TINKER – Software Tools for Molecular Design Version 8.7 June 2019

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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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"Tinker-HP: A Massively Parallel Molecular Dynamics Package for Multiscale Simulations of Large Complex Systems with Advanced Polarizable Force Fields, Louis Lagardère, Luc-Henri Jolly, Filippo Lipparini, Félix Aviat, Benjamin Stamm, Zhifeng F. Jing, Matthew Harger, G. Andres Cisneros, Nohad Gresh, Yvon Maday, Pengyu Ren, Jay W. Ponder, Jean-Philip Piquemal, *Chemical Science*, 9, 956-972, 2017, DOI: 10.1039/c7sc04531j"

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