Electronic Supporting Information

pH-Regulated 'Off-On' Fluorescence Signaling of d-block Metal Ions in Aqueous Media and Realization of Molecular IMP Logic Function

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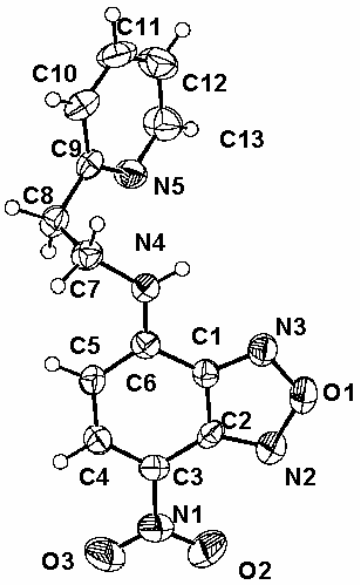

Fig S1. X-ray structure of **1** with atoms represented by thermal ellipsoid at the 50% probability level.

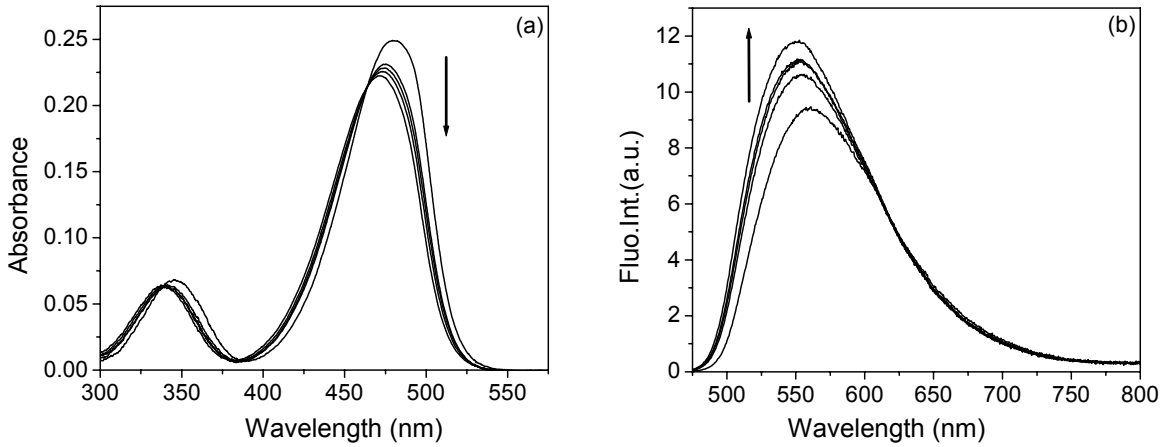

Fig S2. Absorption (a) and fluorescence (b) spectra of **1** (4.9×10^{-6} M) in water upon progressive addition of HCl. $[H^+] = 1 \times 10^{-4} - 2.9 \times 10^{-4}$ M with decreasing absorbance and increasing fluorescence at 525 nm. Excitation wavelength is 460 nm.

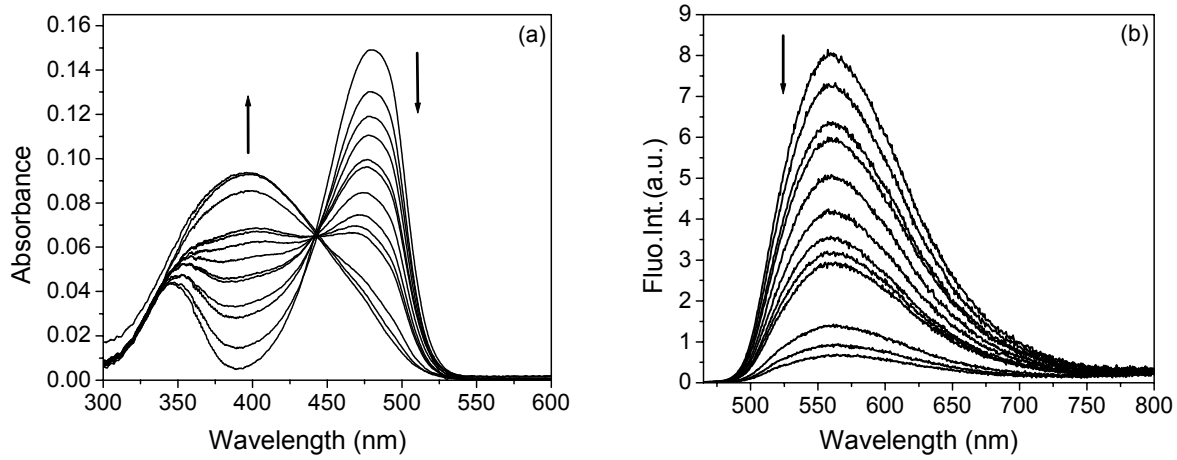

Fig S3. Absorption (a) and fluorescence (b) spectra of **1** (4.9×10^{-6} M) in water upon progressive addition of NaOH. $[OH^{-}] = 0.16 \times 10^{-4} - 5.0 \times 10^{-4}$ M with decreasing absorbance and fluorescence at 525 nm. Excitation wavelength is 440 nm.

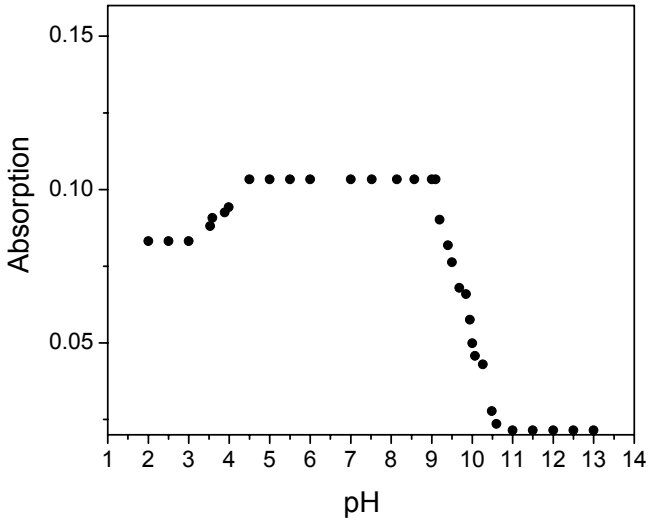

Fig S4. A typical plot showing the change in the absorbance of **1** as a function of pH at 480 nm.

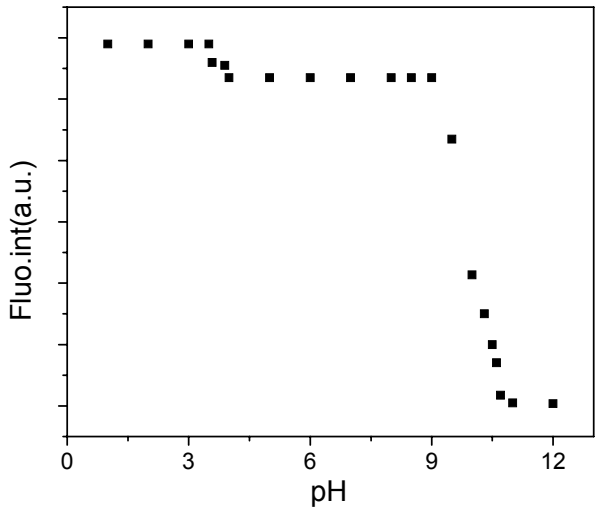

Fig S5. A typical plot showing the change in the fluorescence intensity of **1** as a function of pH .

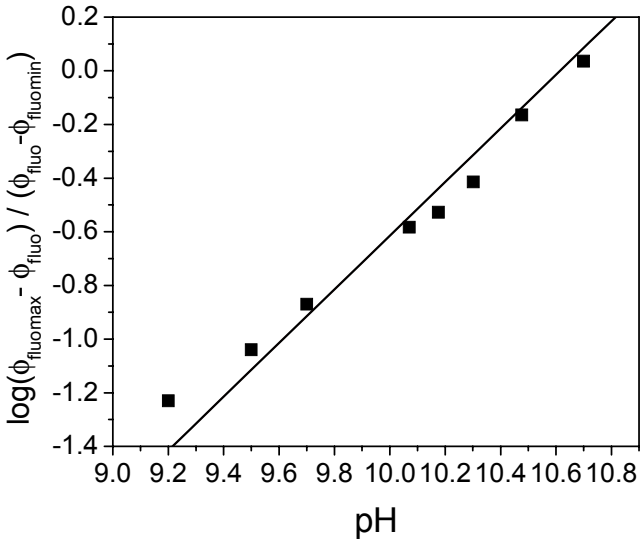

Fig S6. A typical plot from which the pK_a value for the deprotonation of **1** was estimated.

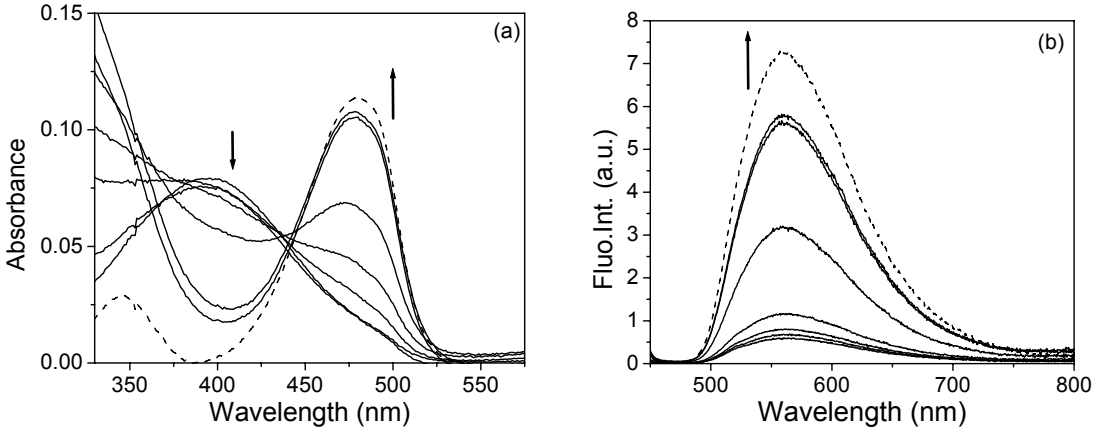

Fig S7. Absorption (a) and fluorescence (b) spectra of **1** (4.9×10^{-6} M) at pH 10.7 and upon subsequent addition of Cu^{2+}. $[Cu^{2+}] = 2 \times 10^{-4} - 9.5 \times 10^{-4}$ M. Dashed line represents the corresponding spectra of **1** at pH 7. Excitation wavelength is 440 nm.

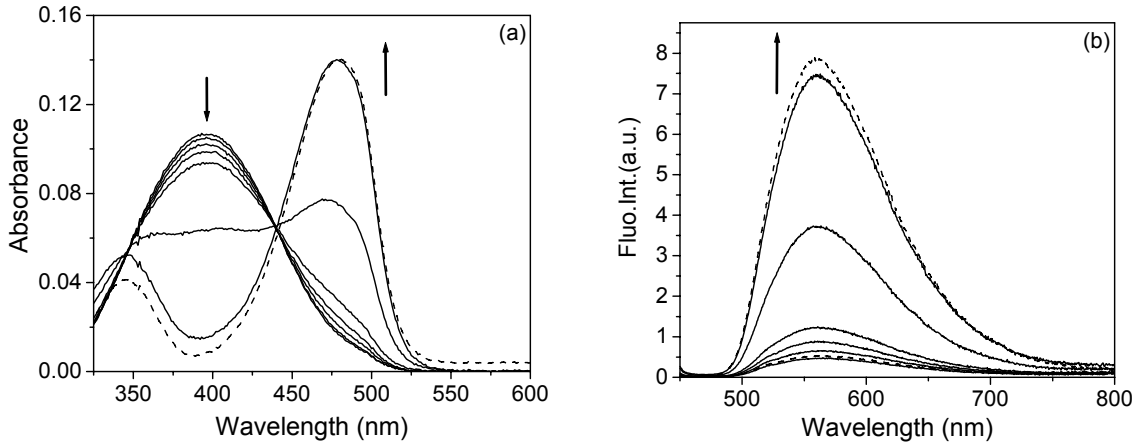

Fig S8. Absorption (a) and fluorescence (b) spectra of **1** (4.9×10^{-6} M) at pH 10.7 and upon subsequent addition of Zn^{2+}. $[Zn^{2+}] = 5.7 \times 10^{-5} - 9 \times 10^{-4}$ M. Dashed line represents the corresponding spectra of **1** at pH 7. Excitation wavelength is 440 nm.

Table S1: Fluorescence response of **1**[a] and the measured binding constant values (K) at pH 10.7 for different metal ions.

Metal ions[b]	[Salt]/ [M][c]	I/I_0[d]	K ($10^3 M^{-1}$) [e]
Ni^{2+}	7×10^{-4}	13.65	1.2
Cu^{2+}	9.5×10^{-4}	9.66	1.5
Zn^{2+}	9×10^{-4}	16.08	5.5
Fe^{3+}	7.7×10^{-4}	9.16	[f]
Mn^{2+}	8.2×10^{-4}	10.8	[f]

[a]Concentration of **1** = 4.9×10^{-6} M. [b]Perchlorate salts of the metals are used. [c]The concentration of the metal salt for which maximum fluorescence enhancement is observed. [d]I_0 corresponds to the fluorescence intensity of **1** at pH 10.7 and I corresponds to observed maximum fluorescence enhancement value after the addition of metal ions at the same pH. [e]K values are calculated from the absorption data. [f]Since no clear isosbestic point was observed in these cases, reliable K values could not be calculated.