Supporting Information for:

**Ground and Excited State Electronic Spectra of Perylenediimide Dimers with Flexible and Rigid Geometries in DNA Conjugates**

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Fig. S1. (a) UV melting curves monitored at 260 nm and (b) the $A^{0-1}/A^{0-0}$ band intensity ratio for hairpins 2AT, 2TA and 2AA in phosphate buffer.
**Fig. S2.** Long wavelength region of the CD spectra of the hairpins 2AT, 2TA, 2AA and 2TT in phosphate buffer.

**Fig. S3.** Circular dichroism spectra of hairpin dimer (H8)$_2$ and duplex A:T in buffer.
Fig. S4. (a) Temperature dependent CD spectra for 2AT (ca. 1 µM hairpin in 10 mM phosphate buffer with 0.1 M NaCl). (b) Temperature dependence of the 560 nm band intensity. Inset shows derivative of 560 nm heating and cooling curves.

Fig. S5. Fluorescence excitation spectra of the hairpins 2AT, 2TA, 2AA and 2TT monitored at (a) 550 and (b) 660 nm in buffer. The spectra of 2AA and 2TT have been multiplied by a factor of 10 in (a) for clarity.
**Fig. S6.** Fluorescence decay profiles of various oligonucleotide conjugates at 560 (top) and 660 nm (bottom) in buffer.

**Fig. S7.** Time resolved emission spectra of various oligonucleotides in buffer. Sample concentration and experimental conditions same as for fluorescence lifetime measurements.
Fig. S8. (Left) Fluorescence spectra and (right) the ratio of monomer to excimer fluorescence intensities of 2TA and 2TT as a function of temperature in buffer. Bold traces in the middle indicate the fluorescence spectra at 25 °C. Excitation wavelength, 505 nm.

Fig. S9. Transient absorption spectra of hairpin 1A in TE buffer (20 mM Tris, 2 mM EDTA), pH = 7.4, following excitation with 505 nm, 120 fs laser pulses. Inset: transient absorption kinetics at (●●●) 605 nm and at (•••) 708 nm. Nonlinear least-squares fits to the data are also shown (data from Zeidan et al.).
References
