SURP 2025: Phase 1

Note: We understand the majority of you have just started with your SURP Projects. This checkpoint is to make sure that you have started working on your projects and to track your progress.

Instructions:

- Make a copy of this Google Document, complete the necessary fields in the provided form, and have it verified by the professor, including a digital signature.
- Download this document as a **PDF file** (mandatory) and submit it via the designated Google form: https://forms.gle/wmC423e3rucaAR7r7
- Deadline: **11:59 PM, Tuesday, 8th July 2025.**
- This progress tracker will be utilized to verify any resume points, this internship season, for all third-year participants to indicate the SURP 2024 Project as an ongoing project on their resumes.
- Please note that this will hold only if permission is also obtained from the guiding professor in this report.
- In case of any queries, kindly reach out to the EnPoWER Team.

SURP 2025: Phase 1

TO BE FILLED BY THE STUDENT

Details of the student :

Name	**Aryan Kayande**
Roll Number	**23B2174**
Year of Study	**Entering 3rd year**
Contact number	**8983853364**

Details of the project

Project UID	**MD05**
Title of project	**Next-Gen Drug Discovery: Generative and Reinforcement Learning for Designing Anticancer Molecules**
Name of the professor guide	**Prof. Debrabata Maiti**

Progress Update

Project Target
To design and implement a reinforcement learning-based pipeline for molecule optimisation and drug sensitivity prediction using the PaccMannRL framework, while gaining familiarity with foundational reinforcement learning (RL) and large language model (LLM) concepts, and integrating these into a structured codebase.
Progress made & Objectives fulfilled(if any)
Project repository setup completed with version control enabled. Development environment configured with all required dependencies. Completed a review of Reinforcement Learning (RL) fundamentals and Large Language Models (LLMs).

Set up the PaccMannRL model environment and performed preliminary runs on a test dataset. Made initial qualitative observations on reward-based learning behavior. Resolved dependency conflicts and documented all work systematically in the project repository.
The deadline targeted for completing the project
31st July 2025

Future plan

Provide a brief month-wise plan of how you plan to meet the above deadline

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• July 8 – July 15:
  ○ Complete any pending Week 1 activities.
  ○ Design an end-to-end data processing and training pipeline.
  ○ Finalise loss functions, reward structures, and optimisation techniques.
  ○ Distribute sub-tasks and finalise functionalities for the final code package.
• July 16 – July 24:
  ○ Begin module-wise development based on the pipeline structure.
  ○ Integrate and test reinforcement learning functionalities.

- Implement reward progression tracking and validate molecule generation behaviour.

- July 25 – July 31:
  - Final model testing, tuning, and documentation.
  - Prepare final report and presentation.
  - Submit deliverables and project outcomes.

TO BE FILLED BY THE PROFESSOR

Any comments/suggestions/feedback	
Can the student mention the project as an ongoing endeavor on their resume?	**Yes**
Signature of the professor with the date