

Thursday April 4, 2013

Creating an Enrichment Graph for Er Agonist

RUNNING JOB

- 1) Login to Kraken using directions from Tuesday
- 2) Move to the directory in which you copied your files for today's lesson
~> cd \$CUE_SCRATCH/thursday
- 3) See what is in the receptor.txt parameter file
~> less receptors.txt
Receptor Box: Center = 6.085 -0.422 -5.791 (C9 of co-crystallized ETC ligand)
- 4) See what is in the ligand.txt parameter file
~> less ligands_sort.txt
- 5) Unarchive the ligand input files
~> tar xzvf ligands.tgz
- 6) Open job submission script in an editor and look at contents of file
~> vi submit_test.pbs
- 7) Edit email address
 - a. press i to enter insert mode (should say – INSERT – on bottom of screen)
 - b. use arrow buttons to navigate to my email address, delete my address and enter yours
 - c. save and exit document by pressing the esc key then type :wq
 - d. when your job finishes you will receive an email now
- 8) To submit job
~> qsub submit_test.pbs
- 9) To check status
~> qstat -u username
- 10) To see entire queue
~> showq

ANALYZING RESULTS

- 1) Login to the Linux partition
 - a. Restart computer
 - b. When red screen appears, use arrow keys to navigate to the first choice and press enter.
 - c. Username: bcmb422
 - d. Password: %LxB422%
- 2) Open terminal and get files needed for this portion (i.e. the already completed result files and scripts)

Click on terminal icon on top left of the screen

```
~> wget http://cmb.ornl.gov/~sek/result_analysis.tgz  
~> tar xzvf result_analysis.tgz
```

```
~> cd result_analysis
~> tar xzvf out_er_agonist.tgz
```

3) Use python script to extract a sorted list of energies

```
~> cd out
~> python ../scripts/postdocking_vina.py
~> less sorted_results
```

4) Use python script to create data needed for enrichment plot

```
~> python ../scripts/enrichment.py er_agonist
~> less enrichment.txt
```

5) Use gnuplot script to make enrichment graph

```
~> gnuplot ../scripts/plots
~> mv enrichment_er_agonist.eps ..
```

6) Open file folder and navigate to result_analysis folder and double click on er_agonist.eps

EXTRA CREDIT

When your job finishes, do the same process with your result files and plot them on the same graph as the results analyzed here to see the effects of different starting seeds.

HINT: make a new directory which contains a copy of the scripts directory and a directory with your results and repeat the above process. You can use EXCEL to combine both results in one graph or modify the gnuplot plots script to plot both (additional extra credit will be given for this). You can use the directions for the upcoming project to figure out how to archive and download your results.