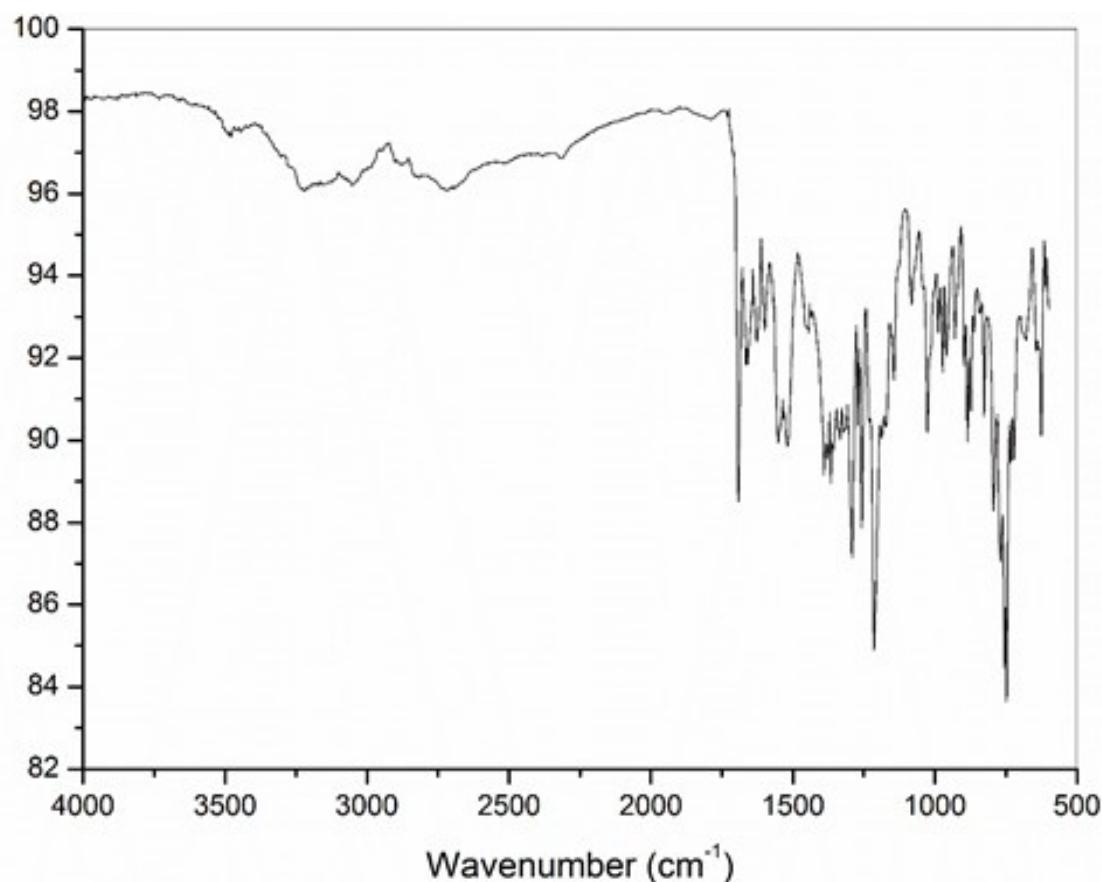


**A novel Schiff base derivative of pyridoxal for the optical sensing of Zn<sup>2+</sup> and cysteine**

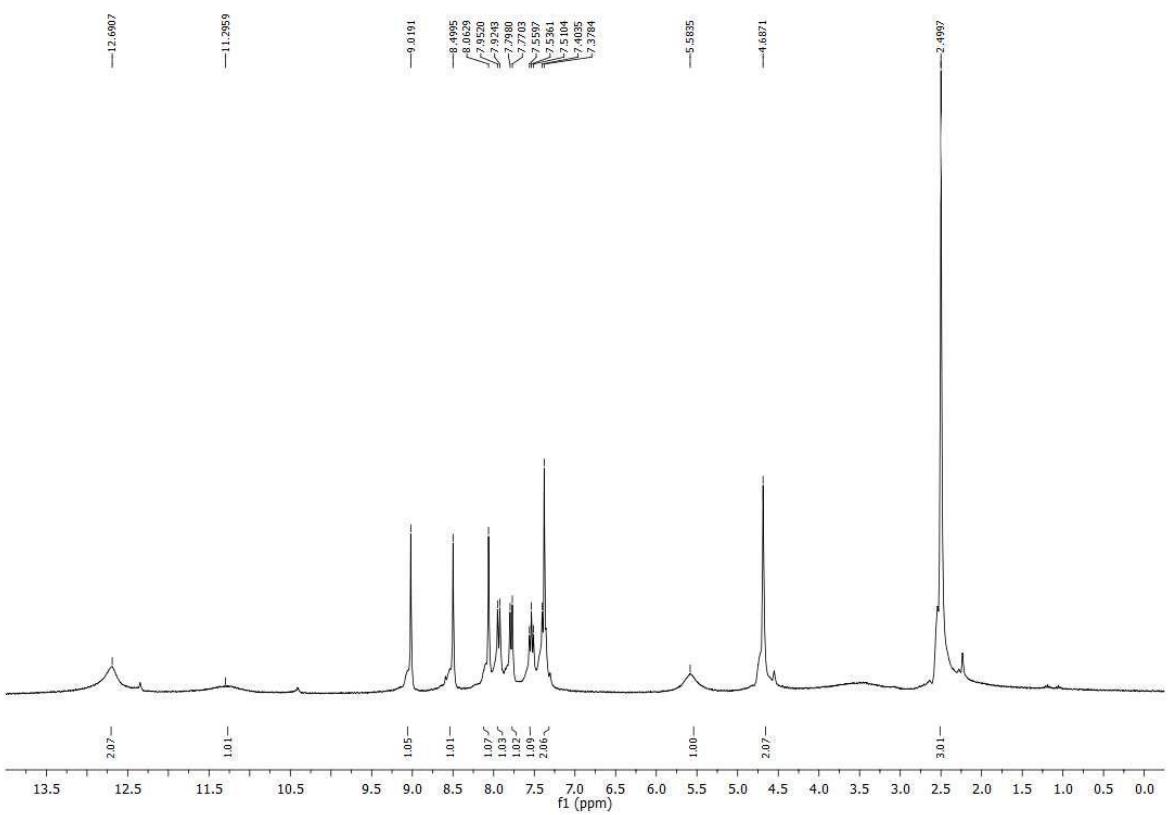
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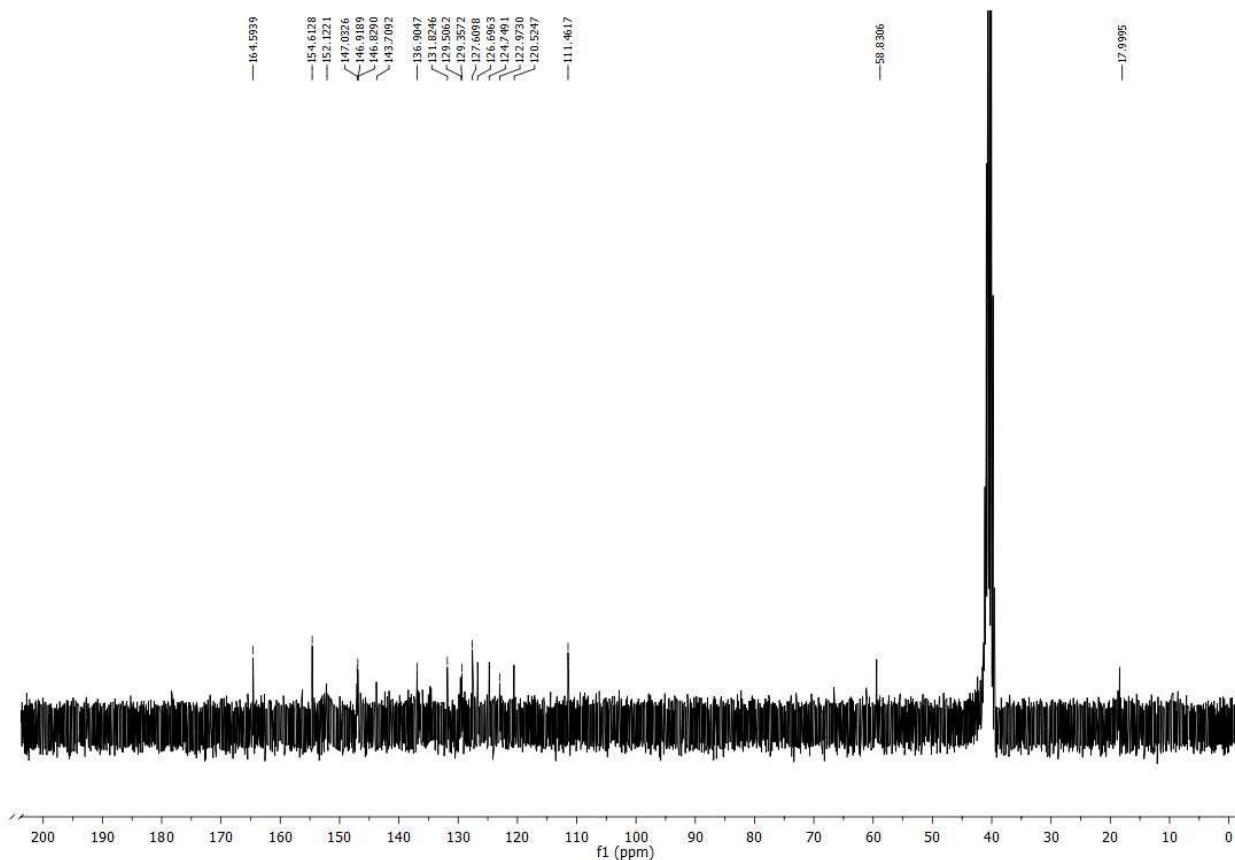
<sup>b</sup> Materials Chemistry Division, School of Advanced Sciences, VIT University, Vellore-632014, India.



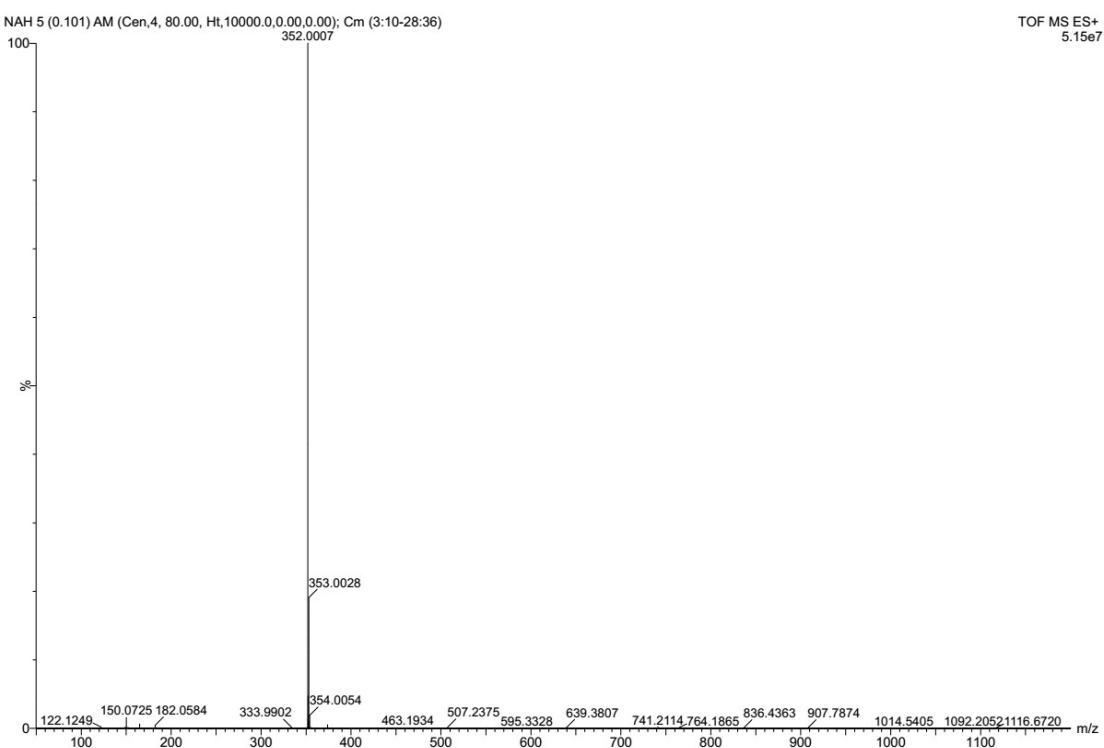
**Fig. S1.** ATR-FTIR spectrum of NPY.



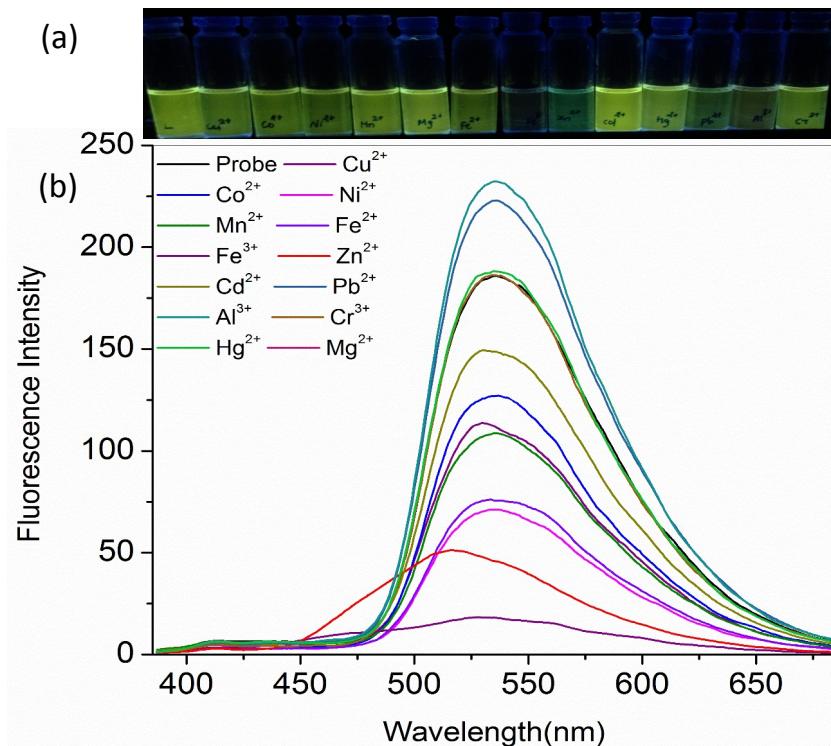
**Fig. S2.**  $^1\text{H}$  NMR spectrum of NPY in  $\text{DMSO}-d_6$ .



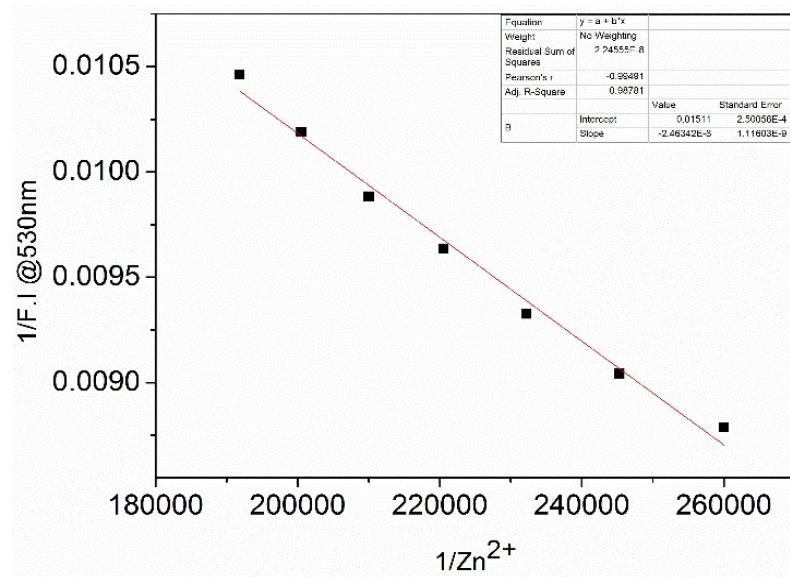
**Fig. S3.**  $^{13}\text{C}$ -NMR spectrum of NPY in  $\text{DMSO}-d_6$ .



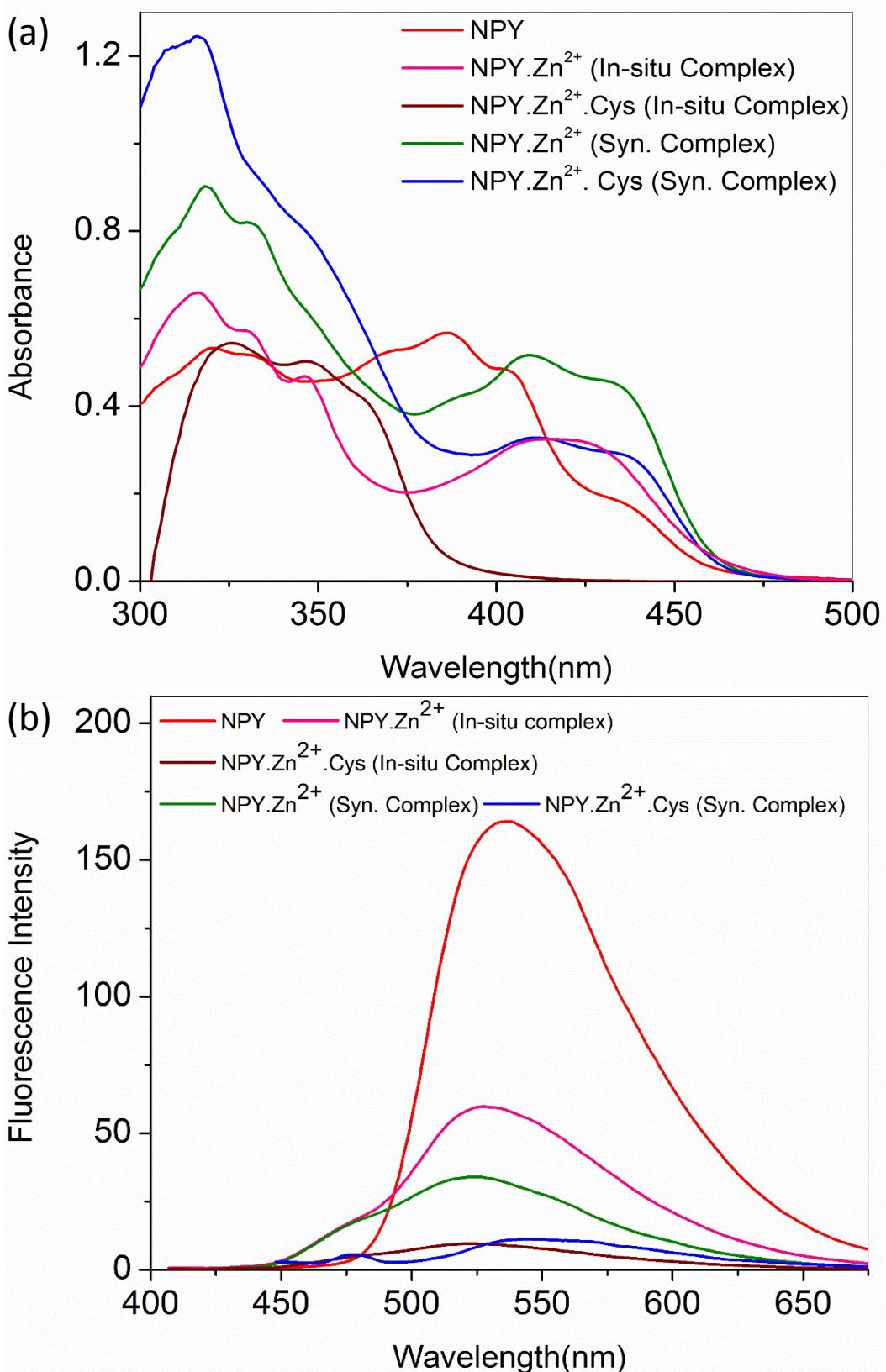
**Fig. S4.** HRMS spectrum of NPY.



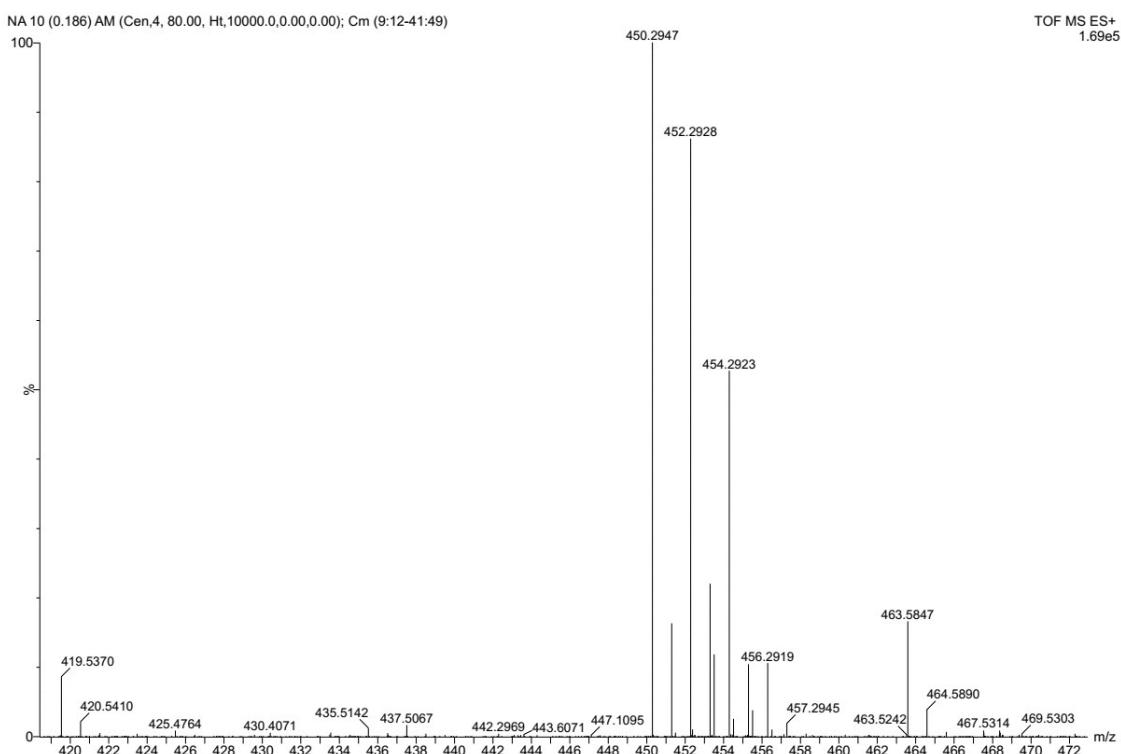
**Fig. S5.** (a) Image of the fluorescence vials of **NPY** (2mL,  $5 \times 10^{-5}$ M, DMSO) with different metal ions under UV-lamp  $\lambda_{\text{exc}} = 375$  nm and the corresponding fluorescence spectra of **NPY** (2mL,  $5 \times 10^{-5}$ M, DMSO) upon the addition of  $Zn^{2+}$  ions and other alkali, alkaline and transition metal ions ( $50\mu\text{l}$ ,  $1 \times 10^{-3}$ M,  $\text{H}_2\text{O}$ ).



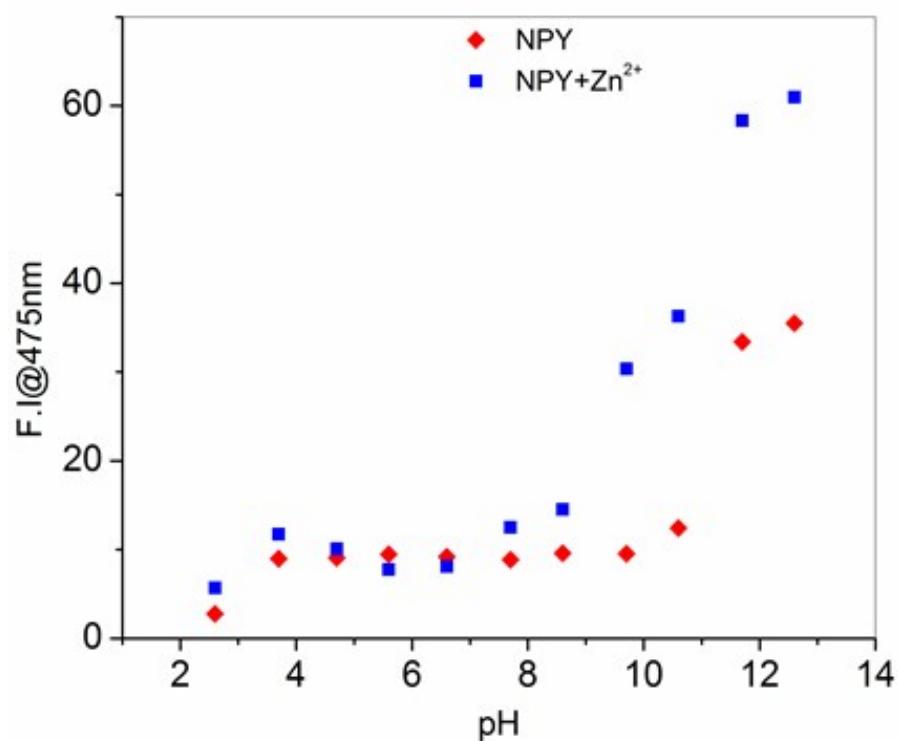
**Fig. S6.** Benesi-Hildebrand expression fitting of fluorescence curve of **NPY** in the presence of  $Zn^{2+}$ .



**Fig. S7.** UV-visible (a) and fluorescence (b) spectra of the *in-situ* prepared **NPY**. $Zn^{2+}$  and **NPY**. $Zn^{2+}$ .Cys complexes, and their corresponding synthesized complexes (Syn. Complex).



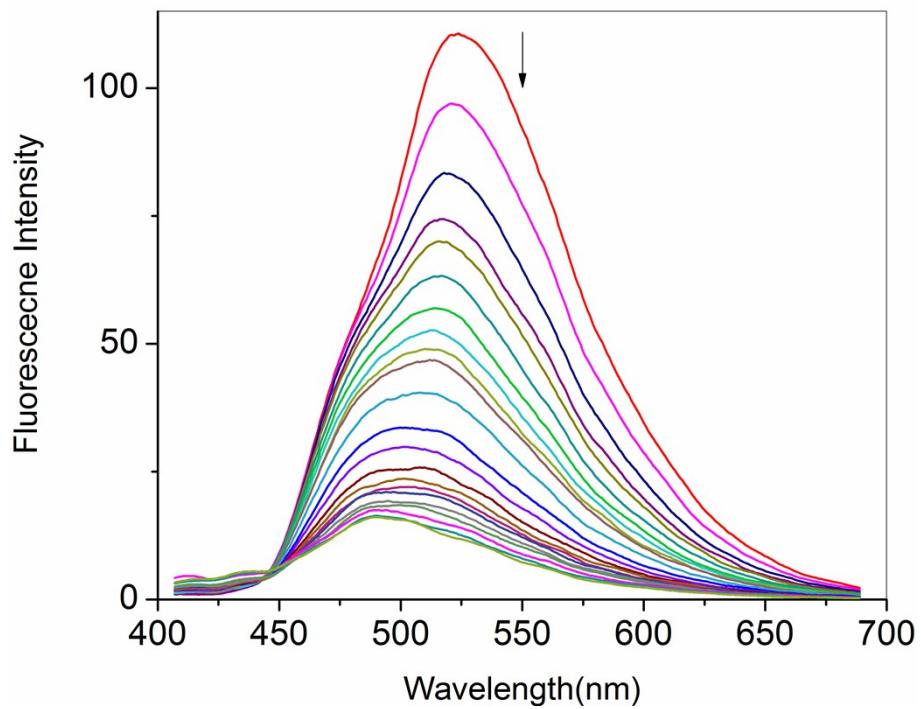
**Fig. S8.** HRMS spectrum of synthesized **NPY**.Zn<sup>2+</sup> complex.



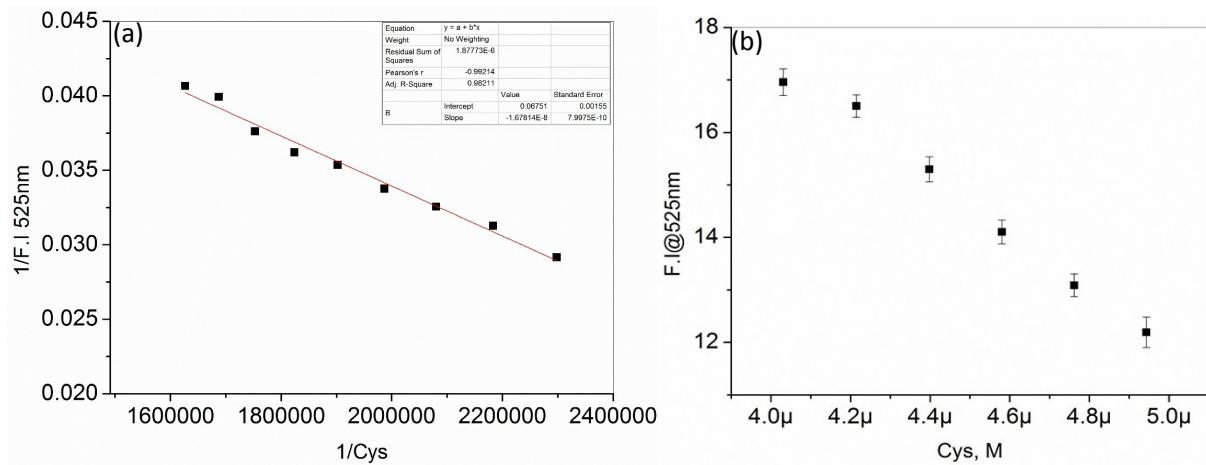
**Fig. S9.** pH effect on the fluorescence intensity at 475 nm of the solution of **NPY** in absence and presence of Zn<sup>2+</sup> ion.



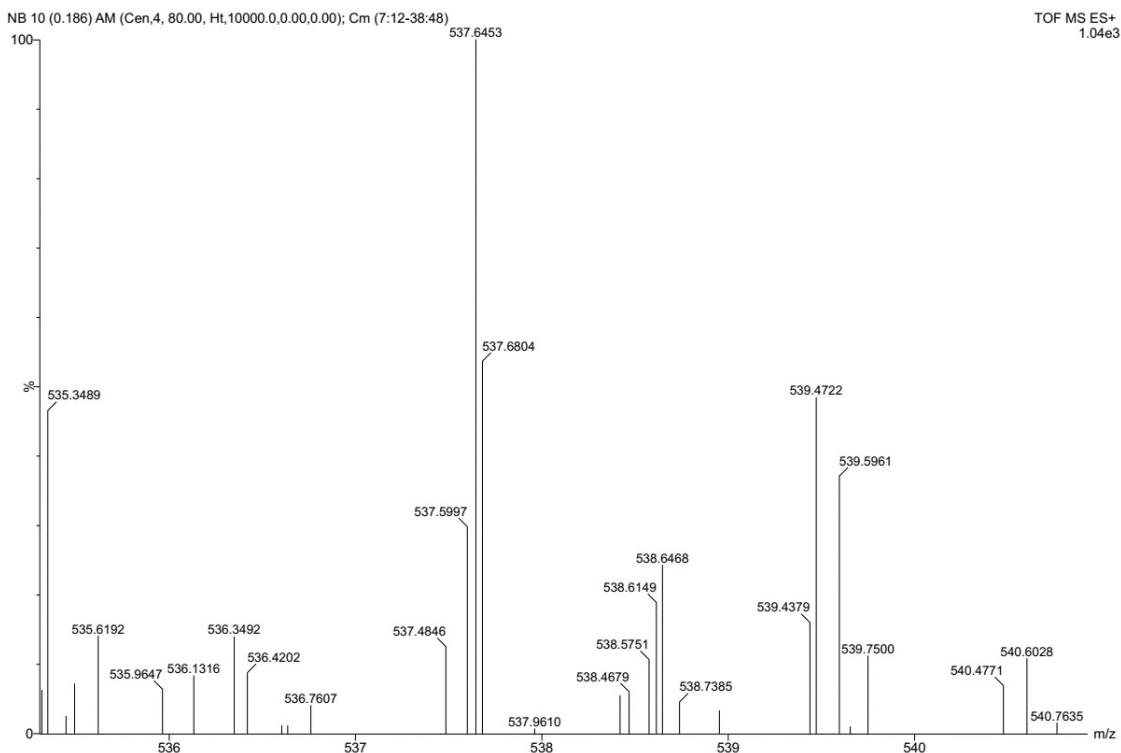
**Fig. S10.** Colour change of NPY (2 mL,  $5 \times 10^{-5}$  M, DMSO) upon the addition of Zn<sup>2+</sup> ions (50  $\mu$ L,  $1 \times 10^{-3}$  M, H<sub>2</sub>O).



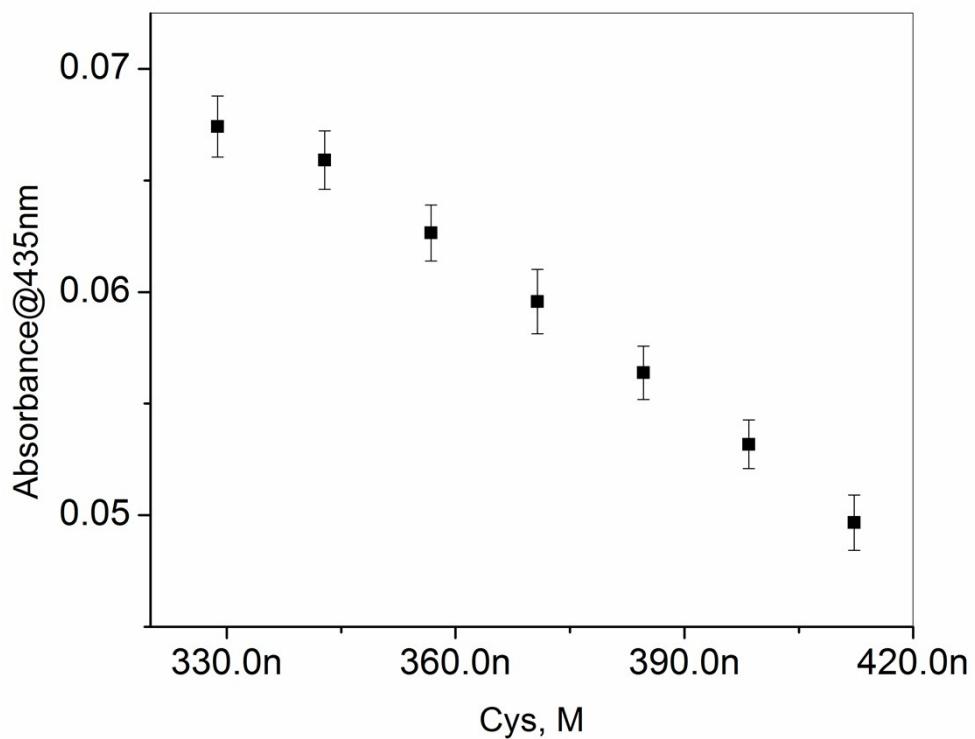
**Fig. S11.** Fluorescence ( $\lambda_{\text{exc}} = 375$  nm) spectral changes of NPY.Zn<sup>2+</sup> complex (2 mL,  $5 \times 10^{-5}$  M, DMSO) upon incremental addition of Cys (4  $\mu$ L,  $1 \times 10^{-4}$  M, H<sub>2</sub>O).



**Fig. S12.** (a). B-H plot of fluorescence curve of **NPY**. $Zn^{2+}$  complex in the presence of Cys.  
(b) Plot of fluorescence intensity of **NPY**. $Zn^{2+}$  complex against [Cys].



**Fig. S13.** HRMS spectrum of the **NPY**. $Zn^{2+}$ .Cys complex.



**Fig. S14.** Linear fit analysis for calculating the detection limit of Cys by using the UV-Vis titration data.

**Table S1.** Comparison table of some earlier reported works of Zn<sup>2+</sup> ion

<b>Systems</b>	<b>Solvent Systems</b>	<b>Analytes</b>	<b>Detection limit</b>	<b>Applications</b>	<b>Ref</b>
Naphthaldehyde-Schiff base	MeOH-buffer	Zn <sup>2+</sup> - turn off	10 μM	-	1
Pyridyl thioether Schiff base	Methanol	Zn <sup>2+</sup> -Turn-on	0.078μM	-	2
Pyridineamine schiff base	HEPES buffer	Zn <sup>2+</sup> -turn on	1.91×10 <sup>-6</sup> M	-	3
Coumarin Schiff base	DMF:H <sub>2</sub> O	Zn <sup>2+</sup> - Turn on	2.59×10 <sup>-6</sup> M	-	4
Naphthyl hydrazide conjugate	THF:H <sub>2</sub> O	Zn <sup>2+</sup> Colorimetry Al <sup>3+</sup> Fluorescence	3.1 nM 0.92 nM	Intracellular Imaging	5
Vanillin Schiff base	DMSO:H <sub>2</sub> O	Zn <sup>2+</sup> -Turn On	0.018 μM	Live cell imaging	6
Triazole Schiff base	DMSO:H <sub>2</sub> O	Zn <sup>2+</sup> -Turn on	4.2×10 <sup>-7</sup> M	Live cell imaging	7
Trian Schiff base	EtOH:H <sub>2</sub> O	Zn <sup>2+</sup> - Turn on	4.89×10 <sup>-8</sup> M		8
<b>Naphthyl hydrazide with pyridoxal</b>	<b>DMSO:H<sub>2</sub>O</b>	<b>Zn<sup>2+</sup> and Cysteine</b>	<b>8.73×10<sup>-7</sup> M and 6.63×10<sup>-7</sup> M</b>	<b>Live cell imaging</b>	<b>This work</b>

**Table S2.** Comparison of various reported official methods for Zn<sup>2+</sup> detection.

<b>S.No</b>	<b>Methods</b>	<b>LOD</b>	<b>Ref</b>
1	Potentiometry	0.0005 M	9
2	Stripping voltammetry	0.9 μgL <sup>-1</sup>	10
3	FAAS	0.05 μgL <sup>-1</sup>	11
4	ICP-MS	0.20 μgL <sup>-1</sup>	12
5	AAS	0.35 μgL <sup>-1</sup>	13

6	IC-ICP-AES	0.07 ng/g	14
7	Colorimetry	$1.15 \times 10^{-7}$ M	15

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