Journal of Molecular Graphics and Modelling

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2. Best, S.A., Merz, K.M. Jr., and Reynolds, C.H. Free energy perturbation study of octanol/water partition coefficients: Comparison with continuum GB/SA calculations. *J. Phys. Chem. B* 1999, **103**, 714-726.

3. Gao, J. Methods and applications of combined quantum mechanical and molecular mechanical potentials. In: *Reviews in computational chemistry,* Lipkowitz, K.B., and Boyd, D.B., Eds., VCH Publishers, New York, 1995, Vol. 7, pp. 119-185.

4. Allen, M.P., and Tildesley, D.J. *Computer simulation of liquids.* Clarendon, Oxford, 1987.

5. Spartan, version 4.1.1, 1993, Wavefunction, Inc., Irvine, Calif.

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