GBr^6: a Parameterization-Free, Accurate, Analytical Generalized Born Model HARIANTO TJONG, HUAN-XIANG ZHOU, Department of Physics and Institute of Molecular Biophysics and School of Computational Science, Florida State University, Tallahassee, Florida 32306 — The Poisson-Boltzmann (PB) equation is widely used for modeling electrostatic effects for macromolecules. Generalized Born (GB) models have been developed to mimic PB results at substantial lower computational cost. Here we report an analytical GB model that reproduces PB results with high accuracy. The analytical approach is adapted from Gallicchio and Levy (J. Comput. Chem 25:479, 2004), but we implement an improvement of the Coulomb-field approximation proposed by Grycuk (J. Chem. Phys. 119:9, 2003). Benchmarked against PB results, our GB model has an average error of only 0.5% for a representative set of 55 proteins and of 0.4% and 0.2%, respectively, for folded and unfolded conformations of cytochrome b_{562} sampled in molecular dynamics simulations. The dependencies of the electrostatic solvation free energy on solute and solvent dielectric constants and on salt concentration are fully accounted for in this model.

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