Supporting Information

Facially-Selective Thymine-Thymine Photodimerization in TTT Triads

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Experimental Section

All nucleotides were prepared on an Expedite 8909 DNA synthesizer using standard phosphoramidite chemistry, followed by purification with reversed-phase HPLC and characterization by MALDI-TOF mass spectrometry. UV-visible spectra were recorded on an Agilent 8453 spectrophotometer using a quartz cuvette with a 10 mm light path length.

The thymine photodimerization studies were conducted in the pH 7.1 buffer solution of 10 mM phosphate containing 100 mM sodium chloride. Standard buffer solutions containing oligonucleotides were irradiated with monochromatic 280 nm light at room temperature in 1 cm path length quartz cuvettes and stirred continuously during irradiation. The light source was a 150 W xenon arc lamp (PTI), and the irradiation wavelength was controlled by a monochromator (PTI Model 101) with a 2.5mmslit width (ca. 10 nm bandwidth) so that the total energy incident on the sample solution was 2 mW. Aliquots were taken from the irradiated solution at 5 min intervals and analyzed by HPLC using a Microsorb-MV C18 reversed-phase column (250 × 4.6 mm) with a column temperature of 60 °C.

Table S1. M/z values of hairpin conjugates determined by MALDI–TOF mass spectrometry.

Hairpin	T_m (°C)[a]	m/z	
		Calculated	Measured
AA_6	48.6	3904.8	3904.7
U_1	47.2	3890.8	3884.8
U_2	46.1	3890.8	3889.3
U_3	47.6	3890.8	3884.4
II_7	50.6	4524.2	4528.8
IA_7	52.7	4526.2	4528.0
AI_7	52.1	4525.2	4531.8
AA_7	55.8	4525.2	4526.3
GI_7	60.3	4496.2	4502.7
GA_7	62.4	4510.2	4511.2
IG_7	67.3	4510.2	4514.7
AG_7	64.8	4511.2	4512.8
GG_7	73.4	4511.2	4513.3

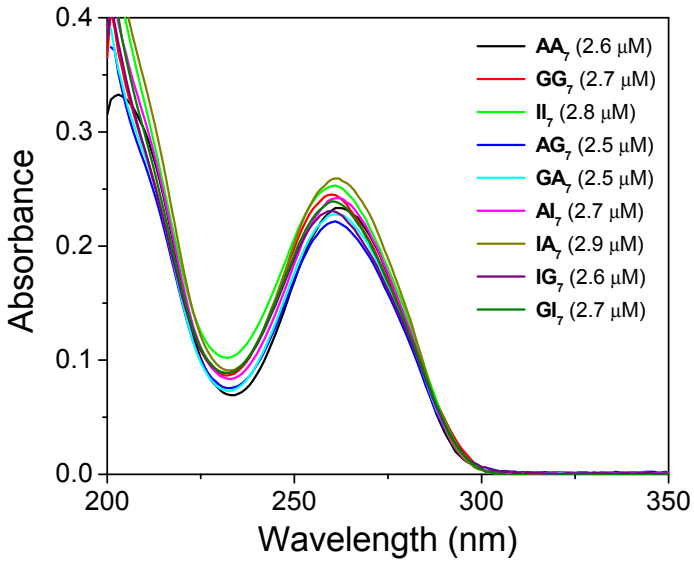

Fig. S1. UV-visible spectra of the hairpin conjugates in 10 mM phosphate buffer (pH 7.2) containing 100 mM NaCl.

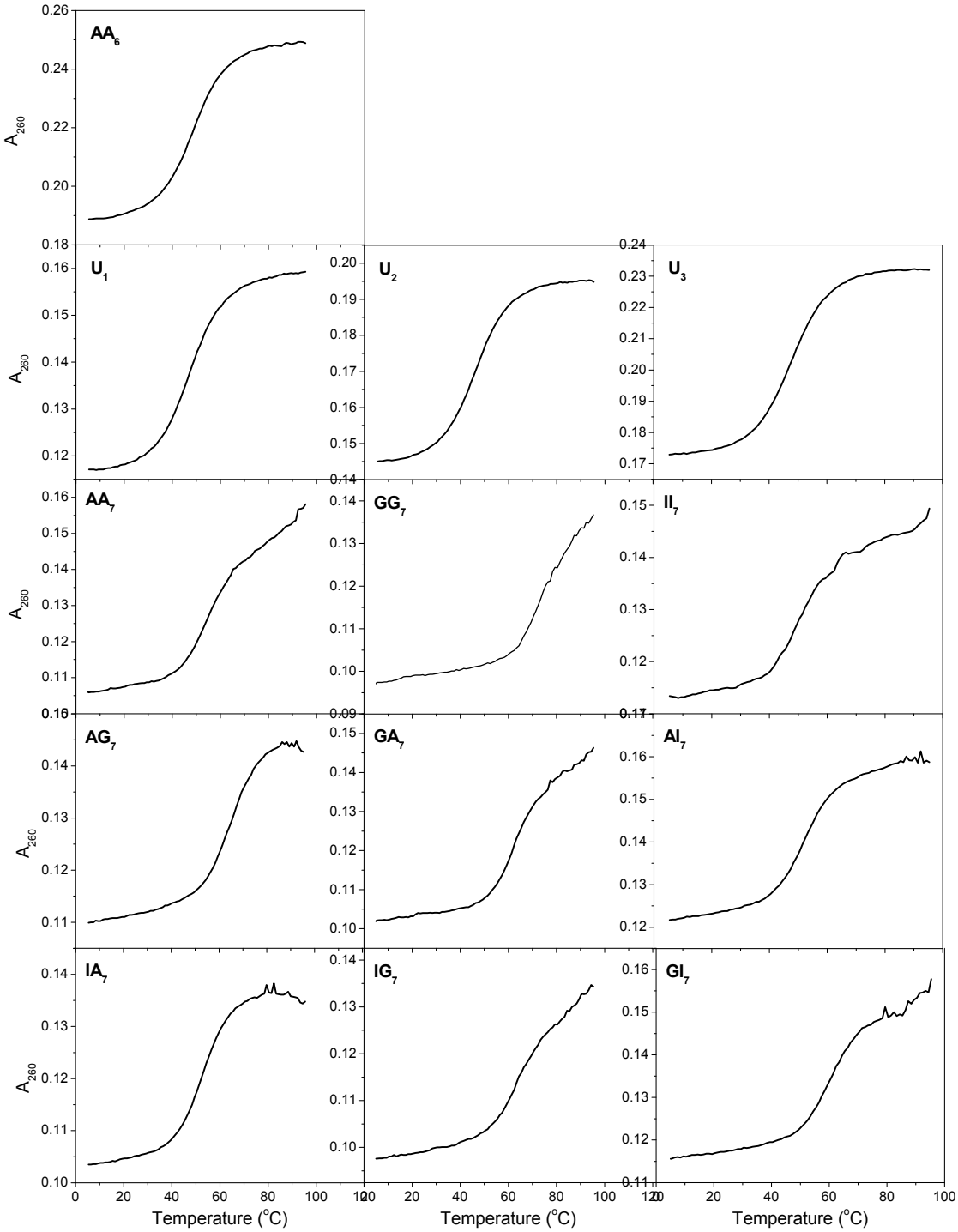

Fig. S2. Thermal denaturation curves monitored at 260 nm for all the hairpin conjugates in 10 mM phosphate buffer (pH 7.2) containing 100 mM NaCl.

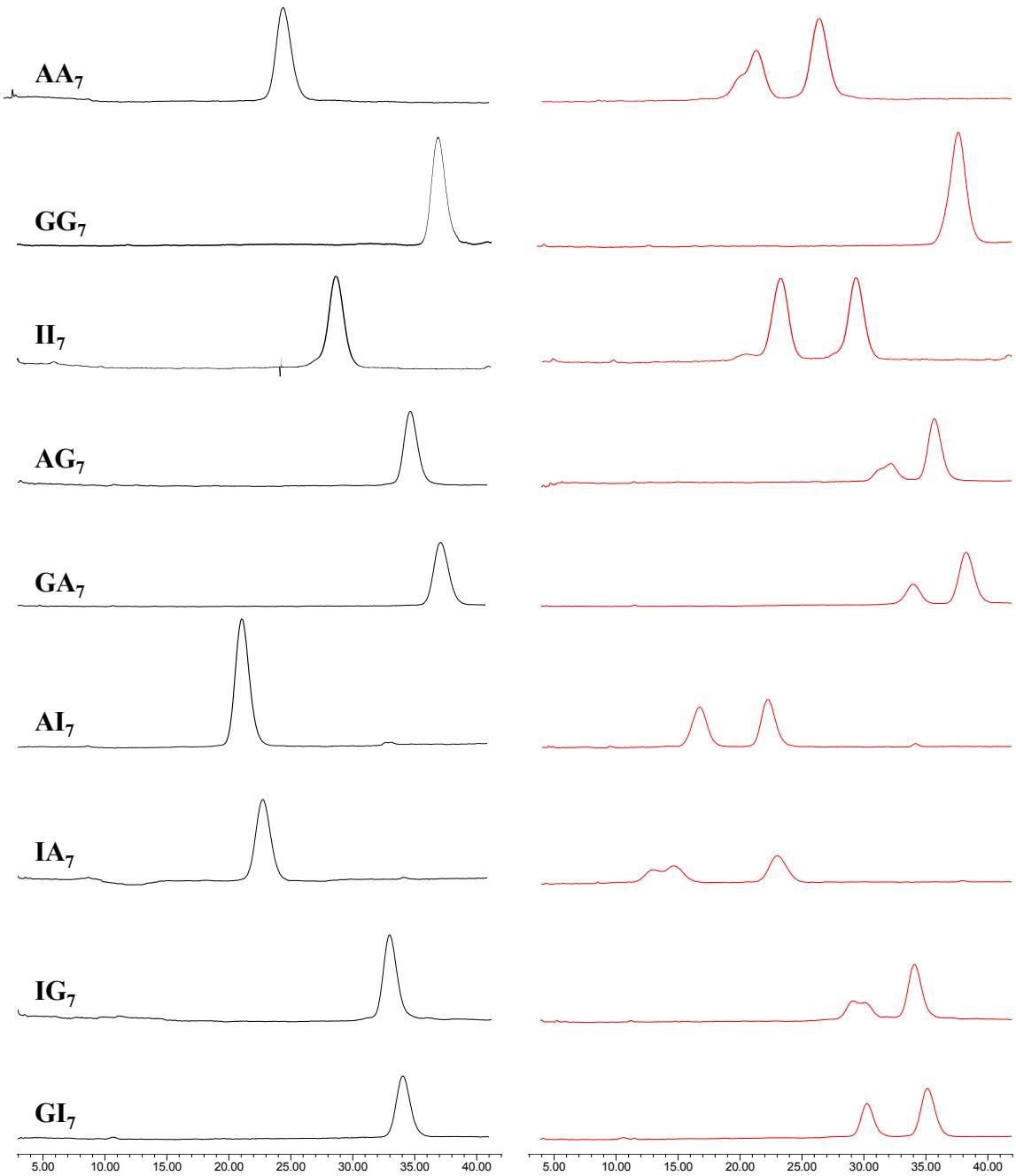

Fig. S3. HPLC traces of the 7 base-pair hairpin conjugates before (left) and after (right) irradiation for 60 minutes at 280 nm.

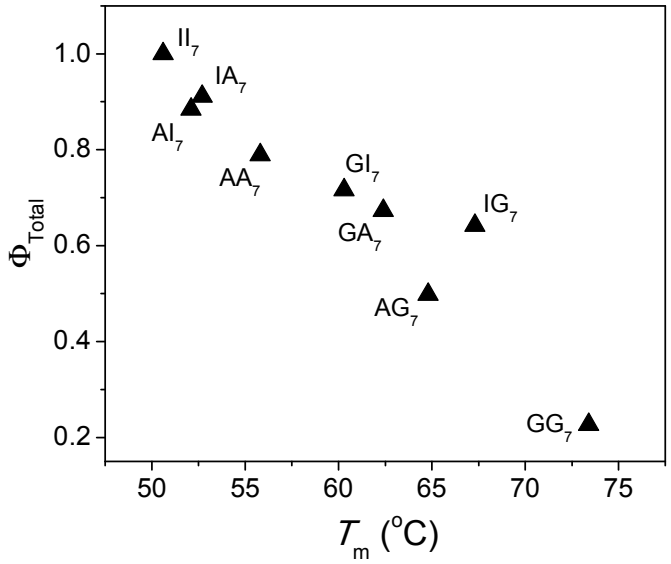

Fig. S4. Plot showing the effect of melting temperature on the total quantum yield of dimerization of the longer (7 base pair) hairpin sequences.