

TINKER – Software Tools for Molecular Design

Version 8.2 June 2017

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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)
- (3) J. W. Ponder, *et al.*, *J. Phys. Chem. B*, **114**, 2549-2564 (2010)
- (4) P. Ren and J. W. Ponder, *J. Phys. Chem. B*, **107**, 5933-5947 (2003)
- (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)
- (7) J. W. Ponder and F. M. Richards, *J. Comput. Chem.*, **8**, 1016-1024 (1987)

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Prof. Jay W. Ponder
Department of Chemistry, Box 1134
Washington University in Saint Louis
One Brookings Drive
Saint Louis, MO 63130 U.S.A.

Phone: 1-314-9354275
Fax: 1-314-9354481
Email: ponder@dasher.wustl.edu