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: Software Tools for Molecular Design, Joshua A. Rackers, Zhi Wang, Chao Lu,
Marie L. Laury, Louis Lagardère, Michael J. Schnieders, Jean-Philip Piquemal, Pengyu Ren and
(DOI: 10.1021/acsc.jtc.8b00529; PMCID: PMC6335969)”

Considering the use of the specific Tinker-HP code, included in the Tinker distribution, any
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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, Noahd Gresh, Yvon Maday, Pengyu Ren, Jay W. Ponder, Jean-Philip Piquemal,
Chemical Science, 9, 956-972, 2017, DOI: 10.1039/c7sc04531j”

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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