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Supporting Information

A turn off and reversible fluorescence probe (HNAPP) for Zn(II) ion towards inorganic phosphate ions (H_2P and HP) at physiological pH†

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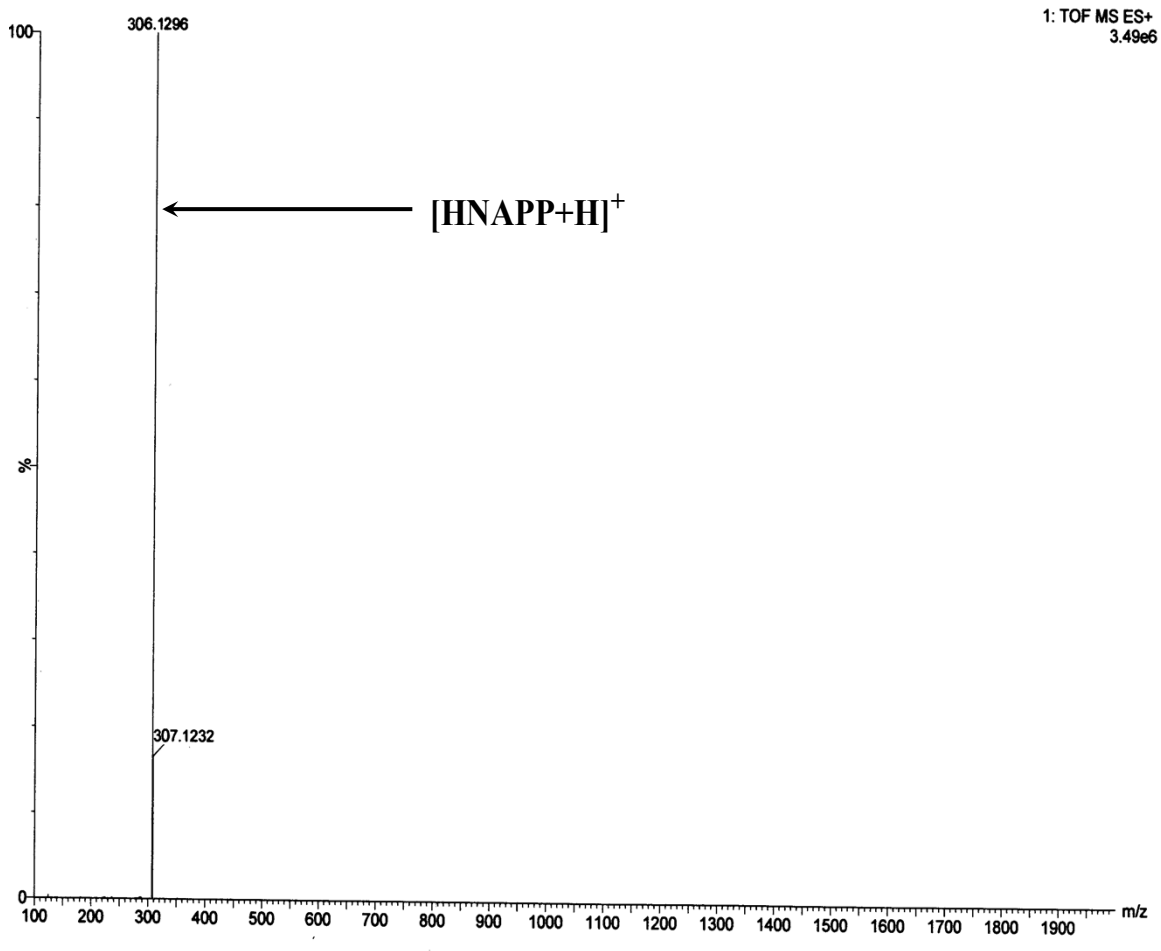

Fig. S1 High-resolution mass spectrum of a solution containing HNAPP in acetonitrile.

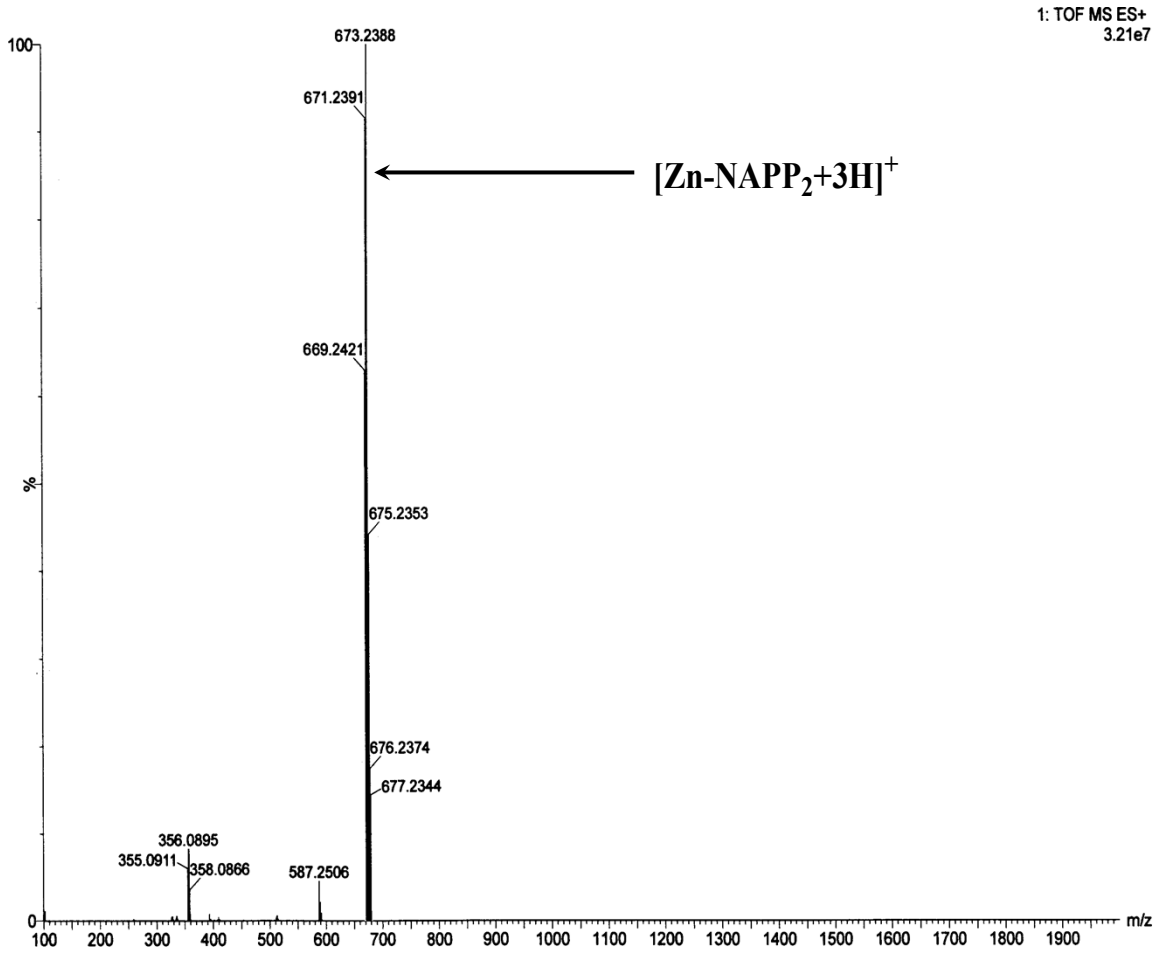

Fig. S2 High-resolution mass spectrum of a solution containing Zn-$NAPP_2$ in acetonitrile.

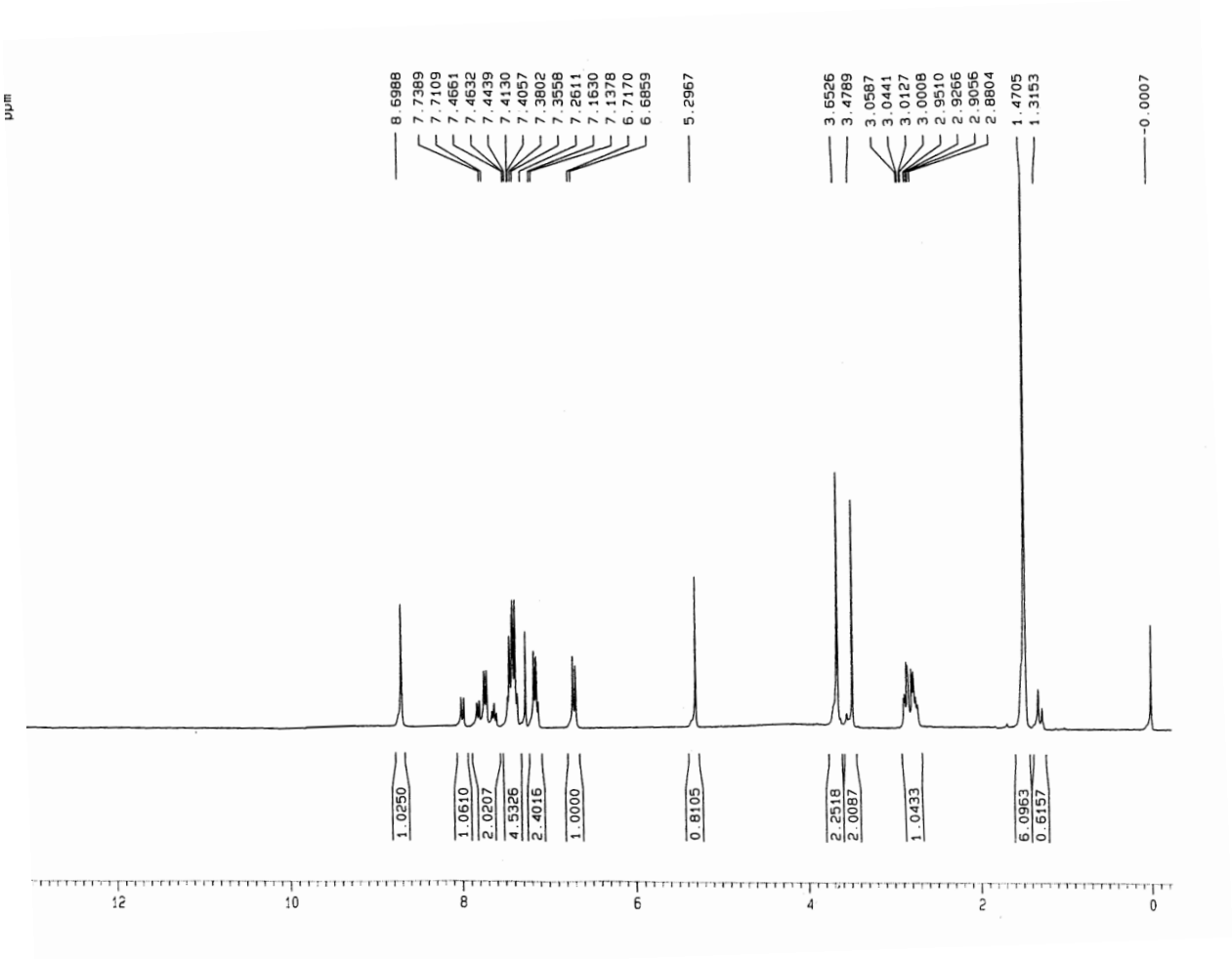

Fig. S3 The ^{1}H NMR spectra of Zn-$NAPP_2$ with their spectral nature of both aromatic and aliphatic region.

Table S1 Selected parameters for the vertical excitation (UV-Vis absorptions) of enol form and keto form of HNAPP; electronic excitation energies (eV) and oscillator strengths (*f*), configurations of the low-lying excited states; calculation of the S_0–S_1 energy gaps based on optimized ground-state geometries (UV-Vis absorption)

Tautomeric Form	Electronic Transitions	Composition	Excitation energy	Oscillator strength (*f*)	CI	λ_{theo} (nm)
ENOL	$S_0 \rightarrow S_1$	HOMO → LUMO	3.0818eV	0.4255	0.70344	405
KETO	$S_0 \rightarrow S_1$	HOMO→LUMO	3.9945eV	0.5897	0.68807	315

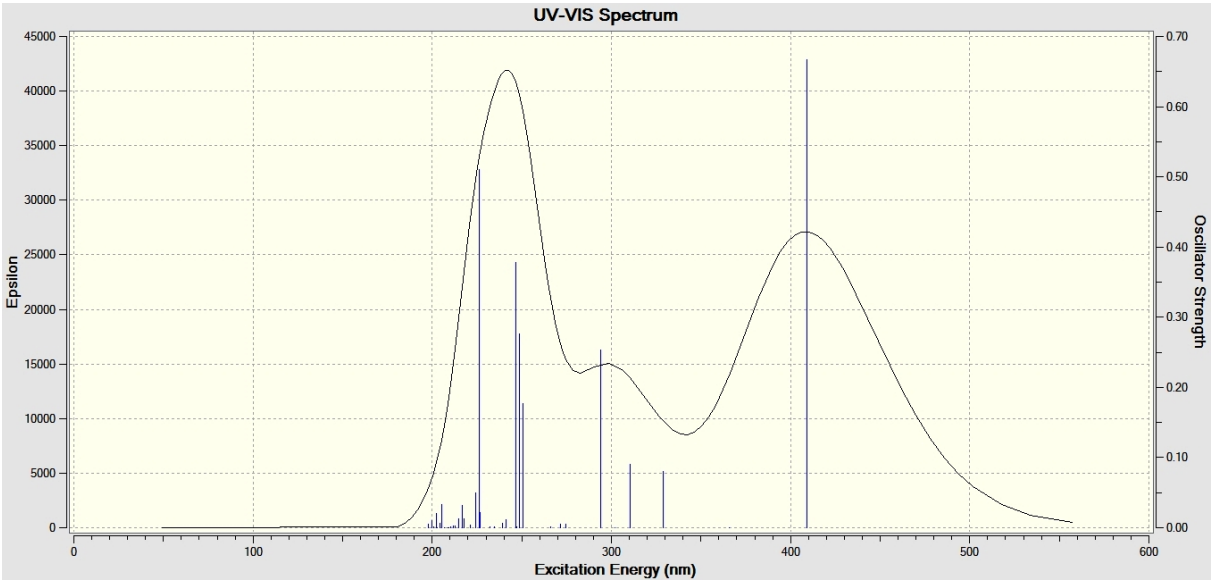

Fig. S4. The theoretical UV-Vis spectra for HNAPP of ENOL form.

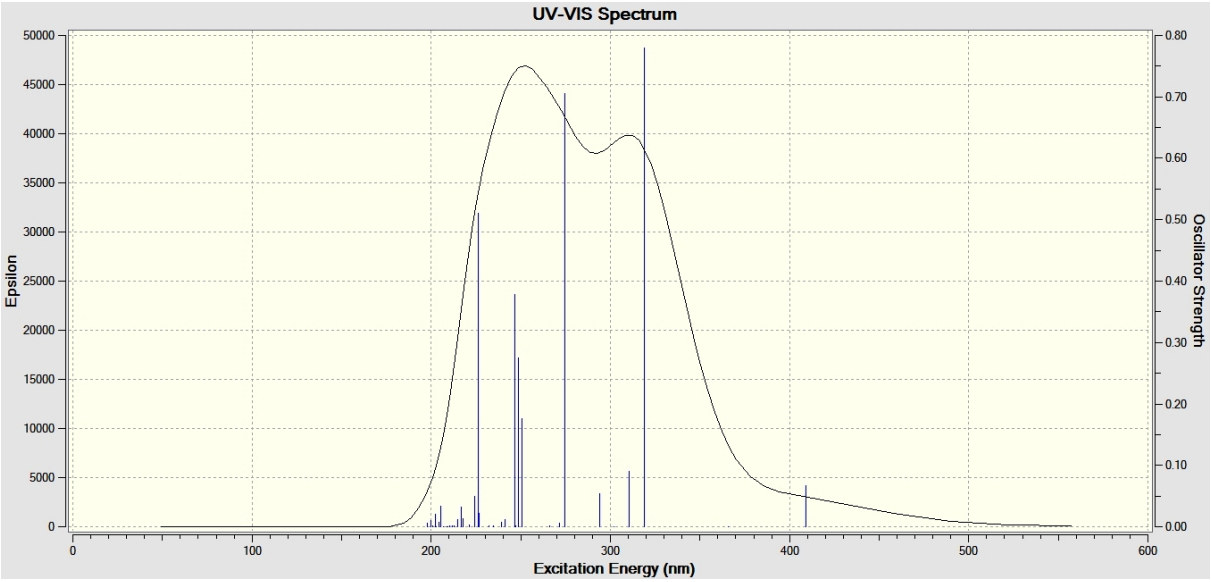

Fig. S5. The theoretical UV-Vis spectra for HNAPP of KETO form.

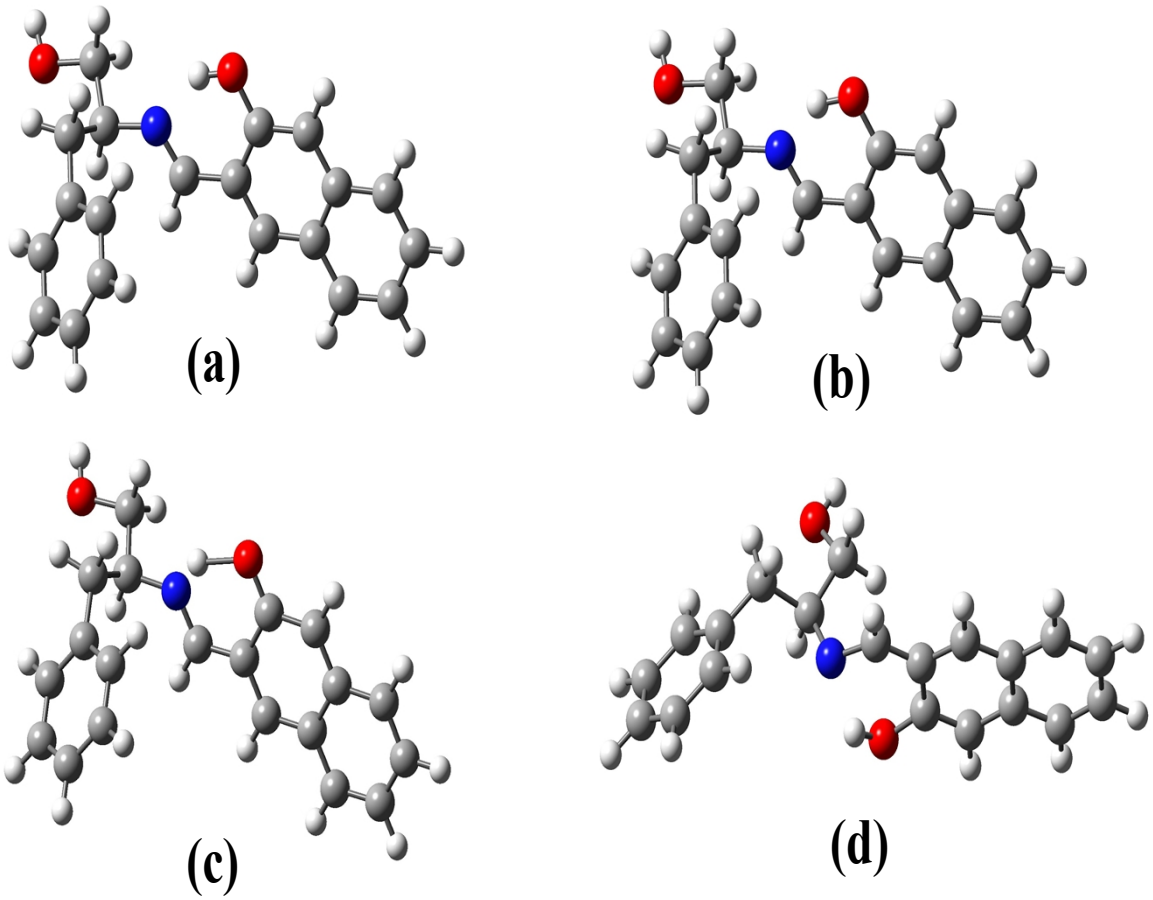

Fig. S6 The optimized ground state structure (S_0) of HNAPP in DMF (a), MeOH (b) and DCM (c); The optimized structure of first excited state (S_1) of HNAPP in DCM (d); [N: Blue, O: Red, C: Grey and H: White atom].

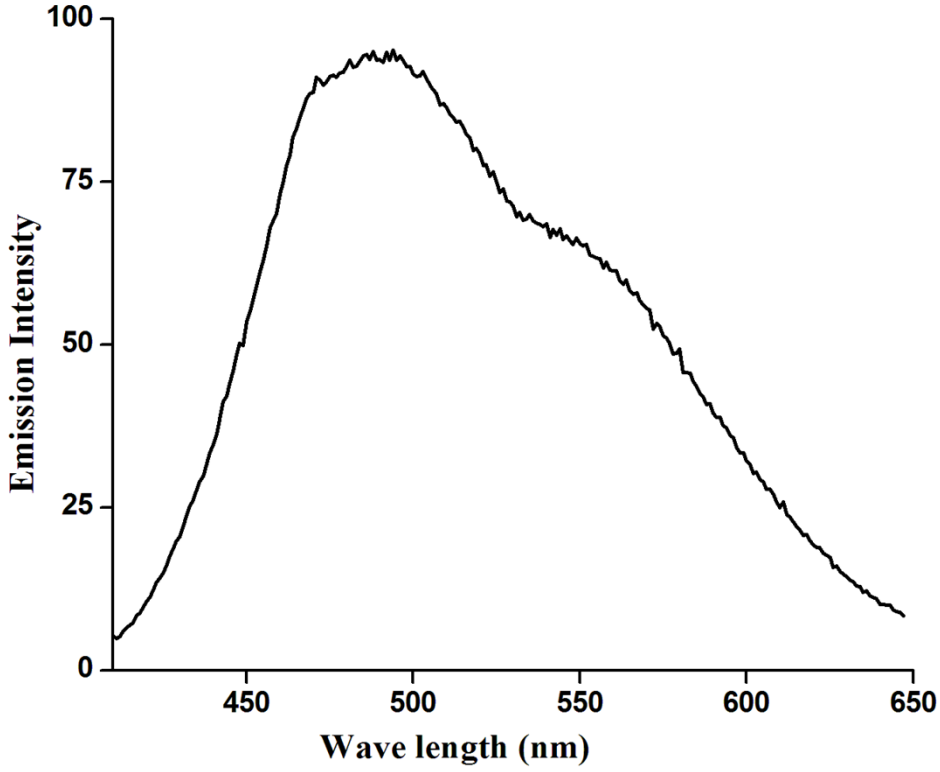

Fig.S6 Emission spectra of HNAPP in DCM at room temperature.