

Fig. S1 FT-IR spectrum of MOF 1.

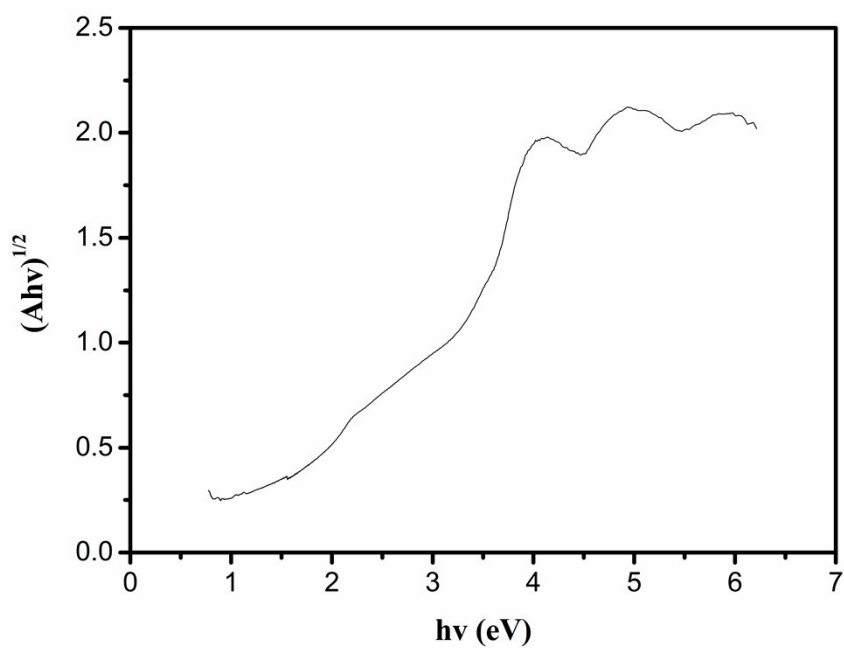


Fig. S2 Diffuse reflectance UV-*vis* spectrum of $(Ah\nu)^{1/2}$ vs photon energy ($h\nu$) for 1.

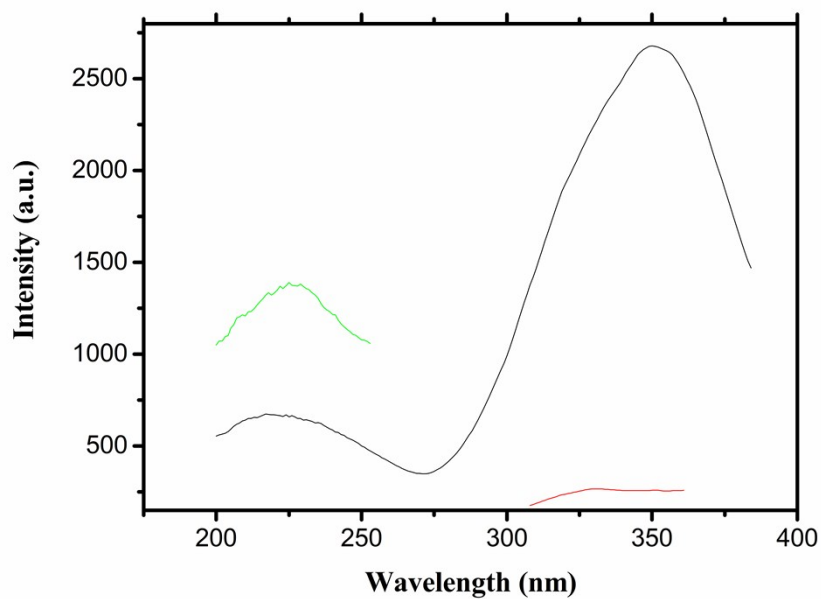


Fig. S3 The excitation spectra of H₂5-asba (red), Bimb (green) and MOF 1 (black).

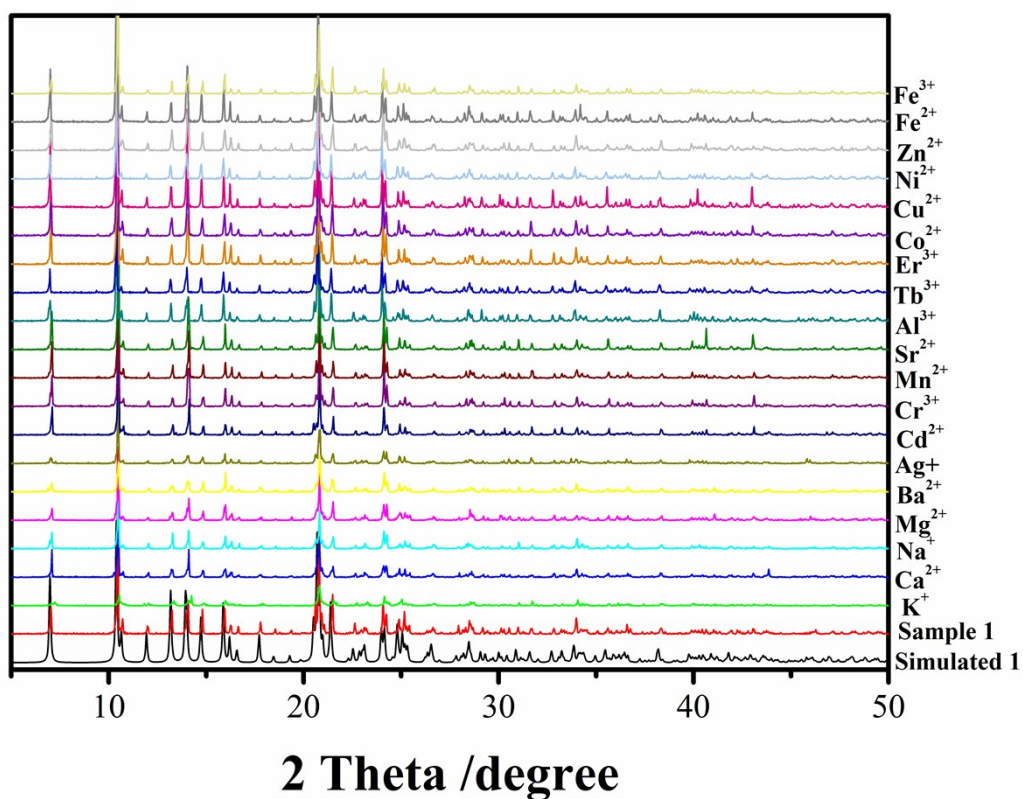


Fig. S4 A variety of PXRD patterns of the samples after immersion in different aqueous metal ion solutions for about five hours, the PXRD pattern of the bulk sample 1 and the simulated XRD pattern of 1 calculated from single-crystal X-ray data with Mercury 1.4.2.

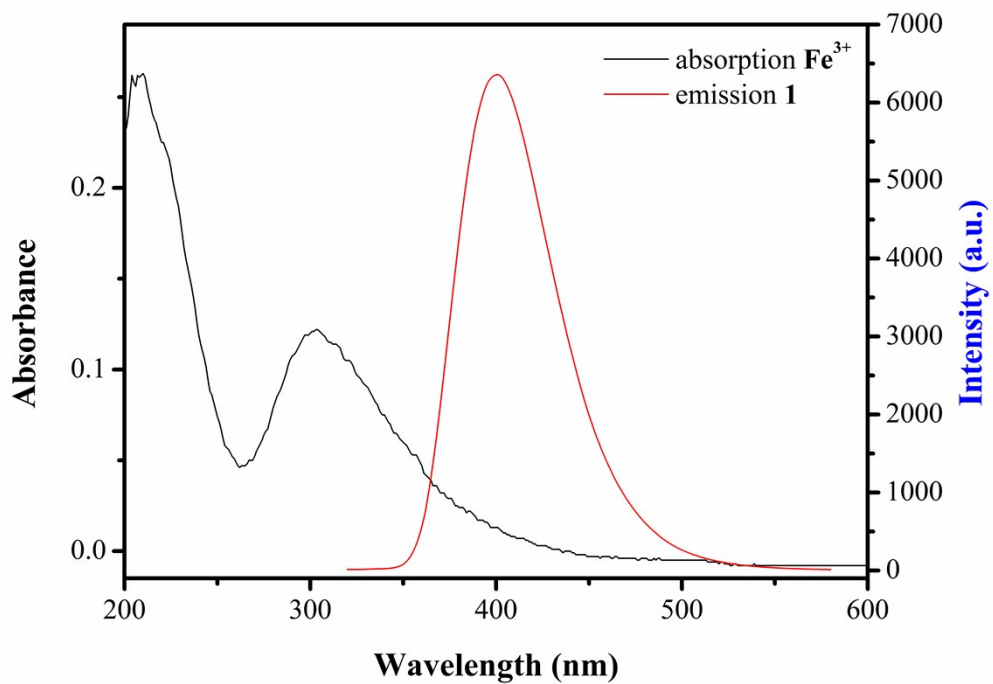
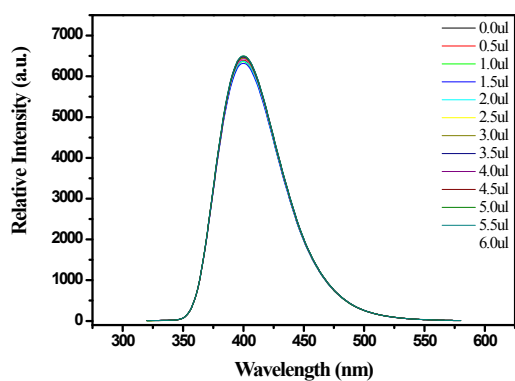
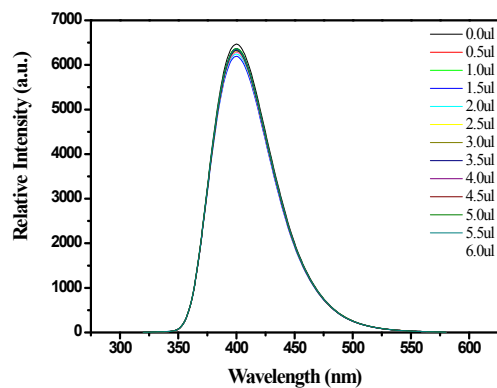


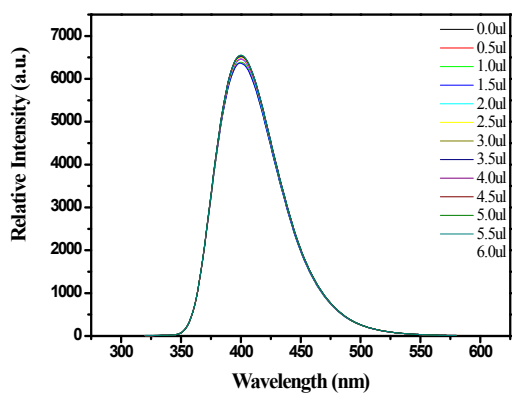
Fig. S5 Spectral overlap between the absorption spectrum of aqueous Fe³⁺ solution and the emission spectrum of **1** in aqueous medium.



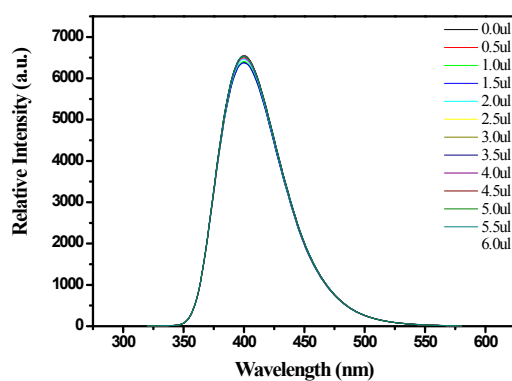
BZ



PL

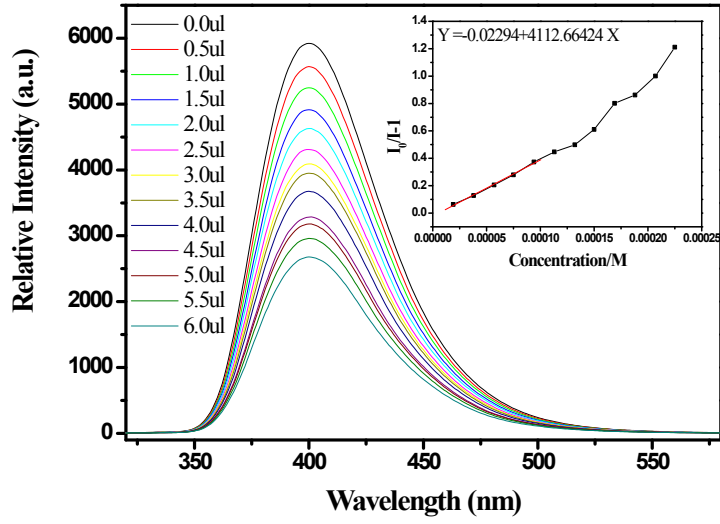


MB

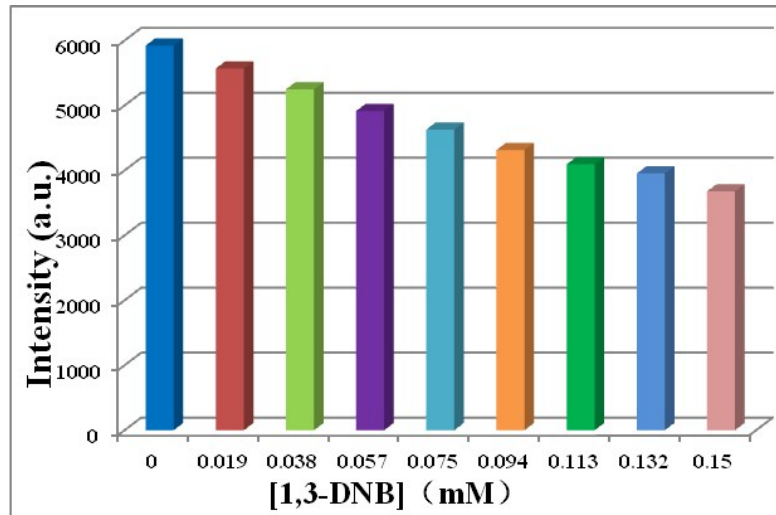


CB

Fig. S6 Photoluminescence spectra of the aqueous suspensions of **1** with incremental addition of various methanol solutions of benzene compounds (0.075 M). The volumes of methanol solutions of benzene compounds added are indicated in the legend.

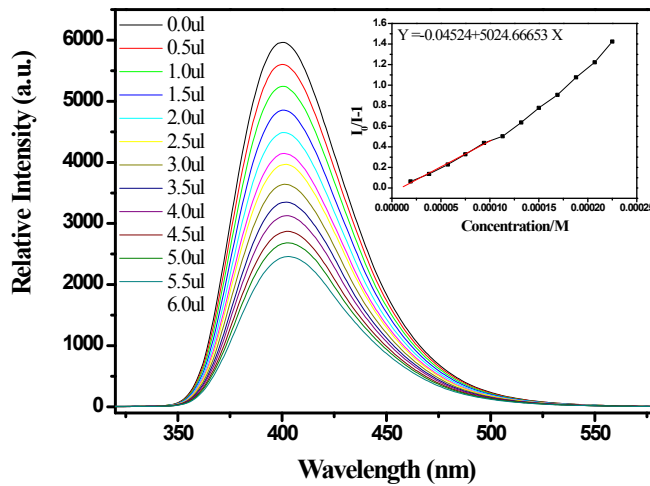


(Top)

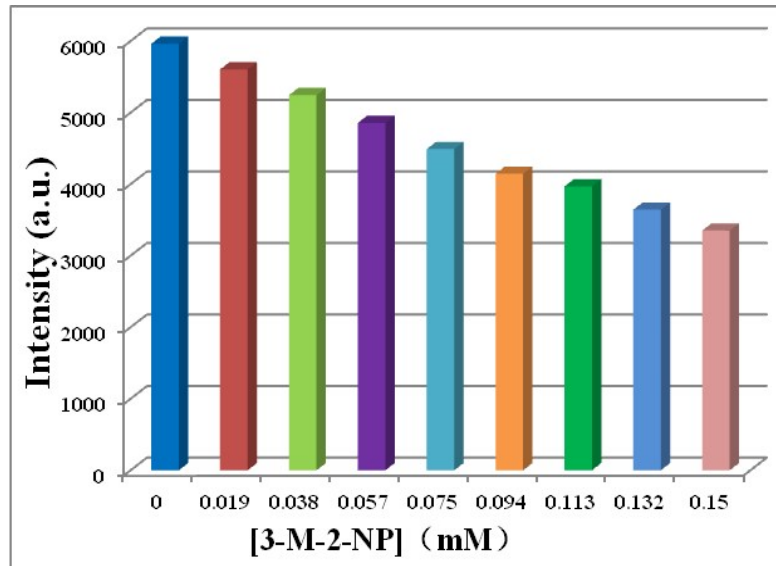


(Bottom)

1, 3-DNB

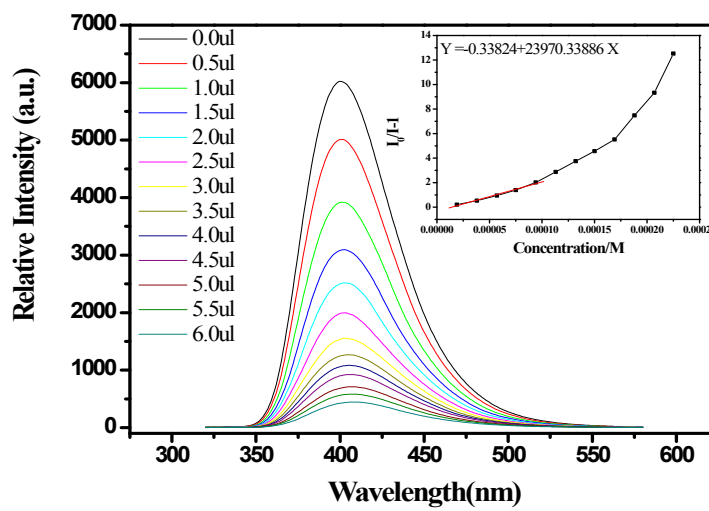


(Top)

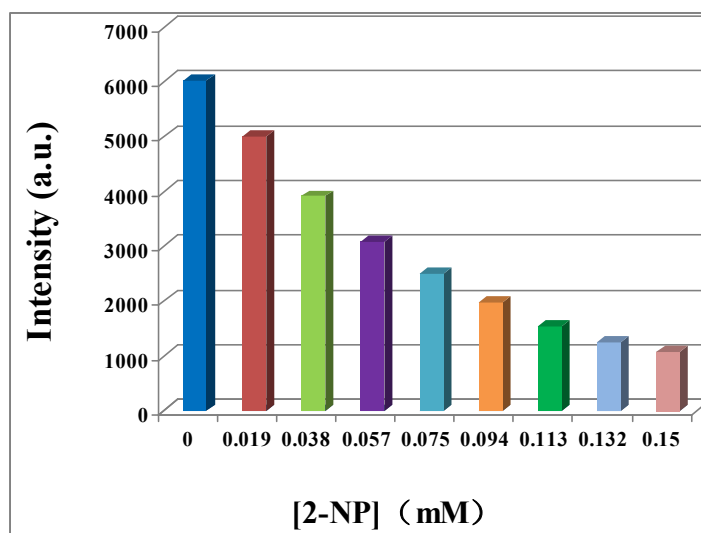


(Bottom)

3-M-2-NP

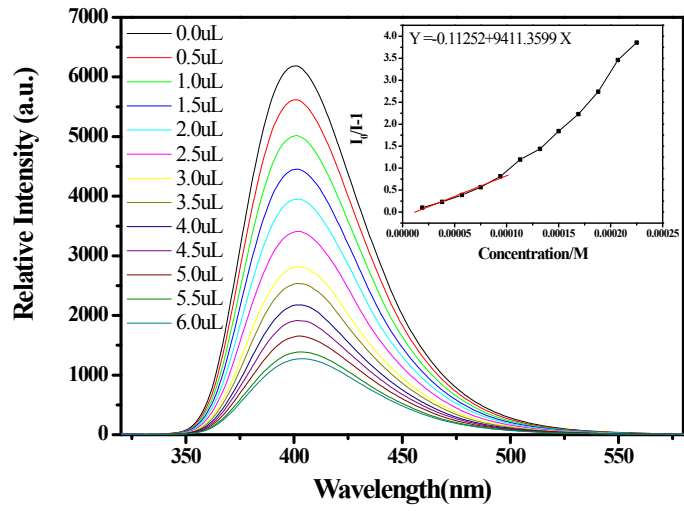


(Top)

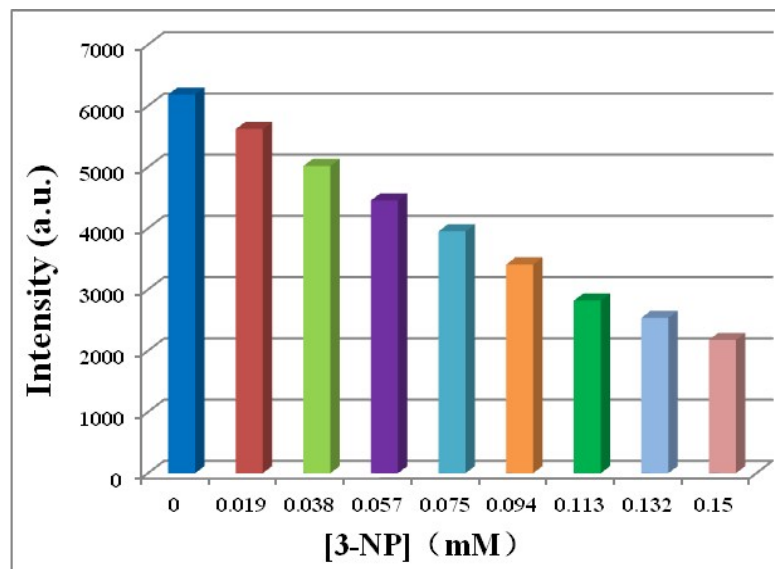


(Bottom)

2-NP

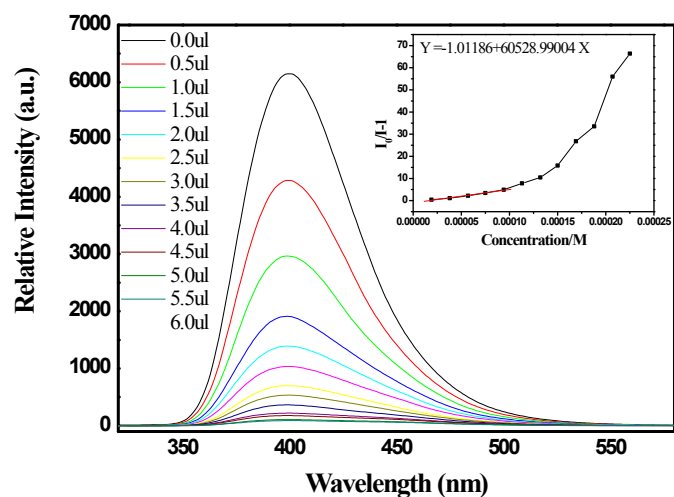


(Top)

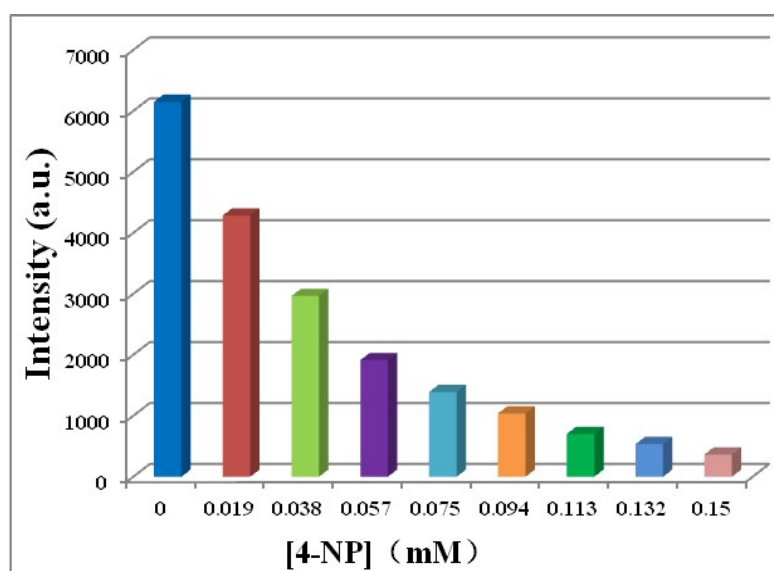


(Bottom)

3-NP



(Top)



(Bottom)

4-NP

Fig. S7 Photoluminescence spectra and the best linear fit of I_0/I_{-1} versus concentration (**Top**), the relative intensity of the maximum emission (**Bottom**) of MOF 1 dispersed in water with incremental addition of the corresponding NACs in methanol. The volumes of methanol solution of the corresponding NACs added are indicated in the legend.

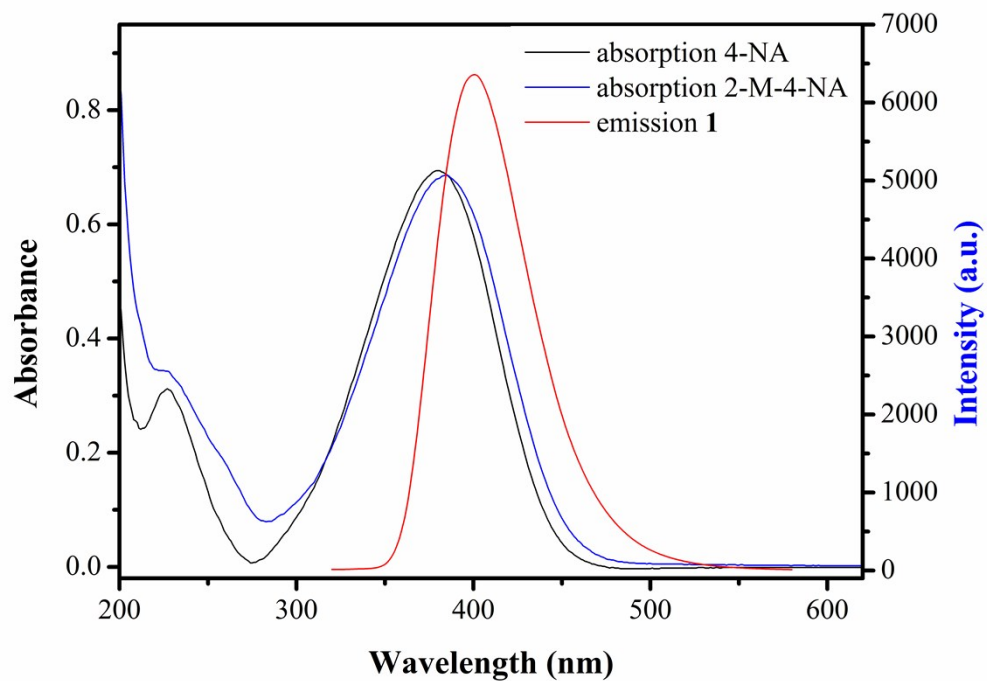


Fig. S8 Spectral overlap between the absorption spectra of 4-NA/2-M-4-NA and the emission spectrum of **1** in aqueous medium.

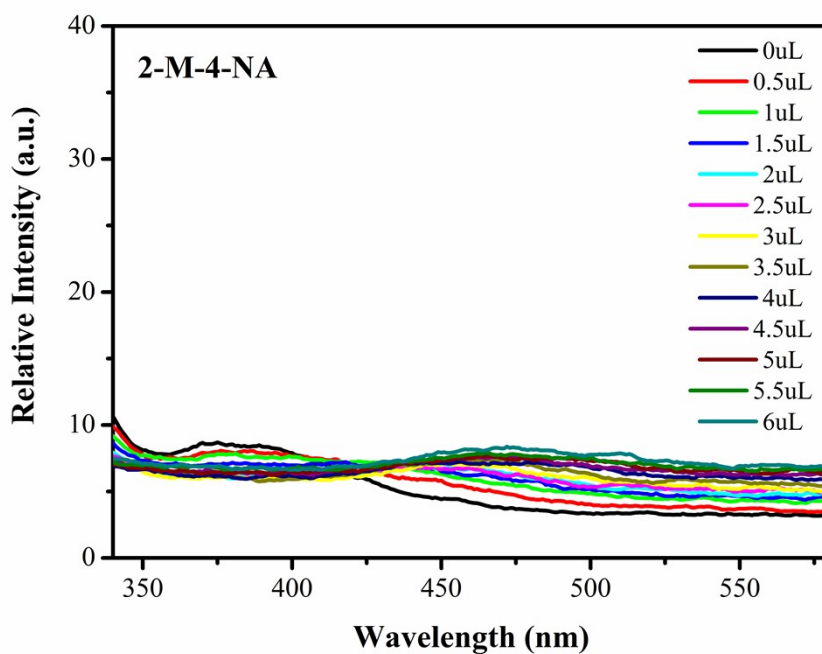
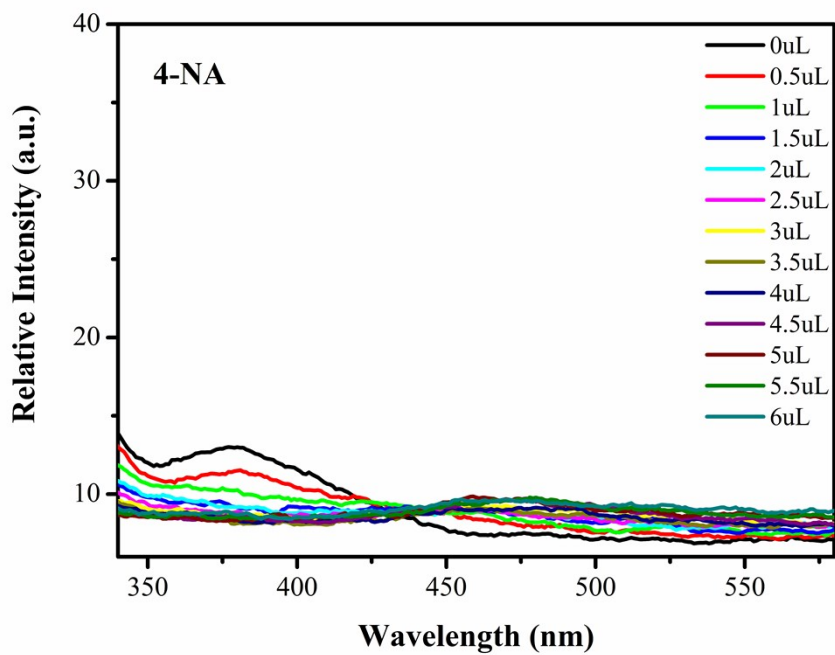


Fig. S9 Fluorescence emission spectra of the aqueous solution of 4-NA and 2-M-4-NA by incrementally adding methanol solution of 4-NA and 2-M-4-NA (0.075 M) into 2 ml of water ($\lambda_{\text{ex}} = 300$ nm). The volumes of methanol solution of 4-NA and 2-M-4-NA added are indicated in the legend.

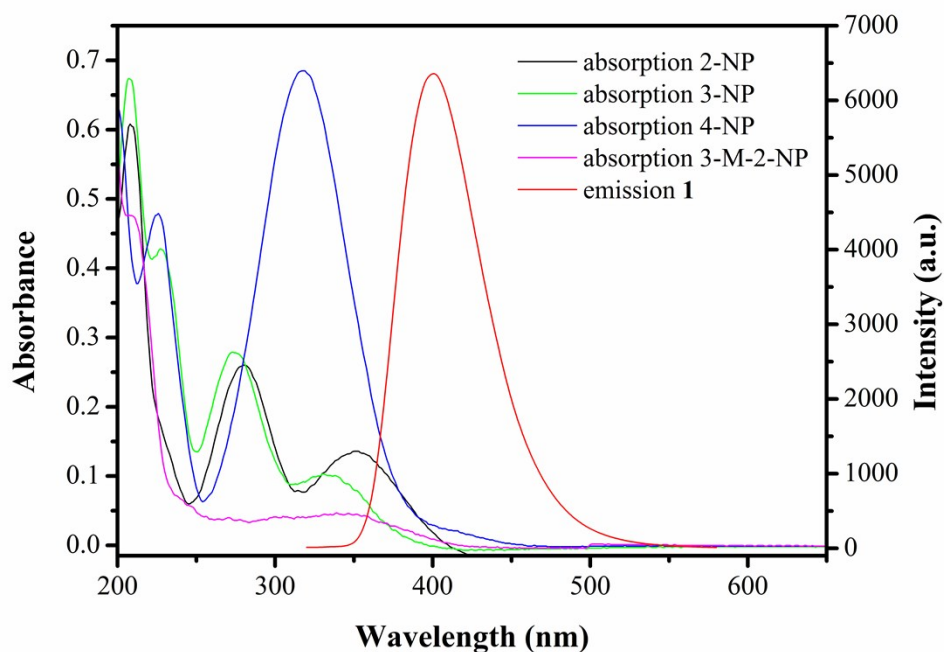


Fig. S10 Spectral overlap between the absorption spectra of analytes 2-/3-/4-NP, 3-M-2-NP and the emission spectrum of **1** in aqueous medium.

Table S1. The Stern–Volmer constants (K_{SV}) for some NACs

NACs	$K_{SV}/(L/mol)$	NACs	$K_{SV}/(L/mol)$
2-NP	$2.4 \cdot 10^4$	3-NP	$9.4 \cdot 10^3$
4-NP	$6.1 \cdot 10^4$	3-M-2-NP	$5.0 \cdot 10^3$
1, 3-DNB	$4.1 \cdot 10^3$		

Table S2 pH of the aqueous metal ion-containing suspensions of **1** (0.075 mM) and the aqueous suspension of **1**.

MOF 1 /Metal ion	pH	Metal ion	pH
MOF 1	7.04	Sr^{2+}	6.87
Na^+	7.00	Co^{2+}	6.83
Mg^{2+}	6.77	Ni^{2+}	6.55
Al^{3+}	5.43	Cu^{2+}	6.48
K^+	7.00	Zn^{2+}	5.33
Ca^{2+}	6.91	Ag^+	6.86
Cr^{3+}	5.53	Cd^{2+}	6.67
Mn^{2+}	6.61	Ba^{2+}	6.94
Fe^{3+}	4.26	Eu^{3+}	6.61
Fe^{2+}	6.22	Tb^{3+}	6.70