



Project Proposal for Ph.D.

Project Details (The research problem must clearly indicate the need for an interdisciplinary approach)

Project Title	Mechanism-Aware and Physics-Informed AI Framework for Antimicrobial Peptide Discovery
Project Summary (Minimum 500 and maximum 2000 characters)	Antimicrobial resistance (AMR) is a critical global health challenge, necessitating the development of new therapeutic strategies such as antimicrobial peptides (AMPs). However, rational AMP design remains difficult due to fragmented scientific knowledge, complex biophysical interactions, and the limited interpretability of existing AI approaches. The objective of this project is to develop an algorithm that systematically discovers novel AMPs. To this end, we intend to: (a) model the causal relations of AMPs; (b) use these causal models to generate new AMPs; (c) systematically compare the newly generated AMPs with existing ones; and (d) evaluate the degree of novelty of the discovered AMPs with respect to existing AMPs. For AMP modeling, approaches that capture causal relationships will be used. Using these models, scientific literature will be systematically transformed into causal knowledge representations, enabling explicit encoding of relationships between peptide properties, microbial interactions, and functional outcomes. These structured representations will guide AI models in generating candidate peptides while incorporating mechanistic reasoning and physicochemical constraints. To ensure physical and biological plausibility, selected candidates will be evaluated using molecular dynamics simulations to analyze peptide–membrane interactions at the molecular scale. An active learning strategy will iteratively refine the model by selecting the most informative candidates for simulation, thereby improving efficiency and reducing computational cost. Additionally, interpretable and interactive interfaces will be developed to provide insights into the design rationale and underlying mechanisms. By combining AI, biophysics and design, this work aims to establish a reliable and interpretable framework for antimicrobial peptide discovery, with potential impact on combating AMR.

Ph.D. Supervisors*
(Supervisor 1 and Supervisor 2 cannot be from the same department of IITD)

Role	Name of Faculty	Academic Unit in IITD/Institute/University	Email ID (Official)
Supervisor 1*	Prof. Garima Rani	Biochemical Engineering and Biotechnology (IITD)	garimarani@iitd.ac.in
Supervisor 2	Prof. Sonal Keshwani	Department of Human Centered Design (IIIT-Delhi)	sonal.keshwani@iitd.ac.in

*Supervisor 1 must be from IIT, Delhi.
+All cells in this table are mandatory fields that need to be filled by faculty for consideration of proposal.
\$The date of superannuation of supervisors should be at least three years from the date of registration of selected candidates.

Project requirements (Student qualifications, experience required, etc)
*The candidate will be shortlisted based on common shortlisting criteria decided by ScRC (SIRe)

- Degree in Bioengineering/Computational Biology/Physics/Computer Science or allied subjects with >=70% in undergraduate and postgraduate.
- Good understanding of programming language, research experience on working with biological systems will be of advantage, knowledge of ML/AI algorithms will be a huge plus
- Valid JRF qualification

Source of fellowship/funding and project number (CSIR/UGC/DBT/ICMR/ICAR/NEET-PG/DST-INSPIRE/IRD/FITT Project details, if any)
Candidate with his/her own fellowship

Role of Faculty Members involved:	
Supervisor-1	Guidance on the biophysical and microbiological aspects of the project, including physics-informed modeling and molecular dynamics simulations for validating peptide–membrane interactions and ensuring biological relevance.
Supervisor-2	Guidance on the choice and use of knowledge representation frameworks, automating the AMP modeling, and development of interpretable AI systems for AMP discovery and novelty evaluation.
	Both supervisors will jointly contribute to the overall direction, integration and execution of the project.

Note :-

1. Approval from the respective DRC/CRC/ScRC of your Department/Centre/School will be required for using the "Full-time Institute Assistantship (Category-wise) (FIA)" for selecting the students in SRe.
2. Declaration:- Faculty members, please ensure that you have at least 3 years of service left before superannuation along with adequate sitting space & lab facilities for the SRe student.
3. PI/s are also encouraged to submit joint proposals with AIIMS, NII, JNU and institutes with which IITD has an existing MoU. If the Co-PI (Supervisor 2) is from outside IITD, kindly share his/her detailed CV.
4. If a research scholar is to be considered for selection under the project fellowship, then the project should have a minimum of two-year duration remaining.
5. A candidate applying with a valid JRF/INSPIRE/any national level fellowship should have at least two-year validity from the date of joining the Ph.D. program.
6. The third supervisor’s name (if required) can be added only after the formation of Student Research Committee (SRC) subject to a strong recommendation of SRC and subsequent approval from the competent authority.
7. If Institute fellowship is being sought, then DRC approval of the parent department of Supervisor 1 is required at the time of selection.