

TINKER – Software Tools for Molecular Design

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Washington University in Saint Louis (WU), The University of Texas at Austin
(UT Austin), and Sorbonne Université (Sorbonne)

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“TINKER 8: A Modular Software Package for Molecular Design and Simulation. Joshua A. Rackers, Marie L. Laury, Chao Lu, Zhi Wang, Louis Lagardère, Jean-Philip Piquemal, Pengyu Ren, Jay W. Ponder, *Journal of Chemical Theory and Computation*, 14, 5273-5289, 2018, DOI 10.1021/acs.jctc.8b00529”

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“Tinker-OpenMM: Absolute and Relative Alchemical Free Energies using AMOEBA on GPUs. Matthew Harger, Daniel Li, Zhi Wang Kevin Dalby, Louis Lagardère, Jean-Philip Piquemal, Jay Ponder, Pengyu Ren, *Journal of Computational Chemistry*, 38, 2047-2055, 2017, DOI 10.1002/jcc.24853”

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