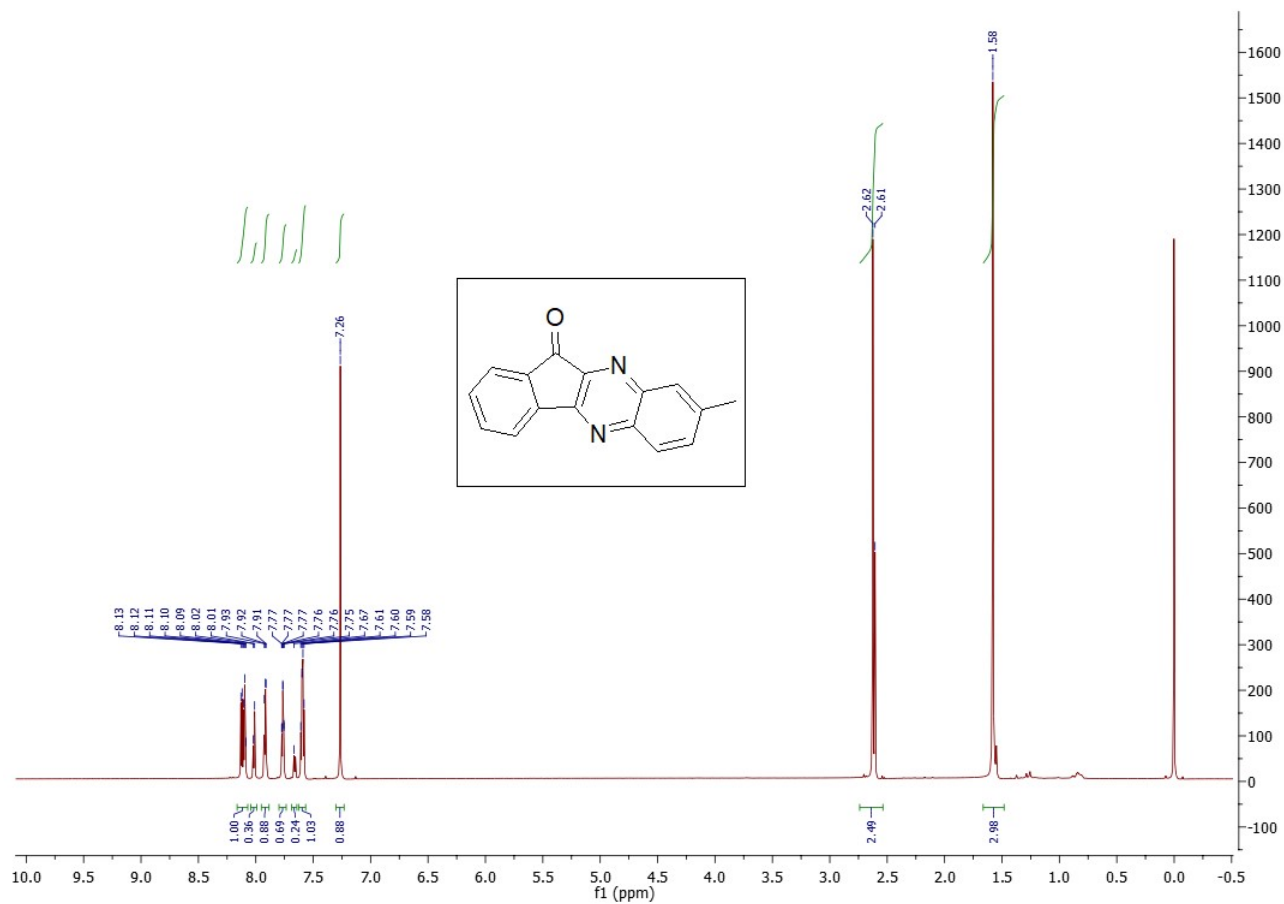


**Synthesis of Quinoxaline-Hydrazinobenzothiazole Based Probe-A Single Point  
Detection of Cu<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup> and Hg<sup>2+</sup> Ions in Real Water Samples**

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Engineering, Dindigul – 624622, Tamil Nadu, India.*



**Figure S1**  $^1\text{H}$  NMR of Quinox in  $\text{CDCl}_3$  (400 MHz)

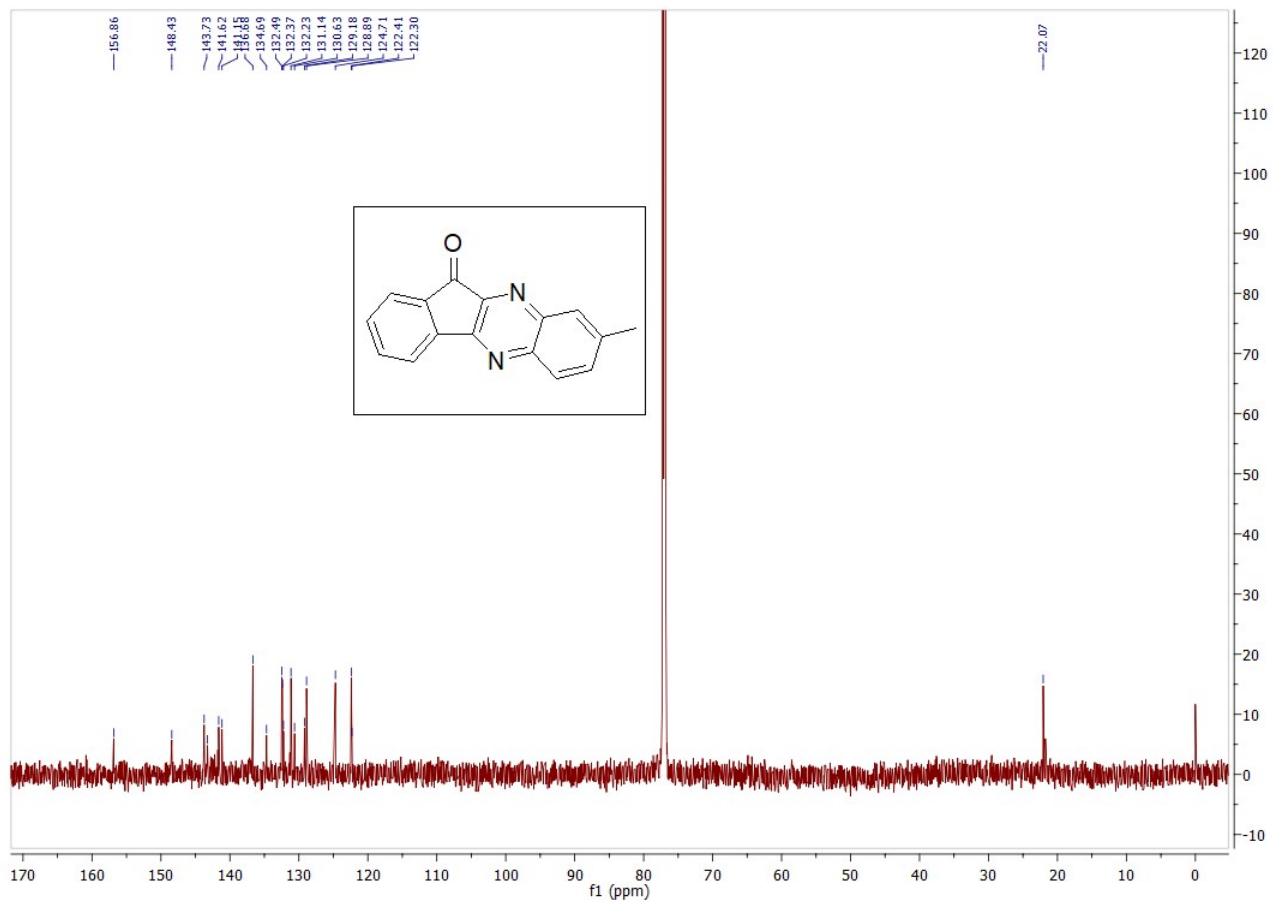
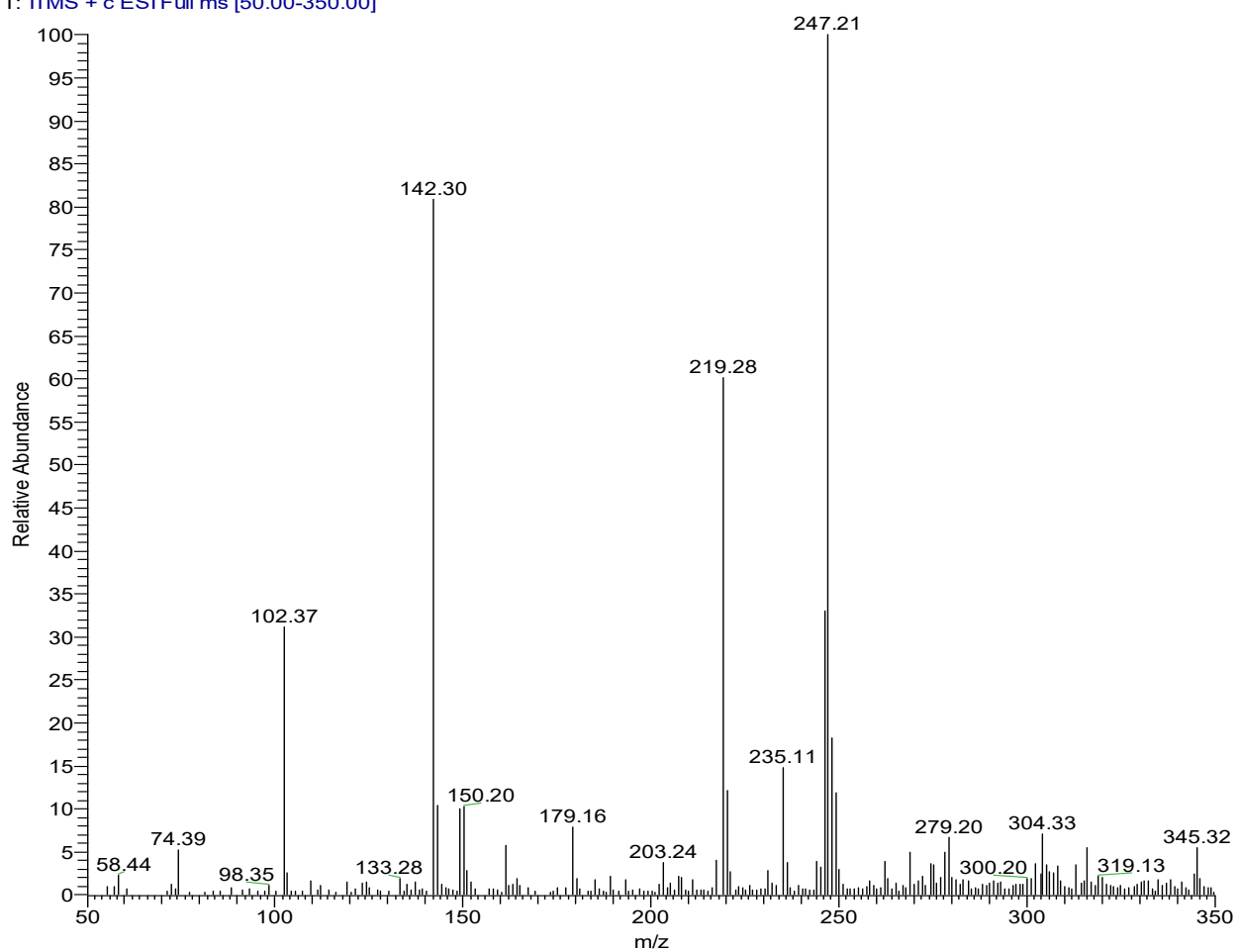
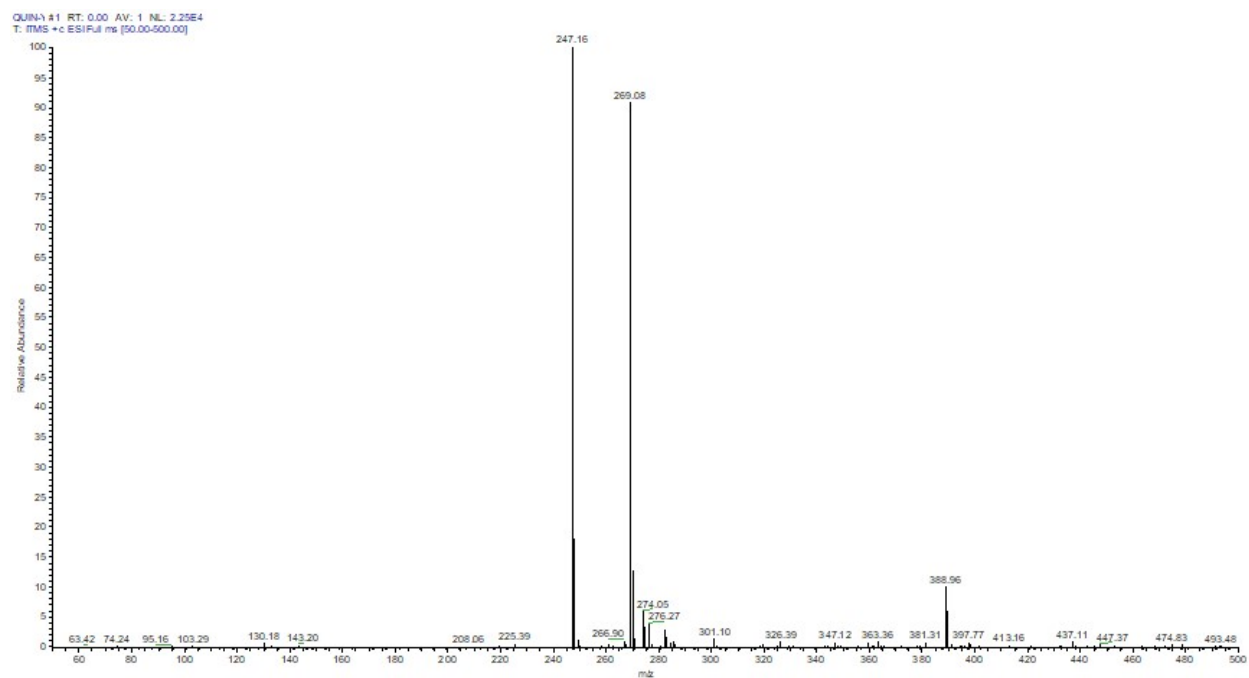


Figure S2 <sup>13</sup>C NMR of Quinox in CDCl<sub>3</sub> (100 MHz)

NH #1 RT: 0.00 AV: 1 NL: 7.92E3  
T: ITMS + c ESI Full ms [50.00-350.00]



**Figure S3** ESI-MS spectrum of Quinox



**Figure S4** HRMS spectrum of **Quinox**

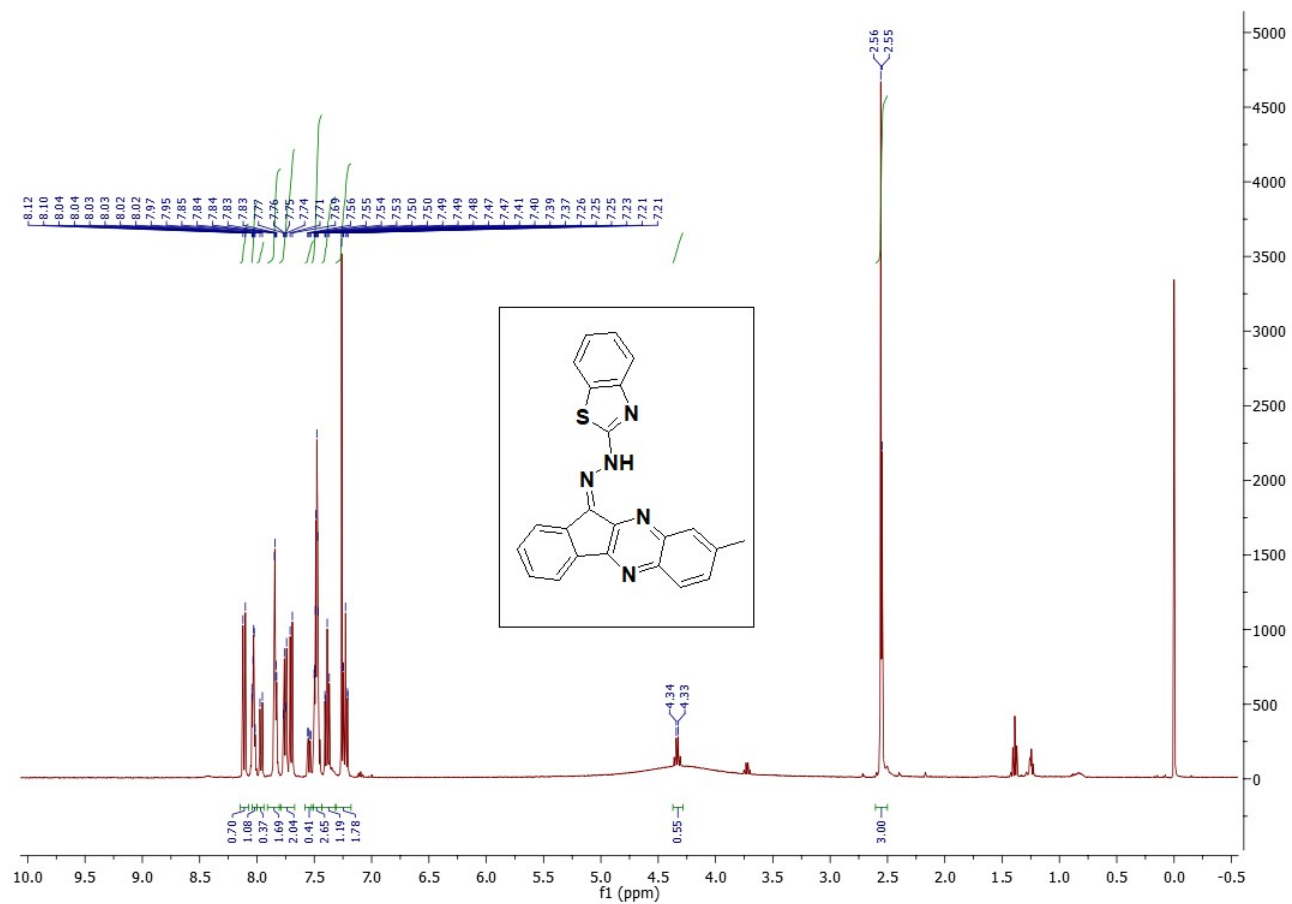


Figure S5  $^1\text{H}$  NMR of Quinox-hBT in  $\text{CDCl}_3$  (400 MHz)

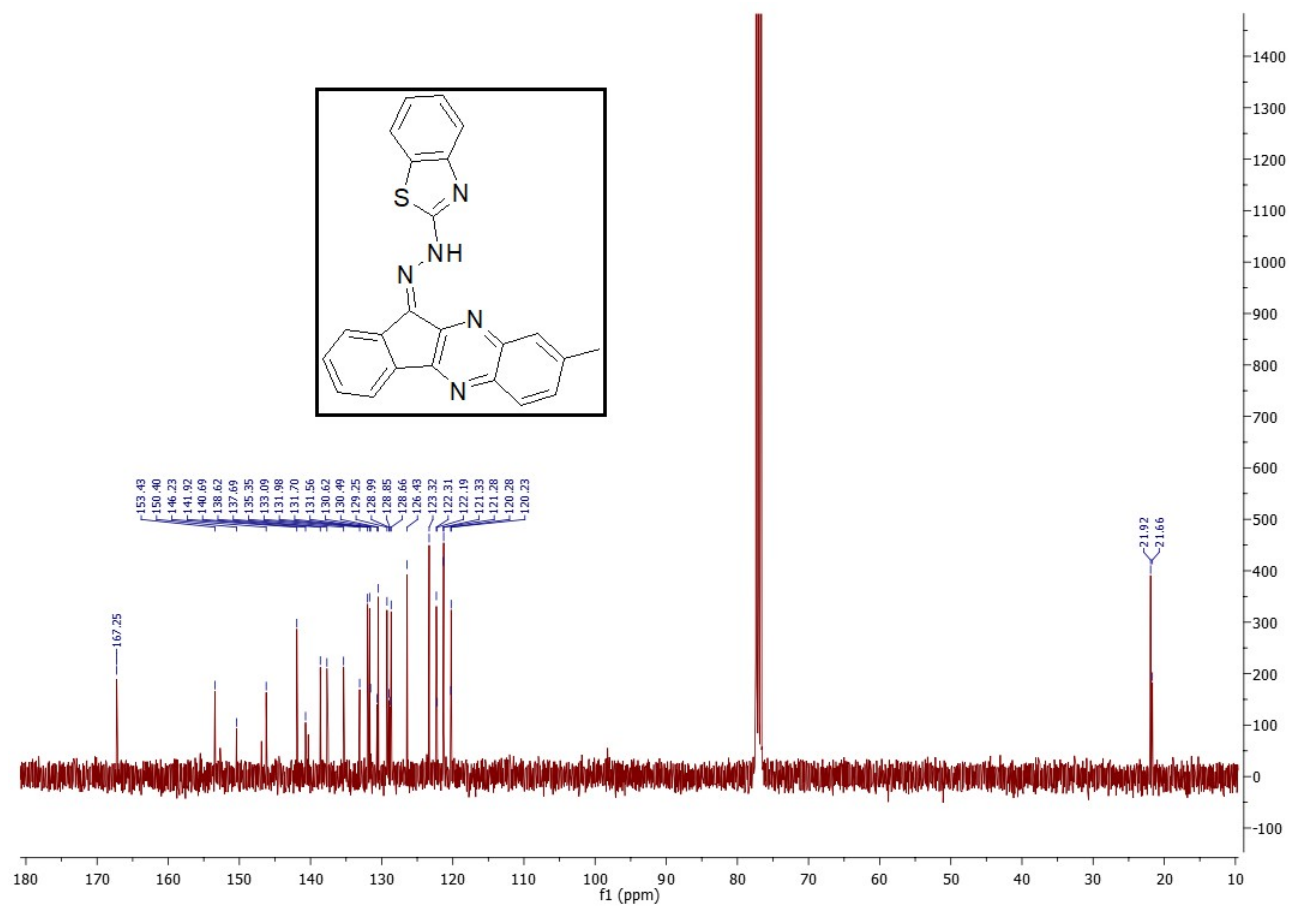
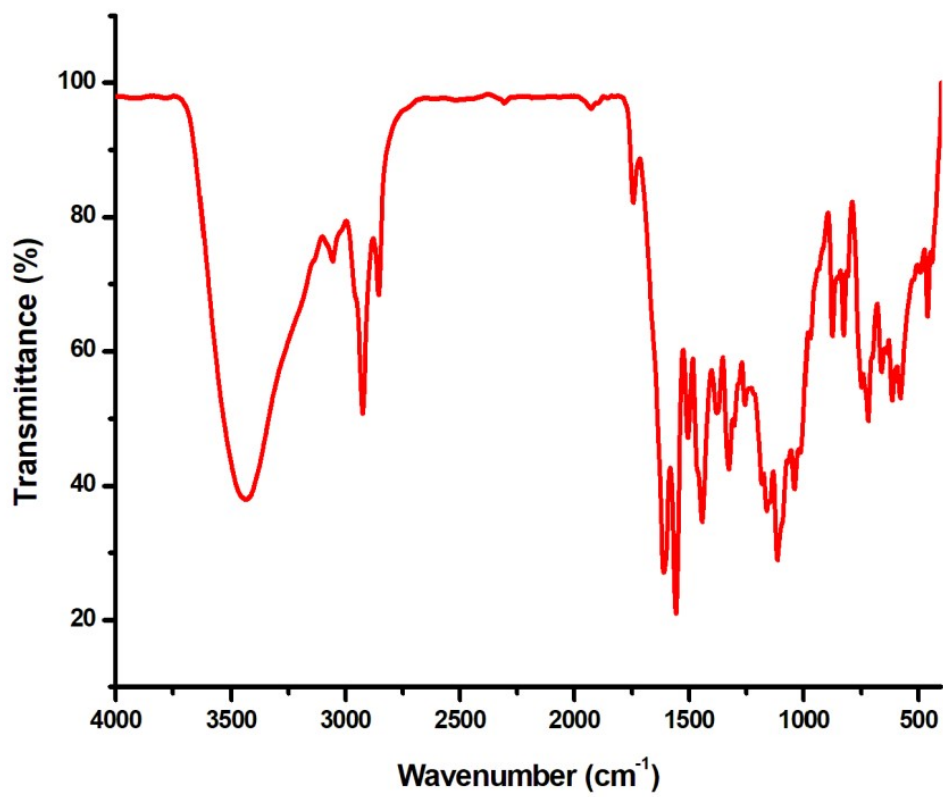


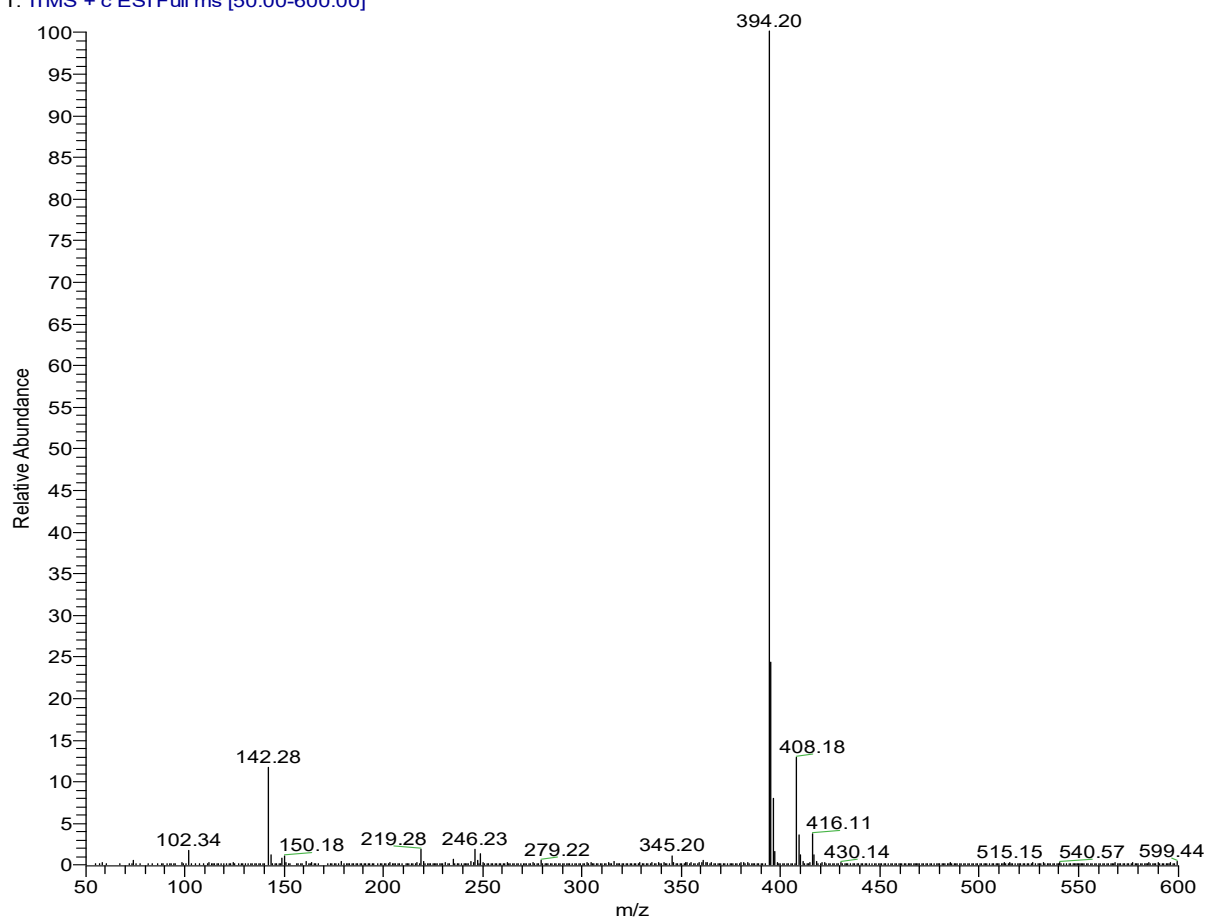
Figure S6 <sup>13</sup>C NMR of Quinox-hBT in CDCl<sub>3</sub> (100 MHz)



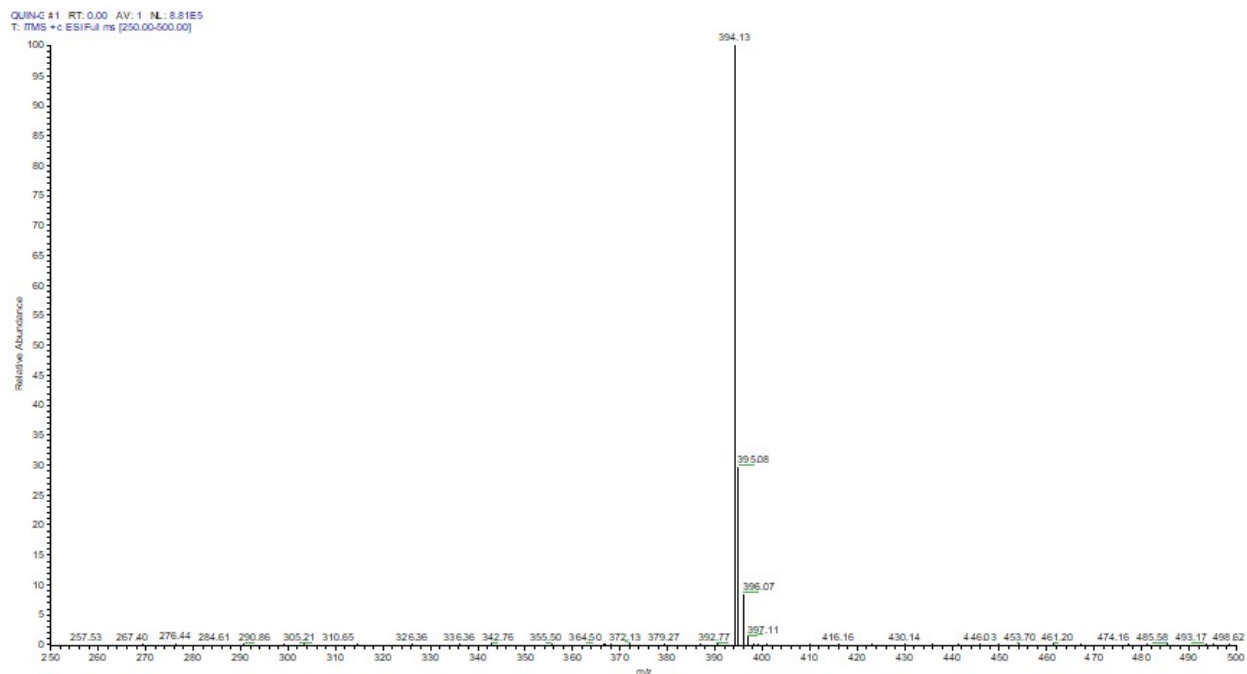
**Figure S7** FTIR spectrum of **Quinox-hBT**



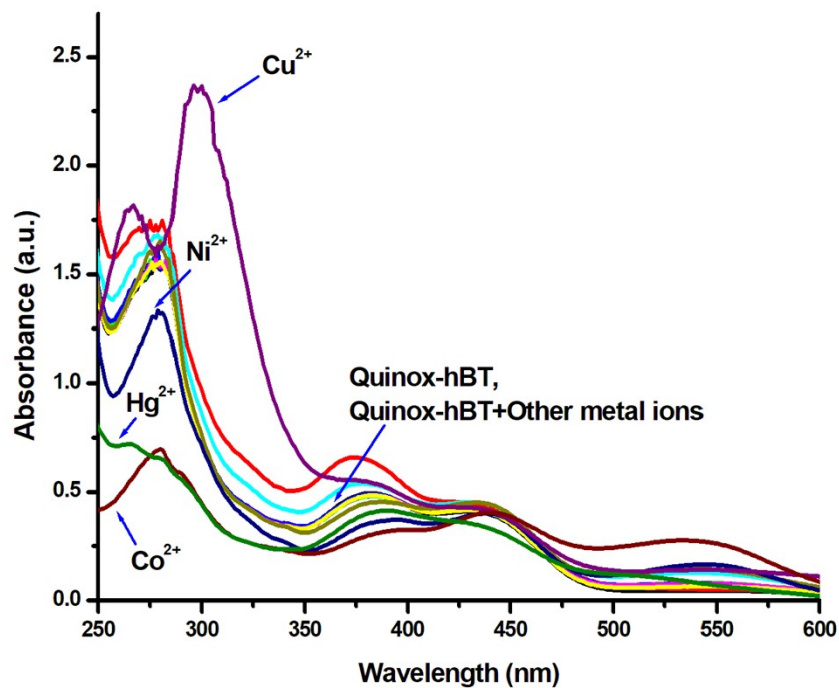
NHBT #1 RT: 0.00 AV: 1 NL: 3.15E4  
T: ITMS + c ESI Full ms [50.00-600.00]



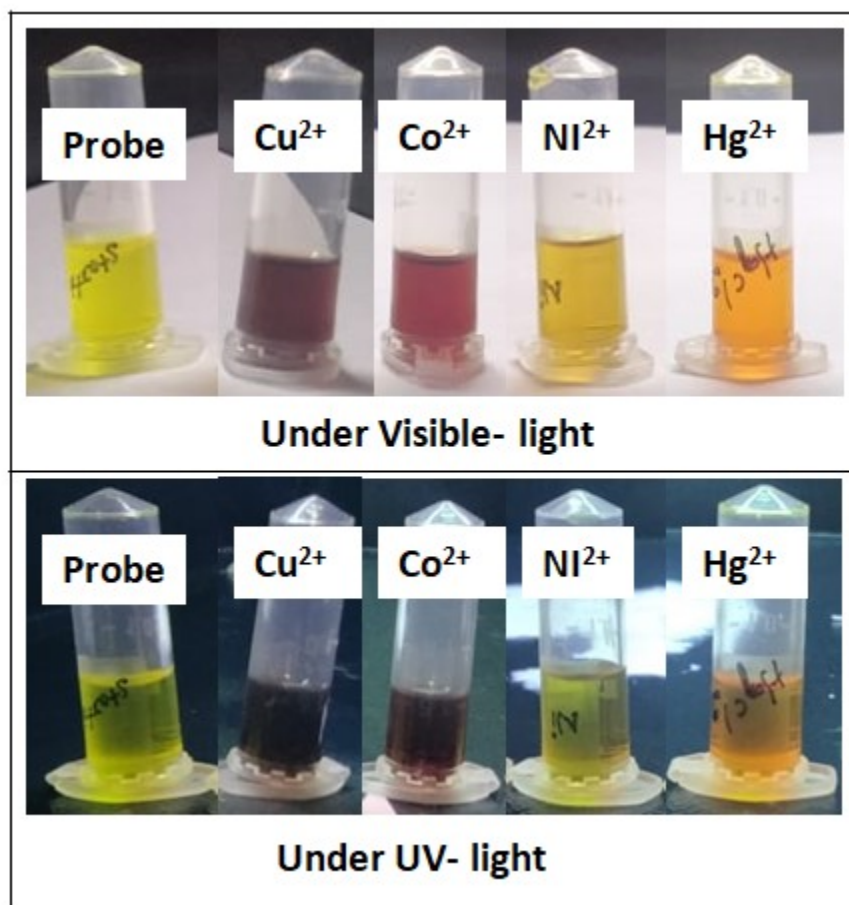
**Figure S8** ESI-MS spectrum of **Quinox-hBT**



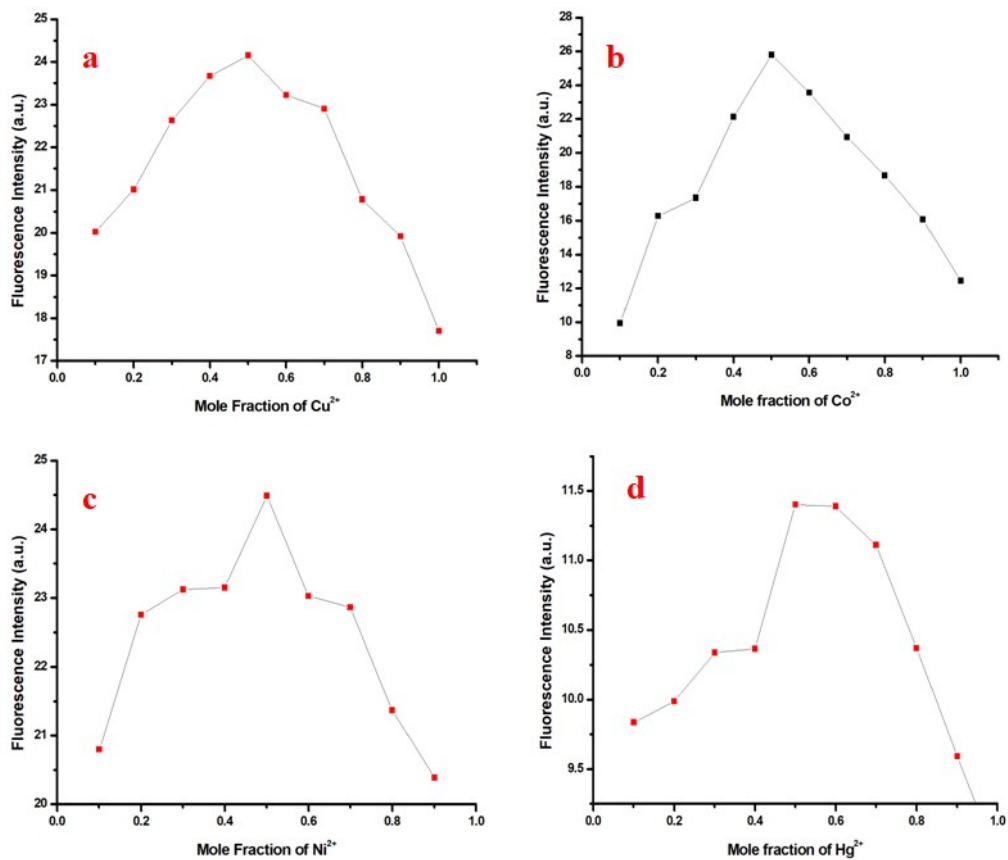
**Figure S9** HRMS spectrum of Quinox-hBT



**Figure S10** UV-Visible spectra of Quinox-hBT ( $1.0 \times 10^{-6}$  M) with addition of different metal ions ( $1.0 \times 10^{-6}$  M) in THF:H<sub>2</sub>O (1:9, v/v) (pH 7.4, 20 mM HEPES buffer)



**Figure S11** Color changes of Quinox-hBT after addition of Cu<sup>2+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup> and Hg<sup>2+</sup> ions



**Figure S12** Job's plot of Quinox-hBT with (a) Cu<sup>2+</sup>, (b) Co<sup>2+</sup>, (c) Ni<sup>2+</sup>, & (d) Hg<sup>2+</sup> ions

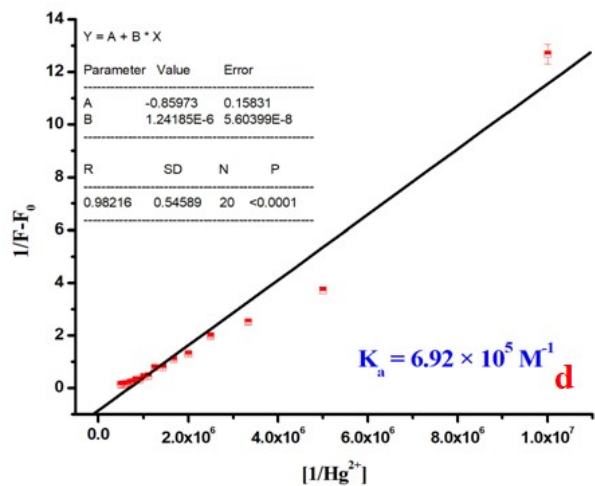
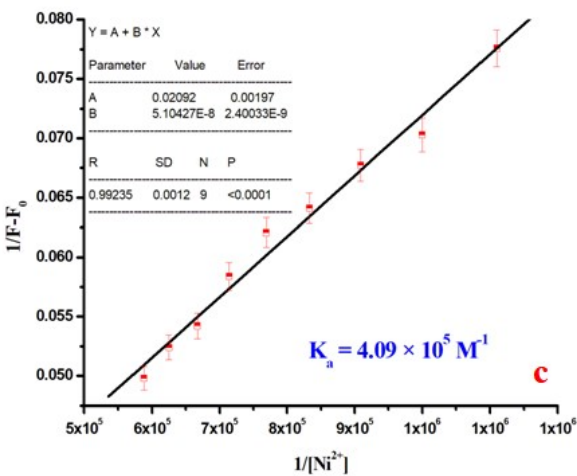
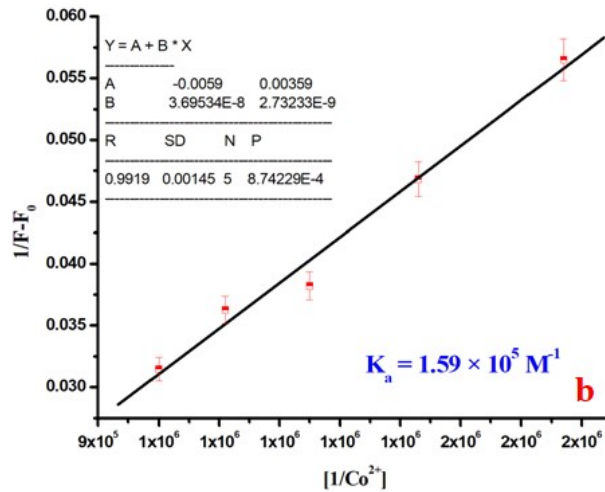
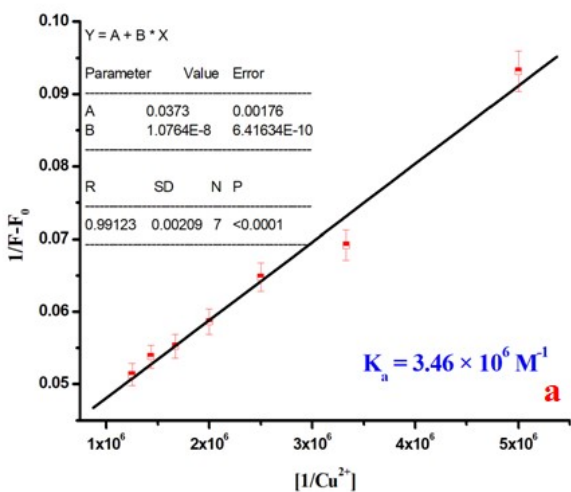
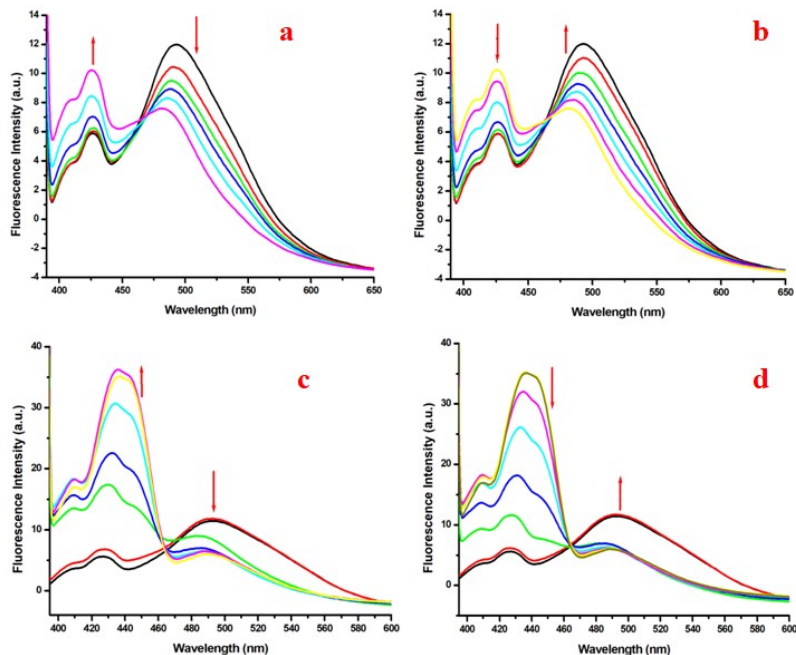
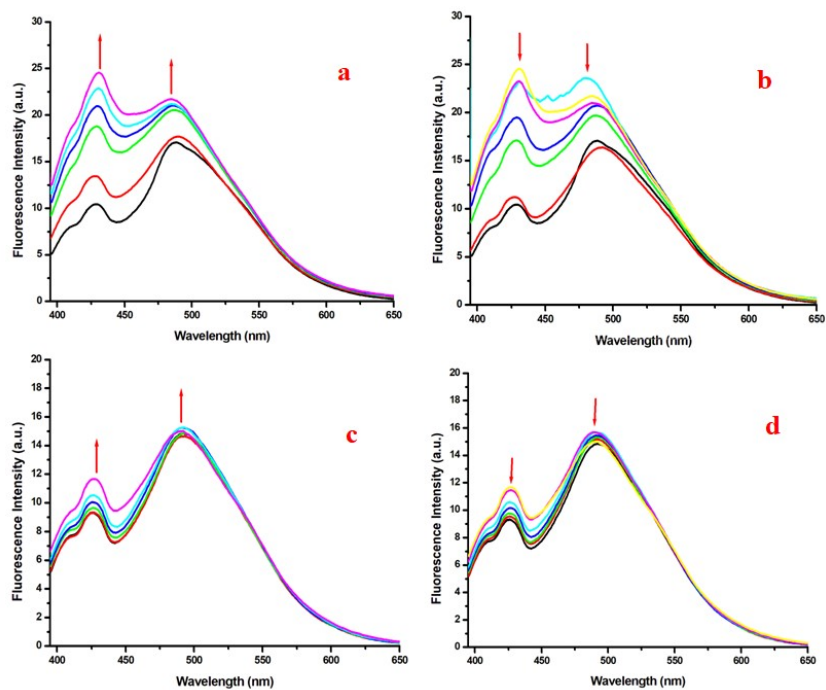


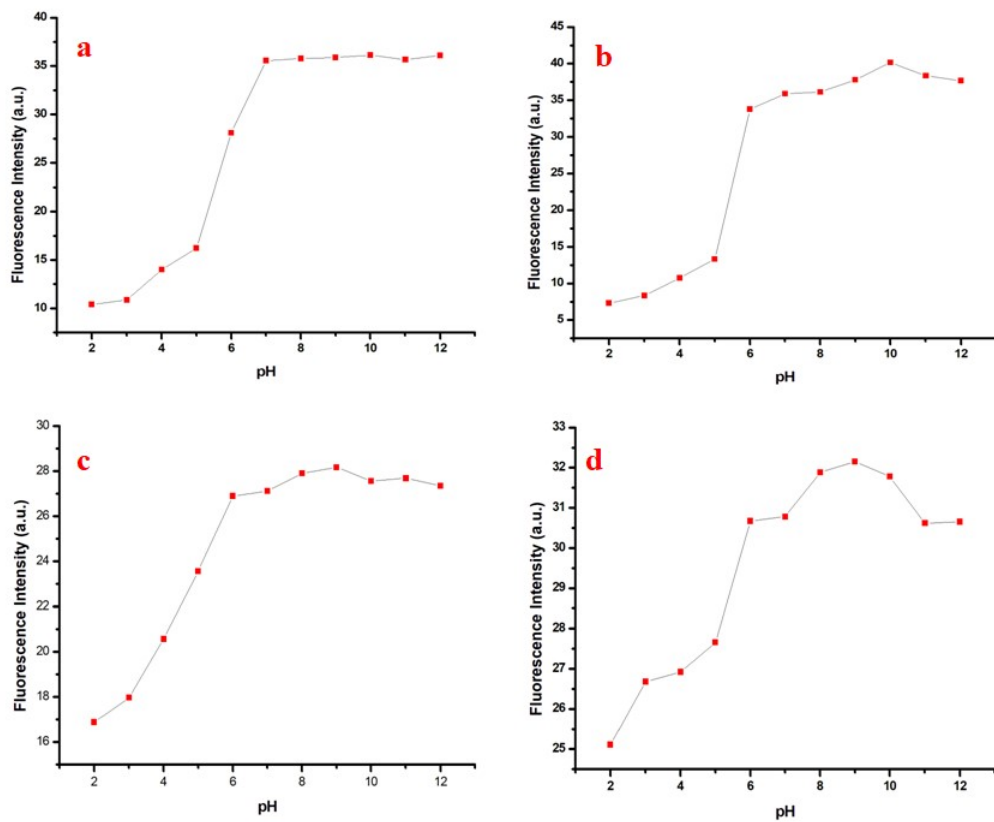
Figure S13 Benesi-Hildebrand plot of Quinox-hBT with (a)  $\text{Cu}^{2+}$ , (b)  $\text{Co}^{2+}$ , (c)  $\text{Ni}^{2+}$ , & (d)  $\text{Hg}^{2+}$  ions



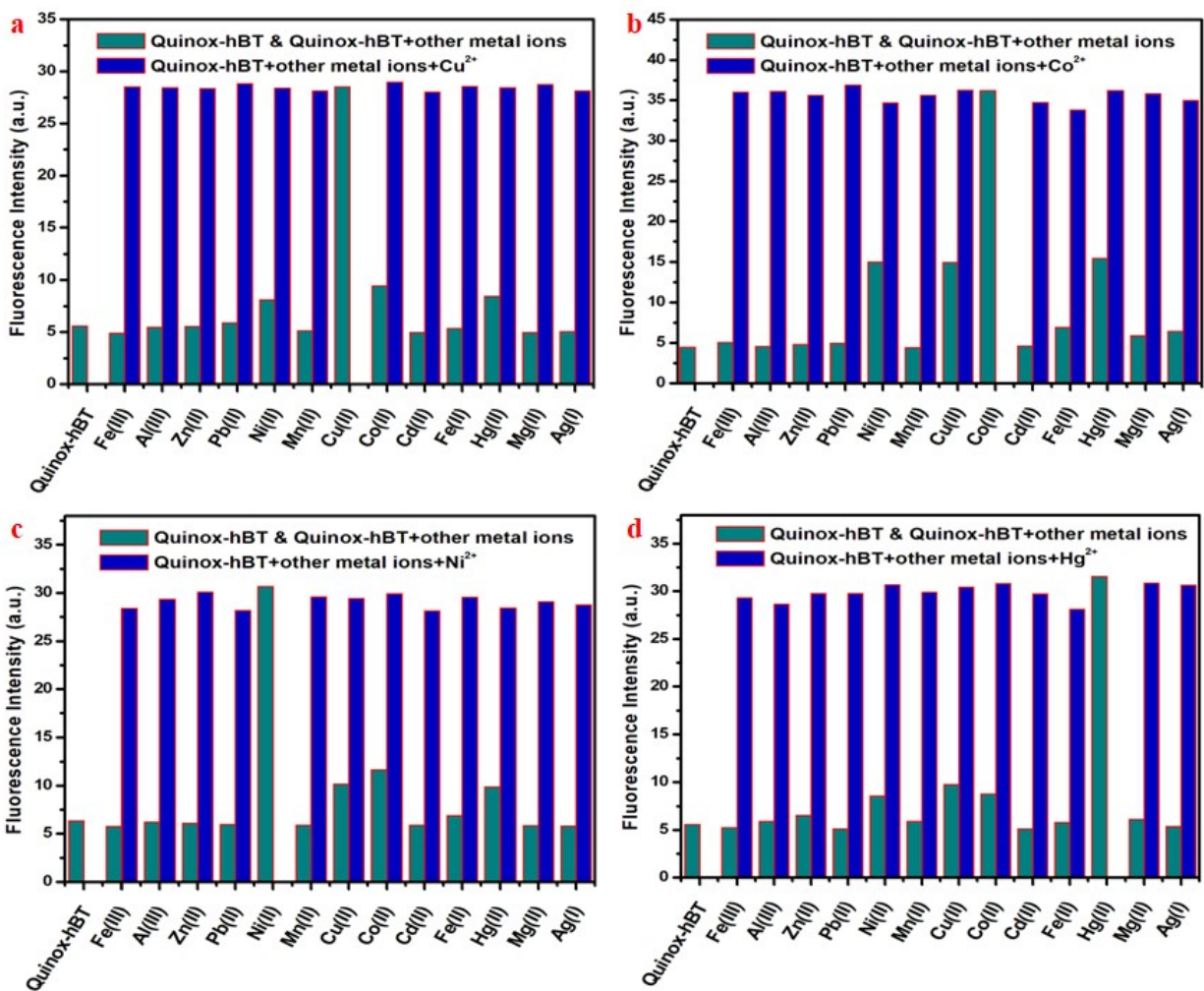
**Figure S14** Fluorescence response of (a) **Quinox-hBT**+ $\text{Cu}^{2+}$ , (b) **Quinox-hBT**+ $\text{Cu}^{2+}$ + $\text{S}^{2-}$ , (c) **Quinox-hBT**+ $\text{Co}^{2+}$  and (d) **Quinox-hBT**+ $\text{Co}^{2+}$ +EDTA



**Figure S15** Fluorescence response of (a) **Quinox-hBT**+ $\text{Ni}^{2+}$ , (b) **Quinox-hBT**+ $\text{Ni}^{2+}$ +EDTA, (c) **Quinox-hBT**+ $\text{Hg}^{2+}$  and (d) **Quinox-hBT**+ $\text{Hg}^{2+}$ + $\text{S}^{2-}$

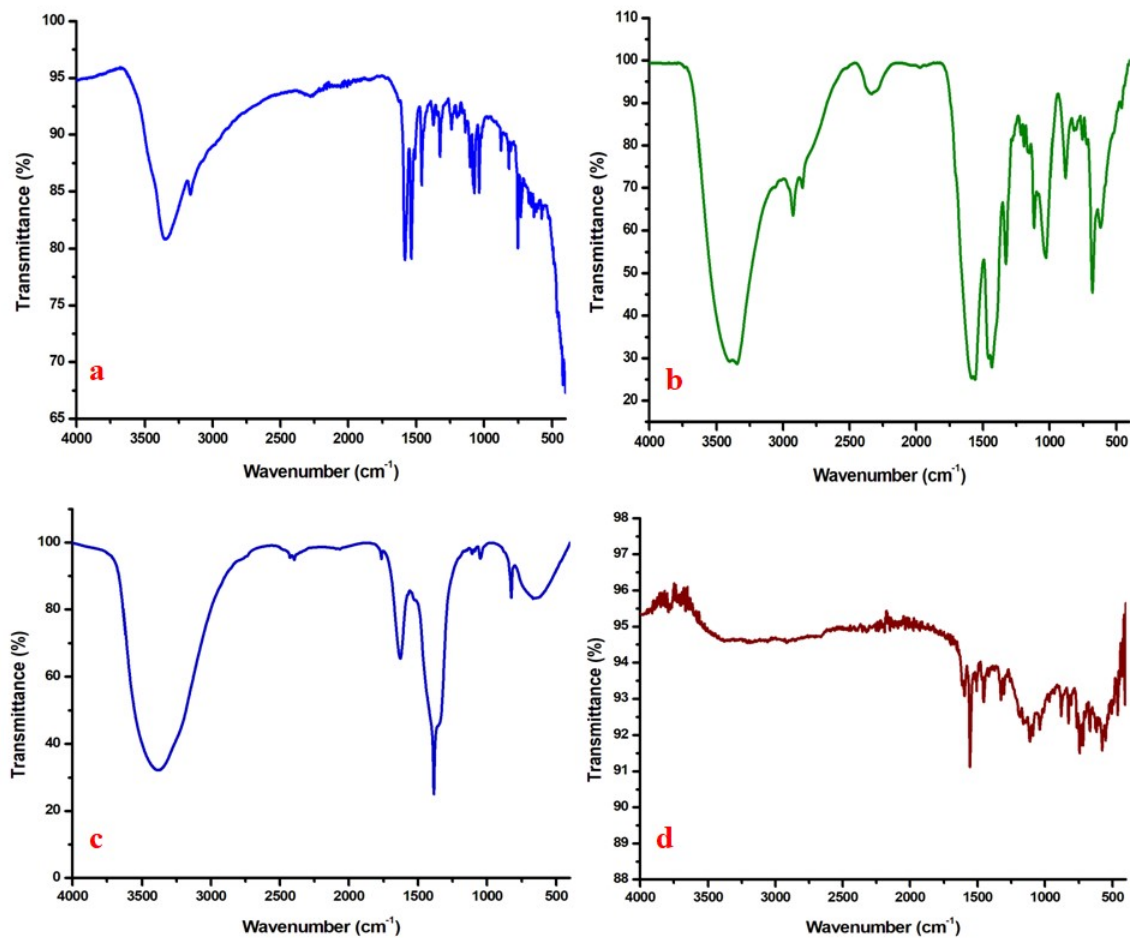


**Figure S16** pH effect on Quinox-hBT with (a) Cu<sup>2+</sup>, (b) Co<sup>2+</sup>, (c) Ni<sup>2+</sup>, & (d) Hg<sup>2+</sup> ions



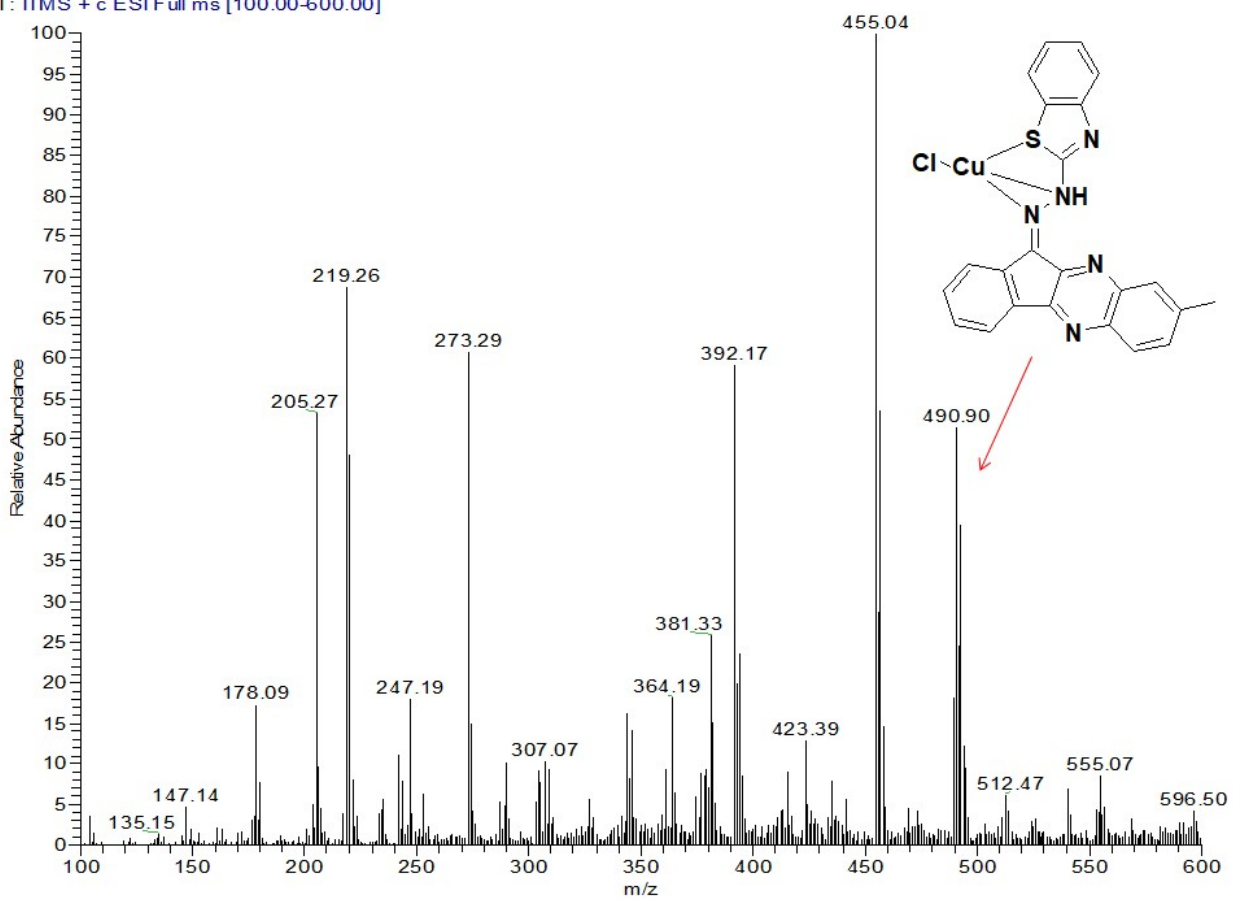
**Figure S17** Competitive bar plot of fluorescence response of **Quinox-hBT** with (a) Cu<sup>2+</sup>, (b) Co<sup>2+</sup>, (c) Ni<sup>2+</sup>, & (d) Hg<sup>2+</sup> ions in presence of Co-metal ion.





**Figure S18** Comparative FTIR spectrum of **Quinox-hBT** with (a) Cu<sup>2+</sup>, (b) Co<sup>2+</sup>, (c) Ni<sup>2+</sup>, & (d) Hg<sup>2+</sup> ions

NHBT-CU #1 RT: 0.00 AV: 1 NL: 2.70E4  
T: ITMS + c ESI Full ms [100.00-600.00]



**Figure S19** ESI-Mass spectrum of **Quinox-hBT+Cu<sup>2+</sup>**

NHBT-CO #1 RT: 0.00 AV: 1 NL: 2.58E4  
T: ITMS + c ESI Full ms [100.00-600.00]

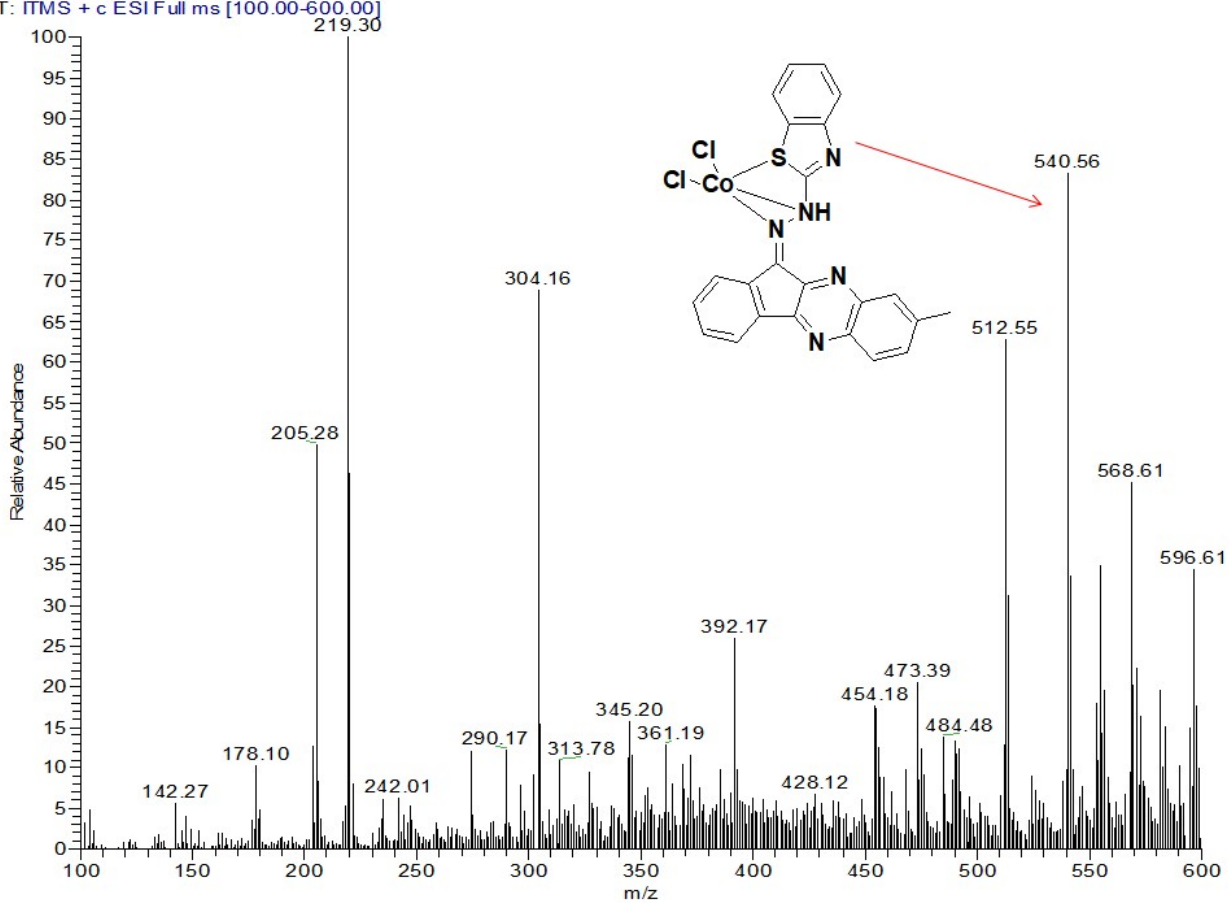


Figure S20 ESI-Mass spectrum of Quinox-hBT+Co<sup>2+</sup>

NHBT-N #1 RT: 0.00 AV: 1 NL: 1.76E5  
T: ITMS + c ESI Full ms [100.00-600.00]

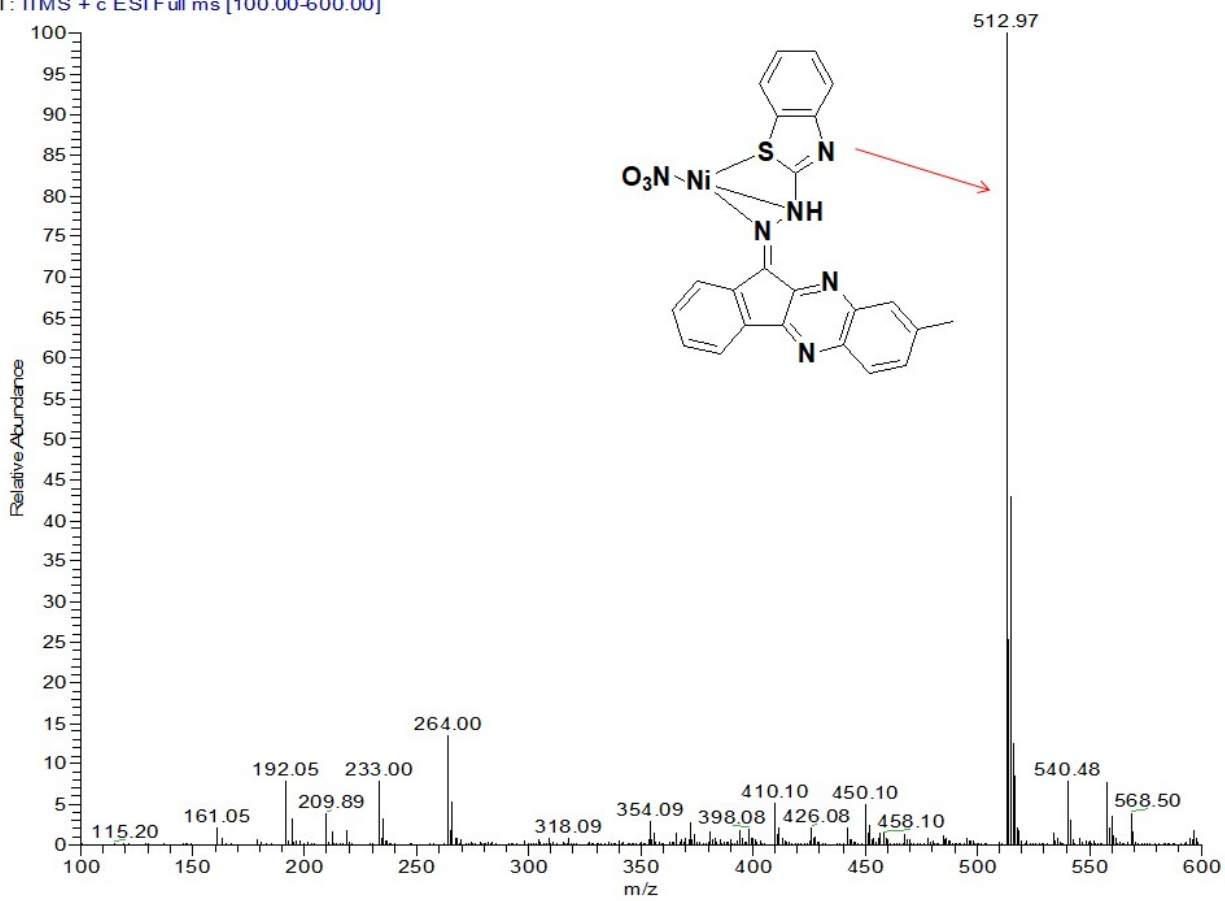


Figure S21 ESI-Mass spectrum of Quinox-hBT+Ni<sup>2+</sup>

NHBT-HG #1 RT: 0.00 AV: 1 NL: 1.69E4  
T: ITMS + c ESI Full ms [400.00-700.00]

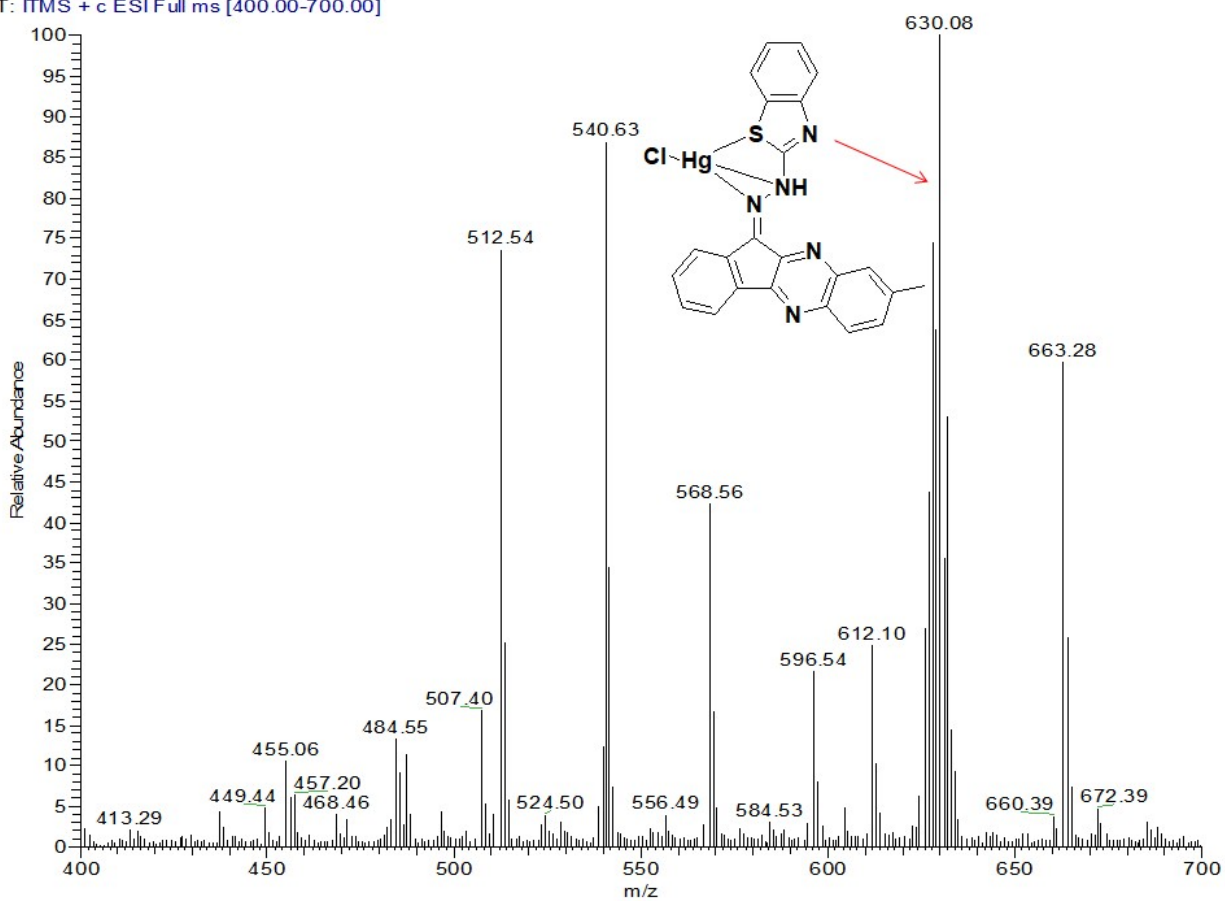


Figure S22 ESI-Mass spectrum of Quinox-hBT+Hg<sup>2+</sup>