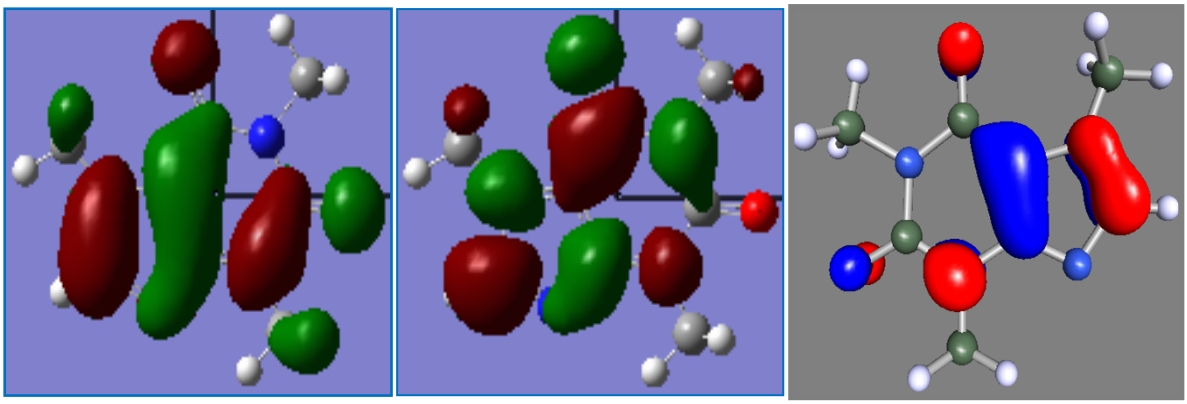
Electronic Supplementary Material (ESI) for RSC Advances.



(a) (b) (c)

Fig. S1. (a) HOMO (b) LUMO of bare caffeine A using GAUSSIAN 09 and (c) HOMO of caffeine A with TURBOMOLE 6.4 Software calculated at MP2/6-311++G(d,p) level.

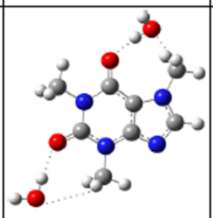
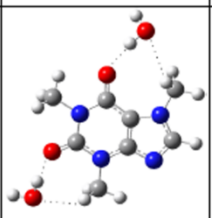
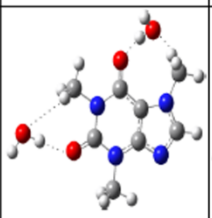
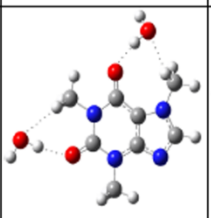
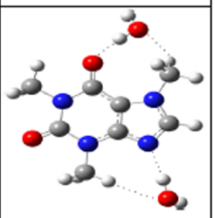
Relative energy (kJ/mol)	(0.00)	(0.00)	(0.86)	(0.86)	(1.94)
Structure	 I	 II	 III	 IV	 V

Fig. S2 Optimized structures and relative energies (kJ/mol) of the lowest-energy caff$_1$-(H$_2$O)$_2$ complexes at B3LYP/6-31+G(d) level.