Supporting Information for
Watson-Crick Base Pairing, Electronic and Photophysical Properties of Triazole Modified Adenine Analogues: A Computational Study

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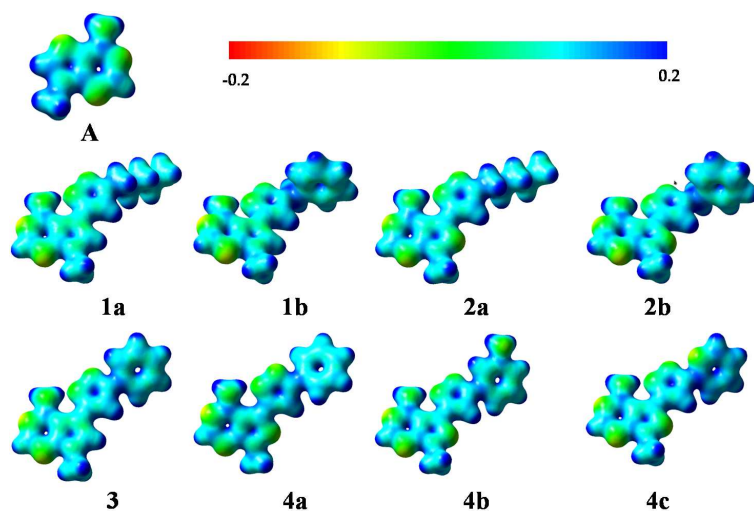
Figure S1: Molecular Electrostatic Potentials (MEPs) are mapped onto the surfaces. Red denotes negative potential and blue positive potential.

Table S1: Intramolecular $N-H\cdots N$ hydrogen bond donor-acceptor distances in triazole adenine analogues calculated in B3LYP/6-31++g(d,p) level

Analogues	1a	1b	2a	2b	3	4a	4b	4c
$N-H\cdots N$ distance (Å)	2.883	2.885	2.922	2.924	2.888	2.930	2.926	2.927

Optical absorptions in Adenine
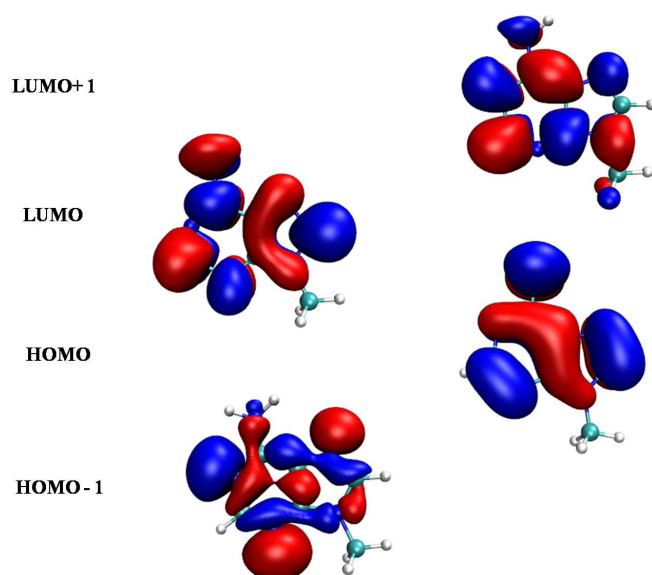
Figure S2: Calculated frontier molecular orbitals of adenine

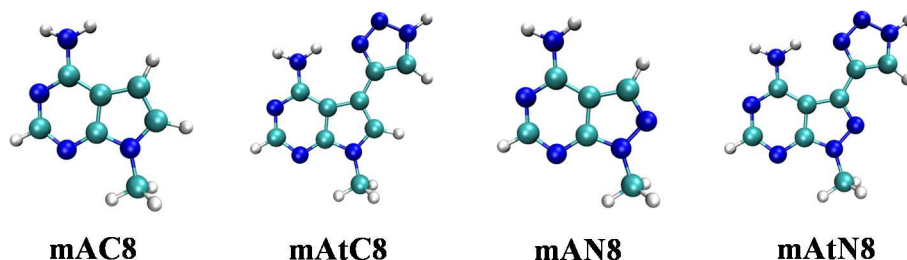**mAC8**   **mAtC8**   **mAN8**   **mAtN8**

Figure S3: B3LYP/6-31++G(d,p) level optimized structures of model structures. Atom colour code: blue (N), cyan (C), white (H).

Details of the model structures

We have replaced the substituents, that are attached to the triazole ring in the analogues, by a hydrogen atom to get two different model structures such as mAtC8 (in which purine 8-position consists of a carbon atom) and mAtN8 (in which a nirogen atom has been incorporated at the purine 8-position). Further, by replacing the triazole rings in mAtC8 and mAtN8 with a hydrogen atom, we arrive at the parent backbone structures, mAC8 and mAN8 respectively. The ground state geometry of all four model structures are optimized in the B3LYP/6-31++G(d,p) level of theory in gas phase and their fully optimized structures are shown in Figure S3. Vertical excitation energies, oscillator strengths and state assignments for three lowest singlet transitions (in methanol) of these model structures are shown in Table S2. Absorption spectra of model structures are shown in Fig. S4. Relevant molecular orbitals dominating these excitations are depicted in Fig S5.

Table S2: Three lowest vertical excitation energies (E), oscillator strengths (f) and state assignments (with % contribution) of model structures in methanol.

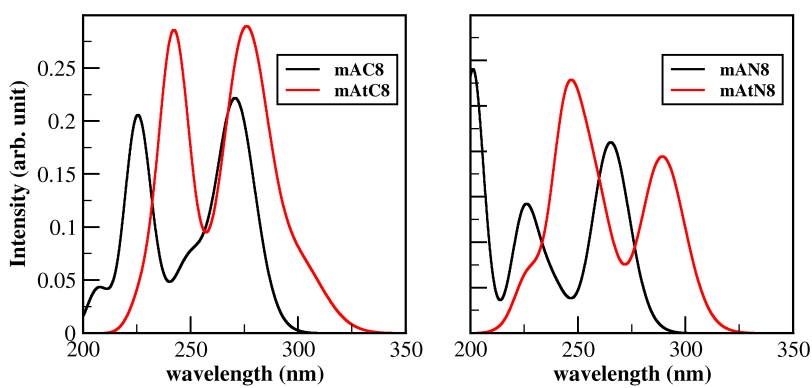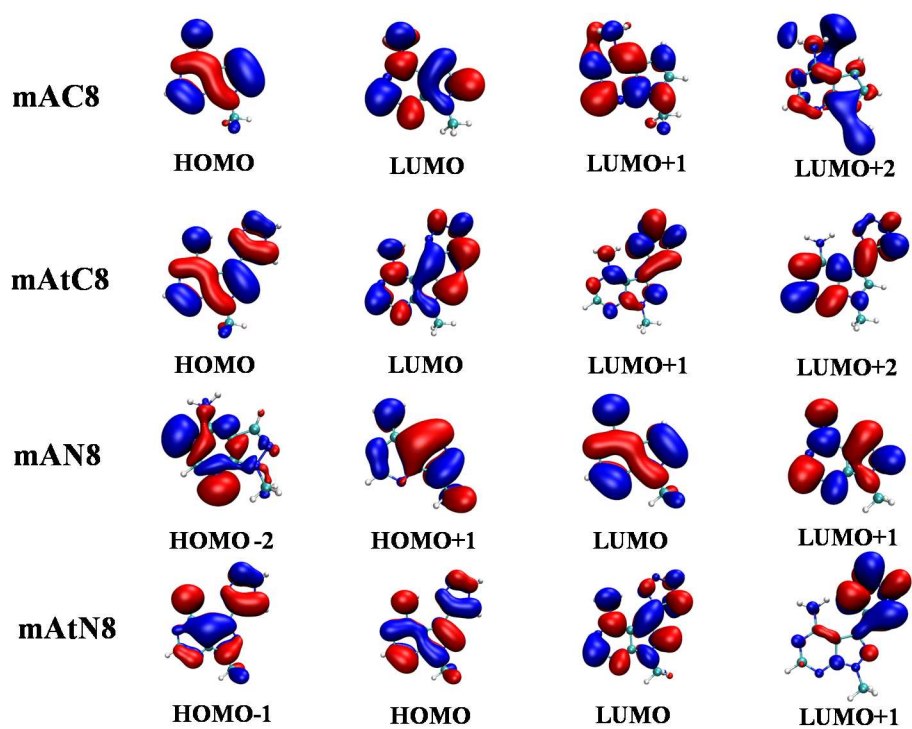| Analogues	E(eV)	f	Assignment
mAC8	4.58	0.219	H $\to$ L (90%), $\pi - \pi^*$
	4.95	0.041	H $\to$ L+1 (74%), $\pi - \pi^*$
	4.98	0.028	H $\to$ L+2 (94%), $\pi - \pi^*$
mAtC8	4.11	0.059	H $\to$ L (87%), $\pi - \pi^*$
	4.45	0.206	H $\to$ L+1 (86%), $\pi - \pi^*$
	4.60	0.114	H $\to$ L+2 (87%), $\pi - \pi^*$
mAN8	4.67	0.210	H $\to$ L (89%), $\pi - \pi^*$
	5.00	0.001	H-2 $\to$ L (96%), $n - \pi^*$
	5.21	0.048	H-1 $\to$ L (52%), $\pi - \pi^*$
mAtN8	4.29	0.194	H $\to$ L (92%), $\pi - \pi^*$
	4.79	0.099	H-2 $\to$ L (82%), $\pi - \pi^*$
	4.81	0.034	H-1 $\to$ L (59%), $\pi - \pi^*$

Figure S4: Absorption spectra of model structures

Figure S5: Calculated frontier molecular orbitals of model structures