Supporting information

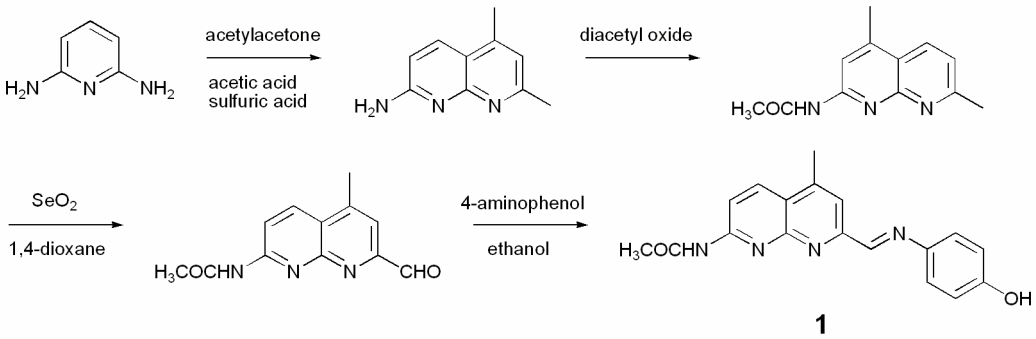
Materials and methods

All chemicals were purchased from commercial suppliers and used without further purification. All reactions were performed under an argon atmosphere with the solvents purified with standard methods.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer. Chemical shifts are reported in ppm using tetramethylsilane (TMS) as the internal standard. Mass spectra were obtained on an LCQ Decaxp PLUS mass spectrometer.

All spectral characterizations were carried out in HPLC-grade solvents at 20 °C within a 10 mm quartz cell. UV-Vis absorption spectra were measured with a TU-1901 double-beam UV-Vis Spectrophotometer, and fluorescence spectra were determined on a Hitachi F-4500 spectrometer.

Synthetic route and characterization of 1



Scheme S1 synthetic route of **1**

Pale-yellow block-shaped crystals of **1** large enough for single crystal X-ray diffraction were grown by slow volatilization of their CH_2Cl_2 solution in air.

Characterization of **1**: ESI-MS $[M+1]^+$ 321 (100). ^{1}H-NMR: δ_H (400 MHz; DMSO; Me_4Si) 11.06 (s, 1H, -OH), 9.75 (s, 1H, NH), 8.64 (m, 1H, naph), 8.52 (m, 1H, naph), 8.37 (m, 1H, naph), 8.02 (s, 1H, CH=N), 7.36 (d, 2H, phenyl), 7.06 (d, 2H, phenyl), 2.70 (s, 3H, CH_3), 2.18 (s, 3H, $COCH_3$). ^{13}C-NMR: δ_C (100 MHz, DMSO): 170.65, 157.49, 154.95, 146.94, 141.65, 136.52, 123.72,120.92,117.90,116.35,115.29,24.66,18.36.

The experiemntal details about cell imaging

MCF-7 cells (gifted from the center of cells, Peking Union Medical College) were cultured in culture media (DMEM/F12 supplemented with 10% FBS, 50 unit/mL penicillin, and 50 μg/mL of streptomycin) at 37 ℃ under a humidified atmosphere containing 5% CO_2. MCF-7cells were seeded in Culture Dishes containing a microscope slide for confocal laser scanning microscopy (CLSM) observations for 24 h, then the culture media was washed with PBS and the cells were incubated with 10^{-3} μmol of compound **1** solution (the volume ratio of ethanol and water is 4 to 6) and 1 mL PBS for 30 min at 37 ℃. After the medium was removed, the cells were carefully washed with PBS thrice. In order to increase Zn^{2+} concentration in cells interior, 2×10^{-2} μM of Zn^{2+} water solution was added to the same Culture Dishes. The fluorescent images were recorded for cells incubated compound **1** and adding Zn^{2+} water solution.

ORTEP of 1

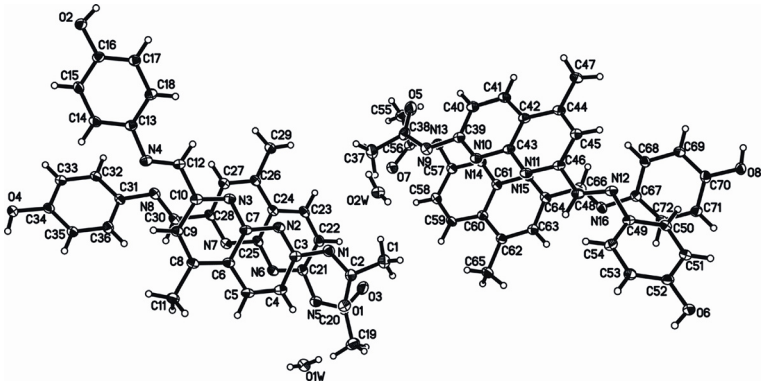


Figure S1. ORTEP of **1**, with thermal ellipsoids drawn at the 30% probability level.

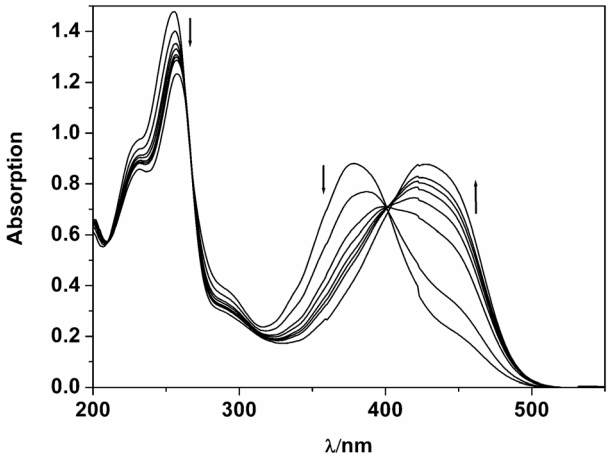


Fig. S2 Changes in absorption spectra of **1** (5.0×10^{-5}M) in ethanol upon addition of Zn^{2+}. The ratio of zinc to **1** is 12 equiv.

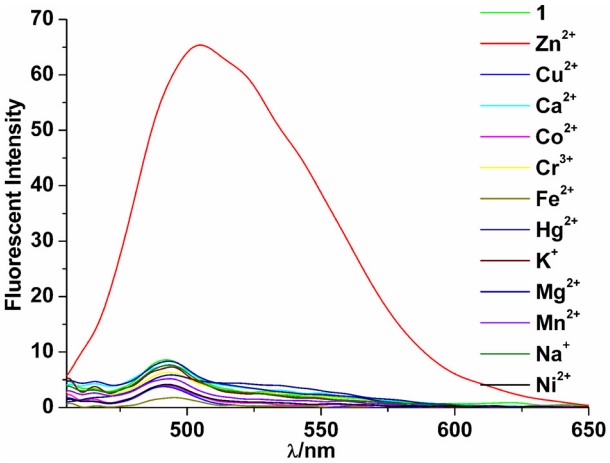


Fig. S3 Fluorescence spectra change of **1** (5.0×10^{-5} M) upon addition of different metal cations (12 equiv) in ethanol solution.

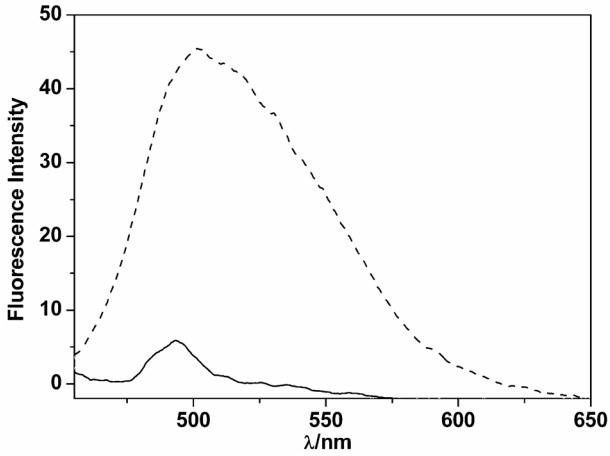


Fig. S4 Emission spectra of **1** upon excitation at 370 nm in ethanol (solid line: before addition of $Zn(NO_3)_2$; dot line: after addition of $Zn(NO_3)_2$).

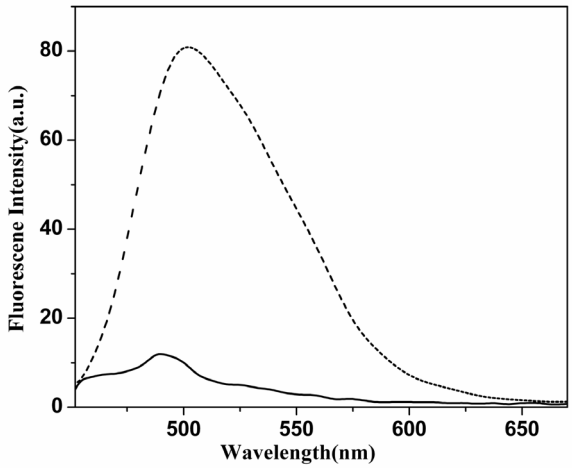


Fig. S5 Emission spectra of **1** upon excitation at 370 nm in ethanol (solid line: before addition of $Zn(CH_3COO)_2$; dot line: after addition of $Zn(CH_3COO)_2$.

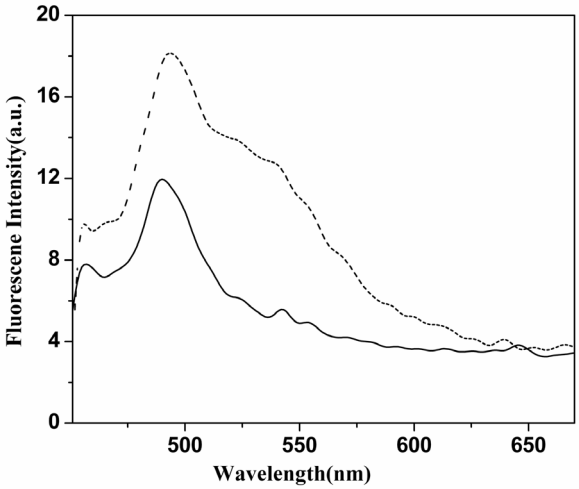


Fig. S6 Emission spectra of **1** upon excitation at 370 nm in ethanol (solid line: before addition of $ZnSO_4$; dot line: after addition of $ZnSO_4$).

Table S1. Binding Ratio and Binding Constant of **1** with Zn(II), Cu(II), Co(II) and Ni(II)[a]

metal ions	Binding Ratio	Binding Constant (L^2/mol^2)
Zn(II)	2	4.41×10^{10}
Cu(II)	2	10.0×10^{10}
Co(II)	2	1.31×10^{10}
Ni(II)	2	6.67×10^{9}

[a] Binding Ratio values were estimated from the absorption spectroscopy data. The absorption peak of Fe^{2+} is blue-shifted and the spectrum overlapped greatly that of **1**.

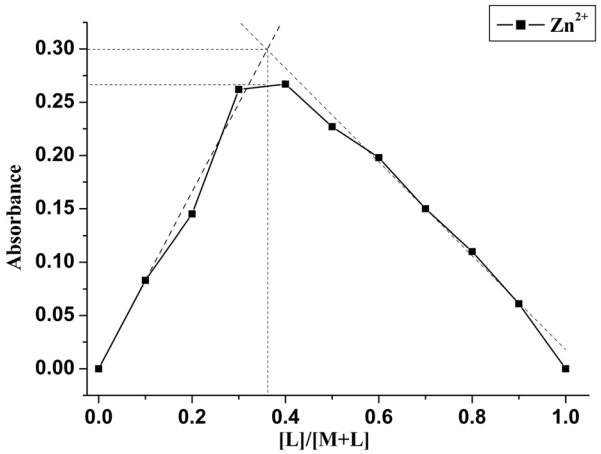


Fig. S7 Molar ratio-extinction curve of Zn^{2+}.

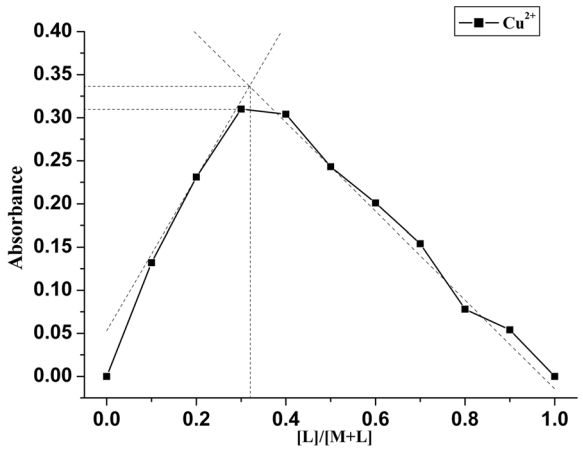


Fig. S8 Molar ratio-extinction curve of Cu^{2+}.

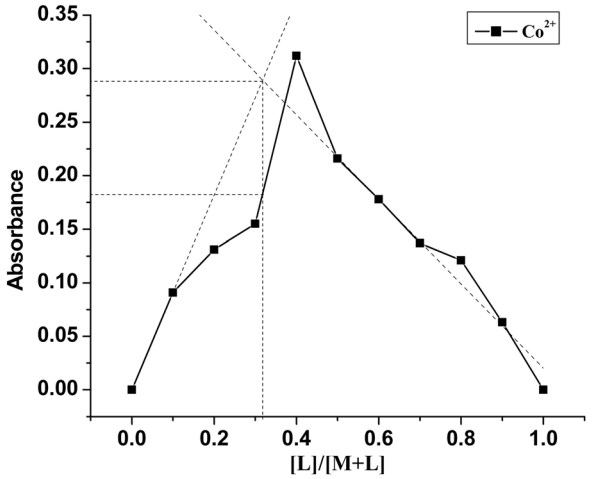


Fig. S9 Molar ratio-extinction curve of Co^{2+}.

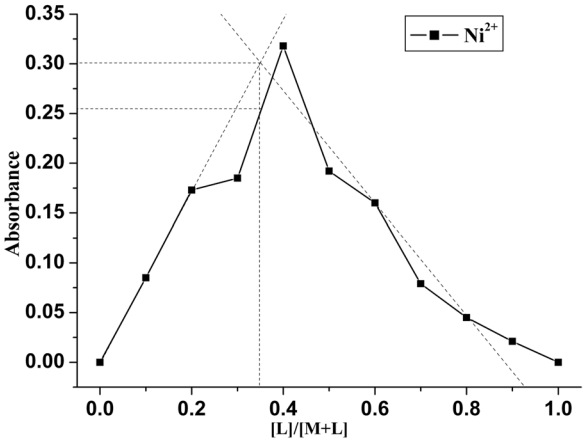


Fig. S10 Molar ratio-extinction curve of Ni^{2+}.

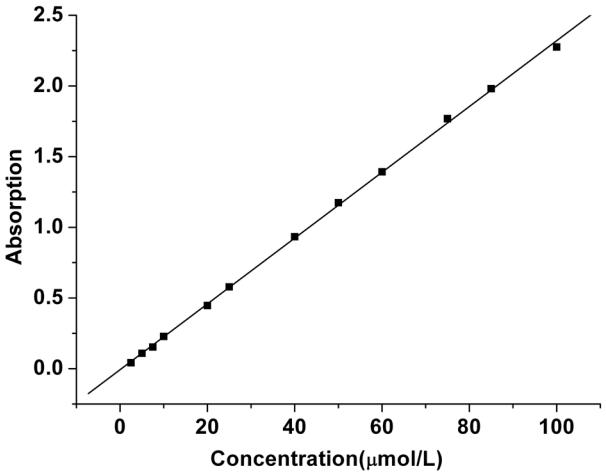


Fig. S11 Absorption Intensity of different concentrations of **1**(the absorption intensity is at 370 nm).

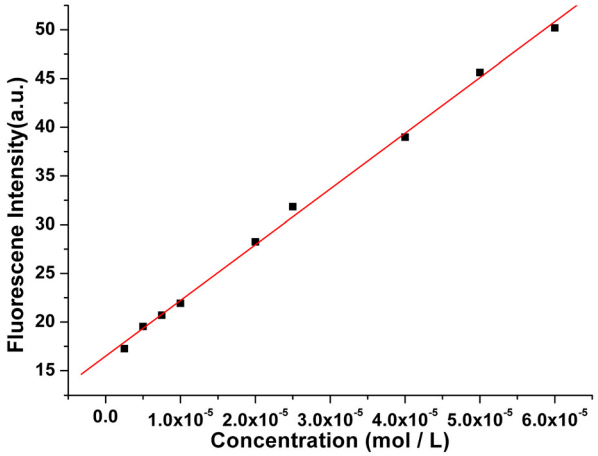


Fig. S12 Fluorescence intensity of different concentrations of **1** and Zn^{2+} (the emission intensity is at 505 nm).