

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:

1. Allawi, H.T. & SantaLucia, J., Jr. (1997) *Biochemistry* **36**, 10581–10594.
2. SantaLucia, J., Jr. (1998) *Proc. Natl. Acad. Sci. USA* **95**, 1460–1465.
3. Bommarito, S., Peyret, N., & SantaLucia, J., Jr. (2000) *Nucleic Acids Res.* **28**, 1929–1934.

TABLE 3. Comparison of melting temperature predictions for different duplexes of fragmented subtilisin E gene between the proposed model and $T_m = 81.5 + 0.41(\% GC) - 500/L + 16.6 \log [\text{Na}^+]$.

Sequence positions	Overlap length	Percent GC	Melting temperature ($^{\circ}\text{C}$)	
			Annealing model	Howley <i>et al.</i> (1)
819-828	10	50	26	30
1013-1022	10	30	17	22
529-538	10	60	32	35
804-828	25	52	61	61
779-828	50	50	72	71
729-828	100	55	81	78

Data shown is for $[\text{Na}^+] = 0.05 \text{ M}$ and an initial template mole fraction $x_A^0 = 2.7 \times 10^{-8}$ that corresponds to a DNA concentration of 10 mg/liter, typical for DNA shuffling.

References:

1. Howley, P.M., Israel, M.F., Law, M., & Martin, M.A. (1979) *J. Biol. Chem.* **254**, 4876–4883.

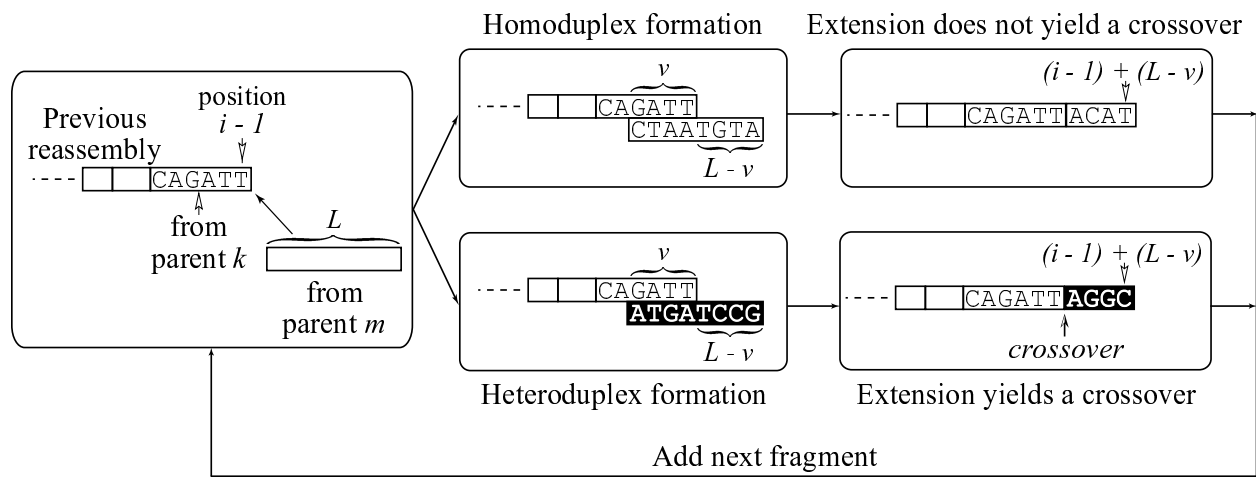


FIGURE 6