

Cybermedia Center, Osaka University

Virtual Screening for High Specificity Inhibitors of SSH-2

Joshua Wei
7/27/2012

Week 5: Amber Screening of SSH-1 and SSH-3

- AMBER scoring is continuing to run on the Milk cluster.
- SSH-1 should be done within a week.
- SSH-3, however, is progressing much more slowly. More nodes can be dedicated to this job after SSH-1 finishes.
- A small fix was added to the Amber script, `slice_redistribute.pl`, resolving the error that did not allow the SSH2 mol2 files to be downloaded from the Jakarta ROOT folder.
- PRL-2 is still running on the Rocks cluster.

Future Plans

- AMBER scoring takes significantly longer for SSH-1 than SSH-2. There are more nodes assigned to SSH-1, but it should not have such a significant impact.
- Also, various slices are encountering errors running antechamber. We will work on resolving these and rerunning the specific slices.
- Lack of nodes continue to be a limiting factor in our progress. Reducing the box size around the docking site may speed up the job's progress, but it is unsure how much this will affect the results.

Cultural Exploration!



Bonus Slide!



Acknowledgements

- UCSD Bioengineering
 - Dr. Jason Haga
- Cybermedia Center, Osaka University
 - Dr. Susumu Date
 - Dr. Kiyoshi Kiyokawa
- UCSD PRIME Program
 - Jim Galvin
 - Dr. Peter Arzberger
 - Teri Simas
 - Dr. Gabriele Wienhausen
 - Tricia Taylor