

Cybermedia Center, Osaka University

Virtual Screening for High Specificity Inhibitors of SSH-2

Joshua Wei
7/5/2012

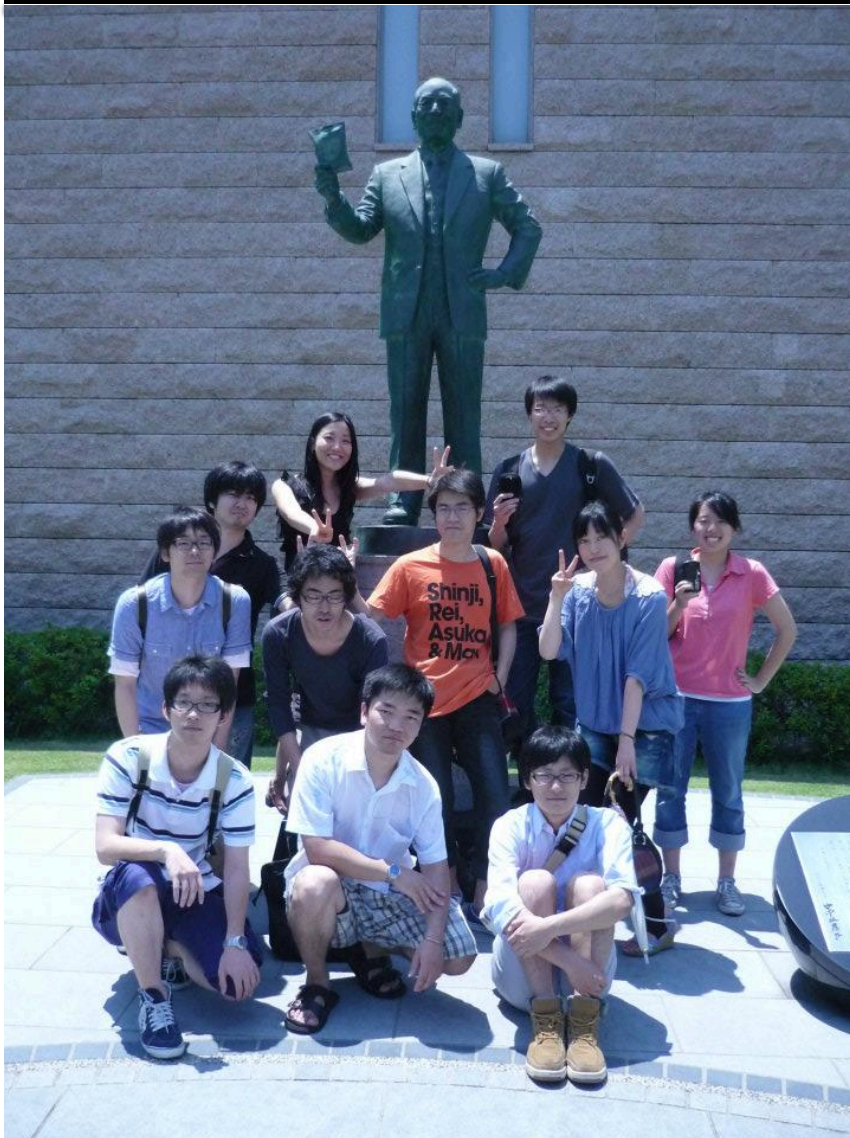
Week 2: Submitting Dock Jobs of Dual Specificity Phosphatases

- Models for SSH1 and SSH3 were remodeled because the previously generated ones were too inaccurate to prove useful.
- Olivia is running dock for DUSP19 and DUSP 21.
- Rocks has been inconsistent with jobs, dropping jobs with no indication or error notification. Several programs have been reinstalled to try to fix the problem, but nothing has changed since.
- PRL-2 is ready to Dock once the Milk nodes that Olivia is using opens up.

Future Plans

- Future plans include docking SSH1, SSH3, and PRL-2. SSH1 and SSH3 still need to be Dock prepped.
- We are also seeing if other clusters can be used to run jobs in parallel since all the nodes on the Milk cluster have been occupied.
- Fixing the problems with running jobs on Rocks is on the highest priority as it is the second fastest after Milks
- We will hopefully start looking into ways to implement Phase, a pharmacophore generation program.

Cultural Exploration!



And more food!

