Virtual Screening Procedure

- First, I transferred the files to Bridges using sync_virtual_screen.sh
- Then, I logged onto Bridges and executed the command `sbatch vina_multithread.job'
- Next, I transferred the results to my own computer using sync_virtual_screen.sh
- Finally, I performed some preliminary analysis on an ipython notebook, AnalyzeVS.ipynb, also exported to html format.

References

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- [Morris et al, 2008a] Presentation: Using AutoDock 4 for Virtual Screening (Handouts, PDF document, 1.1 MB)
  - http://autodock.scripps.edu/faqs-help/tutorial/using-autodock4-for-virtual-screening/VSTutorial2.2008.pdf
  - This presentation also describes some virtual screening success stories
- [Morris et al, 2008b] Instructions: Using AutoDock 4 for Virtual Screening (PDF document, 464 KB)
  - http://autodock.scripps.edu/faqs-help/tutorial/using-autodock4-for-virtual-screening/UsingAutoDock4forVirtualScreening_v4.pdf
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