

Photobehaviour of methyl-pyridium and quinolinium iodides derivatives, free and complexed with DNA. A case of bisintercalation.

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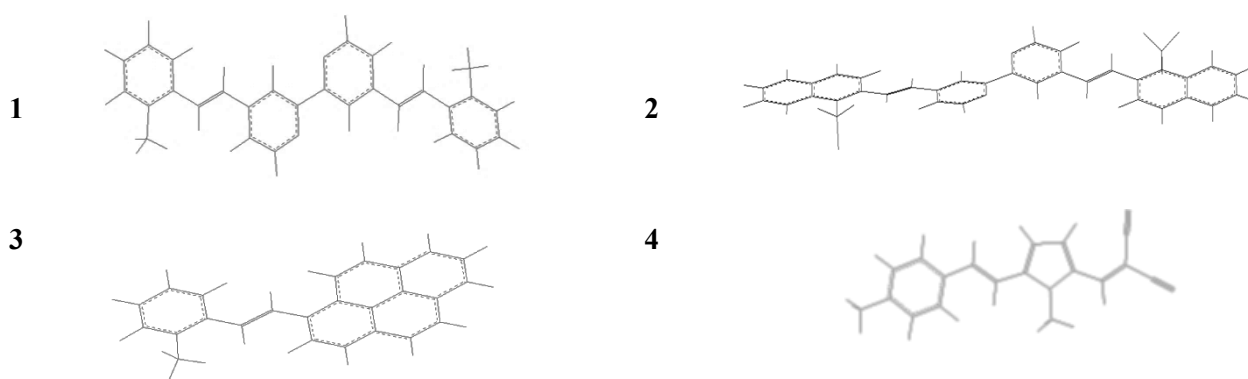
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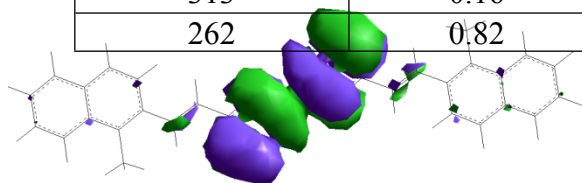
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Electronic Supplementary Information: computational results, decay kinetics by pump probe absorption spectroscopy plots to determine binding constants by absorption and fluorimetric titrations and linear dichroic signals..

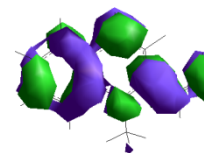


Scheme ESI 1- A conformers of compounds 1-4.

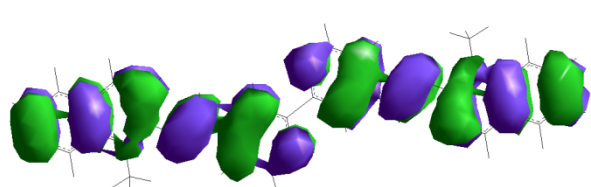
λ (nm)	f	configuration	coeff.
355	2.80	H-1 \rightarrow L+1, H-2 \rightarrow L	0.47, -0.47
313	0.16	H \rightarrow L	0.59
262	0.82		



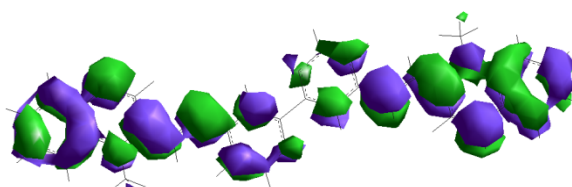
HOMO



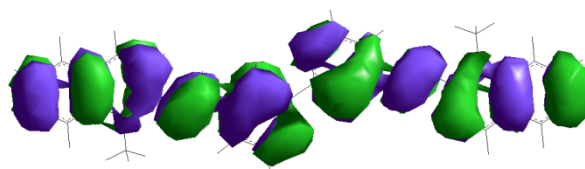
LUMO



HOMO - 1



LUMO + 1



HOMO -2

Figure ESI 1- Molecular orbitals of compound **2** as derived by ZINDO/S method. Inserted table: the HOMO-1 –LUMO+1 and HOMO-2 - LUMO configurations contribute to the main electronic transition with high coefficients.

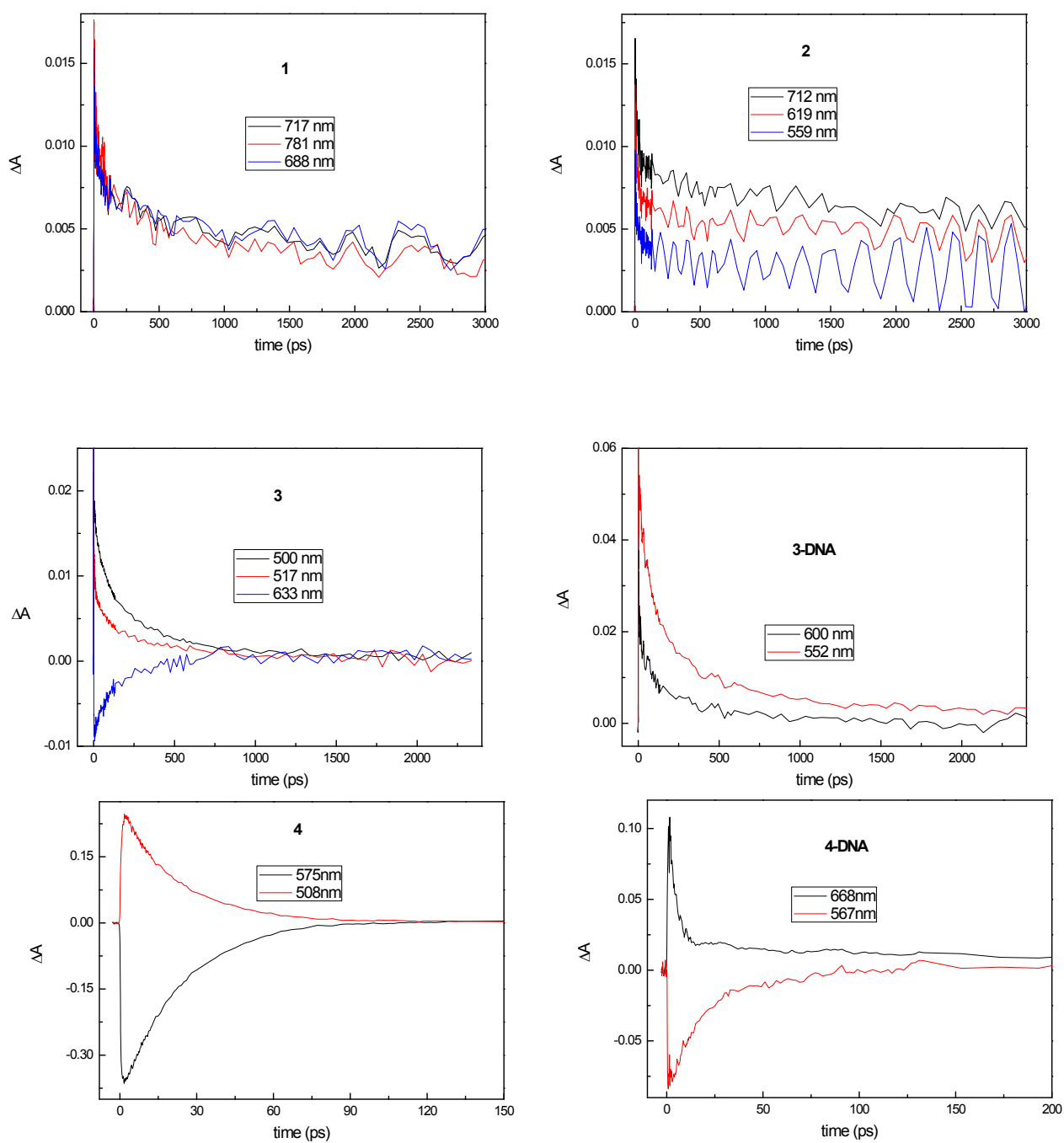


Figure ESI 2- Decay kinetics by pump probe absorption spectroscopy of compounds **1-4** and complexes **3-DNA** and **4-DNA** in W (Insets of Figure 3).

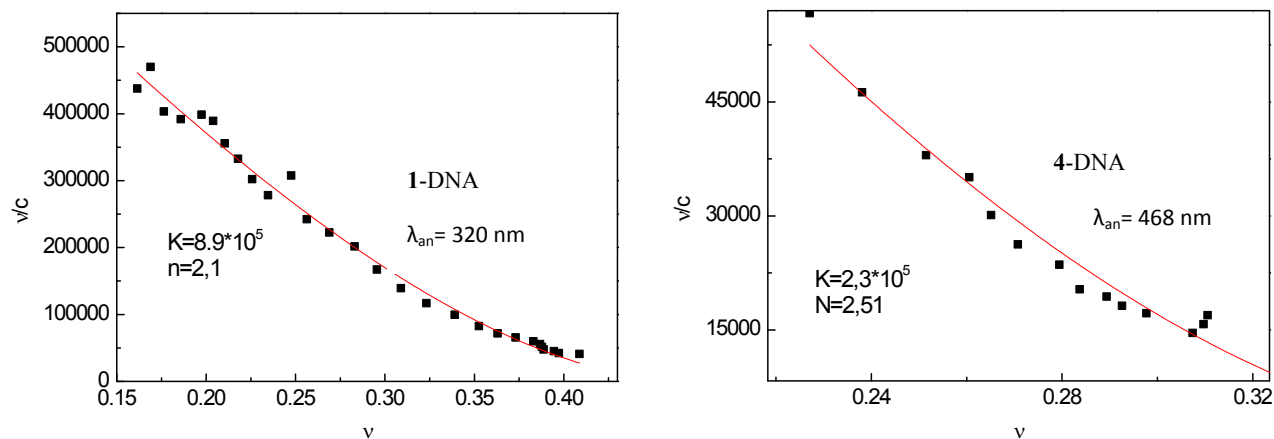


Figure ESI 3- McGhee von Hippel plots to determine binding constants from spectrophotometric titrations according to eq. 1, for complexes **1-DNA** and **4-DNA** in W (Insets of Figure 4).

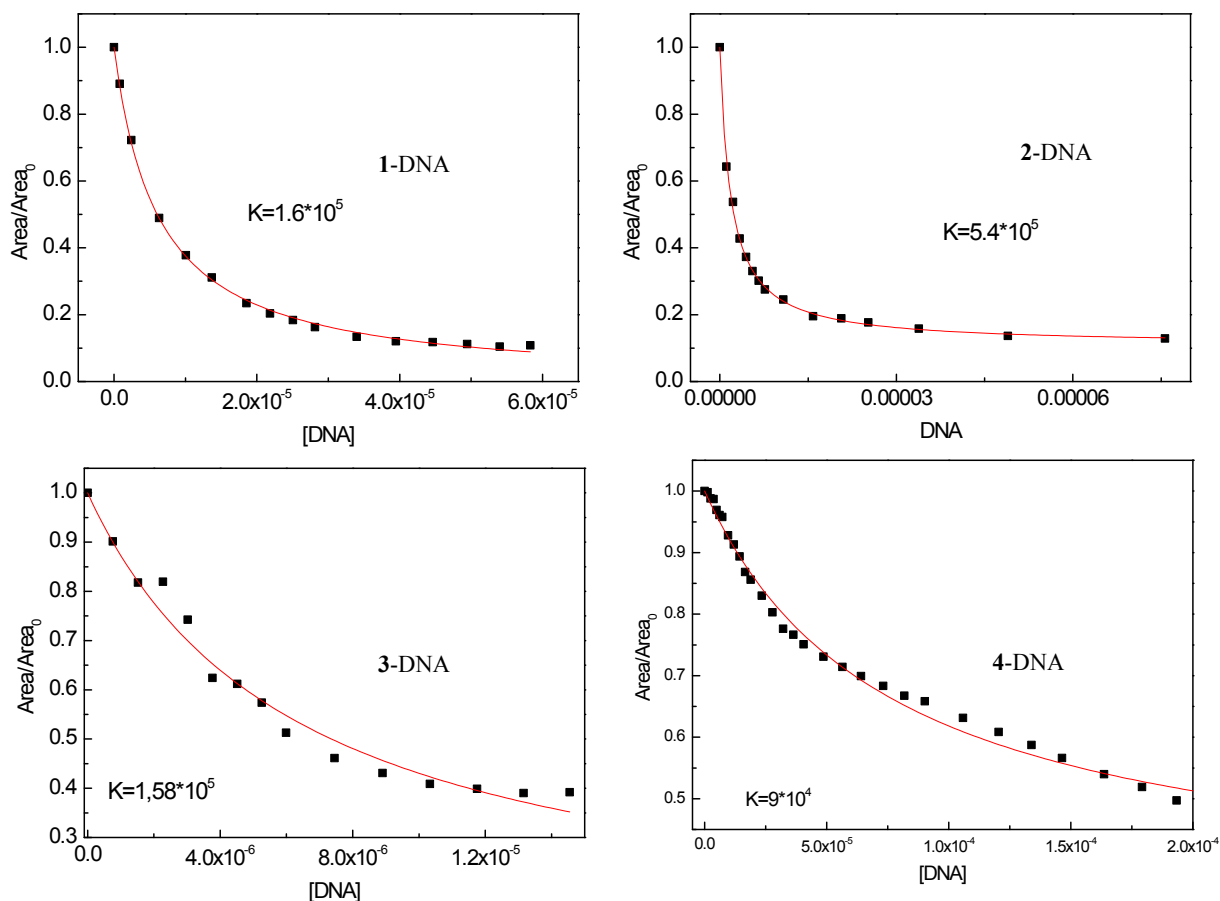
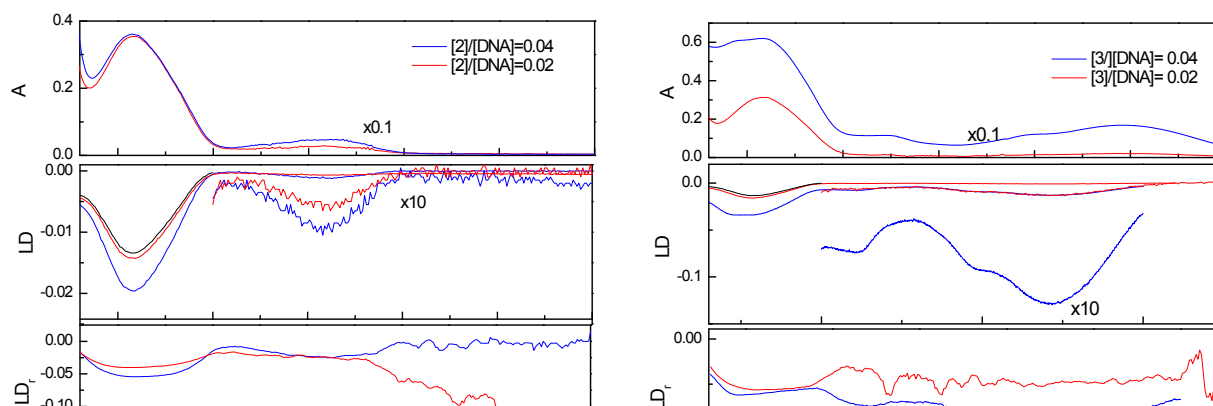


Figure ESI 4- Stern-Volmer plots to determine binding constants from fluorimetric titrations according to eq. 2, for complexes **1,2,3,4-DNA** in W (Insets of Figure 5).



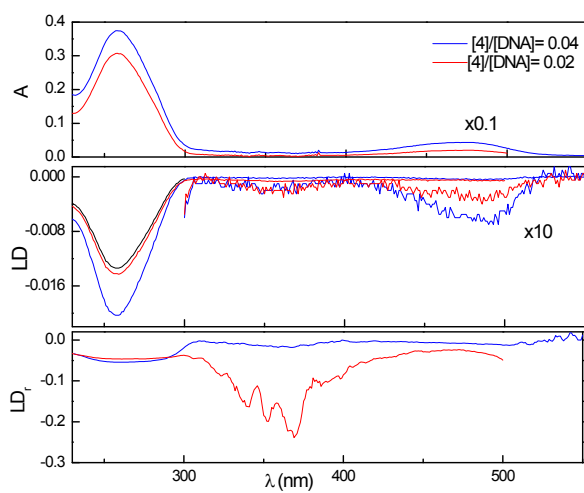


Figure ESI 5- Absorption LD and LD_r signals of compounds **2-4** with [ligand]/[DNA] ratio of 0.04 and 0.02.