Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences
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Photobehaviour and DNA interaction of styrylquinolinium salts bearing thiophene substituents

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Supplementary data

1. double elix preparation

Decamer d(CGTACGTACG)2 purchased from GENSET was HPLC grade pure. The concentration of single strand was determined spectrophotometrically in water using the absorption coefficient at 260 nm ε_{260}= 1.05 × 10^5 M^{-1} cm^{-1}. Then DNA was lyophilized and dissolved in 0.02 M Tris-HCl (pH 7.4) and 0.2 M NaCl to obtain the double helix. The optical melting curve was registered at 260 nm with a temperature increase of 0.5°C/min. starting from 8°C. The melting transition starts above 30°C thus, under our experimental conditions, the duplex state is prevalent. DNA concentration is expressed throughout molar duplex concentrations.

2. Complexation UV difference absorption spectra

The interactions of cations **1-3** with the decamer d(CGTACGTACG)2 were first investigated by UV- Vis difference spectra at constant duplex concentration, on increasing the ligand concentration.

In order to exclude ligand-ligand interactions such as aggregation, etc., the linearity of the Lambert-Beer law was verified in the examined concentration range for all ligands **1-3**. In the absence of interactions with the decamer, difference spectra should exhibit no absorbance in the ligand characteristic absorption wavelength range. Here we report the absorbance values and the UV difference spectra registered for compounds **1-3** at different ratios of [Comp]/[DNA].

Table A1: Description of solutions A-H for the **1**/DNA system used to record the difference absorption spectra of Fig. A1 (the absorbance value at 440 nm is also reported).

	[Comp 1]	[DNA]	[Comp1]/[DNA]	$A_{(440\ nm)}$	cell
A	0	8.6x10^{-6}	0	-	1cm
B	2.15x10^{-6}	8.6x10^{-6}	0.25	-0.008	1cm
C	4.3x10^{-6}	8.6x10^{-6}	0.5	-0.017	1cm
D	8.6x10^{-6}	8.6x10^{-6}	1	-0.031	1cm
E	1.72x10^{-5}	8.6x10^{-6}	2	-0.07	1cm
F	2.58x10^{-5}	8.6x10^{-6}	3	-0.12	1cm
G	3.44 x10^{-5}	8.6x10^{-6}	4	-0.17	1cm
H	5.16 x10^{-5}	8.6x10^{-6}	6	-0.26	1cm

Table A2: Description of solutions A-H for the **2**/DNA system used to record the difference absorption spectra of Fig. A2 (the absorbance value at 410 nm is also reported).

	[Comp 2]	[DNA]	[Comp2]/[DNA]	$A_{(410\ nm)}$	cell
A	0	8.6x10^{-6}	0	–	1cm
B	2.15x10^{-6}	8.6x10^{-6}	0.25	0.02	1cm
C	4.3x10^{-6}	8.6x10^{-6}	0.5	0.01	1cm
D	8.6x10^{-6}	8.6x10^{-6}	1	0.005	1cm
E	1.72x10^{-5}	8.6x10^{-6}	2	-0.001	1cm
F	2.58x10^{-5}	8.6x10^{-6}	3	-0.02	1cm
G	3.44 x10^{-5}	8.6x10^{-6}	4	-0.03	1cm
H	5.16 x10^{-5}	8.6x10^{-6}	6	-0.06	1cm

Table A3 Description of solutions **A-H** for the **3**/DNA system used to record the difference absorption spectra of Fig. A3 (the absorbance value at 424 nm is also reported).

	[Comp **3**]	[DNA]	[Comp**3**]/[DNA]	$A_{(424\ nm)}$	cell
A	0	8.6x10^{-6}	0	-	1cm
B	2.15x10^{-6}	8.6x10^{-6}	0.25	-	1cm
C	4.3x10^{-6}	8.6x10^{-6}	0.5	-	1cm
D	8.6x10^{-6}	8.6x10^{-6}	1	-	1cm
E	1.72x10^{-5}	8.6x10^{-6}	2	-0.001	1cm
F	2.58x10^{-5}	8.6x10^{-6}	3	-0.007	1cm
G	3.44 x10^{-5}	8.6x10^{-6}	4	-0.013	1cm
H	5.16 x10^{-5}	8.6x10^{-6}	6	-0.02	1cm

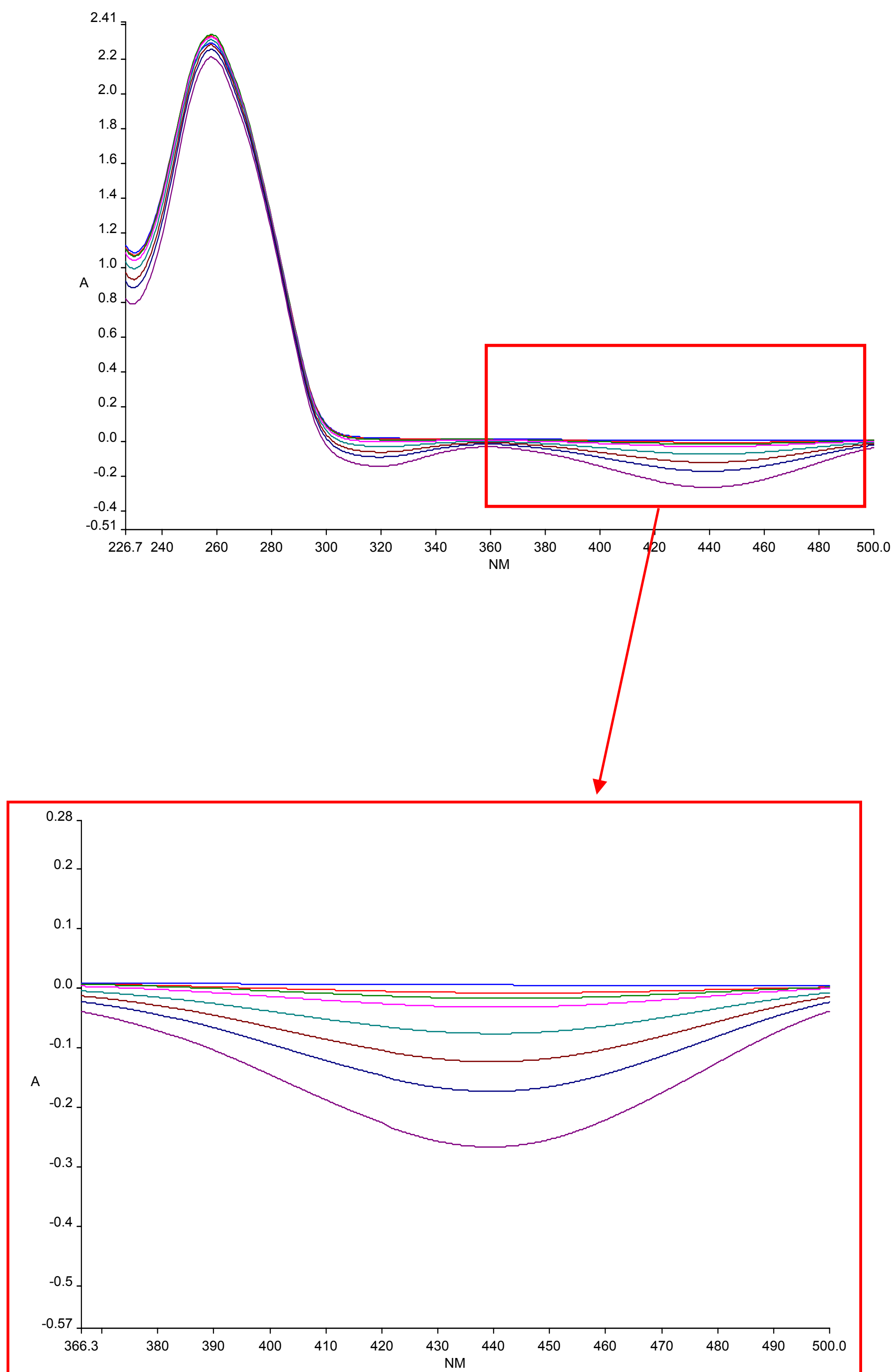
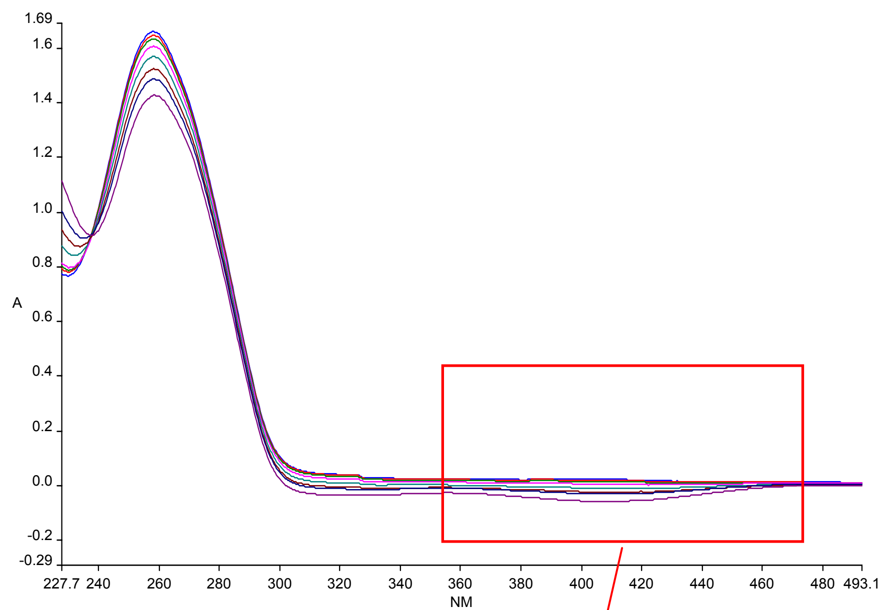


Fig. A1: Difference absorption spectrum of **1**/ DNA system recorded after successive additions of ligand **1** (solutions **A-H** of Table A1).



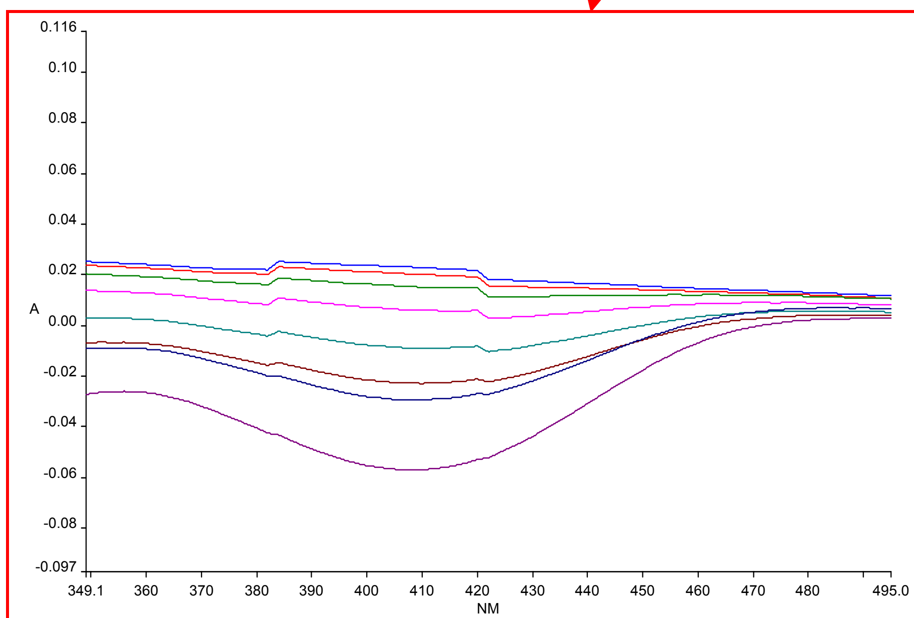


Fig. A2: Difference absorption spectrum of **2**/ DNA system recorded after successive additions of ligand **2** (solutions **A-H** of Table A2).

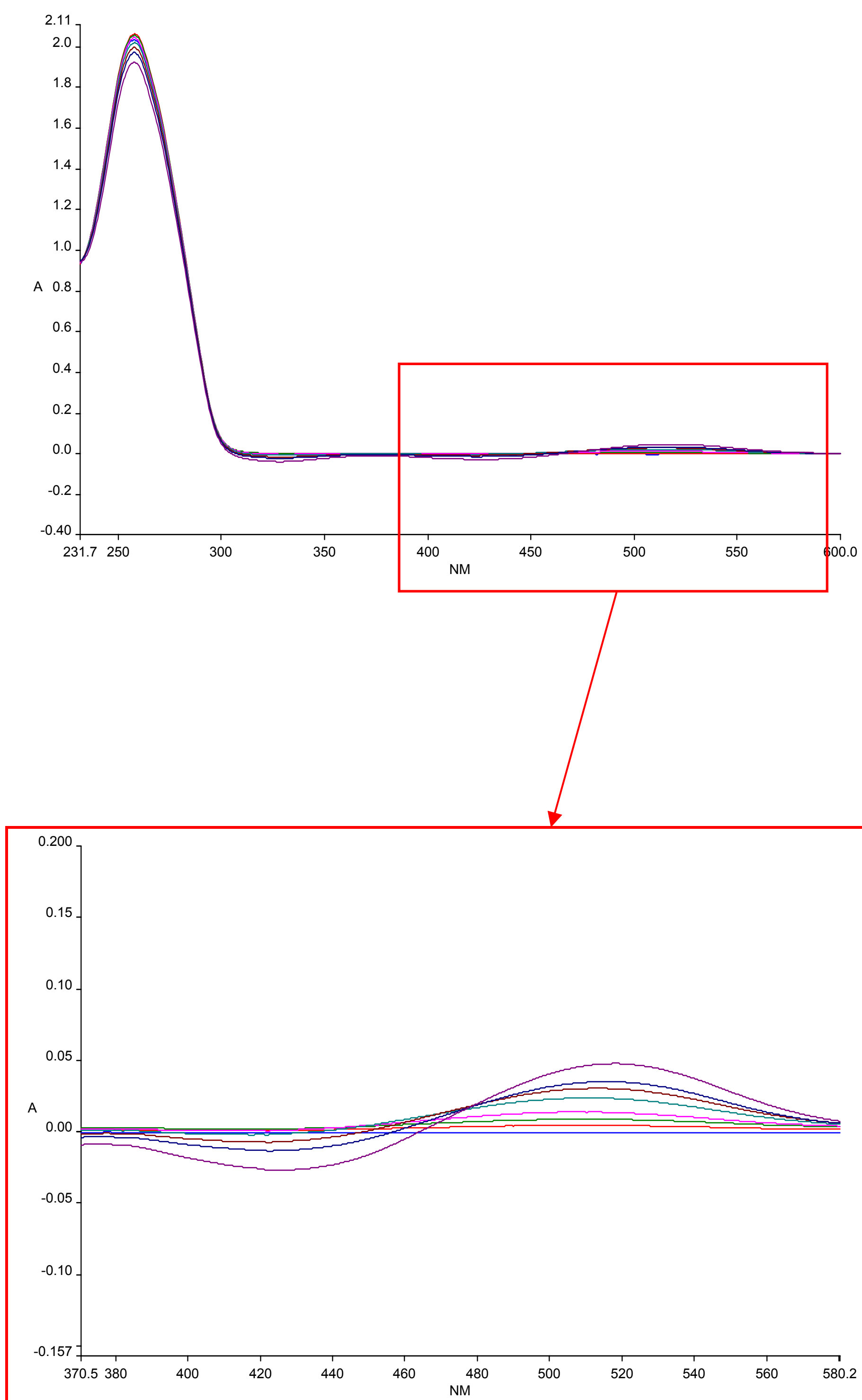


Fig. A3: Difference absorption spectrum of **3**/ DNA system recorded after successive additions of ligand **3** (solutions **A-H** of Table A3).

3. Absorption and fluorescence titrations.

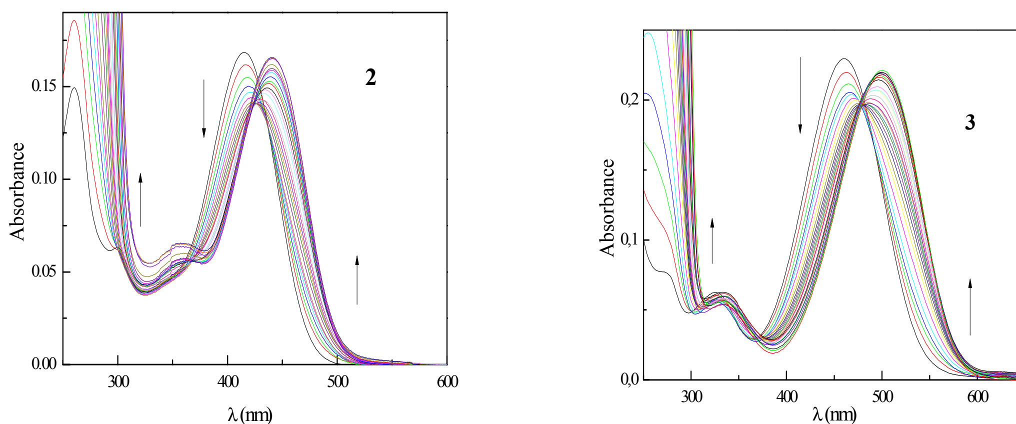


Fig. A4: Absorption spectra of the ligands **2** and **3** (corrected for dilution) recorded after successive additions of a DNA solution up to 8×10^{-4} M.

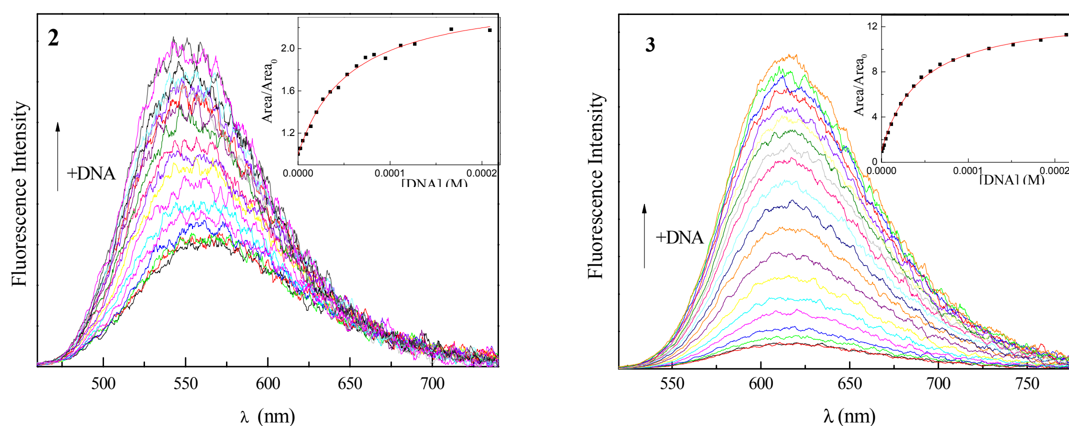


Fig. A5: Fluorescence spectra of the ligands **2** and **3** (corrected for dilution) recorded after successive addition of a DNA solution up to 2×10^{-4} M. The inset shows the fitting of the fluorescence spectra areas according to eq. 2.

4. Spectral properties of the DNA-ligand complexes.

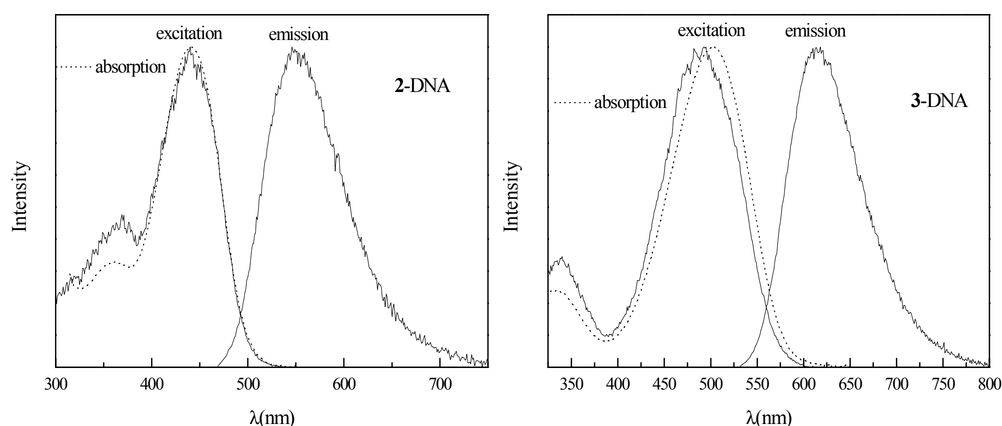


Fig. A6: Normalized absorption and fluorescence excitation and emission spectra of the **2**- and **3**-DNA complexes in buffered (ETN) water.