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”

Considering the use of the specific Tinker-OpenMM code, included in the Tinker distribution, any
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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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