Supplementary Material (ESI) for Molecular BioSystems

Stacking interaction in the middle and at the end of a DNA helix studied with non-natural nucleotides

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Supplementary information

Table S1 Thermodynamic parameters for DNA duplex formations measured in 1 M NaCl–phosphate buffer[a]

Sequence (5′ → 3′)	$-\Delta H°$ (kcal mol^{-1})	$-\Delta S°$ (cal mol^{-1}K^{-1})	$-\Delta G°_{37}$ (kcal mol^{-1})	T_m (°C)
GTGTAA^{phe}ATGTC / GACATFTACAC	76.5±1.9	216±6	9.53±0.22	49.6
GTGTTA^{phe}TTGTC / GACAAFAACAC	79.0±1.5	225±5	9.10±0.14	47.4
GTGTGA^{phe}GTGTC / GACACFCACAC	74.4±1.9	205±6	10.9±0.3	56.6
GTGTCA^{phe}CTGTC [b] / GACAGFGACAC	73.4	203	10.4	54.9
GTGTCA^{naph}CTGTC [b] / GACAGTGACAC	76.5	209	11.5	60.2
GTGTAAATGTC / GACATTTACAC	97.1±1.8	276±5	11.6±0.2	54.1
GTGTTATTGTC / GACAATAACAC	86.2±1.5	242±5	11.0±0.1	54.1

(Table S1 continued)

Sequence (5′ → 3′)	$-\Delta H°$ (kcal mol^{-1})	$-\Delta S°$ (cal mol^{-1}K^{-1})	$-\Delta G°_{37}$ (kcal mol^{-1})	T_m (°C)
GTGTGAGTGTC / GACACTCACAC	92.6±2.3	256±7	13.2±0.3	61.0
GTGTCACTGTC [b] / GACAGTGACAC	89.0	248	12.6	57.4
GTGTCACTGTC [b] / GACAGFGACAC	69.5	199	7.4	42.9
GTGTAC^{phe}ATGTC / GACATFTACAC	76.0±1.4	215±4	9.25±0.14	48.5
GTGTTC^{phe}TTGTC / GACAAFAACAC	75.1±1.9	214±6	8.91±0.23	47.1
GTGTGC^{phe}GTGTC / GACACFCACAC	82.7±1.3	231±4	11.2±0.1	55.6
GTGTCC^{phe}CTGTC / GACAGFGACAC	67.5±5.9	185±18	10.2±0.2	59.0
GTGTCC^{naph}CTGTC / GACAGFGACAC	75.1±4.8	207±15	11.4±0.2	60.8
GTGTACATGTC / GACATGTACAC	89.4±1.7	250±5	11.9±0.2	56.8
GTGTTCTTGTC / GACAAGAACAC	82.6±1.7	229±5	11.5±0.2	56.8
GTGTGCGTGTC / GACACGCACAC	89.6±1.8	243±5	14.3±0.2	66.3
GTGTCCCTGTC / GACAGGGACAC	85.7±3.5	235±10	12.9±0.3	65.3
GTGTCCCTGTC / GACAGFGACAC	64.3±3.9	180±12	7.84±0.16	45.2

[a]Data was obtained using the buffer containing 1 M NaCl, 10 mM Na_2HPO_4 (pH 7.0), and 1 mM Na_2EDTA. The error values were calculated from the difference between the parameters determined by the T_m^{-1} *versus* log (C_t/4) plot and curve fitting to the two-state model. T_m was calculated at 100 μM.

[b]Data are derived from the reference 19.

Table S2 Thermodynamic parameters of self-complementary DNA duplexes measured in 1 M NaCl–phosphate buffer[a]

Sequence (5′ → 3′)	$-\Delta H°$ (kcal mol^{-1})	$-\Delta S°$ (cal mol^{-1}K^{-1})	$-\Delta G°_{37}$ (kcal mol^{-1})	T_m (°C)
Core sequence 1				
ATGCGCAT[b]	62.0	171	9.3	54.3
$\underline{\text{A}}$ATGCGCAT[b]	64.6	175	10.2	60.9
$\underline{\text{A}^{\text{phe}}}$ATGCGCAT[b]	53.9	138	11.1	72.5
$\underline{\text{A}^{\text{naph}}}$ATGCGCAT[b]	56.8	146	11.5	72.7
$\underline{\text{A}}$ATGCGCAT$\underline{\text{T}}$[b]	75.8	208	11.2	61.2
ATGCGCAT$\underline{\text{A}}$[b]	63.1	171	10.0	60.1
ATGCGCAT$\underline{\text{A}^{\text{phe}}}$[b]	56.2	148	10.1	64.1
ATGCGCAT$\underline{\text{A}^{\text{naph}}}$[b]	53.1	138	10.3	66.8
$\underline{\text{T}}$ATGCGCAT$\underline{\text{A}}$	73.6±2.8	203±9	10.7±0.2	59.8
$\underline{\text{C}}$ATGCGCAT	65.9±3.2	183±10	9.48±0.15	55.1
$\underline{\text{C}^{\text{phe}}}$ATGCGCAT	69.2±1.7	170±5	11.3±0.1	65.5
$\underline{\text{C}^{\text{naph}}}$ATGCGCAT	65.4±2.0	174±6	11.3±0.2	66.6
$\underline{\text{C}}$ATGCGCAT$\underline{\text{G}}$	74.3±2.7	206±8	10.9±0.3	59.9
ATGCGCAT$\underline{\text{C}}$	63.8±2.9	177±8	8.94±0.09	53.5
ATGCGCAT$\underline{\text{C}^{\text{phe}}}$	64.0±2.6	173±8	10.3±0.1	61.6
ATGCGCAT$\underline{\text{C}^{\text{naph}}}$	57.6±2.2	153±6	10.3±0.2	63.9
$\underline{\text{G}}$ATGCGCAT$\underline{\text{C}}$	73.0±4.8	203±15	10.3±0.2	57.3
Core sequence 2				
TGCGCA[b]	47.4	129	7.6	50.3
$\underline{\text{A}}$TGCGCA[b]	55.0	151	8.2	51.4
$\underline{\text{A}^{\text{phe}}}$TGCGCA	55.1±2.3	145±7	10.2±0.2	64.1
$\underline{\text{A}^{\text{naph}}}$TGCGCA	51.5±3.3	133±10	10.2±0.2	67.1
$\underline{\text{A}}$TGCGCA$\underline{\text{T}}$[b]	62.0	171	9.3	54.3
TGCGCA$\underline{\text{A}}$	48.2±4.0	132±12	7.39±0.25	47.6
TGCGCA$\underline{\text{A}^{\text{phe}}}$	48.6±3.4	131±11	7.96±0.16	53.0
TGCGCA$\underline{\text{A}^{\text{naph}}}$	46.7±2.6	126±8	7.77±0.10	50.9
$\underline{\text{T}}$TGCGCA$\underline{\text{A}}$	57.4±4.0	158±13	8.64±0.18	52.9
$\underline{\text{C}}$TGCGCA	57.1±3.4	159±10	7.66±0.13	48.1
$\underline{\text{C}^{\text{phe}}}$TGCGCA	57.3±6.0	154±9	9.49±0.09	59.0
$\underline{\text{C}^{\text{naph}}}$TGCGCA	52.6±3.0	140±9	9.35±0.18	61.5
$\underline{\text{C}}$TGCGCA$\underline{\text{G}}$	62.3±5.1	171±15	9.36±0.18	56.5
TGCGCA$\underline{\text{C}}$	37.8±2.8	98.6±9.0	6.92±0.19	49.5
TGCGCA$\underline{\text{C}^{\text{phe}}}$	55.7±2.0	151±6	8.49±0.16	53.1
TGCGCA$\underline{\text{C}^{\text{naph}}}$	54.4±2.9	148±9	8.78±0.15	54.1
$\underline{\text{G}}$TGCGCA$\underline{\text{C}}$	58.7±1.9	156±6	9.94±0.05	62.3

(Table S2 continued)

Sequence (5′ → 3′)	−ΔH° (kcal mol^{-1})	−ΔS° (cal mol^{-1}K^{-1})	−ΔG°$_{37}$ (kcal mol^{-1})	T_m (°C)
Core sequence 3				
GTGCGCAC	58.7±1.9	156±6	9.94±0.05	62.3
AGTGCGCAC	70.2±1.7	189±3	11.5±0.2	65.1
A^{phe}GTGCGCAC	65.7±2.8	171±8	12.7±0.2	74.0
A^{naph}GTGCGCAC	66.6±1.3	174±4	12.9±0.2	73.8
AGTGCGCACT	75.7±1.6	204±4	12.5±0.1	67.3
GTGCGCACA	71.9±1.7	194±5	11.9±0.1	66.3
GTGCGCACA^{phe}	68.4±2.7	184±8	11.5±0.2	65.6
GTGCGCACA^{naph}	67.0±3.1	178±9	11.9±0.3	68.5
TGTGCGCACA	72.2±2.5	193±7	12.5±0.1	69.1
CGTGCGCAC	69.2±1.7	188±5	10.9±0.1	62.1
C^{phe}GTGCGCAC	73.5±1.6	196±4	12.9±0.1	70.5
C^{naph}GTGCGCAC	71.6±2.3	190±7	12.8±0.2	71.3
CGTGCGCACG	79.8±2.1	214±6	13.5±0.2	70.7
GTGCGCACC	67.5±1.8	182±5	10.9±0.1	63.2
GTGCGCACC^{phe}	71.7±1.8	192±5	12.3±0.1	68.3
GTGCGCACC^{naph}	67.6±2.2	179±6	12.1±0.2	69.5
GGTGCGCACC	76.0±2.5	203±7	13.1±0.2	70.9
Core sequence 4				
CTGCGCAG	62.3±5.1	171±15	9.36±0.18	56.5
ACTGCGCAG	70.4±3.4	192±10	10.9±0.2	61.7
A^{phe}CTGCGCAG	67.9±2.9	179±9	12.4±0.2	71.3
A^{naph}CTGCGCAG	76.0±2.7	203±7	13.1±0.1	70.5
ACTGCGCAGT	82.2±2.0	225±6	12.3±0.2	64.0
CTGCGCAGA	65.9±1.9	180±6	10.3±0.1	59.5
CTGCGCAGA^{phe}	60.7±2.3	161±7	10.9±0.2	65.4
CTGCGCAGA^{naph}	66.4±3.1	178±9	11.2±0.2	64.8
TCTGCGCAGA	78.1±3.2	214±10	11.8±0.2	62.6
CCTGCGCAG	61.7±2.8	167±9	10.0±0.2	59.3
C^{phe}CTGCGCAG	76.6±2.2	207±6	12.5±0.2	66.6
C^{naph}CTGCGCAG	73.0±3.1	195±9	12.6±0.2	69.1
CCTGCGCAGG	78.3±2.0	212±6	12.7±0.2	67.5
CTGCGCAGC [c]	nd.	nd.	nd.	nd.
CTGCGCAGC^{phe}	58.5±3.6	155±10	10.4±0.3	64.0
CTGCGCAGC^{naph}	54.7±4.1	144±12	10.2±0.3	65.2
GCTGCGCAGC [c]	nd.	nd.	nd.	nd.

[a] Data was obtained using the buffer containing 1 M NaCl, 10 mM Na_2HPO_4 (pH 7.0), and 1 mM Na_2EDTA. T_m was calculated at 100 μM.

[b] Data are derived from the references 10 and 18.

[c] Parameters could not be determined because of the unusual melting behavior.

Table S3 Thermodynamic parameters of DNA duplexes forming 2 or 3 nucleotide dangling ends measured in 1 M NaCl–phosphate buffer[a]

Sequence (5′ → 3′)	$\Delta H°$ (kcal mol^{-1})	$\Delta S°$ (cal mol^{-1}K^{-1})	$\Delta G°_{37}$ (kcal mol^{-1})	T_m (°C)
$\underline{A_2}$ATGCGCAT [b]	-65.0	-176	-10.3	61.3
$\underline{A_3}$ATGCGCAT [b]	-65.5	-178	-10.4	60.4
$\underline{A^{phe}{}_2}$ATGCGCAT [b]	-63.5	-165	-12.2	72.8
$\underline{A^{phe}{}_3}$ATGCGCAT	-73.1±2.5	-194±7	-12.9±0.1	71.5
$\underline{A^{naph}{}_2}$ATGCGCAT [b]	-64.9	-168	-12.9	76.7
$\underline{A^{naph}{}_3}$ATGCGCAT	-78.6±2.2	-206±6	-14.6±0.3	76.7
$\underline{C_2}$ATGCGCAT	-68.0±3.1	-188±9	-9.63±0.07	56.3
$\underline{C_3}$ATGCGCAT	-72.2±3.5	-202±10	-9.62±0.05	54.9
$\underline{C^{phe}{}_2}$ATGCGCAT	-70.7±3.9	-191±12	-11.5±0.2	64.7
$\underline{C^{phe}{}_3}$ATGCGCAT	-64.8±2.9	-173±9	-11.1±0.2	65.6
$\underline{C^{naph}{}_2}$ATGCGCAT	-66.3±2.6	-178±7	-11.3±0.3	65.2
$\underline{C^{naph}{}_3}$ATGCGCAT	-62.2±1.7	-165±5	-11.3±0.3	67.0

[a] Melting curve was obtained with the buffer containing 1 M NaCl, 10 mM Na_2HPO_4 (pH 7.0), and 1 mM Na_2EDTA. T_m was calculated at 100 μM.
[b] Data are derived from the references 10 and 18.

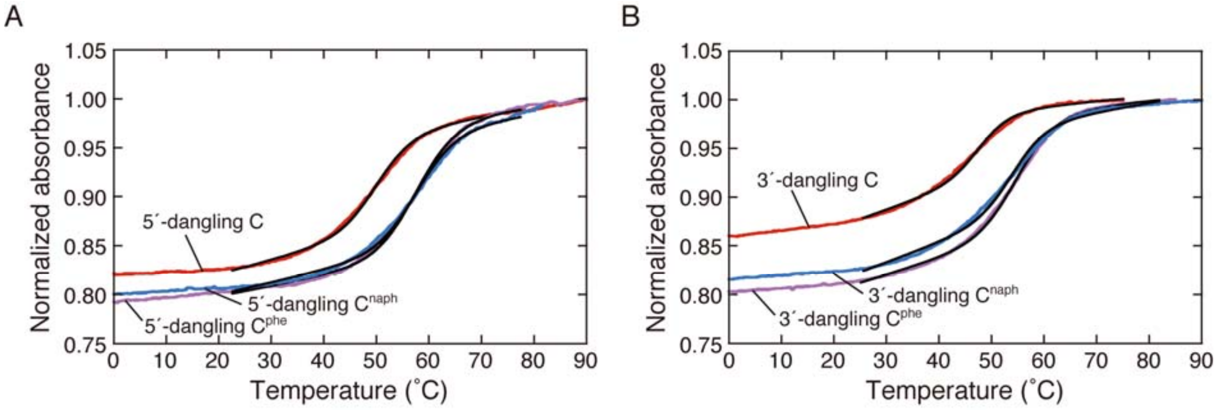

Fig. S1 Melting curve of the DNA duplexes forming a dangling end of C (red), C^{phe} (violet), or C^{naph} (blue) at the 5′ end (A) or the 3′ end (B) of the core sequence of ATGCGCAT, monitored at 260 nm. The curves were obtained with 10 μM DNA in 1 M NaCl–phosphate buffer. The fits to a two–state model are indicated in a black line.