
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

- Selected best models out of the predicted structures
 - Began energy minimization:
 - Categorized proteins into levels of priority based on how well the structure is folded
 - Loop modeled the best DSP's
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Next week's goals

- Continue to optimize the protein models
 - Dock the models with the ligands
 - Currently not enough nodes working on milk cluster – hopefully it will be up soon
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Culture in Japan

