

Electronic Supplementary Information (ESI)

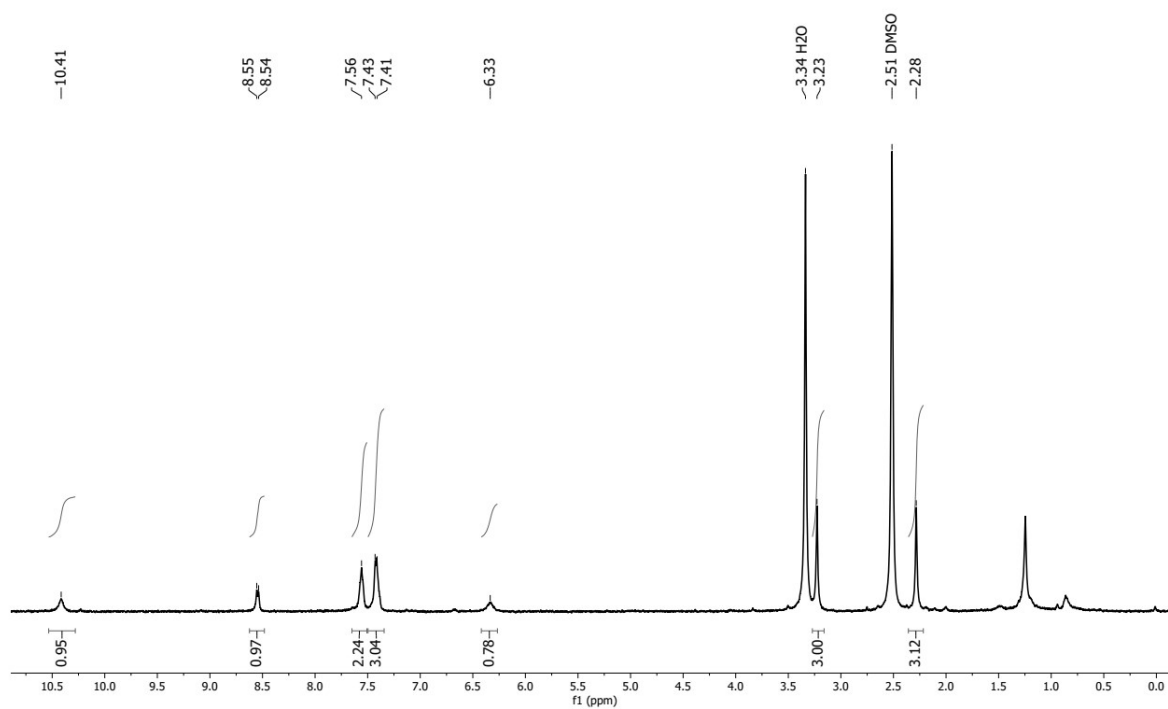
**A Dual Colorimetric Chemosensor for Hg(II) and Cyanide ions in Aqueous Media based on Nitrobenzoxadiazole (NBD)-Antipyrine Conjugate with INHIBIT logic gate behaviour**

Thangaraj Anand and Muniappan Sankar\*

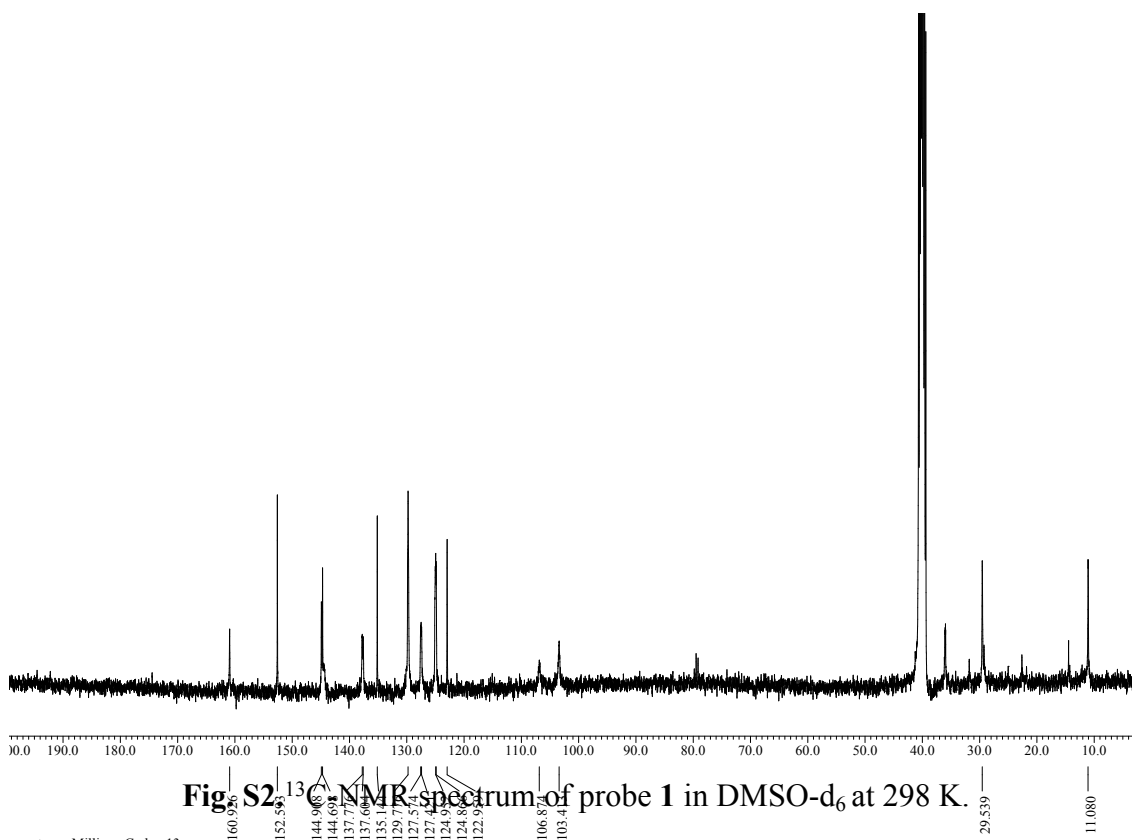
*Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee-247667, India.*

**Table of Contents**

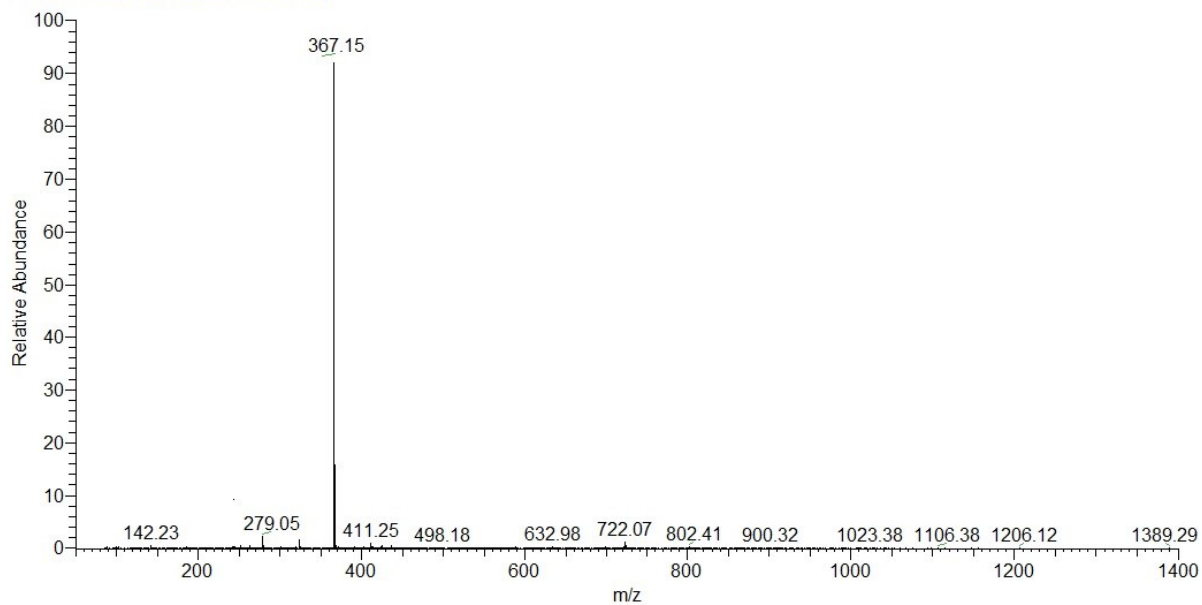
		Page No
<b>Fig. S1.</b>	<sup>1</sup> H NMR spectrum of sensor <b>1</b> in DMSO-d <sub>6</sub> at 298 K.	2
<b>Fig. S2.</b>	<sup>13</sup> C NMR spectrum of probe <b>1</b> in DMSO-d <sub>6</sub> at 298 K.	3
<b>Fig. S3.</b>	ESI-MS spectrum of Probe <b>1</b> in positive ion mode.	3
<b>Fig. S4.</b>	The colour change of probe <b>1</b> (2 mL, 1×10 <sup>-5</sup> M) after the addition of various metal ions and anions (50 μL, 1×10 <sup>-3</sup> M) in aqueous methanol medium (1:1, v/v) observed by naked eyes.	4
<b>Fig. S5a.</b>	The Job's plot; mole fraction of probe <b>1</b> vs change in absorbance during Hg <sup>2+</sup> addition.	5
<b>Fig. S5b.</b>	ESI-MS spectrum of probe <b>1</b> with Hg <sup>2+</sup> ion positive ion mode.	5
<b>Fig.S6a.</b>	Binding constants of binding of probe <b>1</b> with Hg <sup>2+</sup> ion.	6
<b>Fig.S6b</b>	Change in absorbance of sensor <b>1</b> with different concentrations of Hg <sup>2+</sup> in aqueous methanol solution.	6
<b>Fig. S7.</b>	Bar chart illustrates the absorbance changes (abs 50 nm) of probe <b>1</b> with Hg <sup>2+</sup> ion in the presence of other metal ions in aqueous methanol.	7
<b>Fig.S8</b>	Fluorescence spectra of probe <b>1</b> with metal ions in CH <sub>3</sub> OH:H <sub>2</sub> O (1:1, v/v)	7
<b>Fig. S9a.</b>	Job's plot: the mole fraction of sensor <b>1</b> vs change in absorbance during CN <sup>-</sup> ions addition.	8
<b>Fig. S9b.</b>	ESI-MS spectrum of sensor <b>1</b> with CN <sup>-</sup> ions in negative ion mode.	8
<b>Fig. S10a.</b>	Binding constant of binding of probe <b>1</b> with CN <sup>-</sup> ion.	9
<b>Fig. S10b.</b>	The plot of absorbance changes of sensor <b>1</b> during the addition of CN <sup>-</sup> ions in aqueous methanol solution.	9
<b>Fig. S11.</b>	Bar chart illustrates the absorbance changes (abs 485nm) of probe <b>1</b> with CN <sup>-</sup> ion in the presence of other anions in aqueous methanol.	10
<b>Fig. S12.</b>	<sup>1</sup> H NMR spectrum of <b>1</b> in DMSO-d <sub>6</sub> upon addition of CN <sup>-</sup> ions.	10

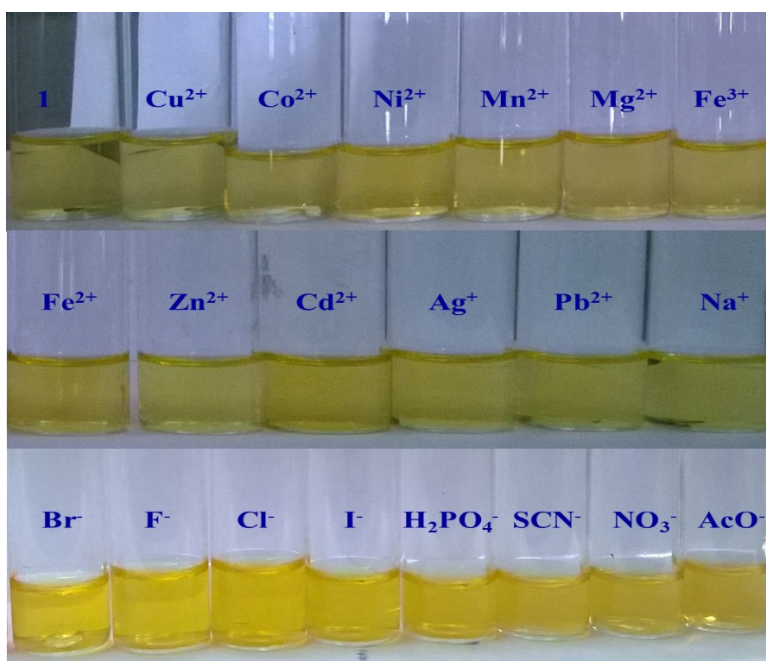


**Fig. S1.**  $^1\text{H}$ -NMR spectrum of sensor **1** in  $\text{DMSO-d}_6$  at 298 K

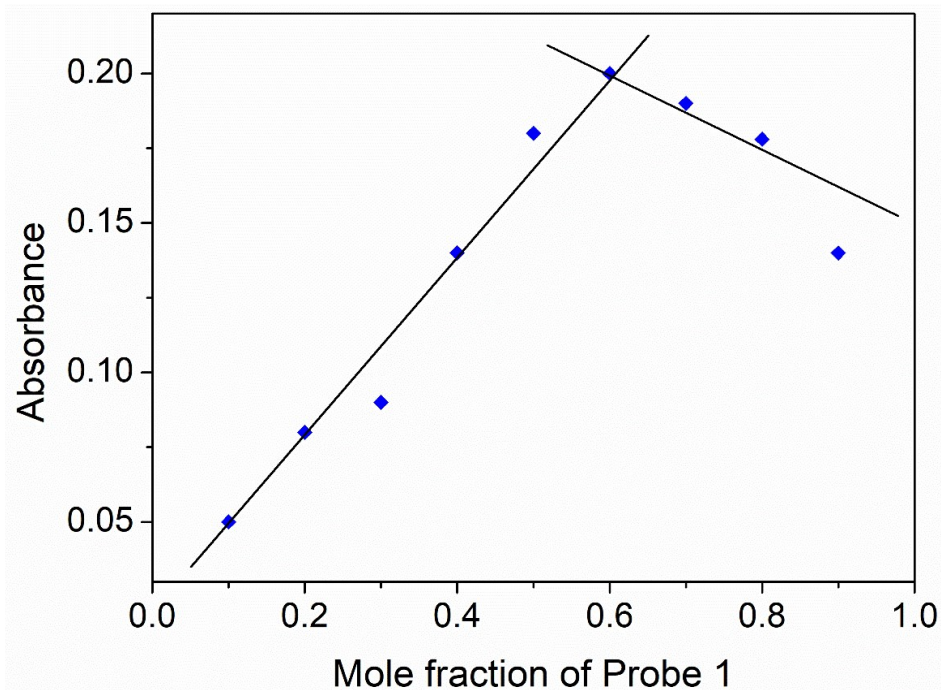


DM03 #15 RT: 0.21 AV: 1 NL: 4.24E4  
 T: ITMS + c ESI Full ms [50.00-1400.00]



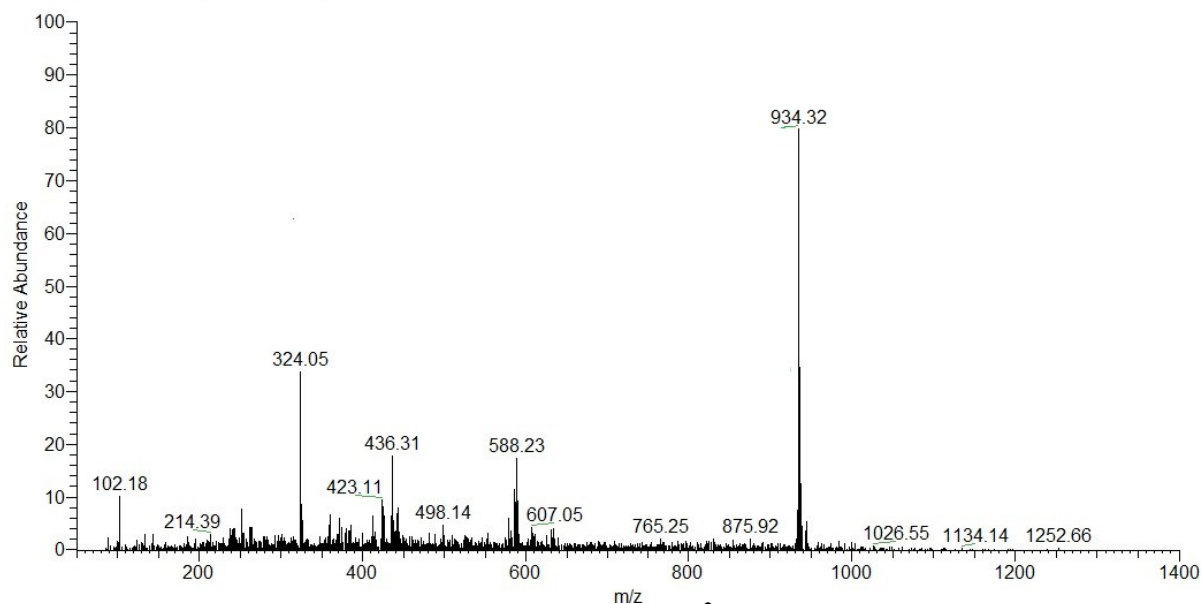


**Fig. S4.** The colour change of probe **1** (2 mL,  $1 \times 10^{-5}$  M) after the addition of various metal ions and anions (50  $\mu$ L,  $1 \times 10^{-3}$  M) in aqueous methanol medium (1:1, v/v) observed by naked eyes.

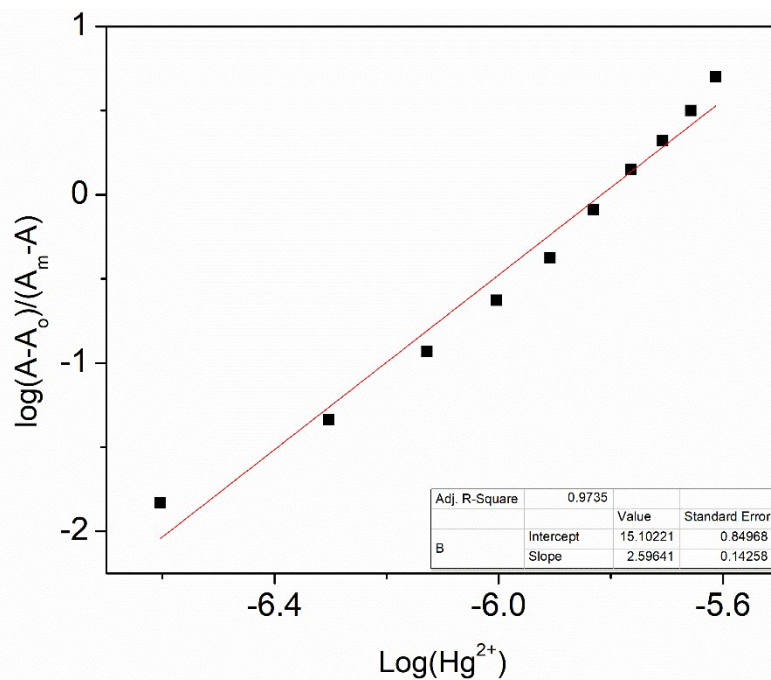


**Fig. S5a.** Job's plot; mole fraction of sensor **1** vs change in absorbance during  $\text{Hg}^{2+}$  addition.

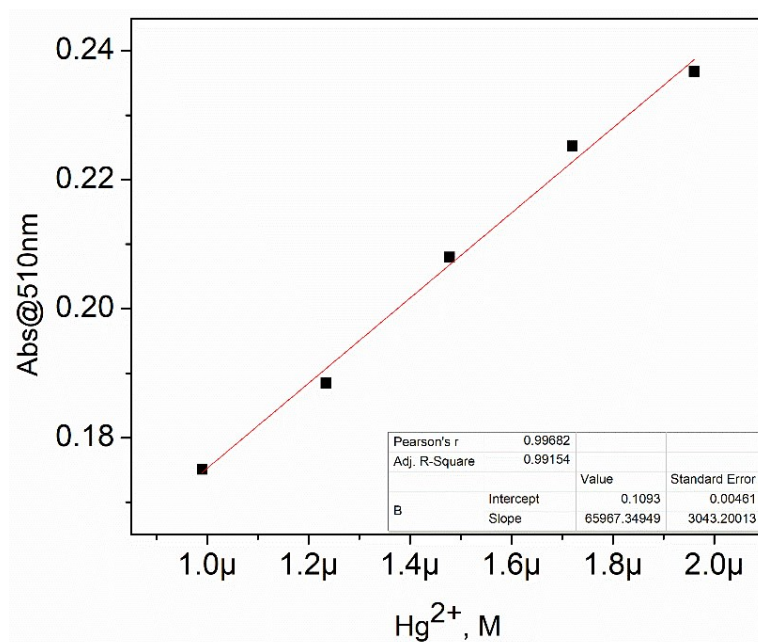
DM05 #63 RT: 0.92 AV: 1 NL: 2.62E3  
T: ITMS + c ESI Full ms [50.00-1400.00]



**Fig.S5b.** ESI-MS spectrum of probe **1** with  $\text{Hg}^{2+}$  ion positive ion mode.

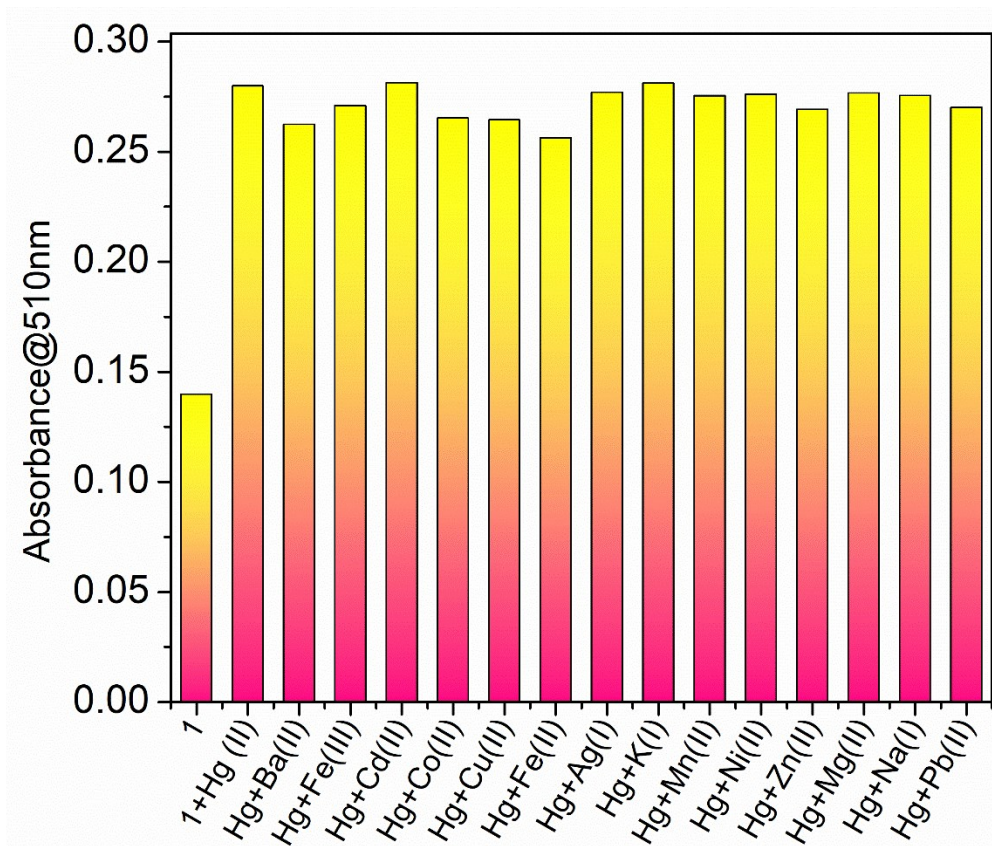


**Fig.S6a.** Binding constants of binding of probe **1** with  $\text{Hg}^{2+}$  ion.

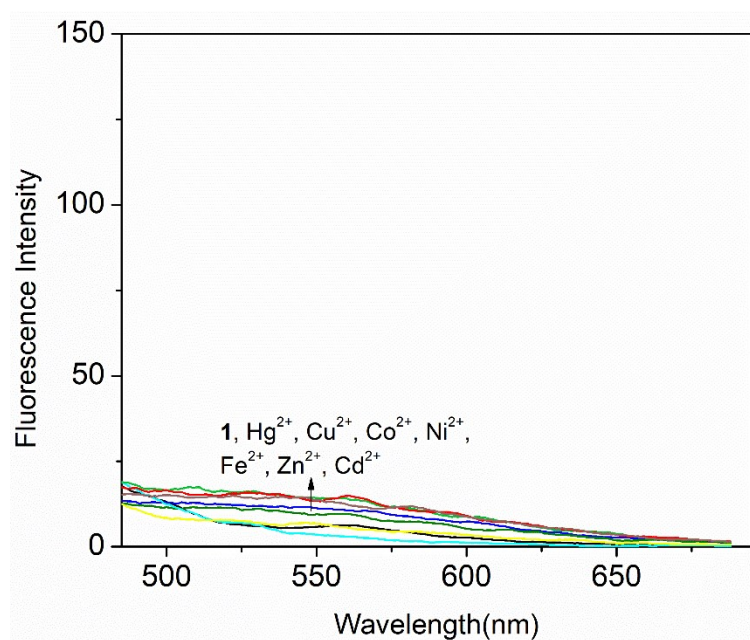


**Fig. S6b.** Change in absorbance of sensor **1** with different concentrations of  $\text{Hg}^{2+}$  in aqueous methanol solution.

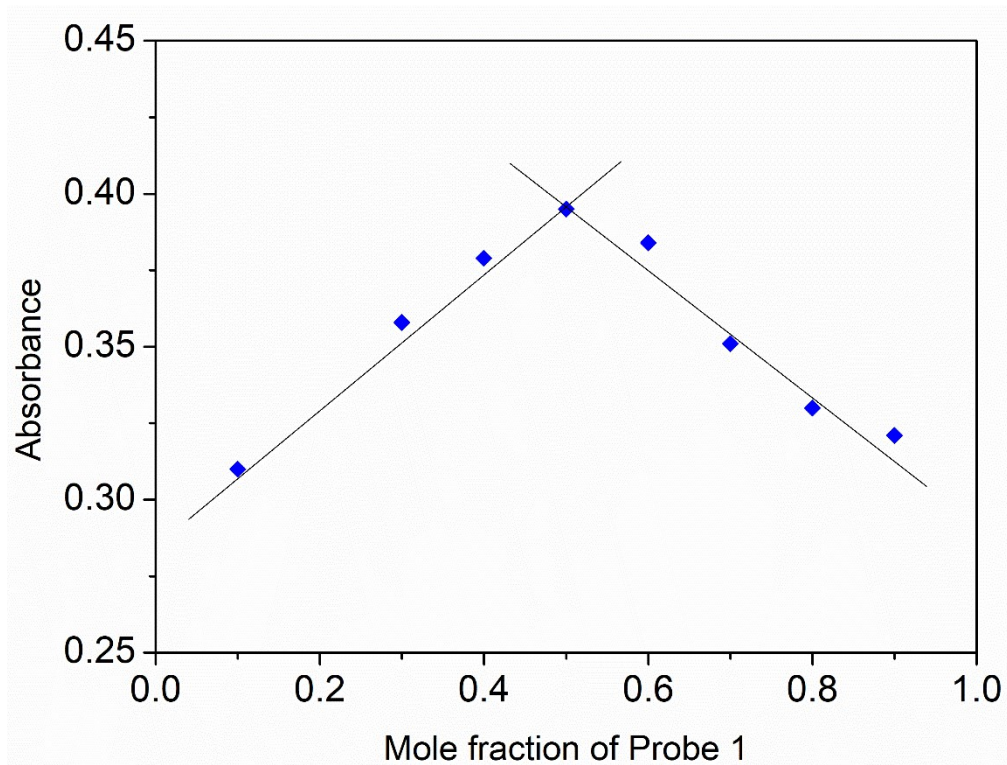




**Fig. S7.** Bar chart illustrates the absorbance changes (abs 510 nm) of probe **1** (2 mL, 1 × 10<sup>-5</sup> M) with Hg<sup>2+</sup> (50 μL, 1 × 10<sup>-3</sup> M) ion in the presence of other metal ions (50 μL, 1 × 10<sup>-3</sup> M) in aqueous methanol medium (1:1, v/v).

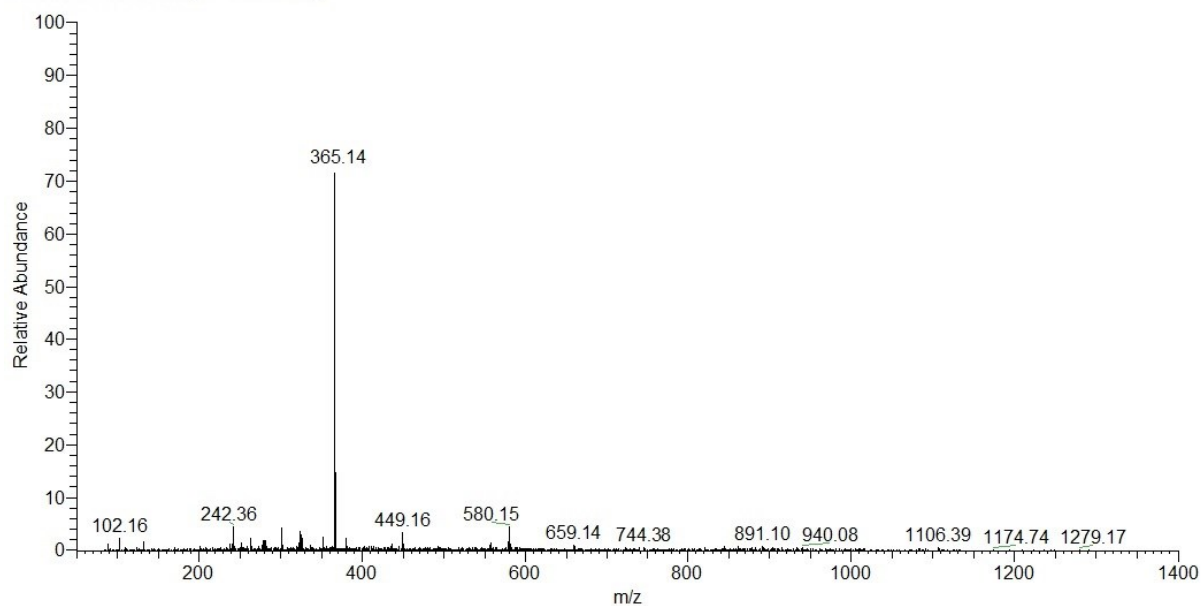


**Fig.S8.** Fluorescence spectra of probe **1** (2 mL, 1 × 10<sup>-5</sup> M) with metal ions in CH<sub>3</sub>OH:H<sub>2</sub>O (1:1, v/v) excited at 450 nm.



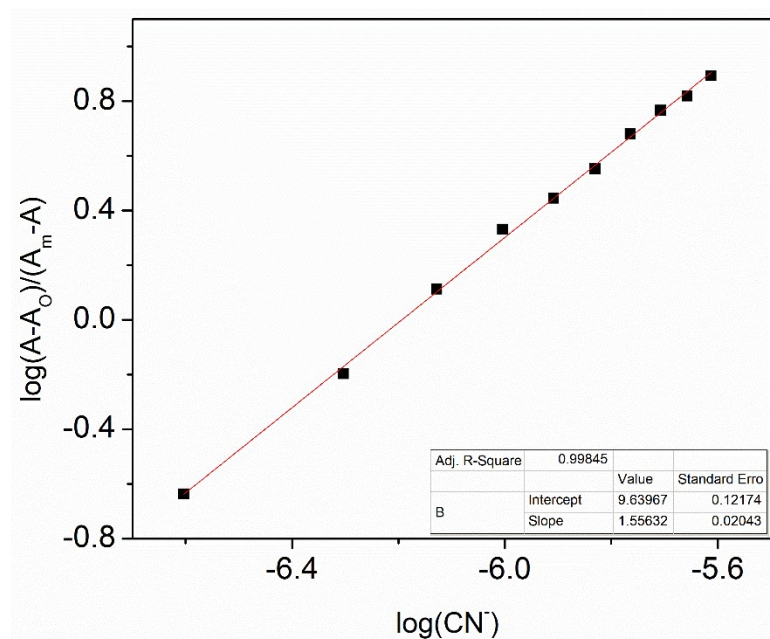
**Fig. S9a.** Job's plot: the mole fraction of sensor **1** vs change in absorbance during  $\text{CN}^-$  ions addition.

DM01 #12 RT: 0.17 AV: 1 NL: 1.88E2  
T: ITMS - c ESI Full ms [50.00-1400.00]

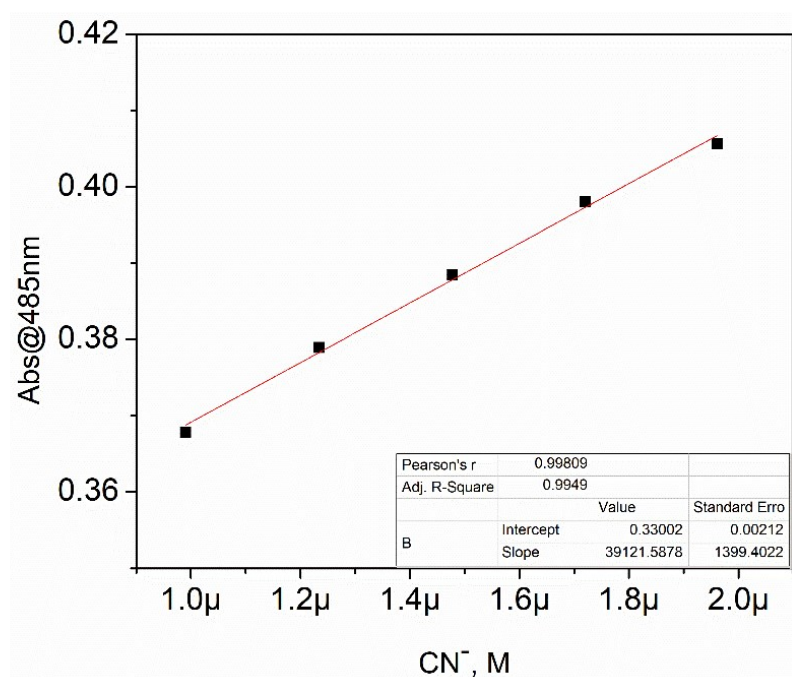


**Fig. S9b.** ESI-MS spectrum of sensor **1** with  $\text{CN}^-$  ions in negative ion mode.

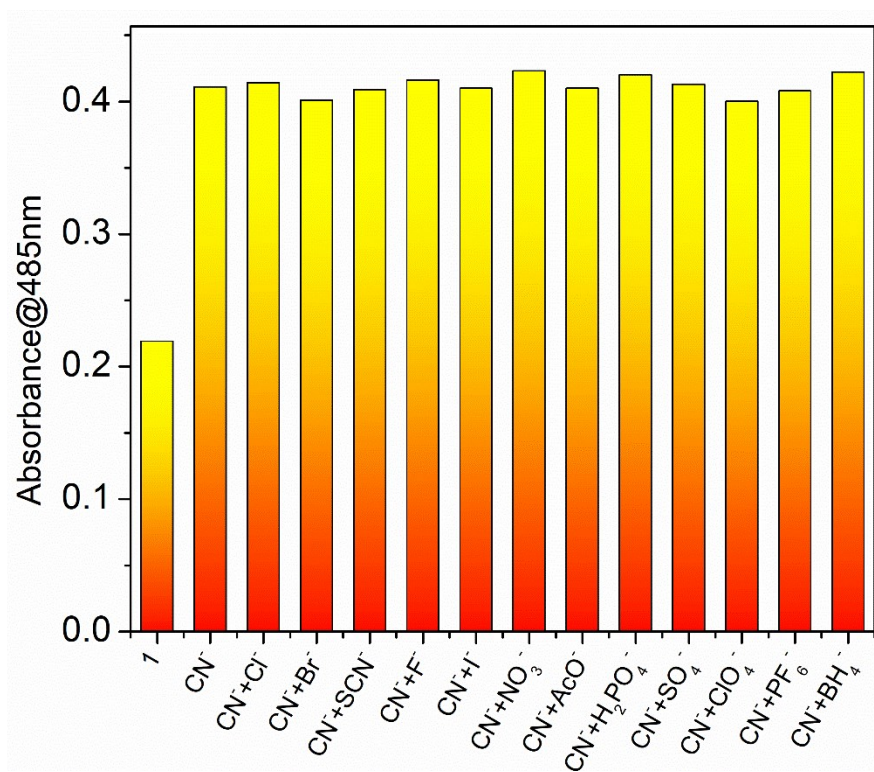




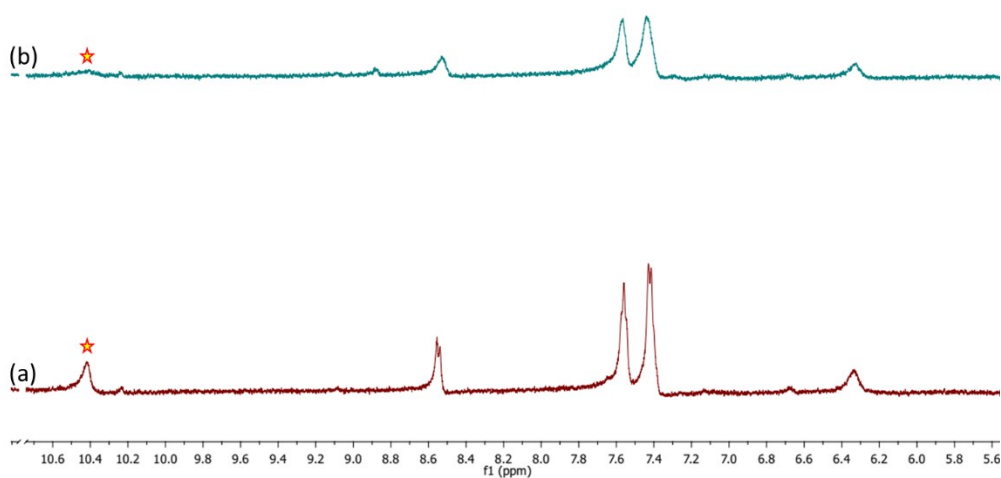
**Fig.S10a.** Binding constant of binding of probe **1** with  $\text{CN}^-$  ion.



**Fig. S10b.** The plot of absorbance changes of sensor **1** during the addition of  $\text{CN}^-$  ions in aqueous methanol solution.



**Fig. S11.** Bar chart illustrates the absorbance changes (abs 485nm) of probe **1** (2 mL,  $1 \times 10^{-5}$  M) with CN<sup>-</sup> (50  $\mu$ L,  $1 \times 10^{-3}$  M) ion in the presence of other anions (50  $\mu$ L,  $1 \times 10^{-3}$  M) in aqueous methanol medium (1:1, v/v).



**Fig. S12.** <sup>1</sup>H NMR spectrum of sensor **1** in DMSO-d<sub>6</sub> with the addition of CN<sup>-</sup> ions.