Supplementary information

G-rich VEGF aptamer with locked and unlocked nucleic acid modifications exhibits a unique G-quadruplex fold

Maja Marušič[1], Rakesh N. Veedu[2,*], Jesper Wengel[3] and Janez Plavec[1,4,5,*]

[1] Slovenian NMR Center, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia

[2] School of Chemistry & Molecular Biosciences, University of Queensland, St Lucia, Brisbane, 4072 Australia

[3] Nucleic Acid Center, Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark

[4] EN-FIST Center of Excellence, SI-1000 Ljubljana, Slovenia

[5] Faculty of Chemistry and Chemical Technology, University of Ljubljana, SI-1000 Ljubljana, Slovenia

Supplementary Figures

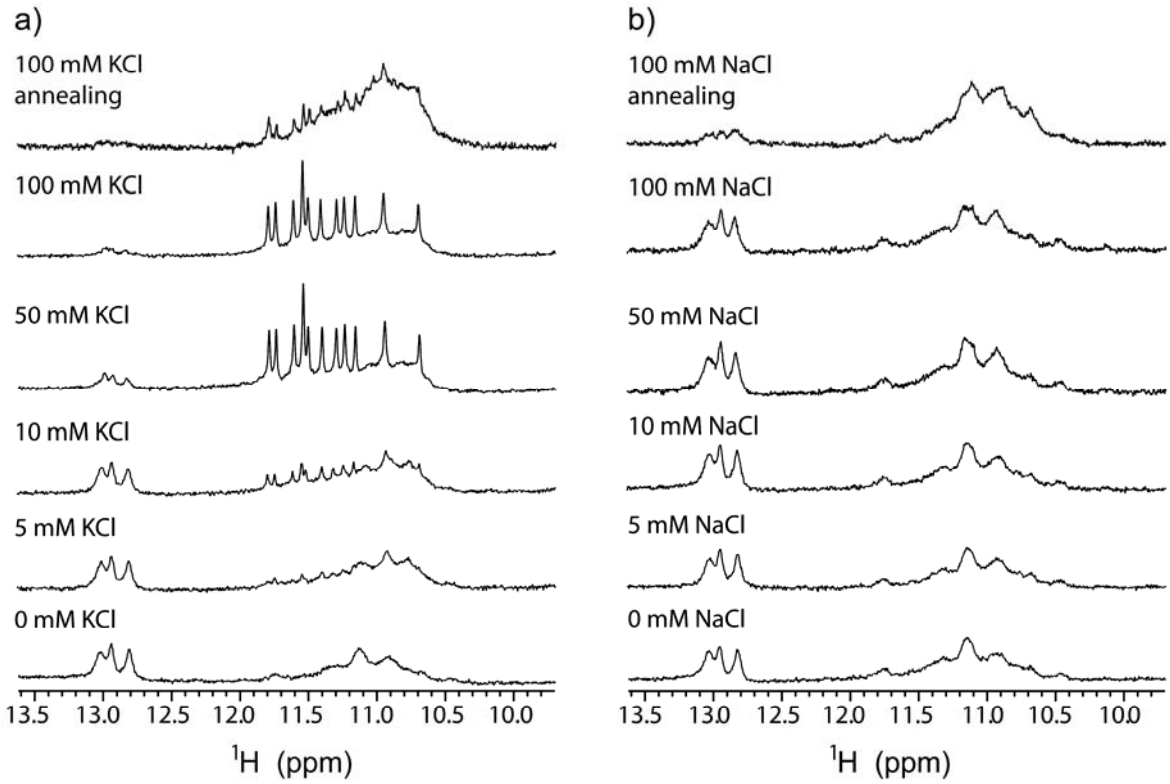

Figure S1: The imino region of the 1D ^{1}H NMR spectra of RNV66 recorded at different concentrations of a) K^+ and b) Na^+ ions and after fast annealing. Spectra were recorded at 600 MHz, 25 °C in 10% ^2H_2O, 10 mM TE buffer with pH 7 and oligonucleotide concentration of 1.0 mM.

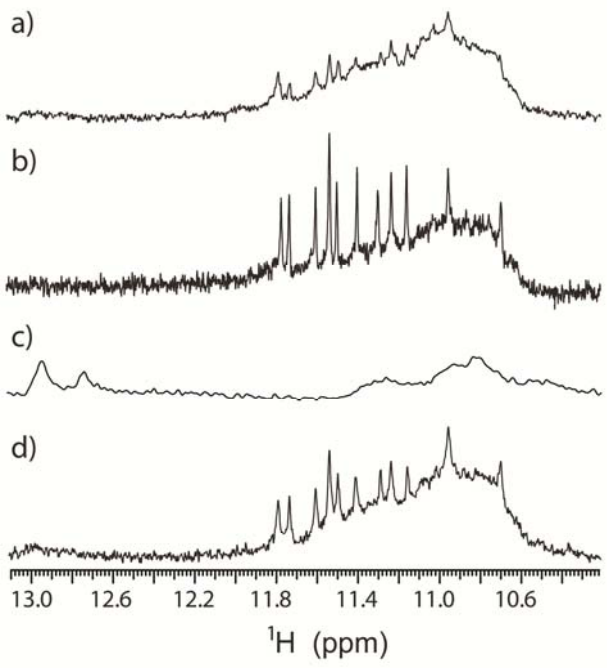

Figure S2: The imino region of 1D ^{1}H NMR spectra of RNV66 recorded after a) fast annealing, b) slow annealing with dilution from 1 to 0.5 mM oligonucleotide concentration c) after removal of K^+ ions and d) upon increase of K^+ ions concentration to 100 mM in a single step. Spectra were recorded at 600 MHz (a and d) or 800 MHz (b and c), 25 °C in 10% ^2H_2O, 100 mM K^+, 10 mM TE buffer with pH 7 and oligonucleotide concentration of 1.0 mM (a and c).

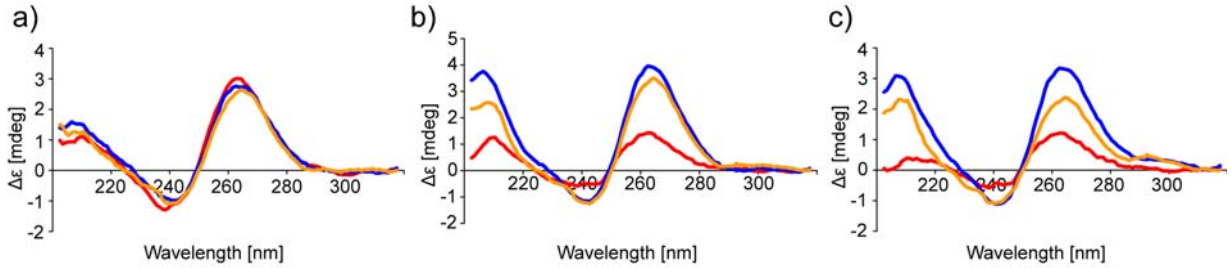

Figure S3: CD spectra of a) RNV66, b) RNV70 and c) V7t1 recorded at 25 °C in 10 mM KPi buffer with pH 7 and 5 μM oligonucleotide concentration. Red, blue and orange curves represent CD spectra acquired at 0 mM K^+, 50 mM K^+ and 50 mM K^+ after annealing, respectively.

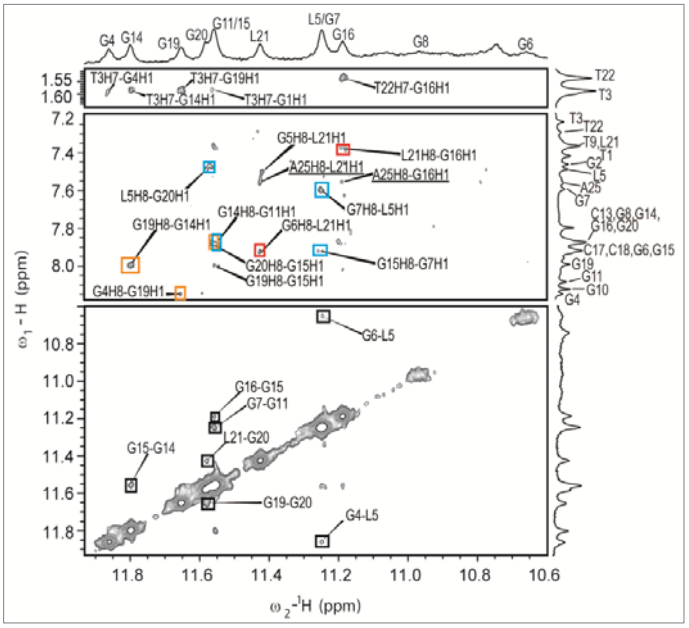

Figure S4: Imino-H7, imino-aromatic and imino-imino regions of 2D NOESY spectrum (τ_m = 250 ms) of RNV66 with resonance assignment indicated along 1D traces. Cross-peaks labelled with red, blue and orange rectangles correspond to NOE interactions between imino and aromatic protons of G6-G8-G16-L21, L5-G7-G15-G20 and G4-G11-G14-G19 quartets, respectively. Cross-peaks labelled with black rectangles indicate connections between sequential residues in the G-quadruplex core. NMR spectrum was recorded at 600 MHz, 0 °C in 10% ^2H_2O, 50 mM K^+, 10 mM KPi buffer with pH 7 and oligonucleotide concentration of 0.5 mM.

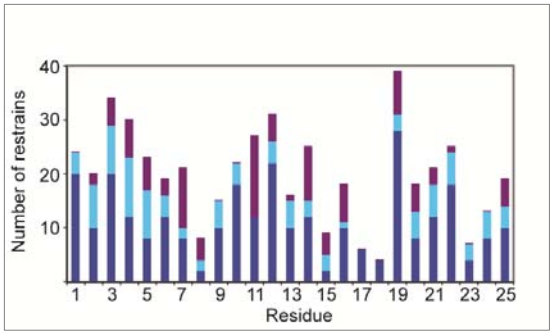

Figure S5: Number of restraints per residue used in SA calculations. Intra-residue, sequential and long range restraints are shown in dark blue, light blue and magenta, respectively.

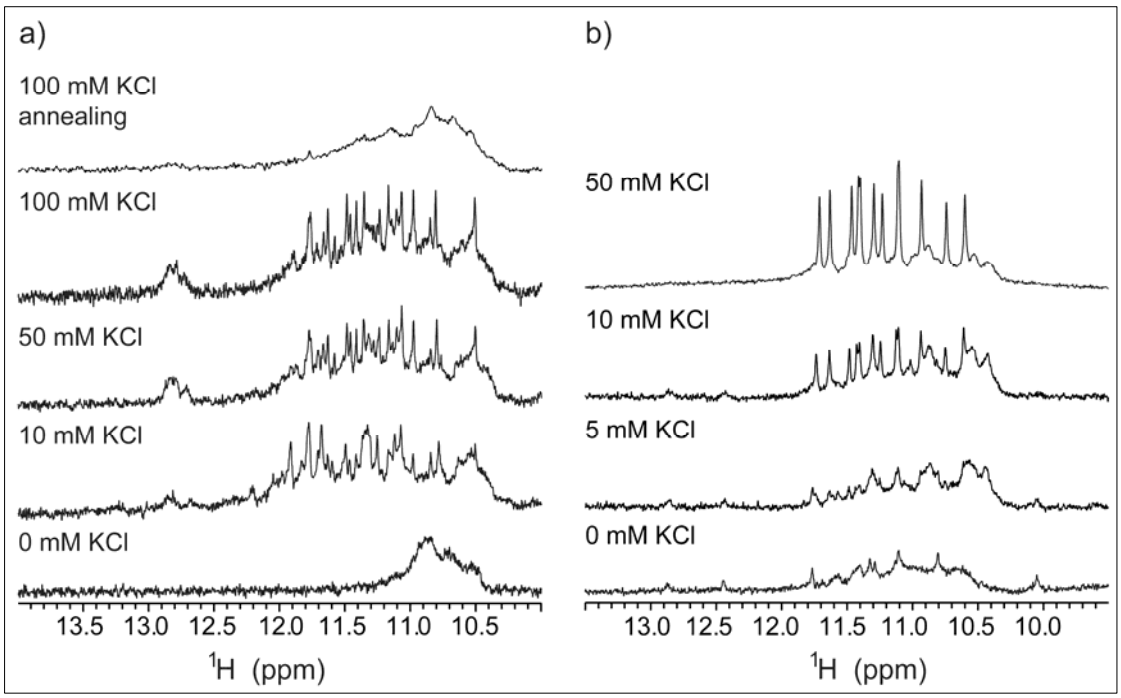

Figure S6: The imino region of 1D ^{1}H NMR spectra of a) V7t1 and b) RNV70 recorded at different concentrations of K^+ ions and after slow annealing. Spectra were recorded at 600 MHz, 25 °C in 10% ^2H_2O, 10 mM KPi buffer with pH 7 and oligonucleotide concentration of 0.8 (V7t1) and 1 (RNV70) mM.

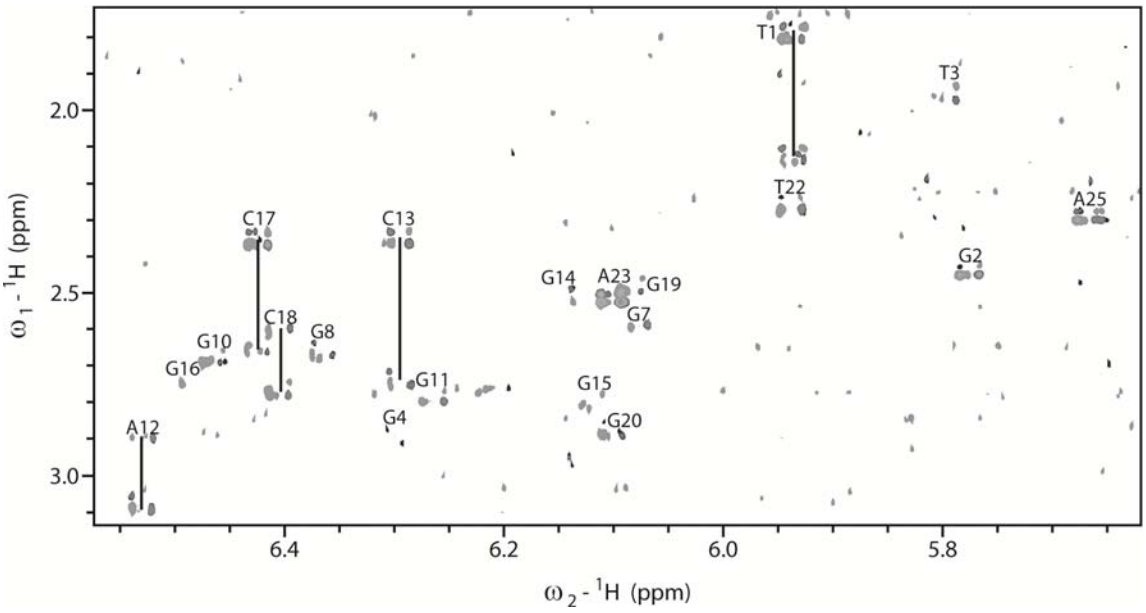

Figure S7: 2D DQF- COSY spectrum of RNV66 at 800 MHz, 25 °C in 50 mM K^+, 10 mM KPi buffer with pH 7 and oligonucleotide concentration of 1 mM.

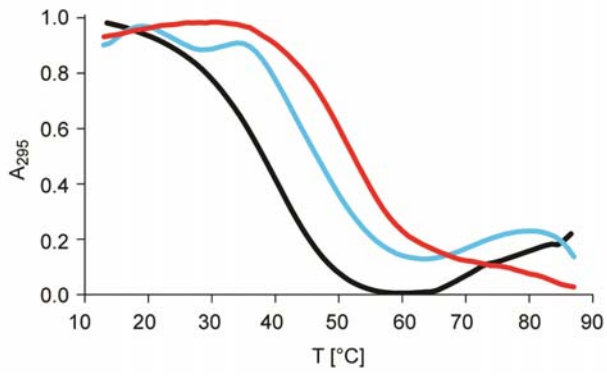

Figure S8: UV melting curves of RNV66 (red), RNV70 (blue) and V7t1 (black) recorded in 10 mM KPi buffer with pH 7 and 5 μM oligonucleotide concentration.

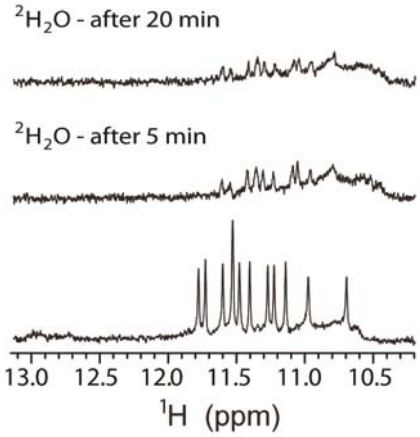

Figure S9: The imino region of 1D ^1H NMR spectra of RNV66 recorded after exchange from H_2O to ^2H_2O. Spectra were recorded at 800 MHz, 25 °C in 50 mM K^+, 10 mM KPi buffer with pH 7 and oligonucleotide concentration of 1 mM.