

Supporting Information

Cooperative Effects of Cytosine Methylation on DNA Structure and Dynamics

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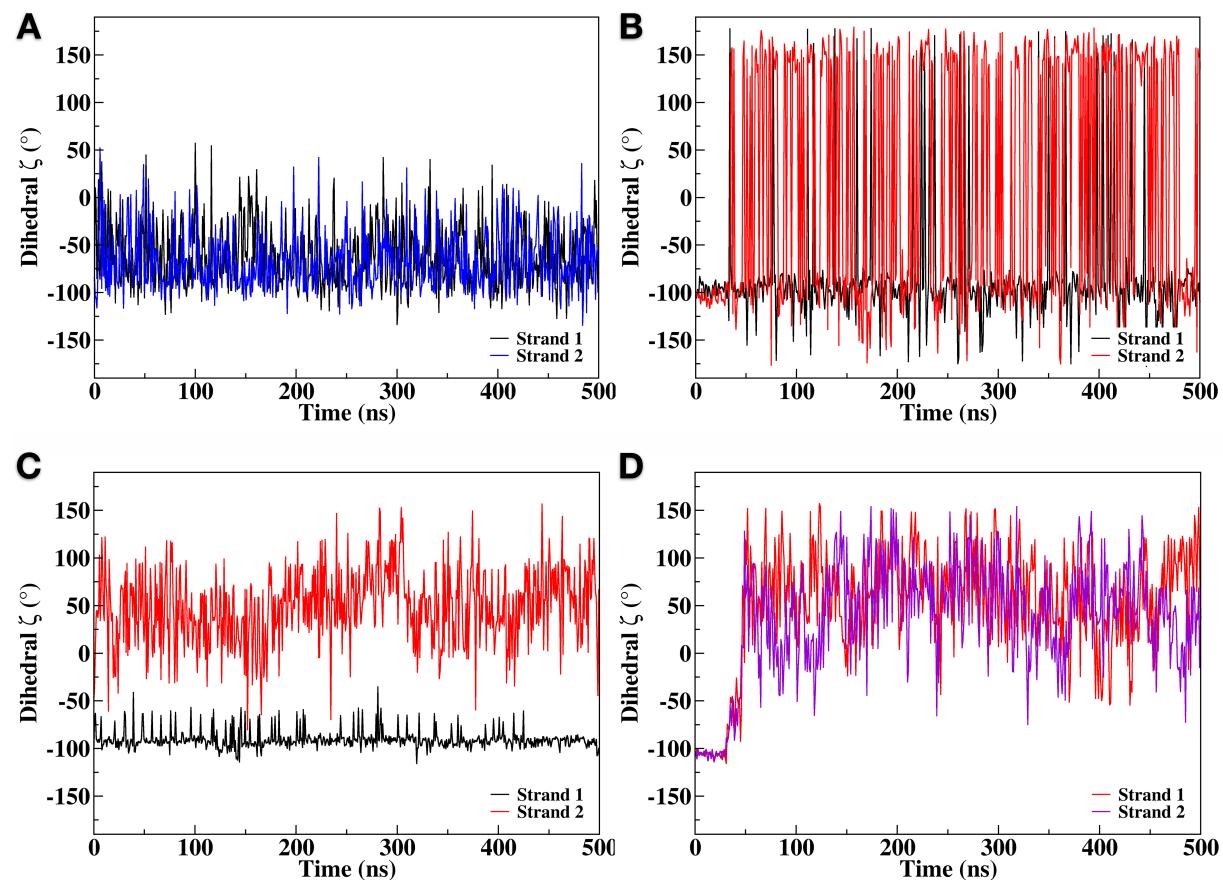


Figure S1 : Time series of torsional angle ζ for model DNA. A : Unmethylated DNA, B : Single methylated DNA, C : Hemi-methylated DNA, D : Methylated DNA.

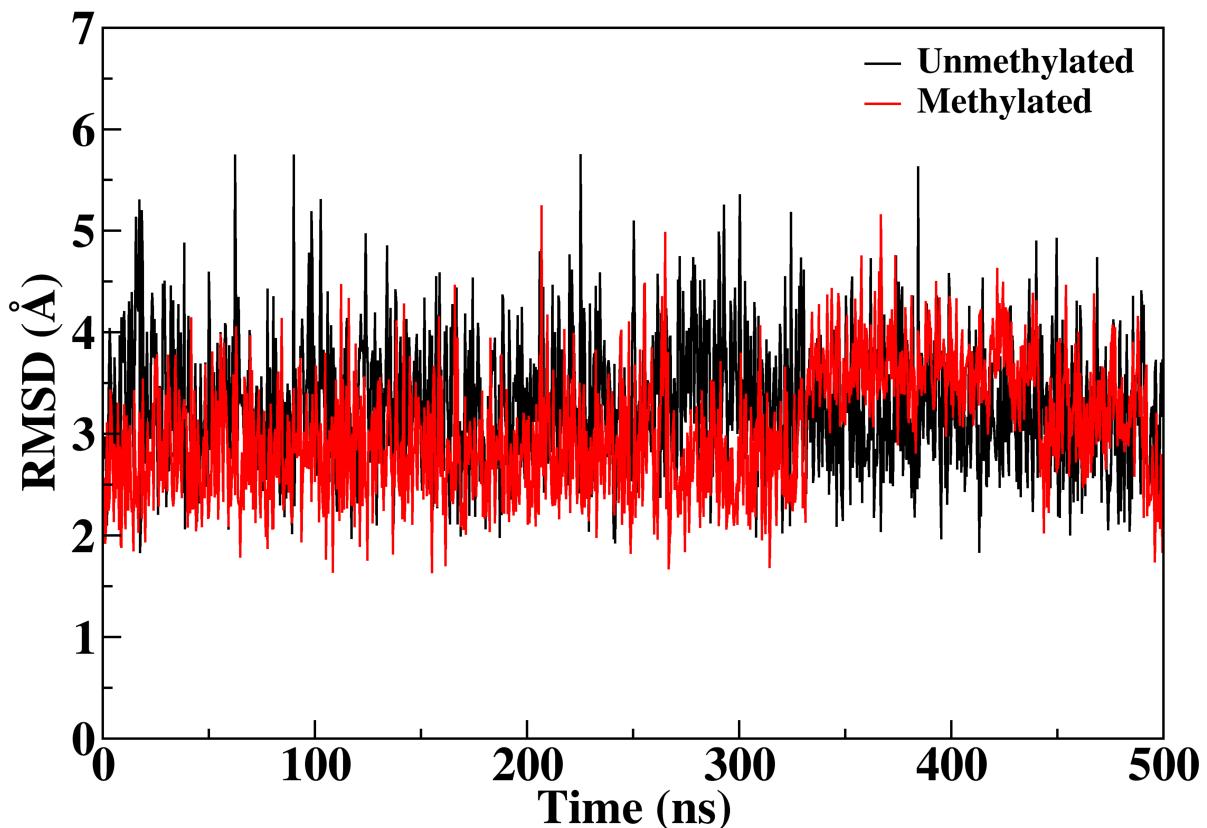


Figure S2 : Time series of the RMSD for APC gene un-methylated (black) and methylated (red).

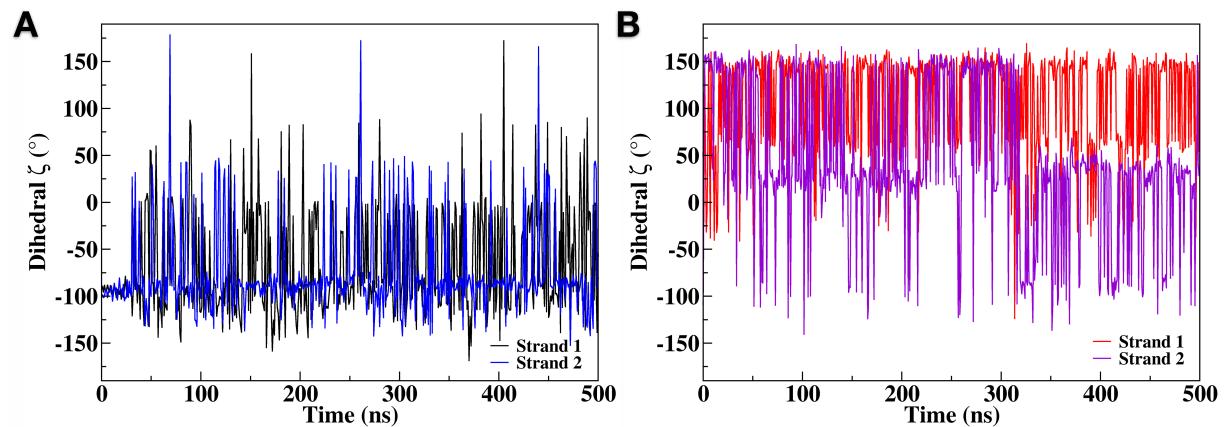


Figure S3 : Time series of torsional angle ζ in DC or in 5-mC for APC promoting region. A : Un-methylated APC promoting region, B : Methylated APC promoting region.

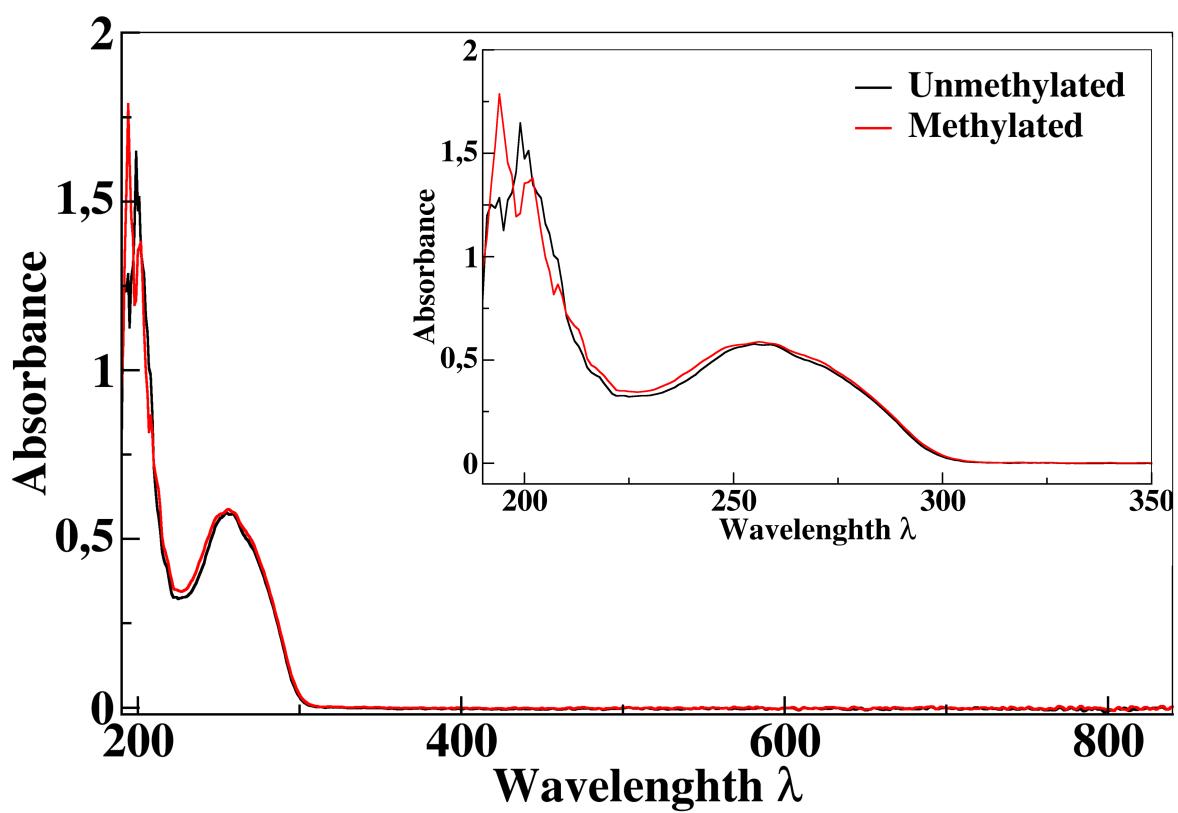


Figure S4 : Spectrum (UV-Vis) of APC promoting region unmethylated (black) or methylated (red).

Name	Atom type	Charge
P	P	1.158386879
OP1	O2	-0.786433121
OP2	O2	-0.786433121
O5	OS	-0.367634121
C5'	CT	-0.124613121
H5'	H1	0.085450879
H5''	H1	0.085450879
C4'	CT	0.381806879
O4'	OS	-0.530837121
C1'	CT	0.184391879
H1	H2	0.157954879
N1	N*	-0.220418121
C6	CM	0.018923879
H6	H4	0.254180879
C5	CM	-0.265800121
C4	CA	0.842233879
N4	N2	-1.014376121
H41	H	0.422986879
H42	H	0.422986879
N3	NC	-0.855177121
C2	C	0.893149879
O2	O	-0.696222121
C3'	CT	0.264619879
H3'	H1	0.109296879
C2'	CT	-0.230318121
H2'	HC	0.077348879
H2''	HC	0.077348879
O3'	OS	-0.556918121
H4'	H1	0.010153879
C01	CT	-0.241364121
H03	H1	0.076623879

H04	H1	0.076623879
H02	H1	0.076623879

Table S1 : Atom types and RESP charges for the 5-mC