

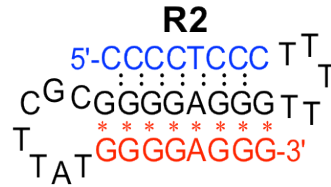
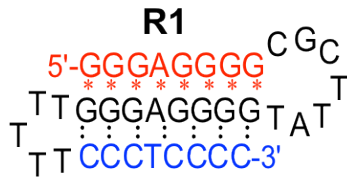
Supporting Information for:

Alternative DNA structure formation in the mutagenic human *c-MYC* promoter

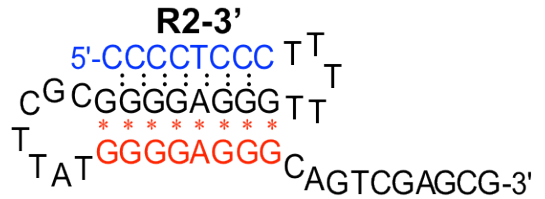
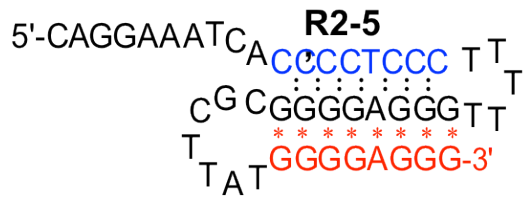
Imee Marie A. del Mundo, Maha Zewail-Foote, Sean M. Kerwin and Karen M. Vasquez

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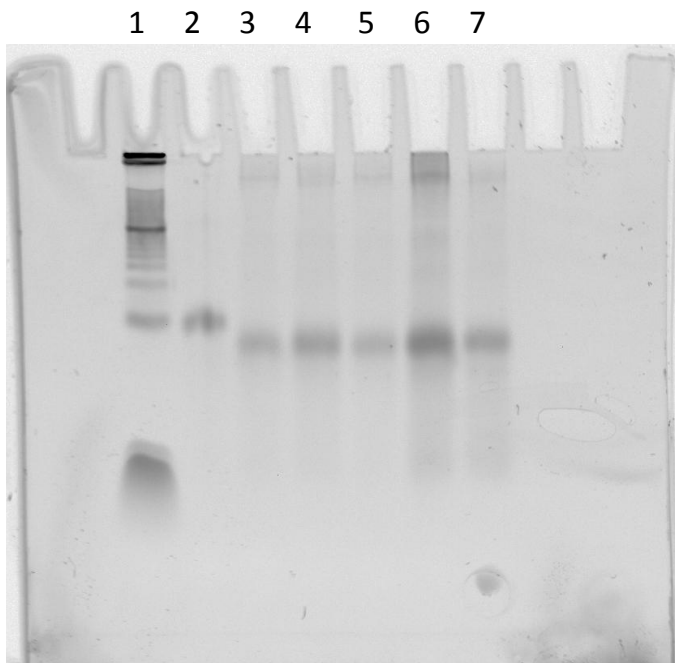
SI- 1. Predicted folding topologies under triplex/H-DNA-forming conditions.



* Hoogsteen
: Watson-Crick



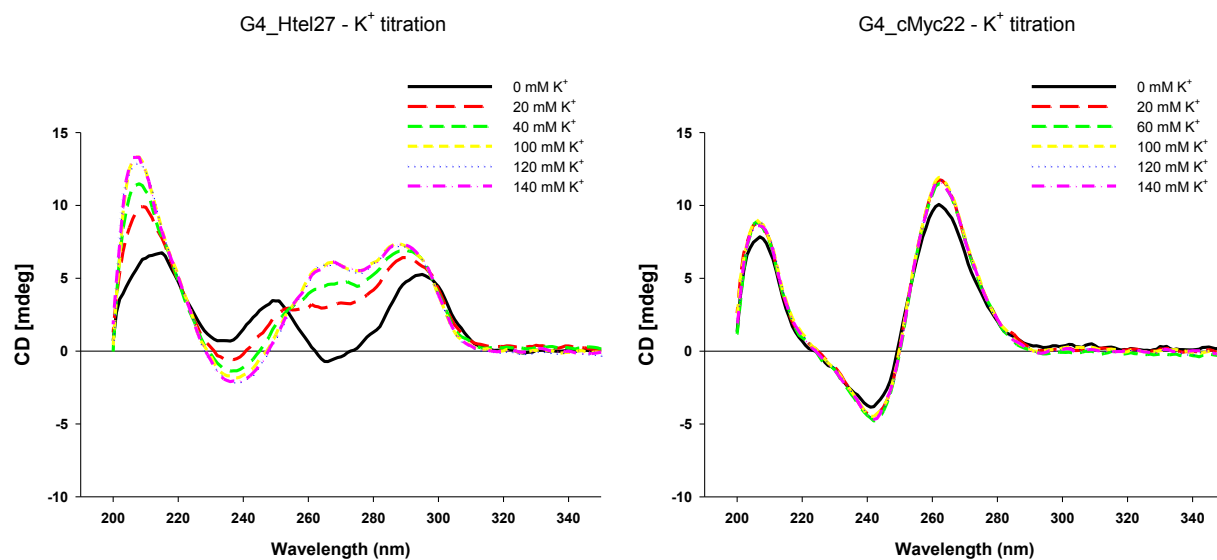
SI- 2. Similar gel mobilities were observed with R2 independent of DNA concentration.



PAGE gel of R2 and R2-ino with Mg^{2+} .

- 1) MWM (10 bp ladder)
- 2) R2-ino (1 μ M)
- 3) R2 (1 μ M)
- 4) R2 (0.2 μ M)
- 5) R2 (1 μ M)
- 6) R2 (20 μ M)
- 7) R2 (99 μ M)

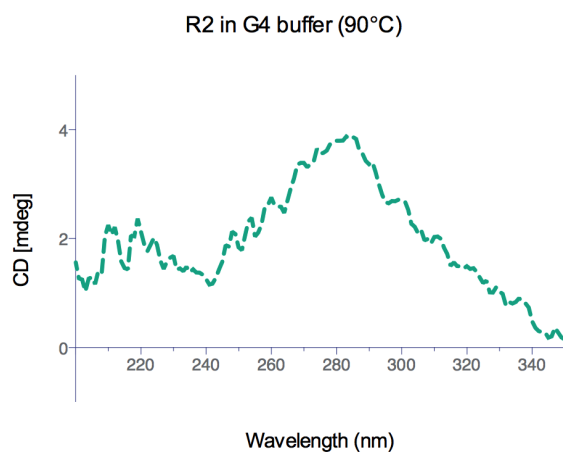
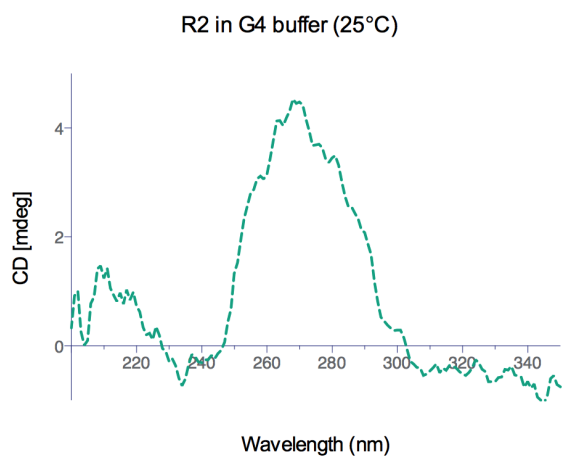
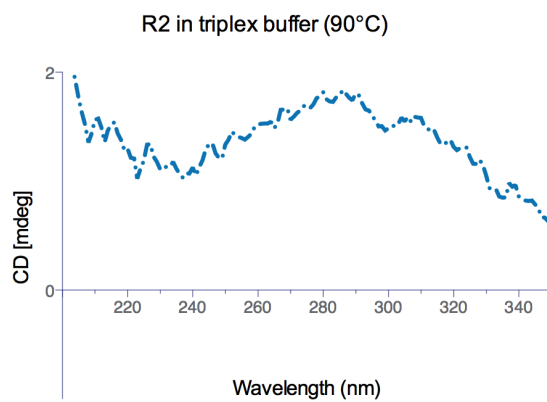
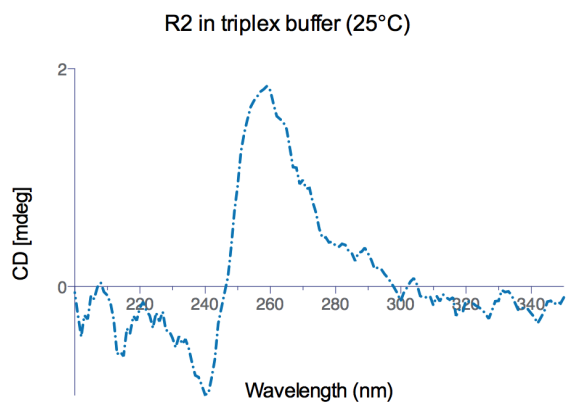
SI- 3. K⁺ titration into known G4-DNA-forming sequences initially annealed under H-DNA-forming conditions (G4-Htel27, antiparallel G4-DNA; G4-cMyc22, parallel G4-DNA).



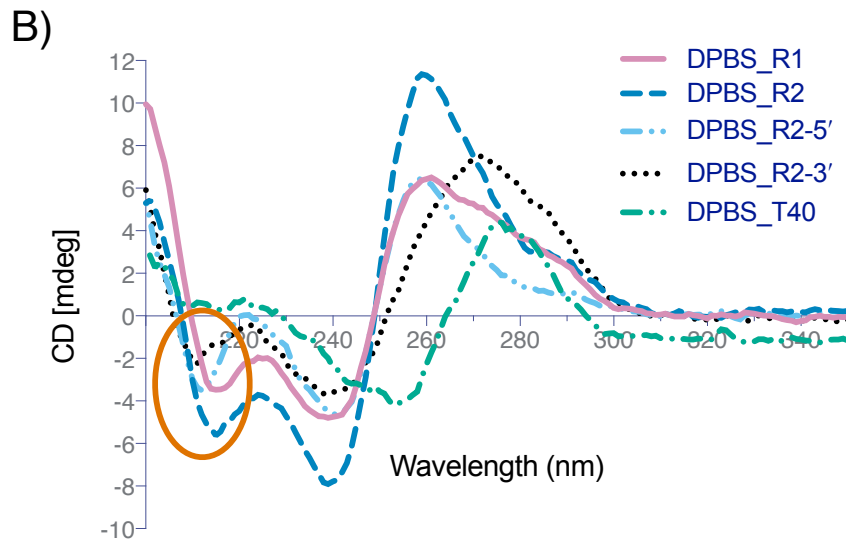
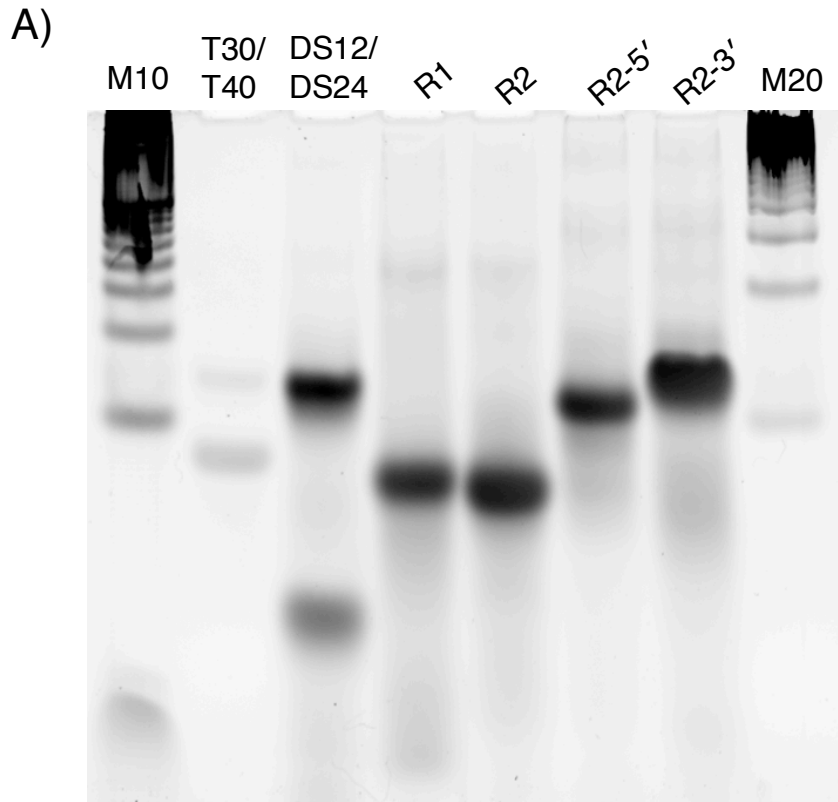
G4-Htel27 : 5'-TTA GGG TTA GGG TTA GGG TTA GGG TTA-3'

G4-cMyc22 : 5'-TGA GGG TGG GTA GGG TGG GTT A-3'

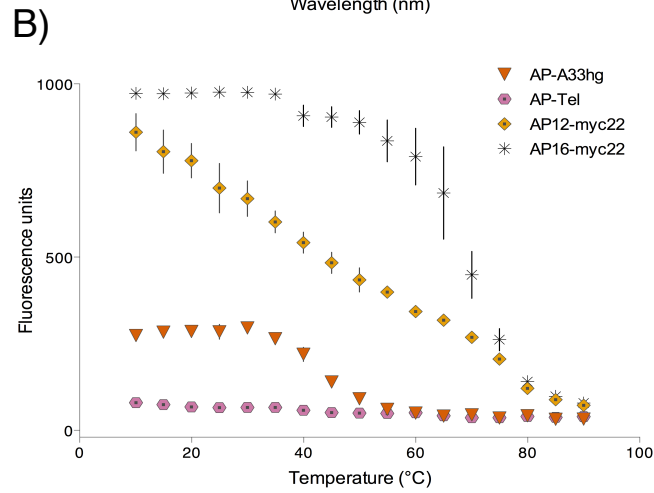
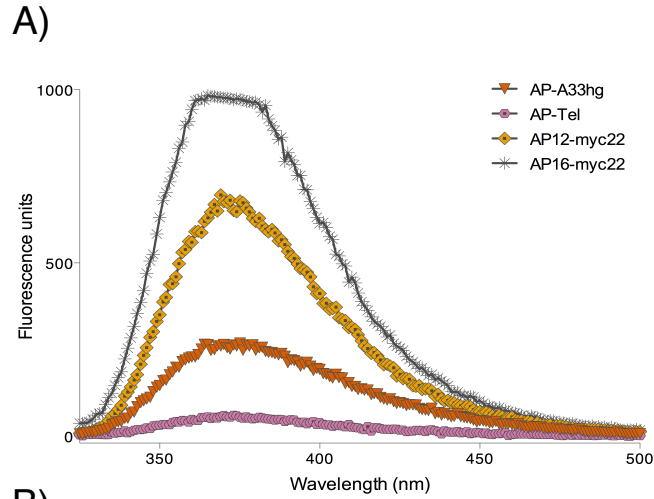
SI- 4. CD structures obtained at 25°C are structure-related. The structures at 90°C are similarly in random coil/denatured states.



SI- 5. Native gel and CD spectroscopy results under Dulbecco's Phosphate Buffered Saline (DPBS) showing that motifs **A**) also folded intramolecularly and **B**) possess the triplex CD signature.

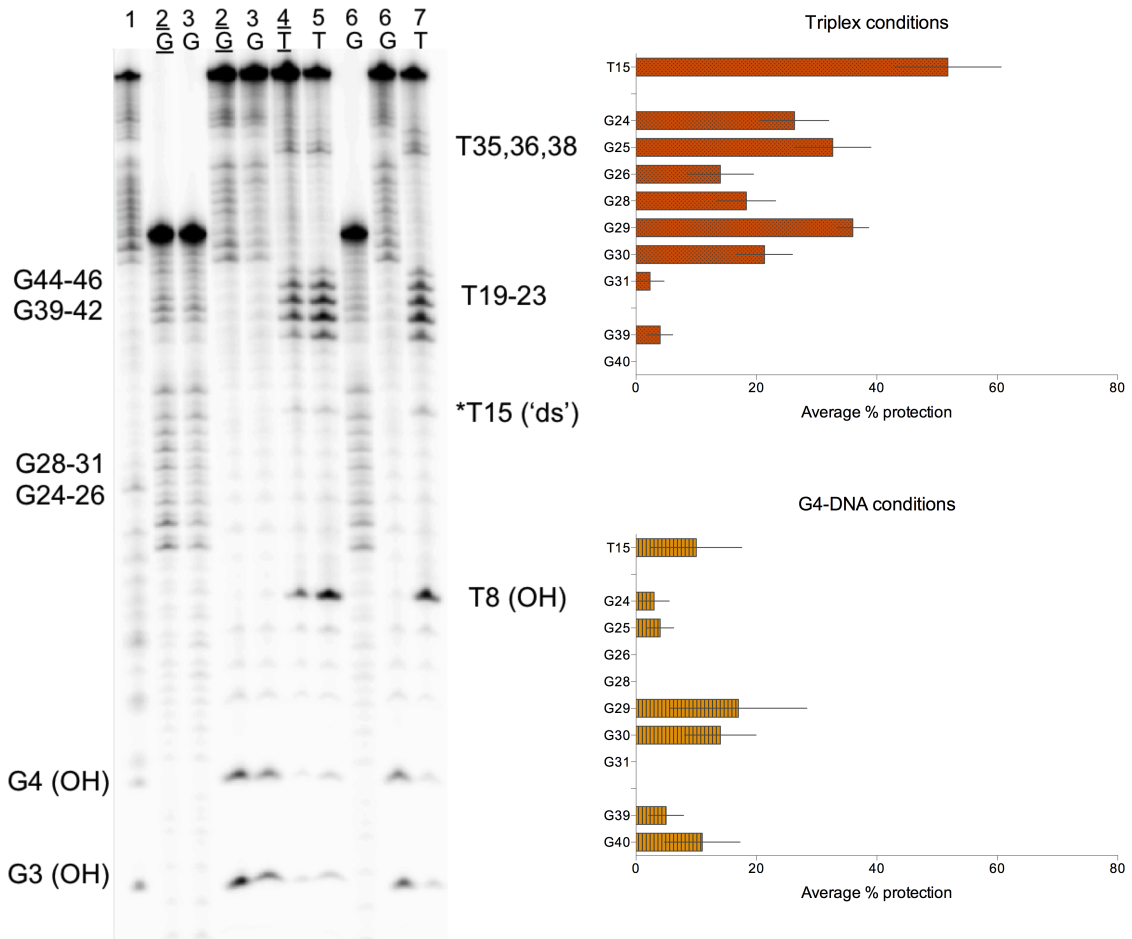


SI- 6. Comparison of the temperature-dependent fluorescence of AP-A33hg under G4-DNA-forming conditions with 2AP-substituted, control G4-DNA-forming sequences (AP12-myc22, AP16-myc22, AP-Tel). AP-A33hg was **A)** only 30% as intense but **B)** had a similar temperature-dependent profile as that of AP16-myc22. Intensity comparison suggests that 2AP may participate in a 2-nt loop.



AP16-myc22: 5'-TGA GGG T GGG TA GGG 2AP GGG TT A-3'	1-nt loop
AP12-myc22: 5'-TGA GGG T GGG T2AP GGG T GGG TT A-3'	2-nt loop
AP-Tel: 5'-GGGG TT GGGG T2AP GGGG TT GGGG-3'	2-4-nt loop
AP-33hg: CCCCTCCC TTTTT GGGAGGGG CGCTTAT GGGG2APGGG	1-2-nt loop

SI- 7. A representative denaturing gel image after chemical modification of R2-5' (primary data) under H-DNA/triplex- or G4-DNA-forming conditions. Lane 1=untreated; lanes 2-5=triplex conditions; lanes 6-7=G4 conditions; lanes 2 and 4 (underlined)=boiled samples. Average % protection was calculated as described in the Methods section.



SI- 8. Polyacrylamide gel electrophoresis of structure-forming DNA in the **A)** presence and **B)** absence of Mg^{2+} . **C)** CD spectroscopy results show the presence of the triplex signature (negative peak at ~ 220 nm) in the presence and absence of Mg^{2+} .

