SUPPLEMENTARY DATA

Characterization of DNA with an 8-Oxoguanine Modification

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Temperature-dependent melts by UV spectroscopy. The UV melting experiments were performed on a Cary UV 300 Bio UV-visible Spectrophotometer (Varian Inc., Palo Alto, CA) equipped with a Cary Temperature Controller. The melting of the ODNs were monitored at 260 and/or 275 nm in the temperature range of 0 - 90 °C at a heating rate of 1.0 °C/min with a data interval of 0.4 °C. The transition temperature (T_M) was determined by the analysis of the first derivative and shape of the melting curves. The nature of complex formation of the ODNs was studied by performing the UV melts as a function of their total strand concentration (3 – 70 μM).

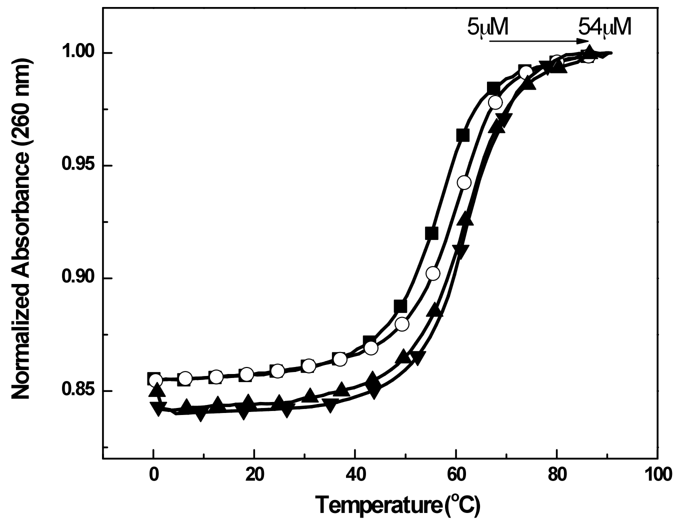
Thermal denaturation by differential scanning calorimetry. Calorimetric enthalpies for the helix to coil transitions of the ODNs were acquired on a VP-DSC differential scanning calorimeter (MicroCal, LLC, Northampton, MA). In a typical DSC experiment, ~ 200 μM of total strand concentration of the ODN solution in the sample cell (0.506 mL cell volume) was scanned from 0 – 90 °C at a rate of 45 °C/hr with buffer in the reference cell. A buffer vs. buffer scan was also done under similar conditions and subtracted from the subsequent experimental runs. A 16 sec filter period was used for all the data acquisitions. The resulting thermograms were plotted as heat capacity (C_p) vs. temperature profiles using Origin 7.0 software provided with the instrument. Analysis of the integrated plots of the anomalous C_p vs. temperature curves ($\int \Delta C_p/\mathrm{d}T$) and normalization for the number of moles, yields the molar calorimetric enthalpy (ΔH_{cal})

using a non-two state cursor initiation model. Calculation of the Gibbs free energy for the transition at 20°C, assuming negligible entropy contributions from the strand concentration, used Equation 1:

$$\Delta G_{cal}(T) = \Delta H_{cal}\left[1 - \left(\frac{T}{T_M}\right)\right] \qquad (1)$$

The molar calorimetric entropy (ΔS_{cal}) was calculated from integration of the ΔC_p/T versus T curves and the G (from Equation 1), enthalpy values using the Gibbs equation:

$$\Delta G_{cal}(T) = \Delta H_{cal} - T\Delta S_{cal} \qquad (2)$$



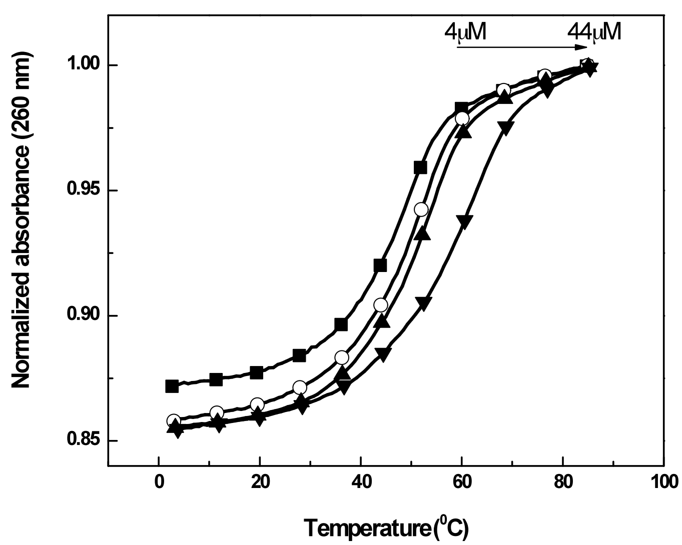


Figure S1: Strand dependence of (top) GAGAGCGCTCTC and (bottom) GAGA-oxoG-CGCTCTC in 100 mM sodum phosphate buffer (pH 7.0)

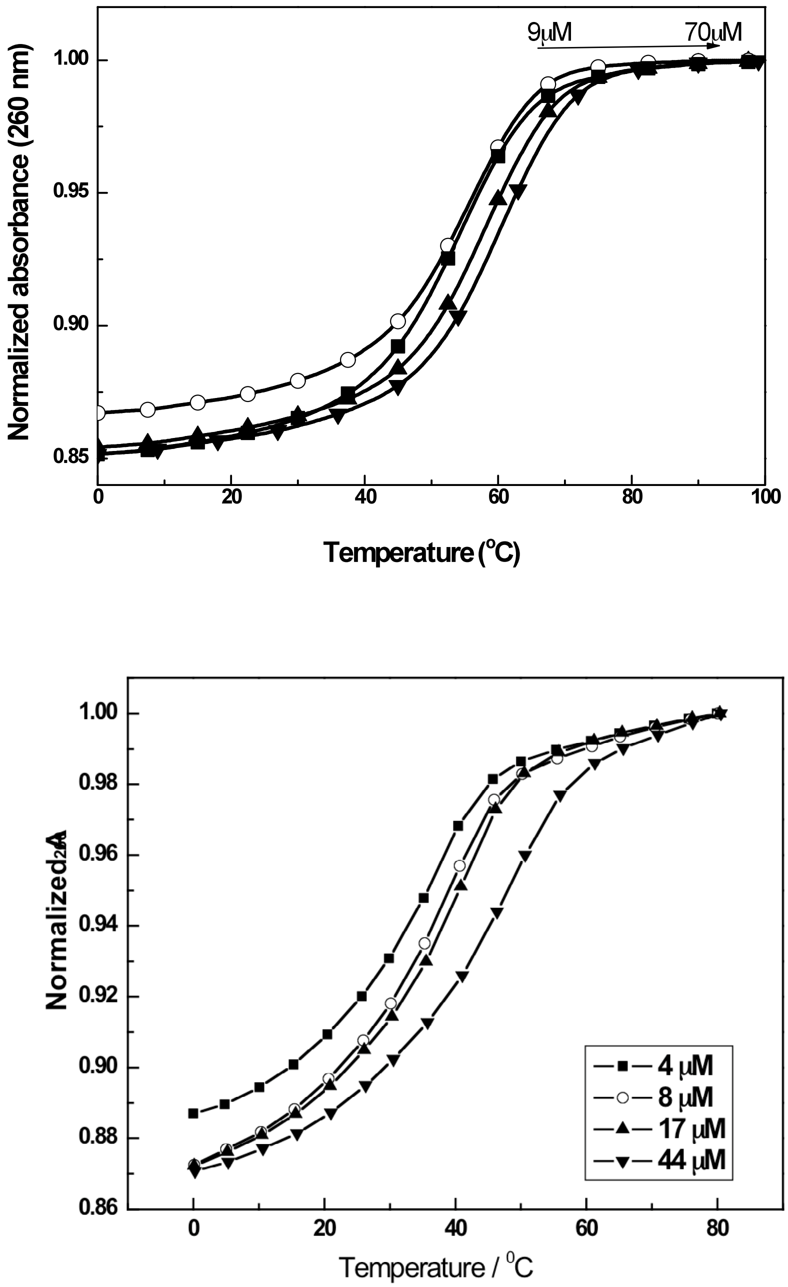


Figure S2: Strand dependence of GCGAATTCGC (top) and GCGAATTCXC (bottom) in 100 mM sodium phosphate buffer (pH 7.0)

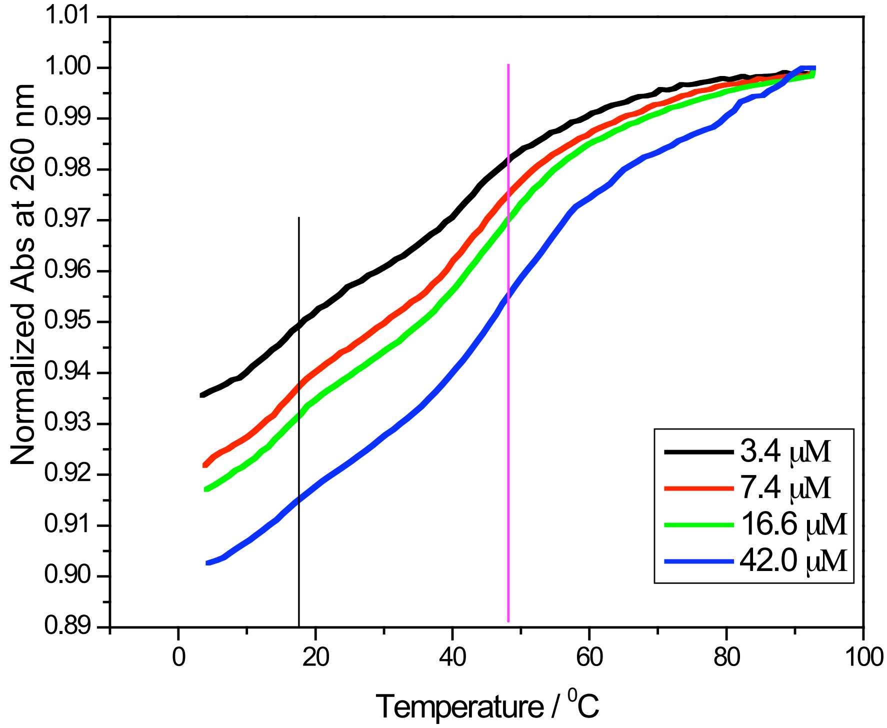


Figure S3: Strand dependence of CGCGTTTTC-oxoG-CG in 100 mM sodium phosphate buffer (pH 7.0)

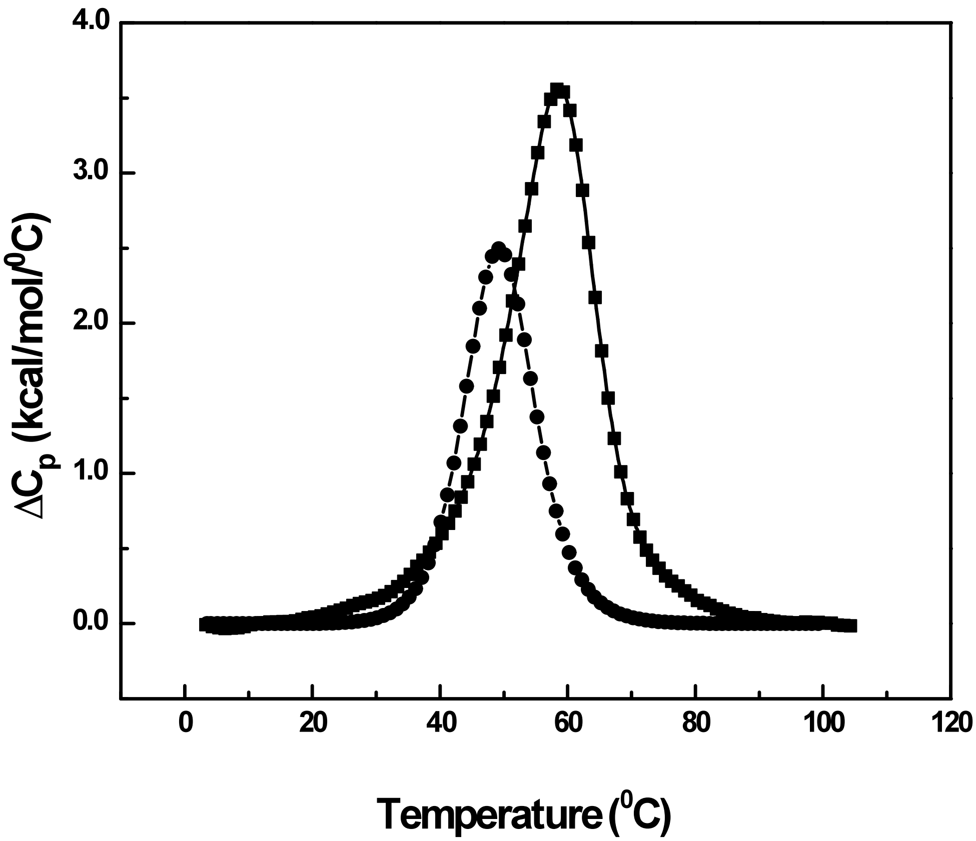


Figure S4: DSC thermograms for the melting of GCGAATTCGC (■) and GCGAATTC-oxoG-C (●) at ~ 200 μM in 100 mM phosphate buffer (pH 7.0)

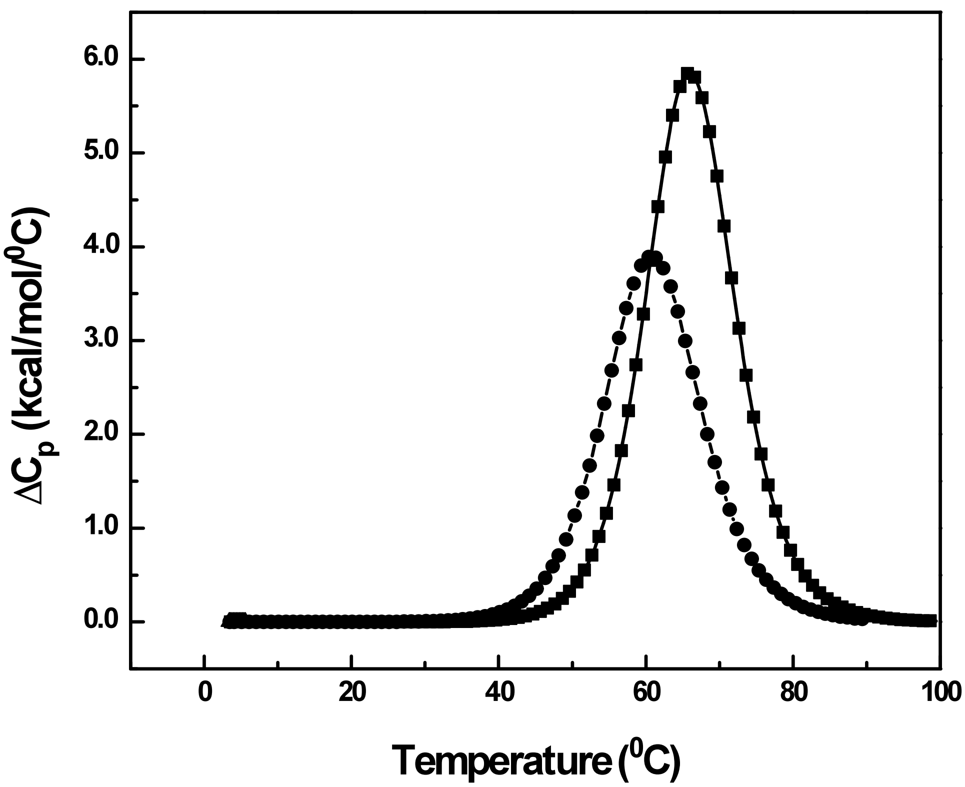
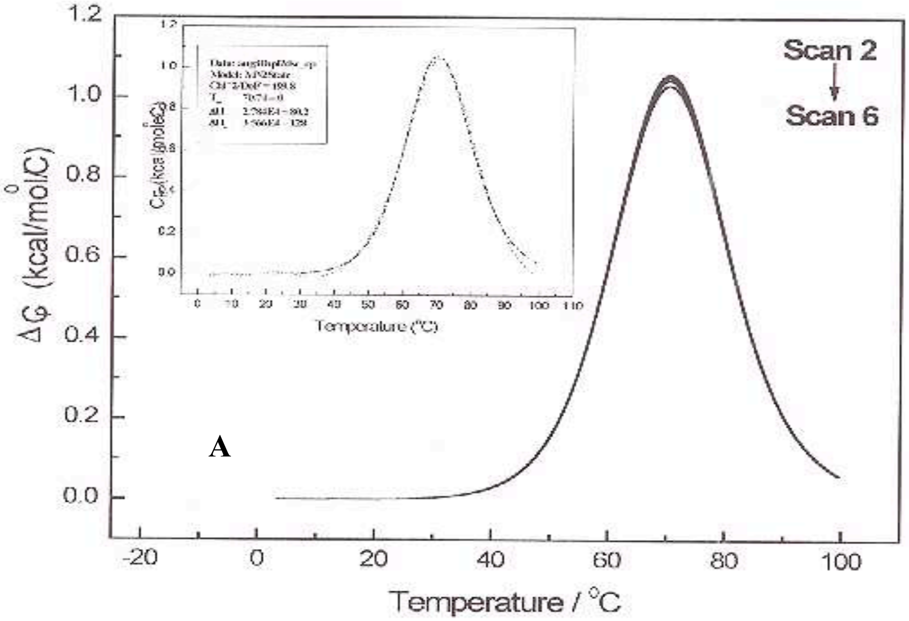


Figure S5: DSC thermograms for the melting of GAGAGCGCTCTC (■) and GAGA-oxoG-CGCTCTC (●) at ~ 200 μM in 100 mM phosphate buffer (pH 7.0)



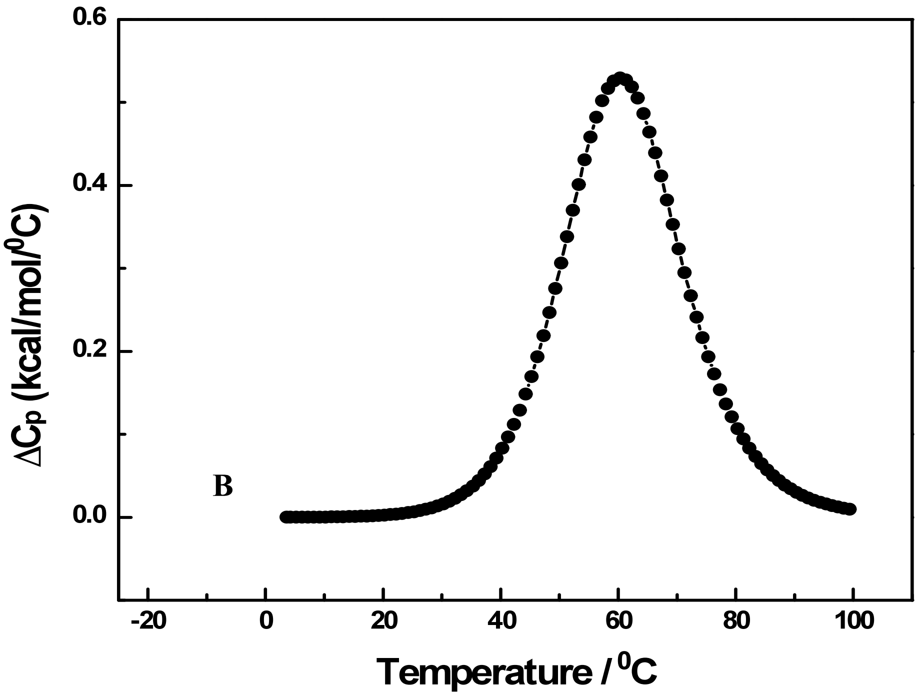


Figure S6: DSC thermograms for the melting of CGCGTTTTCGCG (A) and CGCGTTTTC-oxoG-CG (B) at ~ 200 μM in 100 mM phosphate buffer (pH 7.0)