TINKER – *Software Tools for Molecular Design*

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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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