Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Photochemistry and DNA-affinity of some pyrimidine-substituted styryl-azinium iodides

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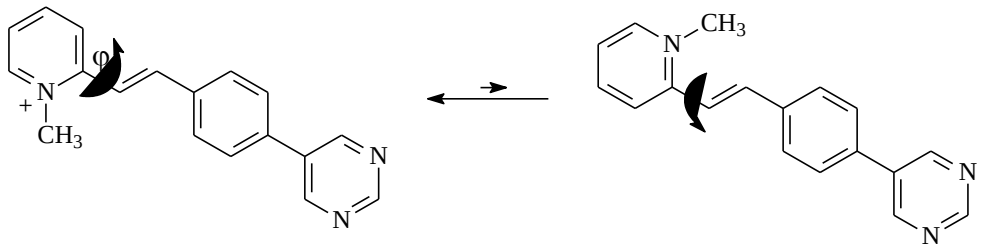
Electronic Supplementary Information: computational results, linear dichroism spectra and fitting of the .



conformer **B** conformer **A**

Scheme ESI 1 Conformers of compound **1**

Table ESI 1 Computed parameters for the ground state and the first electronic transitions of compounds **1**-**3**: formation enthalpy ($\Delta H_f°$, kcal mol^{-1}), relative conformational abundance at 293 K (%), dipole moment (D) in the ground (μ_g) and excited (μ_e) states, dihedral angle (φ, degrees), absorption wavelength (λ, nm) and oscillator strength (f).

Compound	$\Delta H_f°$	%	φ	μ_g	μ_e	λ	f	configuration	coeff.
1(A)	257.948	1.4	54.39°	20.32	6.55	348	0.96	H→L	0.64
						262	0.59	H→L+1	-0.62
1(B)	255.460	98.6	2.59°	19.23	8.80	363	1.63	H→L	0.66
						259	0.23	H→L+1	0.62
2(A)	270.821	0.6	-42.18°	16.48	1.81	365	1.46	H→L	0.65
						245	0.59	H→L+1, H-2→L	0.46, -0.33
2(B)	267.827	99.4	-4.20°	15.50	3.65	371	1.93	H→L	0.66
						257	0.19	H→L+1, H-2→L	0.35, 0.48
3	243.035	100	-27.34°	18.90	10.77	338	1.59	H→L	0.67
						220	0.36	H→L+1	-0.61

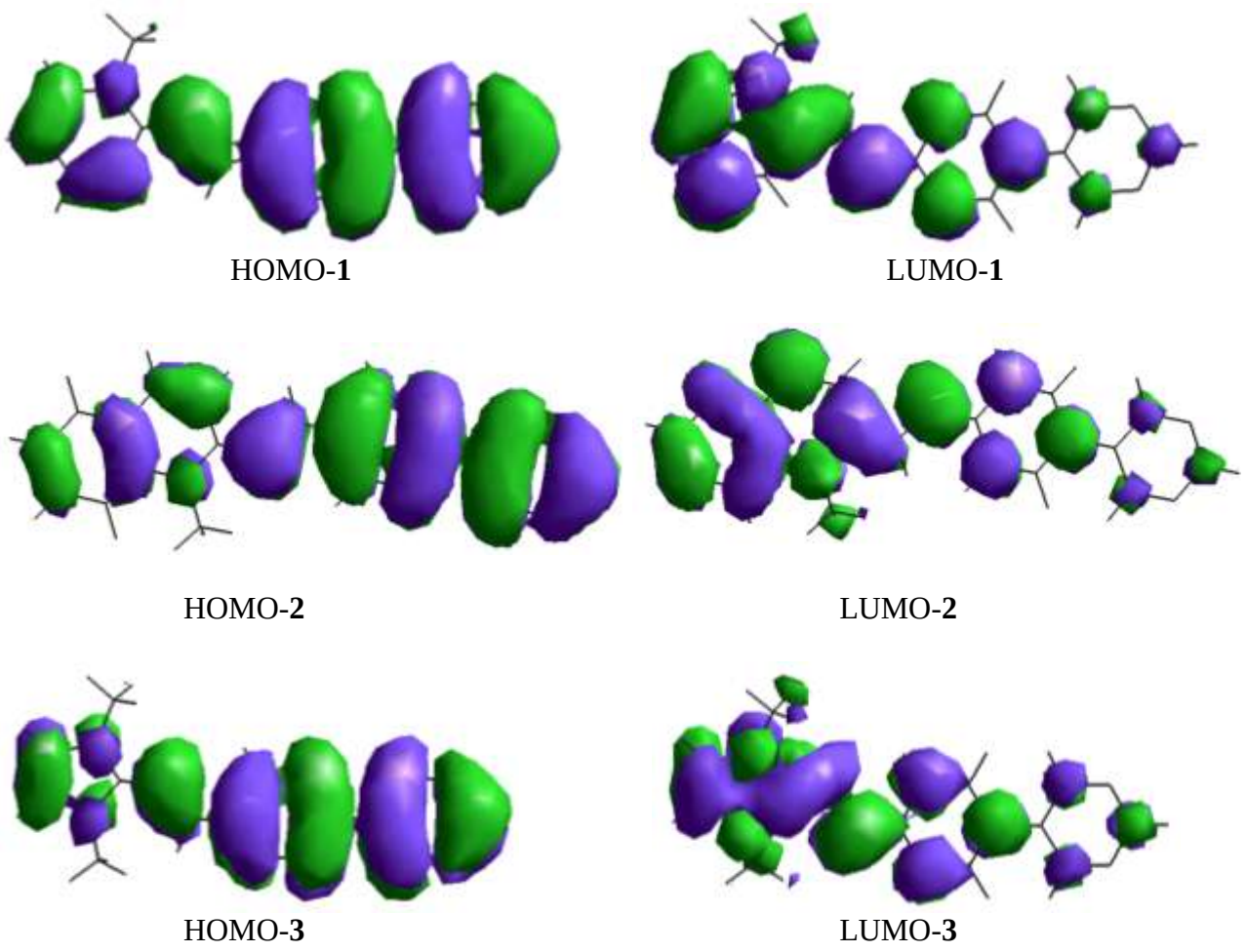


Fig. ESI 1 Molecular orbitals of **1** as derived by ZINDO/S method. The HOMO-LUMO configuration contributes to the main electronic transition with the highest coefficient.

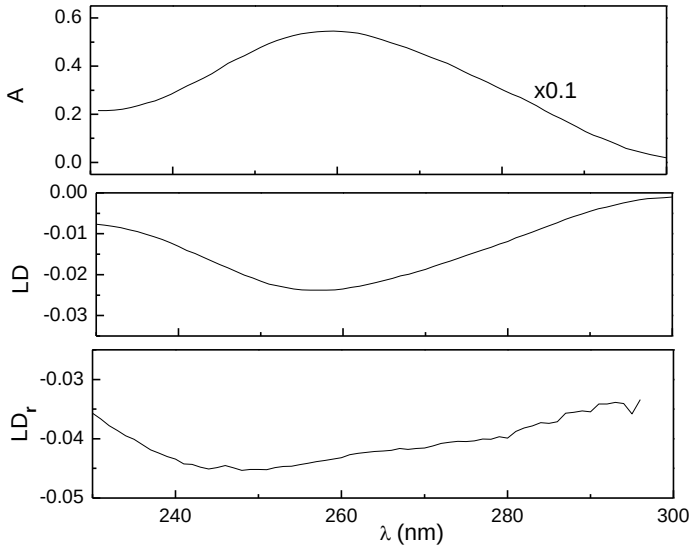


Fig. ESI 2 Absorption, linear dichroism (LD) and reduced LD_r spectra for salmon DNA.

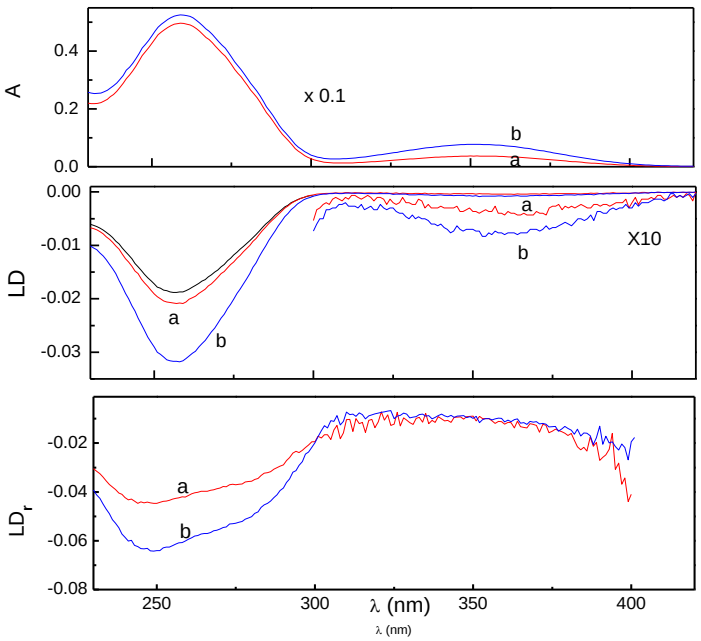


Fig. ESI 3 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **1**-DNA at a [ligand]/[DNA] ratio of 0.04 (a) and 0.08 (b). LD for DNA is shown for comparison, black trace.

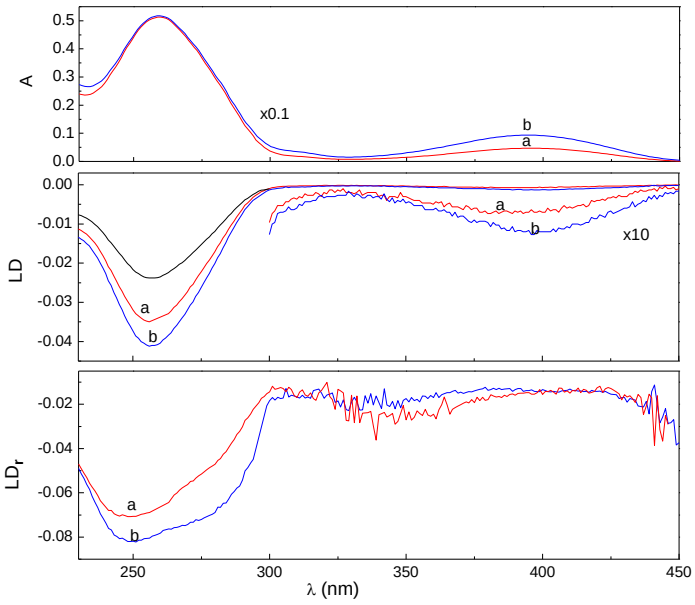


Fig. ESI 4 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **2**-DNA at a [ligand]/[DNA] ratio of 0.04 (a) and 0.08 (b). LD for DNA is shown for comparison, black trace.

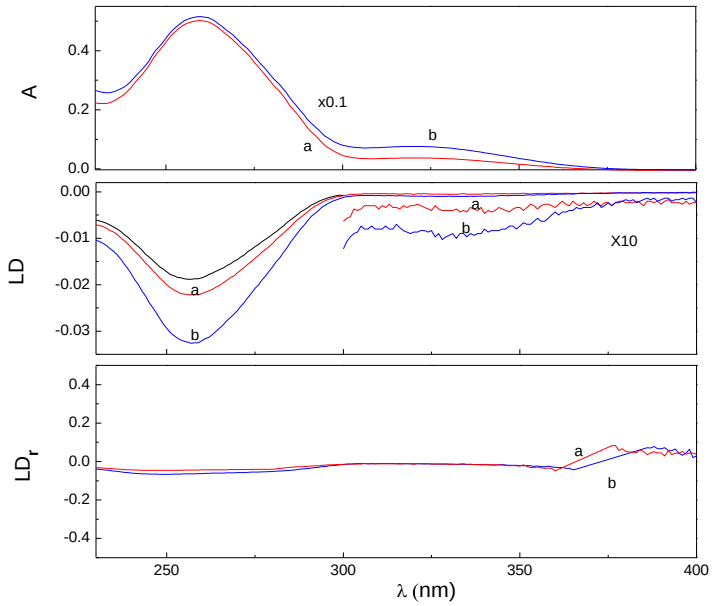


Fig. ESI 5 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **3**-DNA at a [ligand]/[DNA] ratio of 0.04 (a) and 0.08 (b). LD for DNA is shown for comparison, black trace.

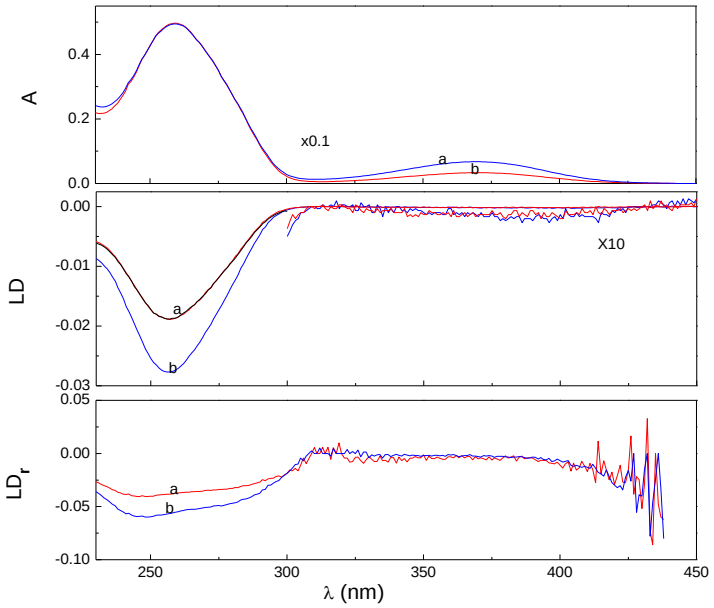


Fig. ESI 6 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **4**-DNA at a [ligand]/[DNA] ratio of 0.04 (a) and 0.08 (b). LD for DNA is shown for comparison, black trace.

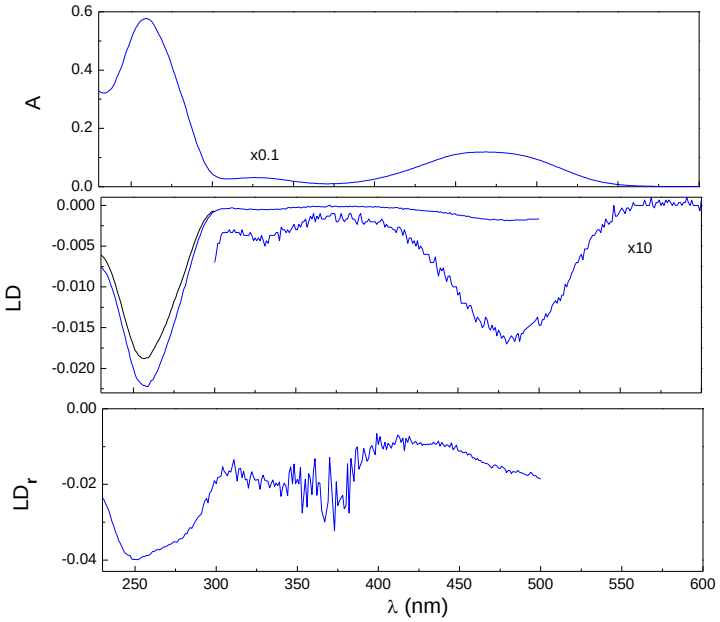


Fig. ESI 7 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **5**-DNA at a [ligand]/[DNA] ratio of 0.08. LD for DNA is shown for comparison, black trace.

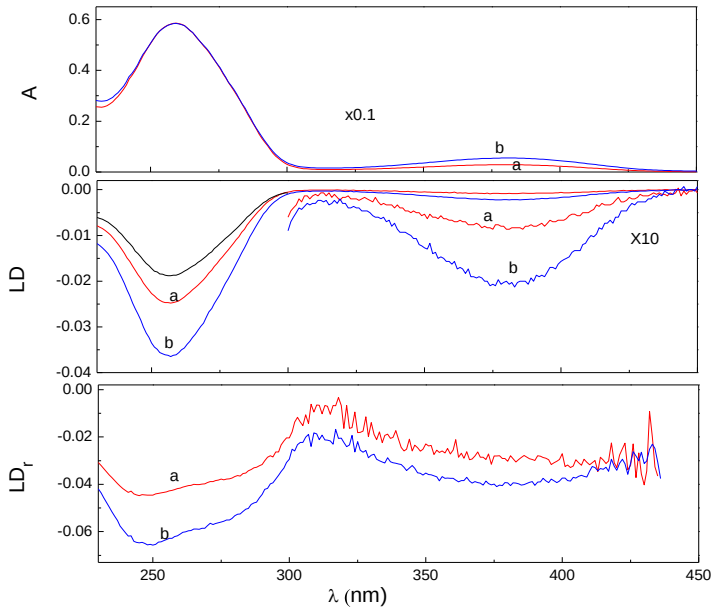


Fig. ESI 8 Absorption, linear dichroism (LD) and reduced LD_r spectra for the complex **6**-DNA at a [ligand]/[DNA] ratio of 0.04 (a) and 0.08 (b). LD for DNA is shown for comparison, black trace.

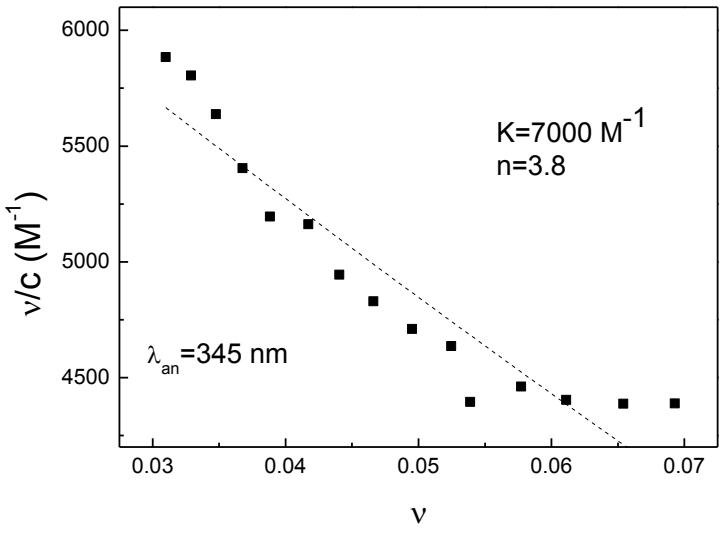


Fig. ESI 9 Plot to obtain the association constant of the **1**-DNA complex according to the eq. 1.

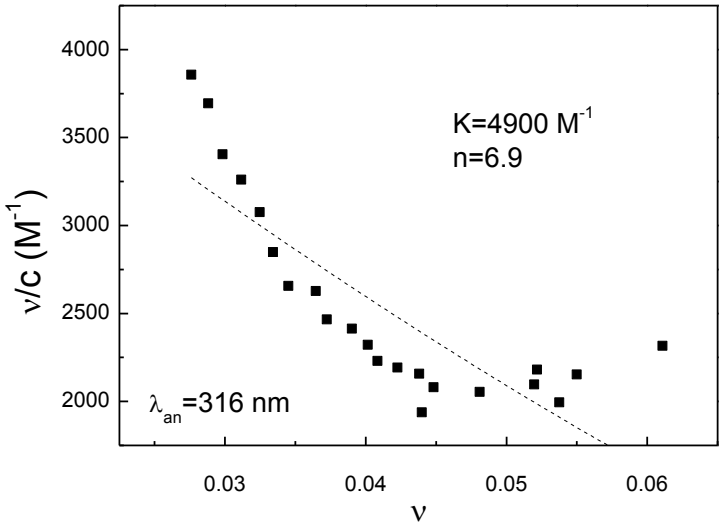


Fig. ESI 9 Plot to obtain the association constant of the **3**-DNA complex according to the eq. 1.