

SUPPLEMENTARY MATERIAL

***KRAS* promoter oligonucleotide with decoy activity dimerizes into a unique topology consisting of two G-quadruplex units**

Peter Podbevšek^{1,2} and Janez Plavec^{1,2,3,*}

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

² EN-FIST Centre of Excellence, Trg Osvobodilne fronte 13, SI-1000 Ljubljana, Slovenia

³ Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia

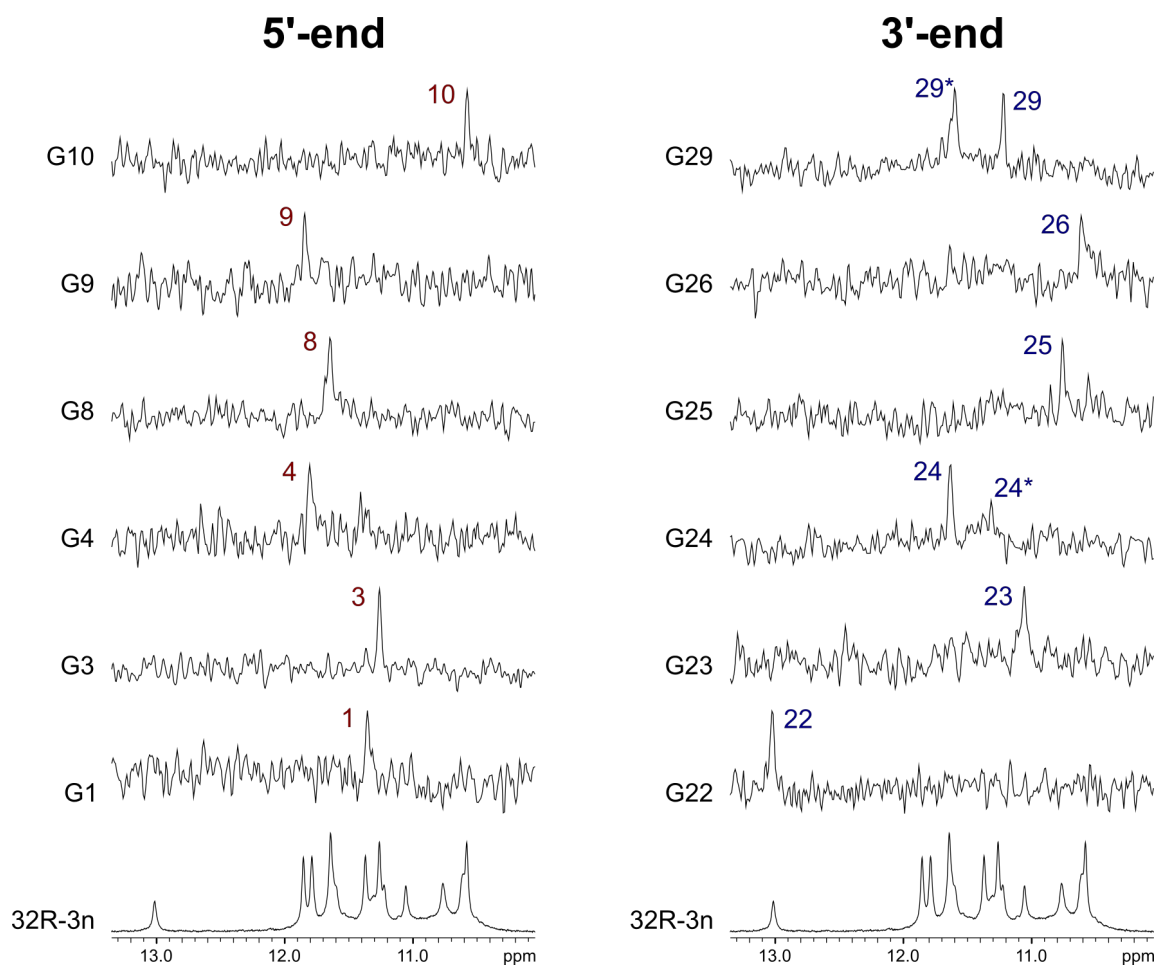
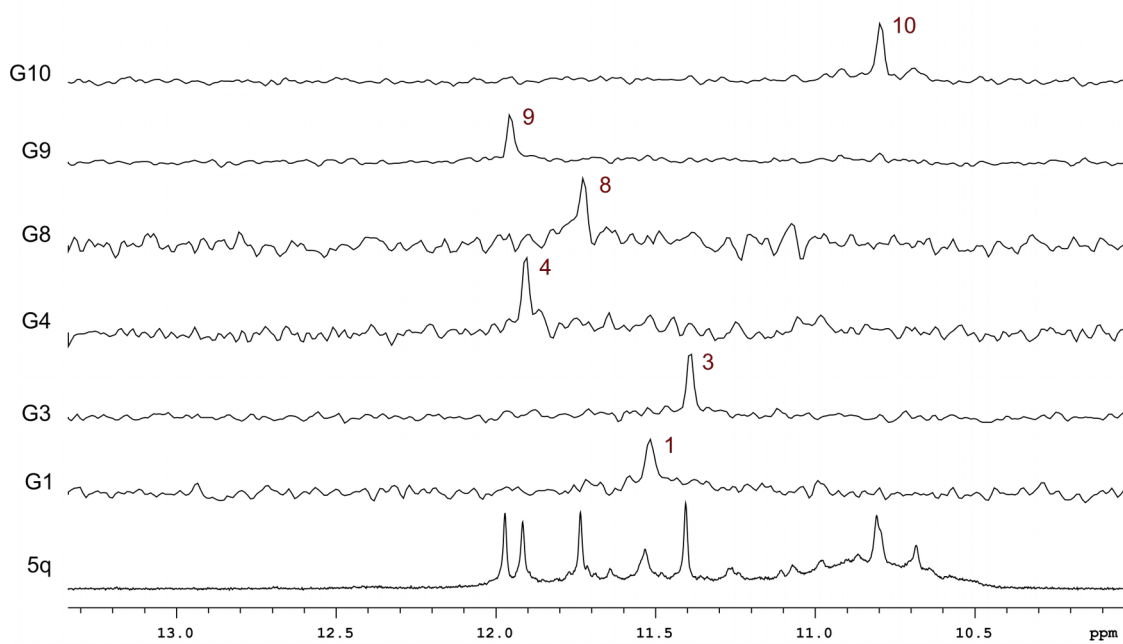


Figure S1. Imino regions of 1D ^1H NMR spectra of the parent 32R-3n and 1D ^{15}N -edited HSQC spectra of ^{15}N site specific labeled guanines of the 5'- and 3'-end G-quadruplex forming regions.

5q



3q

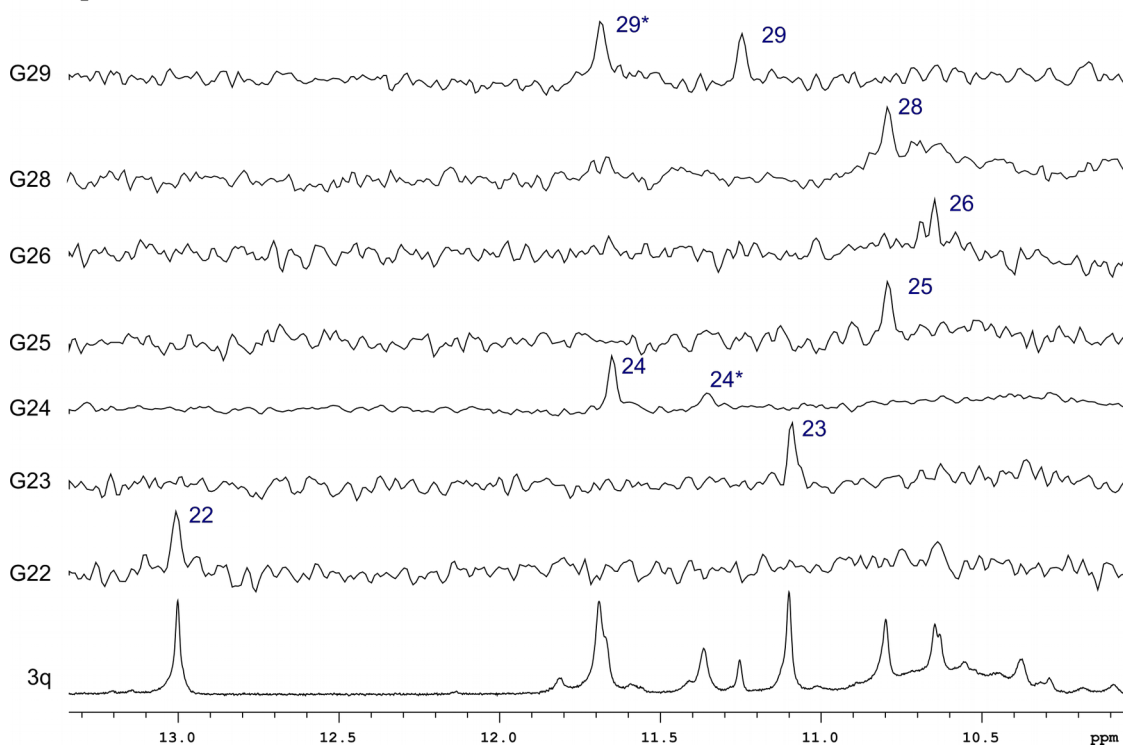


Figure S2. Imino regions of 1D ^1H NMR spectra of 5q and 3q and 1D ^{15}N -edited HSQC spectra of ^{15}N site specific labeled guanines of the 5'- and 3'-end G-quadruplex forming regions.

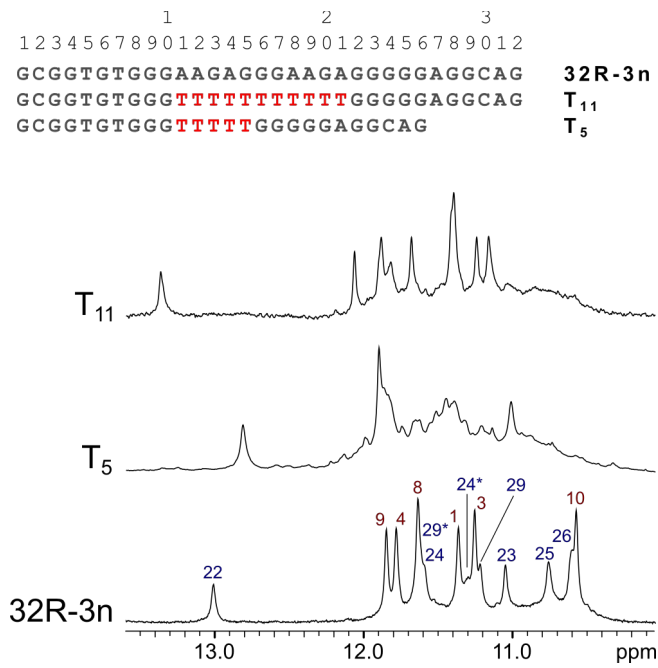
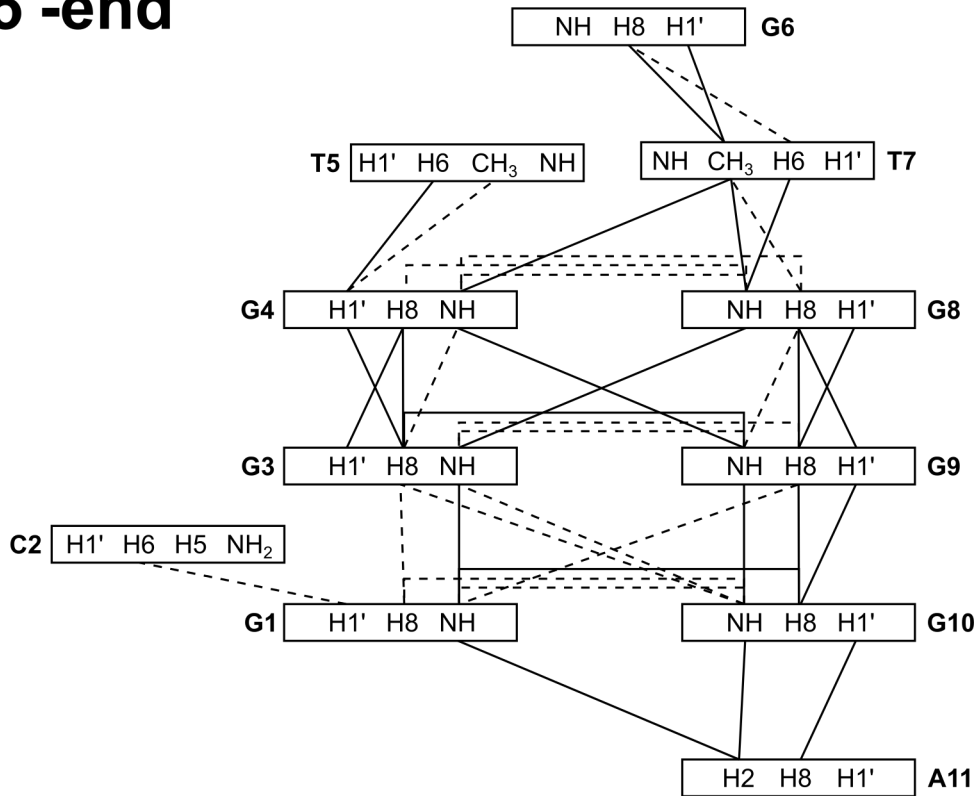


Figure S3. Imino regions of 1D ¹H NMR spectra of oligonucleotides with T₁₁ and T₅ elements in comparison to the parent 32R-3n.

5'-end



3'-end

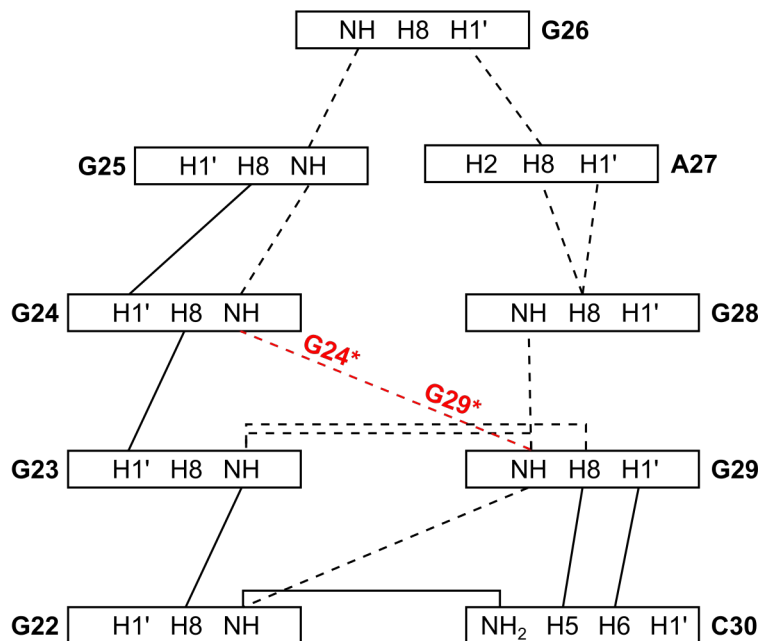


Figure S4. A diagram of strong (solid line) and weak (dashed line) NOE connectivities for the two G-quadruplex units. Due to the symmetric nature of both structures the connectivities in the diagram do not distinguish between inter- and intra-strand contacts.

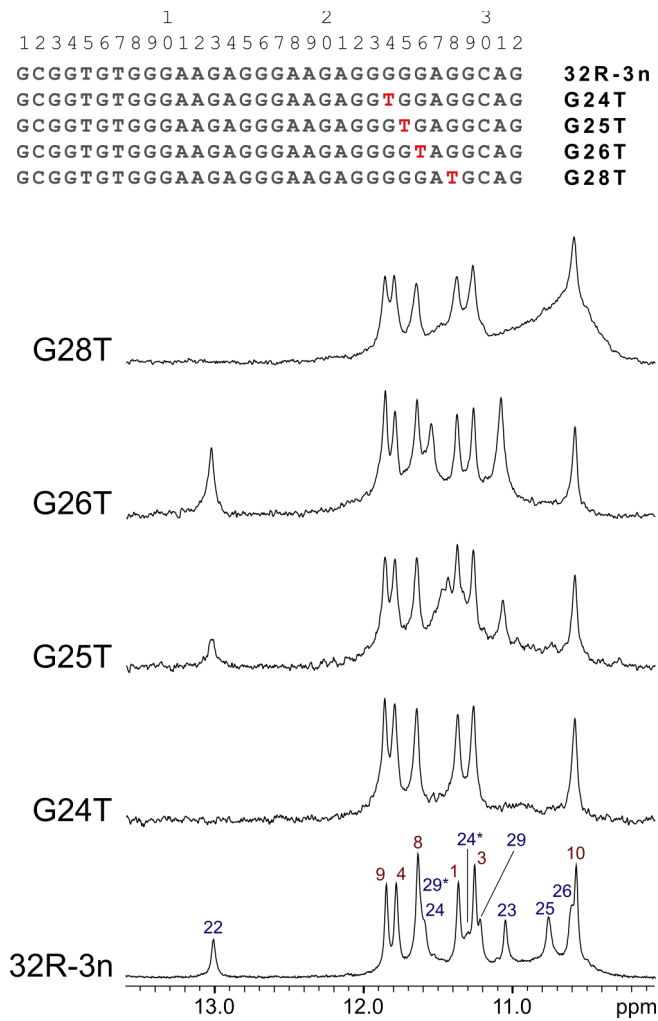
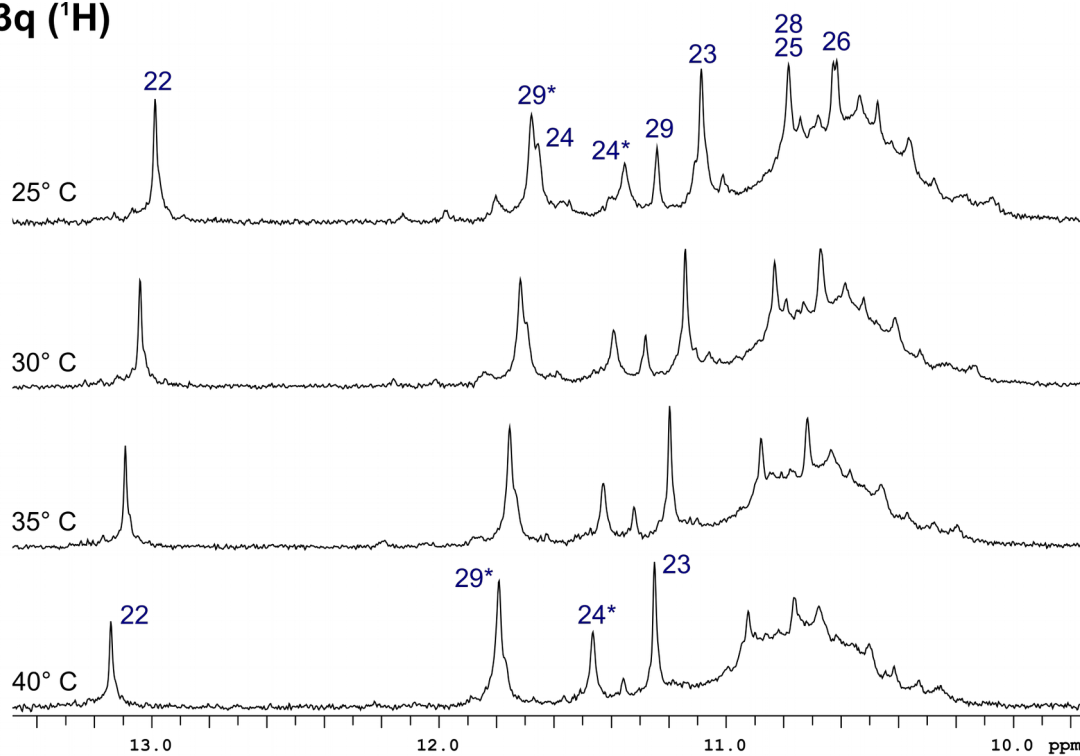


Figure S5. Imino regions of 1D ¹H NMR spectra of oligonucleotides with G24T, G25T, G26T and G28T substitutions in comparison to the parent 32R-3n.

3q (¹H)



3q (¹⁵N-edited HSQC)

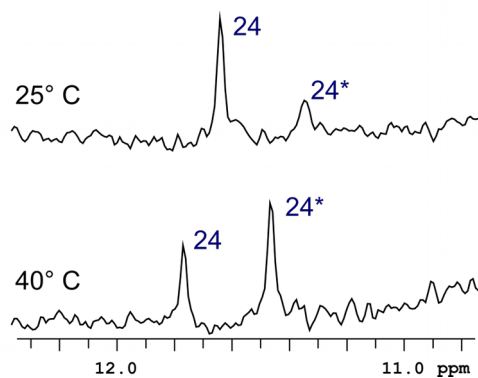


Figure S6. Imino regions of 1D ¹H NMR spectra of 3q and ¹⁵N-edited HSQC of G24 site specific ¹⁵N labeled 3q at different temperatures.

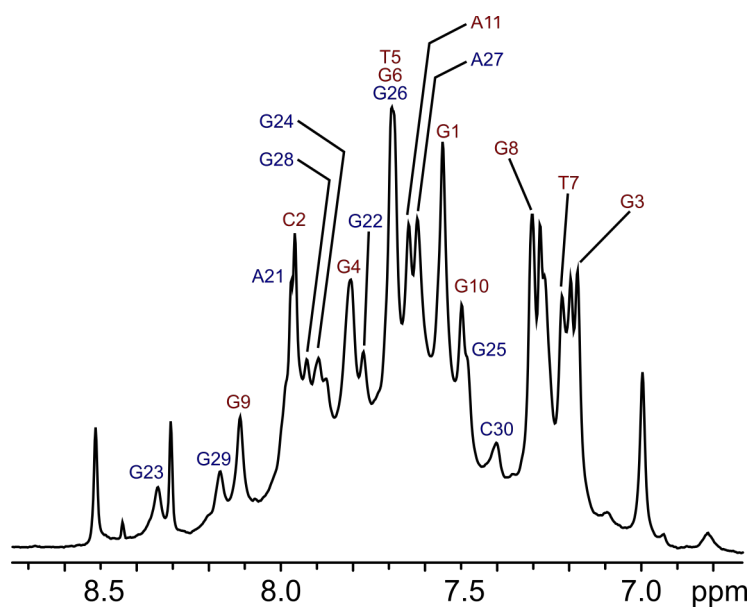


Figure S7. Aromatic region of 1D ¹H NMR spectrum of 32R-3n with assignments.

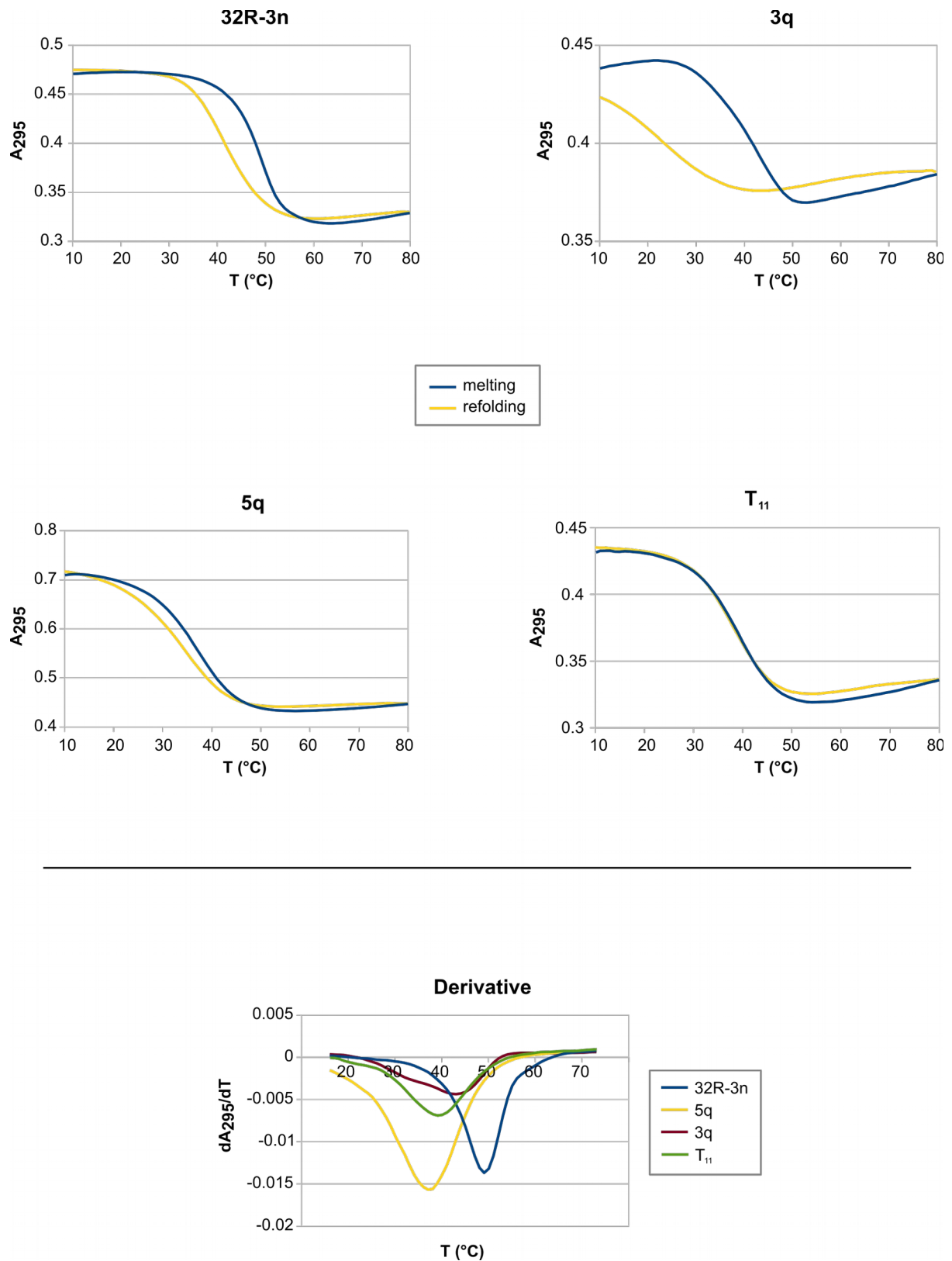


Figure S8. UV melting and refolding curves for 32R-3n, 5q, 3q and T₁₁, and a graph with the first derivative of the melting curves.