

# **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 Universités (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, **2018.**”

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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, J. Comput. Chem., **2017**, 38, **2047-2055.**”

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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, **2017.**”

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