

# Thermodynamic Coupling of the Loop and Stem in Unusually Stable DNA Hairpins Closed by CG Base Pairs

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Contents:

1. Thermodynamic parameters measured by UV melting<sup>a</sup>

Sequence	$\Delta H^\circ$ (kcal mol <sup>-1</sup> )	$\Delta S^\circ$ (cal mol <sup>-1</sup> K <sup>-1</sup> )	$\Delta G_{37}^\circ$ (kcal mol <sup>-1</sup> )	$T_M$ (°C)	$\Delta\Delta G_{37}^\circ$ (kcal mol <sup>-1</sup> )	$\Delta T_M$ (°C)
cGCAg	-33.0±1.3	-94.4±3.7	-3.69±0.12	76.1±0.7		
c(C3)GCAg	-30.6±3.4	-91.7±10.6	-2.12±0.10	60.3±1.5	1.57±0.16	-15.8±1.6
cG(C3)CAg	-31.3±2.0	-88.8±5.9	-3.71±0.18	78.8±1.1	-0.02±0.21	2.7±1.3
cGC(C3)Ag	-35.6±0.6	-102.5±2.3	-3.79±0.07	74.0±1.5	-0.10±0.13	-2.1±1.6
cGCA(C3)g	-36.0±0.9	-103.5±2.6	-3.92±0.09	74.9±0.2	-0.23±0.15	-1.2±0.7
cGCA(C3)(C3)g	-34.6±2.4	-103.4±7.6	-2.55±0.08	61.8±1.1	1.13±0.14	-14.3±1.3
cGCACg	-33.0±1.0	-97.0±3.0	-2.96±0.10	67.5±0.3		
c(C3)GCACg	-29.1±1.1	-89.7±3.2	-1.35±0.07	52.1±0.5	1.61±0.12	-15.4±0.6
cG(C3)CACg	-37.5±3.4	-110.2±10.2	-3.30±0.24	67.0±0.7	-0.34±0.26	-0.5±0.8
cGC(C3)ACg	-37.6±1.3	-111.7±4.0	-3.02±0.10	64.0±0.6	-0.05±0.15	-3.5±0.7
cGCA(C3)Cg	-32.7±5.5	-105.8±2.2	-2.39±0.07	59.6±0.3	0.57±0.13	-7.9±0.4
cGCAC(c3)g	-34.2±1.8	-102.8±5.3	-2.36±0.13	60.0±0.3	0.60±0.16	-7.5±0.4
c(2AP)CACg	-31.3±1.0	-94.6±3.7	-2.04±0.04	58.6±0.7	0.92±0.11	-8.9±0.7
c(DAP)CACg	-27.8±0.8	-83.6±2.6	-1.83±0.05	58.9±0.5	1.13±0.11	-8.6±0.6
gGCACc	-26.5±1.0	-82.0±2.9	-1.08±0.12	50.2±1.4		
g(C3)GCACc	-24.1±0.5	-75.1±1.7	-0.85±0.11	48.3±1.7	0.23±0.16	-1.9±2.2
gG(C3)CACc	-32.3±1.4	-98.0±4.2	-1.88±0.08	56.2±0.5	-0.80±0.14	6.0±1.5
gGC(C3)ACc	-29.6±0.5	-91.0±1.6	-1.43±0.04	52.7±0.5	-0.34±0.12	2.5±1.5
gGCA(C3)Cc	-27.8±1.6	-86.4±4.9	-1.04±0.15	49.0±1.4	0.05±0.19	-1.2±2.0
gGCAC(C3)c	-30.5±3.3	-95.2±10.7	-0.99±0.04	47.6±1.4	0.09±0.13	-2.7±2.0
g(2AP)CACc	-22.0±1.7	-69.4±5.6	-0.44±0.09	43.5±1.6	0.64±0.15	6.7±2.1
g(DAP)CACc	-15.3±3.2	-48.4±10.0	-0.29±0.11	43.0±2.3	0.79±0.16	-7.2±2.6
gGCAc	-14.4±2.4	-44.5±7.6	-0.63±0.38	51.3±8.9		
g(C3)GCAc	-24.5±1.5	-75.8±4.9	-0.94±0.06	49.5±1.5	-0.31±0.39	-1.8±9.1
gG(C3)CAc	-17.9±2.1	-55.7±6.3	-0.62±0.19	48.1±3.0	0.01±0.42	-3.2±9.4
gGC(C3)Ac	-16.3±3.8	-51.6±11.5	-0.42±0.36	41.8±4.3	0.22±0.53	-9.5±9.9
gGCA(C3)c	-31.5±1.3	-95.0±3.9	-2.01±0.09	58.2±0.81	-1.38±0.39	6.9±9.0
tGCACa	-28.8±0.6	-88.6±1.3	-1.34±0.22	52.1±2.3		
t(C3)GCACa	-18.6±4.1	-57.2±3.5	-0.78±0.17	51.3±4.9	0.56±0.28	-0.9±5.4
tGCAC(C3)a	-30.7±1.2	-95.3±4.0	-1.15±0.17	48.9±2.2	0.19±0.28	-3.2±3.1
aGCAcT	-21.3±3.2	-66.8±10.5	-0.58±0.17	45.7±2.9		
a(C3)GCAcT	-24.2±1.0	-77.2±3.5	-0.30±0.08	40.9±1.2	0.28±0.19	-4.8±3.2
aGCAC(C3)t	-19.9±1.3	-63.8±4.0	-0.10±0.14	38.5±2.6	0.49±0.22	-7.2±3.9

<sup>a</sup> Solutions were P<sub>10</sub>E<sub>0.1</sub> (pH 7.0). Parameters are the average of at least three independently prepared samples between 1 and 60 μM C<sub>T</sub>, and errors are standard deviations. The T<sub>M</sub> was constant between 1 and 60 μM C<sub>T</sub>. Experiments were carried out as described in the main paper.  $\Delta\Delta G_{37}^\circ$  values are referenced to the entry at the top of each grouping. All sequences are DNA.