
Optimizing Models of Dual-Specificity Phosphatases (DSPs)

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Project goals

- Run DOCK with the tertiary structures of DSP's modeled by students from PRIME 2011 to determine how well ligands bind to the models
 - Choose the best model based on DOPE score
 - Minimize energy using UCSF Chimera
 - Improve loops near the active site using loop modeler
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Project Progress

- Began docking SSH-1 and SSH-3 on milk cluster; expected to finish docking and begin Amber over the weekend
- Just for fun: attempt to come up with a script that will label and zip up the application folders generated by dock

Next week's goals

- Run Amber on SSH-1
- Continue working on code

Culture in Japan

