Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

for

Synthesis, crystal structure and remote allosteric binding properties of cone thiacalix[4]pseudocrown receptors bearing anthraquinone function and different arms

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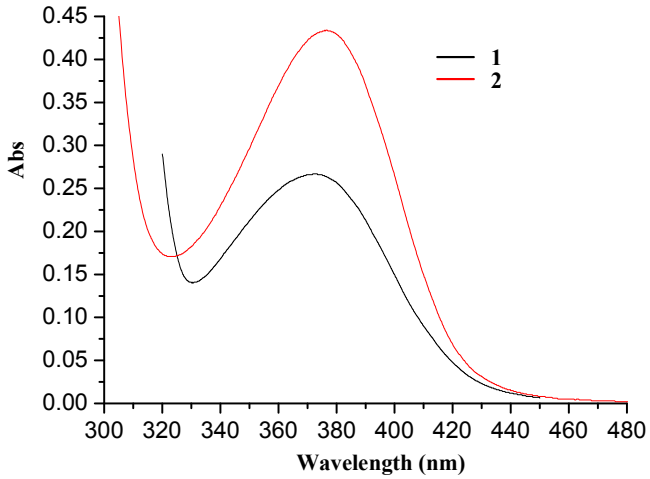


Fig. S1 The UV-vis spectra of receptors **1** and **2** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v).

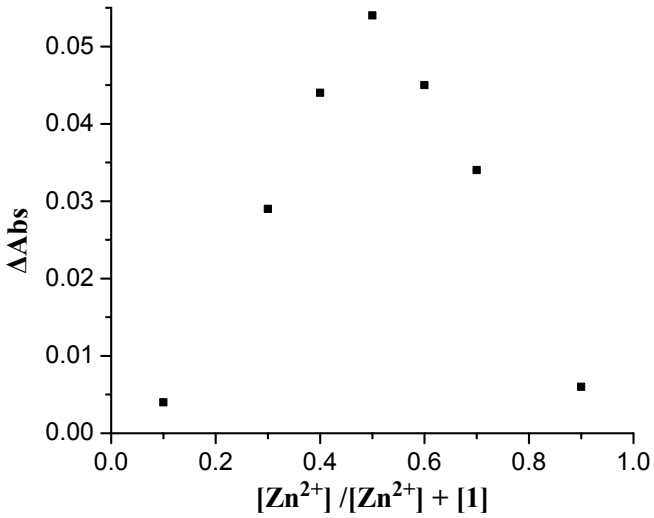


Fig. S2 The Job's plot of **1** with Zn^{2+}.

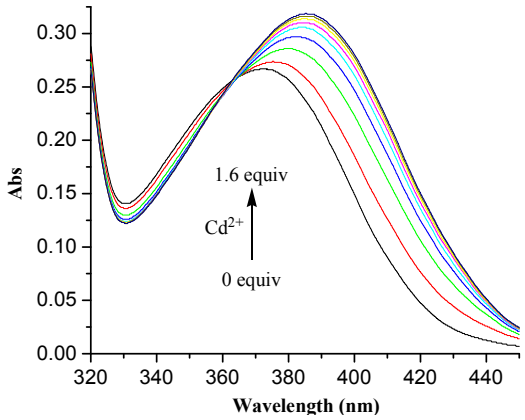


Fig. S3 Changes in the UV-vis spectrum of **1** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Cd^{2+} ions.

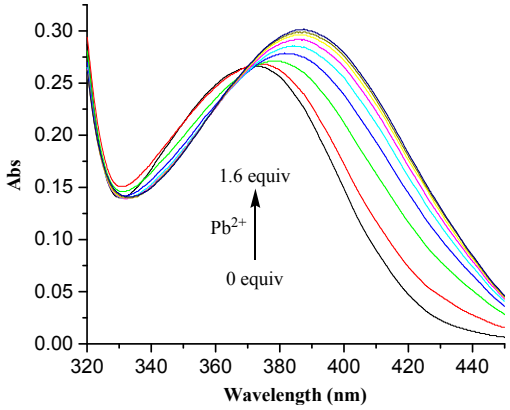


Fig. S4 Changes in the UV-vis spectrum of **1** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Pb^{2+} ions.

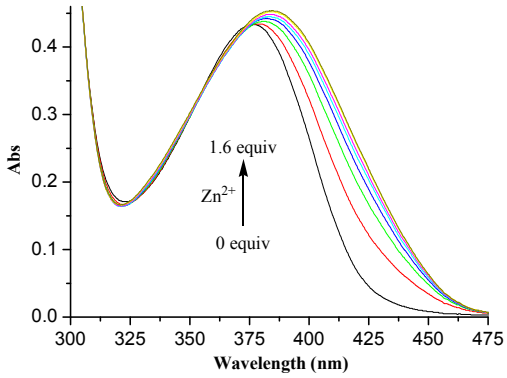


Fig. S5 Changes in the UV-vis spectrum of **2** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Zn^{2+} ions.

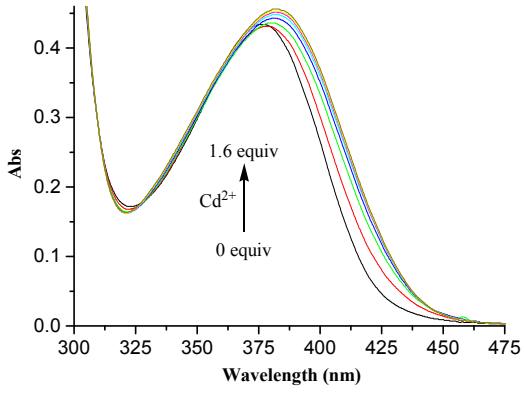


Fig. S6 Changes in the UV-vis spectrum of **2** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Cd^{2+} ions.

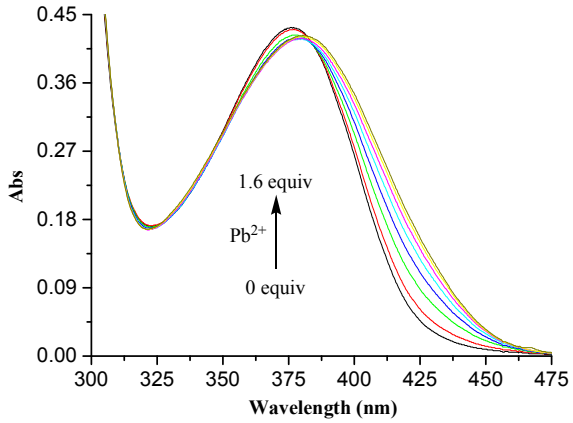


Fig. S7 Changes in the UV-vis spectrum of **2** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Pb^{2+} ions.

Table S1 The association constants of **1** and **2** with Zn^{2+}, Cd^{2+} and Pb^{2+} ions

Receptor	Cation	$\Delta\lambda$/nm	log*Ks*
1	Zn^{2+}	27	5.73
	Cd^{2+}	13	5.74
	Pb^{2+}	15	5.90
2	Zn^{2+}	9	5.09
	Cd^{2+}	6	5.24
	Pb^{2+}	5	5.67

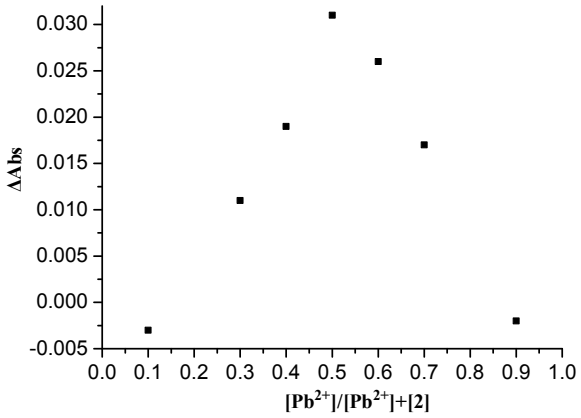


Fig. S8 The Job's plot of **2** with Pb^{2+}.

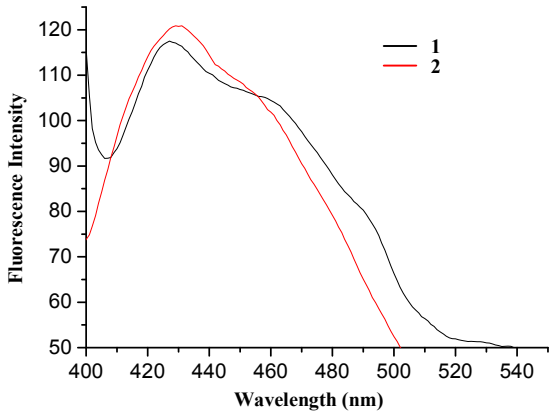


Fig. S9 The fluorescence spectra of receptors **1** and **2** excited at 375 nm in CH_2Cl_2/MeCN (1:1, v/v).

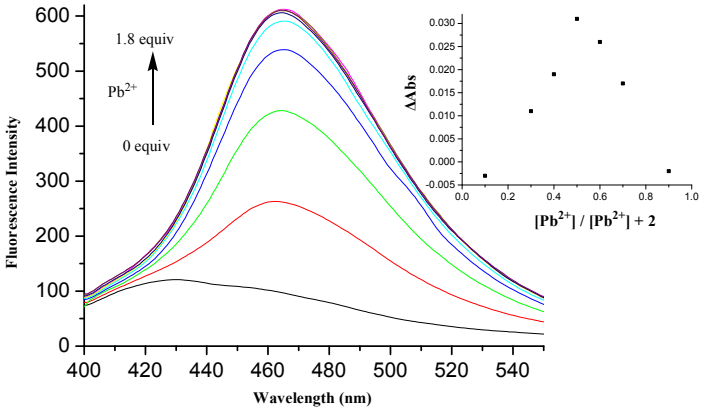


Fig. S10 Changes in the fluorescence emission spectrum of receptor **2** (5.0×10^{-5} M) in CH_2Cl_2/MeCN (1:1, v/v) upon addition of Pb^{2+} ions with an excitation at 375 nm. The inset shows the Job's plot of **2** with Pb^{2+}.

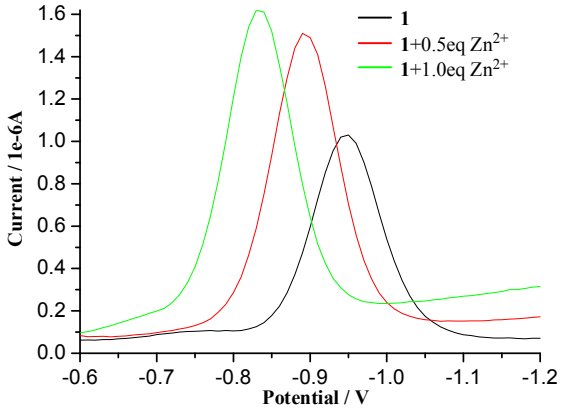


Fig. S11 Electrochemical response of receptor **1** upon addition of an increasing amount of Zn^{2+} ions (5.0×10^{-2} M).

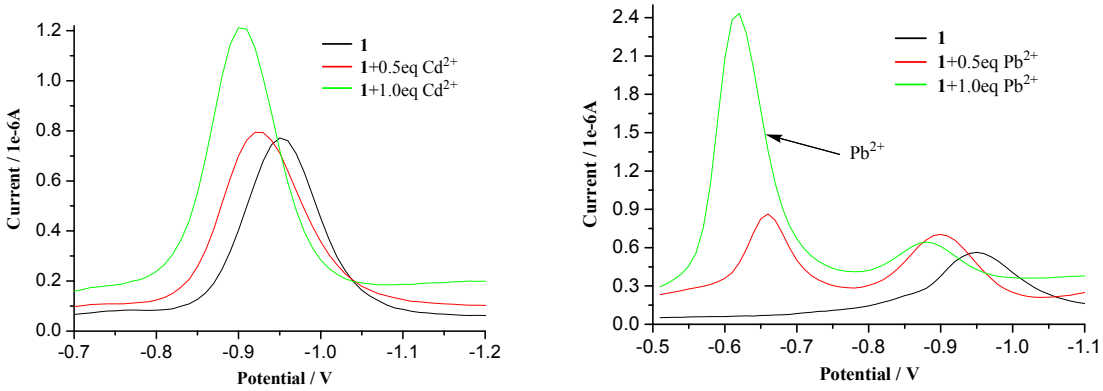


Fig. S12 Electrochemical response of receptor **1** upon addition of an increasing amount of Cd^{2+} and Pb^{2+} ions (5.0×10^{-2} M).

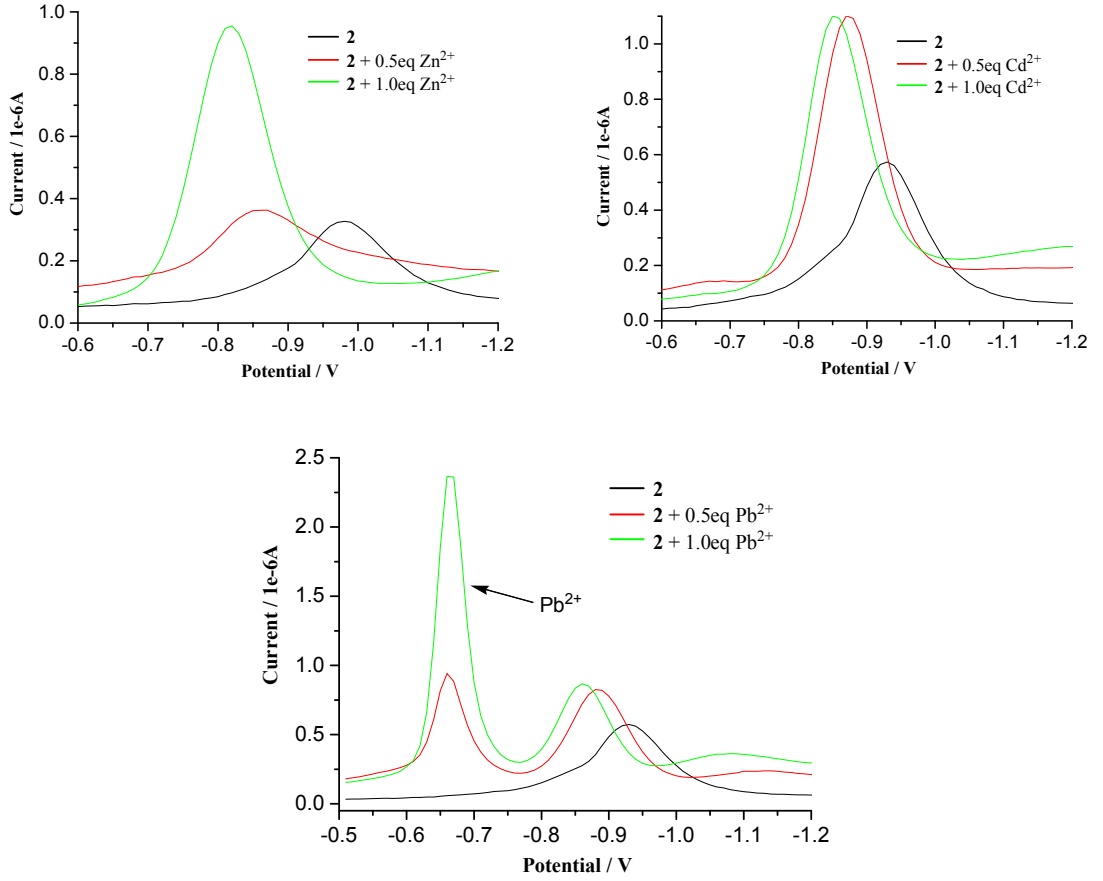


Fig. S13 Electrochemical response of receptor **2** upon addition of an increasing amount of Zn^{2+}, Cd^{2+} and Pb^{2+} ions (5.0×10^{-2} M).

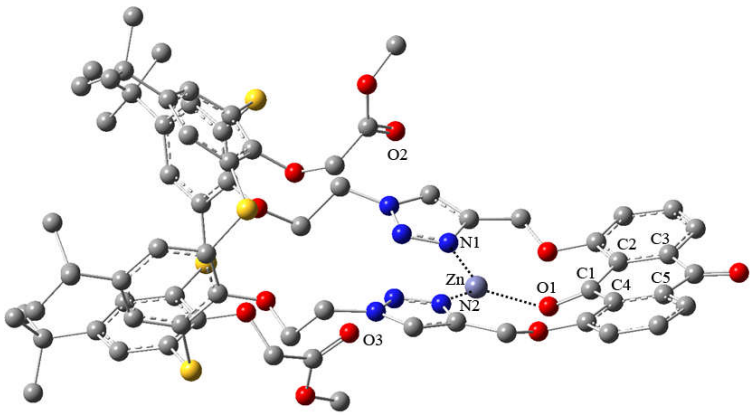


Fig. S14 An optimized structure (AM1/3-21G) of [**2**·Zn^{2+}].

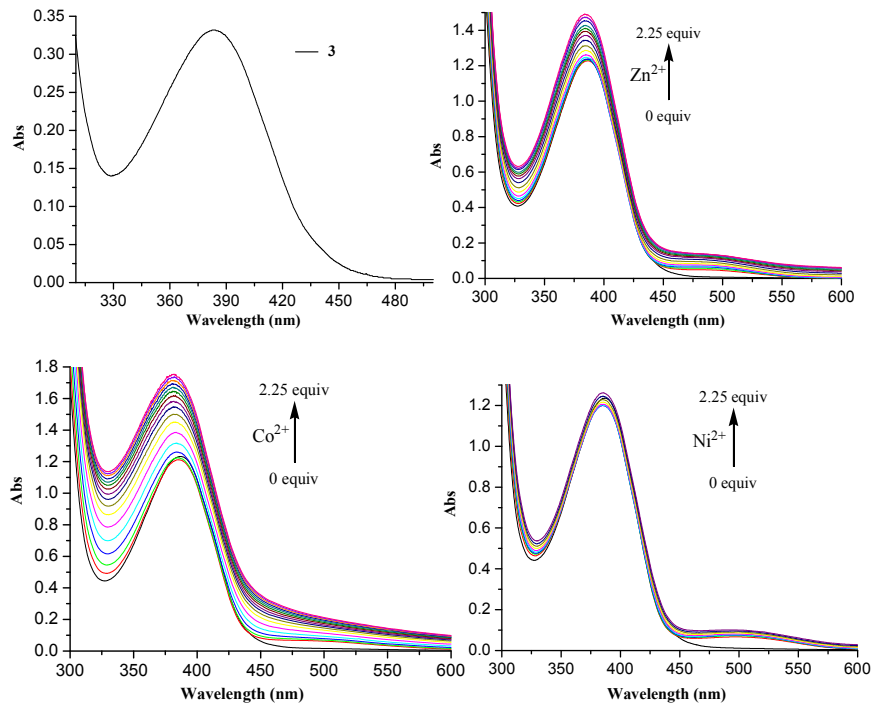


Fig. S15 UV-vis spectrum and its changes of **3** (5.0×10^{-5} M) in THF/H_2O (9:1, v/v) at pH 7.4 in HEPES upon addition of Zn^{2+}, Co^{2+} and Ni^{2+} ions (5.0×10^{-3} M).

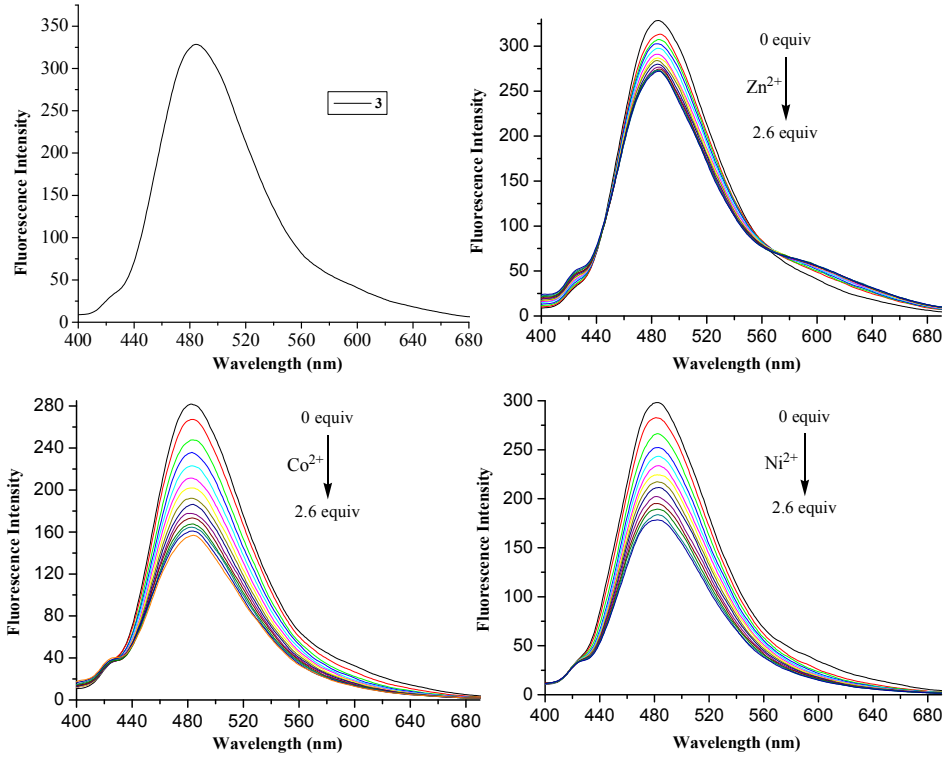
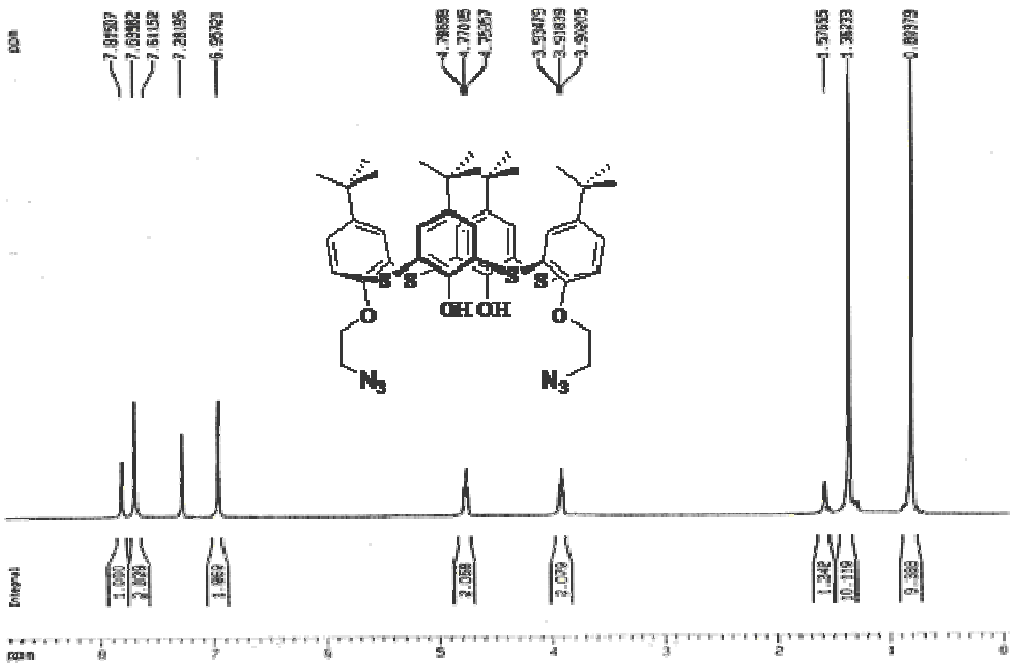
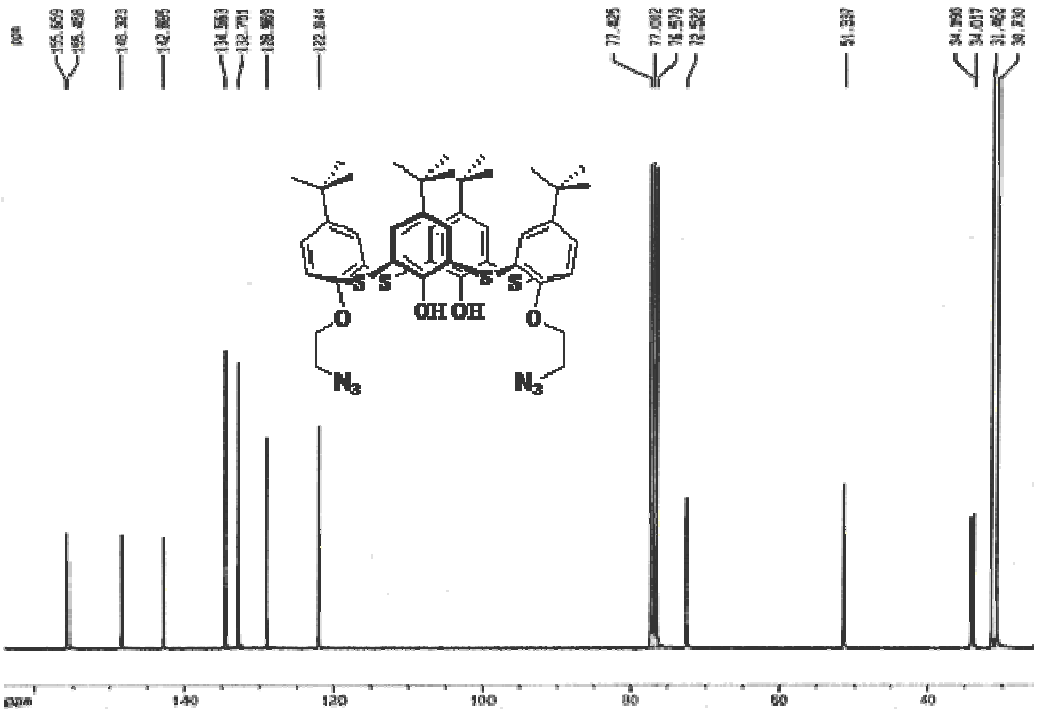


Fig. S16 Fluorescence emission spectrum and its changes of **3** (5.0×10^{-5} M) in THF/H_2O (9:1, v/v) at pH 7.4 in HEPES upon addition of Zn^{2+}, Co^{2+} and Ni^{2+} ions (5.0×10^{-3} M).

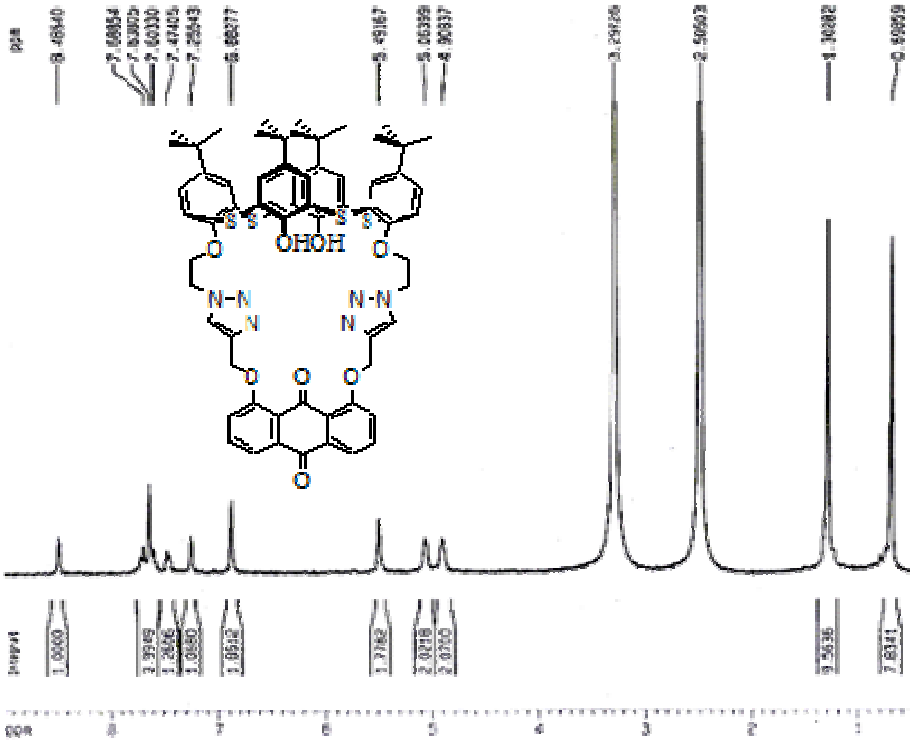
^{1}H NMR, ^{13}C NMR and ESI-MS spectra of I and 1-3:



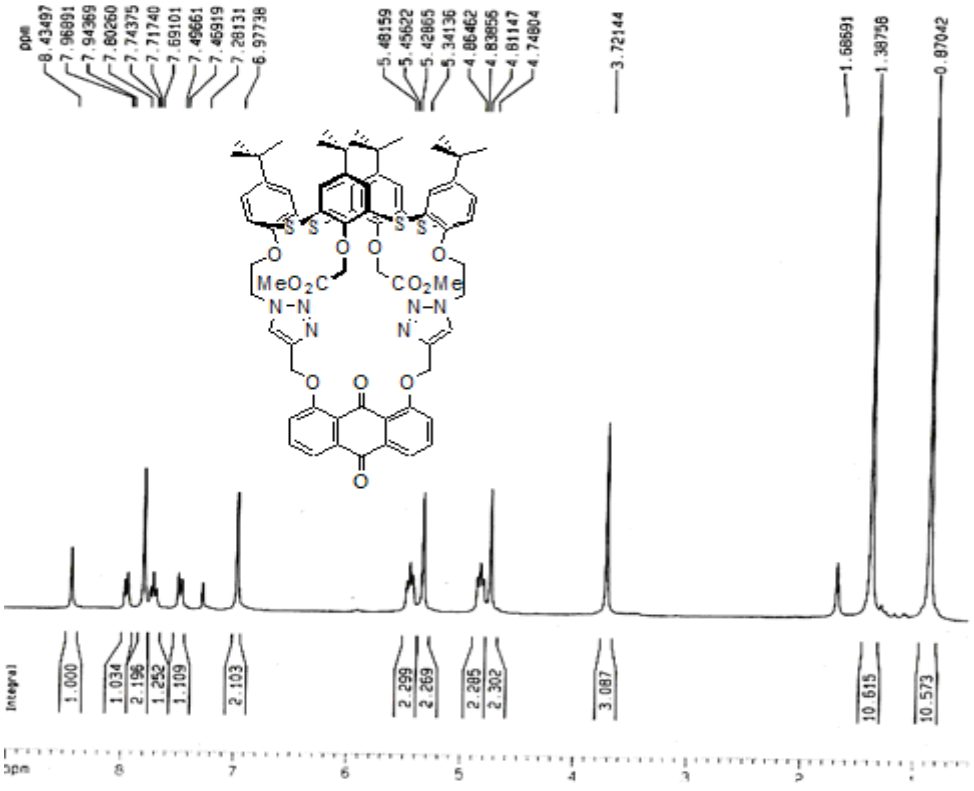
^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **I**



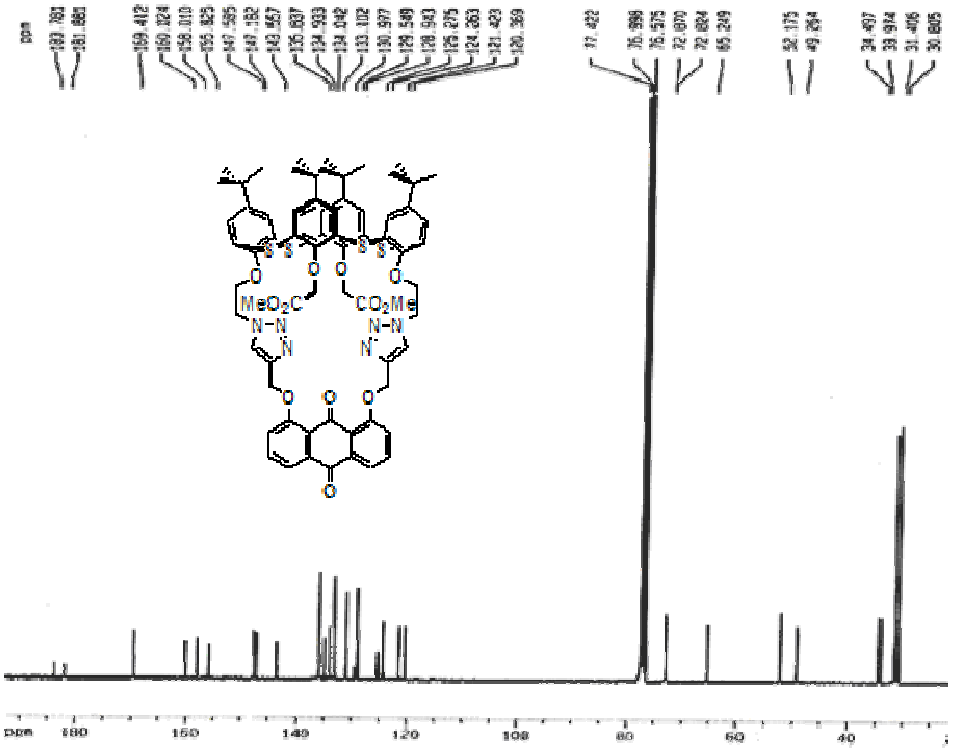
^{13}C NMR ($CDCl_3$, 75 MHz) spectrum of **I**



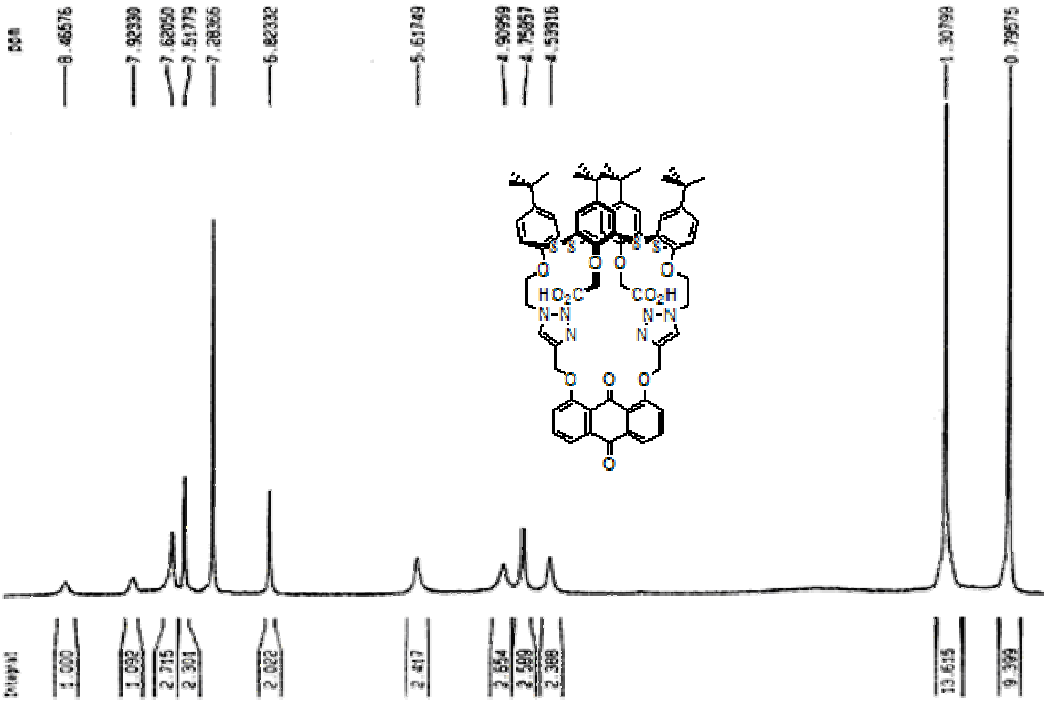
^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **1**



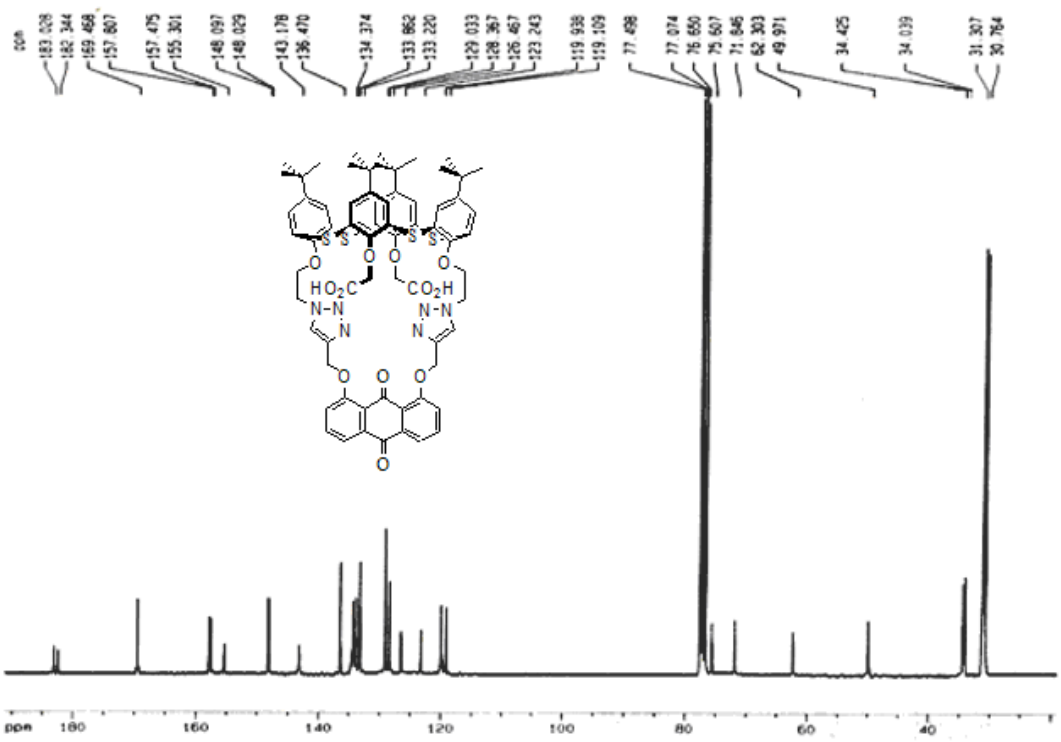
^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **2**



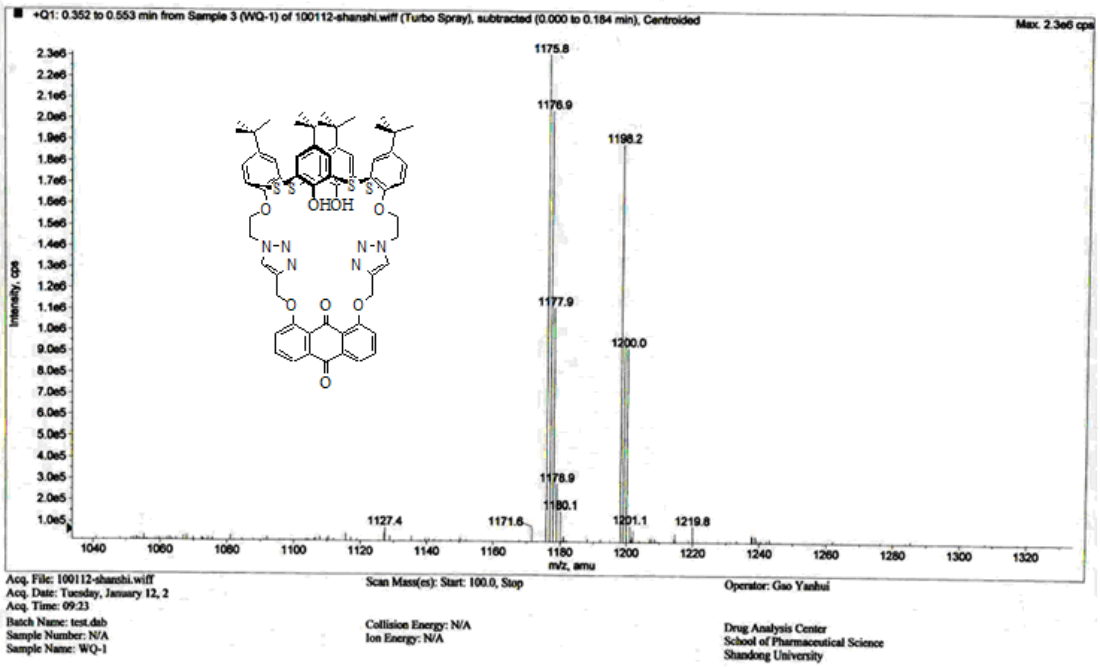
^{13}C NMR ($CDCl_3$, 75 MHz) spectrum of **2**



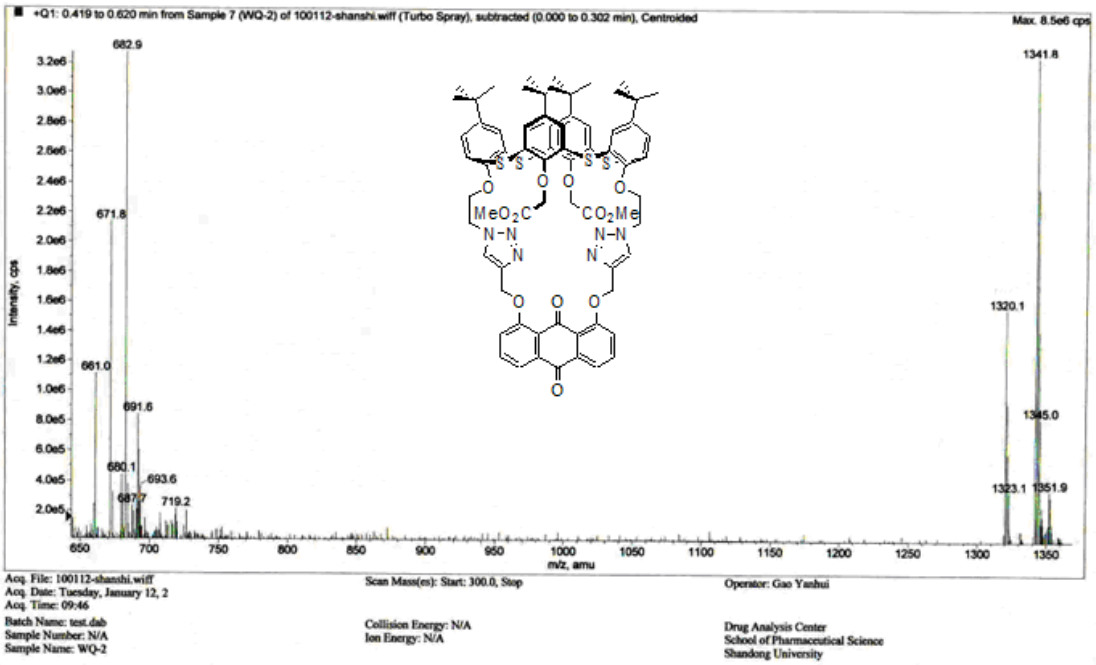
^{1}H NMR ($CDCl_3$, 300 MHz) spectrum of **3**



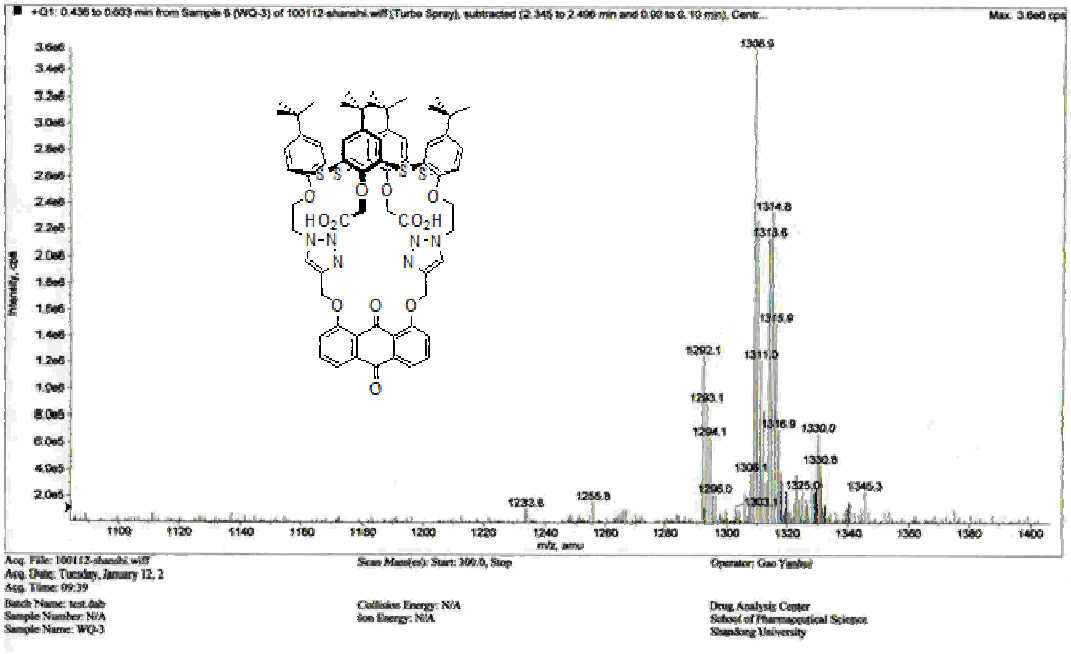
^{13}C NMR ($CDCl_3$, 75 MHz) spectrum of **3**



ESI-MS spectrum of **1**



ESI-MS spectrum of **2**



ESI-MS spectrum of **3**