

Supporting Information for:

**Perylenediimide-Linked DNA Dumbbells: Long-Distance Electronic Interactions and
Hydrophobic Association upon Base-Pair Melting**

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Table S1. m/z values for dumbbell precursors **P6-P10**, **P13** and **P16** and the corresponding dumbbells **D6-D10**, **D13** and **D16** determined by MALDI-TOF mass spectrometry.

n^a	Dumbbell Precursors		Dumbbells	
	Calculated	Measured	Calculated	Measured
6	4859.4	4852.3	4841.1	4839.1
7	5476.8	5475.7	5458.8	5458.0
8	6094.2	6092.6	6076.2	6075.5
9	6711.7	6702.5	6693.7	6688.5
10	7329.1	7326.6	7311.1	7311.4
13	9181.3	9178.1	9163.3	9161.5
16	11033.5	11033.6	11015.5	11016.3

^a n = number of A-T base pairs in the dumbbell precursor or dumbbell.

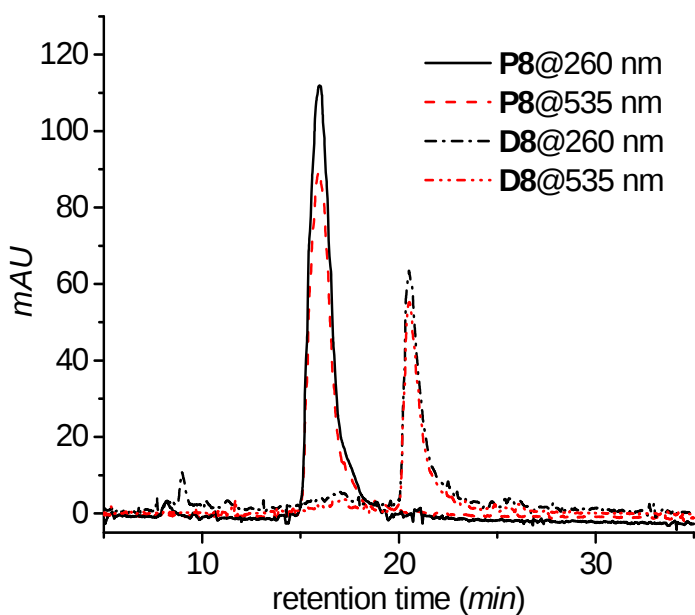


Figure S1. HPLC traces of 8 layer dumbbell **D8** before and after ligation reaction, monitored at both DNA and PDI absorbance wavelengths. Gradient: 12% - 25% acetonitrile in 30 min.

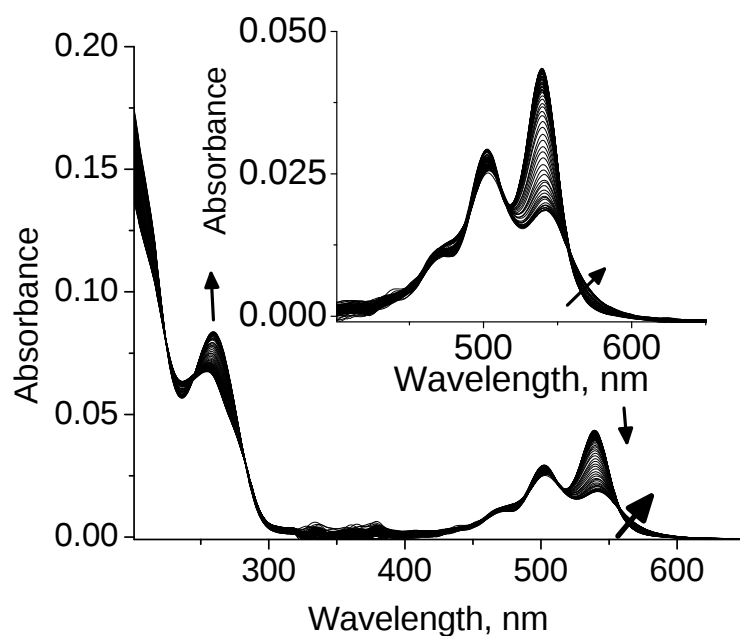


Figure S2. Temperature dependent absorption spectra of PDI conjugate **D8** (1 μ M) in 10 mM phosphate buffer (pH 7.2). Arrows indicate changes which occur upon heating from 5 to 95 $^{\circ}$ C in 5 $^{\circ}$ C steps.

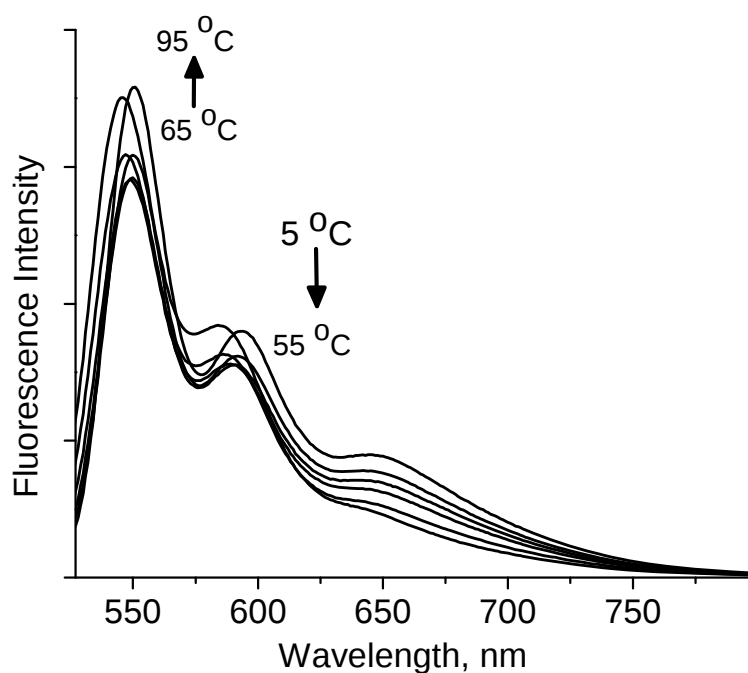


Figure S3. Temperature dependent fluorescence emission spectra for dumbbell **D8** in aqueous buffer. Arrows indicate changes which occur upon heating from 5 to 55 $^{\circ}$ C and from 65 to 95 $^{\circ}$ C in 5 $^{\circ}$ C steps.

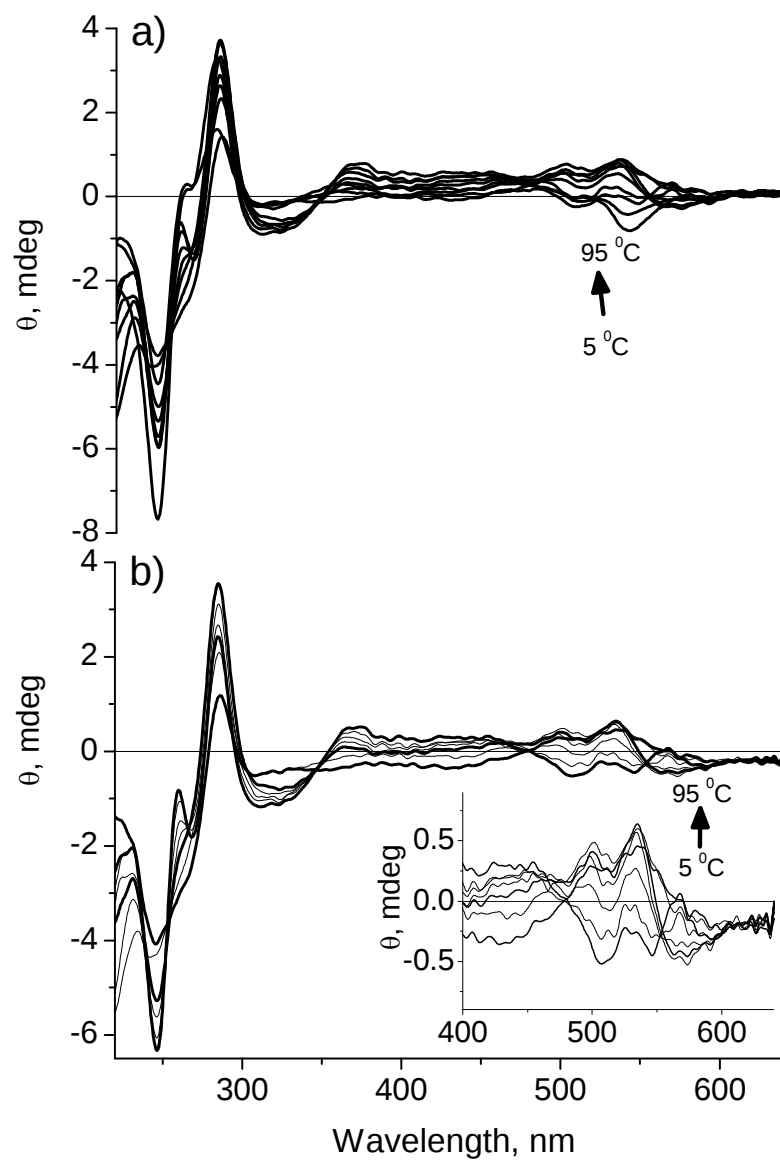


Figure S4. (a) Temperature dependent CD spectra of PDI dumbbell conjugates (a) **D8** and (b) **D13** in 10 mM phosphate buffer (pH 7.2). Arrows indicate changes which occur upon heating from 5 to 95 °C in 5 °C steps.

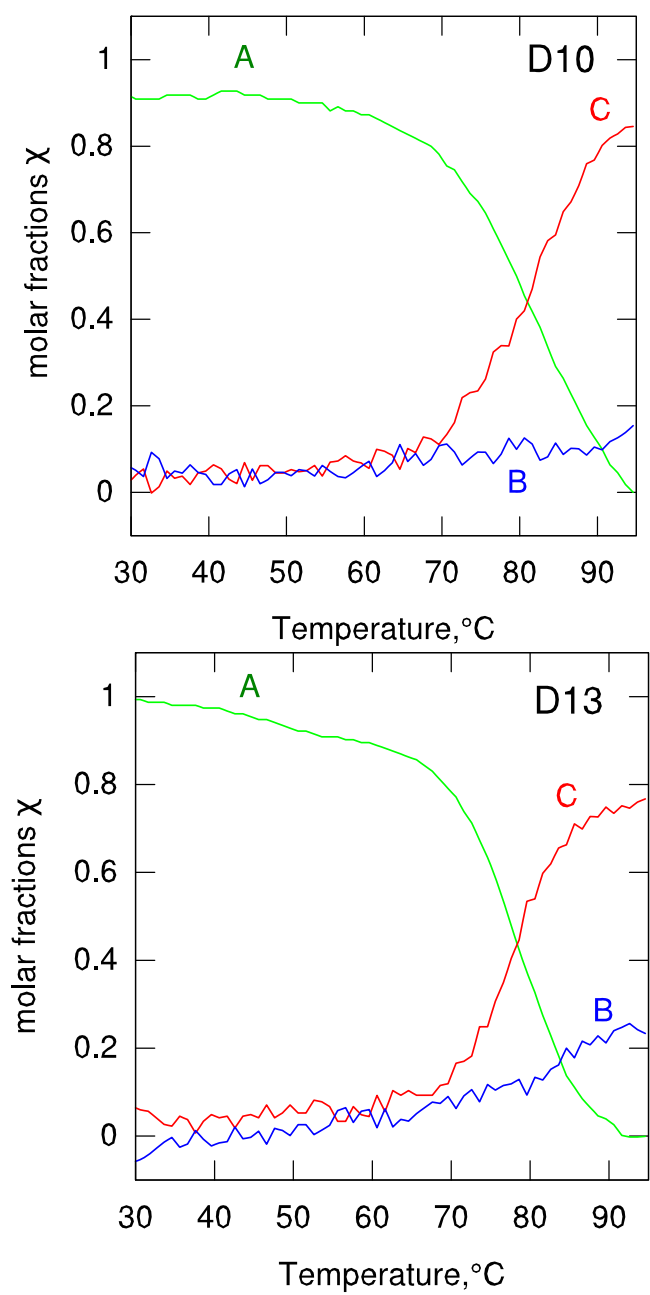


Figure S5. Temperature dependence of the mole fractions of species A, B, and C (Scheme 2) for (a) **D10** and (b) **D13**.