Optimizing Models of Dual-Specificity Phosphatases (DSPs)

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08/03/12
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

• Run AMBER to generate another list of binding scores
Project Progress

• Finished first run of AMBER for SSH-1

• Located problematic files in AMBER

• Removed problematic files in AMBER and reran AMBER

• Look into writing a script to expedite the process
Next week’s goals

• Finish running AMBER on SSH-1

• Begin running AMBER on SSH-3
Culture in Japan
Acknowledgments:

- Cybermedia Center, Osaka, Japan
  - Date-sensei
- UC San Diego, La Jolla, USA
  - Dr. Haga
  - Dr. Wienhausen
  - Dr. Arzberger
  - Teri Simas
- NSF grant IOSE-0710726
- Wendy Kwok Eureka! Scholarship