

TINKER – Software Tools for Molecular Design

Version 7.1 February 2015

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TINKER is a modular program package for molecular mechanics-based potential energy calculations, geometry optimization, molecular dynamics simulation, distance geometry and structural analysis.

Selected References for the TINKER Package:

- (1) Y. Shi, *et al.*, *J. Chem. Theory Comput.*, **9**, 4046-4063 (2013)
- (2) P. Ren, C. Wu and J. W. Ponder, *J. Chem. Theory Comput.*, **7**, 3143-3161 (2011)
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- (5) R. V. Pappu, R. K. Hart and J. W. Ponder, *J. Phys. Chem. B*, **102**, 9725-9742 (1998)
- (6) C. E. Kundrot, J. W. Ponder and F. M. Richards, *J. Comput. Chem.*, **12**, 402-409 (1991)
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