References

- [1] Pande, V. S.; Beauchamp, K. A.; Bowman, G. R. Everything You Wanted to Know about Markov State Models but Were Afraid to Ask. Methods (San Diego, Calif.) 2010, 52 (1), 99–105. https://doi.org/10.1016/j.ymeth.2010.06.002.
- [2] Chodera, J. D.; Noé, F. Markov State Models of Biomolecular Conformational Dynamics. Current Opinion in Structural Biology 2014, 25, 135–144. https://doi.org/10.1016/j.sbi.2014.04.002.
- [3] Xie, B.; Clark, J. D.; Minh, D. D. L. Efficiency of Stratification for Ensemble Docking Using Reduced Ensembles. Journal of Chemical Information and Modeling 2018, 58 (9), 1915–1925. https://doi.org/10.1021/acs.jcim.8b00314.

Some software

- For MD analysis
  - MDTraj: http://mdtraj.org/1.9.3/index.html
  - ProDy: http://prody.csb.pitt.edu/tutorials/trajectory_analysis/trajectory.html

- For Markov State Models
  - MSMBuilder: http://msmbuilder.org/3.8.0/
  - PyEMMA: http://emma-project.org/latest/