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

The progress this week is to do a basic analysis on the two systems, including RMSD,RMSF, water path, specific helices, and volume of the active site.

There is some technical difficulty in loading the full length of the trajectory, but SyBing says I can try their supercomputer located in another side of the campus next week. This week, I was able to shorten my trajectory for some basic analysis, but not the complete trajectory of 250 nano-second.

Goal for next week

Work on more analysis work using a supercomputer with a full length of 250 ns along with the scripts from UCSD. I'm touring the experimental lab next Monday and Tuesday. I still need to talk to Rina about my project on dengues.

Community project: T-shirt painting



