

# References on Ligand Parameters

- [5] Wang, J.; Wolf, R. M.; Caldwell, J. W.; Kollman, P. A.; Case, D. A. Development and Testing of a General Amber Force Field. *Journal of Computational Chemistry* 2004, 25 (9), 1157–1174. <https://doi.org/10.1002/jcc.20035>.
- [6] Mobley, D. L.; Bannan, C. C.; Rizzi, A.; Bayly, C. I.; Chodera, J. D.; Lim, V. T.; Lim, N. M.; Beauchamp, K. A.; Slochower, D. R.; Shirts, M. R.; Gilson, M. K.; Eastman, P. K. Escaping Atom Types in Force Fields Using Direct Chemical Perception. *J. Chem. Theory Comput.* 2018, 14 (11), 6076–6092. <https://doi.org/10.1021/acs.jctc.8b00640>.

# Additional Resources

- Resource for alchemical binding free energy calculations ([http://www.alchemistry.org/wiki/Main\\_Page](http://www.alchemistry.org/wiki/Main_Page))
- Thermodynamic cycle in YANK (<http://getyank.org/latest/theory.html>)