

Title: Effect of Interior Loop Length on the Thermal Stability and pK_a of i-Motif DNA

Byline: Samantha M. Reilly[†], Rhianna K. Morgan[‡], Tracy A. Brooks[‡], & Randy M. Wadkins^{†,*}

[†]Department of Chemistry and Biochemistry, University of Mississippi, University, MS 38677

[‡]Department of BioMolecular Sciences, University of Mississippi, University, MS 38677

*Corresponding Author: rwadkins@olemiss.edu

SUPPORTING INFORMATION

The excluded volume of PEG-i-motif complexes was calculated using the shift in T_m value of the i-motif in 40% PEG using the following equation (see reference 48).

$$T_M = T_M^o + \frac{RT_M^o{}^2}{\Delta H} (\Delta V_{EX}) * C_p$$

where T_M is the average melting temperature in 40% PEG, T_M^o is the average melting temperature without PEG, R is the gas constant, C_p is the molar concentration of polymer, ΔH is the enthalpy of folding (-30 kcal/mol = -5 kcal/mol per base * 6 bases for the i-motif), and ΔV_{EX} is the calculated excluded volume. The results are given in table S1 and are in reasonable agreement with data on triplex DNA reported by Spink and Chaires (ref. 48).

Table S1: Calculated Excluded Volume of PEG-i-motif DNA complexes

Oligo	40% PEG-300 (L/mol)	40% PEG-600 (L/mol)	40% PEG-1500 (L/mol)	40% PEG-3350 (L/mol)
Mod1T1	0.2	0.5	3.3	7.2
Mod1T3	0.4	1.2	2.5	7.6
Mod1T10	0.6	2.2	6.8	16.3