

## Supplementary Information S2. The physical structural properties of dinucleotides in DNA

**Table S2-1.** The original values of the six properties for the 16 dinucleotides in DNA. See Eq.8 and the relevant text for further explanation.

Dinucleotide	Physical structural property					
	Rise $P_1$	Roll $P_2$	Shift $P_3$	Slide $P_4$	Tilt $P_5$	Twist $P_6$
AA	7.65	2.26	1.69	0.026	0.020	0.038
AC	8.93	3.03	1.32	0.036	0.023	0.038
AG	7.08	2.03	1.46	0.031	0.019	0.037
AT	9.07	3.83	1.03	0.033	0.022	0.036
CA	6.38	1.78	1.07	0.016	0.017	0.025
CC	8.04	1.65	1.43	0.026	0.019	0.042
CG	6.23	2.00	1.08	0.014	0.016	0.026
CT	7.08	2.03	1.46	0.031	0.019	0.037
GA	8.56	1.93	1.32	0.025	0.020	0.038
GC	9.53	2.61	1.20	0.025	0.026	0.036
GG	8.04	1.65	1.43	0.026	0.019	0.042
GT	8.93	3.03	1.32	0.036	0.023	0.038
TA	6.23	1.20	0.72	0.017	0.016	0.018
TC	8.56	1.93	1.32	0.025	0.020	0.038
TG	6.38	1.78	1.07	0.016	0.017	0.025
TT	7.65	2.26	1.69	0.026	0.020	0.038

**Table S2-2.** The values obtained by the standard conversion of Eq.9 from Table S2-1. See Eqs.8-9 and the relevant text for further explanation.

Dinucleotide	Physical structural property					
	Rise $P_1$	Roll $P_2$	Shift $P_3$	Slide $P_4$	Tilt $P_5$	Twist $P_6$
AA	-0.11	0.11	1.59	0.06	0.09	0.50
AC	1.04	1.29	0.13	1.50	1.19	0.50
AG	-0.62	-0.24	0.68	0.78	-0.28	0.36
AT	1.17	2.51	-1.02	1.07	0.83	0.22
CA	-1.25	-0.62	-0.86	-1.38	-1.01	-1.36
CC	0.24	-0.82	0.56	0.06	-0.28	1.08
CG	-1.39	-0.29	-0.82	-1.66	-1.38	-1.22
CT	-0.62	-0.24	0.68	0.78	-0.28	0.36
GA	0.71	-0.39	0.13	-0.08	0.09	0.50
GC	1.59	0.65	-0.35	-0.08	2.30	0.22
GG	0.24	-0.82	0.56	0.06	-0.28	1.08

GT	1.04	1.29	0.13	1.50	1.19	0.50
TA	-1.39	-1.51	-2.24	-1.23	-1.38	-2.37
TC	0.71	-0.39	0.13	-0.08	0.09	0.50
TG	-1.25	-0.62	-0.86	-1.38	-1.01	-1.36
TT	-0.11	0.11	1.59	0.06	0.09	0.50

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