

TABLE 2. Enthalpic (kcal/mol) and entropic (cal/mol·K) nearest-neighbor parameters for matches and single-nucleotide mismatches at 37°C and $[\text{Na}^+] = 1.0 \text{ M}$ compiled by J. SantaLucia Jr.

Nucleotide matches			Single nucleotide mismatches														
NN Pair	ΔH	ΔS	NN Pair	ΔH	ΔS	NN Pair	ΔH	ΔS	NN Pair	ΔH	ΔS	NN Pair	ΔH	ΔS	NN Pair	ΔH	ΔS
AA / TT	-7.9	-22.2	AA / TA	1.2	1.7	GG / CG	-6.0	-15.8	GA / CG	-0.6	-1.0	TA / AC	3.4	8.0	AG / TT	1.0	0.9
AT / TA	-7.2	-20.4	CA / GA	-0.9	-4.2	TG / AG	1.6	3.6	GG / CA	0.5	3.2	TC / AA	7.6	20.2	AT / TG	-2.5	-8.3
TA / AT	-7.2	-21.3	GA / CA	-2.9	-9.8	AT / TT	-2.7	-10.8	TA / AG	0.7	0.7	AC / TT	0.7	0.2	CG / GT	-4.1	-11.7
CA / GT	-8.5	-22.7	TA / AA	4.7	12.9	CT / GT	-5.0	-15.8	TG / AA	3.0	7.4	AT / TC	-1.2	-6.2	CT / GG	-2.8	-8.0
GT / CA	-8.4	-22.4	AC / TC	0.0	-4.4	GT / CT	-2.2	-8.4	AA / TC	2.3	4.6	CC / GT	-0.8	-4.5	GG / CT	3.3	10.4
CT / GA	-7.8	-21.0	CC / GC	-1.5	-7.2	TT / AT	0.2	-1.5	AC / TA	5.3	14.6	CT / GC	-1.5	-6.1	GT / CG	-4.4	-12.3
GA / CT	-8.2	-22.2	GC / CC	3.6	8.9	AA / TG	-0.6	-2.3	CA / GC	1.9	3.7	GC / CT	2.3	5.4	TG / AT	-0.1	-1.7
CG / GC	-10.6	-27.2	TC / AC	6.1	16.4	AG / TA	-0.7	-2.3	CC / GA	0.6	-0.6	GT / CC	5.2	13.5	TT / AG	-1.3	-5.3
GC / CG	-9.8	-24.4	AG / TG	-3.1	-9.5	CA / GG	-0.7	-2.3	GA / CC	5.2	14.2	TC / AT	1.2	0.7			
GG / CC	-8.0	-19.9	CG / GG	-4.9	-15.3	CG / GA	-4.0	-13.2	GC / CA	-0.7	-3.8	TT / AC	1.0	0.7			

Average values for double mismatches (1): $\Delta H = 2.8 \text{ kcal/mol}$, $\Delta S = 6.5 \text{ cal/mol}\cdot\text{K}$.

Average values for initiation cost (2): $\Delta H = 2.4 \text{ kcal/mol}$, $\Delta S = 1.3 \text{ cal/mol}\cdot\text{K}$.

Average values for dangling ends contribution (3): $\Delta H = -2.5 \text{ kcal/mol}$, $\Delta S = -7.0 \text{ cal/mol}\cdot\text{K}$.

Sodium concentration correction for N -nucleotide duplex (2): $\Delta S = (0.368 \text{ cal/mol}\cdot\text{K}) \cdot N \cdot \ln [\text{Na}^+]$.

References:

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3. Bommarito, S., Peyret, N., & SantaLucia, J., Jr. (2000) *Nucleic Acids Res.* **28**, 1929–1934.