Coulombic Free Energy and Salt Ion Association Per Phosphate of All-atom Models of DNA Oligomer: Dependence on Oligomer Size

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Supplementary Information

All-atom NLPB calculation details. Table S1 shows grid dimension and sizes for all three all-atom model. Amber force field[1] was used to generate atomic charges and radii. Other parameters used in calculations are: nonlinear PBE; multiple Debye-Huckel sphere boundary conditions, 2.0 Å mobile ion radius, solute dielectric constant 2.0, solvent dielectric constant 78.54, "molecular" surface definition, harmonic average smoothing, solvent probe radius 1.4 Å, temperature 298.15 °K.

Table S1. Grid Sizes and Spacings for All-atom NLPB Calculations

File/Model	Grid dimensions	Grid spacings before focusing (Å/grid)^3	Grid lengths before focusing Å^3	Grid spacings after focusing (Å/grid)^3	Grid lengths after focusing Å^3
CGATTAGATAGC	129x129x193	0.625x0.625x0.547	80x80x105	0.391x0.391x0.391	50x50x75
1DUF and 1CS2	97x97x129	0.833x0.833x0.938	80x80x120	0.573x0.573x0.547	55x55x70

References

(1) D.A. Case, T.E. Cheatham, III, T. Darden, H. Gohlke, R. Luo, K.M. Merz, Jr., A. Onufriev, C. Simmerling, B. Wang and R. Woods, The Amber biomolecular simulation programs. *J. Computat. Chem.*, **2005**, *26*, 1668-1688 .