

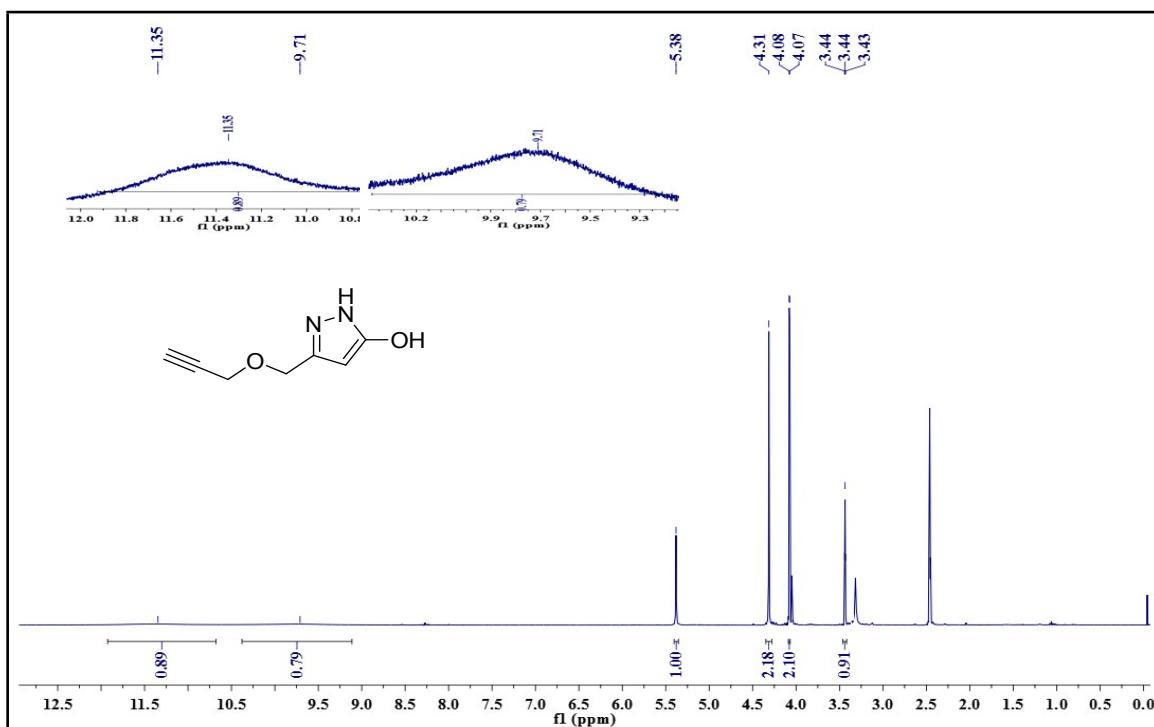
**Triazole-appended pyrano[2,3-*c*]pyrazolone based colorimetric chemosensors for  
recognition of Fe<sup>3+</sup> ions and their molecular logic gate behavior**

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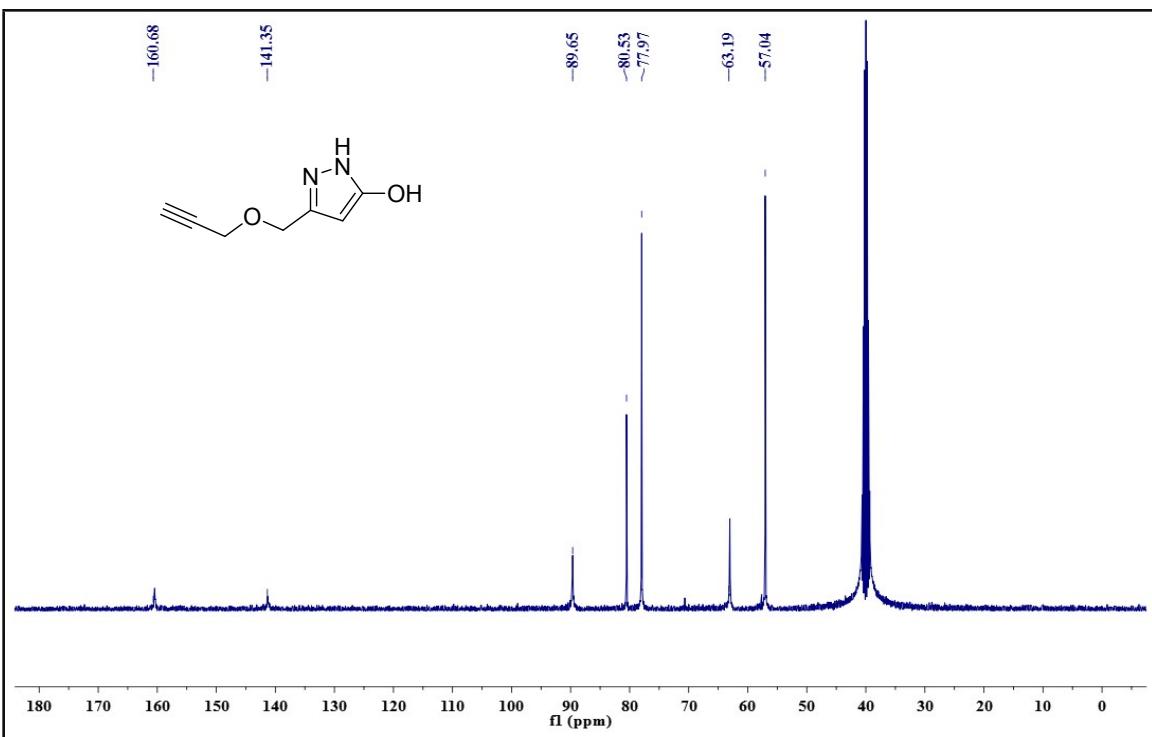
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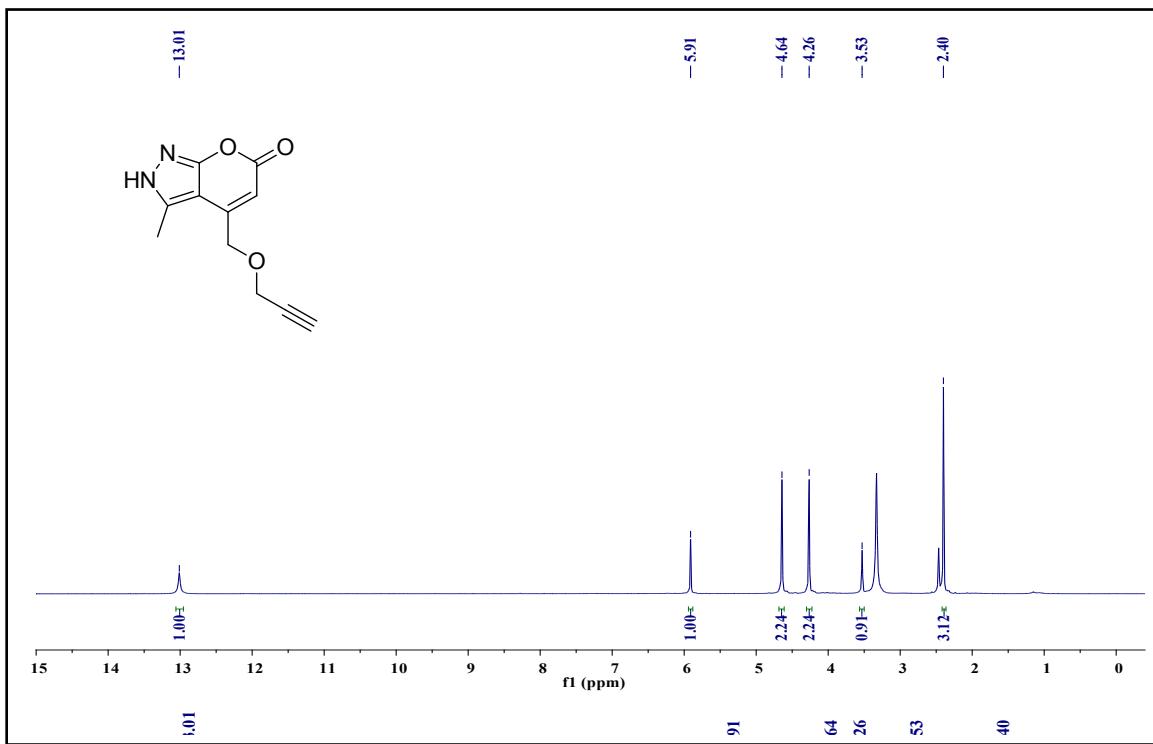
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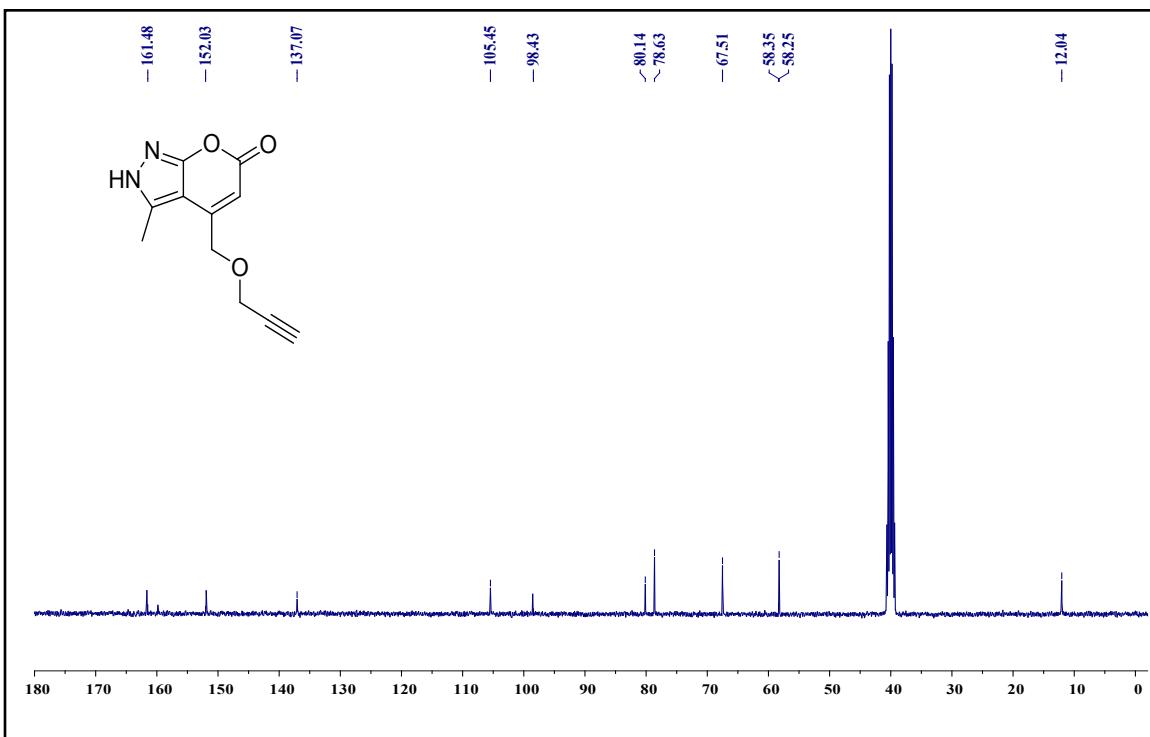
**Fig. S1** <sup>1</sup>H NMR spectra of compound 2b (DMSO-d<sub>6</sub>, 400 MHz)



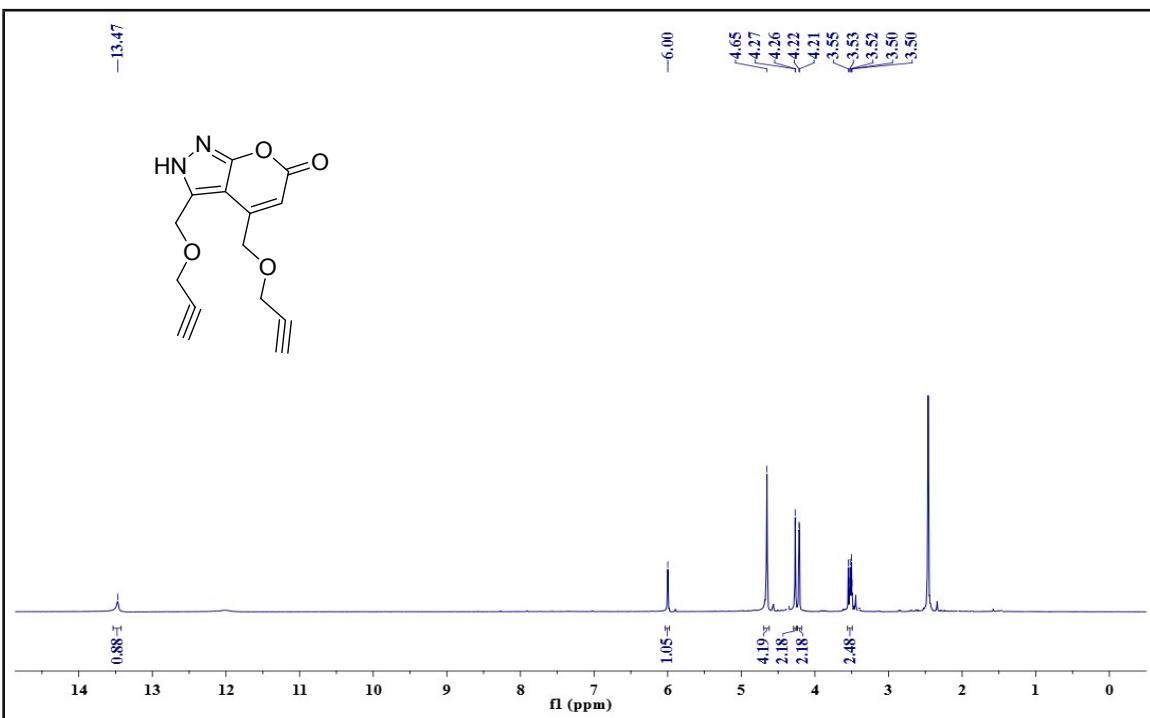
**Fig. S2**  $^{13}\text{C}$  NMR spectra of compound **2b** (DMSO- $d_6$ , 100 MHz)



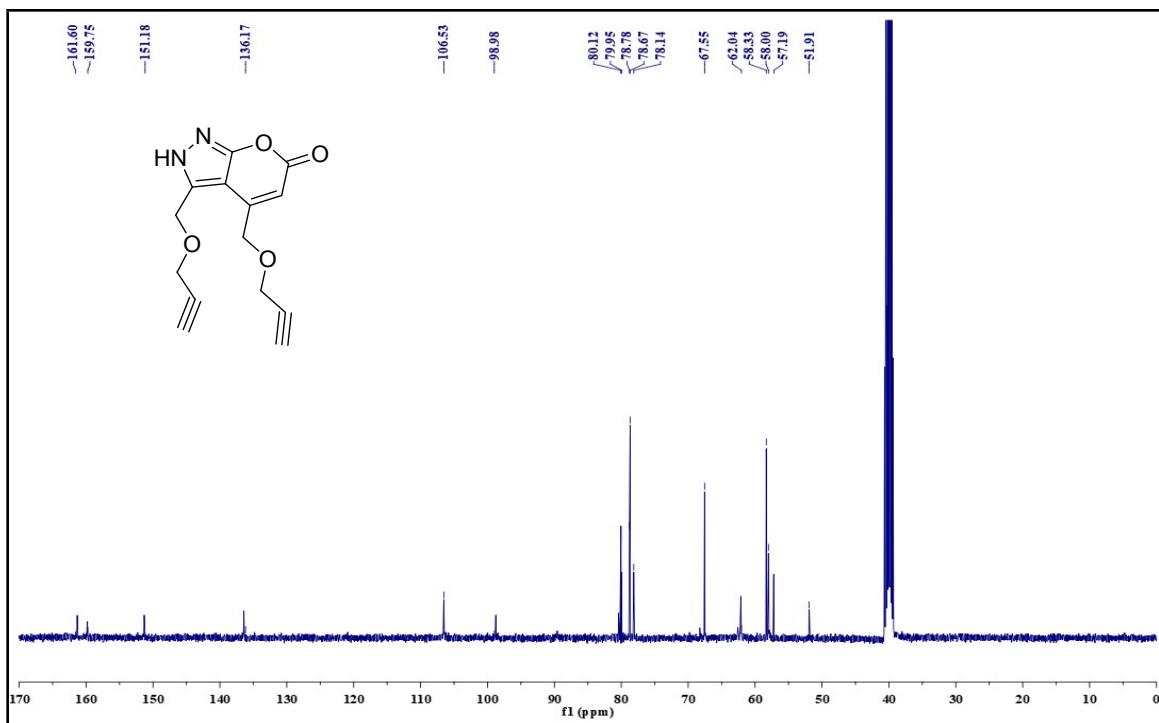
**Fig. S3**  $^1\text{H}$  NMR spectrum of compound **3a** (DMSO- $d_6$ , 400 MHz)



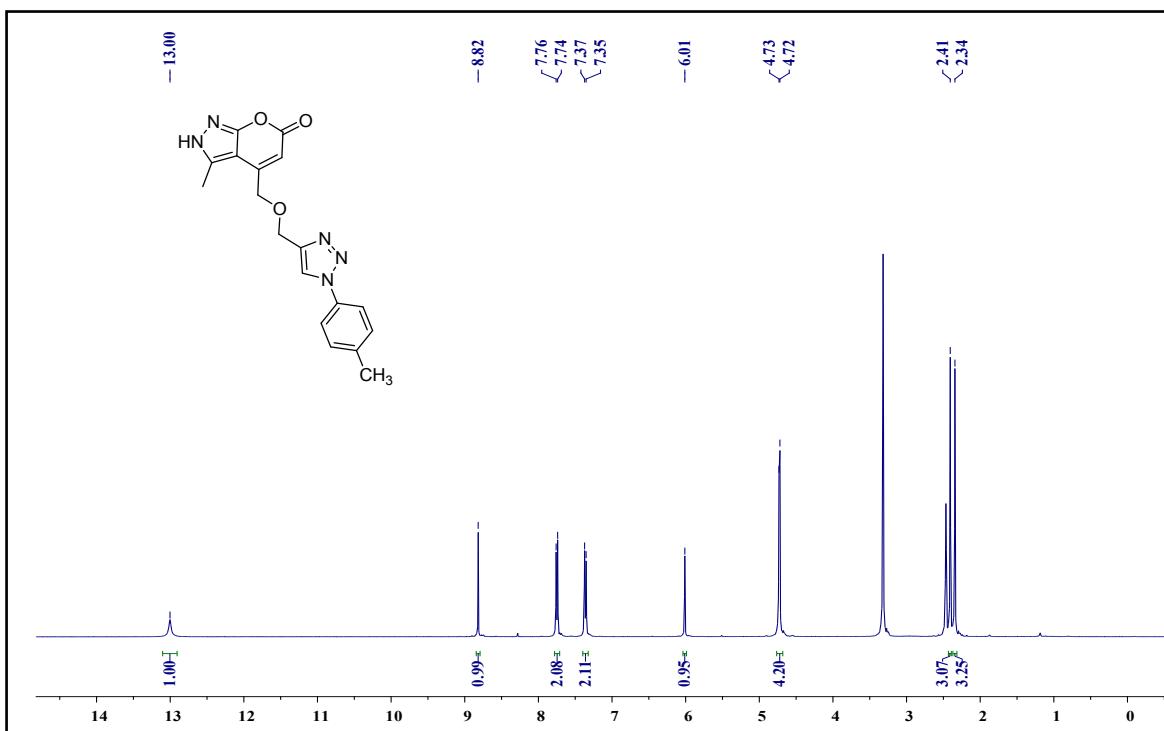
**Fig. S4**  $^{13}\text{C}$  NMR spectrum of compound **3a** (DMSO- $d_6$ , 100 MHz)



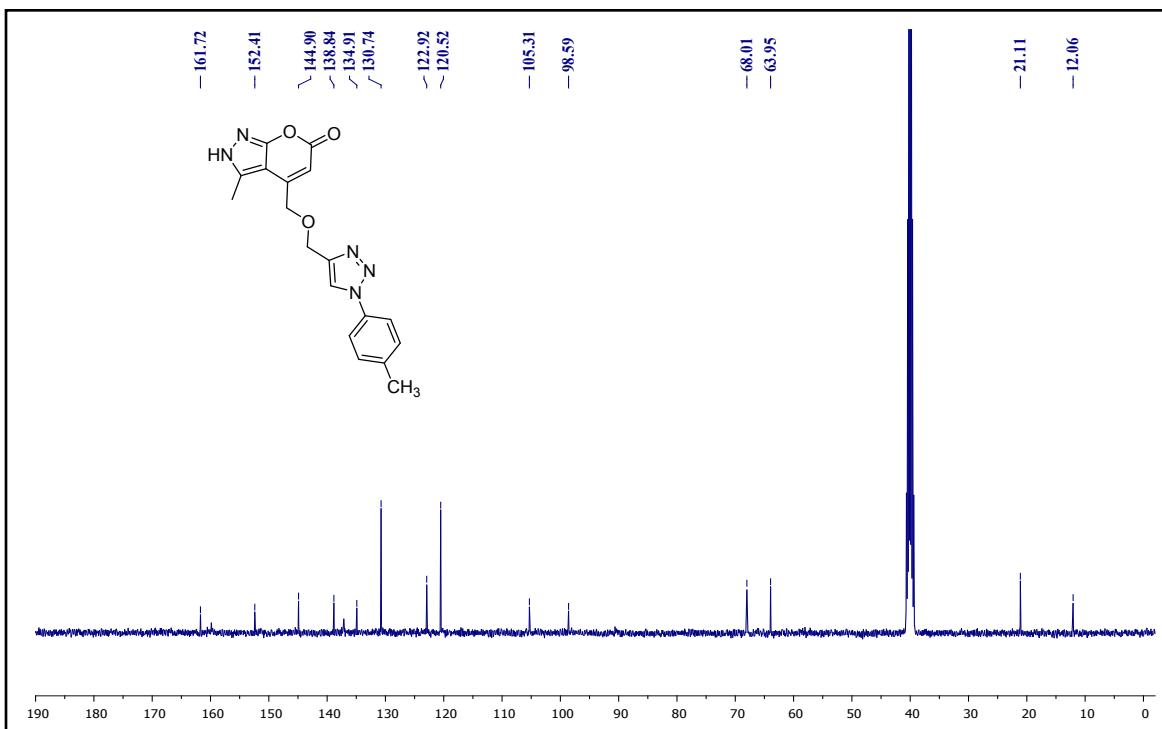
**Fig. S5**  $^1\text{H}$  NMR spectra of compound **3b** (DMSO- $d_6$ , 400 MHz)



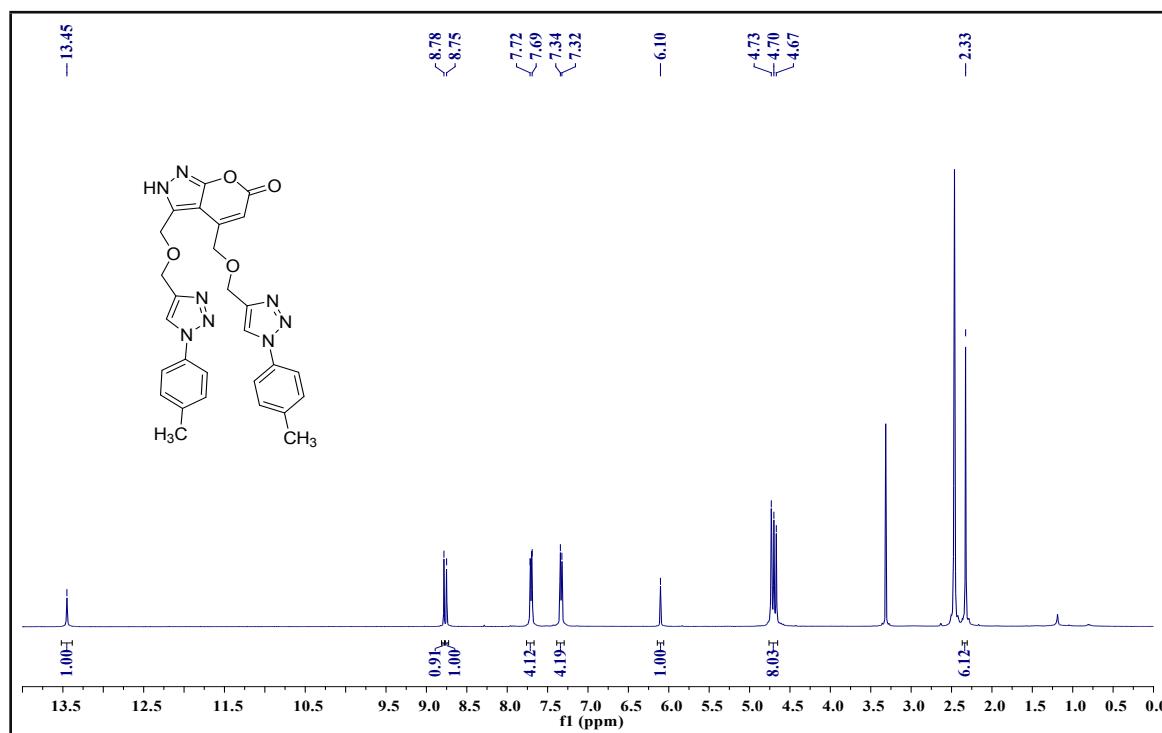
**Fig. S6**  $^{13}\text{C}$  NMR spectra of compound **3b** (DMSO- $d_6$ , 100 MHz)



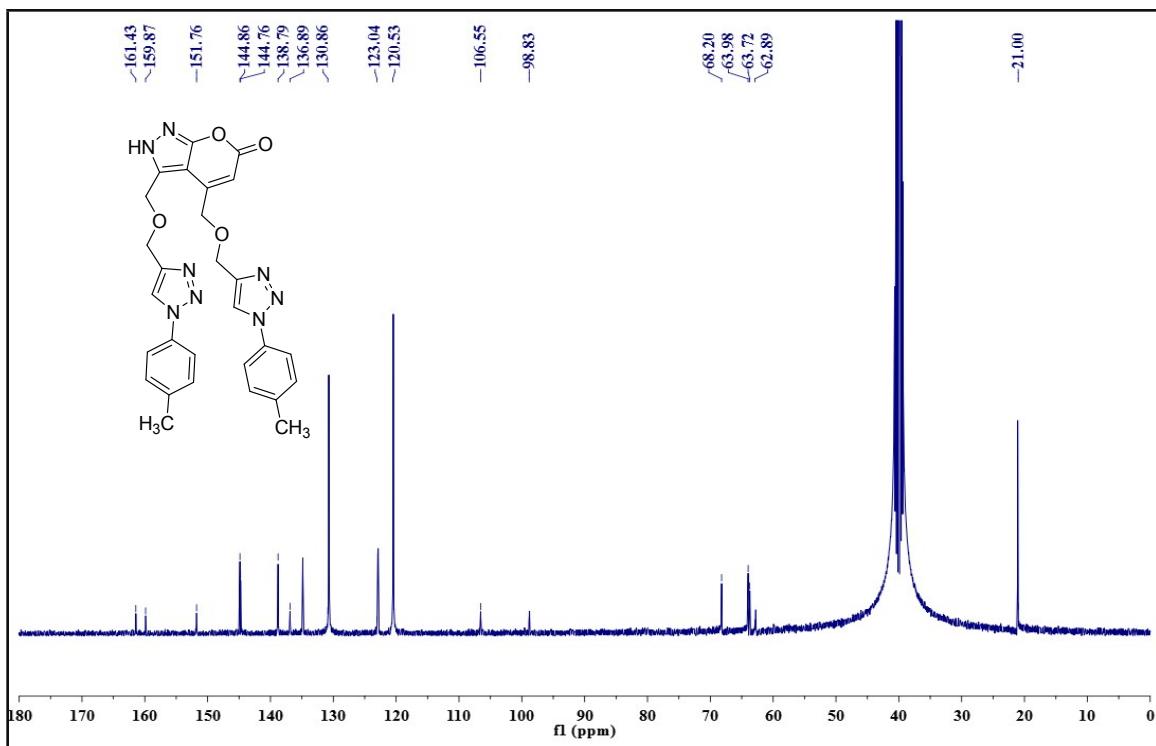
**Fig. S7**  $^1\text{H}$  NMR spectra of compound **4a** (DMSO- $d_6$ , 400 MHz)



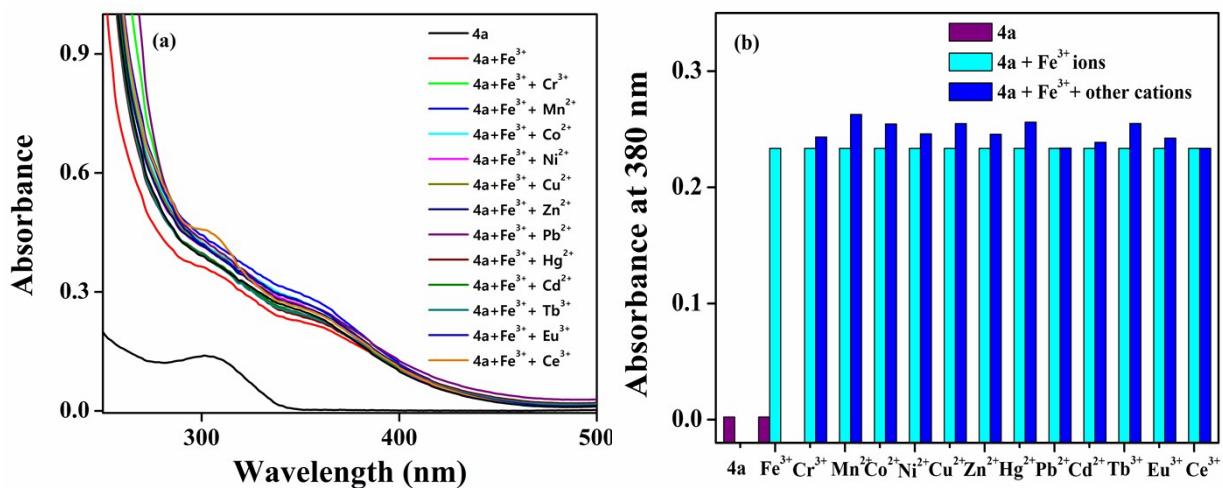
**Fig. S8**  $^{13}\text{C}$  NMR spectra of compound **4a** (DMSO- $d_6$ , 100 MHz)



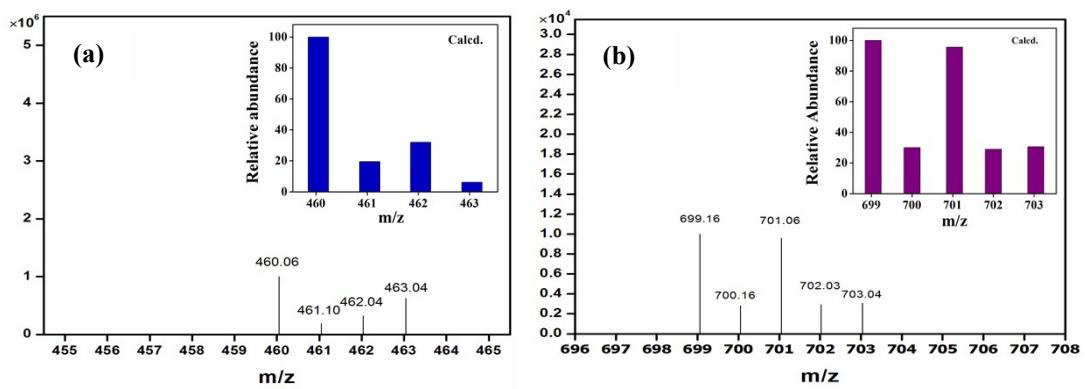
**Fig. S9**  $^1\text{H}$  NMR spectra of compound **4b** (DMSO- $d_6$ , 400 MHz)



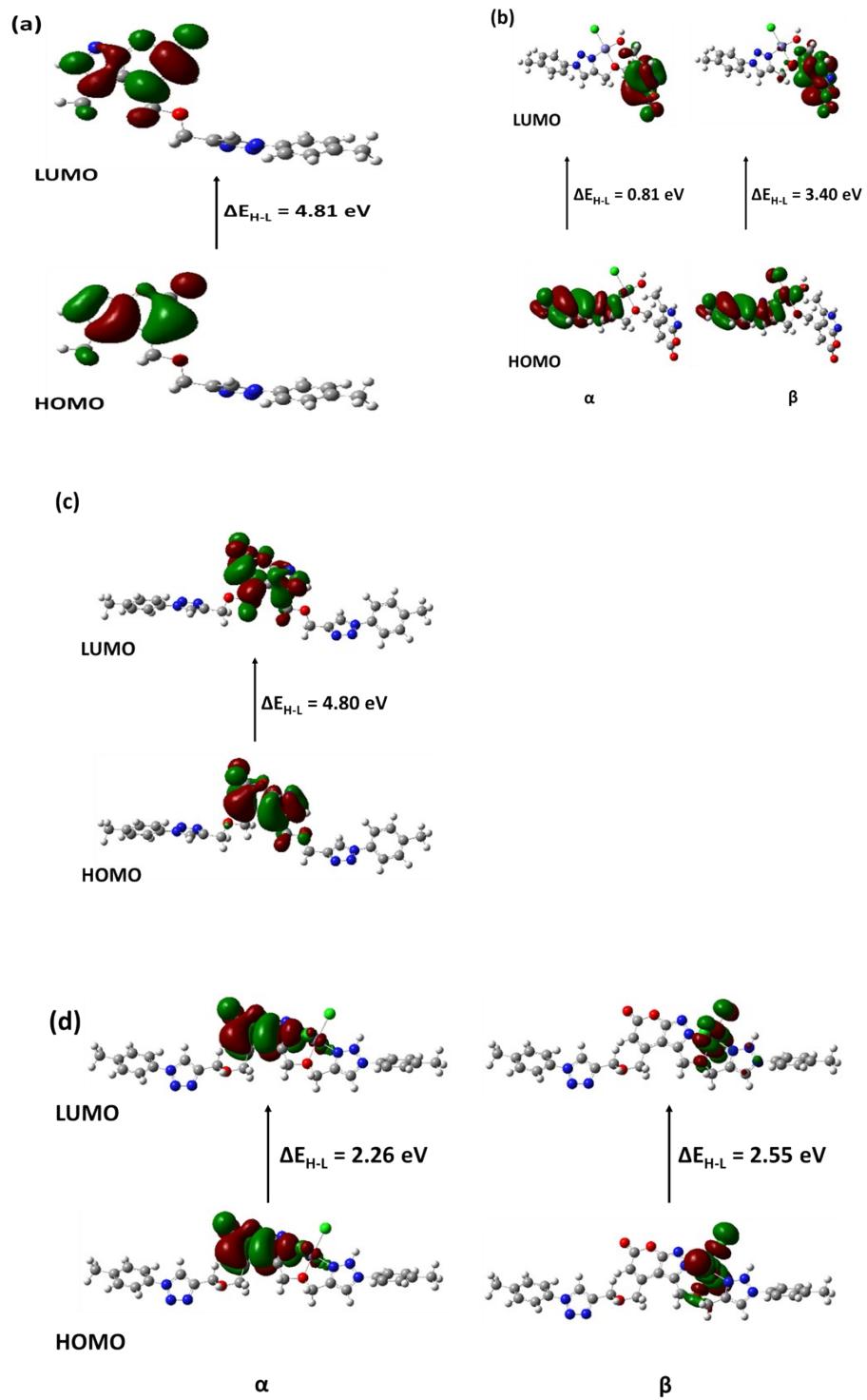
**Fig. S10**  $^{13}\text{C}$  NMR spectra of compound **4b** ( $\text{DMSO}-d_6$ , 100 MHz)



**Fig. S11 (a)** UV-Vis spectral changes for 1:10 mixture of chemosensor **4a** (10  $\mu\text{M}$ ,  $\text{MeOH}/\text{H}_2\text{O}$ , 8:2, v/v) and different metal ions, **(b)** Absorbance data for 1:10 mixture of chemosensor **4a** and different metal ions obtained at wavelength of 380 nm.



**Fig. S12 Mass-spectrum of (a) 4a-Fe<sup>3+</sup> complex and (b) 4b-Fe<sup>3+</sup> complex.**



**Fig. S13 Frontier molecular orbitals of (a) 4a, (b) 4a- $\text{Fe}^{3+}$ , (c) 4b and (d) 4b- $\text{Fe}^{3+}$**