

Thiacalix[4]crown based optical chemosensor for Fe³⁺, Li⁺ and cysteine: A Fe³⁺/Li⁺ ions synchronized allosteric regulations

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- S2 UV-vis spectra of **2** in the presence of different metal ions
- S3 Calculations for detection limit
- S4 Competitive fluorescence response of 2-Fe³⁺ complex
- S5 ¹H NMR Spectrum of **2**
- S6 ¹H NMR Spectrum of **2** (Expanded)
- S7 ¹³C NMR Spectrum of **2**
- S8 Mass Spectrum of **2**

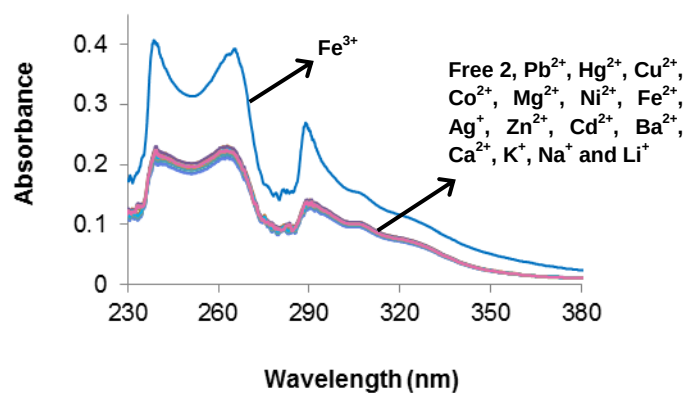


Figure S1. UV-vis spectra of **2** (1.0 μM) in the presence of various metal ions (16 equiv each) in THF:H₂O; (9:1, v/v) buffered with HEPES, pH = 7.0.

Calculations for detection limit:

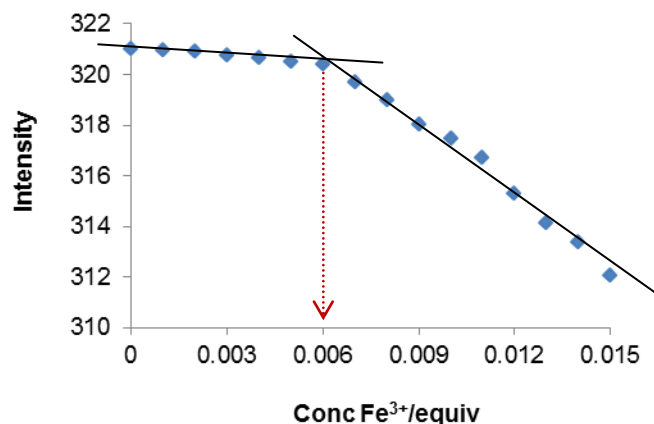


Figure S2. Figure showing the fluorescence intensity at 356 nm as a function of Fe³⁺ ions concentration.

To determine the detection limit, fluorescence titration of compound **2** with ferric ions was carried out by adding aliquots of ferric solution of minimum concentration and the fluorescence intensity as a function of Fe³⁺ ions added was then plotted. From this graph the equivalents used at which there was a sharp change in the fluorescence intensity multiplied with the concentration of receptor **2** gave the detection limit.

Equation used for calculating detection limit (DL):

$$DL = C_L \times E_T$$

C_L = Conc. of Ligand; E_T = Equiv. of Titrant at which change observed.

Thus;

$$DL = 5 \times 10^{-6} \times 0.006 = 0.03 \times 10^{-6} = 3 \times 10^{-8}$$

or

$$= 30 \times 10^{-9} = 30 \text{ nanomolar}$$

Similar procedure was utilized for calculating the detection limits of Li⁺ and cysteine.

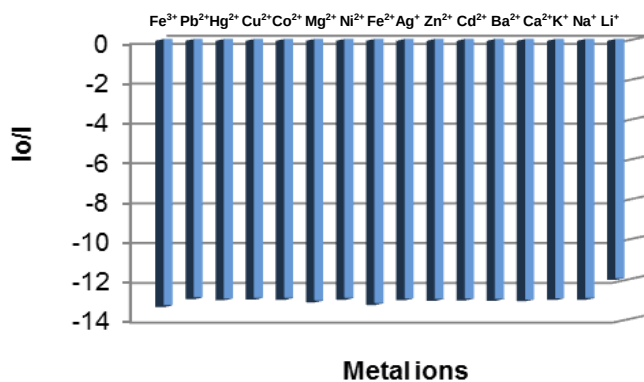
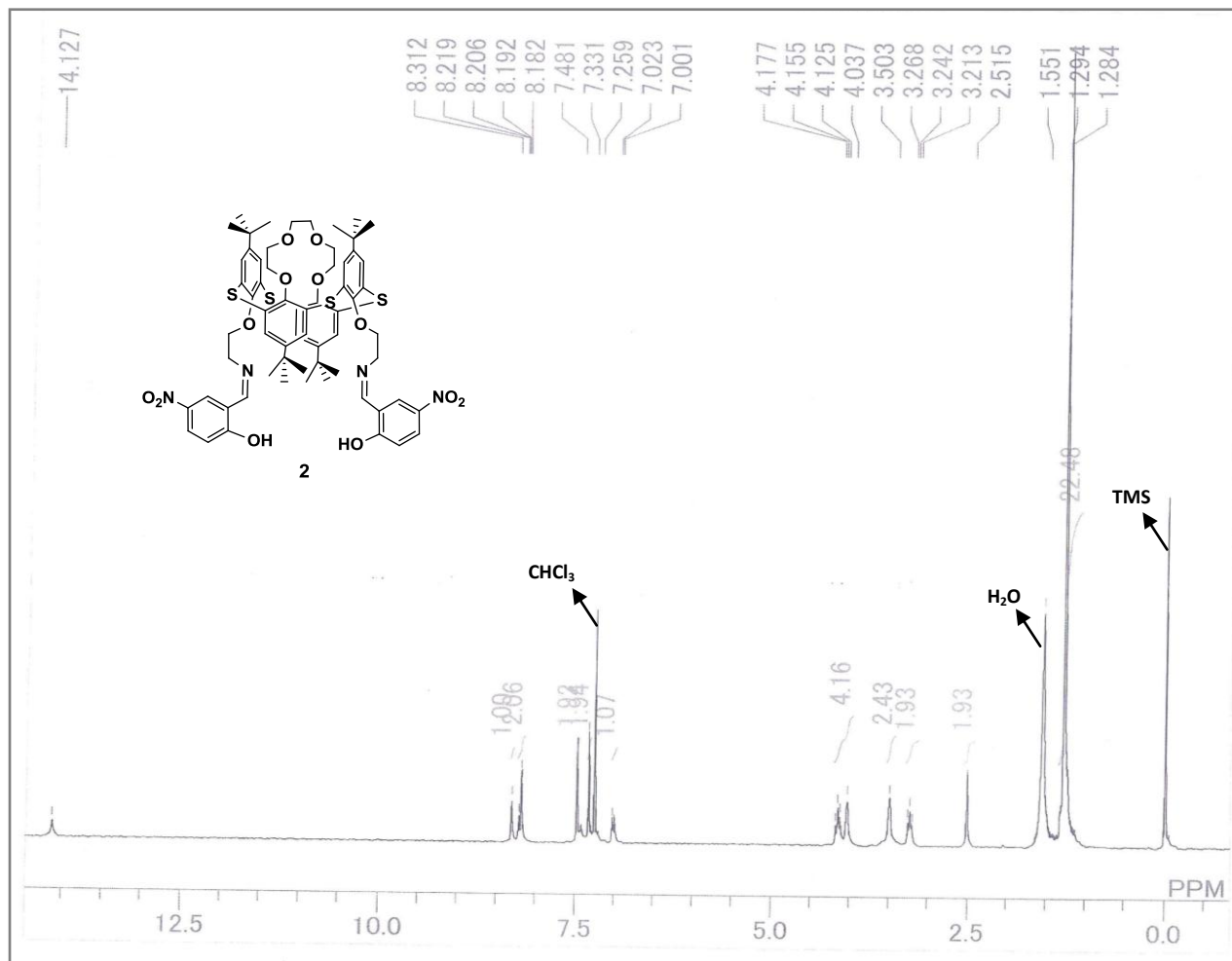
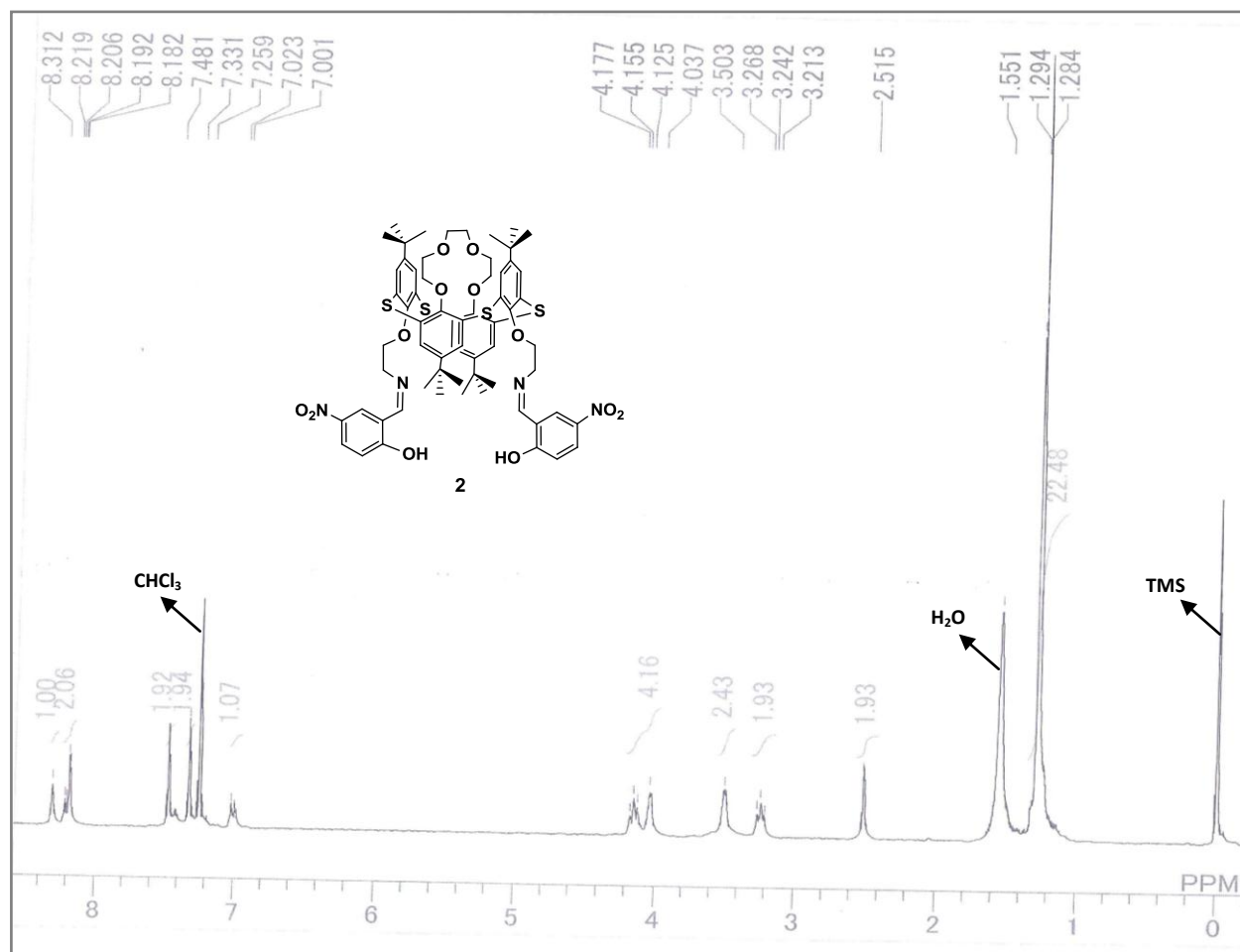


Figure S3. Fluorescence response of **2** (5.0 μM) with Fe^{3+} ions (20 equiv) in $\text{THF}:\text{H}_2\text{O}$; (9:1, v/v) buffered with HEPES, pH = 7.0; λ_{ex} = 300 nm in the presence of other metal ions (20 equiv each). Bars represent selectivity (I_0/I); I_0 and I denote the fluorescence intensity at 356 nm before and after the addition of metal ions, respectively.

^1H NMR spectrum of **2** (Full Scale)



^1H NMR spectrum of **2**



Mass spectrum of **2**.

