Thermodynamic stability and folding kinetics of the major G-quadruplex and its loop-isomers formed in the Nuclease Hypersensitive Element in the human c-Myc promoter

-Effect of loops and flanking segments on the stability of parallel-stranded intramolecular G-quadruplexes

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SUPPORTING INFORMATION

TITLE RUNNING HEAD: Stability and kinetics of c-Myc promoter G4 loop-isomers

Table S1. ΔG_{25} values for the c-Myc G-quadruplex loop-isomers formed by the extended and truncated DNA sequences, determined in the presence of 10 mM Li_3PO_4 (pH=7) containing different concentrations of K^+. The same experiment conditions as described for Table 2 were used.

	ΔG_{25} (kJ/mol)	**ΔG_{25}** (kJ/mol)	**ΔG_{25}** (kJ/mol)	**ΔG_{25}** (kJ/mol)
DNA\[K^+]	**2mM**	**5mM**	**10mM**	**20mM**
14/23	-14.8	-20.08	-23.58	-29.98
11/23	-12.59	-15.03	-19.84	-25.43
14/20	-11.40	-15.00	-16.86	-22.93
11/20	-7.12	-9.16	-11.80	-16.98
T14/23T	-16.20	-19.40	-20.62	-24.72
T11/23T	-13.19	-17.35	-18.87	-24.16
T14/20T	-11.71	-16.19	-19.28	-21.45
T11/20T	-8.70	-13.70	-16.11	-19.19

Figure legends

Figure S1. Hysteresis was observed between CD melting (black) and annealing (red) curves of 11/20 with a temperature gradient of 0.5 °C/min. The presence of hysteresis between melting and annealing profiles indicates the molecule is not at thermodynamic equilibrium during melting and annealing processes. Conditions: 10 mM Li_3PO_4 (pH=7), 2 mM [K^+].

Figure S2. The imino regions of 1D ^{1}H NMR spectra of the completely truncated sequences for the four loop-isomers of the major c-Myc G-quadruplex. The DNA sequences of 14/23TR, 11/23TR, 14/20TR, 11/20TR are shown at the bottom. The completely truncated sequences did not show good quality ^{1}H NMR spectra. Experimental conditions: 25°C, 30 mM K^+-phosphate, 70 mM KCl, pH 7.0, 0.2 mM DNA.

Figure S3. The CD melting (red) and annealing (black) curves of 11/20 and 11/23 loop-isomers with different temperature gradients. Hysteresis between the melting and annealing curves were observed for 11/20 (A) and 11/23 (B) with temperature gradients of 2 °C/min (upper) and 4 °C/min (lower). A higher level of hysteresis was observed for 11/20 as compared to 11/23. Conditions: 10 mM Li_3PO_4 (pH=7), 2 mM [K^+].

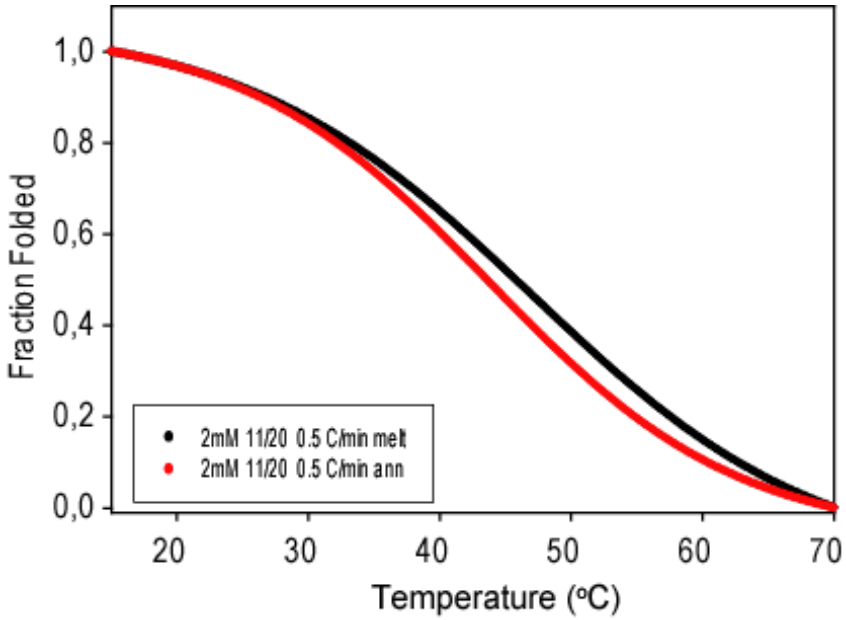
1,0
0,8
0,6
0,4
0,2
0,0
Fraction Folded
2mM 11/20 0.5 C/min melt
2mM 11/20 0.5 C/min ann
20
30
40
50
60
70
Temperature (°C)

Figure S1.

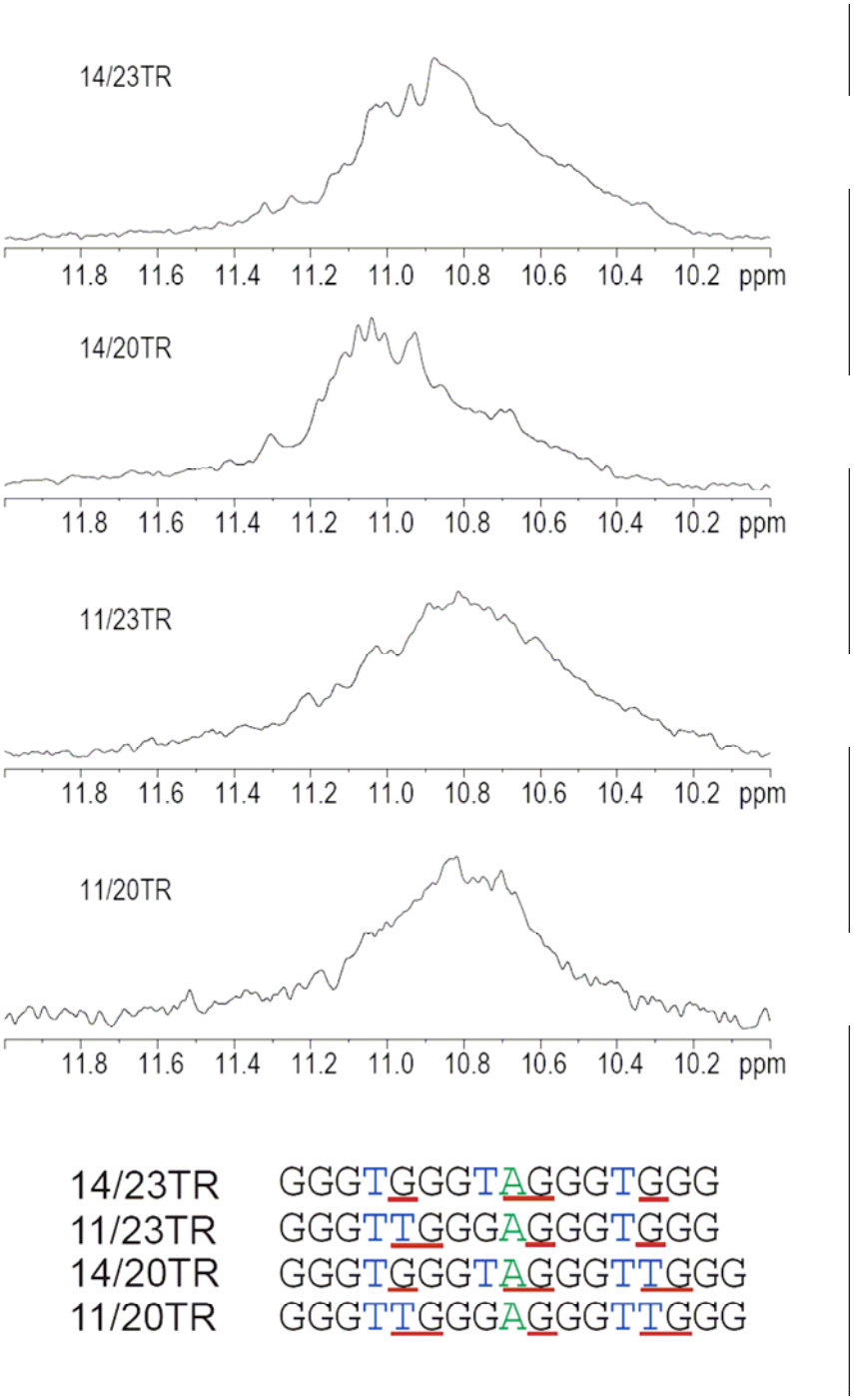
14/23TR
11.8 11.6 11.4 11.2 11.0 10.8 10.6 10.4 10.2 ppm
14/20TR
11.8 11.6 11.4 11.2 11.0 10.8 10.6 10.4 10.2 ppm
11/23TR
11.8 11.6 11.4 11.2 11.0 10.8 10.6 10.4 10.2 ppm
11/20TR
11.8 11.6 11.4 11.2 11.0 10.8 10.6 10.4 10.2 ppm
14/23TR GGGTGGGTAGGGTGGG
11/23TR GGGTTGGGAGGGTGGG
14/20TR GGGTGGGTAGGGTTGGG
11/20TR GGGTTGGGAGGGTTGGG

Figure S2.

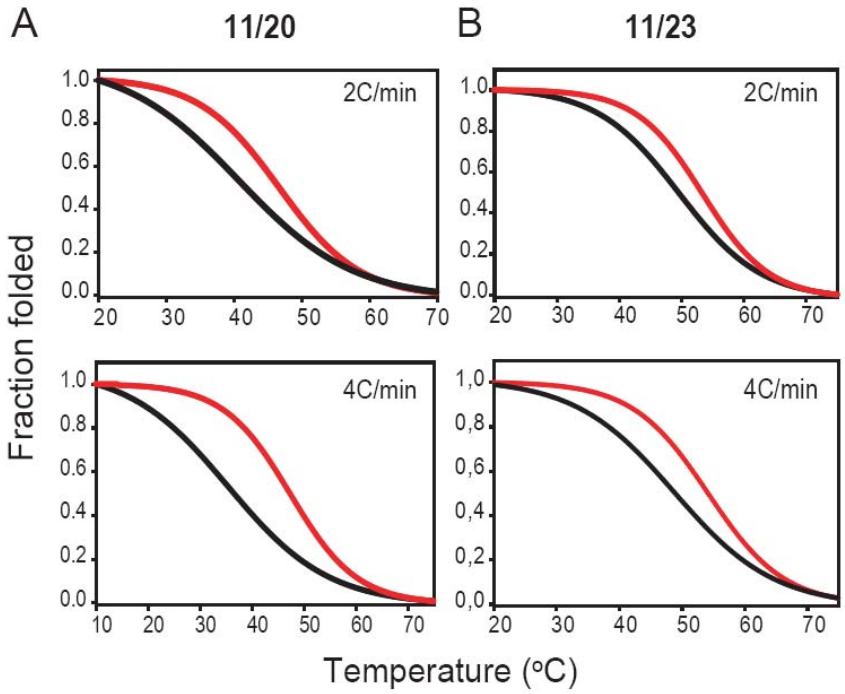
A
11/20
B
11/23
2C/min
2C/min
4C/min
4C/min
Fraction folded
Temperature (°C)

Figure S3.