Supporting Information

„C5-Methylation of Cytosine in B-DNA thermodynamically and kinetically stabilizes BI"

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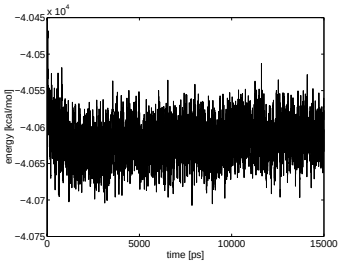
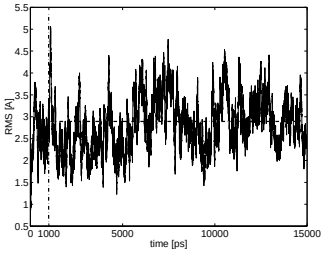
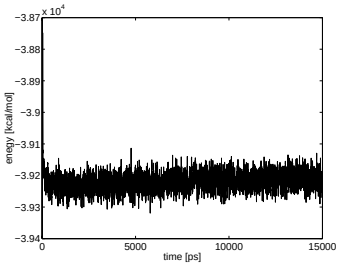
Total Energy and RMSd values of the published simulations

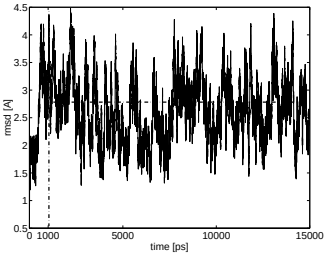
(a) simulation of d(GCGCGCGCGCGC)$_2$



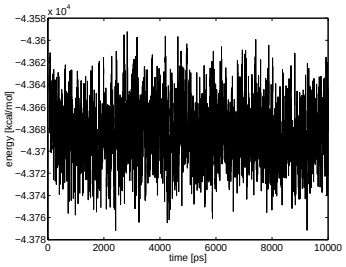


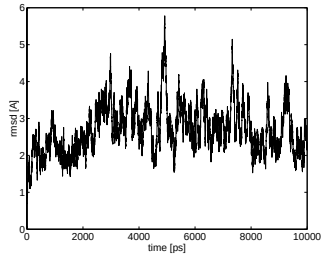
(b) simulation of d(G5mCG5mCG5mCG5mCG5mCGC)$_2$



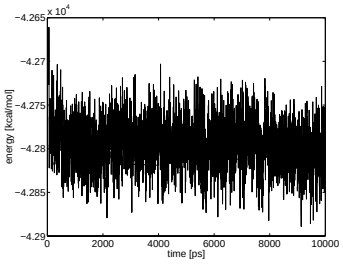


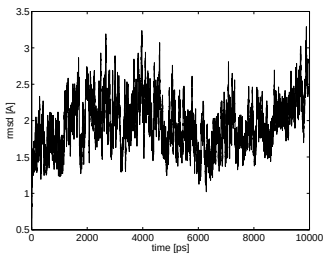
(c) simulation of d(ACGACGACGACGA)$_2$





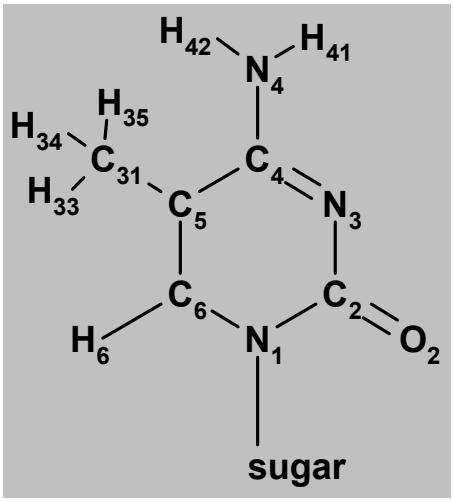
(d) simulation of d(A5mCGA5mCGA5mCGA5mCGA)$_2$





Parameterization of 5-Methyl-Cytosine

Geometry optimization and ab initio electrostatic potential calculation were carried out for 1,5-dimethylcytosine with GAUSSIAN98 at HF/6-31+G(d) level of theory. Charges were derived using the RESP (Restrained ElectroStatic Potential) charge fitting procedure: From the charges for the nucleotide cytosine given in the force field the charge for the base alone were calculated to be -0.0631, thus the overlapping 1-methylgroup was forced to have a charge of +0.0631, and the whole residue to be neutral. One missing force field parameter (for the angle CA-CM-CT, 70.0/120.0) was added in analogy to existing parameters.



RESP-Charges		
Atoms	**dC (parm99)**	**5mC**
N1	-0.0339	0.0141
C2	0.7959	0.7754
O2	-0.6548	-0.6227
N3	-0.7748	-0.7175
C4	0.8439	0.6091
N4	-0.9773	-0.8758
H41/H42	0.4314	0.3996
C5	-0.5222	-0.0616
H5/C31	0.1863 (H5)	-0.235 (C31)
H33-H35		0.0777
C6	-0.0183	-0.192
H6	0.2293	0.2106

Fig.1: Left: Scheme of 5-methylcytosine with atom names. Right: RESP derived charges for 5-methylcytosine, second column: default AMBER-charges for cytosine; third column: new charge-set for 5-methylcytosine.