

Cybermedia Center, Osaka University

Virtual Screening for High Specificity Inhibitors of SSH-2

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7/19/2012

Week 4: Amber Screening of SSH-1 and SSH-3

- Several problems arose when trying to start AMBER, but they have been solved.
- AMBER scoring successfully started for SSH-3 on the Milks cluster.
- Vicky has AMBER running for SSH-1 on Milks as well.
- DUSP19 and DUSP21 are almost done, which will free up more nodes. We will decide on whether to allocate more nodes to ongoing jobs or to run a third AMBER job for another protein.
- PRL-2 is still running on the Rocks cluster, but now with more nodes to speed up the process.

Future Plans

- AMBER scoring takes considerably longer than the grib based scoring we have been running before, so we may want to focus on completing SSH-1 and SSH-3 first by allocating more nodes to these jobs.
- The perl script for sending the AMBER jobs to the clusters does not work as conveniently as desired. However, since the script works, this is a low priority fix.
- A script was generated that helps to sort the resulting data folders, but useful improvements include being able to take into account duplicate copies and having alternative ways to check whether the docking is finished for a given folder.

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