

Electronic Supplementary Information

Synthesis, Structural Characterization, and Multichannel Anion and Cation Sensing Studies of a Bifunctional Ru(II) Polypyridyl-Imidazole Based Receptor

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Table S1 Selected bond distances (Å) and bond angles (deg) for **1**

Bond distances(angstrom)	
Ru1-N1	2.079(5)
Ru1-N4	2.069(6)
Ru1-N8	2.044(6)
Ru1-N9	2.067(6)
Ru1-N10	2.037(6)
Ru1-N11	2.029(6)
Bond angles(degree)	
N1-Ru1-N4	78.8(2)
N1-Ru1-N8	173.8(3)
N1-Ru1-N9	95.5(2)
N1-Ru1-N10	87.6(2)
N1-Ru1-N11	95.5(2)
N4-Ru1-N8	99.3(2)
N4-Ru1-N9	83.4(2)
N4-Ru1-N10	96.8(2)
N4-Ru1-N11	172.9(2)
N8-Ru1-N9	78.4(3)
N8-Ru1-N10	98.5(2)
N8-Ru1-N11	86.9(2)
N9-Ru1-N10	176.8(2)
N9-Ru1-N11	101.5(2)
N10-Ru1-N11	78.6(2)

Table S2 Spectrophotometric and fluorometric detection limit of **1** in MeCN and H₂O

	Detection Limit / M		
Absorption		In MeCN	In H ₂ O
	F ⁻	4.34×10 ⁻⁹	
	AcO ⁻	1.03×10 ⁻⁸	
	H ₂ PO ₄ ⁻	2.30×10 ⁻⁶ 1.89×10 ⁻⁵	
	Fe ²⁺	6.68×10 ⁻⁹	2.18×10 ⁻⁷
Emission			
	F ⁻	8.19 ×10 ⁻⁹	4.75×10 ⁻⁵
	AcO ⁻	1.19×10 ⁻⁸	
	H ₂ PO ₄ ⁻	1.99×10 ⁻⁶ 1.90×10 ⁻⁵	
	Fe ²⁺	6.78×10 ⁻⁹	2.38×10 ⁻⁷

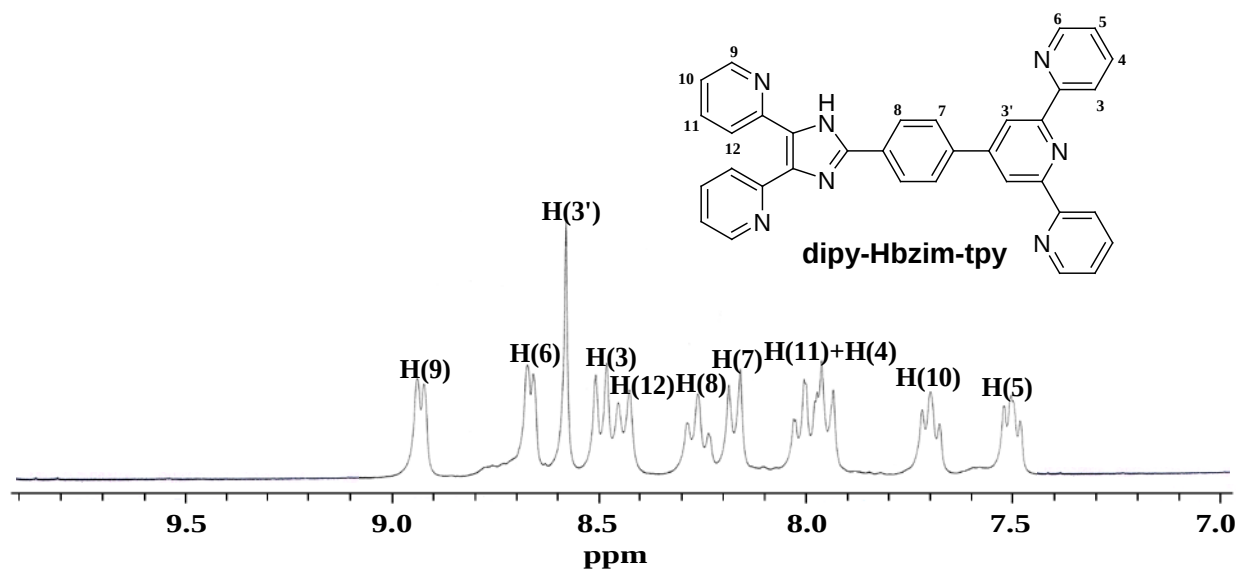


Fig. S1. ^1H NMR (300 MHz) spectrum of **dipy-Hbzim-tpy** in $\text{DMSO}-d_6$.

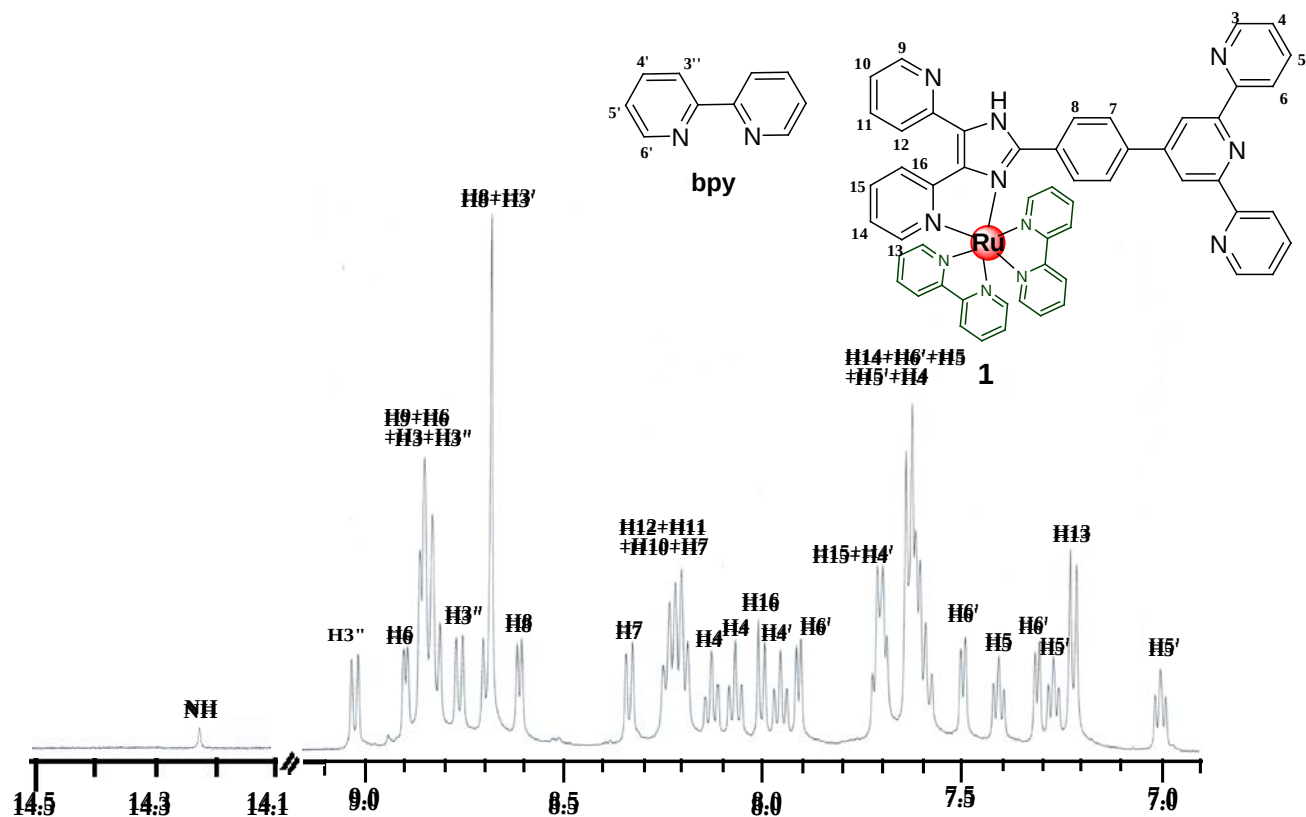


Fig. S2 ^1H NMR (500 MHz) spectrum of **1** in $\text{DMSO}-d_6$.

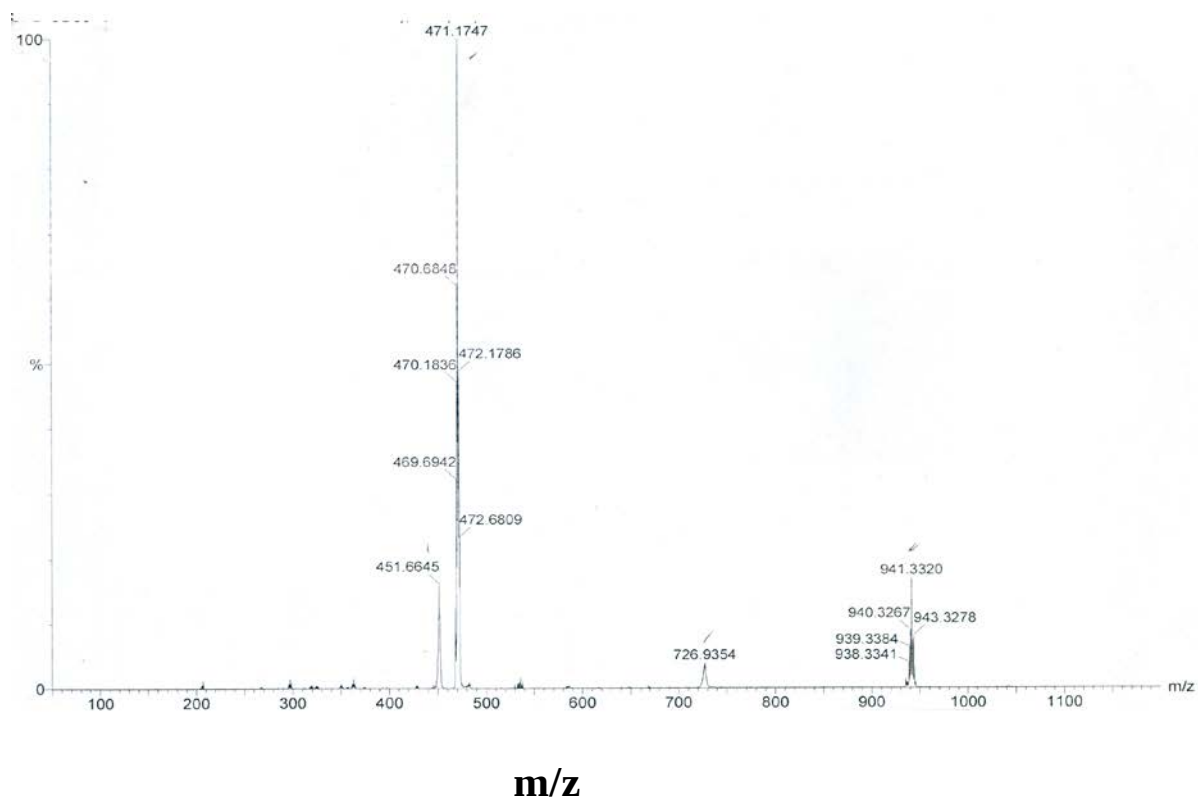


Fig. S3 Experimental ESI mass spectrum of **1** in acetonitrile.

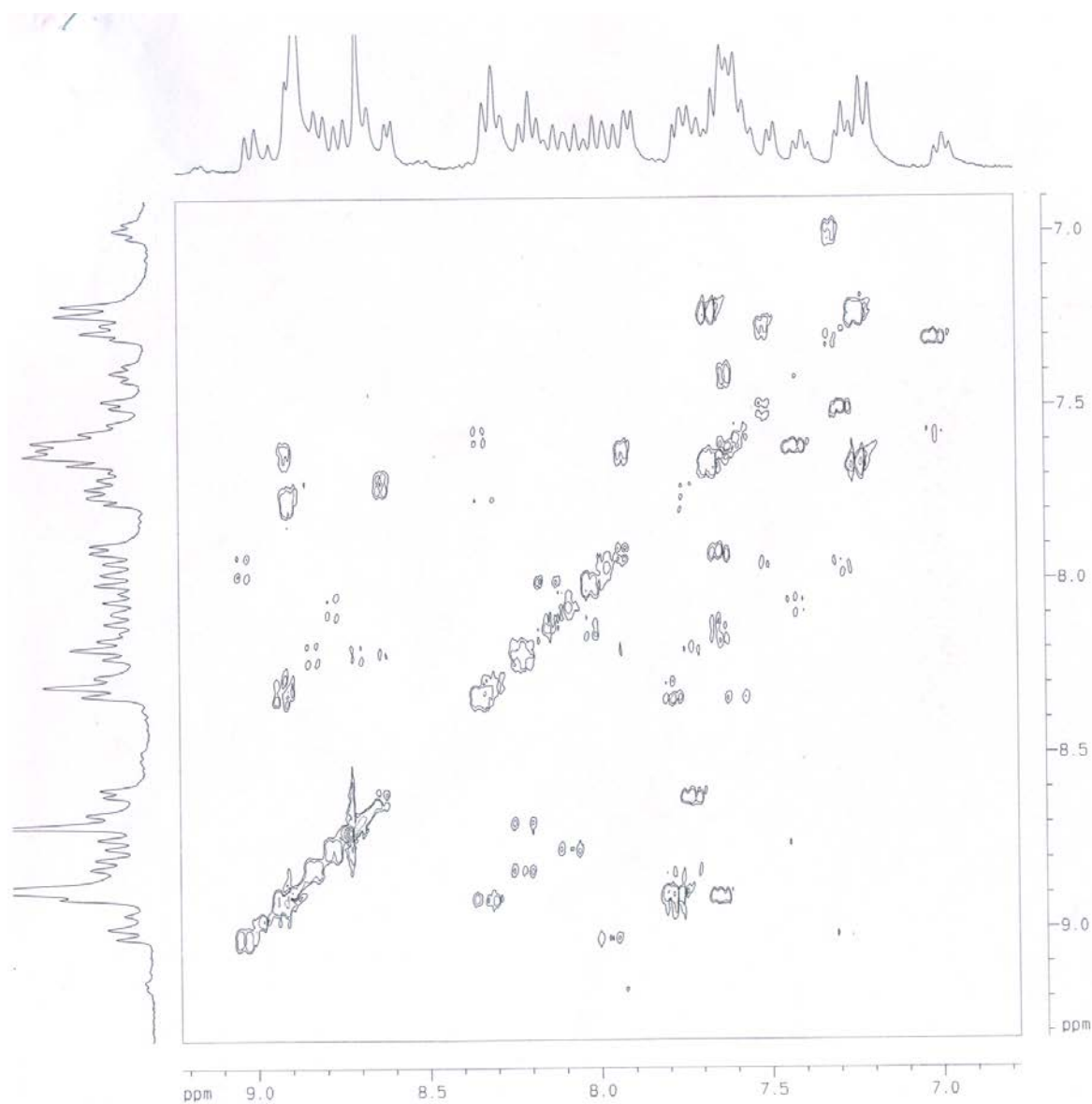


Fig. S4 ^1H - ^1H COSY spectrum of **1** $\text{DMSO}-d_6$.

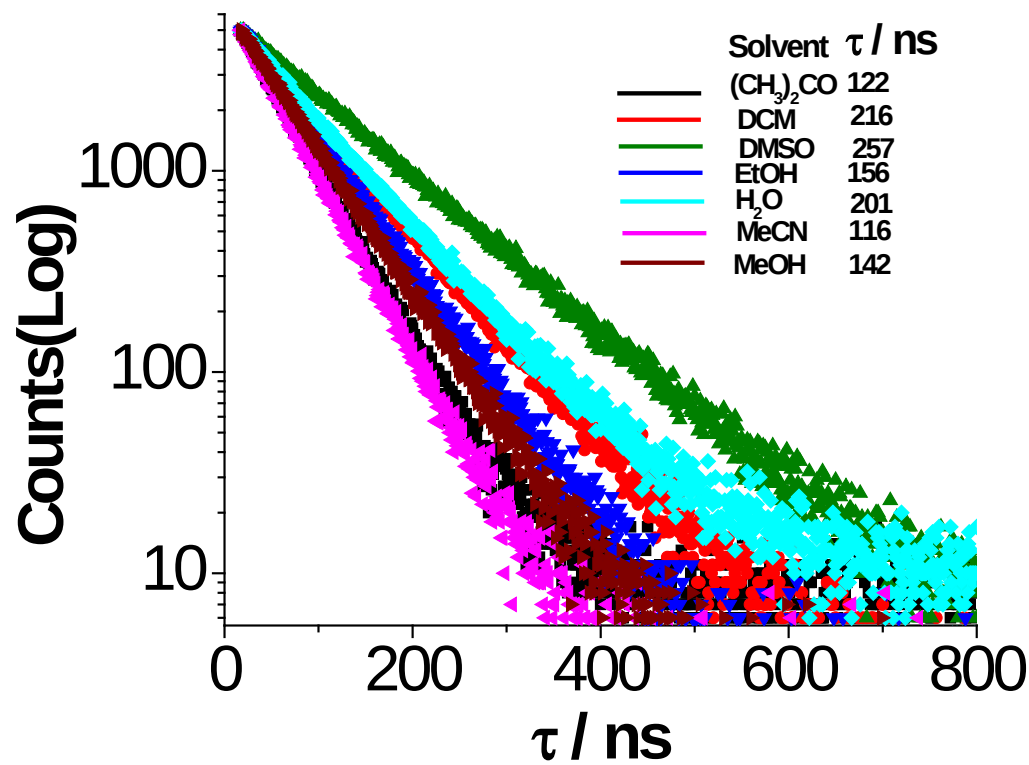


Fig. S5 Time-resolved luminescence decay profiles of **1** at room temperature in different solvents. Lifetimes of **1** in different solvents are given in the inset of the figure.

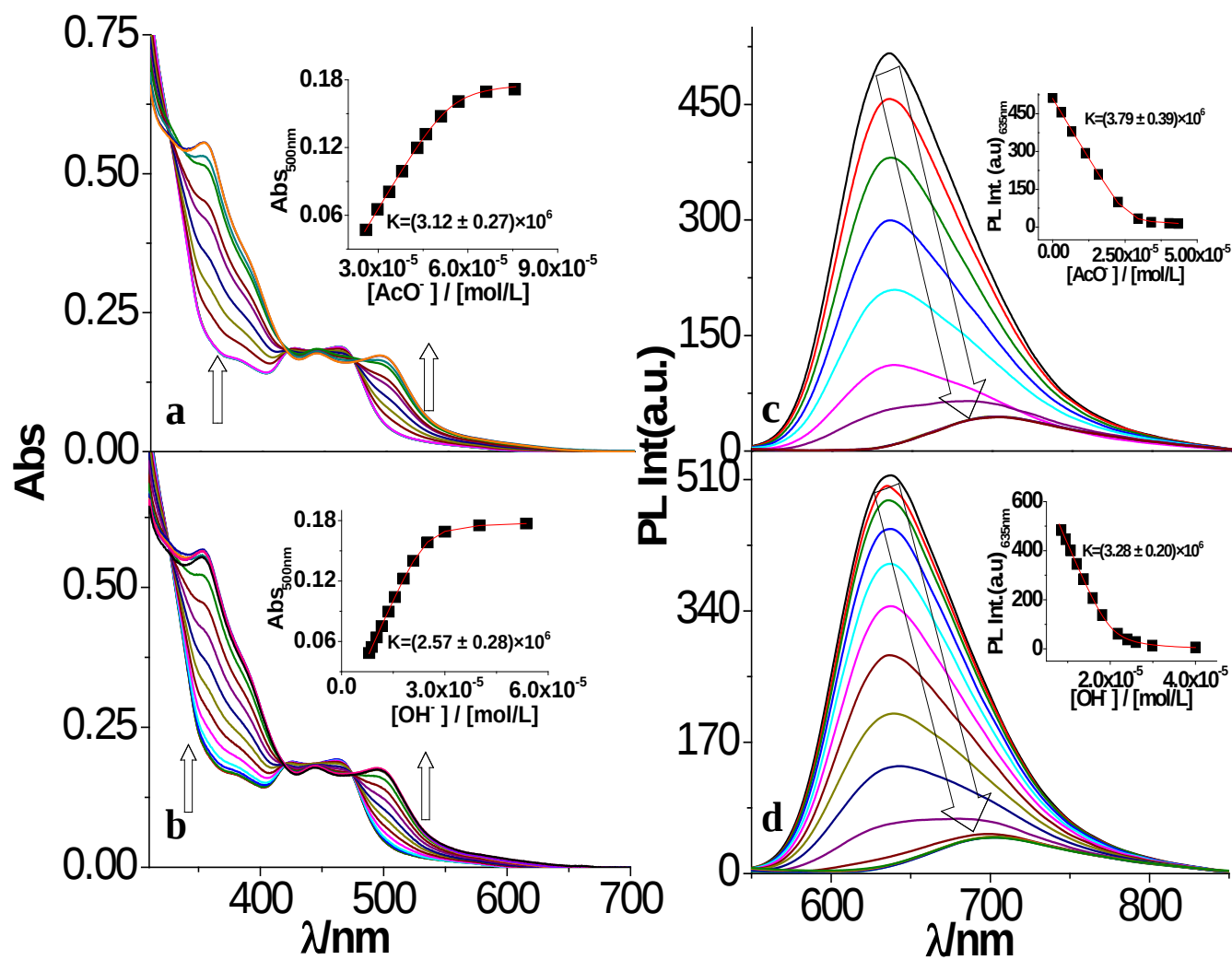


Fig. S6 Changes in UV-vis absorption and photoluminescence spectra of **1** in acetonitrile upon addition of AcO^- (a and c, respectively) and OH^- (b and d, respectively) ions.

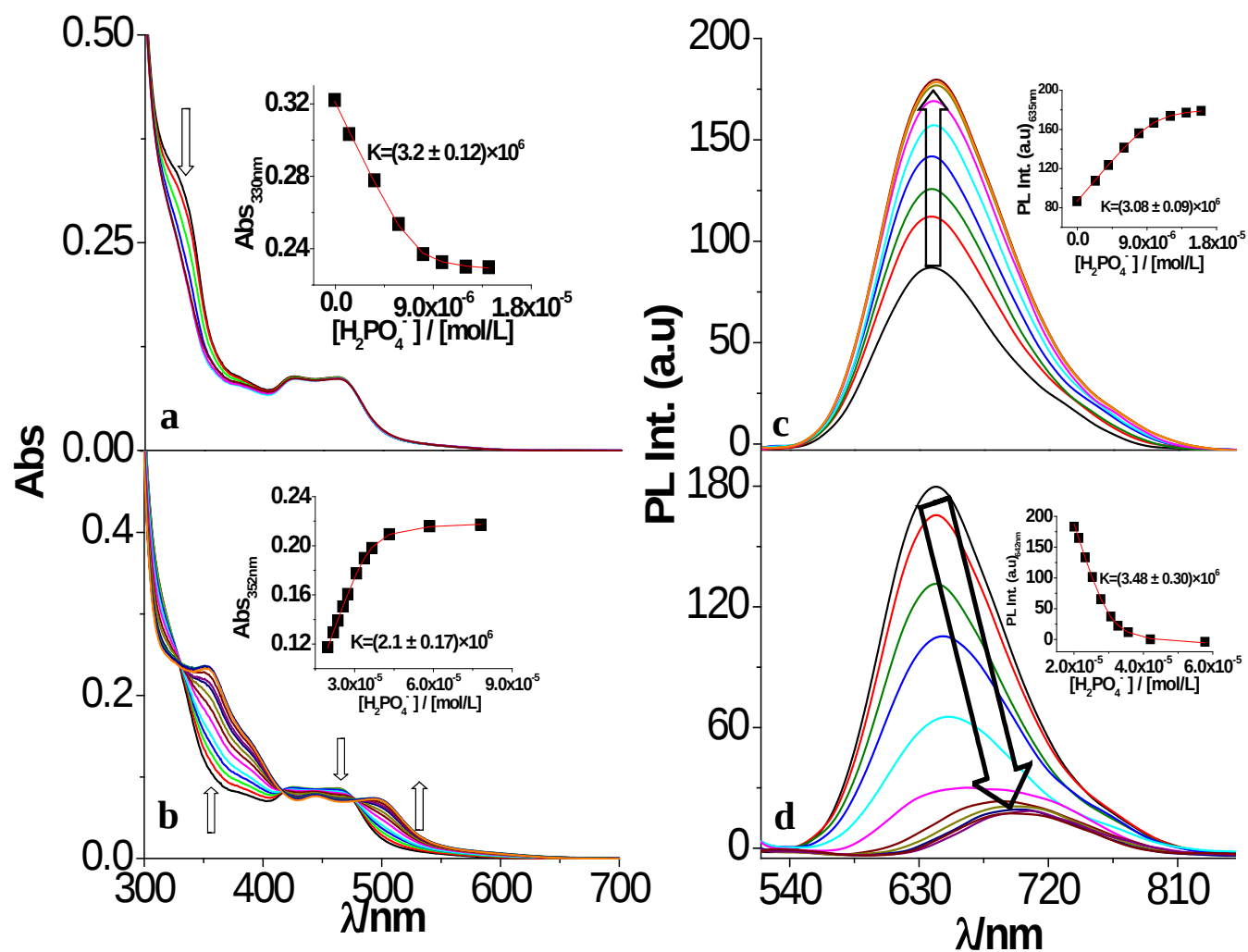


Fig. S7 Changes in UV-vis absorption (a and b) and photoluminescence (c and d) spectra of **1** in acetonitrile upon incremental addition of H_2PO_4^- .

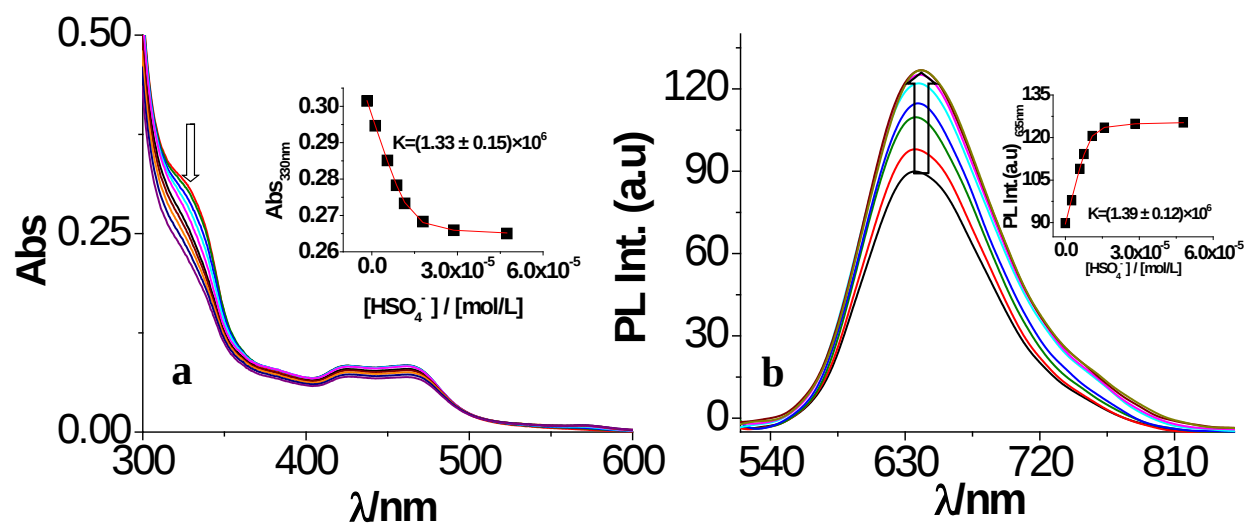


Fig. S8 Changes in UV-vis absorption (a) and photoluminescence (b) spectra of **1** in acetonitrile upon addition of HSO_4^- ion.

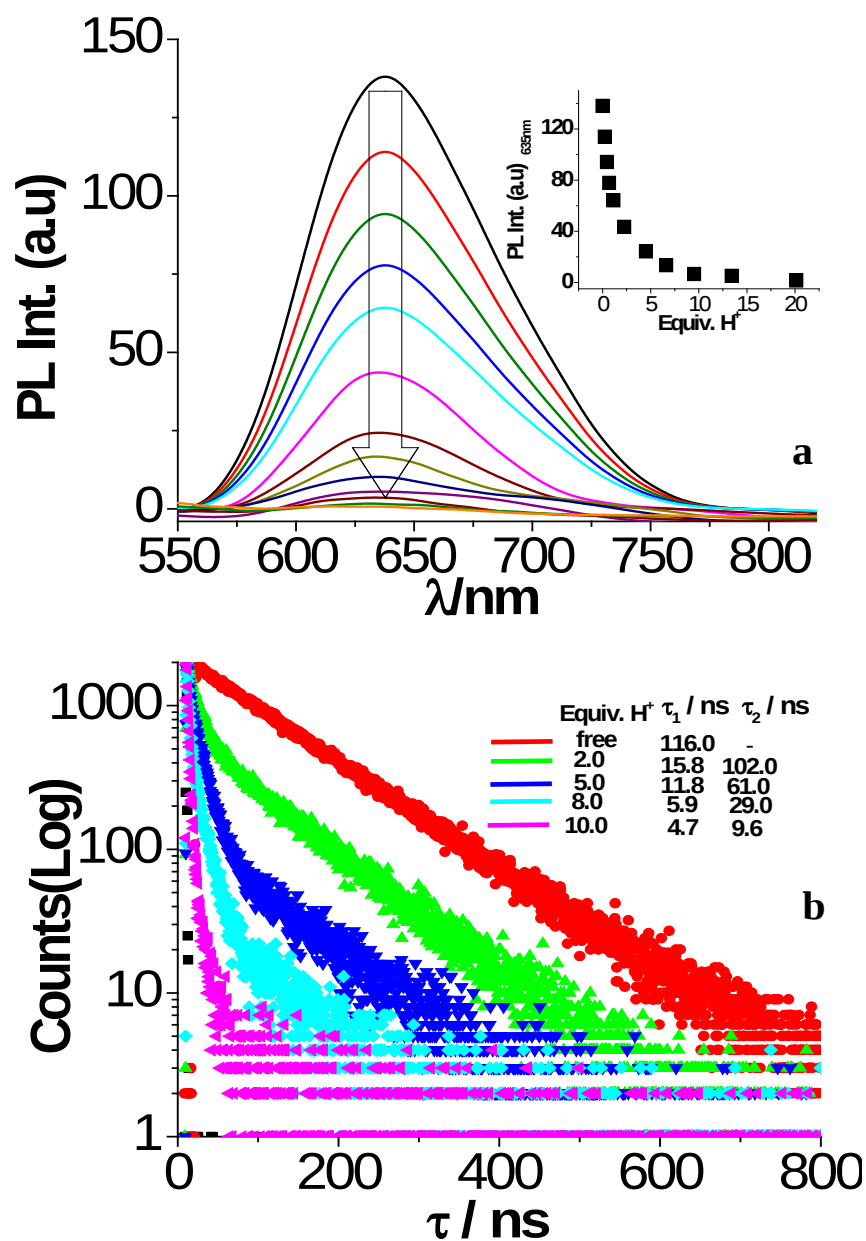


Fig. S9 Changes in photoluminescence spectra (a) and time-resolved luminescence decay profiles (b) of **1** in acetonitrile at room temperature on incremental addition of HClO_4 . The inset shows the change of emission intensity (a) and lifetimes (b) of **1** as a function of the equivalent of HClO_4 added.

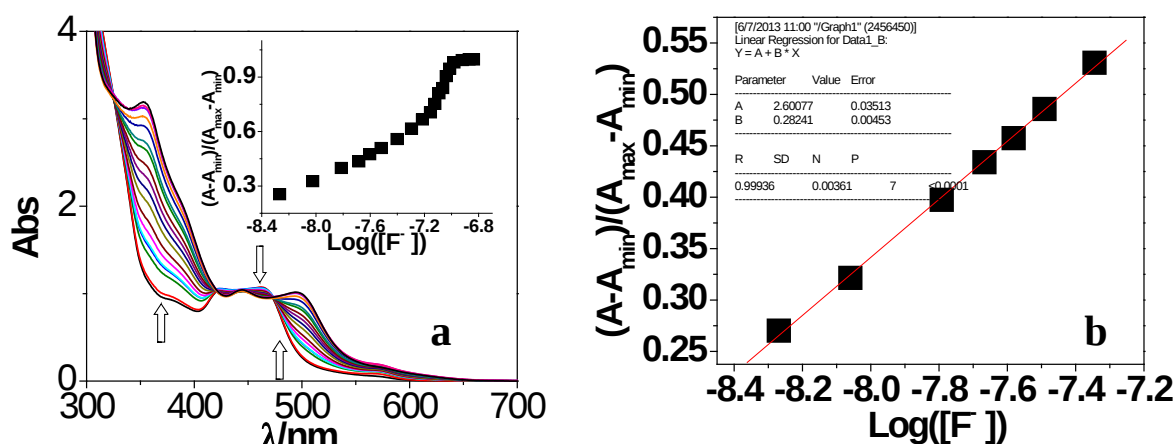


Fig. S10 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with F^- (5.0×10^{-3} M) in acetonitrile. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{F}^-])$, the calculated detection limit of receptor is 4.34×10^{-9} M.

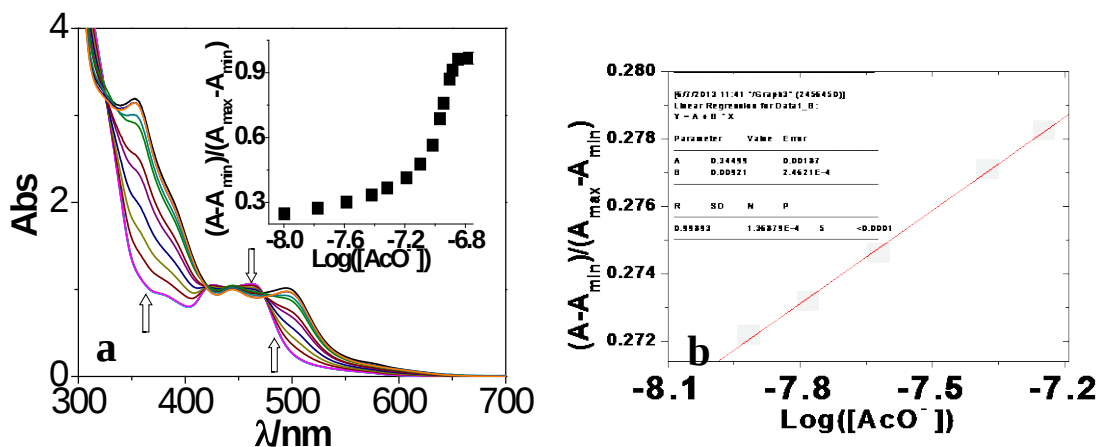


Fig. S11 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with AcO^- (5.0×10^{-3} M) in acetonitrile. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{AcO}^-])$, the calculated detection limit of receptor is 1.03×10^{-8} M.

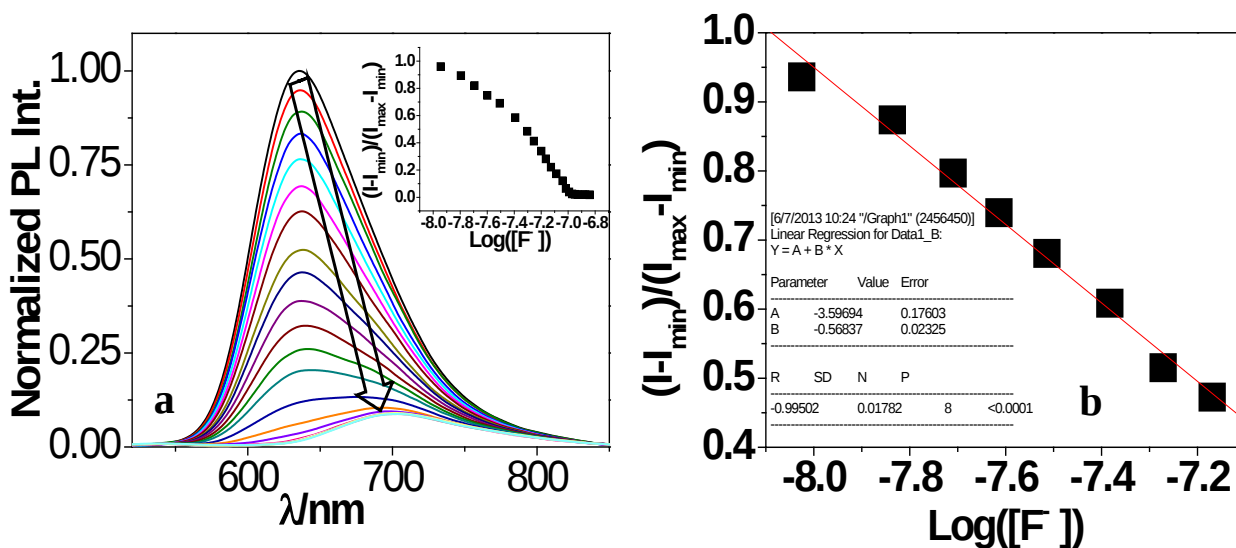


Fig. S12 (a) Luminescence changes during the titration of **1** (2.0 × 10⁻⁵ M) with F⁻ (5.0 × 10⁻³ M) in acetonitrile, inset: Normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of (I-I_{min})/(I_{max}-I_{min}) vs Log([F⁻]), the calculated detection limit of receptor is 8.19 × 10⁻⁹ M.

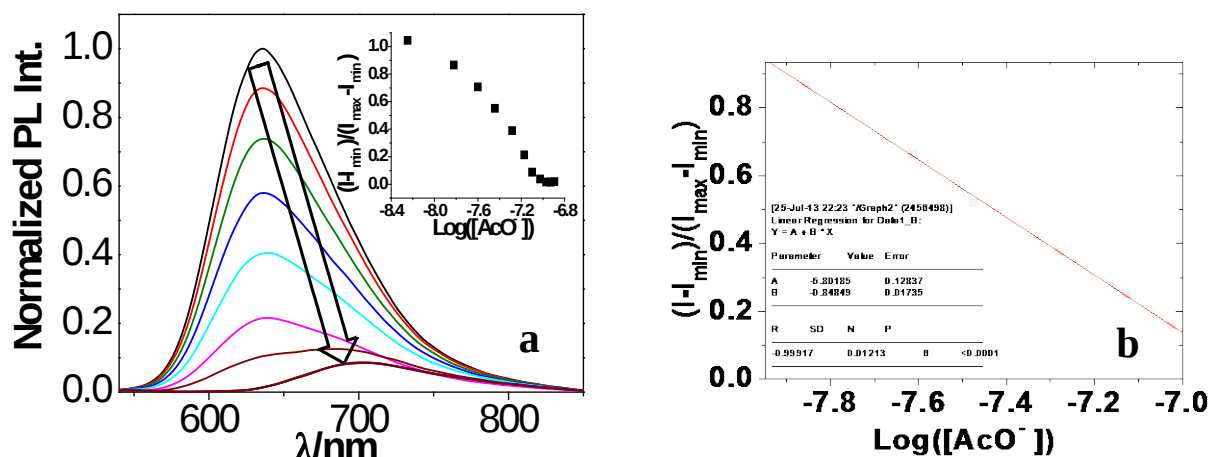


Fig. S13 (a) Luminescence changes during the titration of **1** (2.0 × 10⁻⁵ M) with AcO⁻ (5.0 × 10⁻³ M) in acetonitrile, inset: Normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of (I-I_{min})/(I_{max}-I_{min}) vs Log([AcO⁻]), the calculated detection limit of receptor is 1.19 × 10⁻⁸ M.

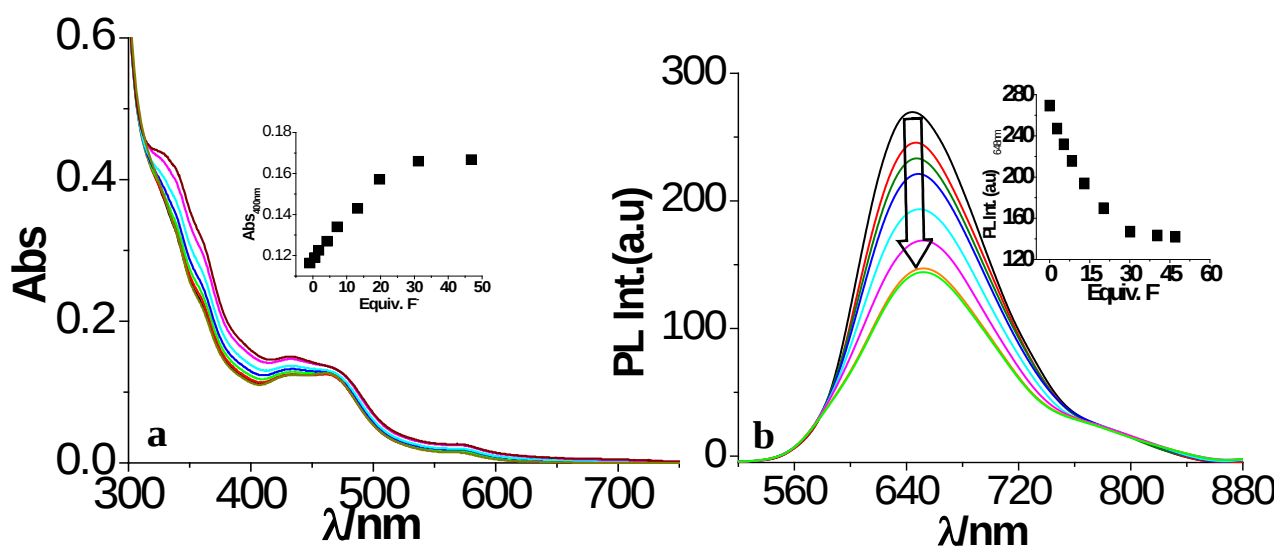


Fig. S14 Changes in UV-vis absorption (a) and photoluminescence spectra (b) of **1** in water upon addition of F^- ion.

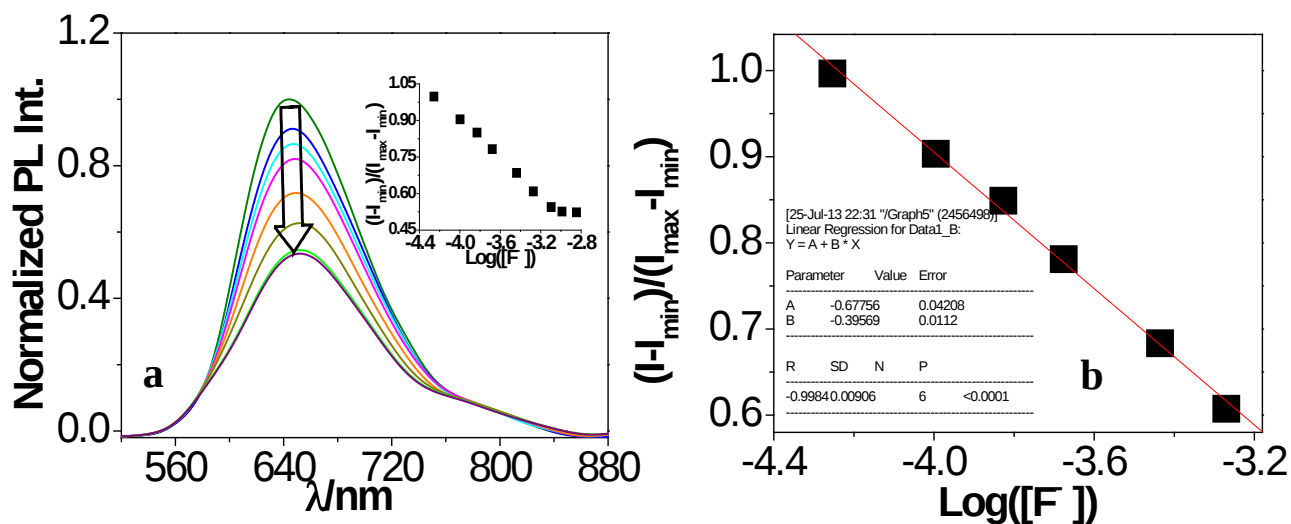


Fig. S15 (a) Luminescence changes during the titration of **1** (2.0×10^{-5} M) with F^- (5.0×10^{-3} M) in water, inset: Normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of $(I-I_{min})/(I_{max}-I_{min})$ vs $\text{Log}([F^-])$, the calculated detection limit of receptor is 4.75×10^{-5} M.

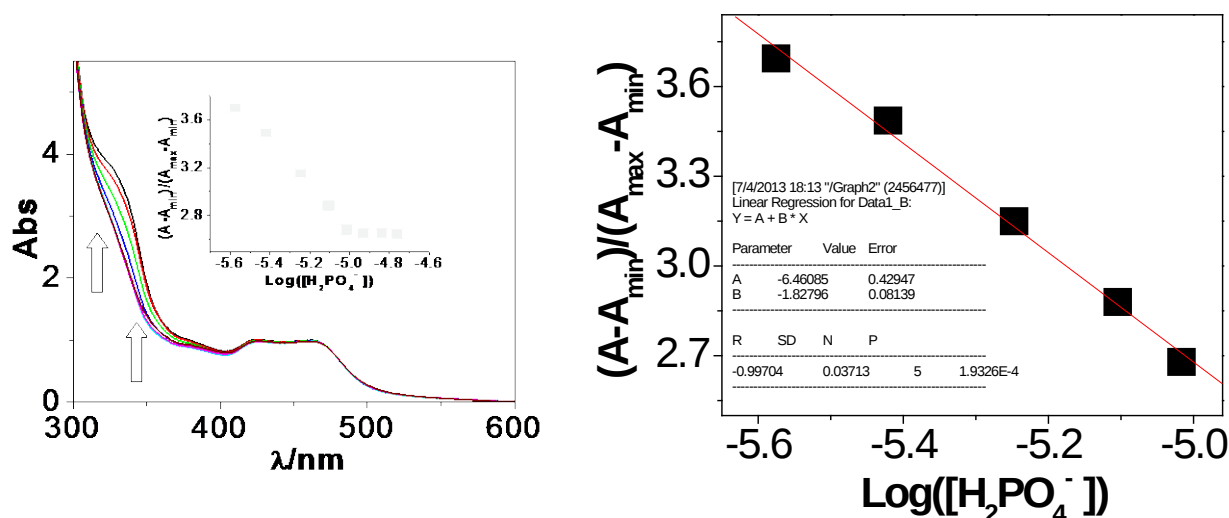


Fig. S16 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with H_2PO_4^- (5.0×10^{-3} M) in acetonitrile. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{H}_2\text{PO}_4^-])$, the calculated detection limit of receptor is 2.30×10^{-6} M.

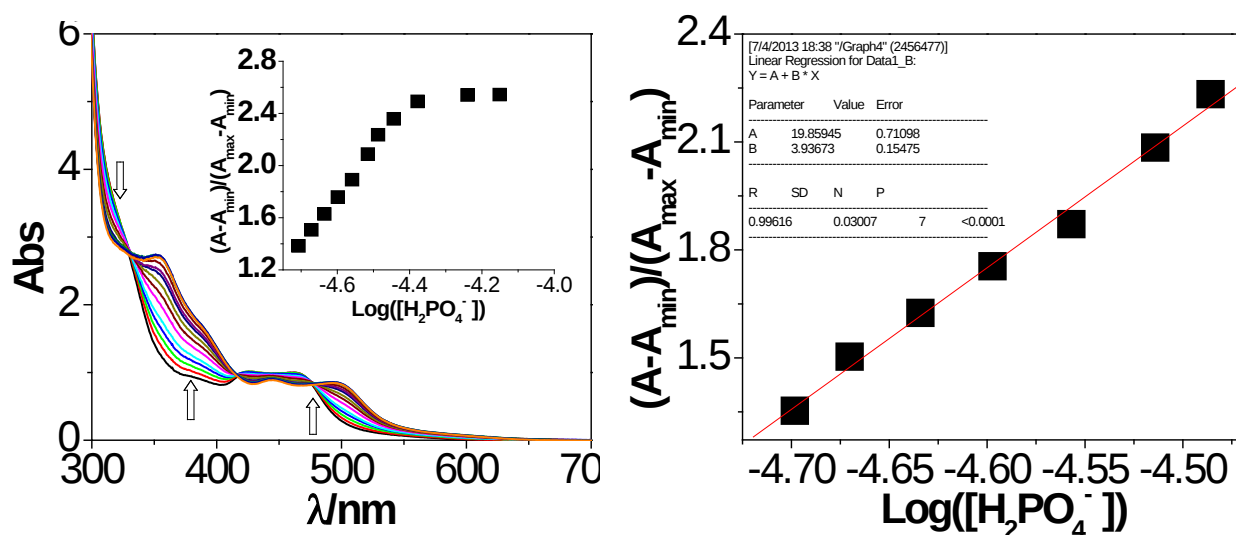


Fig. S17 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with H_2PO_4^- (5.0×10^{-3} M) in acetonitrile. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{H}_2\text{PO}_4^-])$, the calculated detection limit of receptor is 1.89×10^{-5} M.

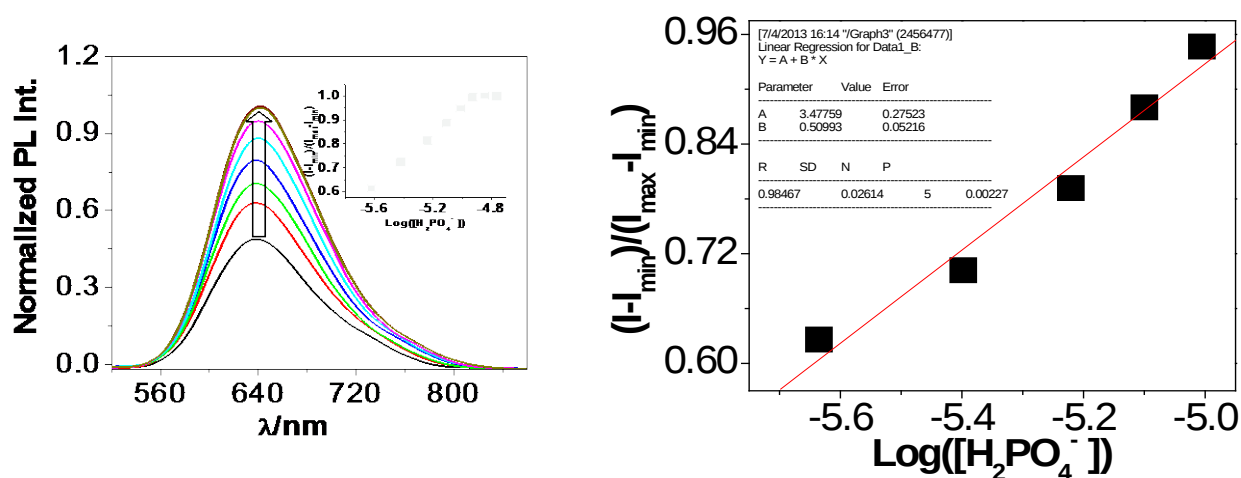


Fig. S18 (a) Luminescence changes during the titration of **1** (2.0 × 10⁻⁵ M) with H₂PO₄⁻ (5.0 × 10⁻³ M) in acetonitrile, inset: normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of $(I - I_{\min}) / (I_{\max} - I_{\min})$ vs $\text{Log}([H_2PO_4^-])$, the calculated detection limit of receptor is 1.99 × 10⁻⁶ M.

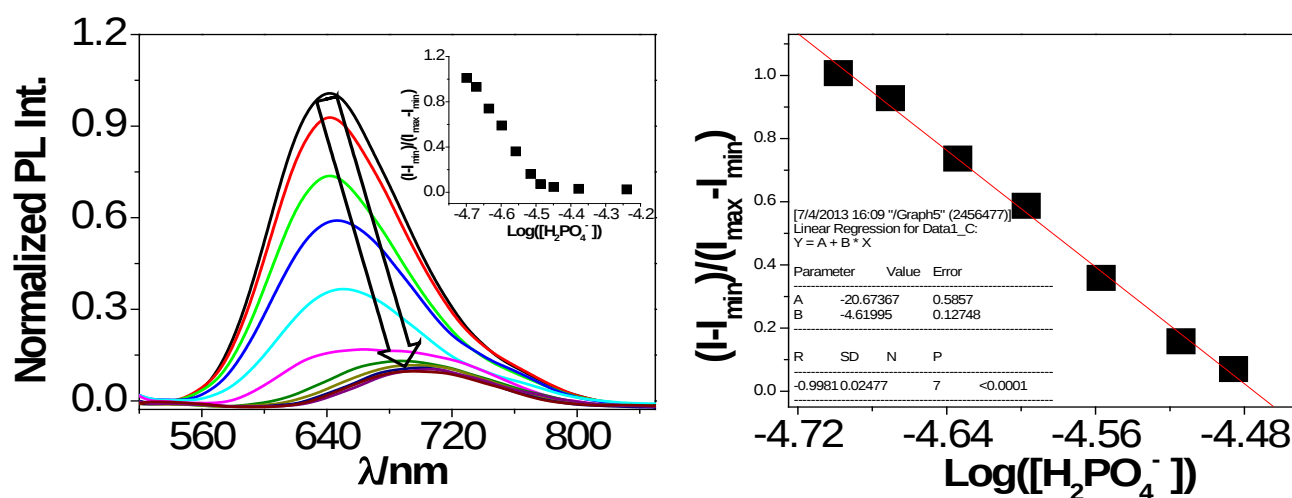


Fig. S19 (a) Luminescence changes during the titration of **1** (2.0 × 10⁻⁵ M) with H₂PO₄⁻ (5.0 × 10⁻³ M) in acetonitrile, inset: normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of $(I - I_{\min}) / (I_{\max} - I_{\min})$ vs $\text{Log}([H_2PO_4^-])$, the calculated detection limit of receptor is 1.90 × 10⁻⁵ M.

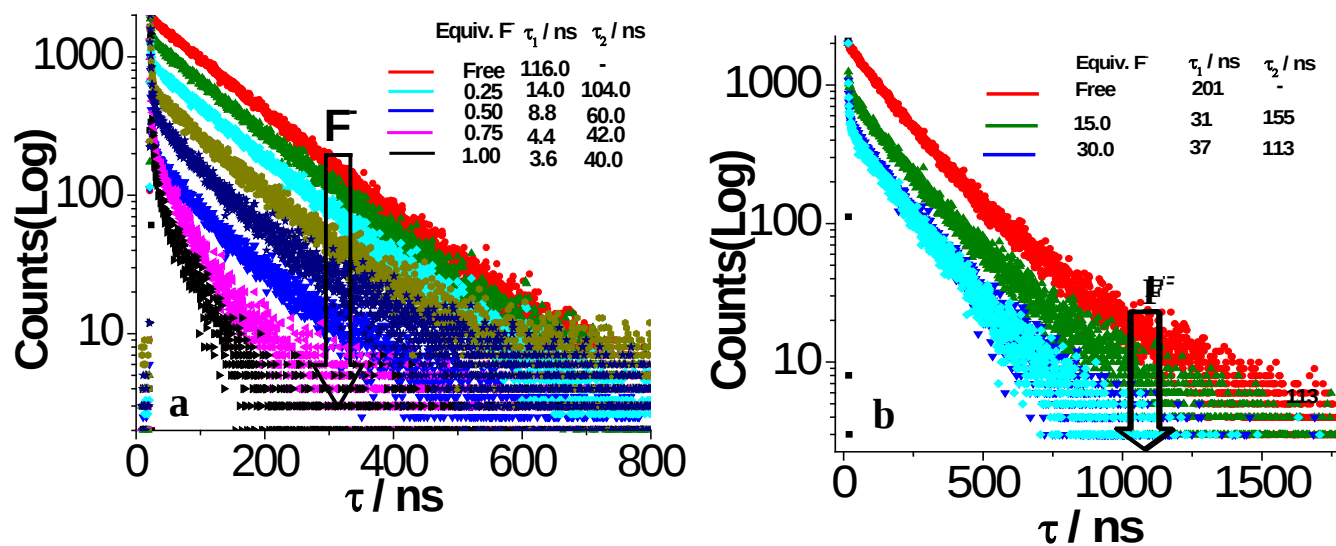


Fig. S20 Changes in time resolved luminescence decay profiles of **1** upon addition of F^- in its acetonitrile (a) and aqueous (b) solution. Lifetimes values are also given in the inset of the figure.

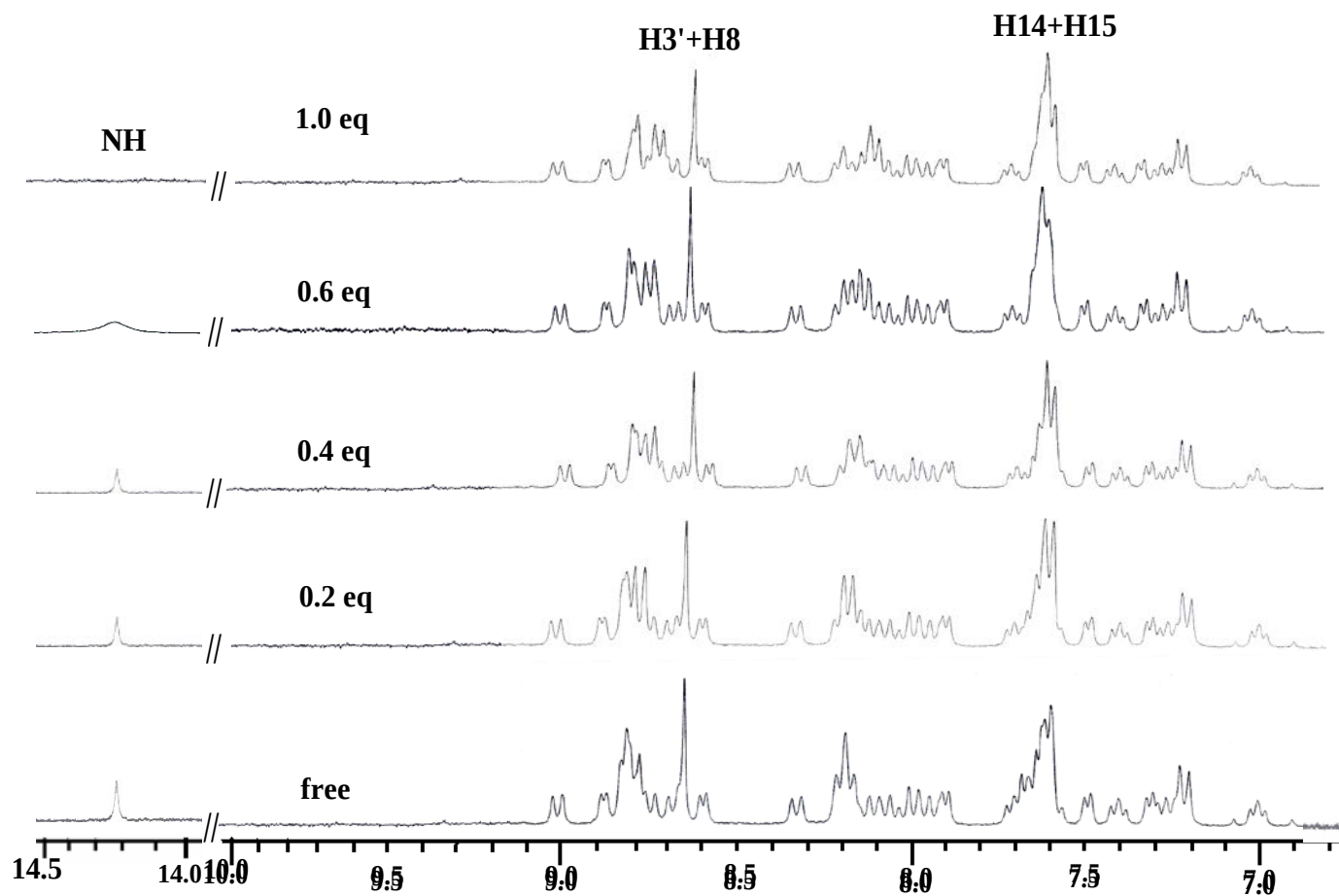


Fig. S21 ¹H NMR titration of **1** in DMSO-*d*₆ solution (5.0×10^{-3} M) upon addition of F⁻ ion (1.25×10^{-1} M, 0–1 equiv).

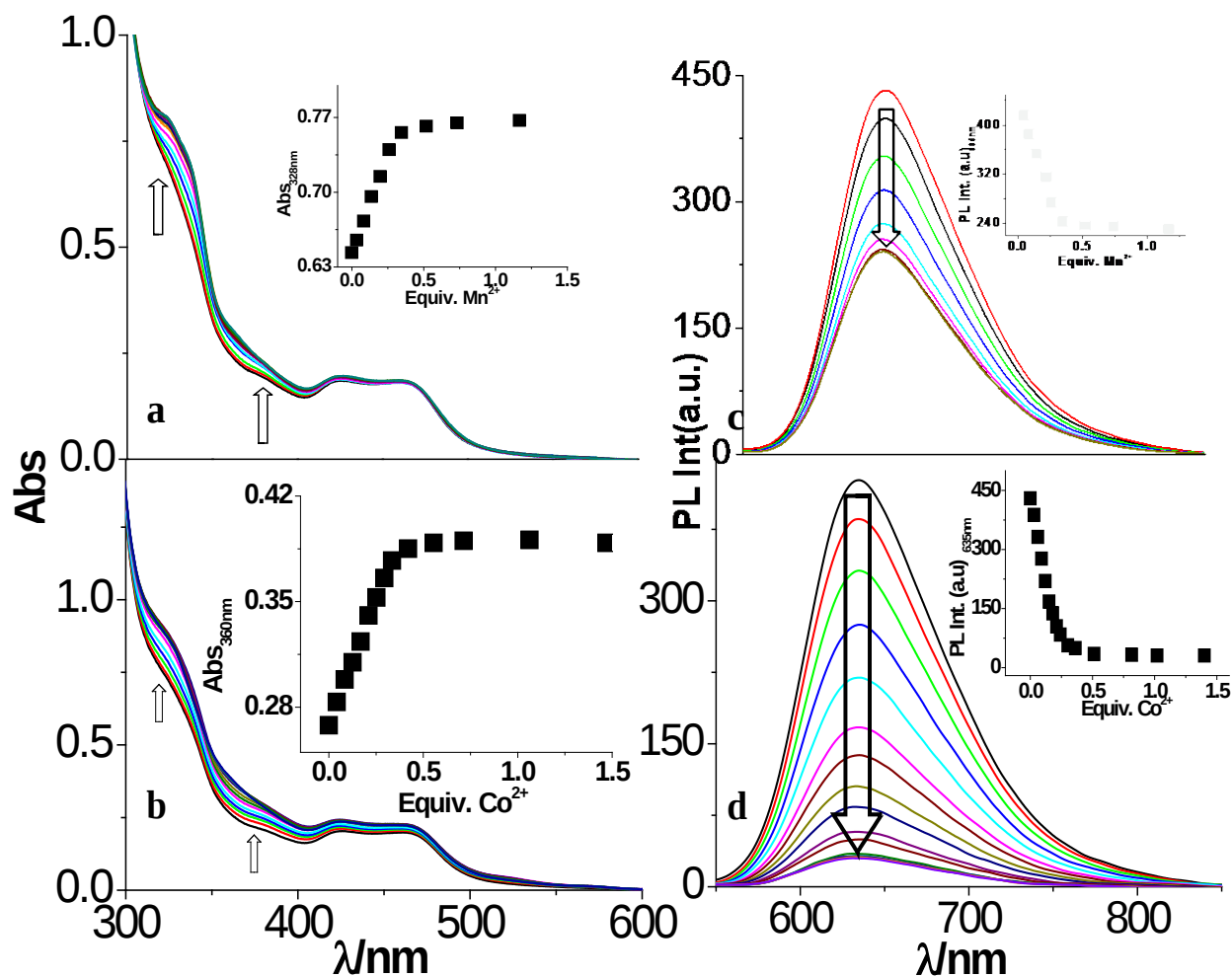


Fig. S22 Changes in UV-vis and photoluminescence spectra of **1** in acetonitrile upon addition of $\text{Mn}(\text{ClO}_4)_2$ (a and c, respectively) and $\text{Co}(\text{ClO}_4)_2$ (b and d, respectively). The inset shows the change of absorption and emission intensity as a function of the equivalent of Mn^{2+} and Co^{2+} ions added.

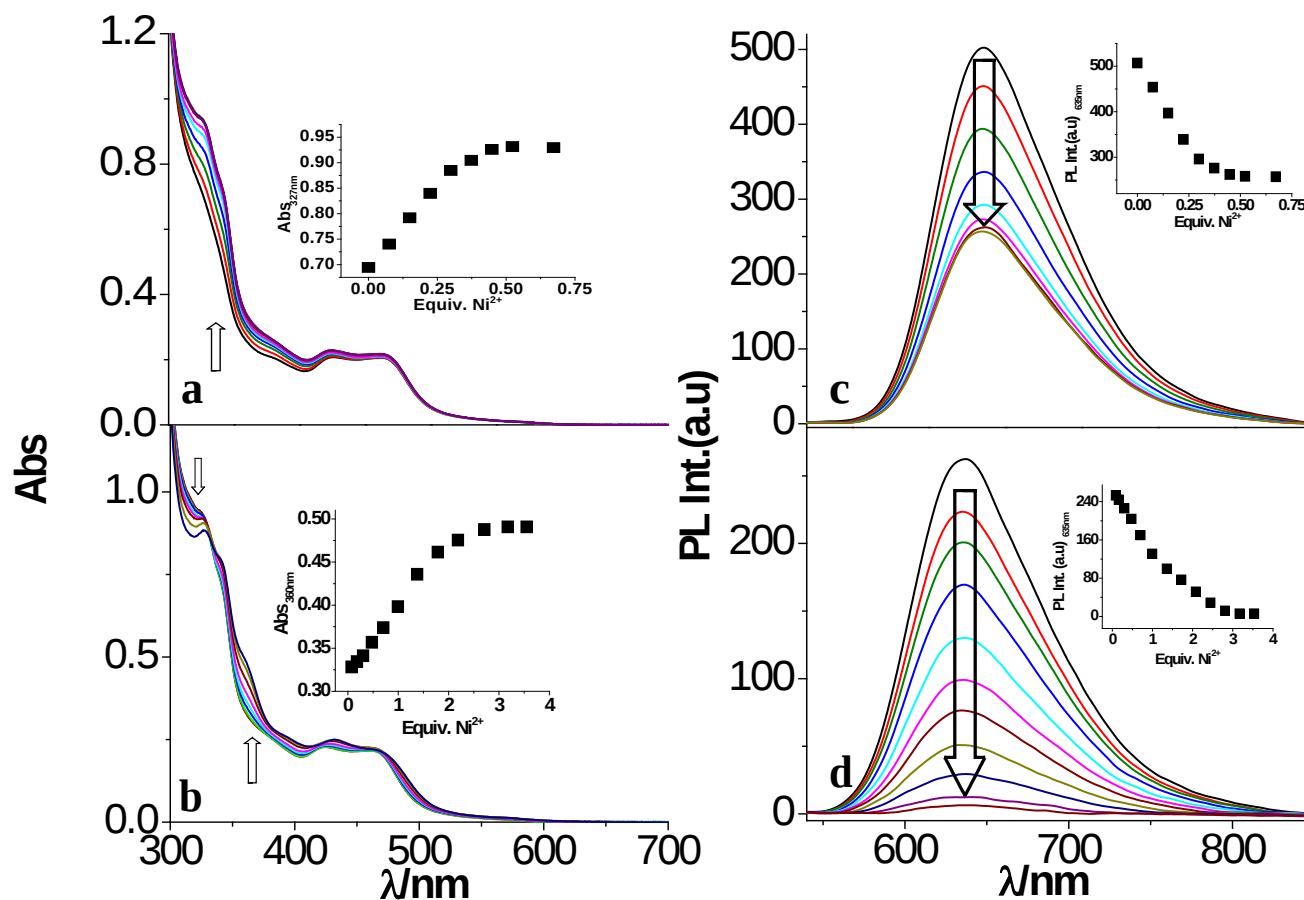


Fig. 23 Changes in UV-vis absorption (a and b) and photoluminescence spectra (c and d) of **1** in acetonitrile upon incremental addition of $\text{Ni}(\text{ClO}_4)_2$. The inset shows the change of absorption and emission intensity as a function of the equivalent of Ni^{2+} ion added.

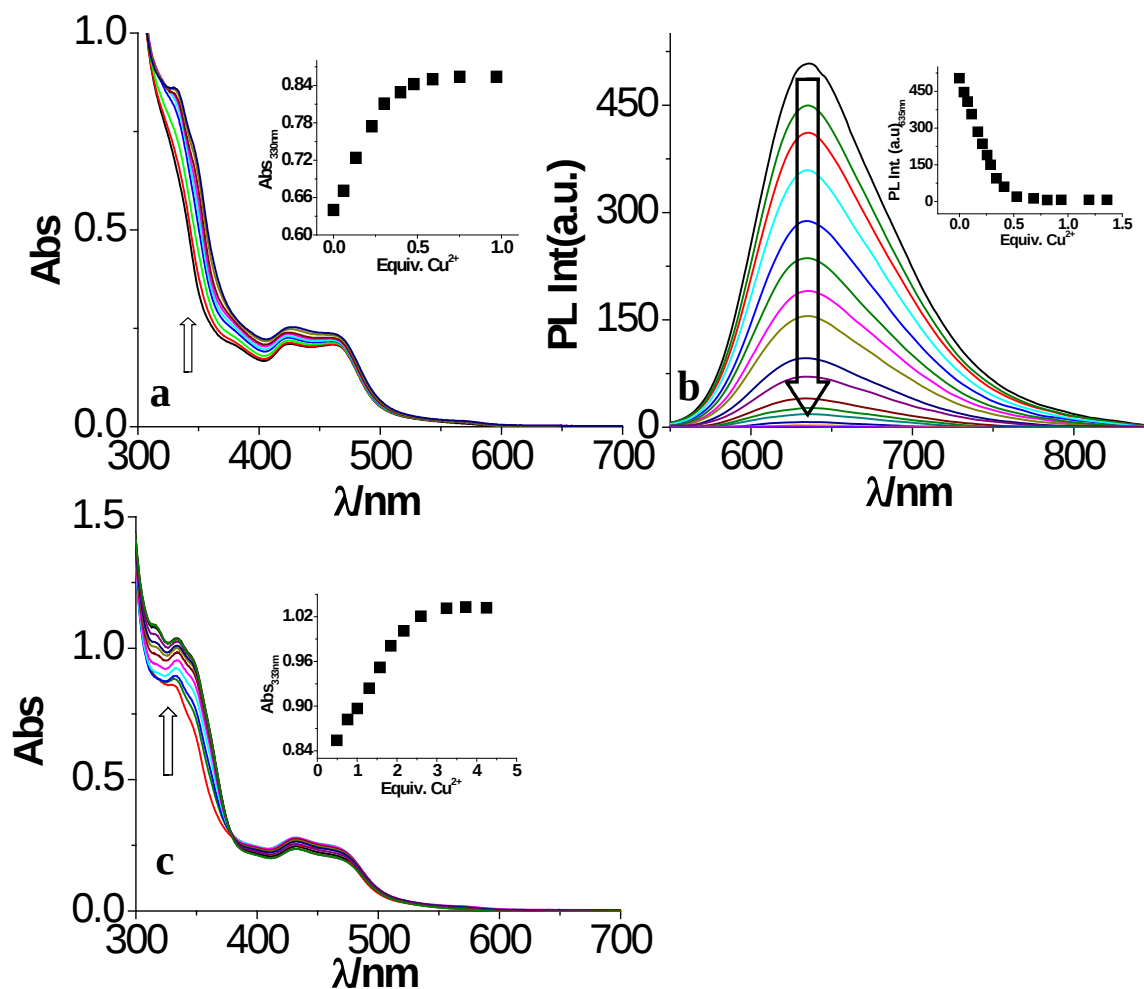


Fig. S24 Changes in UV-vis absorption (a and c) and photoluminescence spectra (b) of **1** in acetonitrile upon addition of $\text{Cu}(\text{ClO}_4)_2$. The inset shows the change of absorption and emission intensity as a function of the equivalent of Cu^{2+} ion added.

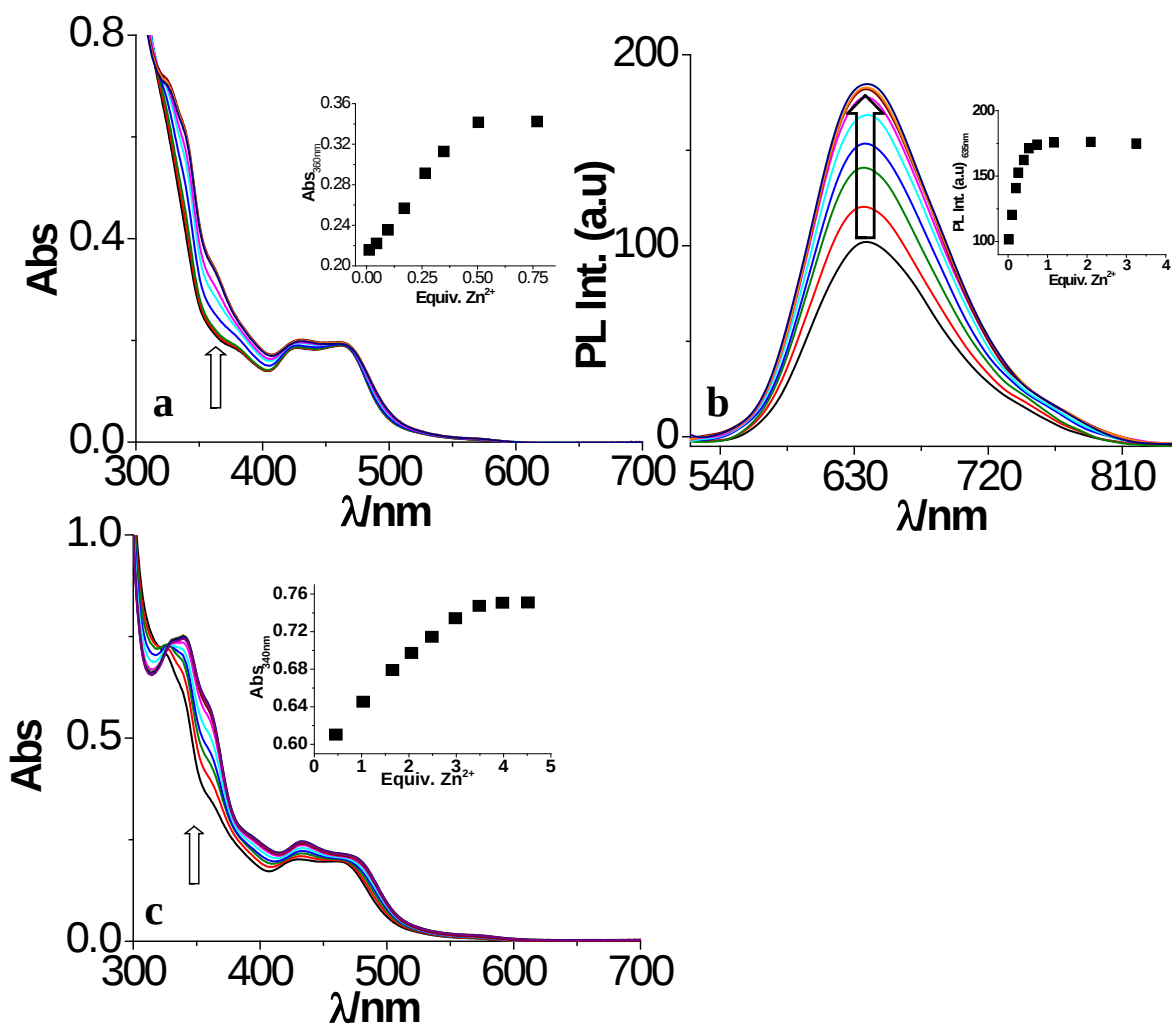


Fig. S25 Changes in UV-vis absorption (a and c) and photoluminescence (b) spectra of **1** in acetonitrile upon addition of $\text{Zn}(\text{ClO}_4)_2$. The inset shows the change of absorption and emission intensity as a function of the equivalent of Zn^{2+} ion added.

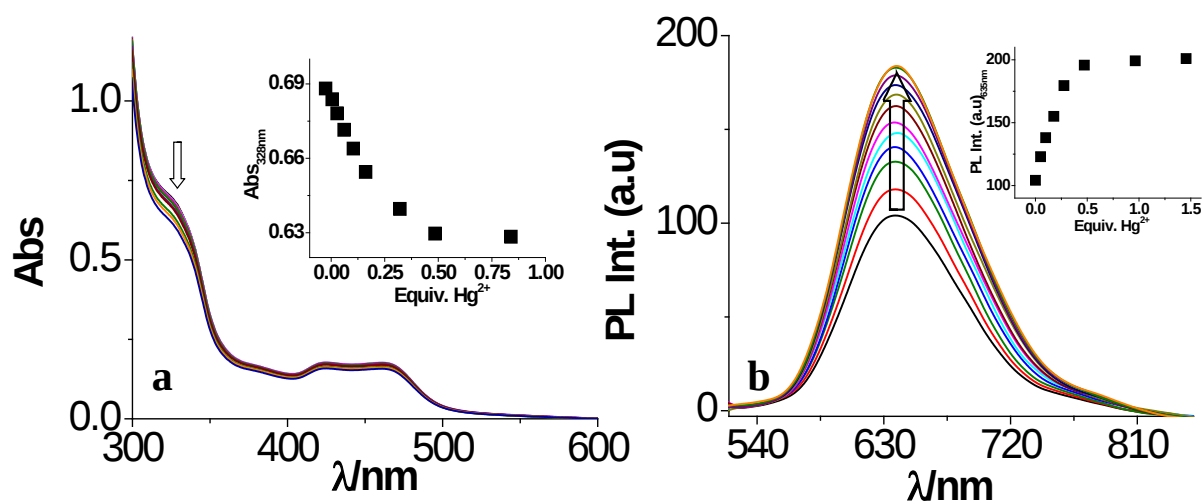


Fig. S26 Changes in UV-vis absorption (a) and photoluminescence (b) spectra of **1** in acetonitrile upon addition of $\text{Hg}(\text{ClO}_4)_2$. The inset shows the change of absorption and emission intensity as a function of the equivalent of Hg^{2+} ion added.

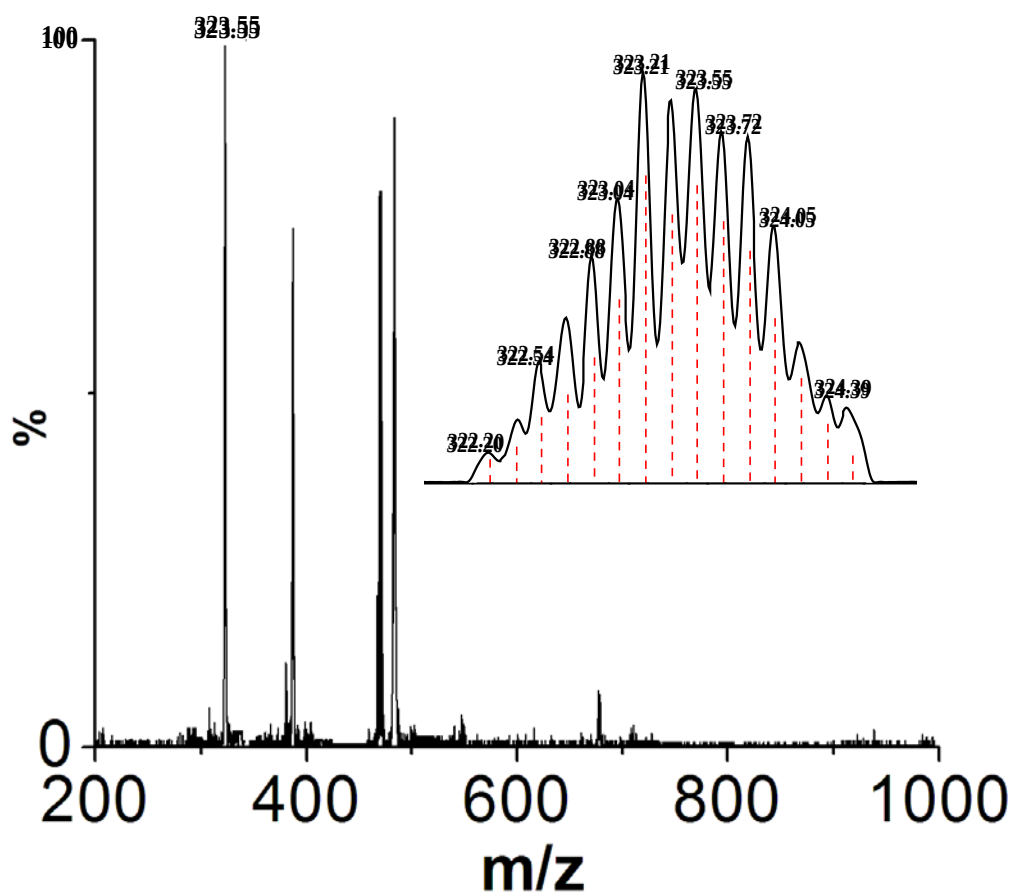


Fig. S27 Experimental ESI mass spectra (positive) for **1** in acetonitrile in the presence Fe^{2+} . Inset shows the observed and simulated isotopic distribution patterns of the peak at $m/z = 323.55$.

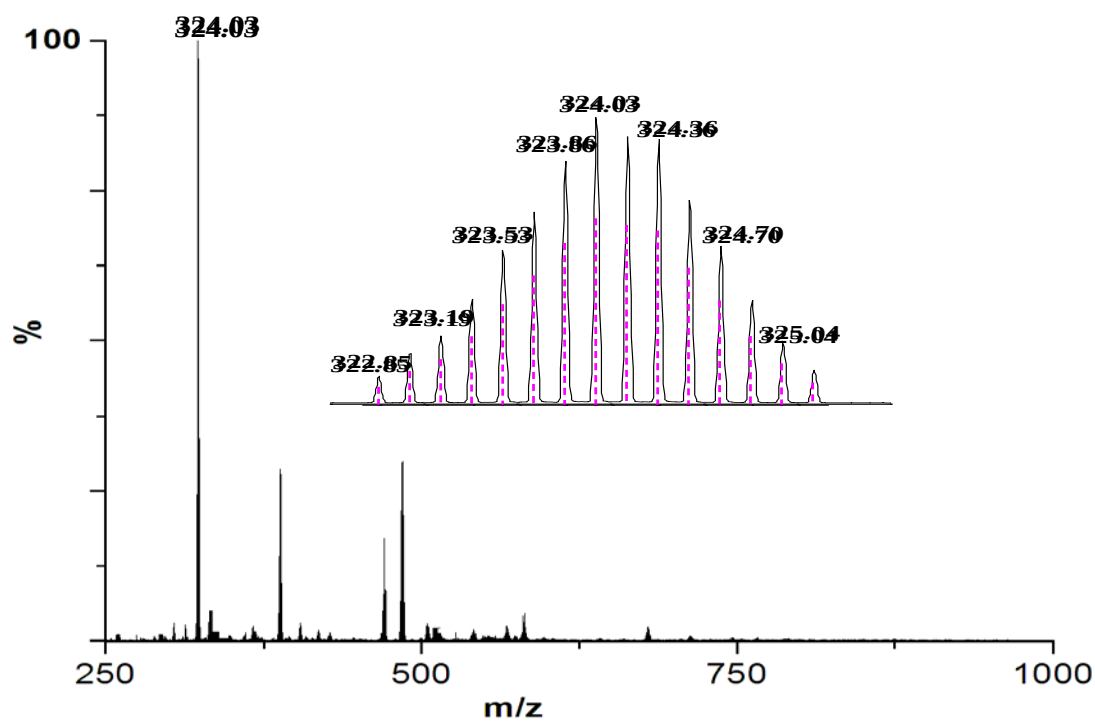


Fig. S28 Experimental ESI mass spectra (positive) for **1** in acetonitrile in the presence Ni^{2+} . Inset shows the observed and simulated isotopic distribution patterns of the peak at $m/z = 324.03$.

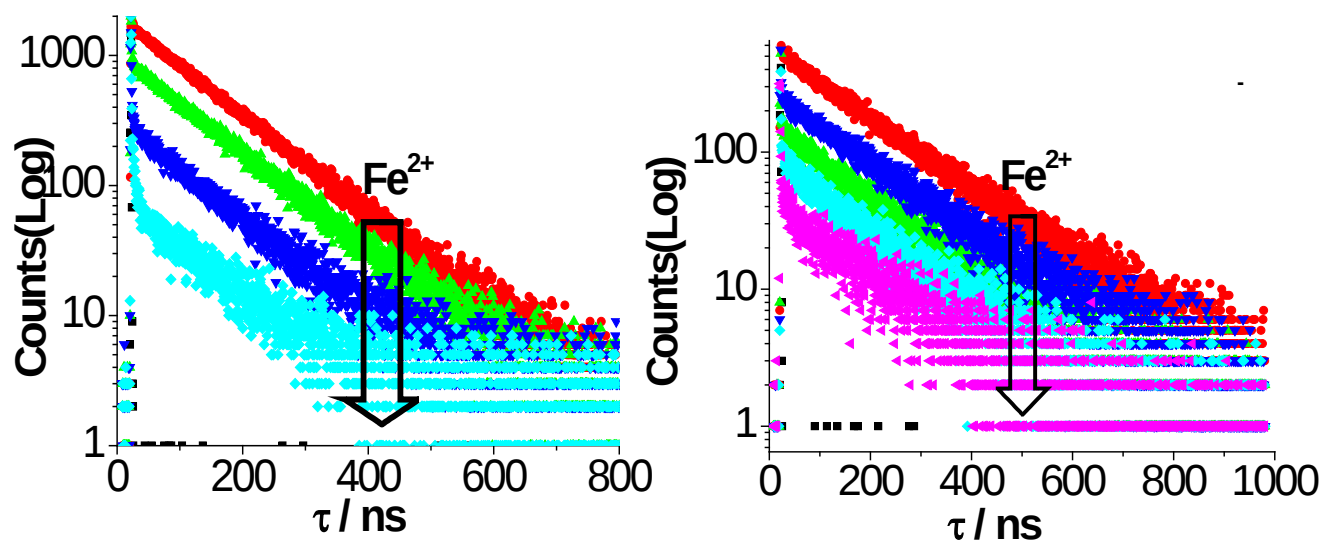


Fig. S29 Changes in time resolved luminescence decay profiles of **1** upon addition of Fe^{2+} ion in its acetonitrile (a) and aqueous (b) solution.

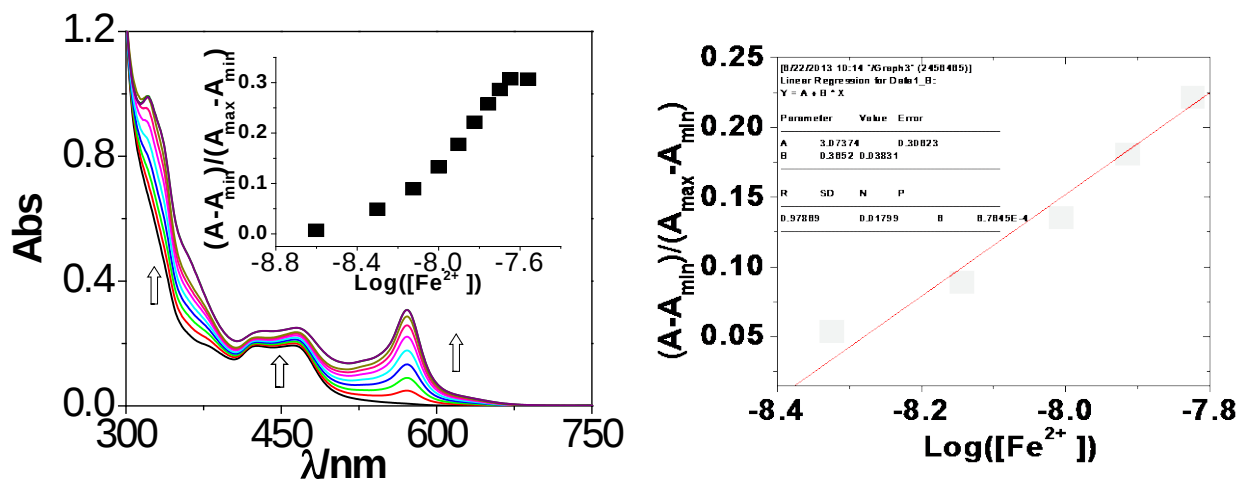


Fig. S30 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with Fe^{2+} (5.0×10^{-3} M) in acetonitrile. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{Fe}^{2+}])$, the calculated detection limit of receptor is 6.68×10^{-9} M.

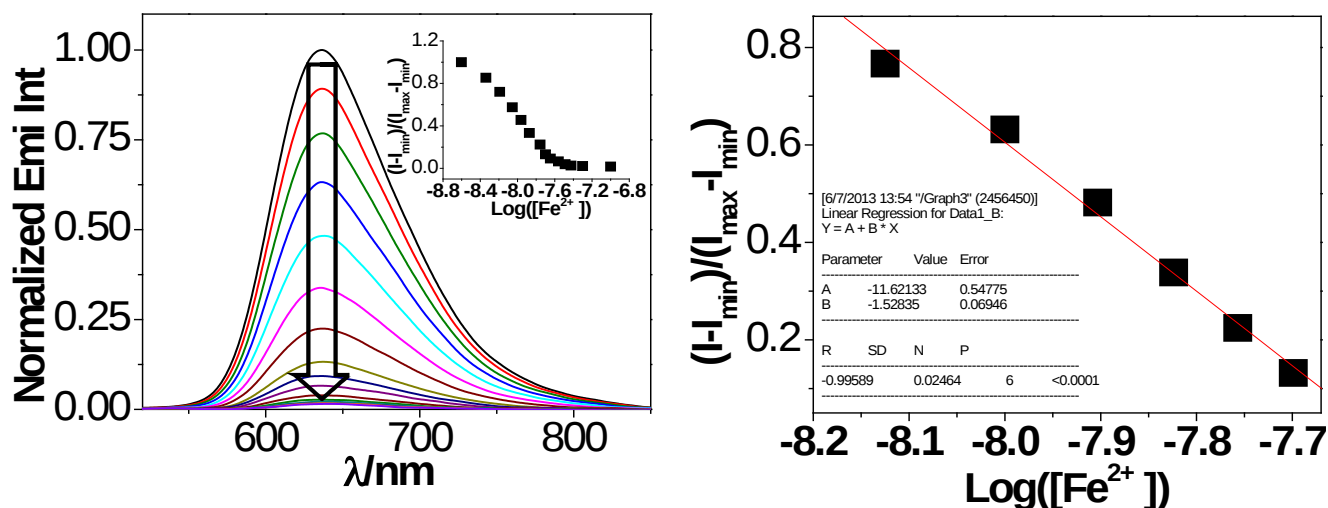


Fig. S31 (a) Luminescence changes during the titration of **1** (2.0×10^{-5} M) with Fe^{2+} (5.0×10^{-3} M) in acetonitrile, inset: normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of $(I-I_{\min})/(I_{\max}-I_{\min})$ vs $\text{Log}([\text{Fe}^{2+}])$, the calculated detection limit of receptor is 6.78×10^{-9} M.

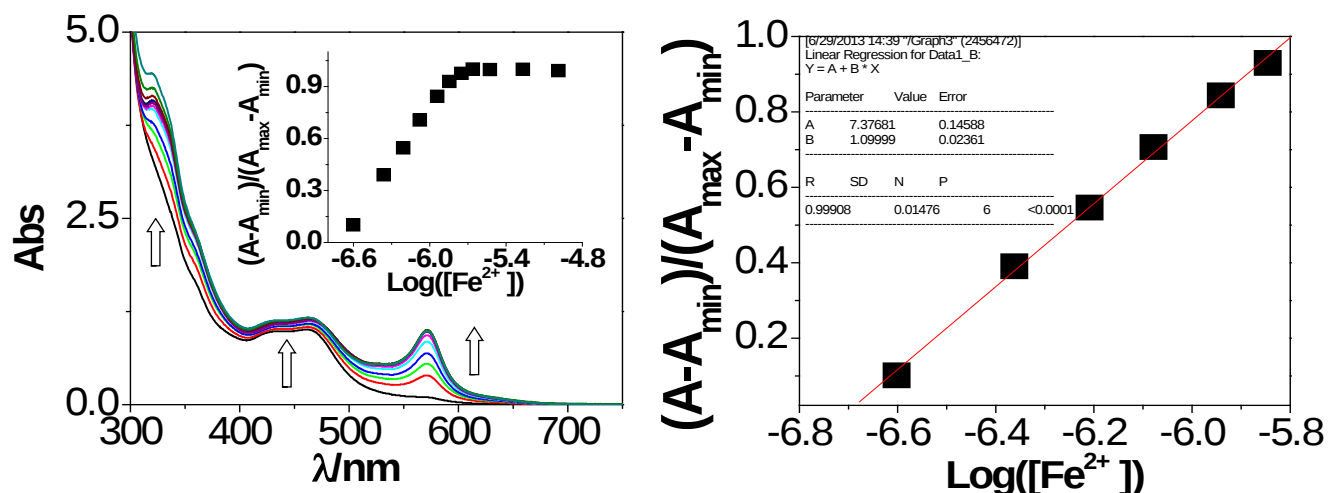


Fig. S32 (a) Absorbance changes during the titration of **1** (2.0×10^{-5} M) with Fe^{2+} (5.0×10^{-3} M) in water. Normalized absorbance between the minimum absorbance and the maximum absorbance. (b) A plot of $(A-A_{\min})/(A_{\max}-A_{\min})$ vs $\text{Log}([\text{Fe}^{2+}])$, the calculated detection limit of receptor is 2.18×10^{-7} M.

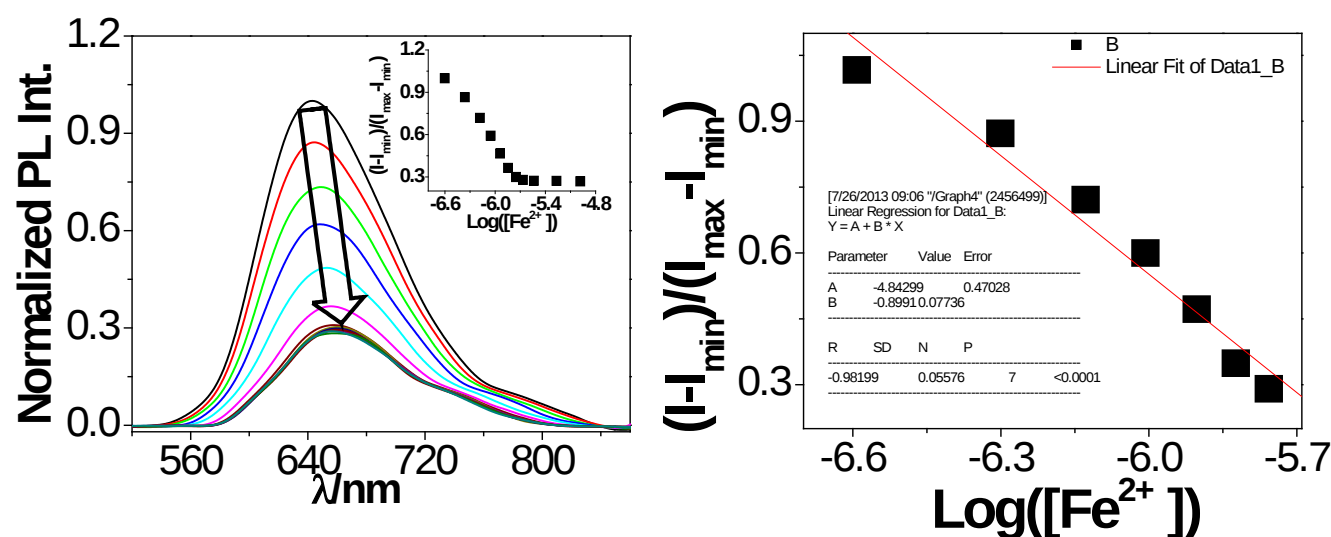


Fig. S33 (a) Luminescence changes during the titration of **1** (2.0×10^{-5} M) with Fe^{2+} (5.0×10^{-3} M) in water, inset: normalized intensity between the minimum intensity and the maximum intensity. (b) A plot of $(I-I_{\min})/(I_{\max}-I_{\min})$ vs $\text{Log}([\text{Fe}^{2+}])$, the calculated detection limit of receptor is 2.38×10^{-7} M.

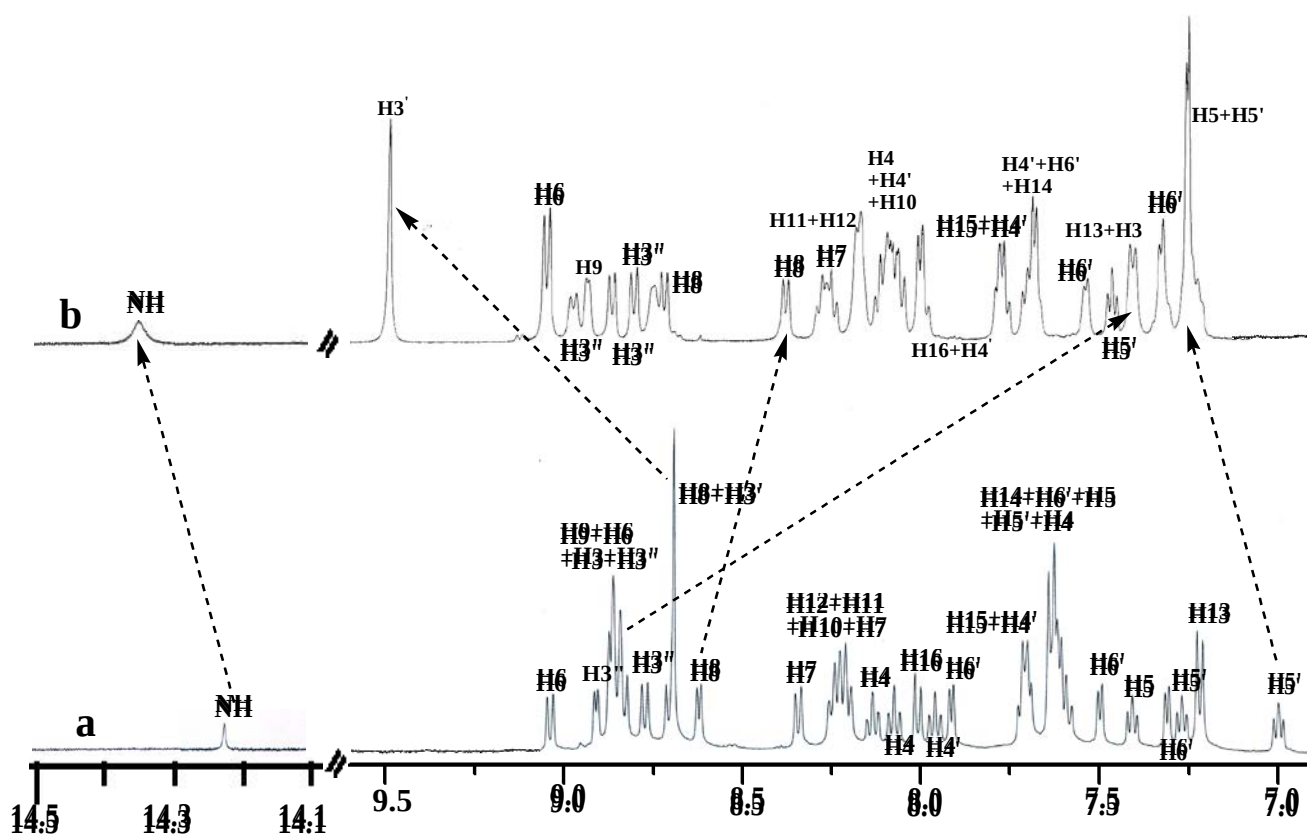


Fig. S34 ^1H NMR spectra of **1** in $\text{DMSO-}d_6$ (5.0×10^{-3} M) in absence (a) and in presence of 0.5 equiv. of Fe^{2+} ion (b).

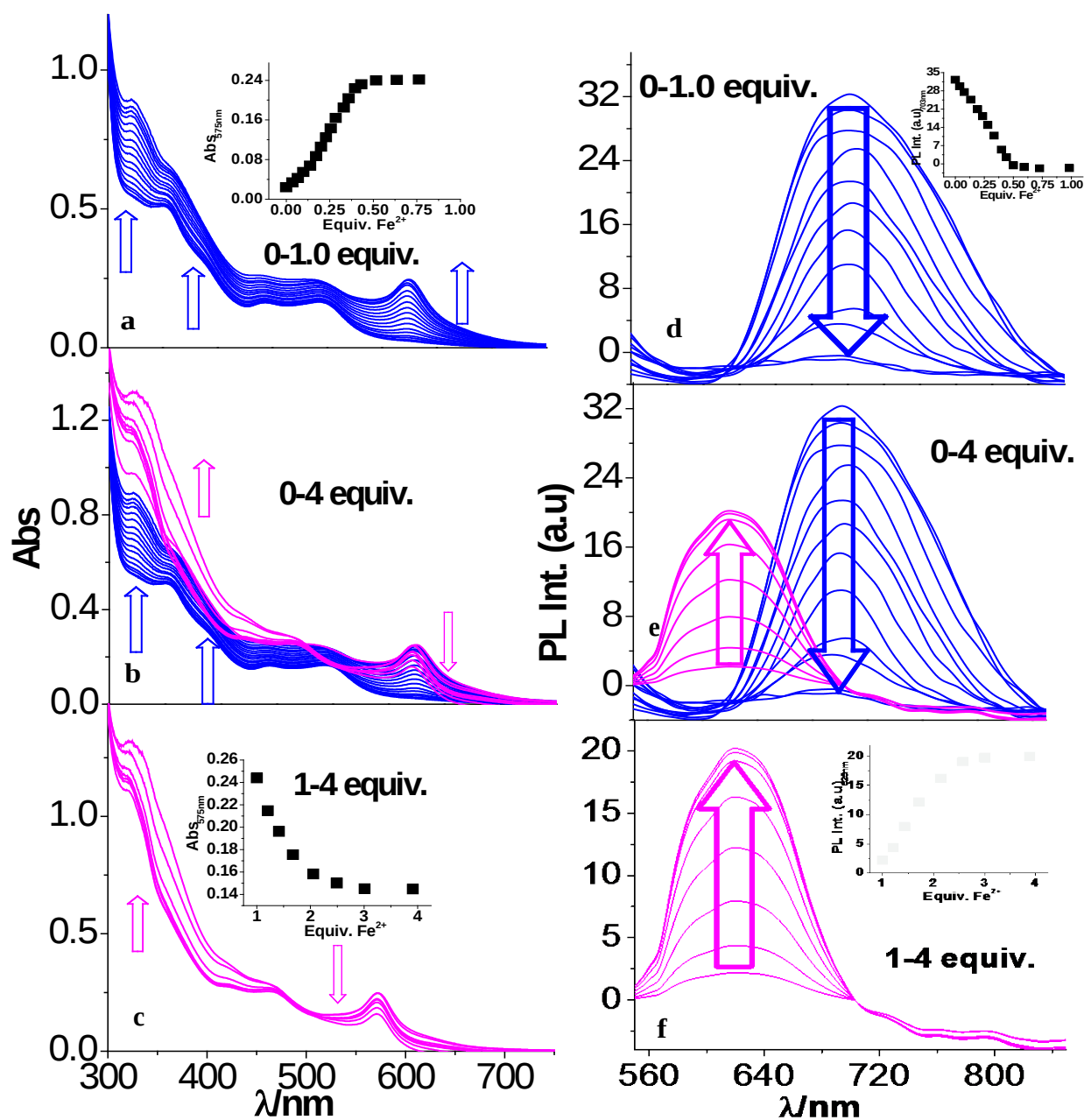


Fig. S35 Changes in UV-vis absorption (a-c) and photoluminescence (d-f) spectra of **1** in acetonitrile upon incremental addition of Fe^{2+} in the presence of 1 equiv. of F^- ion.

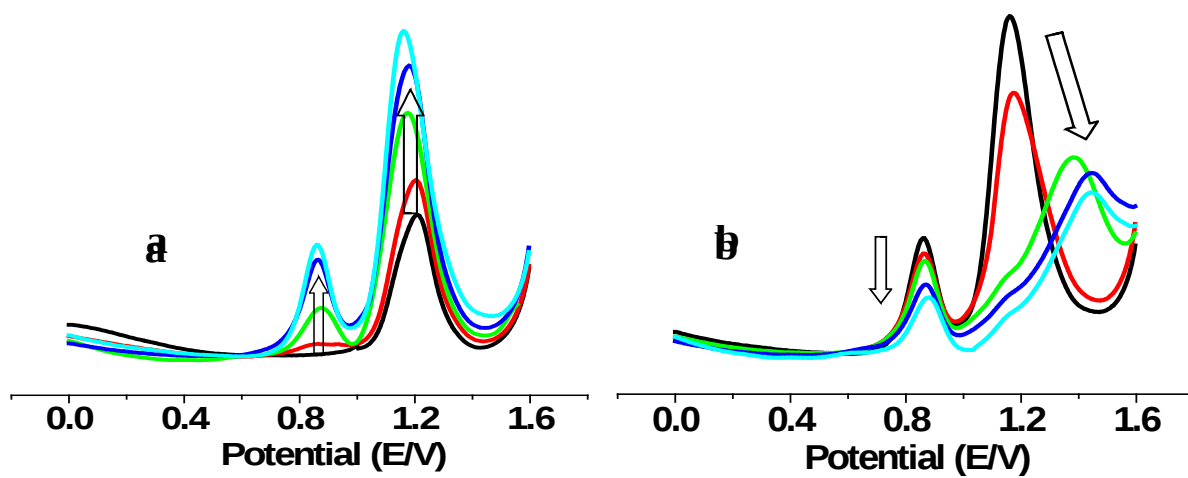


Fig. S36 Changes of SWVs of **1** on incremental addition of F^- (a: 0-2 equiv. and b: 2-10 equiv.) in the presence of 0.5 equiv of Fe^{2+} ion.

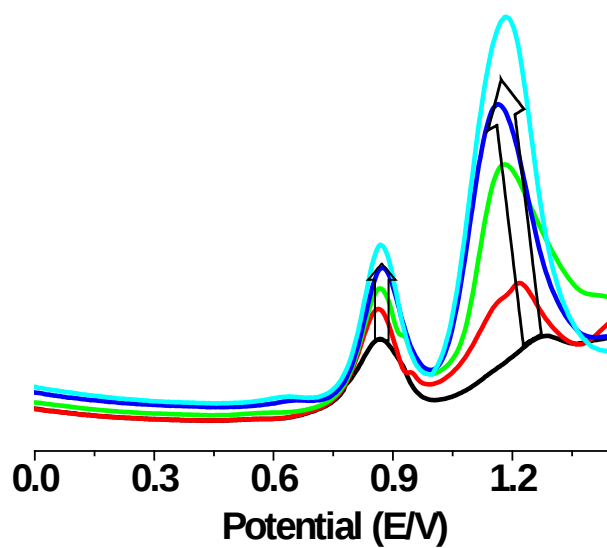


Fig. S37 Changes of SWVs of **1** on incremental addition of Fe²⁺ (0-1 equiv.) in the presence of 1.0 equiv of F⁻ ion.