Table 1 Table S1 - Parameters found by QM calculations for the electrostatic term (Adenosine)

Atom	Charge
CT5	0.1070
CT4	-0.1540
OS1	0.1884
CT3	-0.1800
OH1	0.2754
CT2	-0.1749
OH2	0.2746
CT1	-0.1308
N9	0.0936
C2	-0.0372
NB	0.0910
CB	-0.1779
CA	-0.2025
N2	0.3345
NC	0.0737
CQ	-0.1051
NC	0.1041
CB	-0.1622
H11	0.0029
H12	0.0021
H13	-0.0051
H14	0.0198
H15	0.0219
H16	0.0242
HO2	-0.1818
H2	0.0218
H5	0.0189
HH1	-0.0056
HH2	-0.0185
H5	0.0210
HO1	-0.1394

^{a} Values set in (e).

Table 2 Table S2 - Parameters found by quantum calculations for the electrostatic term (Guanosine)

Atom	Charge
CT5	0.1167
CT4	0.2623
OS1	-0.6018
CT3	0.1919
OH1	-0.6103
CT2	0.2545
OH2	-0.6799
CT1	0.5347
N9	-0.4770
CK	0.4080
NB	-0.5695
CB2	0.0823
C6	0.6851
OO	-0.4786
NA	-0.4684
CA	0.8706
NC	-0.5345
CB1	0.3092
H11	0.0355
H12	0.0085
H13	0.0179
H14	0.0288
H15	0.0442
H16	-0.0080
HO2	0.3217
H2	-0.0005
H5	-0.0548
N2	-0.6042
HO1	0.3151
HH1	0.1907
HH2	0.2065
HH3	0.2031

^{a} Values set in (e).

Table 3 Table S3 - Parameters found by quantum calculations for the electrostatic term (Cytidine)

Atom	Charge
CT5	0.1760
CT4	0.0741
OS1	-0.6852
CT3	0.3906
OH1	-0.6733
CT2	0.3395
OH2	-0.7518
CT1	0.4810
N9	-0.6135
C6	0.7328
OO	-0.5651
NC	-0.6031
CA	0.9115
N2	-0.6180
CM	-0.6013
C1	0.7661
H11	0.0048
H12	0.0379
H13	0.0284
H14	0.0259
H15	0.0082
H16	0.0111
HO2	0.3383
HO1	0.3903
H2	0.0406
HA	-0.0877
H4	0.0159
HH1	0.2188
HH2	0.2069

[a] Values set in (e).

Table 4 Table S4 - Parameters found by quantum calculations for the electrostatic term (Uridine)

Atom	Charge
CT5	0.1405
H12	0.0145
H13	0.0435
CT4	0.1793
H14	0.0165
OS	-0.641
CT1	0.6526
H2	0.0024
CT3	0.4826
H15	0.0310
CT2	0.0874
H16	-0.0002
OH2	-0.7209
HO2	0.3327
N9	-0.685
CC1	0.7428
NA	-0.451
CC2	1.0673
CM1	-0.5025
CM2	0.4332
OO1	-0.529
HH	0.2065
OO2	-0.5428
HA	-0.0699
H4	0.0182

[a] Values set in (e).