Cybermedia Center, Osaka University

# Virtual Screening for High Specificity Inhibitors of SSH-2

# Week 3: Submitting Dock Jobs of Dual Specificity Phosphatases

- Rock cluster was successfully reinstalled, allowing jobs to run without crashing now.
- PRL-2 is running slices. Progress will be checked tomorrow and the number of nodes will be adjusted so that the job is completed
- Olivia created a script for the installation of all the programs, making reinstallation faster.
- DUSP19 and DUSP21 are still running, but should be ready for AMBER scoring soon.
- Vicky is running both SSH-1 and SSH-3 on the Milks cluster.

#### **Future Plans**

- Once DUSP19, DUSP21, SSH-1, SSH-3 and PRL-2 are finished docking, they will be ready for AMBER scoring.
- DUSP19 and DUSP21 should be ready first. AMBER will be tested beforehand to make sure the jobs work properly.
- Other clusters can be prepared and utilized using the new program installation script.
- We will also write a script to sort the results folders so that the data can be more clearly organized.

# **Cultural Exploration!**











## **Bonus Slide!**









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