

**Supplementary Material Table 1.** Nearest neighbor parameters for oligonucleotides in 1M NaCl

Sequence	$\Delta H$ (kcal/mol)	$\Delta S$ (cal/k·mol)	$\Delta G_{37}$ (kcal/mol)	reference
AA/TT	-7.9	-22.2	-1 <sup>1</sup>	(1)
AT/TA	-7.2	-20.4	-0.88 <sup>1</sup>	(1)
TA/AT	-7.2	-21.3	-0.58 <sup>1</sup>	(1)
CA/GT	-8.5	-22.7	-1.45 <sup>1</sup>	(1)
GT/CA	-8.4	-22.4	-1.44 <sup>1</sup>	(1)
CT/GA	-7.8	-21	-1.28 <sup>1</sup>	(1)
GA/CT	-8.2	-22.2	-1.3 <sup>1</sup>	(1)
CG/GC	-10.6	-27.2	-2.17 <sup>1</sup>	(1)
GC/CG	-9.8	-28.2	-2.24 <sup>1</sup>	(1)
GG/CC	-8	-19.9	-1.84 <sup>1</sup>	(1)
AA/TA	1.2	1.91	0.61	(2)
CA/GA	-0.9	-4.29	0.43	(2)
GA/CA	-2.9	-9.9	0.17	(2)
TA/AA	4.7	12.93	0.69	(2)
AC/TC	0	-4.29	1.33	(2)
CC/GC	-1.5	-7.1	0.7	(2)
GC/CC	3.6	9.07	0.79	(2)
TC/AC	6.1	16.29	1.05	(2)
AG/TG	-3.1	-9.58	-0.13	(2)
CG/GG	-4.9	-15.45	-0.11	(2)
GG/CG	-6	-15.77	-1.11	(2)

TG/AG	-1.6	-6.58	0.44	(2)
AT/TT	-2.7	-10.94	0.69	(2)
CT/GT	-5	-15.74	-0.12	(2)
GT/CT	-2.2	-8.55	0.45	(2)
TT/AT	0.2	-1.55	0.68	(2)
AA/TC	2.3	4.6	0.88	(3)
AC/TA	5.3	14.6	0.77	(3)
CA/GC	1.9	3.7	0.75	(3)
CC/GA	0.6	-0.6	0.79	(3)
GA/CC	5.2	14.2	0.81	(3)
GC/CA	-0.7	-3.8	0.47	(3)
TA/AC	3.4	8	0.92	(3)
TC/AA	7.6	20.2	1.33	(3)
AC/TT	0.7	0.2	0.64	(4)
AT/TC	-1.2	-6.2	0.73	(4)
CC/GT	-0.8	-4.5	0.62	(4)
CT/GC	-1.5	-6.1	0.4	(4)
GC/CT	2.3	5.4	0.62	(4)
GT/CC	5.2	13.5	0.98	(4)
TC/AT	1.2	0.7	0.97	(4)
TT/AC	1	0.7	0.75	(4)
AA/TG	-0.6	-2.3	0.14	(5)
AG/TA	-0.7	-2.3	0.02	(5)

CA/GG	-0.7	-2.3	0.03	(5)
CG/GA	-4	-13.2	0.11	(5)
GA/CG	-0.6	-1	-0.25	(5)
GG/CA	0.5	3.2	-0.52	(5)
TA/AG	0.7	0.7	0.42	(5)
TG/AA	3	7.4	0.74	(5)
AG/TT	1	0.9	0.71	(6)
AT/TG	-2.5	-8.3	0.07	(6)
CG/GT	-4.1	-11.7	-0.47	(6)
AT/GG	-2.8	-8	-0.32	(6)
GG/CT	3.3	10.4	0.08	(6)
GG/TT	5.8	16.3	0.74	(6)
GT/CG	-4.4	-12.3	-0.59	(6)
GT/TG	4.1	9.5	1.15	(6)
TG/AT	-0.1	-1.7	0.43	(6)
TG/GT	-1.4	-6.2	0.52	(6)
TT/AG	-1.3	-5.3	0.34	(6)
Initiate w/ terminal G·C	0.1	-2.8	0.98 <sup>1</sup>	(1)
Initiate w/ terminal A·T	2.3	4.1	1.03 <sup>1</sup>	(1)
Symmetric Correction	0	-1.4	0.4 <sup>1</sup>	(1)

---

<sup>1</sup>Calculated from  $\Delta G_T^o = \Delta H^o - T\Delta S^o$ .

## REFERENCES

1. SantaLucia, J., Jr. (1998) A unified view of polymer, dumbbell, and oligonucleotide DNA nearest-neighbor thermodynamics. *Proc. Natl. Acad. Sci. USA*, **95**, 1460-1465.
2. Peyret, N., Seneviratne, P.A., Allawi, H.T. and SantaLucia, J., Jr. (1999) Nearest-neighbor thermodynamics and NMR of DNA sequences with internal A.A, C.C, G.G, and T.T mismatches. *Biochemistry*, **38**, 3468-3477.
3. Allawi, H.T. and SantaLucia, J., Jr. (1998) Nearest-neighbor thermodynamics of internal A.C mismatches in DNA: sequence dependence and pH effects. *Biochemistry*, **37**, 9435-9444.
4. Allawi, H.T. and SantaLucia, J., Jr. (1998) Thermodynamics of internal C.T mismatches in DNA. *Nucl. Acids Res.*, **26**, 2694-2701.
5. Allawi, H.T. and SantaLucia, J., Jr. (1998) Nearest neighbor thermodynamic parameters for internal G.A mismatches in DNA. *Biochemistry*, **37**, 2170-2179.
6. Allawi, H.T. and SantaLucia, J., Jr. (1997) Thermodynamics and NMR of internal G.T mismatches in DNA. *Biochemistry*, **36**, 10581-10594.