Electronic Supplementary Material (ESI) for RSC Advances.

The influence of isolated and penta-hydrated Zn^{2+} on some of the intramolecular proton-transfer process of thymine: a quantum chemical study

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Fig. S1 Schematic drawings of the optimized structures of metalated thymine.

Fig. S2 Relative energy profile of the tautomeric process from Zn^{2+}T8 to Zn^{2+}T5 or Zn^{2+}T4.

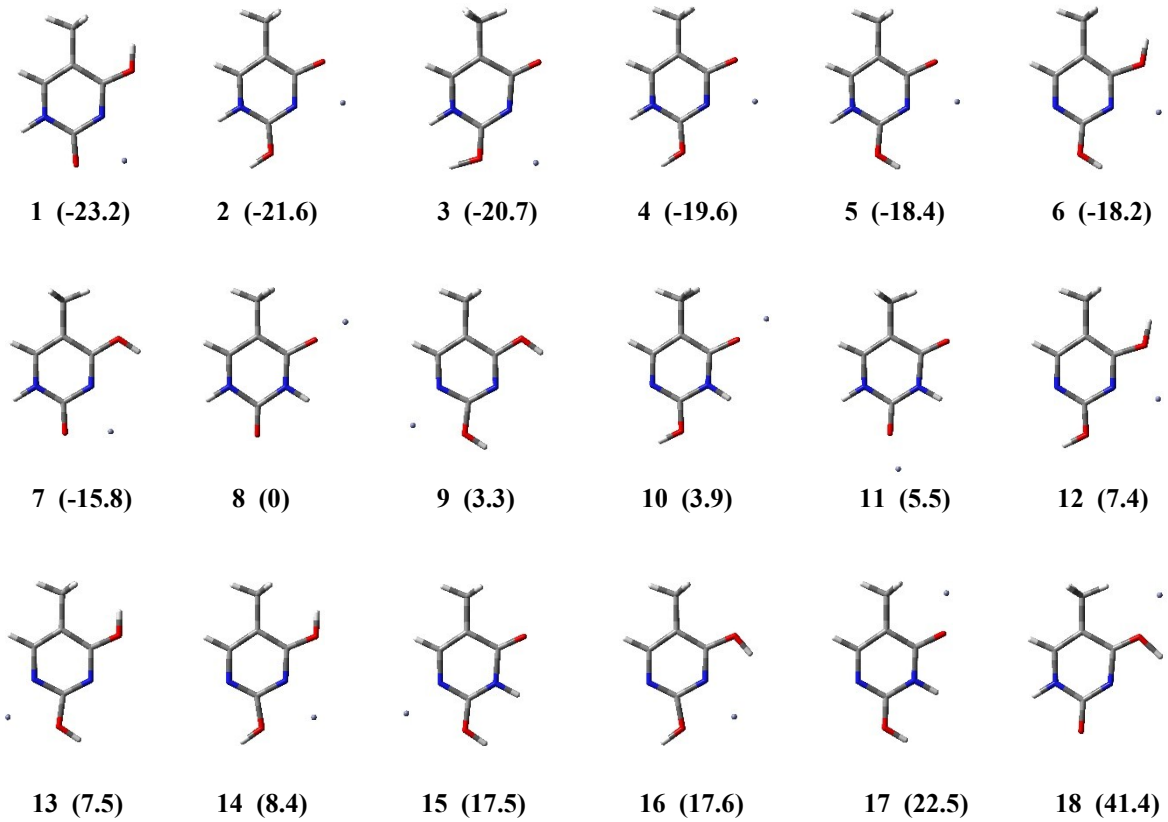

Fig. S1 Schematic drawings of the optimized structures of metalated thymine. Each of the adduct structure covers the tautomeric form of the base and also information on the binding sites. They are sequenced in order of their relative energies according to the canonical structure of thymine with Zn^{2+} which attaches at O8 position. Energies are in kcal mol^{-1}.

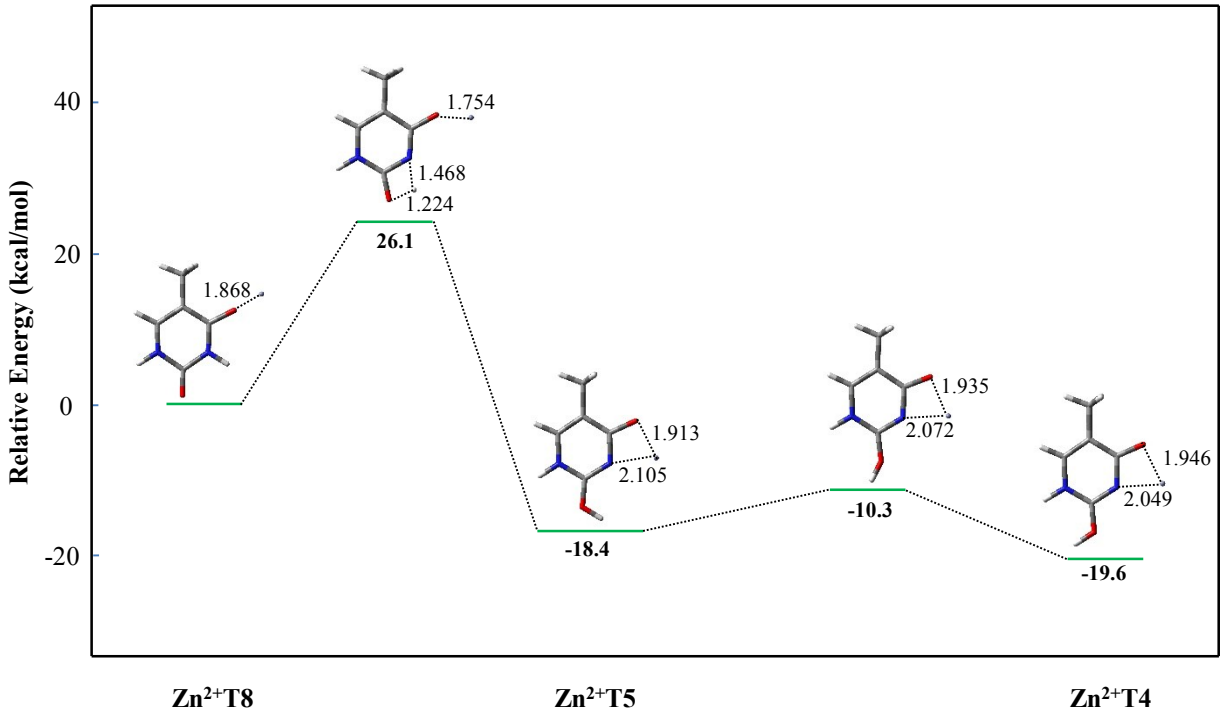

Fig. S2 Relative energy profile of the tautomeric process from Zn^{2+}T8 to Zn^{2+}T5 or Zn^{2+}T4. Zn^{2+}T8→Zn^{2+}T5 is a one step process and Zn^{2+}T8→Zn^{2+}T4 is a two steps process. Bond distances in angstrom.

Table S1 NPA Charge Distribution (au) on the Portion of Zn^{2+}T-nw

Water number	Zn^{2+}	T	water
0	1.333	0.667	–
1	1.697	0.195	0.108
2	1.726	0.129	0.145
3	1.646	0.175	0.179
4	1.624	0.154	0.222