

Developing a Platform to Identify Enzymes that Break Down Psychoactive Drugs

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Introduction

The abuse of psychoactive drugs has become a significant public health concern, with detrimental effects on both individuals and society. Current detection methods of these drugs rely on time-consuming and expensive techniques, underscoring a pressing need for the development of novel, efficient identification methods. In this research, we aim to develop a platform to identify enzymes that break down psychoactive drugs, such as ketamine, into easily and affordably detectable metabolites, to facilitate the development of improved detection techniques.

Research Question

Can we develop a platform to identify bacterial enzymes that break down ketamine and potentially other psychoactive drugs, and can this platform be used to develop efficient detection methods?

Goals

Our aim is to create an intuitive, user-friendly platform that seamlessly integrates with existing lab technologies to identify optimal target sites for various ligands. The platform will continuously retrieve data from the Protein Data Bank (PDB) website, specifically focusing on bacterial enzymes associated with plants, to ensure relevance to our laboratory's research focus.

UI Vision

Name this project

Upload Ligand SMILES

Search for hits

Figure 1. Low fidelity prototype of home page.

Process and Methods

The project has two main components: a computational component and a lab verification component.

We adopted this approach because it allows us to leverage the strengths of computational methods to identify potential enzymes and conduct preliminary docking analyses quickly and efficiently. At the same time, the lab verification component allows us to verify our computational predictions and validate our findings in a real-world setting.

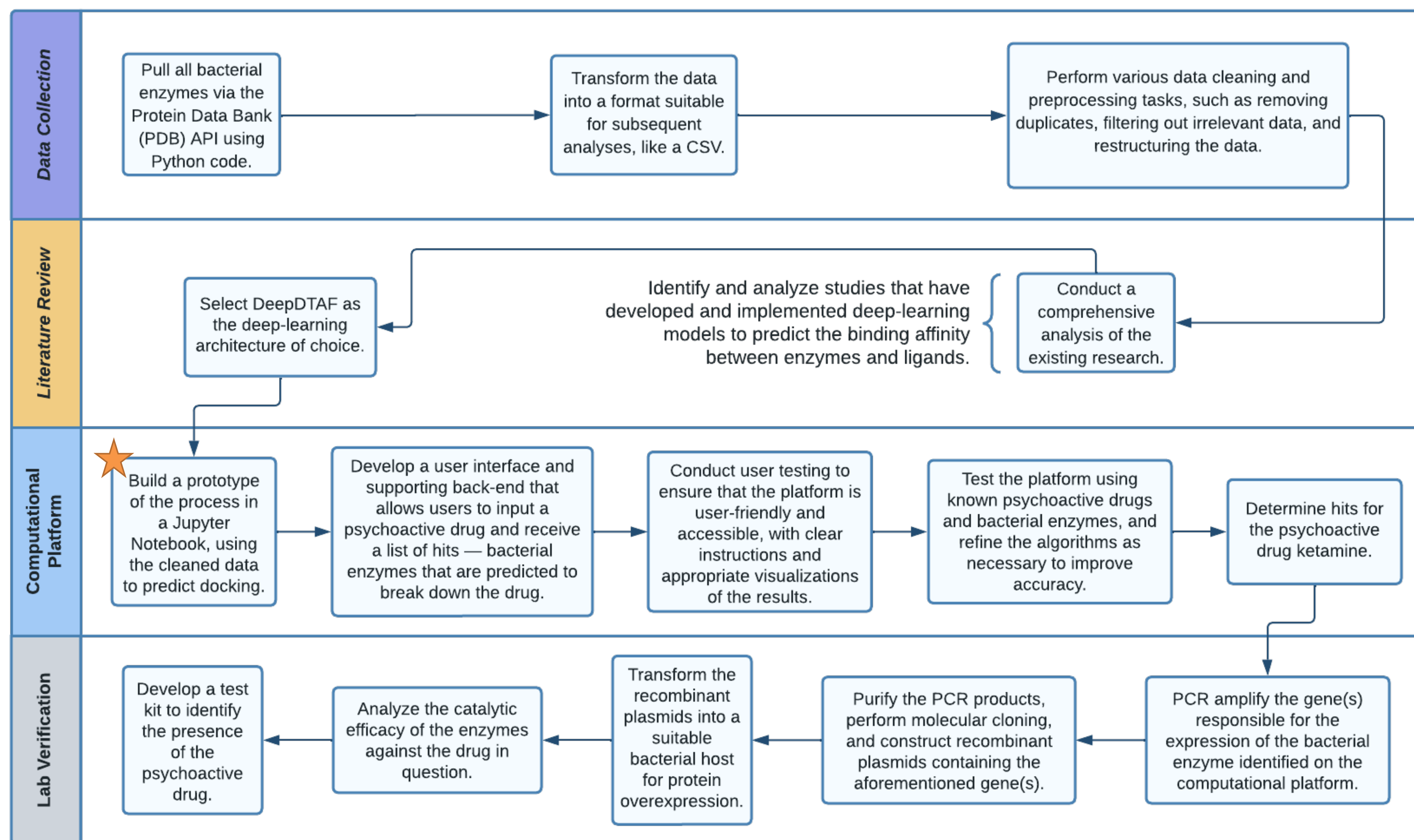


Figure 2. Flowchart of platform development process.

References

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Acknowledgements

This project is being funded by an Undergraduate Research and Fellowships PEAK Experiences Award.