Supporting Information

The Base Flipping of A Form DNA-a Molecular Dynamic Simulation Study

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Content

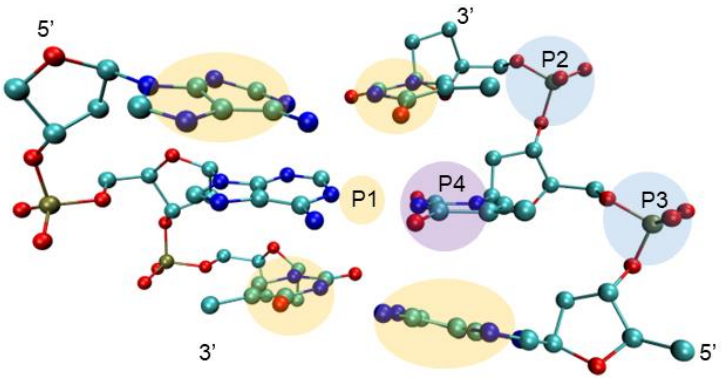

Fig. S1 The definition of the pseudo dihedral angle CPDb. p1 is defined by the mass center of the two flanking base pairs, p2 and p3 are defined by the flanking phosphate groups, and p4 is defined by the five-member ring of the flipping purine (or the entire six-membered ring for a flipping pyrimidine)

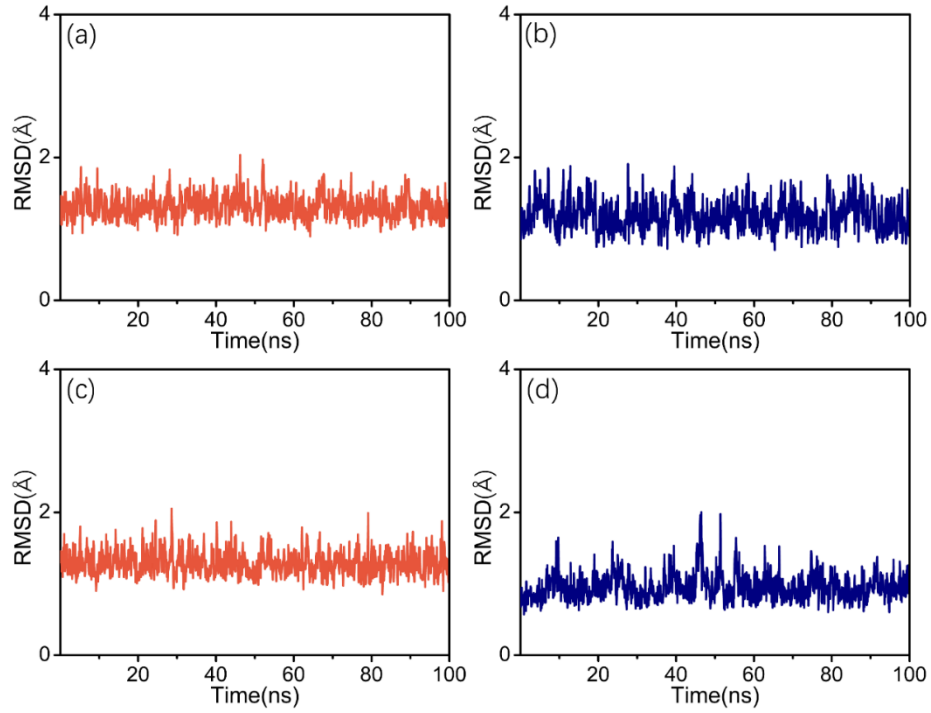

Fig. S2 The RMSD of the DNA system during the 100 ns production simulation (a) B-DNA1: RMSD (1.3 ± 0.3); (b) A-DNA1: RMSD (1.2 ± 0.3) (C) B-DNA2: RMSD (1.3 ± 0.2) and (d) A-DNA2: RMSD (1.0 ± 0.2)

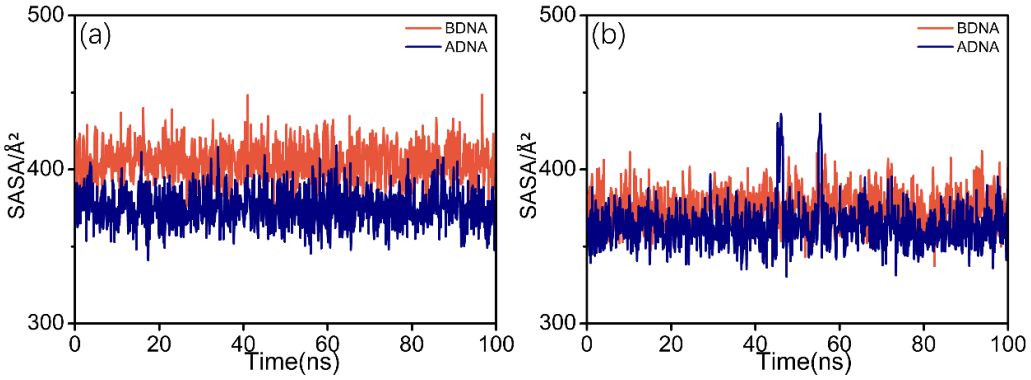

Fig. S3 The solvent-accessible surface areas (SASA) of T7:A18 base pair (DNA1) and C7:G18 base pair during 100ns production simulation (DNA2).

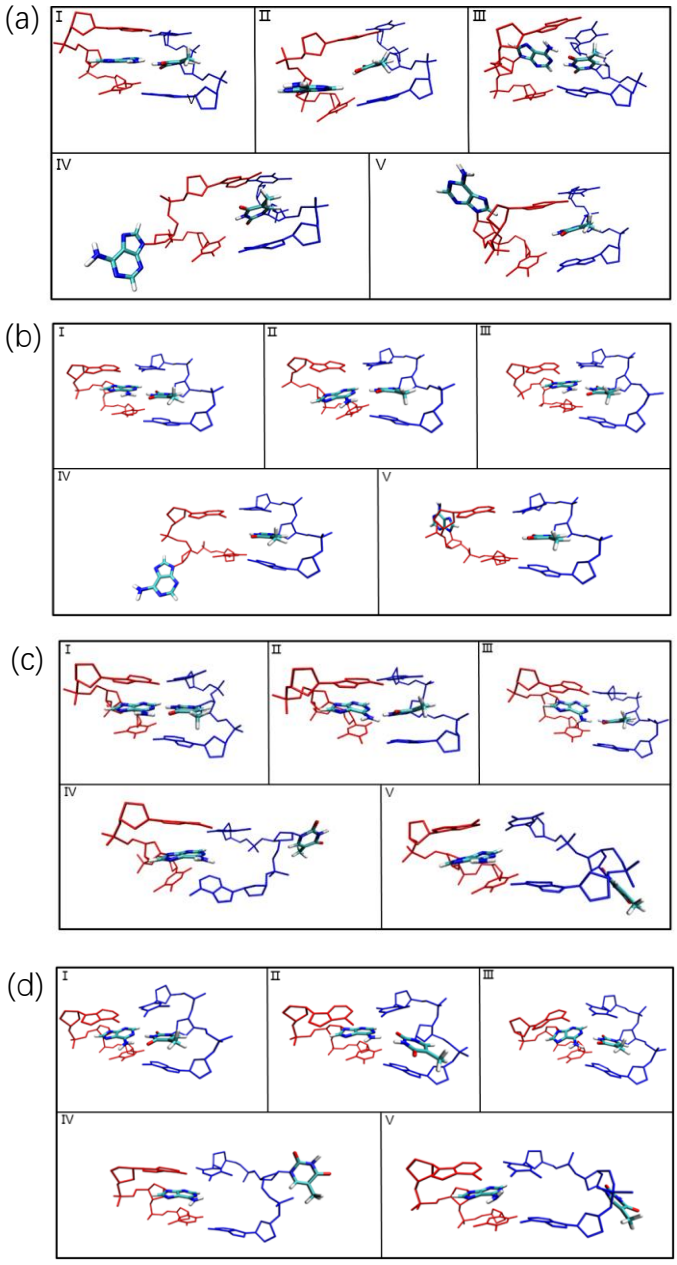

Fig. S4 The representative structures during the flipping process (a) A18 and its adjacent bases of B-DNA1; (b) A18 and its adjacent bases of A-DNA1; (C) T7 and its adjacent bases of B-DNA1 ; (d) T7 and its adjacent bases of A-DNA1, the hydrogen atoms were omitted for clarity, except A18:T7 base pair.

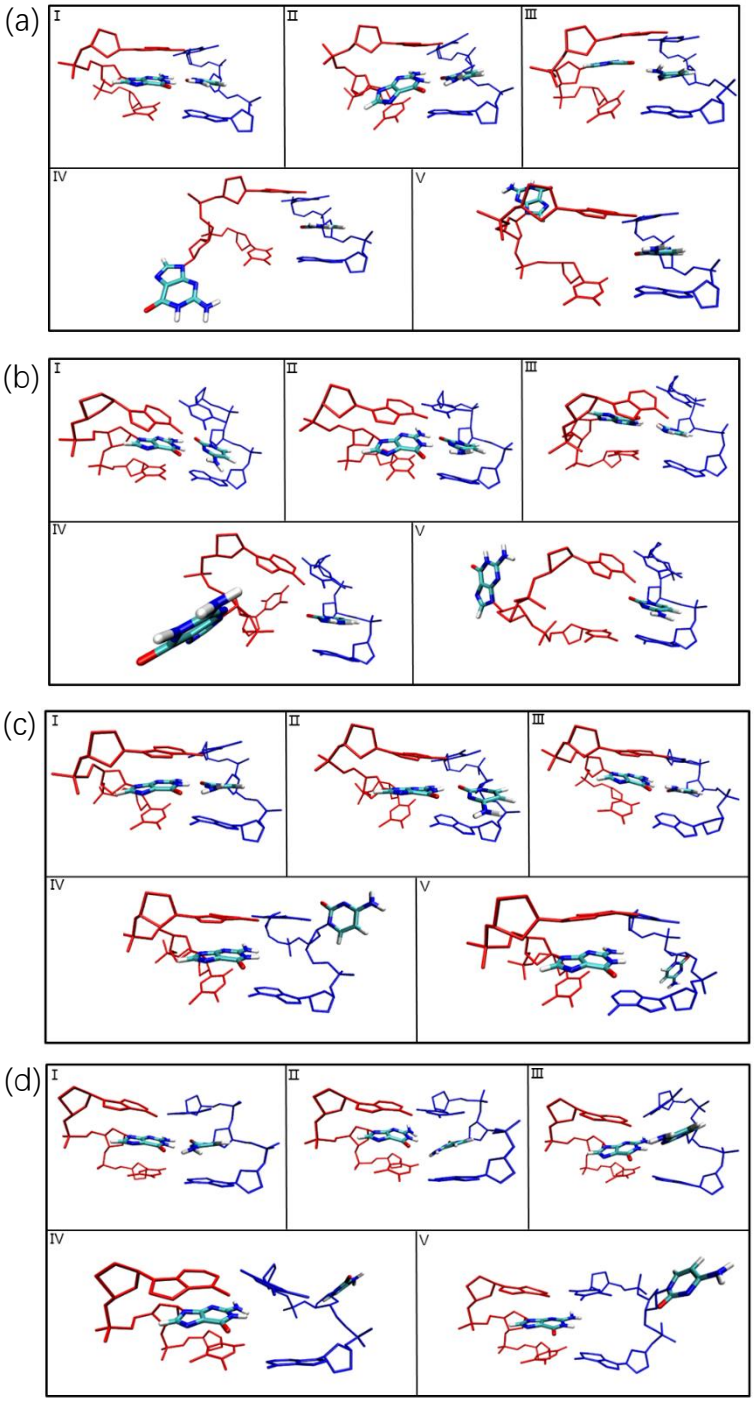

Fig. S5 The representative structures during the flipping process, (a) G18 and its adjacent bases of B-DNA2; (b) G18 and its adjacent bases of A-DNA2; (C) C7 and its adjacent bases of B-DNA2 ; (d) C7 and its adjacent bases of A-DNA2, the hydrogen atoms were omitted for clarity, except G18:C7 base pair.

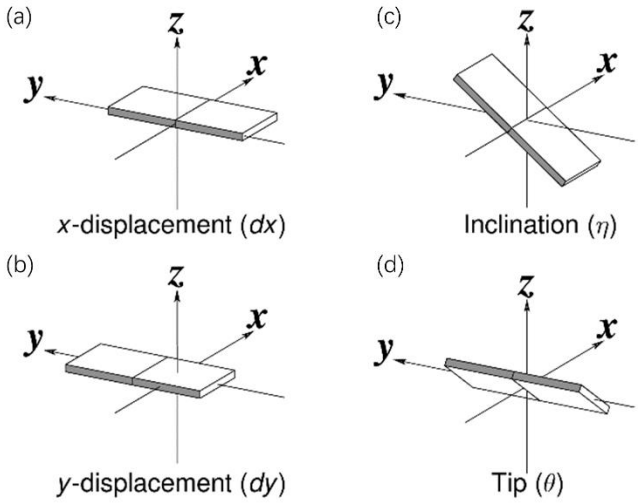

Fig. S6 The structural parameters employed in this paper. Adapted from Lu et al.[1]

Table S1 The interaction energy of T and A bases with adjacent bases for DNA1 (kcal mol^{-1})

	T7:A8[a]	T7:A6[a]	A18:T19[a]	A18:A17[a]	T7:A18[b]
A-DNA1	-4.9±0.7	-6.4±0.7	-6.4±0.8	-6.2±0.8	-11.0±1.2
B-DNA1	-5.4±0.8	-6.7±0.8	-6.7±0.8	-7.2±0.8	-10.9±1.2

[a] represent the π-stacking interaction energy of Adenine or Thymine with adjacent bases.

[b] represent the Watson-Crick hydrogen interaction energy of Adenine and Thymine.

Table S2 The interaction energy of C and G bases with adjacent bases for DNA2 (kcal mol^{-1})

	C7:A8[a]	C7:A6[a]	G18:T19[a]	G18:A17[a]	C7:G18[b]
A-DNA2	-4.8±0.7	-5.7±0.7	-6.4±0.8	-6.3±0.8	-24.1±2.4
B-DNA2	-4.8±0.8	-6.0±0.8	-6.8±1.1	-7.5±0.8	-24.7±1.7

[a] represent the π-stacking interaction energy of Adenine or Thymine with adjacent bases.

[b] represent the Watson-Crick hydrogen interaction energy of Adenine and Thymine.

Table S3 The key structural parameters of the two types DNA[a]

	Xdisp	Ydisp	Inclin	Tip				
A-DNA1	-4.39	0.07	18.5	1.3				
B-DNA1	-0.00	-0.13	3.1	-2.5				
A-DNA2	-4.21	0.33	21.9	1.2				
B-DNA2	0.18	0.05	1.5	0.3				
	Shear	Stretch	Stagger	Buckle	Prople	Opening		
A-DNA1	-0.09	-0.06	-0.06	2.8	-11.6	0.6		
B-DNA1	-0.01	-0.01	0.07	-1.5	-10.2	-0.7		
A-DNA2	0.12	0.00	-0.36	6.9	-9.3	2.2		
B-DNA2	0.29	-0.02	0.03	3.0	-10.3	-1.6		
	Shift	Slide	Rise	Tilt	Roll	Twist	H-rise	H-Twi
A-DNA1	0.00	-1.51	3.34	-0.3	10.6	31.0	2.70	32.8
B-DNA1	0.16	0.24	3.34	1.3	2.6	35.9	3.39	36.1
A-DNA2	-0.28	-1.27	3.35	-0.4	13.0	30.4	2.66	32.9
B-DNA2	-0.02	0.30	3.35	0.3	1.3	36.0	3.39	36.2
	Min-W[a]	Min-D[b]	Maj-W[a]	Maj-D[b]				
A-DNA1	10.2	0.4	4.4	11.1				
B-DNA1	7.3	5.0	10.7	5.7				
A-DNA2	10.2	0.6	3.6	10.3				
B-DNA2	6.9	5.3	11.7	3.2				

[a]The parameters are given in the average value

Reference:

[1] Lu, X-J.; W. K. 3DNA: A versatile, integrated software system for the analysis, rebuilding and visualization of three-dimensional nucleic-acid structures. *Nat. Protoc.* **2008**, 3, 1213-1227.