Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Studying the excited electronic states of Guanine rich DNA quadruplex by quantum mechanical methods: main achievements and perspectives.

Lara Martínez-Fernández, Luciana Esposito and Roberto Improta

Supporting Information **Page**

Table S1. Vertical absorption energies and oscillator strengths for guanine with and without Na^+ atom, by using the coordination geometry depicted below, with a distance of 1 or 2 Angstroms from the tetrad plane, computed at the TD-PCM-M052X/6-31G* level of theory.

		G/Na^+ 1 Å[a]		G/Na^+ 2 Å[b]		G	
		ΔE (eV)	**F**	**ΔE (eV)**	**F**	**ΔE (eV)**	**f**
S_1	ππ* (La)	5.13	0.19	5.17	0.19	5.23	0.18
S_2	ππ* (Lb)	5.72	0.46	5.71	0.46	5.71 (S_3)	0.45

Notes: a) distance from the carbonyl oxygen 2.3 Å. b) distance from the carbonyl oxygen 2.7 Å.

Figure S1. Computed Absorption Spectra (a) for a representative tetrad (b) varying the distance between the central ion (Na^+ in blue and K^+ in red) and the centre of the tetrad computed at the TD-PCM-M052X/6-31G*/M052X/6-31G* level of theory.