

# Deployment of Virtual Clusters on a Commercial Cloud Platform for Molecular Docking & Fault Tolerance

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# Expectations from Previous Week

- ◆ Operate dock6 and estimate the size of all output files (Completed)
- ◆ Support Anthony with dock6 in the Multi-Cloud environment (Completed)
- ◆ Work with Katy to operate dock6 on Hadoop (In Progress)



# Research Progress

- ◆ Supported Anthony to prepare and perform all 3 types of Dock operations (Rigid, Flexible, and Amber Score) on the Multi-Cloud environment
- ◆ Estimated the size of all Dock Outputs
  - ◆ table showed in the next slide
  - ◆ for Amber Scoring: perl splits the ligand file during preparation and creates extra files per ligand, 3646 kb per ligand, 3439 kb general files



# Research Progress

## ◆ Estimated size of Dock Outputs

Type of Docking	Number of Ligands	Size of dock. out	Size of ranked.mol2	Estimated Total Size of output files for 1000 ligands	Size of preparation files per ligand	Size of output files per ligand
Rigid	100	31.9 KB	493.9 KB	5.3 MB	-	-
Flexible	5	8.1 KB	26.8 KB	7.0 MB	-	-
Amber Scoring	5	6.1 KB	27 KB	6.6 MB	3646 KB +3439 KB general files	571.8A KB +564.2 KB general files



# Overall Plan of Action

- ◆ During this last week of my PRIME internship. I mainly completed all the tasks with Dock, and prepared for our Final Presentation in Osaka with the other PRIME students. Although we did not get as far as we planned with our project, but we gained in-depth knowledge about Dock and Hadoop, and created a critical foundation to the job of molecular docking among a virtual cluster. I am more than happy to support the next generation of Prime students to complete the deployment.





*Onsen Trip  
with Shimojo  
Sensei's lab in  
Osaka  
University*



*Final  
Presentation  
Day with  
Ichikawa  
Sensei*







#UCSDPRIME2014

*Universal Studios, Osaka, Japan*





Last day in lab, completion of our internship



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