

Supporting Information

Ratiometric Detection of Hg²⁺ ions: An Allosterically Synchronized Hg²⁺/Li⁺ Switch Based on Thiacalix[4]crown

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- 2 Fluorescence spectra of **4** in the presence of different metal ions.
- 3 UV-vis spectra of **4** in the presence of different metal ions.
- 4 ¹H NMR Spectrum of **2**.
- 5 ¹³C NMR Spectrum of **2**.
- 6 Mass Spectrum of **2**.
- 7 ¹H NMR Spectrum of **3**.
- 8 ¹³C NMR Spectrum of **3**.
- 9 Mass Spectrum of **3**.
- 10 ¹H NMR Spectrum of **4**.
- 11 ¹³C NMR Spectrum of **4**.
- 12 Mass Spectrum of **4**.
- 13 IR Spectrum of **4**.
- 14 ¹H NMR spectra of **4** in CDCl₃/CD₃CN (8:2). (A) Free ligand (B) in presence of 1.0 equiv of mercury perchlorate; (C) in presence of 1.0 equiv of lithium perchlorate.

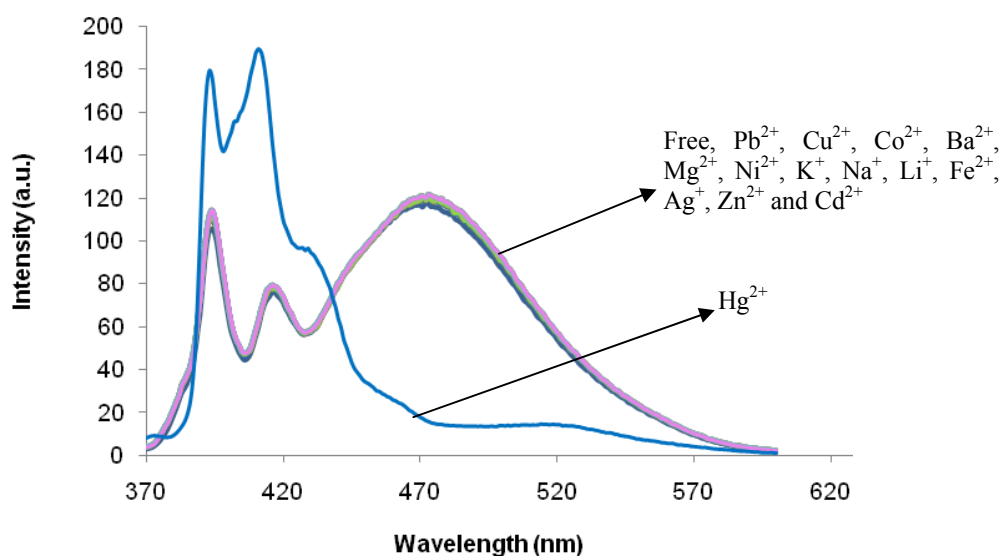


Figure S1. Fluorescence spectra of **1** (1 μM) in response to the presence of different metal ions (10 equiv. each) in THF, $\lambda_{\text{ex}} = 343$ nm.

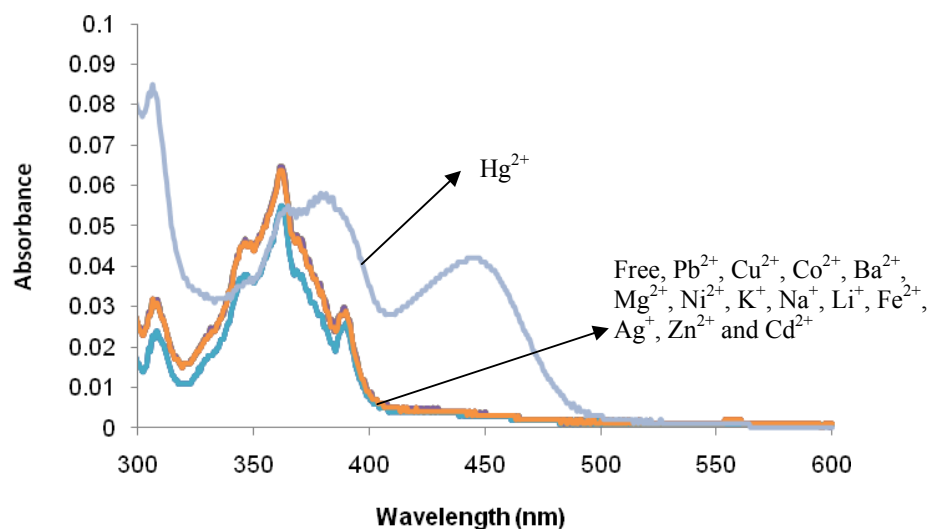
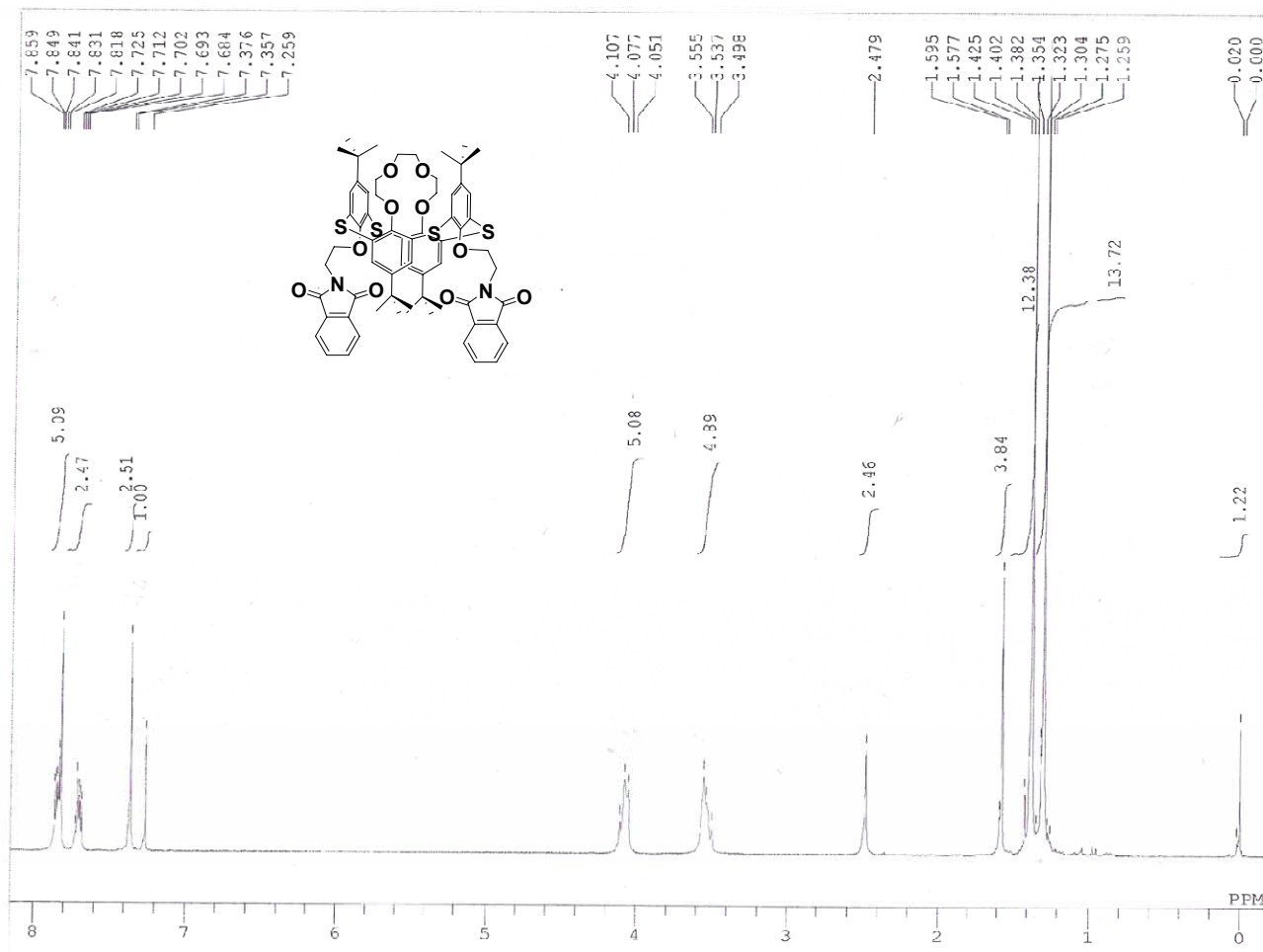
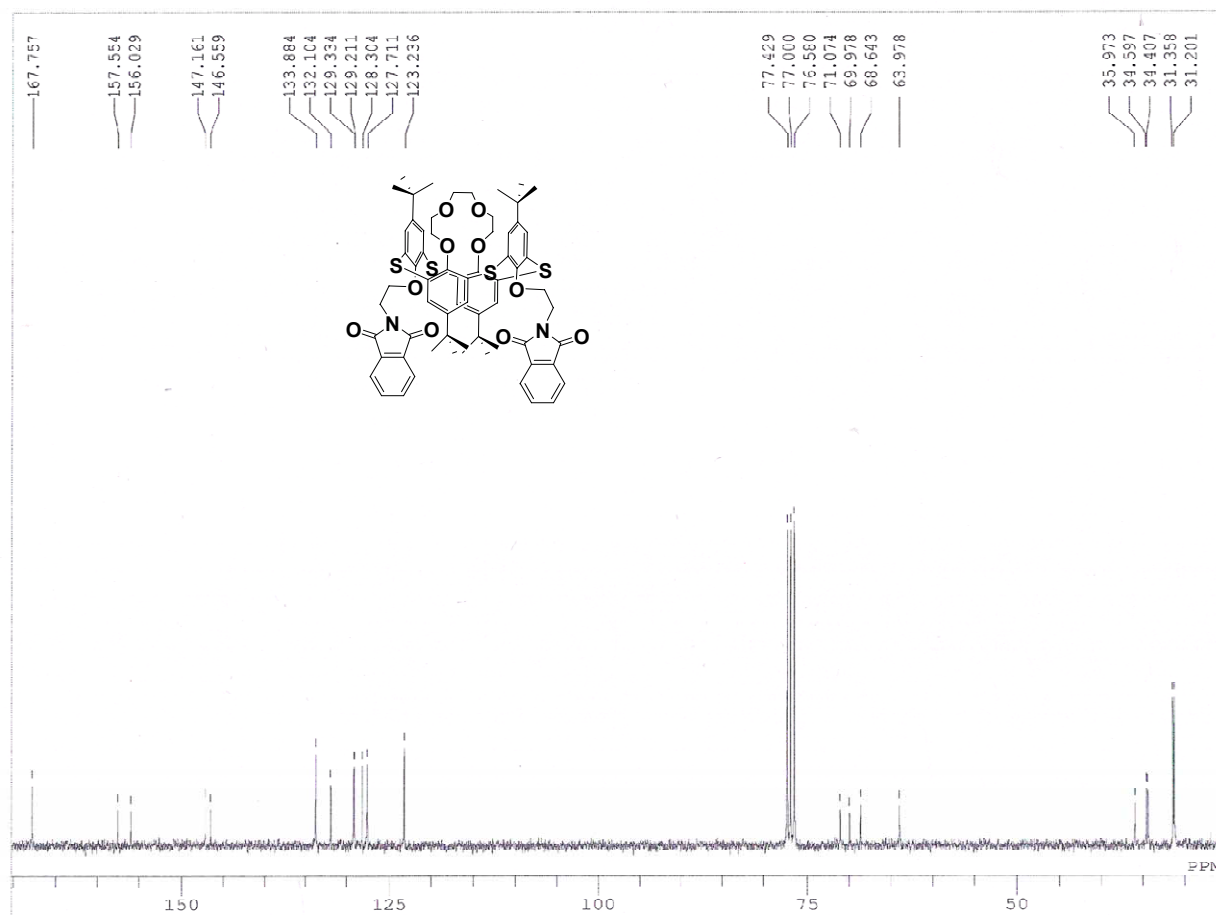


Figure S2. UV-vis spectra of **4** (1 μM) in response to the presence of different metal ions (30 equiv each) in THF.

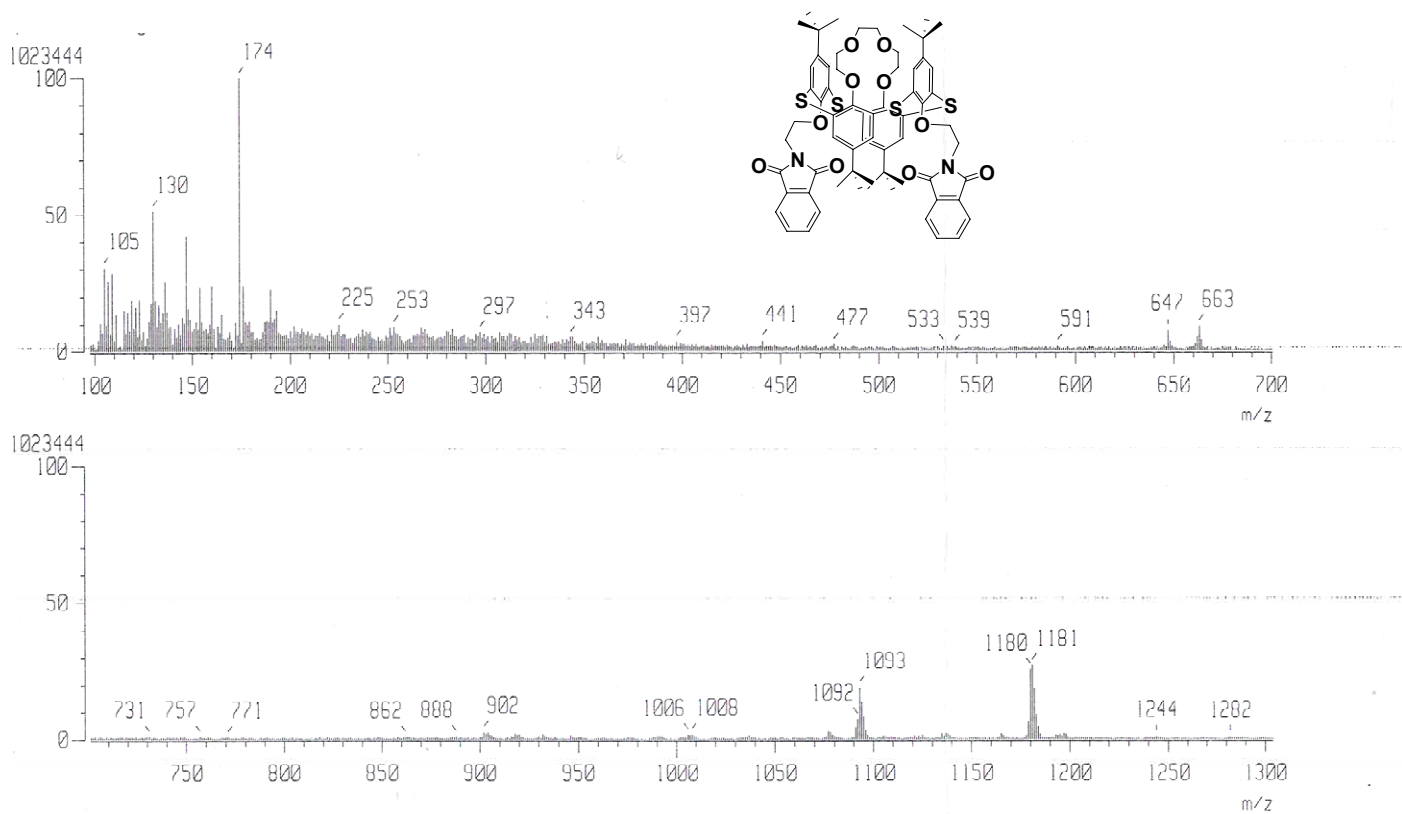
^1H NMR spectrum of compound **2**



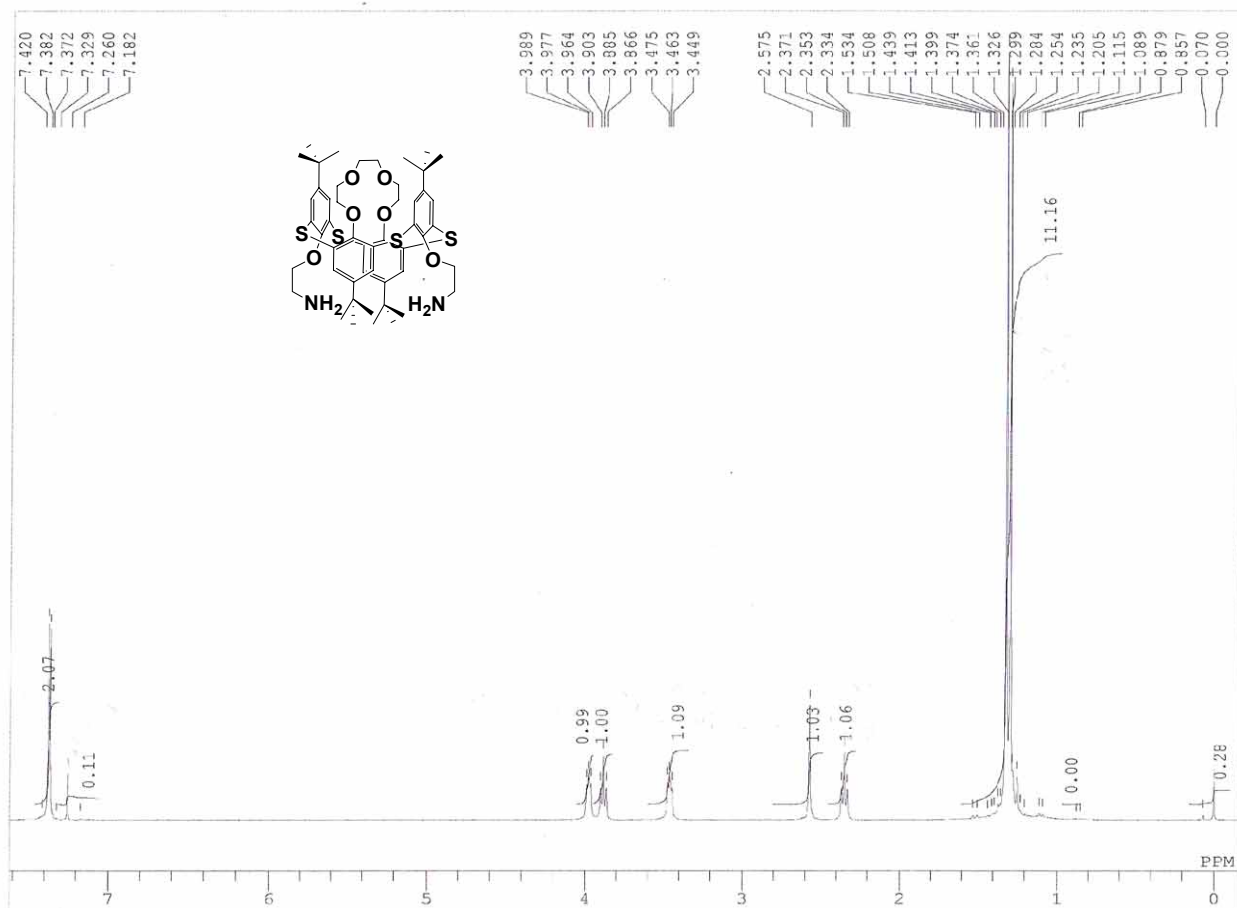
^{13}C NMR spectrum of compound **2**



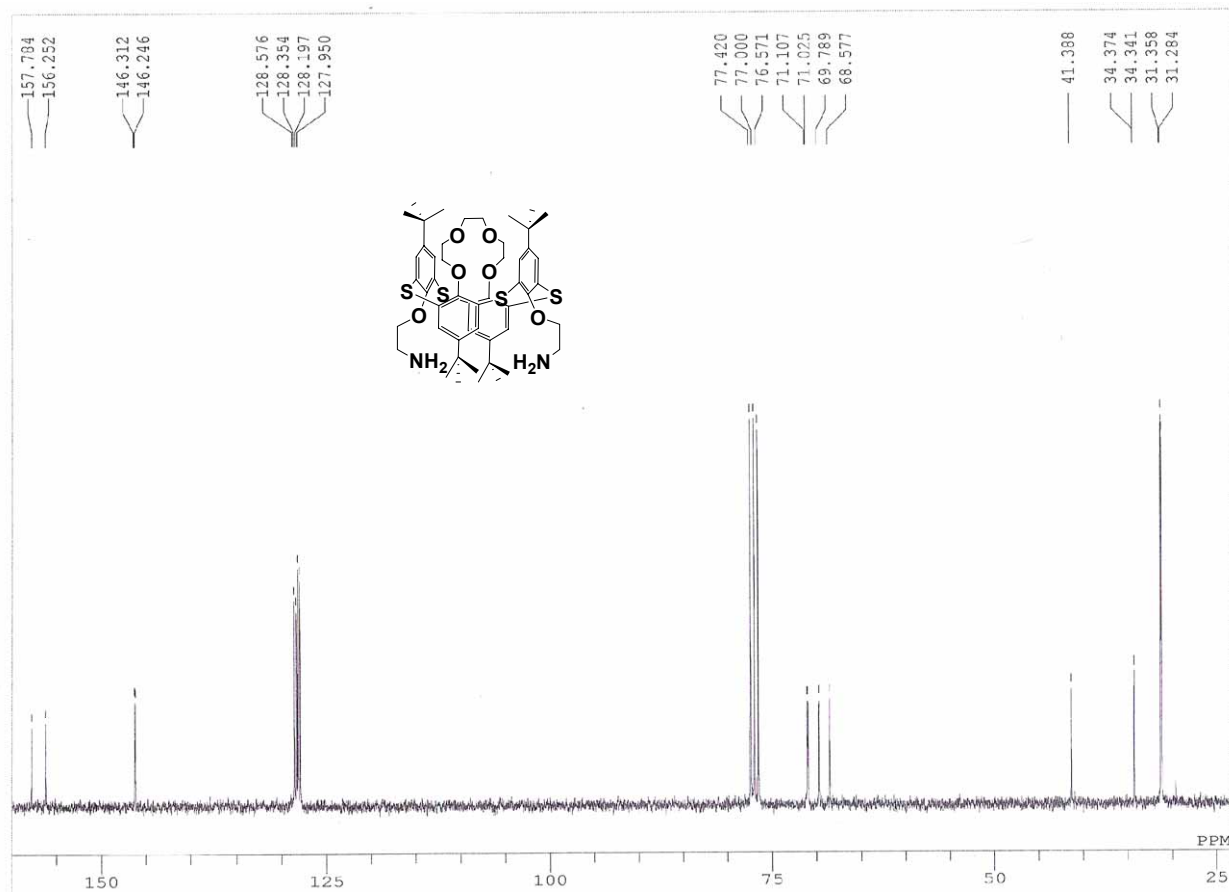
Mass spectrum of compound 2



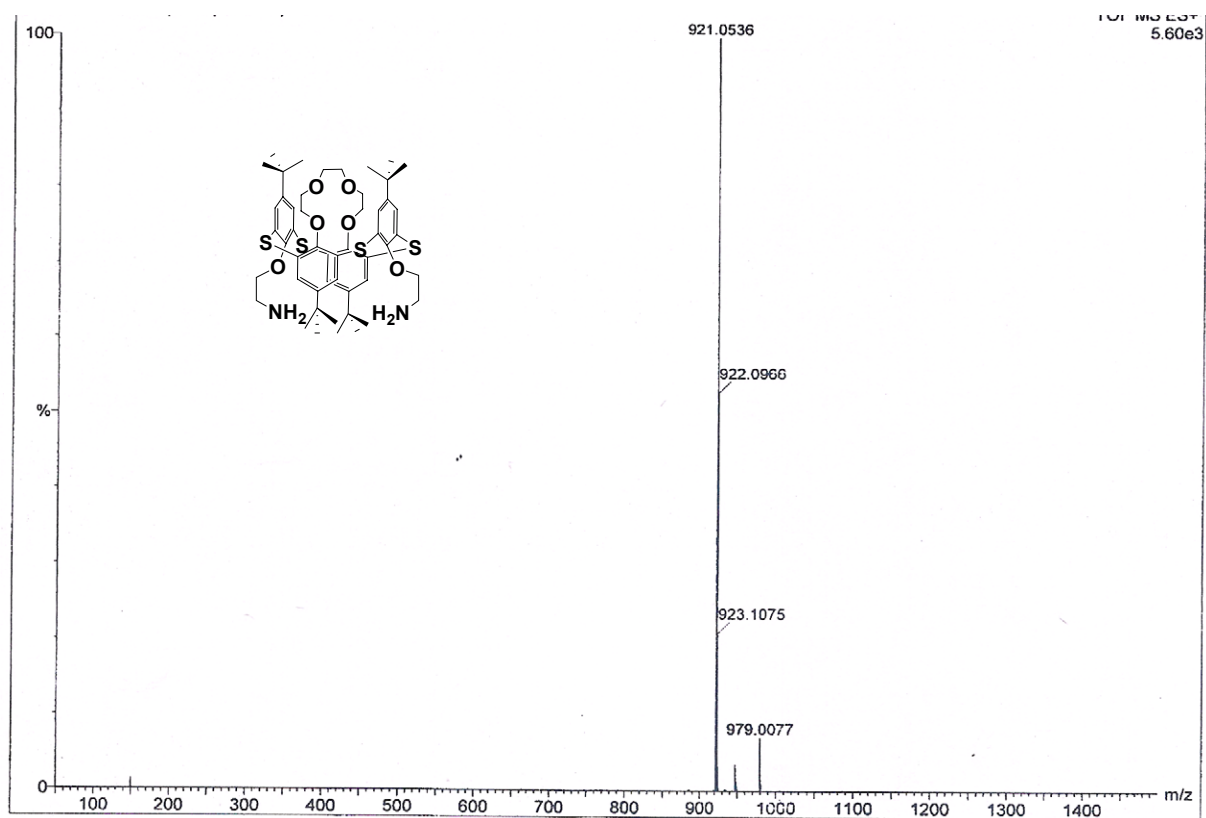
^1H NMR spectrum of compound **3**



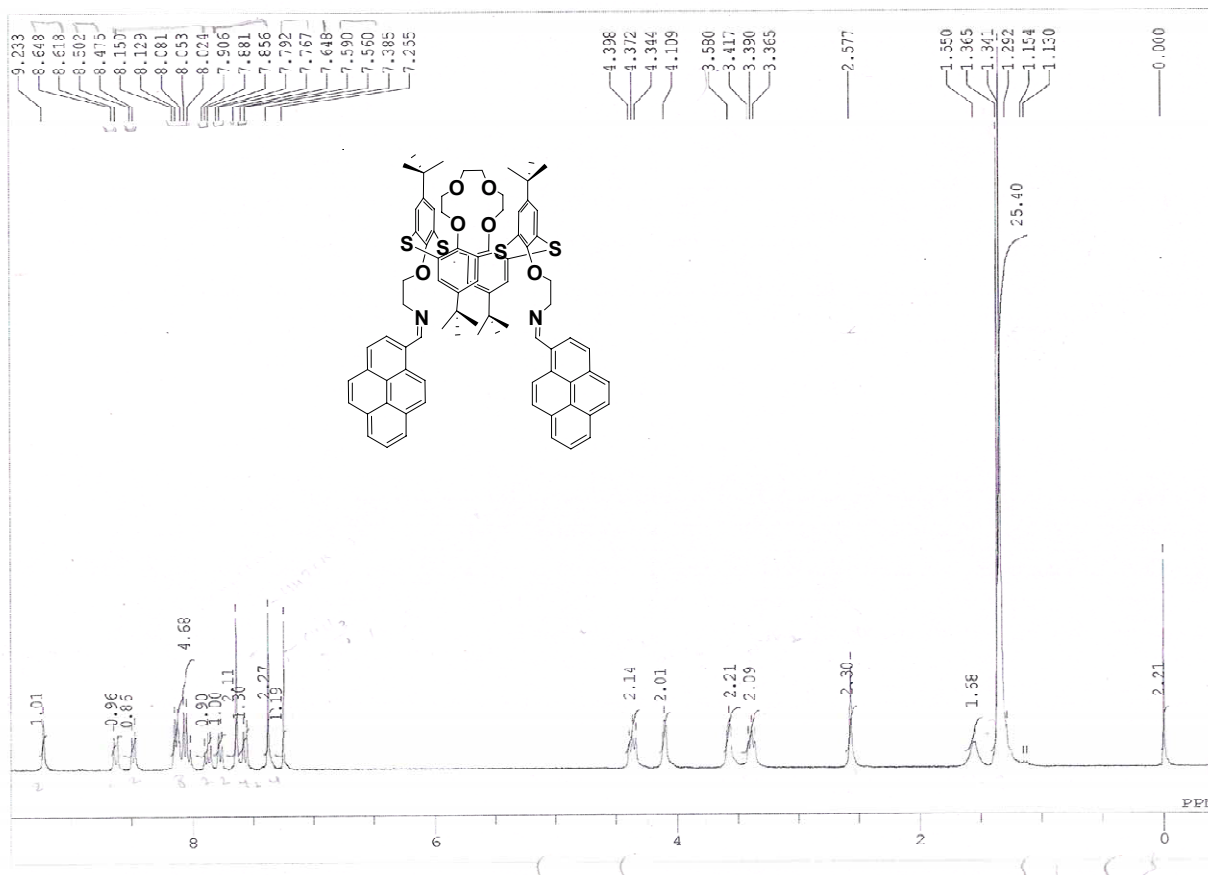
^{13}C NMR spectrum of compound **3**



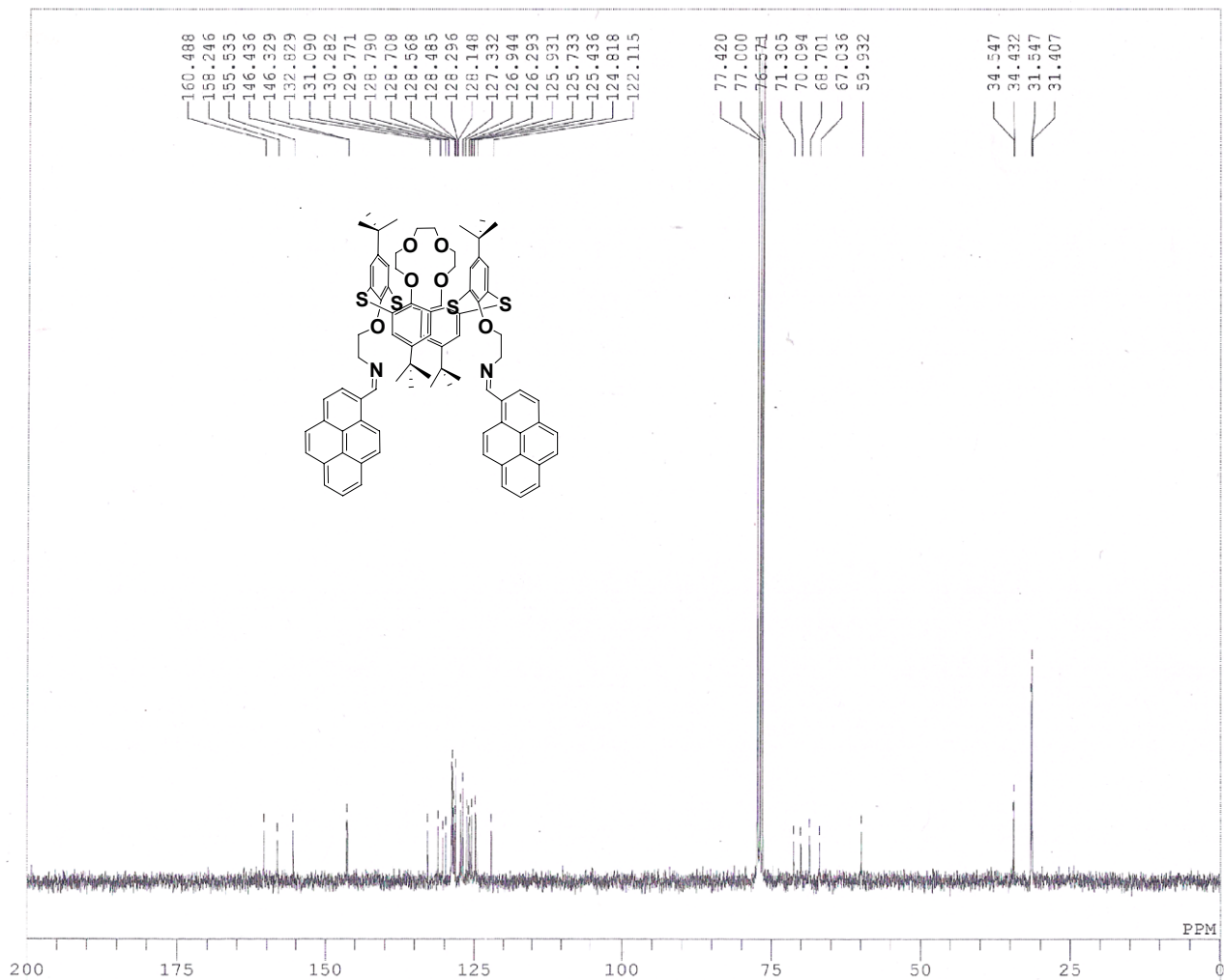
Mass spectrum of compound 3



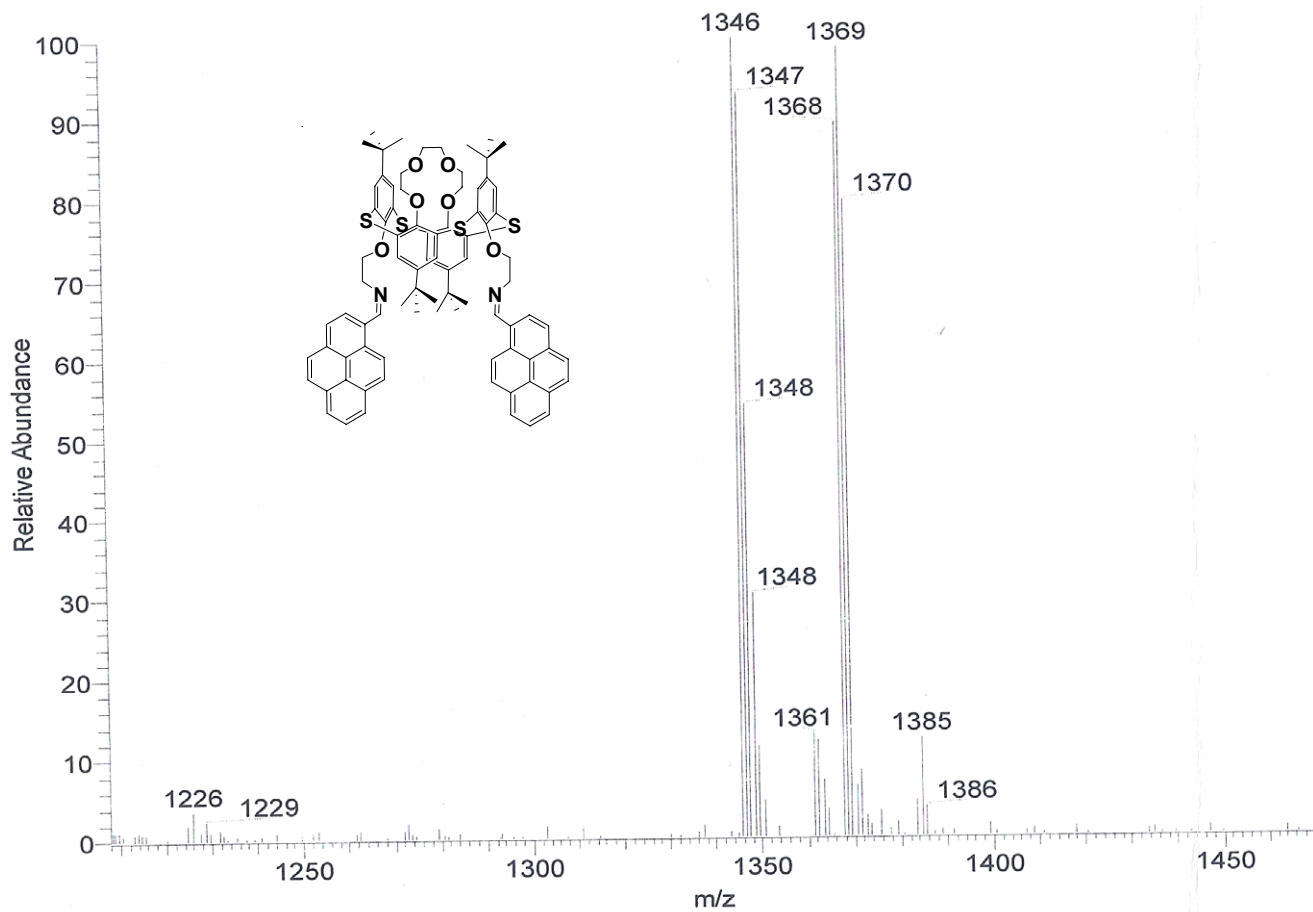
^1H NMR spectrum of compound 4



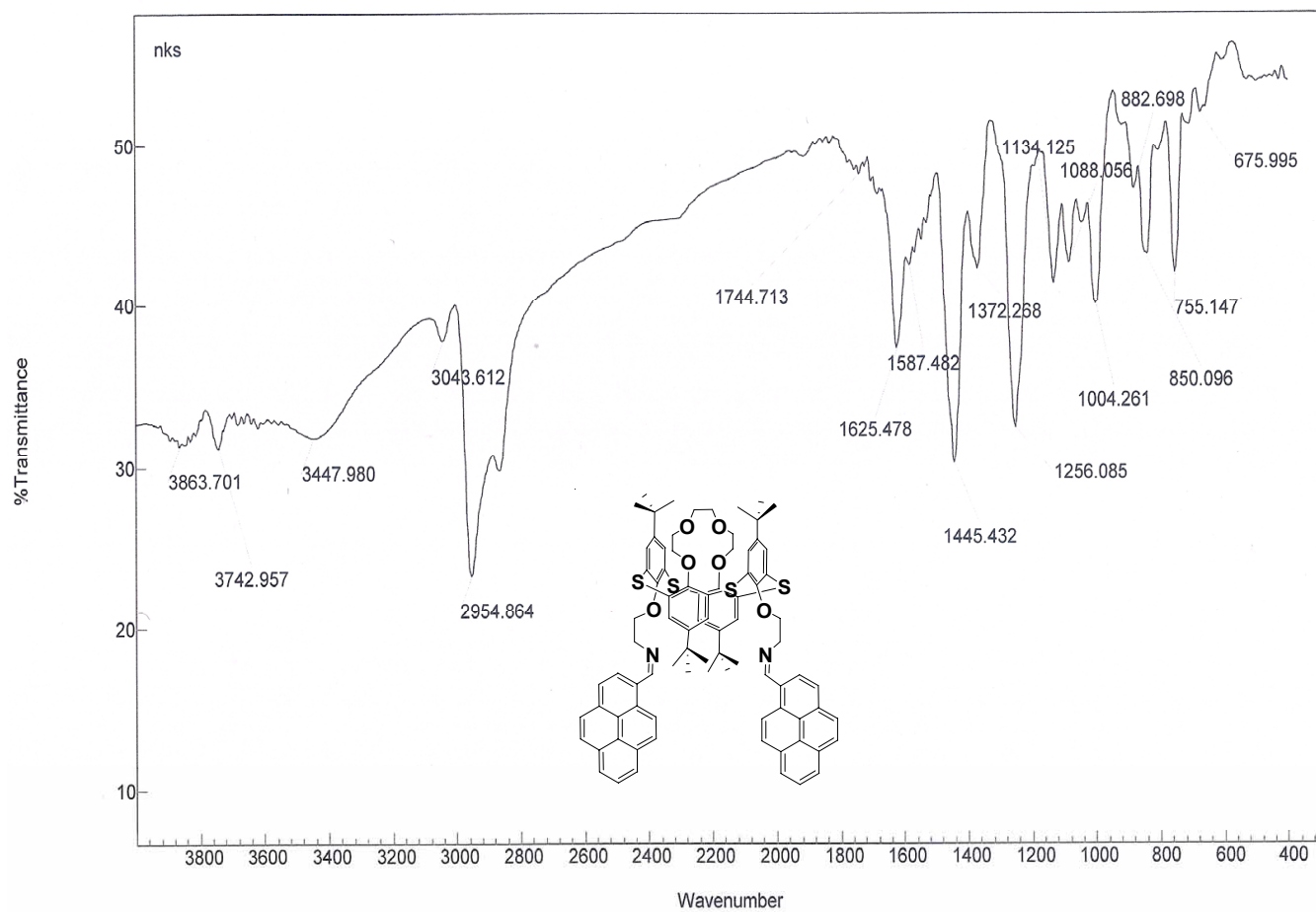
^{13}C NMR spectrum of compound 4

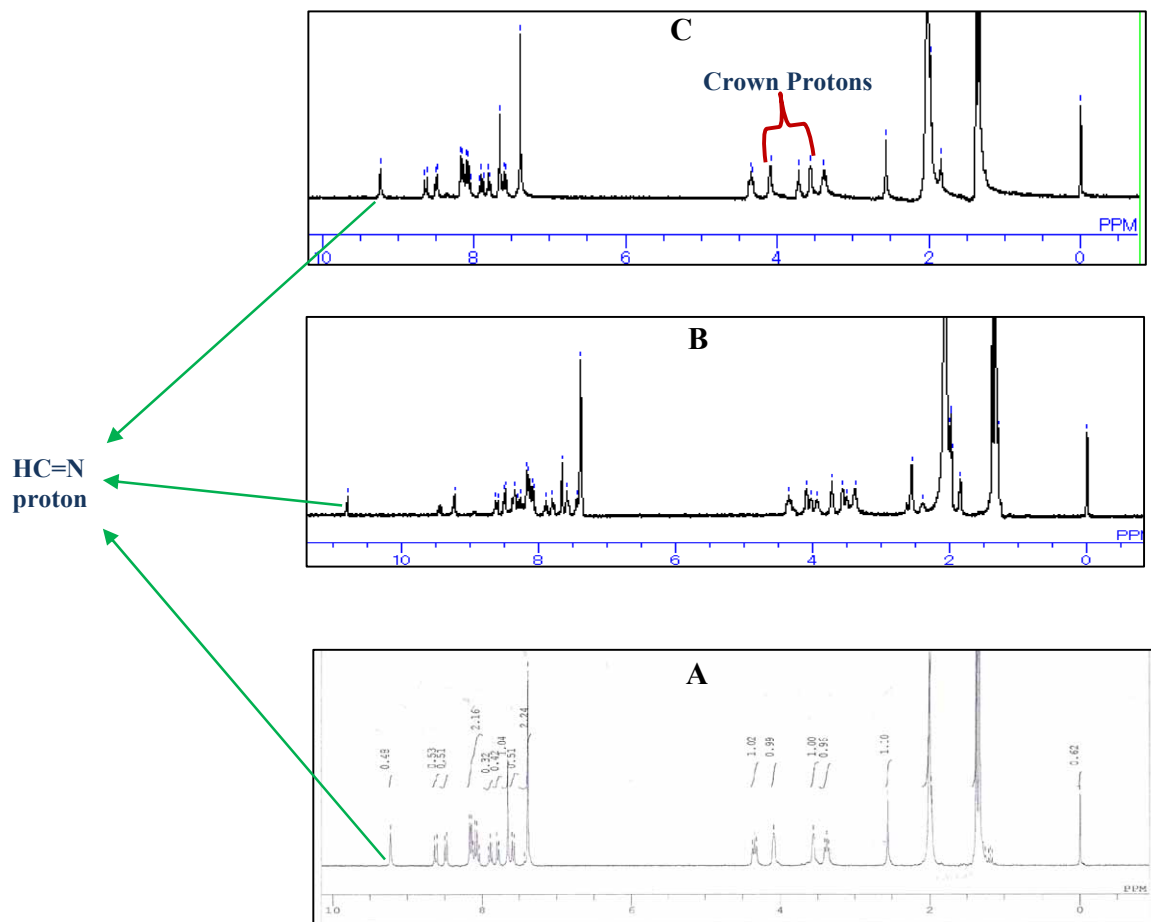


Mass spectrum of compound 4



IR Spectrum of compound 4





^1H NMR spectra of **4** in $\text{CDCl}_3/\text{CD}_3\text{CN}$ (8:2). (A) Free ligand (B) in presence of 1.0 equiv of mercury perchlorate; (C) in presence of 1.0 equiv of lithium perchlorate.