Supporting Information

Constant pH Molecular Dynamics Simulations of Nucleic Acids in Explicit Solvent

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Table S1: Bond Parameters for Protonated Adenine and Cytosine. Parameters were adapted from comparable values from the tautomeric form of cytosine and guanine in CHARMM.[1]

Atom Types	K_b	b_o
CN1 NN2C	350.0	1.335
CN2 NN2C	450.0	1.343
HN2 NN2C	474.0	1.01

Table S2: Angle Parameters for Protonated Adenine and Cytosine. Parameters were adapted from comparable values from the tautomeric form of cytosine and guanine in CHARMM.[1]

Atom Types	K_θ	θ_o
CN4 NN2G CN2	70.0	131.1
NN2G CN4 NN3A	70.0	122.2
CN5 CN2 NN2G	70.0	107.8
NN2 CN1 NN2C	50.0	116.8
NN2C CN1 ON1C	130.0	123.8
CN1 NN2C HN2	37.0	121.2
CN1 NN2C CN2	85.0	119.1
CN2 NN2C HN2	37.0	121.2
CN3 CN2 NN2C	85.0	119.3
NN2C CN2 NN1	81.0	122.3

Table S3: Dihedral Parameters for Protonated Adenine and Cytosine. Parameters were adapted from comparable values from the tautomeric form of cytosine and guanine in CHARMM.[1]

Atom Types	K_δ	n	δ
CN2 NN2G CN4 NN3A	0.2	2	180.0
HN2 NN2G CN4 NN3A	3.6	2	180.0
CN2 NN2G CN4 HN3	4.0	2	180.0
NN2C CN2 NN1 HN1	1.0	2	180.0
CN1 NN2C CN2 CN3	6.0	2	180.0
NN1 CN2 NN2C CN1	2.0	2	180.0
ON1C CN1 NN2C CN2	1.6	2	180.0
NN2 CN1 NN2C CN2	0.6	2	180.0
ON1C CN1 NN2C HN2	3.0	2	180.0
HN2 NN2C CN1 NN2	2.0	2	180.0
CN3 CN2 NN2C HN2	1.0	2	180.0
HN2 NN2C CN2 NN1	2.0	2	180.0