

Cybermedia Center, Osaka University

Virtual Screening for High Specificity Inhibitors of SSH-2

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Week 7: Resolving Issues with Amber Screening

- AMBER scoring is continuing to run on the Milk cluster.
- The SSH-1 job errors have been resolved with the help of the error finding scripts and is ready to be run through rerank.pl and grabtopscores.pl to sort the ligands and cut off the top 10% of the best scoring ligands. This percentage is subject to change, but we are aiming at listing about 20,000 ligands to match the previous years.
- SSH-3 is approaching completion quickly now that the nodes have been reallocated under one job.

Future Plans

- Next, we will rerank the SSH-3 ligands and generate the consensus list of the best scores taking both the grid scores and AMBER scores into account. The final list will be added to the compiled spreadsheet of scores from previous years.
- We are also backing up our files into an external hard drive.
- DUSP 21 is ready for AMBER once we finish SSH-1 and SSH-3
- The PRL-2 job is going to be moved to the Milks cluster, as it has been running abnormally slowly on Rocks.

Cultural Exploration!



Bonus Slide!



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