Suggested steps for MD simulation with explicit water

- 0-propka:
  - Submit your complete PDB file to the PDB2PQR server to assign protonation states. Use the AMBER force field and AMBER output naming scheme.
- 1-model_water:
  - Modify this script and use the Modeller package in OpenMM to add water at the desired salt concentration.
- 2-simulation:
  - Copy your input files onto XSEDE Bridges using the sync_data.sh script.
  - Log into Bridges and submit the simulation onto the GPU-small (sbatch run_small_simulation.job) or GPU-shared queue (sbatch run_simulation.job)
  - Check the queue to see if your job has submitted.
  - When your job is complete, copy your output files from XSEDE Bridges using the sync_data.sh script.

References

- Awale, M.; van Deursen, R.; Reymond, J.-L. MQN-Mapplet: Visualization of Chemical Space with Interactive Maps of DrugBank, ChEMBL, PubChem, GDB-11, and GDB-13. J. Chem. Inf. Model. 2013, 53 (2), 509–518. https://doi.org/10.1021/ci300513m.
- Cross, J. B.; Thompson, D. C.; Rai, B. K.; Baber, J. C.; Fan, K. Y.; Hu, Y.; Humblet, C. Comparison of Several Molecular Docking Programs: Pose Prediction and Virtual Screening Accuracy. Journal of Chemical Information and Modeling 2009, 49 (6), 1455–1474. https://doi.org/10.1021/ci900056c.
- [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
- Sterling, T.; Irwin, J. J. ZINC 15 – Ligand Discovery for Everyone. J. Chem. Inf. Model. 2015, 55 (11), 2324–2337. https://doi.org/10.1021/acs.jcim.5b00559.