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

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Expectations from Previous Week

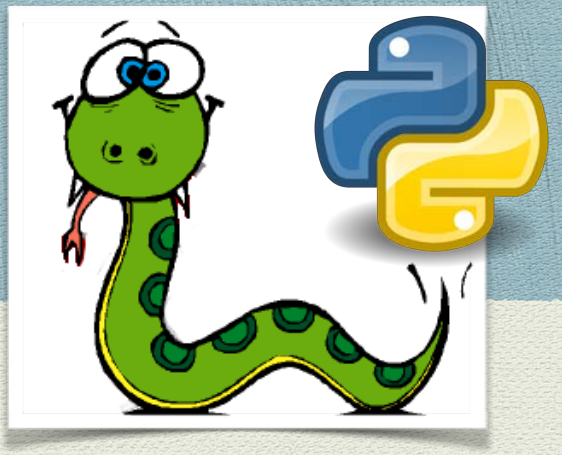
- Continue to learn Python and start coding for splitting of ligand slices (Completed)
- Start screening all ligands for SSH2 protein receptor using DOCK (No longer needed)

Research Progress

- Adjusted Amber Scoring input file "dock.generic.amber.in" to test for most efficient time with accurate result
  - 5-ligand test file test.mol2 was used

Default	26393s (~1.5 hrs/mol)	Result
Max_Ranked_Ligands=500	28499s (~1.6 hrs/mol)	same
Amber_Score_md_Steps=2500	15886s (~0.9 hr/mol)	very different
Amber_Score_md_Steps=3500	20494s (~1.1 hr/mol)	very different
Amber_Score_md_Steps=4000	in progress	in progress

Research Progress



- Reading and learning Python 3.4
- Conducted a rough skeleton of Python codes for splitting ligand slices
- Consulted Intern Thai and Graduate Student Jin Yong for Python coding support
- Performed a series of modification and tests to split test.mol2 into multiples of 2 molecules using Python
- Contacted Dr. Haga and obtained raw ligand slice data from ZINC Database

Overall Plan of Action

- This week I fully focused on learning and writing Python codes. Being able to split the ligand slices is a critical step to our project, without a strong background knowledge of coding and programming languages, thus it was extremely difficult for me. Nevertheless, I sought support from online and book resources, consulted Graduate student and other interns in lab. After 2 weeks of speed learning and support from other, I was finally able to complete the codes. Now I plan to further modify the codes to split the raw data from ZINC database.

Research Expectations

- Organize the tremendous amount of ligand slices obtained from ZINC Database
- Modify and test Python codes to accurately split raw data of ligand slices
- Compare test results from adjusting Amber Score parameters

Above = Takayama Science Town, NAIST

Left = Takoyaki Party in Lab, NAIST

#UCSDPRIME2014

Kobe Port Tower, Kobe

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