TINKER – *Software Tools for Molecular Design*

Version 8.11 June 2024

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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 Jay W. Ponder, ***Journal of Chemical Theory and Computation***, *14*, 5273-5289, 2018.
(DOI: 10.1021/acs.jctc.8b00529; PMCID: PMC6335969)"

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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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"**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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