Structural features of intra- and intermolecular G-quadruplexes derived from telomeric repeats

Supplementary material

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Figure S1: CD and UV spectra of *d(G$_4$T$_2$)$_3$G$_4$* sequence. Spectra were collected at various temperatures in Britton-Robinson buffer supplemented by 200 mM KCl, pH 7.0. The temperatures of collection are 30, 40, 50, 60, 70, 80, 90 and 100°C (direction of heating is marked by arrows). The isosbestic point is observed for stable oligomer and reversible G-quadruplexes at ~ 289 nm (circle).

Figure S2: CD spectra collected at increments of 10 °C during the melting profile measurements. Absorbance at 257 nm at the last scan of spectra is displayed in each panel.

Figure S3: The same gel as in Fig. 2c stained twice with silver. The second staining clearly demonstrates that each oligomer folds into more conformers. Electrophoresis was performed at 20°C.

Figure S4: Electrophoretic separation under the same conditions as was used in the experiment shown in Fig. 2, but the temperature of electrophoretic gel was adjusted with circulating water to 55 °C.

Figure S5: CD and UV melting profiles of G_4T_2 oligomer. The melting curves were obtained with CD spectroscopy at 265 (red line) and 295 nm (black line) and by UV spectroscopy at 295 nm (blue line). Melting curves of G_4T_2 are biphasic. Both UV and CD melting curves at 295 nm display two clear transitions highlighted by arrows and two filled quadrants. The first transition corresponds to the conversion of intramolecular conformers to parallel forms; the band in Figure 2b marked with an asterisk disappears with an increase in temperature. This fact also supports the increase of the CD signal at 265 nm around the temperature where the transformation was observed. Very poor reversibility was observed during sample cooling probably due to the slow kinetic of the formation of anti-parallel conformers. Nevertheless, the second measurement of the melting curve immediately after the first scan practically copies the reversible curves obtained at both wavelengths with CD and 295 nm with UV collections. The second heating and cooling process achieves a reversibility of about 95 %. The third scan was the same as the second one (not shown).

Figure S6: Electrophoresis of G3X and G4X series under the same conditions as in the results depicted in Fig.2a, but polyacrylamide gel contains an additional 30 % PEG 200.

Figure S7: Representative illustration of electrophoretic data evaluation. The projection of objective electrophoretic record is depicted on the x-y plane, and the intensity of the DNA sample on the z-axis. The connection of the most intensive points represents an objective melting curve for the evaluation of thermodynamic parameters.

Figure S8: The demonstration of curve fitting of normalized UV (right) and CD (left) melting curves of G4T2 in the presence of 50 mM KCl and 50 mM NaCl. Pre- and post-unfolding baselines into transition region, $Y_f(T) = Y_f(T_0) + A_f.T$ and $Y_u(T) = Y_u(T_0) + B_f.T$, are represented by the dotted lines. The baseline of intermediate, $Y_i(T) = Y_i(T_0) + C_i.T$ is clearly recognized for biphasic transitions (BC). Non-sigmoidal curve (NS) represents UV measurement in 50 mM KCl at 263 nm. An ideal sigmodial curve representing a two-state mechanism of unfolding is obtained in 50 mM NaCl.

Figure S1.

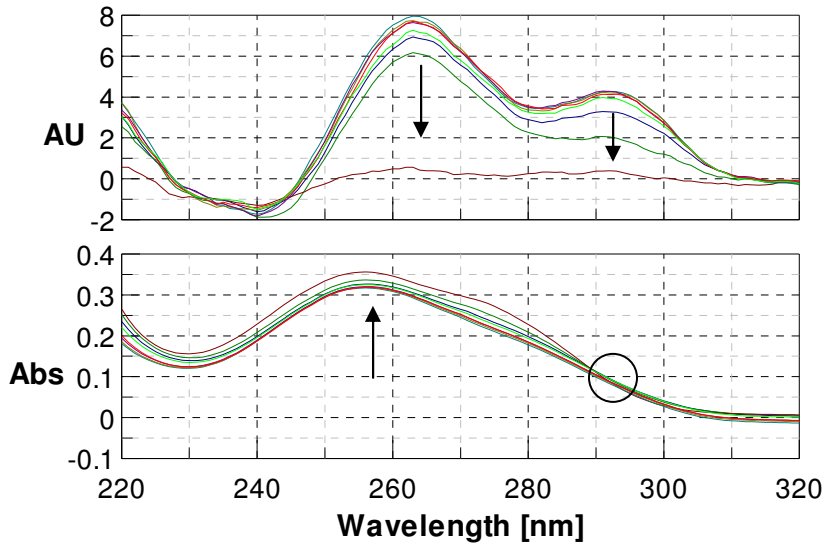

Table S1: Detection of isoelliptic (isodichroic) points in Fig. S2.

50 mM	LiCl	NaCl	KCl
G_3T	+++	+++	+++
G_3T_2	--	+	+++
G_3T_3	--	+++	+
G_3T_2A	-	++	++
G_4T_2	++	+	+
G_4T_3	--	++	++
G_4T_2A	+++	+++	-
G_4T_4	+++	+++	--

The level of the best fitting isoeliptic points is marked by the following labels: (+++), (++), (+), (-) and (--). The best and worst cases are designated by (+++) and (--), respectively.

Figure S2.

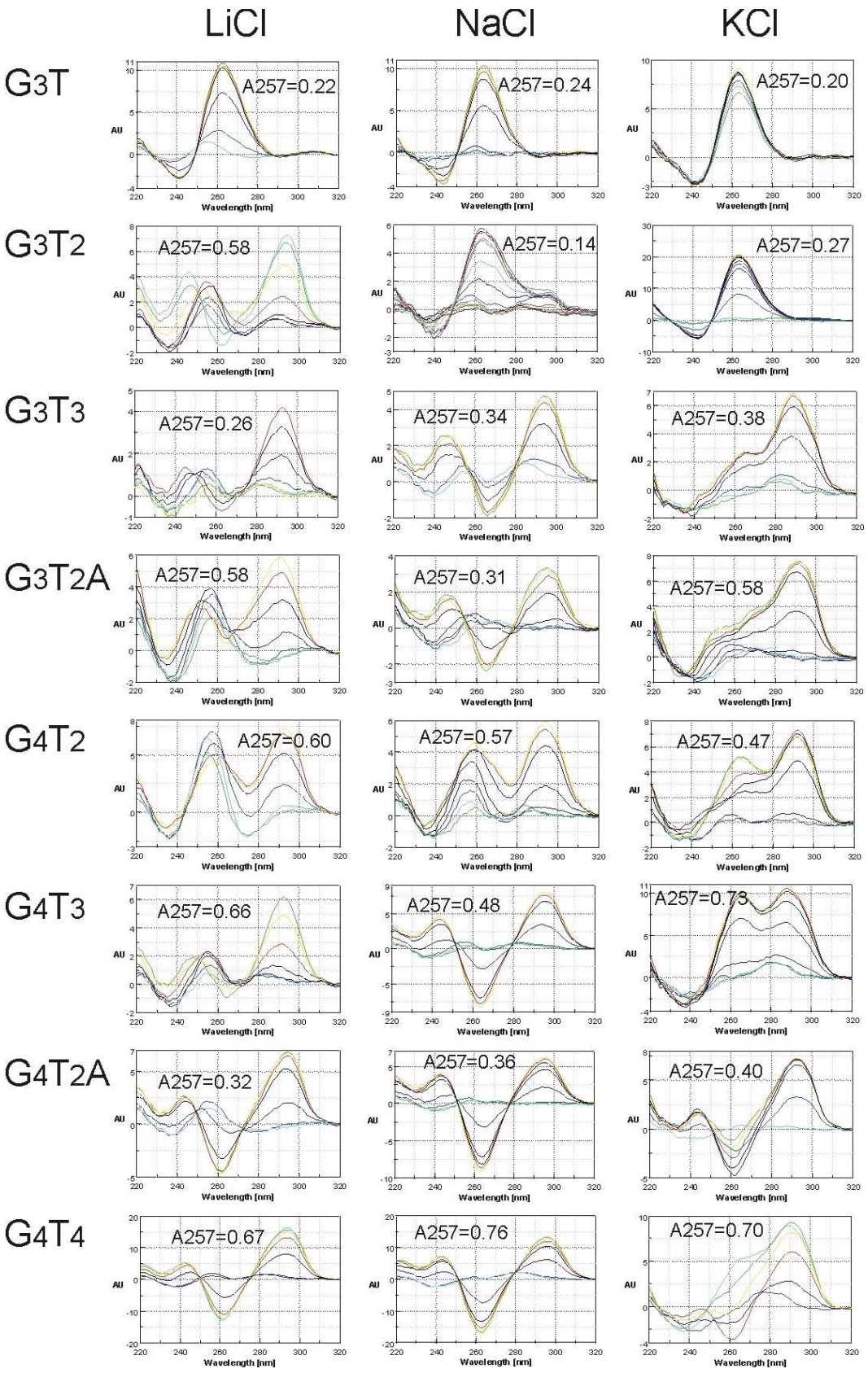
LiCl
NaCl
KCl
G3T
A257=0.22
A257=0.24
A257=0.20
G3T2
A257=0.58
A257=0.14
A257=0.27
G3T3
A257=0.26
A257=0.34
A257=0.38
G3T2A
A257=0.58
A257=0.31
A257=0.58
G4T2
A257=0.60
A257=0.57
A257=0.47
G4T3
A257=0.66
A257=0.48
A257=0.73
G4T2A
A257=0.32
A257=0.36
A257=0.40
G4T4
A257=0.67
A257=0.76
A257=0.70
AU
Wavelength [nm]

Figure S3

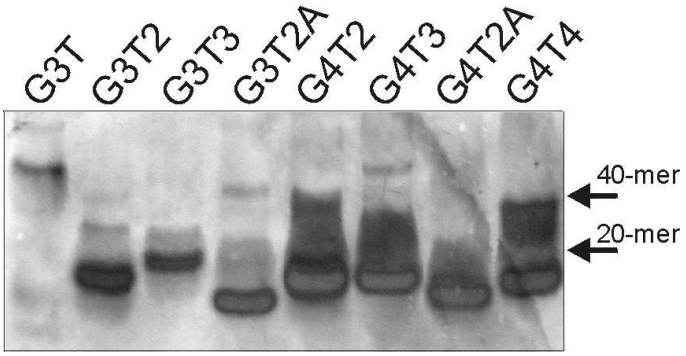

Figure S4

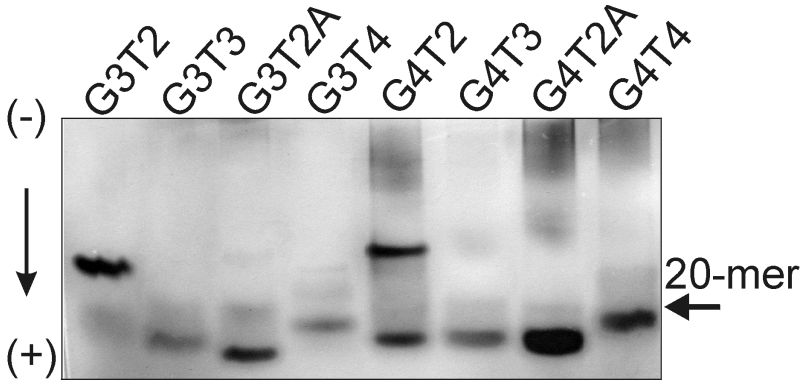

Figure S5

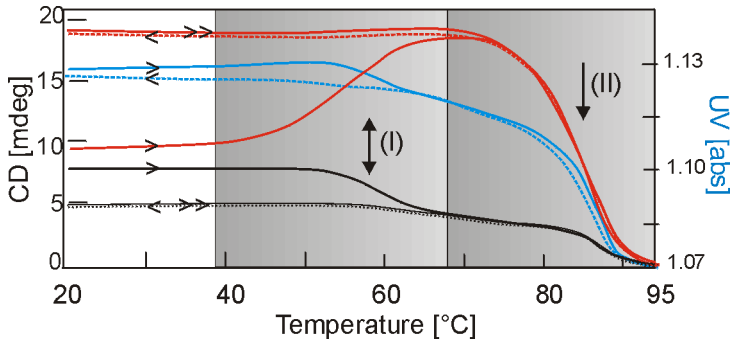

Figure S6

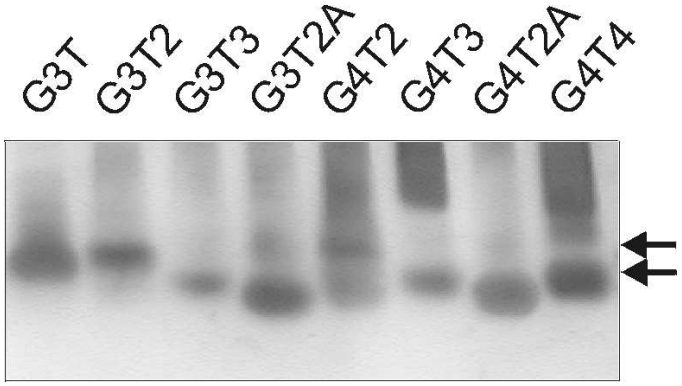

Figure S7

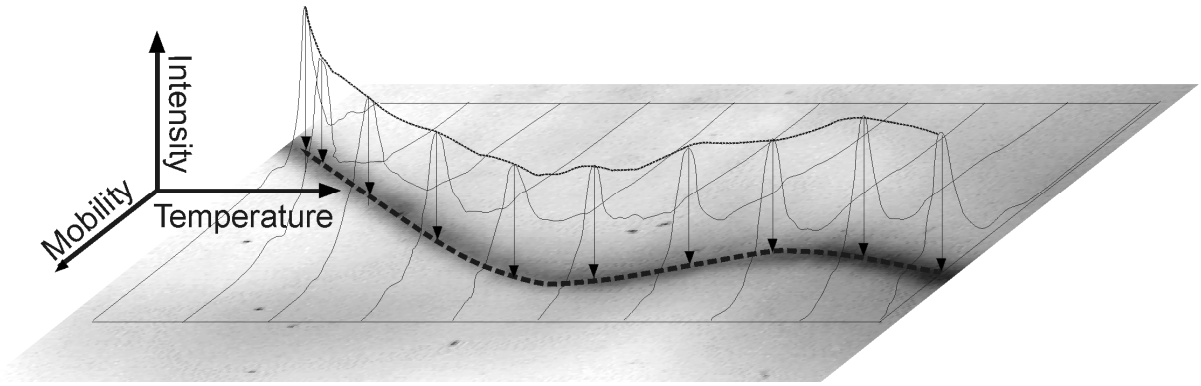

Figure S8