

# Molecular Dynamics: Comparison of the Cytochrome P450 1A2 System

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## Project(s)

My main project is on the molecular dynamic analysis on cytochrome P450 1A2 membrane-bound and waterbox systems.

Another project is on dengue (NS2B/NS3pro) with a master student, Rina. I'll be working on laboratory testing.

### **Progress**

Finish active site analysis using fpocket2 and reading from "Biochemistry of Membrane Transport" on protein lipid interaction.

Study mutated CYP1A2 systems and discuss with my mentor, Luke about setting up a parallel system.

Complete a timeline for my research project for the following 3 weeks.

#### Goal for next week

Calculate the charges of the system and record major structural difference between the two systems.

Write an outline for the final research paper, including all the analysis methods and background information.

Finish reading the selected chapters from "Enzyme assays" and "Evaluation of enzyme inhibitors in drug discovery."

Follow Rina to IPHARM for some experimental work.





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