

Supporting material #1

Parameter	In water	Without water
Cytosine		
C4-N4	1.351	1.381
C2-O2	1.270	1.233
N3-C4	1.359	1.331
N3-C2	1.362	1.383
N1-C2	1.399	1.452
N1-C6	1.369	1.368
N1-H1	1.034	1.020
C5-C6	1.363	1.367
C4-C5	1.434	1.446
C6-H6	1.084	1.070
C5-H5	1.082	1.087
N2-H21	1.023	1.019
N2-H22	1.018	1.016
Thymine		
C2-N1	1.380	1.40689
C2-O2	1.253	1.23008
H3-C3	1.088	1.09021
N1-C6	1.383	1.39317

C6-C5	1.364	1.35991
C5-C4	1.454	1.47675
C5-C5	1.509	1.51498
C5-H51	1.097	1.10037
C5-H52	1.097	1.0997
C5-H53	1.095	1.09977
C2-N3	1.386	1.39865
N3-C4	1.412	1.42935
N3-H3	1.031	1.02235
N1-H1	1.035	1.01873
C4-O4	1.253	1.23426
Guanine		
C2-N3	1.341	1.324
C2-N1	1.388	1.384
C6-N1	1.415	1.469
C5-C6	1.421	1.446
N7-C5	1.397	1.395
N7-C8	1.323	1.317
C8-N9	1.384	1.402
N9-C4	1.377	1.385
C5-C4	1.405	1.406
C4-N3	1.358	1.366

C2-N2	1.355	1.389
N2-H21	1.026	1.026
N2-H22	1.023	1.017
N1-H1	1.035	1.022
C8-H8	1.083	1.086
C6-O6	1.265	1.230
H9-N9	1.033	1.018
Adenine		
N3-C2	1.345	1.350
N1-C2	1.348	1.354
N1-C6	1.369	1.356
C5-C6	1.420	1.417
C7-C5	1.398	1.400
N7-C8	1.331	1.321
N9-C8	1.379	1.397
C4-N9	1.382	1.393
C4-C5	1.404	1.409
N3-C4	1.353	1.346
C2-H2	1.088	1.092
N6-C6	1.351	1.372
N6-H61	1.022	1.017
N6-H62	1.021	1.017

C8-O8	1.084	1.087
N9-H9	1.036	1.018
C2-H2	1.088	1.092