

**Structure of the intramolecular human telomeric G-quadruplex in potassium solution: A novel adenine triple formation.**

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**Supplementary Information**

## Figure Legends.

**Figure S1.** Imino proton assignments of Tel26 using 1D  $^{15}\text{N}$ -filtered experiments on site-specific labeled oligonucleotides. Conditions: 25 mM K-PO<sub>4</sub>, 70 mM KCl, pH 7.0, 25 °C, 0.6-0.7 mM DNA.

**Figure S2.** (A). Determination of stoichiometry by NMR titration for Tel26 in K<sup>+</sup> solution (42). The slope of the fitted line is about 1, meaning that the quadruplex structure that exists in solution is unimolecular. The peak intensities of two resolved peaks at 55 °C (one belonging to the melted, one to the folded forms of Tel26) were used for the calculation. (B). The 1D  $^1\text{H}$  NMR spectra of Tel26 at 0.6 mM and 2.5 mM strand concentrations at 25 °C. Conditions: 25 mM K-PO<sub>4</sub>, 70 mM KCl, pH 7.0.

**Figure S3.** The expanded H8/H6-H1' region with assignments of the non-exchangeable 2D-NOESY spectrum of Tel26. The sequential assignment pathway is shown. Missing connectivities are labeled with asterisks. The H8-H1' NOEs of the *syn* guanines are labeled in red. Conditions: 25 °C, 25 mM K-PO<sub>4</sub>, 70 mM KCl, pH 7.0, 2.5 mM DNA.

**Figure S4.** The expanded H1-H1 region of the exchangeable proton 2D JR-NOESY spectrum of Tel26 in K<sup>+</sup> solution at 1 °C. NOEs are labeled as following: *intra-tetrad NOEs are labeled in green, inter-tetrad NOEs are labeled in blue, sequential NOEs are labeled in black.* Conditions: 1 °C, 25 mM K-PO<sub>4</sub>, 70 mM KCl, pH 7.0, 2.5 mM DNA.

**Figure S5.** Stacking interactions between (A) the top (cyan) and middle (magenta) G-tetrads, which have reversed *syn:syn:anti:syn* and *anti:anti:syn:anti* guanine arrangements, and (B) the middle (magenta) and bottom (blue) G-tetrads, which have the same *anti:anti:syn:anti* G-arrangements.

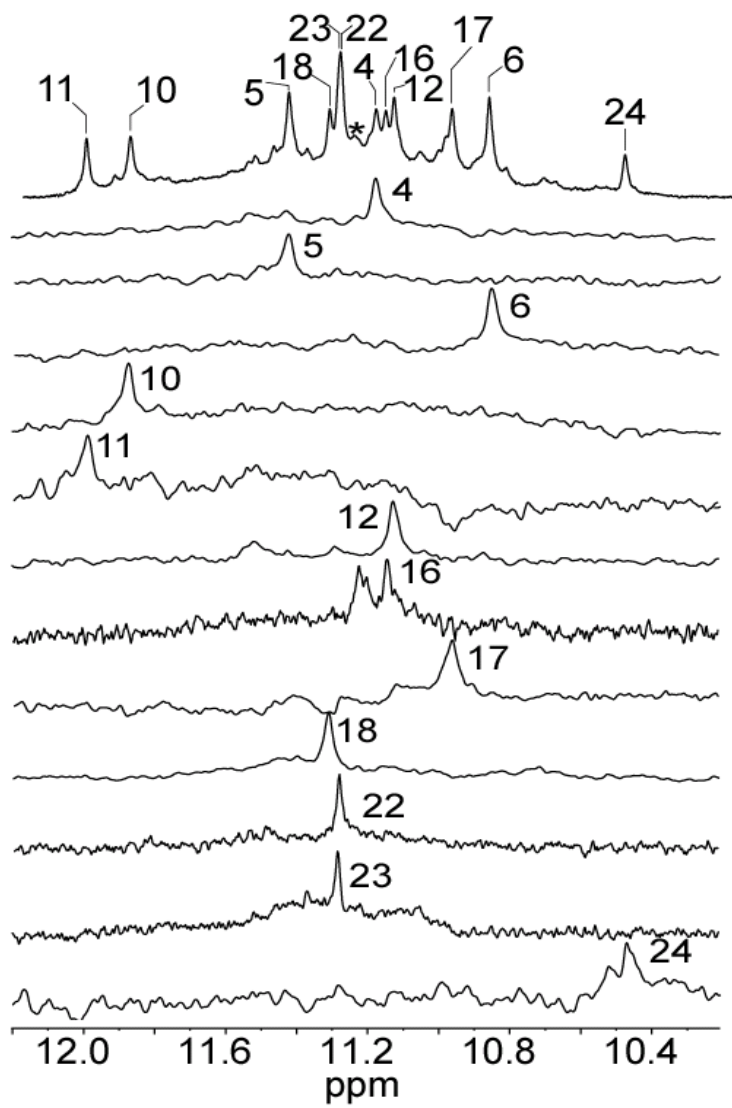
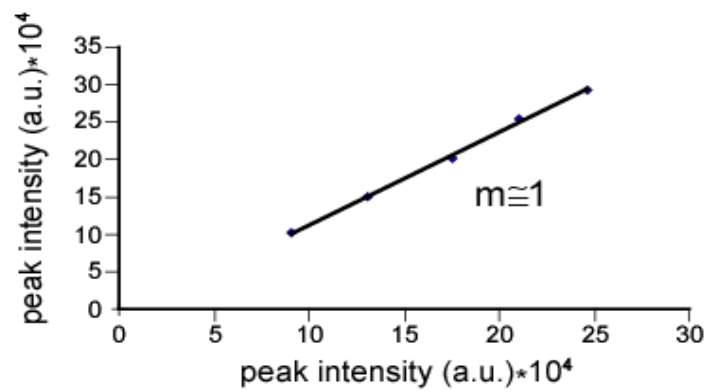


Figure S1.

A



B

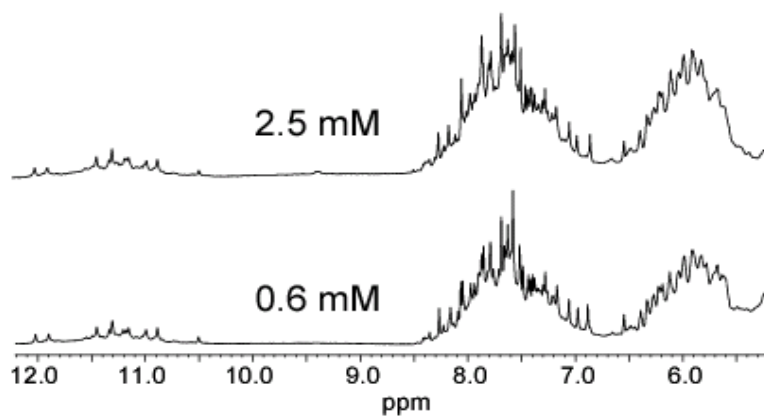


Figure S2.

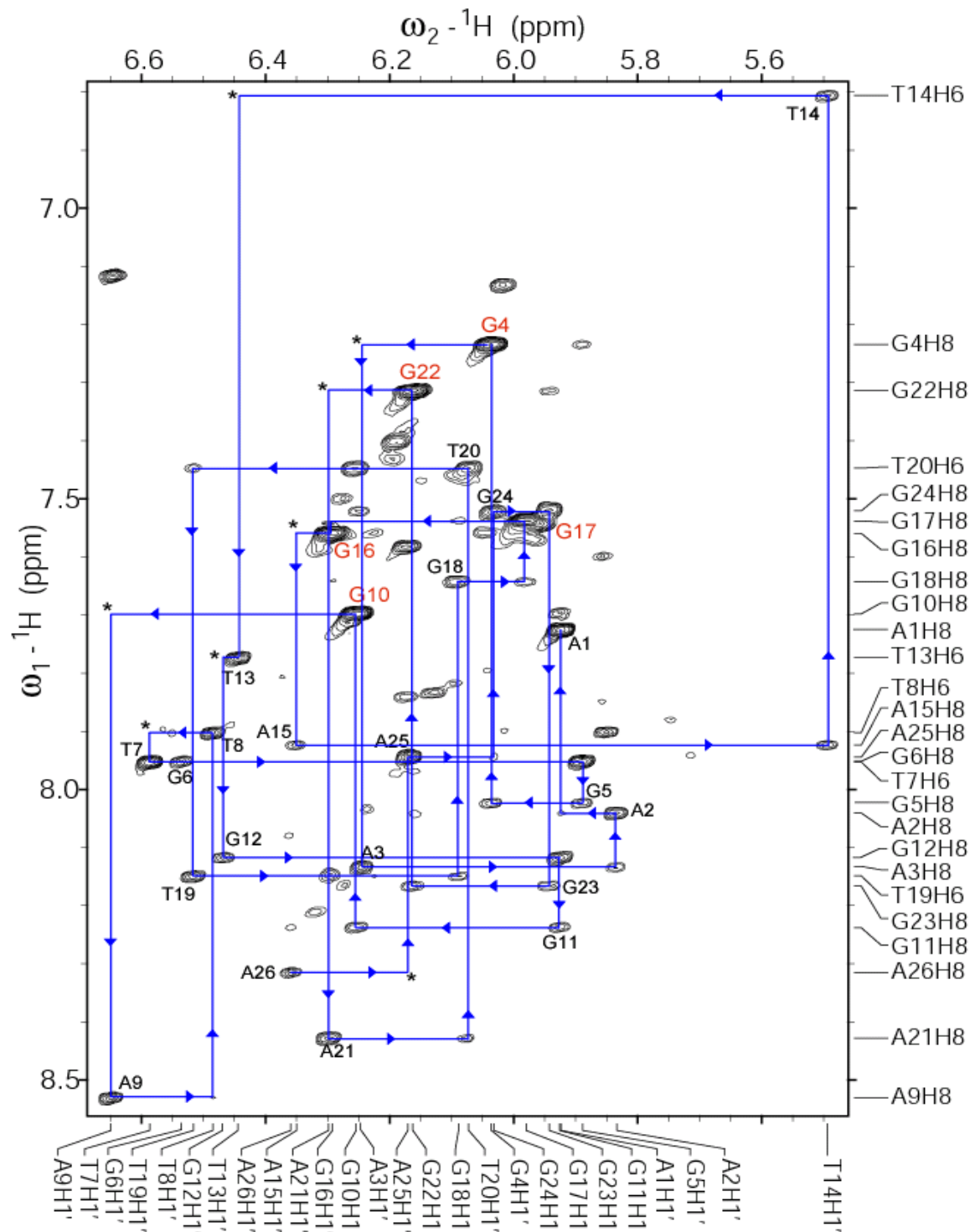


Figure S3.

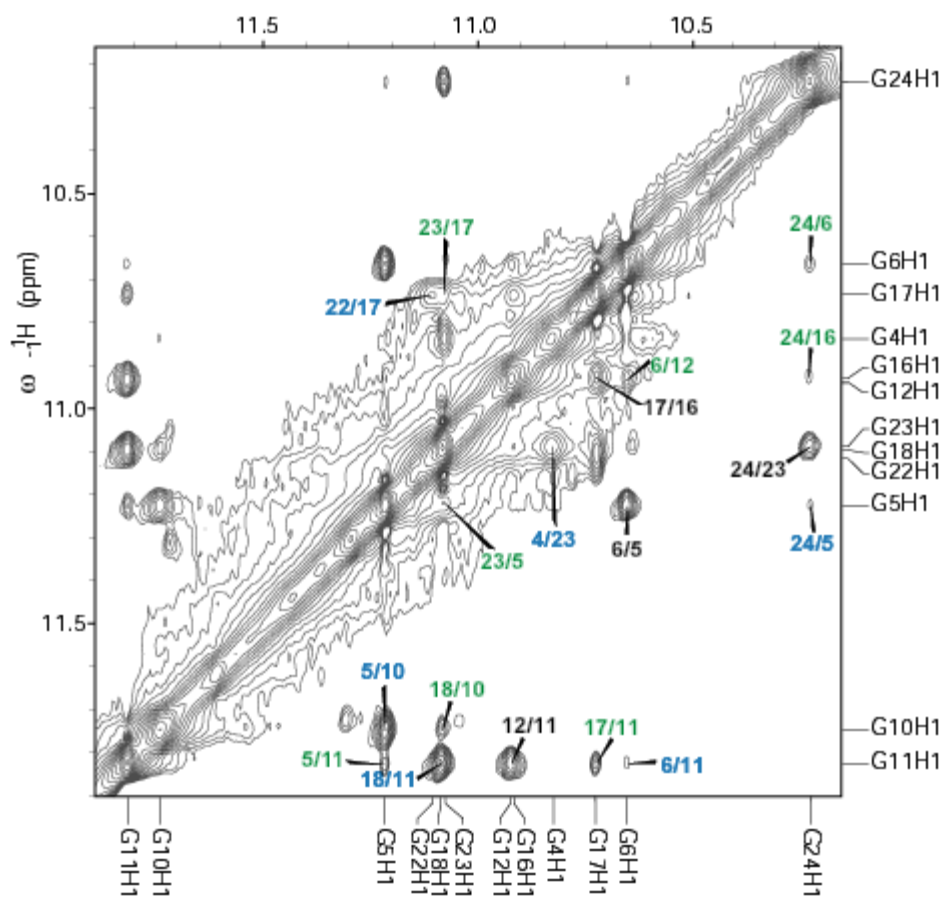


Figure S4.

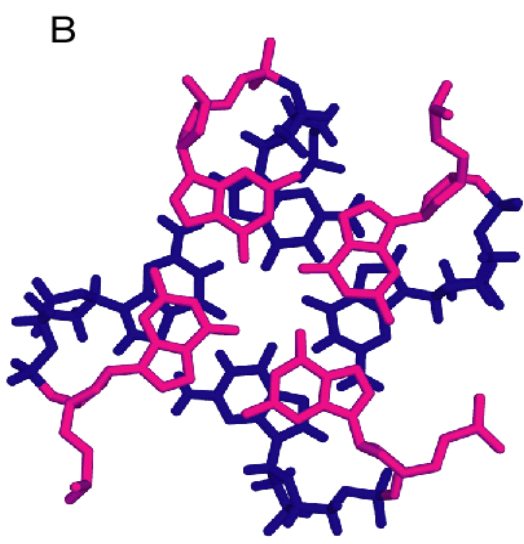
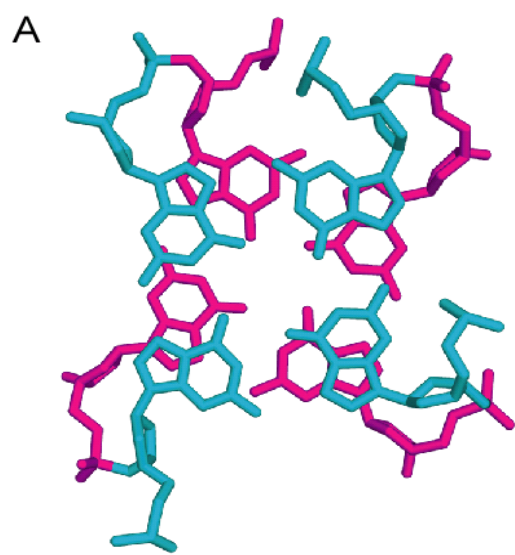


Figure S5.