Master of Technology, **Biotechnology)**   Supervisor: Prof. Ashutosh Mani
Thesis: *Effect of YBX1 gene silencing on the expression of*
Alzheimer's disease-related genes in the HT29 cell line

Kumaon Engineering College   Uttarakhand, India
(Bachelor of Technology, Biochemical Engineering)   2011-2015

Research Interests

Protein structure and dynamics, Protein-membrane Interactions, MD simulation, Enhanced sampling method, AI/ML and Biophysical Experiments

Research Experience

Postdoctoral Research Associate   **(The University of Georgia, Jan 2025 - Present)**
Developing an AI model to predict kinase dynamics and analyse their relationship with co-evolutionary signals
Advisors: Prof. Natrajan Kannan, The University of Georgia
Developing an ML-MD framework to predict the kinase dynamics from its amino acid sequences. Establishing the relationship between dynamics and co-evolutionary signals

Postdoctoral Research   **(IIT Bombay and Monash University, July 2023 - December 2024)**
Development of Gen-AI model to explore amyloidogenicity in antimicrobial peptides: Investigating peptide-membrane interactions [Initiated with Monash Data Future Institute as a research officer]
Advisors: Prof. Lisandra L. Martin (Monash University), Prof. Ajay S. Panwar (IIT Bombay) and Dr. Senthil Arumugam (Monash University)

❖ Developed an ML-MD framework to design novel amyloidogenic antimicrobial peptides. Additionally, developed an in-house genAI model capable of generating stable antimicrobial peptide sequences with amyloidogenic properties.

❖ Simulated lead compounds from generated peptides in bacterial membrane mimetic environments to infer antimicrobial activity.

❖ Implemented a rational MD-based conformational search on lead peptide sequences to predict amyloid-forming oligomers.

❖ Teamwork (IIT Bombay + Monash): Mentored 1 undergraduate and 2 postgraduate students.

Ph.D. Thesis

Identification of helical intermediates in different environments that play a crucial role in the early stages of amyloid formation in antimicrobial (AMP) frog peptides. Utilized a combination of large-scale molecular dynamics simulations, free energy calculations and biophysical experiments.
Supervisors: Prof. Ajay S. Panwar (IIT Bombay), Prof. Lisandra L. Martin (Monash University)

❖ Revealed molecular mechanisms of helical intermediate formation in solution and membrane mimetic environments using MD simulations.

- ❖ Identified helical intermediates in the early stages of peptide self-assembly. Demonstrated that helical intermediates facilitate peptide-peptide interactions and β-sheet transitions using aggregate analysis and free energy calculations.
- ❖ Demonstrated that enhanced amyloid formation in membrane mimetic environments resulted from the promotion of helical intermediates at low concentrations of hydrophobic species.
- ❖ Investigated the role of electrostatic interactions in the disintegration of peptide aggregates on SDS micelle surfaces.
- ❖ Characterized peptide conformations and peptide aggregation extensively in different environments using circular dichroism and plate reader experiments.
- ❖ Investigated disruption of liposomes and giant unilamellar vesicles (GUVs) by uperin AMPs using Total Internal Reflection Fluorescence (TIRF) microscopy.
- ❖ <u>Teamwork (IIT Bombay and Monash)</u>: Collaborated with 1 postdoctoral fellow, 3 PhD students, and 2 undergraduate students on different projects. Co-authored papers with these collaborators. Mentored 3 PhD and 2 undergraduate students.

M.Tech Thesis

Effect of YBX1 gene silencing on the expression of Alzheimer's disease-related genes in the HT29 cell line.
Advisor: Prof. Ashutosh Mani
- ❖ Extensively used the cell culture process to ensure the health and functionality of cell populations.
- ❖ Utilised the Small interfering RNA (siRNA) technique for YBX1 gene silencing in HT29 cells.
- ❖ Investigated the relationship between YBX1 and Alzheimer's disease genes through their expression by quantitative real-time PCR through YBX1 gene silencing in the HT-29 cell line.

Scientific and Technical Skills

Computational skills
1. Simulations
- ● Molecular Dynamics (MD) simulations (GROMACS, NAMD, LAMMPS)
- ● Free energy calculation methods, including Adaptive Biasing Force (ABF) and Steered Molecular Dynamics (SMD)
- ● Large-scale data analysis using Python and Tcl scripting, MDAnalysis

2. Machine learning
PyTorch, Keras and Scikit-learn libraries for AI model development and Statistical data analysis
3. Bioinformatics
Structural and sequence analysis, docking, Biopython (Python library for bioinformatics)
4. Software platforms: Linux, VMD, PyMol, Hex dock and Inkscape
5. Programming: Python, TCL, Shell scripting

Experimental skills
1. Biophysical characterization: Circular dichroism (CD), Plate reader, FTIR and Dynamic light scattering (DLS)
2. Microscopy: Total Internal Reflection Fluorescence (TIRF) microscopy, Image analysis using Python, ImageJ
3. Molecular biology
- ● Lipid vesicle formulation, including micelle, liposome (extrusion method) and GUVs (electro-formation method)
- ● Dye-leakage experiments, ThT assays, peptide-peptide and peptide-lipid interaction
- ● Crystallography, cell culture, transfection, PCR, blotting techniques and RNA extraction method

Publications

1. **Prasad, A. K.,** Samajdar, R., Panwar, A. S., & Martin, L. L. (2024). Origin of Secondary Structure Transitions and Peptide Self-Assembly Propensity in Trifluoroethanol–Water Mixtures. *The Journal of Physical Chemistry B*. **(Link)**

2. **Prasad, A. K.,** Martin, L. L., & Panwar, A. S. (2023). Helical intermediate formation and its role in amyloids of an amphibian antimicrobial peptide. *Physical Chemistry Chemical Physics*, *25*(17), 12134-12147. **(Link)**

3. **Prasad, A. K.**, Tiwari, C., Ray, S., Holden, S., Armstrong, D. A., Rosengren, K. J., ... & Martin, L. L. (2022). Secondary structure transitions for a family of amyloidogenic, antimicrobial uperin 3 peptides in contact with sodium dodecyl sulfate. *ChemPlusChem, 87(1), e202100408*. **(Link)**

4. Ray, S., Holden, S., **Prasad, A. K.**, Martin, L. L., & Panwar, A. S. (2020). Exploring the role of peptide helical stability in the propensity of uperin 3.x peptides toward beta-aggregation. *The Journal of Physical Chemistry B, 124(51), 11659-11670.* **(Link)**

5. **Prasad, A. K.**, Martin, L. L., Panwar, A. S., & Arumugam, S. Rational design of amyloidogenic antimicrobial peptides using BiGAN deep learning model. (*Under preparation*)

Conferences and Workshops

Prasad, A. K., Martin, L. L., and Panwar, A. S. "Peptide disintegration on sodium dodecyl sulfate micelle surfaces " *Lorne Protein 2023 (Poster session), Lorne, Australia*

Prasad, A. K., Martin, L. L., and Panwar, A. S. "Role of α-helices in β-sheet-rich aggregate formation in amphibian antimicrobial peptide" *RACI 2022 National Congress (Poster session), Brisbane, Australia*

Prasad, A. K. and Mani, Ashutosh, "Analysis of Human brain development genes in Alzheimer's disease through gene co-expression network approach" *BioSangam 2018 (Poster session), NIT Allahabad, India*

Teaching experience

Teaching associate   **Monash University, 2022-2023**

- Introduction to Bioinformatics
- Protein Biology: From Sequence to Structure and Disease
- Human Molecular Cell Biology
- Biological Chemistry

Honours and Awards

- Coromandel International Limited Best Thesis Award   IITB-Monash Research Academy

- Department of Biotechnology (DBT) fellowship for Ph.D   Government of India

- Travelling grant for RACI 2022 conference   IIT Bombay, India

- Best poster award to me and my student group in the BMS2021 teaching course   Monash University

References

Prof. Ajay S. Panwar
MEMS Department, IIT Bombay   panwar@iitb.ac.in

Prof. Lisa L. Martin
School of Chemistry, Monash University   lisa.martin@monash.edu

Prof. Ashutosh Mani
Motilal Nehru National Institute of Technology, Allahabad   amani@mnnit.ac.in