



Molecular Dynamics: Comparison of the Cytochrome P450 1A2 System

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July 27, 2012



Project(s)

- My main project is on the molecular dynamic analysis on cytochrome P450 1A2 membrane-bound and waterbox systems. Another project is with a
- Another project is on on dengue (NS2B/NS3pro) laboratory with a master student, Rina. I'll be working on laboratory testing.

Progress

Started working on my introduction and computational methods for my research project along with an outline of my research paper. I've completed clustering analysis and hydration analysis.

Had a conference call with my PI, Rommie and my mentor, Luke from UCSD regarding the progress of my project.

Goal for next week

Complete the binding site analysis using fpocket2 and MOE for my CYP1A2 system. Start membrane density distribution and heme angle calculation using scripts provided by my mentor, Luke.

Finish reading the chapter on protein lipid interaction from “Biochemistry of Membrane Transport.”

Write a short report on the mutation work done on CYP1A2 for further discussion with Luke.

Work on a timeline for my CYP1A2 project.

Discuss with Rina about the wet lab work.

Tropical Spice Garden



Durian Market



Acknowledgments

UCSD PRIME: Pacific RIM Undergraduate Experiences

Co. PI: Gabriele Wienhausen

Co. PI: Peter Arzberger

All PRIME staff members

University of California, San Diego

PI: Rommie E. Amaro

Mentor: Luke Czapla

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Ministry of Science, Technology and Innovation:IPharm

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