Supplementary Material

Gaussian-based smooth dielectric function: A surface-free approach for modeling macromolecular binding in solvents

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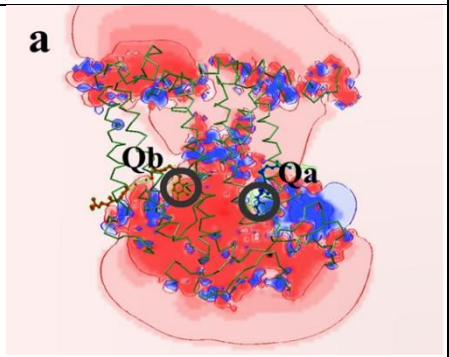
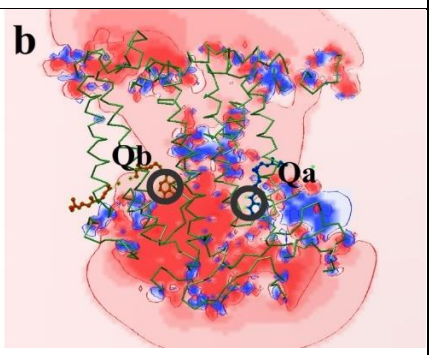
Table S1. Comparisons of performance of traditional 2-dielectric and Gaussian-based methods against experimental data and observable phenomena.

	Traditional 2-dielectric method	Gaussian-based dielectric method
pKa modeling: RMSD (calculated vs experimental) of 89 pKa's of SNase (J. Chem. Theory Comput. 2013, 9, 2126−2136)	2.43 pH units	1.77 pH units
Binding free energy changes upon 105 mutations (calculated vs experimental). (Bioinformatics. 2017 Oct 28. doi: 10.1093/bioinformatics/btx69)	0.62kcal/mol	0.54kcal/mol
Electron transfer in Bacterial Reaction Center: red – negative; blue - positive. Electron is supposed to be transferred from Qa→Qb. In traditional model, the electrostatic potential opposes the transfer, while in Gaussian-based model, it is almost neutral (Qa and Qb have similar potentials).		
Linkage to the physical properties of amino acids ((J. Chem. Theory Comput. 2013, 9, 2126−2136).	Hydrophobic and hydropilic acids are assigned the same dielectric constant	Hydrophobic acids are assigned lower dielectric consatnt as compared with hydrophilic and polar residues