Electronic supplementary information for New Journal of Chemistry

A semi-rigid tricarboxylate ligand based Co(II) coordination polymer: construction and applications in multiple sensing

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Table S1 Selected bond distances (Å) and angles (°) for CP **1**.

CP **1**			
Co(1)–O(2)	2.079(2)	Co(1)–O(9)#2	2.110(2)
Co(1)–O(3)#3	2.123(2)	Co(1)–O(6)#4	2.156(2)
Co(1)–O(8)	2.150(2)	Co(1)–O(9)	2.077(2)
Co(2)–O(4)#5	2.014(2)	Co(2)–O(9)	2.031(2)
Co(2)–O(6)#1	2.081(2)	Co(2)–O(10)	2.088(3)
Co(2)–O(5)#1	2.411(3)	Co(2)–O(1)	1.994(2)
O(9)–Co(1)–O(2)	103.17(8)	O(9)–Co(1)–O(9)#2	81.01(8)
O(2)–Co(1)–O(9)#2	100.37(9)	O(9)–Co(1)–O(3)#3	176.16(8)
O(2)–Co(1)–O(3)#3	80.37(9)	O(9)#2–Co(1)–O(3)#3	96.97(8)
O(9)–Co(1)–O(6)#4	89.75(8)	O(2)–Co(1)–O(6)#4	166.52(9)
O(9)#2–Co(1)–O(6)#4	77.59(8)	O(3)#3–Co(1)–O(6)#4	86.62(8)
O(9)–Co(1)–O(8)	90.32(9)	O(2)–Co(1)–O(8)	92.15(9)
O(9)#2–Co(1)–O(8)	166.10(8)	O(3)#3–Co(1)–O(8)	91.05(9)
O(6)#4–Co(1)–O(8)	91.61(9)	O(1)–Co(2)–O(4)#5	160.82(10)
O(1)–Co(2)–O(9)	100.38(9)	O(4)#5–Co(2)–O(9)	97.42(9)
O(1)–Co(2)–O(6)#1	97.28(9)	O(4)#5–Co(2)–O(6)#1	92.46(9)
O(9)–Co(2)–O(6)#1	81.07(8)	O(1)–Co(2)–O(10)	86.28(10)
O(4)#5–Co(2)–O(10)	84.28(10)	O(9)–Co(2)–O(10)	97.84(11)
O(6)#1–Co(2)–O(10)	176.41(9)	O(1)–Co(2)–O(5)#1	83.46(12)
O(4)#5–Co(2)–O(5)#1	84.50(12)	O(9)–Co(2)–O(5)#1	151.40(9)
O(6)#1–Co(2)–O(5)#1	70.25(9)	O(10)–Co(2)–O(5)#1	110.60(12)
Symmetry Code: #1 –x+1, –y+1, –z+1		#2 –x, –y+2, –z	#3 –x, –y+1, –z
#4 x–1, y+1, z–1		#5 x, y+1, z	

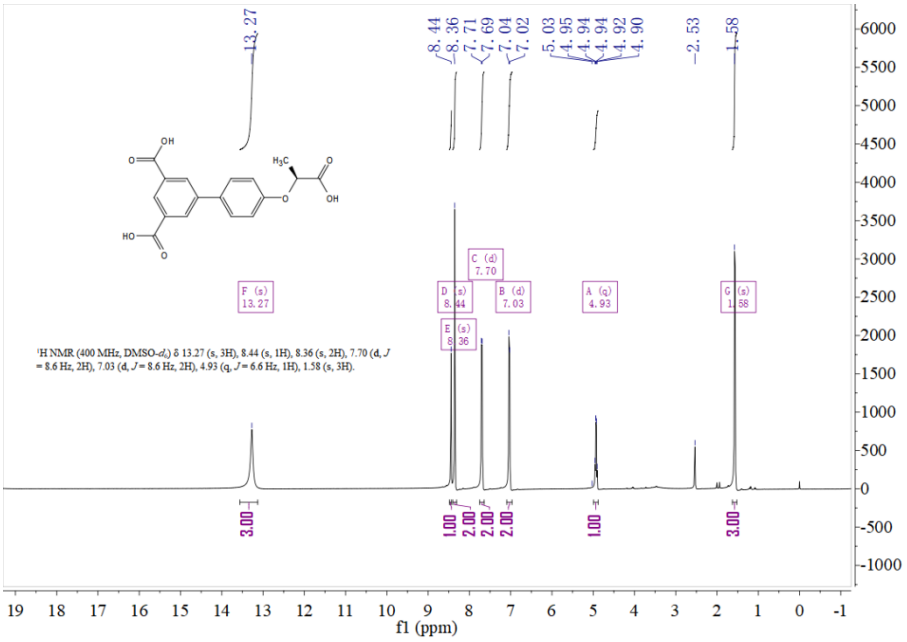


Fig. S1 ^{1}H NMR Spectrum of (R)-H_3cbda.

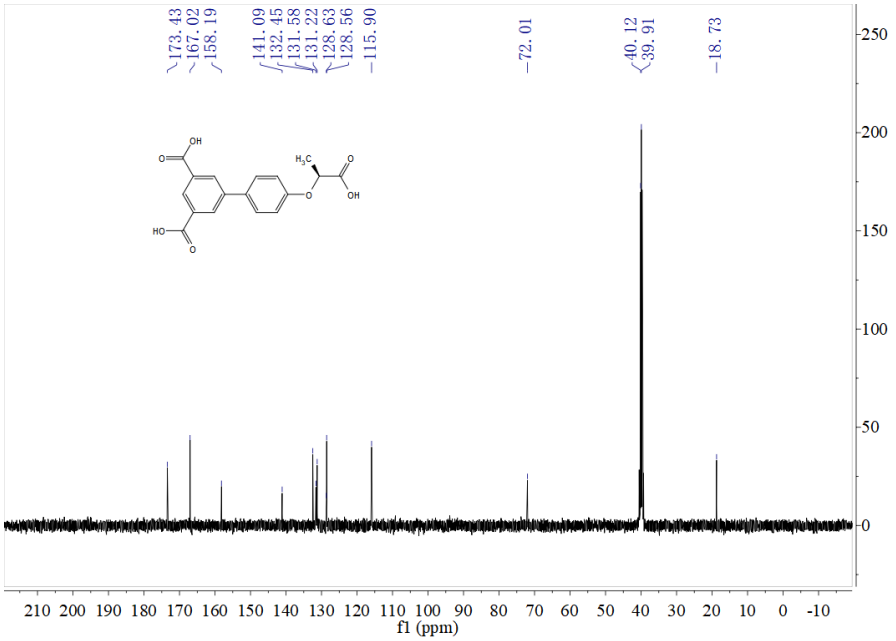


Fig. S2 ^{13}C NMR Spectrum of (R)-H_3cbda.

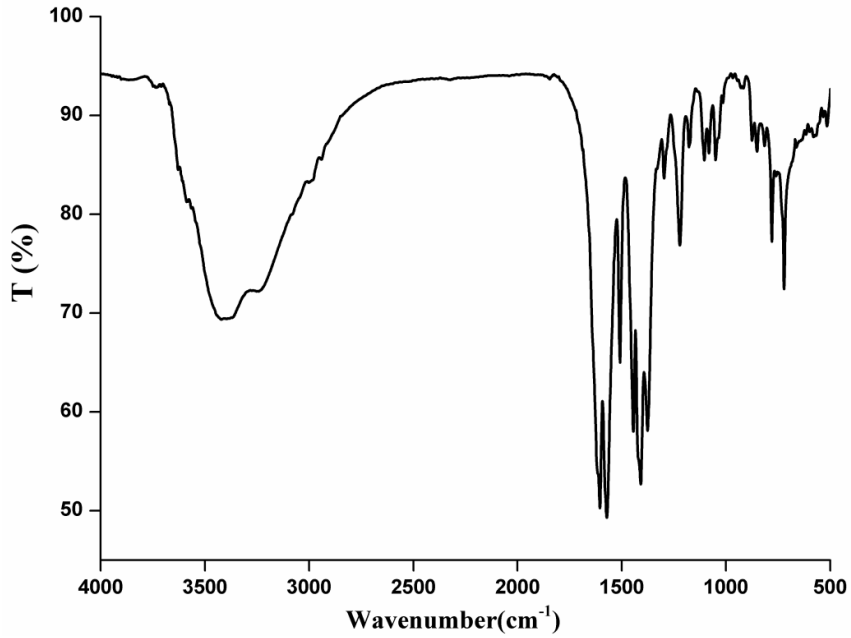


Fig. S3 The IR spectrum of (R)-H_3cbda.

Table S2 Hydrogen bonds (Å, °) in CP **1**.

D–H···*A*	*D*–H	H···*A*	*D*···*A*	∠*D*–H···*A*
O8–H8A···O11	0.742	2.324	3.051	166.68
O8–H8B···O7^{i}	0.693	2.234	2.893	159.50
O9–H9···O10^{ii}	0.933	2.329	3.238	164.86
O10–H10A···O11	0.854	1.890	2.700	158.01
O10–H10B···O7^{iii}	0.851	1.969	2.778	158.22
O11–H11A···O12	1.021	1.671	2.691	177.50
O11–H11B···O2^{iv}	1.025	2.028	3.005	158.47
O11–H11B···O3^{v}	1.025	2.482	3.208	127.29
O12–H12A···O3^{iv}	1.031	1.853	2.874	169.87
O12–H12B···O8^{v}	1.064	2.339	2.993	118.17

Symmetry codes: (i) x−1, y+1, z−1; (ii) −x+1, −y+2, −z; (iii) −x+2, -y+1, −z+1; (iv) x+1, y, z; (v) -x+1, −y+1, −z.

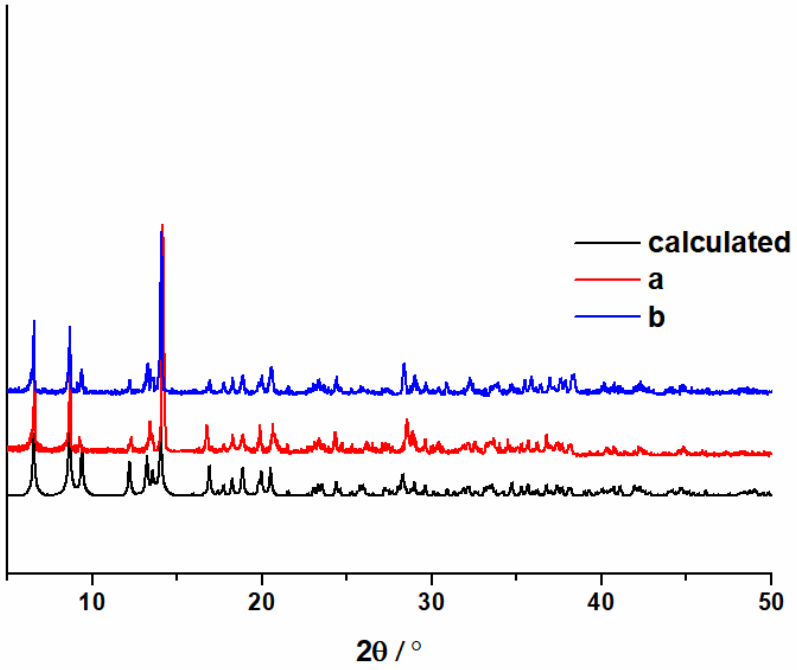


Fig. S4 (a) PXRD pattern of CP **1** before treated with Fe^{3+} ion; (b) PXRD patterns of CP **1** after treated with Fe^{3+} ion.

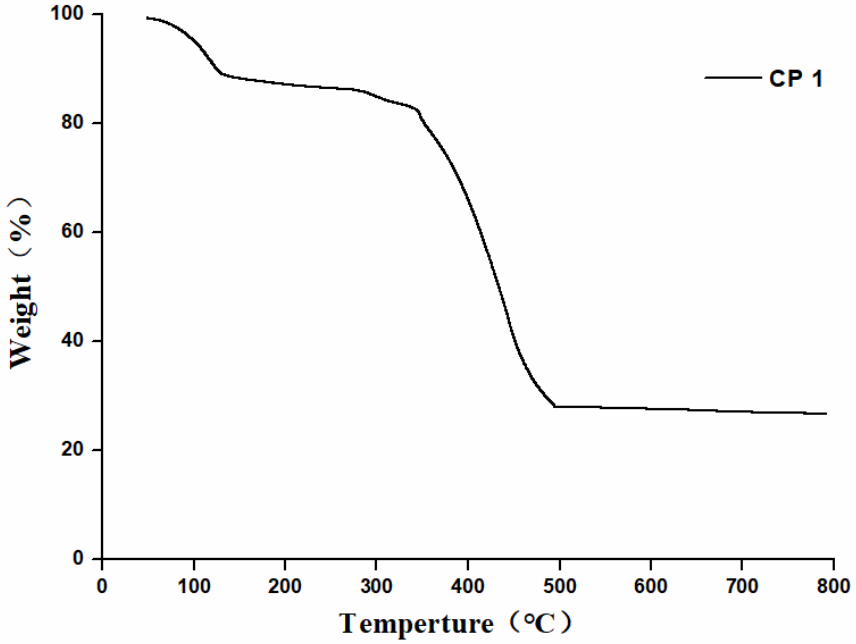


Fig. S5. TGA curve of CP **1**.

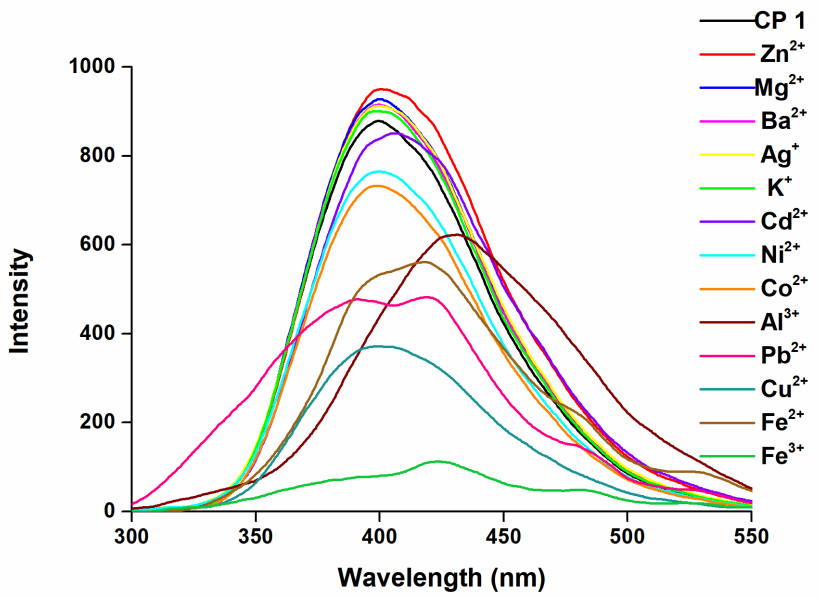


Fig. S6 Luminescence spectra of CP **1** when introducing disparate metal ions.

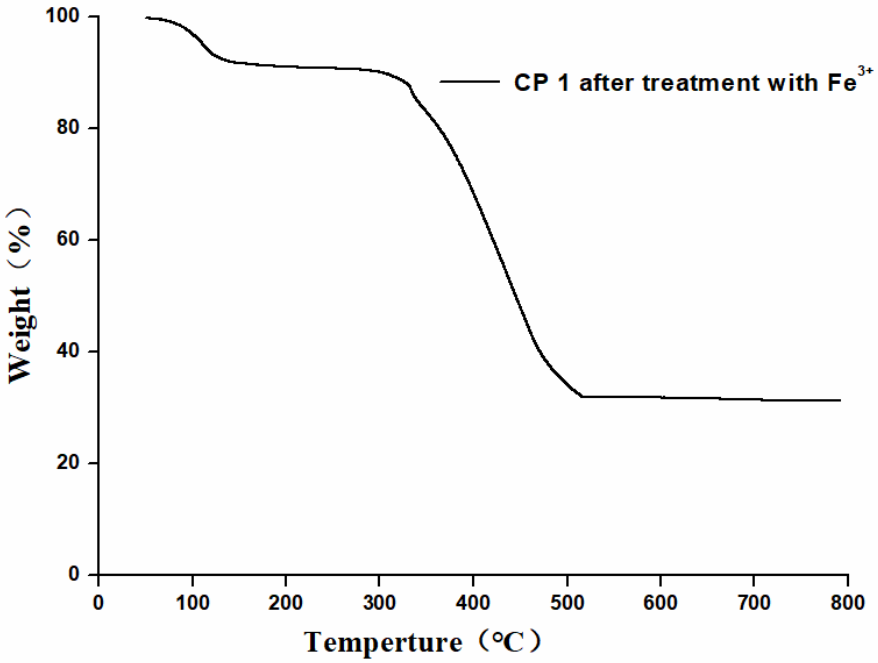


Fig. S7 CP **1** TGA curves after treatment with Fe^{3+}

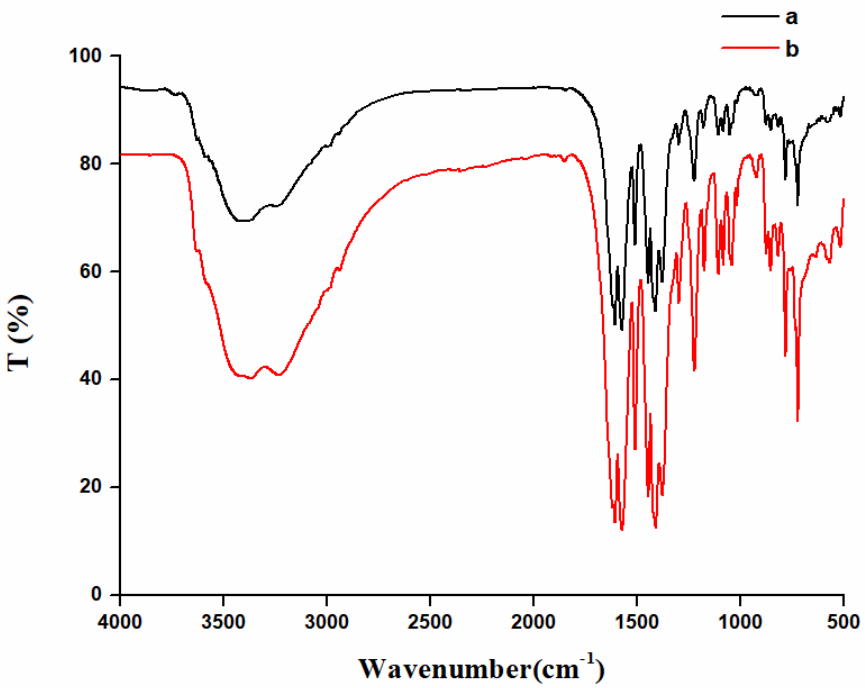


Fig. S8 (a) The IR spectrum of CP **1** before treated with Fe^{3+} ions; (b) The IR spectrum of CP **1** after treated with Fe^{3+} ions.

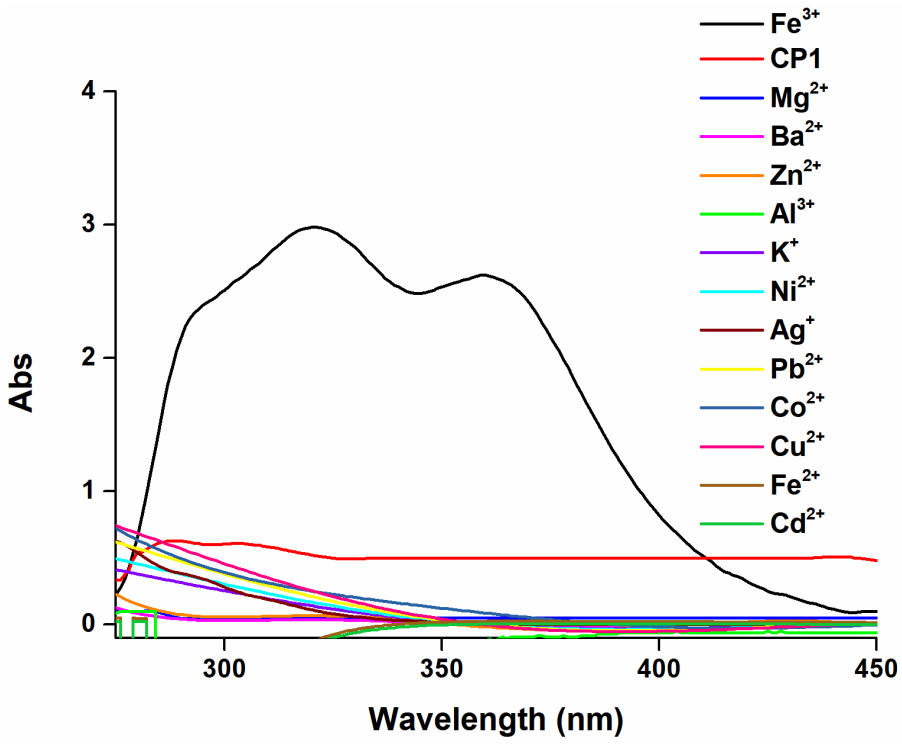


Fig. S9. Absorption spectra of aqueous solution containing $Fe(NO_3)_3$ and other metal Ions (10^{-3} mol/L); red line represents the absorption spectra of CP **1**.

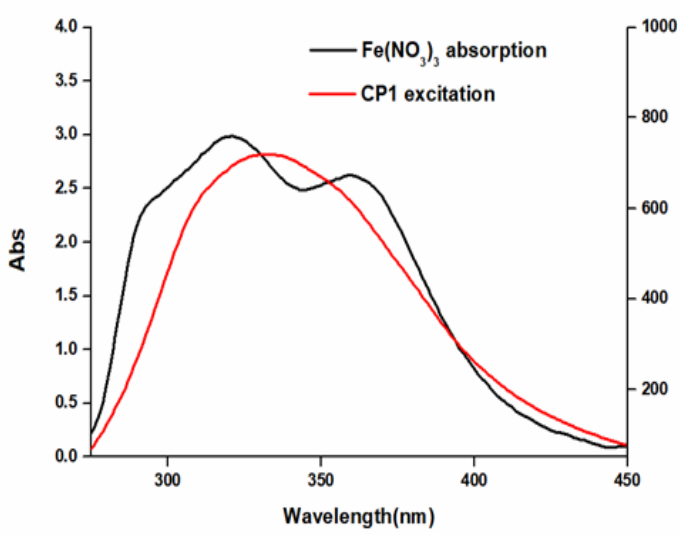


Fig. S10 The absorption spectrum of $Fe(NO_3)_3$ (black) and excitation spectrum (red) spectra of CP **1** suspended stock solution**.**

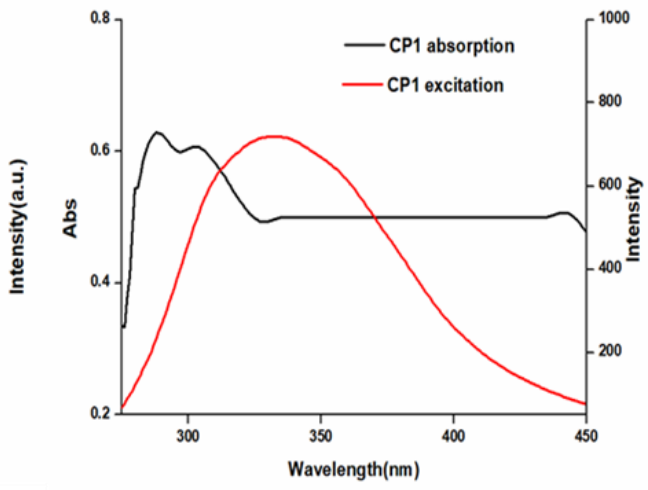


Fig. S11 The absorption spectrum (black) and excitation spectrum (red) of CP **1** suspended stock solution.

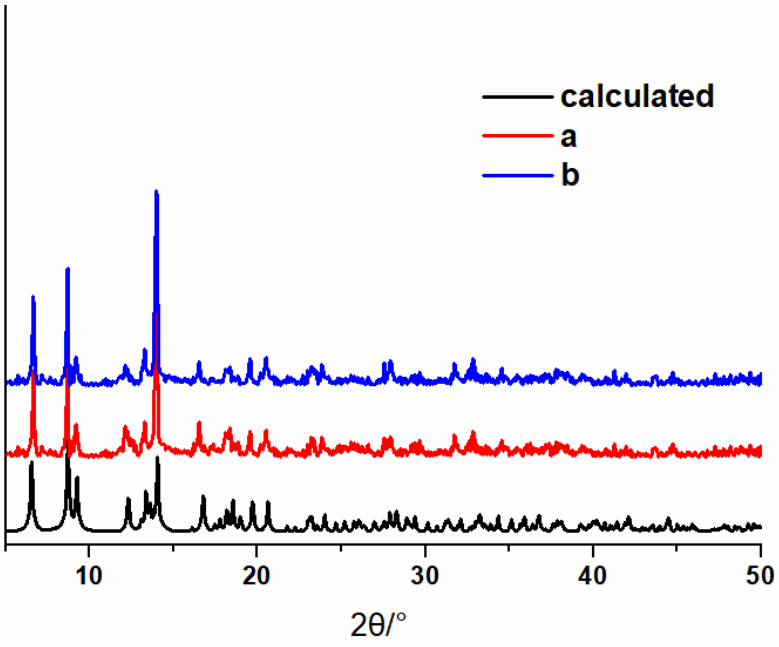


Fig. S12 (a) PXRD pattern of CP **1** before treating with NB; (b) PXRD patterns of CP **1** after treating with NB.

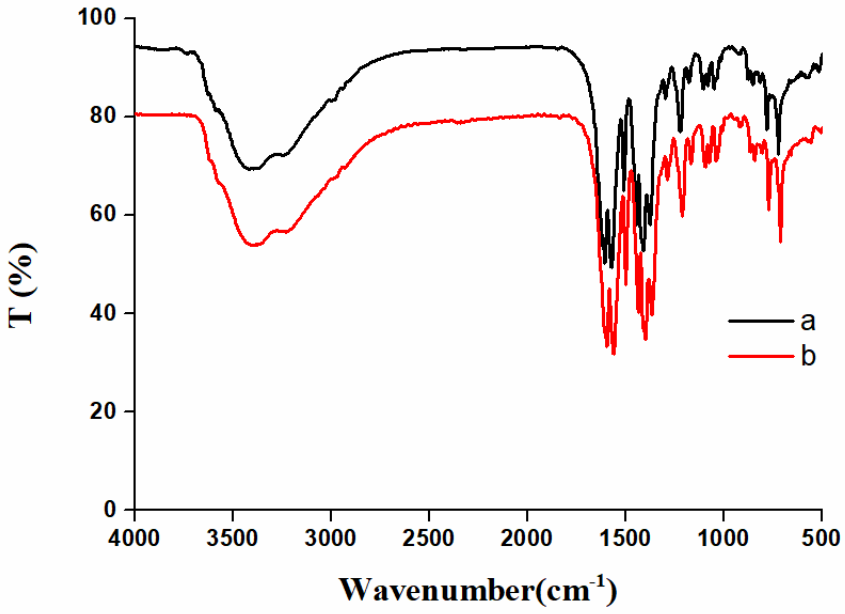
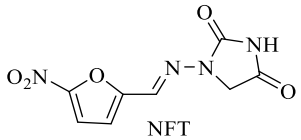
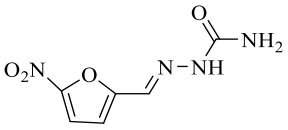


Fig. S13 (a) The IR spectrum of CP **1** before treating with NB; (b) The IR spectrum of CP **1** after treating with NB.

Detection of antibiotics


NFT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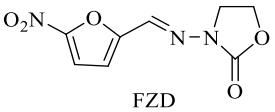
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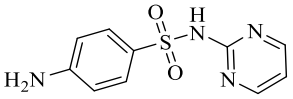
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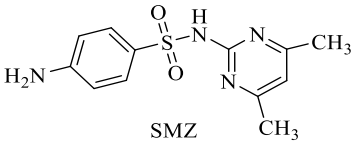
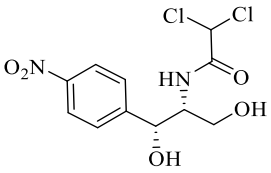

SMZ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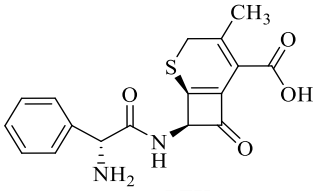
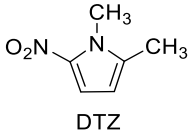

LEX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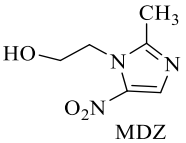
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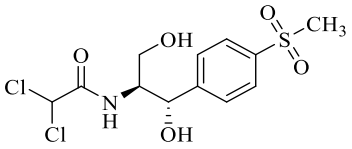
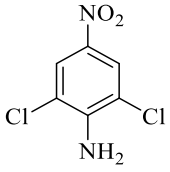
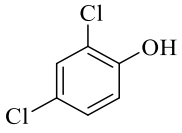
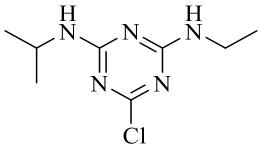
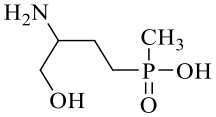

THI

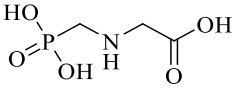
Detection of pesticide


DCN


2,4-dichlorophenol


Atrazine


Glufosinate


Glyphosate

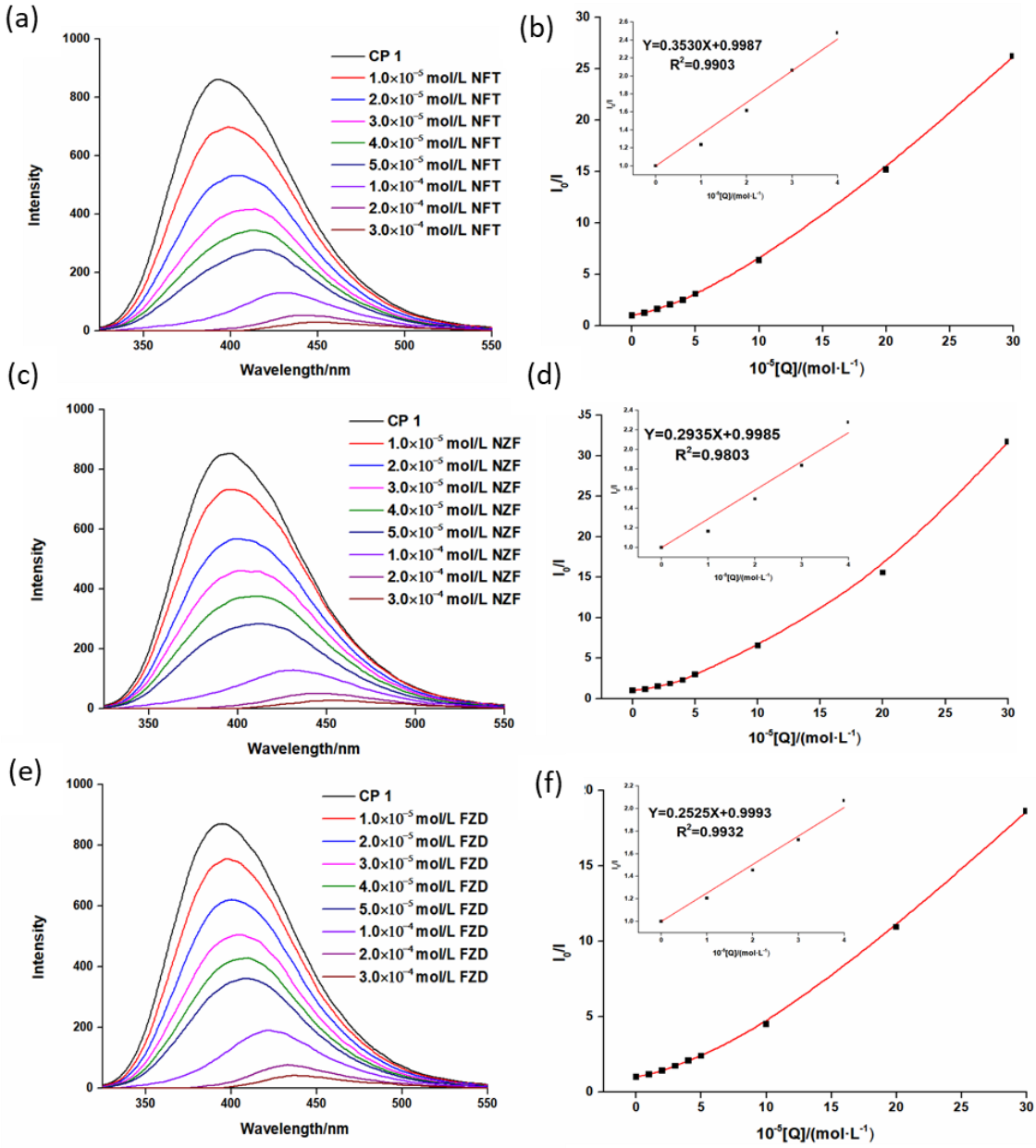


Fig. S14 (a)、(c)、(e) Luminescence spectra of CP **1** when different concentrations of nitrofuran antibiotics were applied; (b)、(d)、(f) the relation curve between relative luminescence intensity and nitrofuran antibiotics concentration. Inset: Linear relationship of I_0/I to concentration of nitrofuran antibiotics.

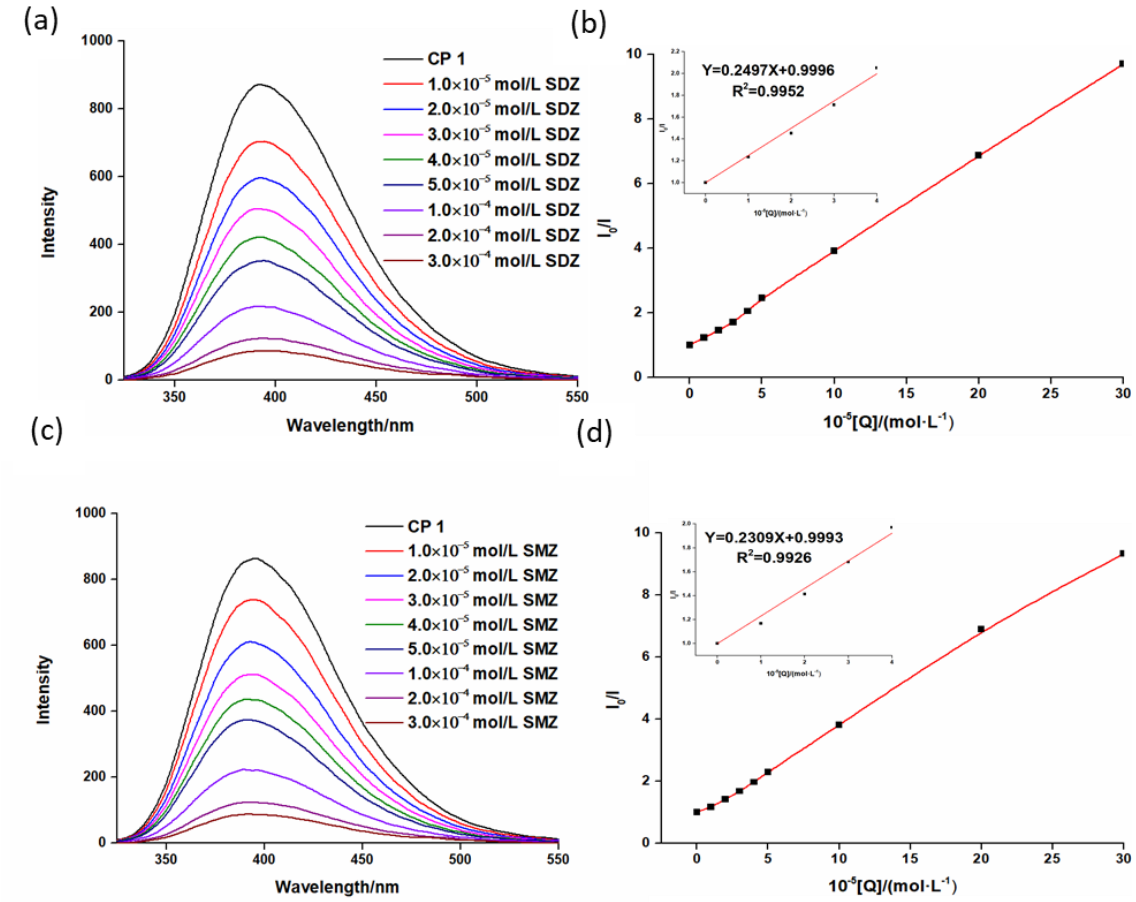


Fig. S15. (a)、(c)Luminescence spectra of CP **1** when different concentrations of sulfa antibiotics were applied; (b)、(d)The relation curve between relative luminescence intensity and sulfa antibiotics concentration. Inset: Linear relationship of I_0/I to concentration of sulfa antibiotics.

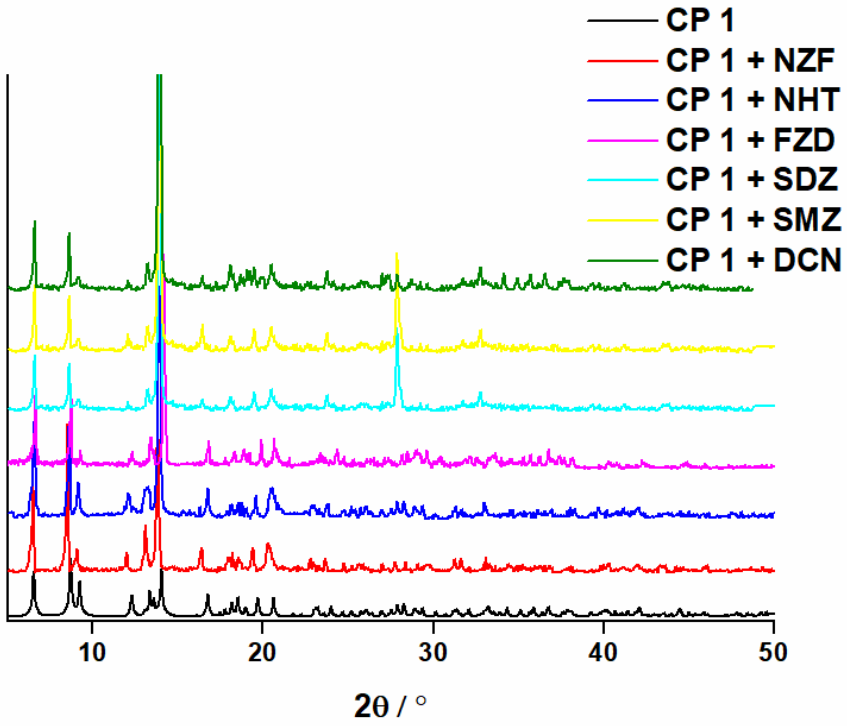


Fig. S16 PXRD patterns of CP 1 before and after treatment with different analytes.

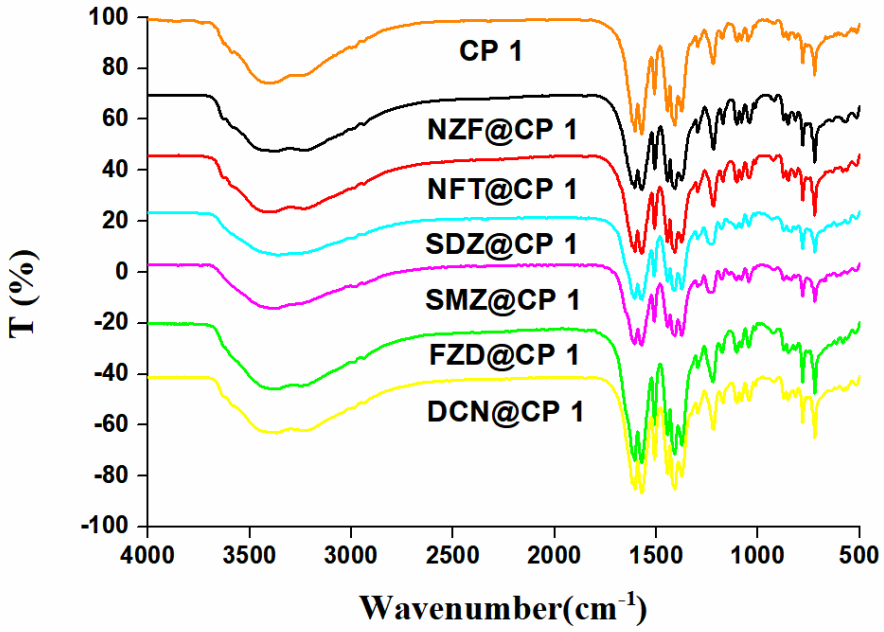


Fig. S17 The IR spectra of CP 1 before and after treatment with different analytes

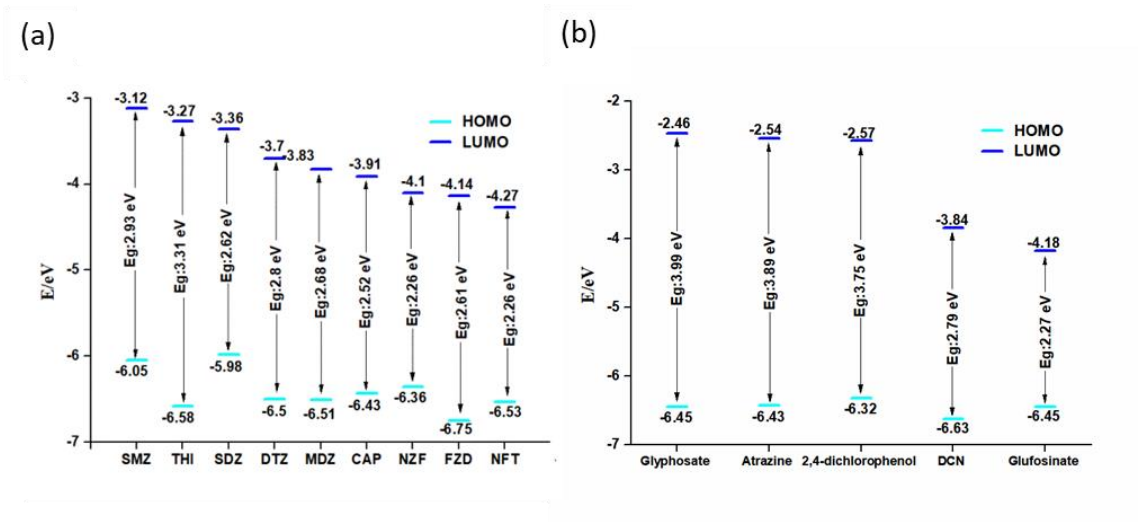


Fig. S18 HOMO and LUMO energies for the selected antibiotics(a) and pesticides(b) calculated by the calculation formula (-|4.78+x|eV).

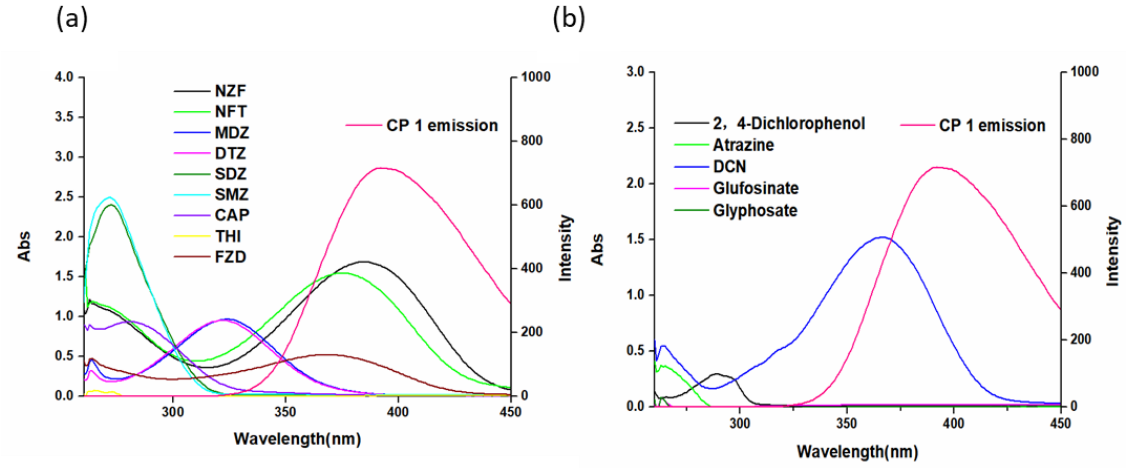


Fig. S19 UV-vis absorption spectra of selected antibiotics(a) and pesticides(b) and the emission spectra of CP **1** in water.