

Supporting Information:

Dewar Lesion Formation in Single- and Double-Stranded DNA is Quenched by Neighboring Bases

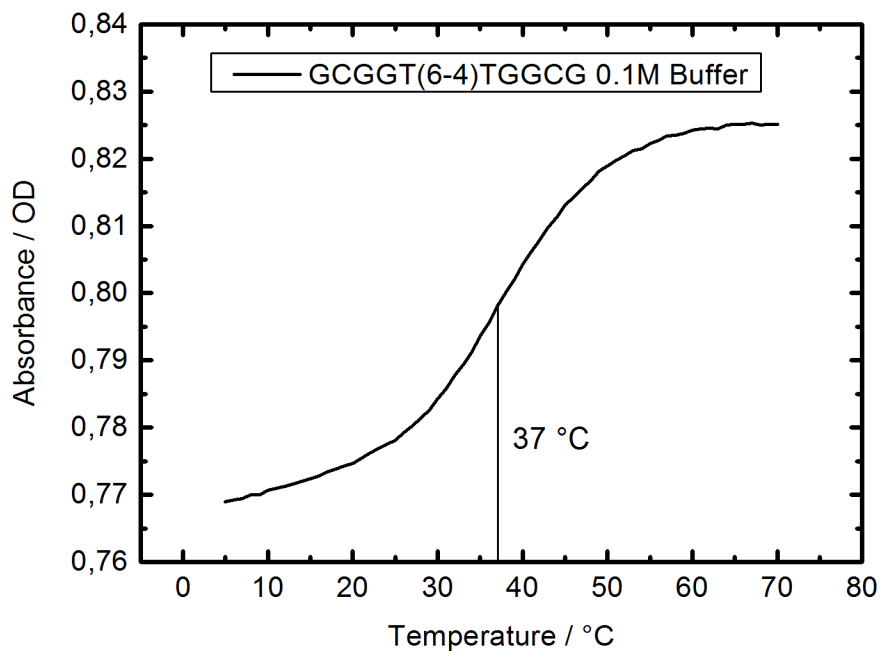
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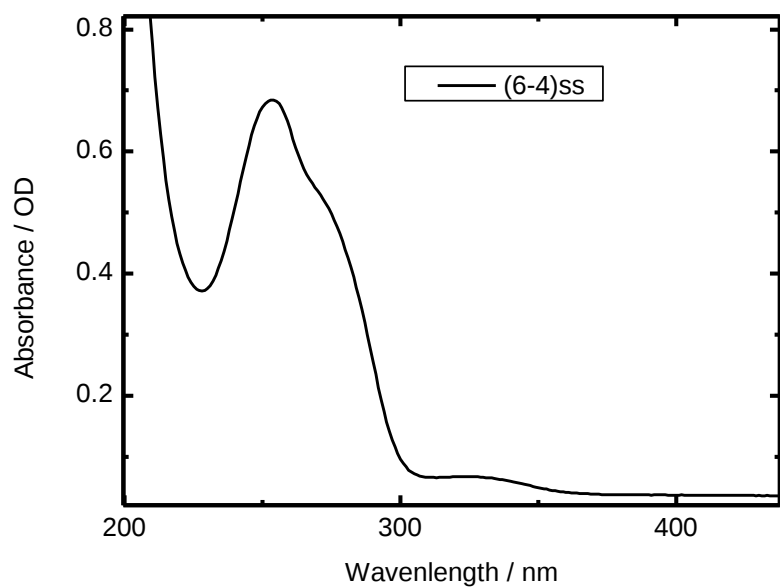
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SI1: Melting curve of the (6-4) ds sample.

The melting curve was recorded with a concentration of 3 μM of the GCGGT(6-4)TGGCG strand. The second derivative of the absorbance vs. temperature plot gives a melting temperature of 37 °C. The concentration of the sample for the time resolved measurement is in the mM regime, which enhances the melting temperature. Therefore the strand forms stable duplexes under the experimental conditions.



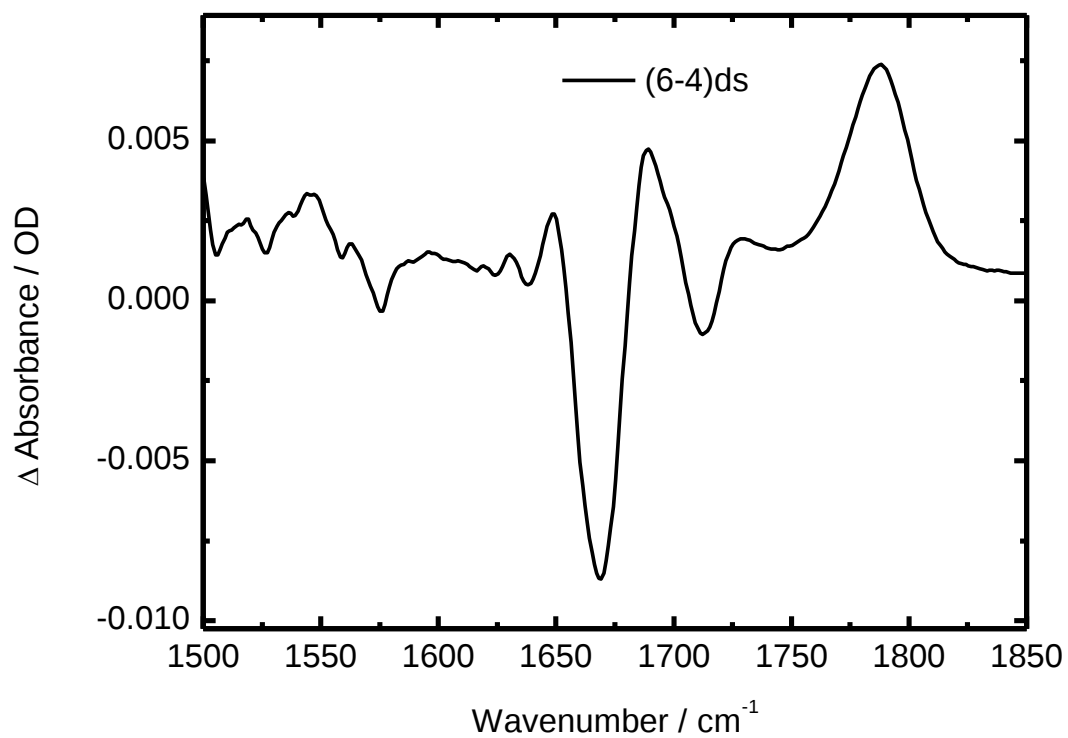
SI2: UV/Vis spectrum of (6-4)ss

The absorbance spectrum of the GGCGT(6-4)TGGCG single strand shows the characteristic absorbance of the 6-4 chromophore at 325 nm. The strong absorbance of the intact bases G and C is observable below 300 nm.

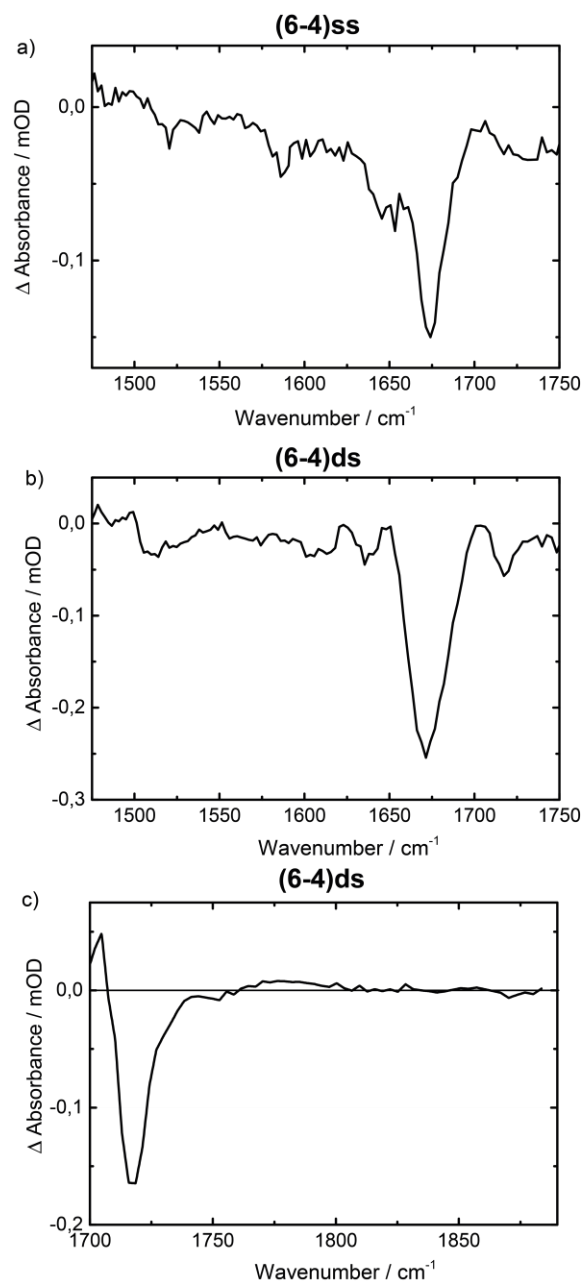
Nucleobase	Single Strand		Double Strand	
	Experiment	Literature	Experiment	Literature
Guanine	1673	1673–1660	1680	1689–1678
Guanine	1583	1590–1575	1581	1590–1575
Cytosine	1651	1655–1647	1650	1655–1647
Cytosine	1502	1506–1498	1503	1506–1498

	Dinucleotide	Single Strand	Double Strand
	Literature	Experiment	Experiment
6-4	1666	1672	1672
	1612	1612	---
	1591	1591	---
	1516	1516	1508

SI3: IR-marker bands for nucleobases in single and double strands as well as for the 6-4 lesion. Literature values taken from Banyay¹ et al., Haiser² et al. and Fingerhut et al.³.



SI4: Stationary IR difference spectrum of illuminated (6-4)ds sample (325 nm, 7 mW, 20 min) showing the Dewar marker band at 1787 cm^{-1} .



SI5: Decay associated difference spectra (DADS) of the long living component for the (6-4)ss (a) and (6-4)ds (b). The spectral region around the Dewar marker band at 1780 cm^{-1} is shown in detail in (c). Data of (c) obtained by averaging the transient spectra between 1 – 2 ns.

Literature

- (1) Banyay, M.; Sarkar, M.; Gräslund, A. A Library of IR Bands of Nucleic Acids in Solution. *Biophys. Chem.* **2003**, *104* (2), 477–488.
- (2) Haiser, K.; Fingerhut, B. P.; Heil, K.; Glas, A.; Herzog, T. T.; Pilles, B. M.; Schreier, W. J.; Zinth, W.; de Vivie-Riedle, R.; Carell, T. Mechanism of UV-Induced Formation of Dewar Lesions in DNA. *Angew. Chem. Int. Ed.* **2011**.
- (3) Fingerhut, B. P.; Herzog, T. T.; Ryseck, G.; Haiser, K.; Graupner, F. F.; Heil, K.; Gilch, P.; Schreier, W. J.; Carell, T.; Vivie-Riedle, R. de; et al. Dynamics of Ultraviolet-Induced DNA Lesions: Dewar Formation Guided by Pre-Tension Induced by the Backbone. *New J. Phys.* **2012**, *14* (6), 065006.