

Molecular Dynamics: Comparison of the Cytochrome P450 1A2 System

Tiffany Sun Universiti Sains Malaysia

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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 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.

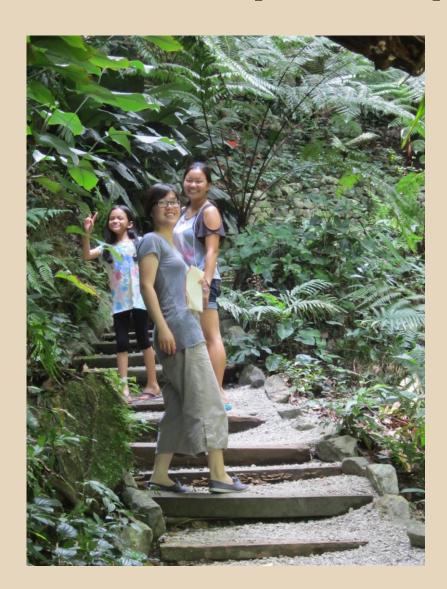
Finish reading the chapter on protein lipid interaction from "Biochemistry of Membrane Transport."

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

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Co. PI: Peter Arzberger

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PI: Rommie E. Amaro

Mentor: Luke Czapla

Universiti Sains Malaysia, Penang

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(School of Pharmaceutical Sciences)

PI: Habibah Wahab

Mentor: Sybing Choi

Ministry of Science, Technology and Innovation: IPharm

Habibah Wahab

Rina Nuwarda