References

- [1] Many parts of today's lecture were adapted from a lecture by David Mobley (https://github.com/MobleyLab/drug-computing/tree/master/uci-pharmsci/lectures/free_energy_basics) under the CC BY 4.0 license. The lecture is part of the Drug Discovery Computing Techniques course (PharmSci 175/275) at UC Irvine.
- [2] Zwanzig, R. High-Temperature Equation of State by a Perturbation Method. I. Nonpolar Gases. Journal of Chemical Physics 1954, 22 (8), 1420.
- [3] Bennett, C. H. Efficient Estimation of Free-Energy Differences from Monte Carlo Data. Journal of Computational Physics 1976, 22 (2), 245–268.
- [4] Shirts, M. R.; Chodera, J. D. Statistically Optimal Analysis of Samples from Multiple Equilibrium States. Journal of Chemical Physics 2008, 129 (12), 124105.

Additional Resources

- Resource for alchemical binding free energy calculations (http://www.alchemistry.org/wiki/Main_Page)
- Thermodynamic cycle in YANK (http://getyank.org/latest/theory.html)