

Cybermedia Center, Osaka University

Virtual Screening for High Specificity Inhibitors of SSH-2

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Week 6: Resolving Issues with Amber Screening

- AMBER scoring is continuing to run on the Milk cluster. Antechamber errors were found to be normal.
- SSH-1 is pretty much finished, but all the error messages still have to be sorted through. Certain ligands will not dock correctly and have to be deleted by locating `amberize_ligand.[#].out`
- SSH-3 is still progressing slowly, but seems relatively error-free.
- The PRL-2 job has been having problems, running the same slice repeatedly. Once the problem is fixed, it should finish soon. However, finishing the AMBER scoring remains higher on our priorities.

Future Plans

- AMBER scoring still takes much too long for SSH-3. We need to resolve all the errors for SSH-1 before we can reallocate the nodes.
- Perl scripts are being written to help resolve the AMBER errors faster. They will look into completed app folders, check the std.err file, and edit the necessary ligand file.
- The PRL-2 app folders have a lot of sorting to be done since so many extra folders were generated. Some previously made scripts could be modified to make this easier.

Cultural Exploration!



Bonus Slide!



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