

Electronic Supporting Information

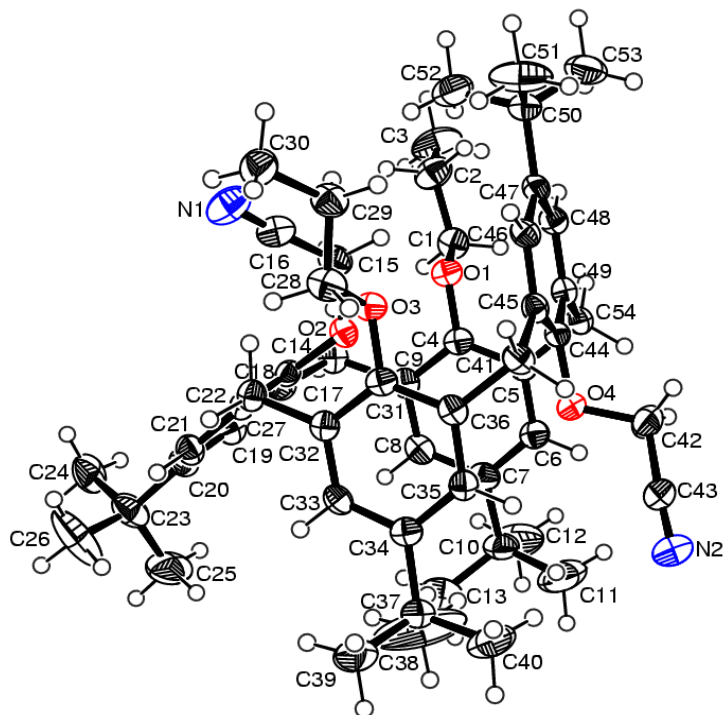
A Ni²⁺ Selective Chemosensor Based on *Partial Cone* Conformation of Calix[4]arene

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- S3** ORTEP diagram of **3**.
- S4** Job's Plot of **5** with Ni²⁺ ions.
- S5** ¹H NMR Spectrum of **2**.
- S6** ¹³C NMR Spectrum of **2**.
- S7** ¹H NMR Spectrum showing mixture of **2** and **3**.
- S8** ¹H NMR Spectrum of **3**.
- S9** Expanded ¹H NMR Spectrum of **3**.
- S10** Mass Spectrum of **3**.
- S11** ¹³C NMR Spectrum of **3**.
- S12** ¹H NMR Spectrum of **4**.
- S13** Expanded ¹H NMR Spectrum of **4**.
- S14** Mass Spectrum of **4**.
- S15** ¹³C NMR Spectrum of **4**.
- S16** ¹H NMR Spectrum of **5**.
- S17** Expanded ¹H NMR Spectrum of **5**.

- S18** Mass Spectrum of **5**.
- S19** ^{13}C NMR Spectrum of **5**.
- S20** ^1H NMR Spectrum of **5** in $\text{CDCl}_3:\text{CD}_3\text{CN}$ (8:2).
- S21** ^1H NMR Spectrum of **5** in $\text{CDCl}_3:\text{CD}_3\text{CN}$ + 2 equiv. Ni^{2+} (8:2).



ORTEP diagram of 3

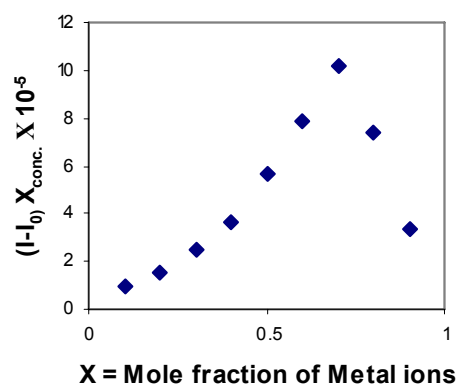
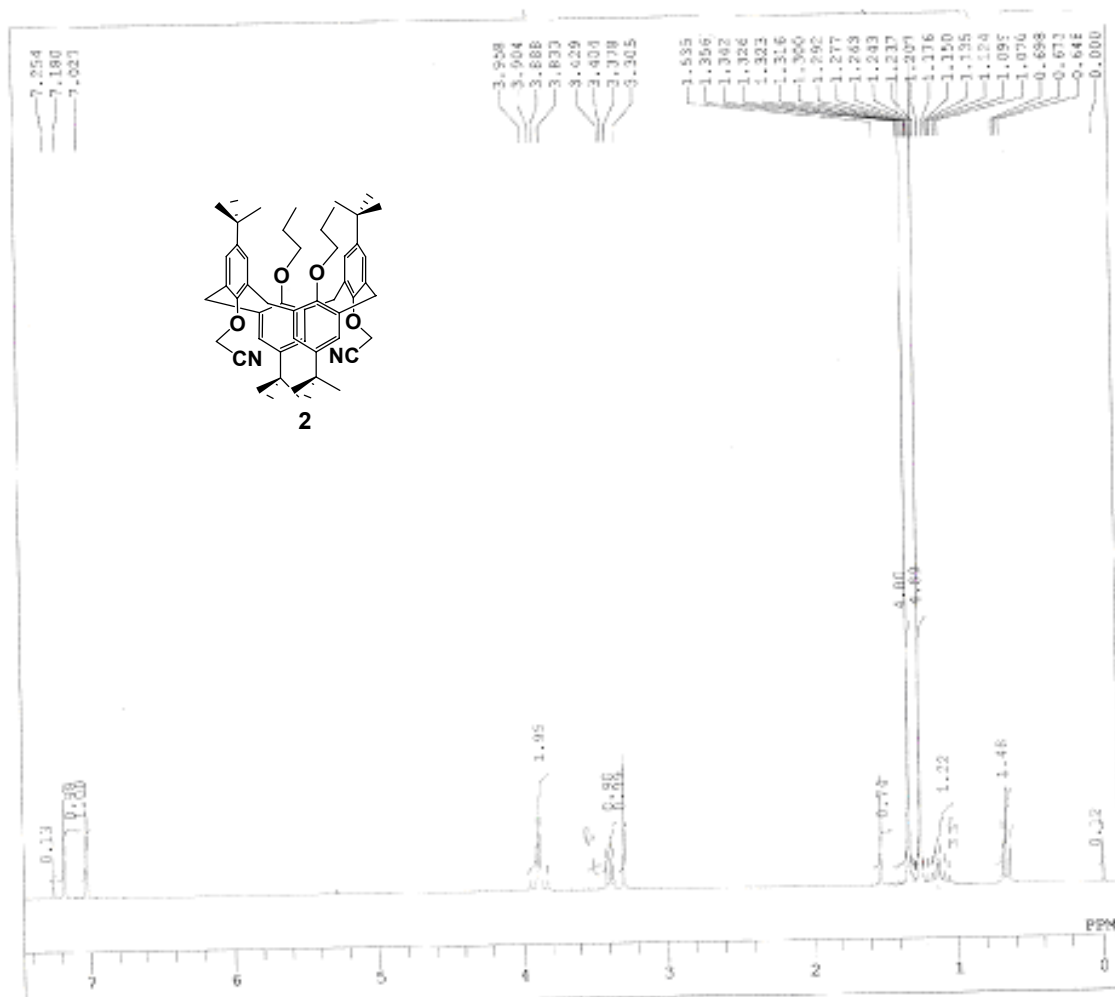


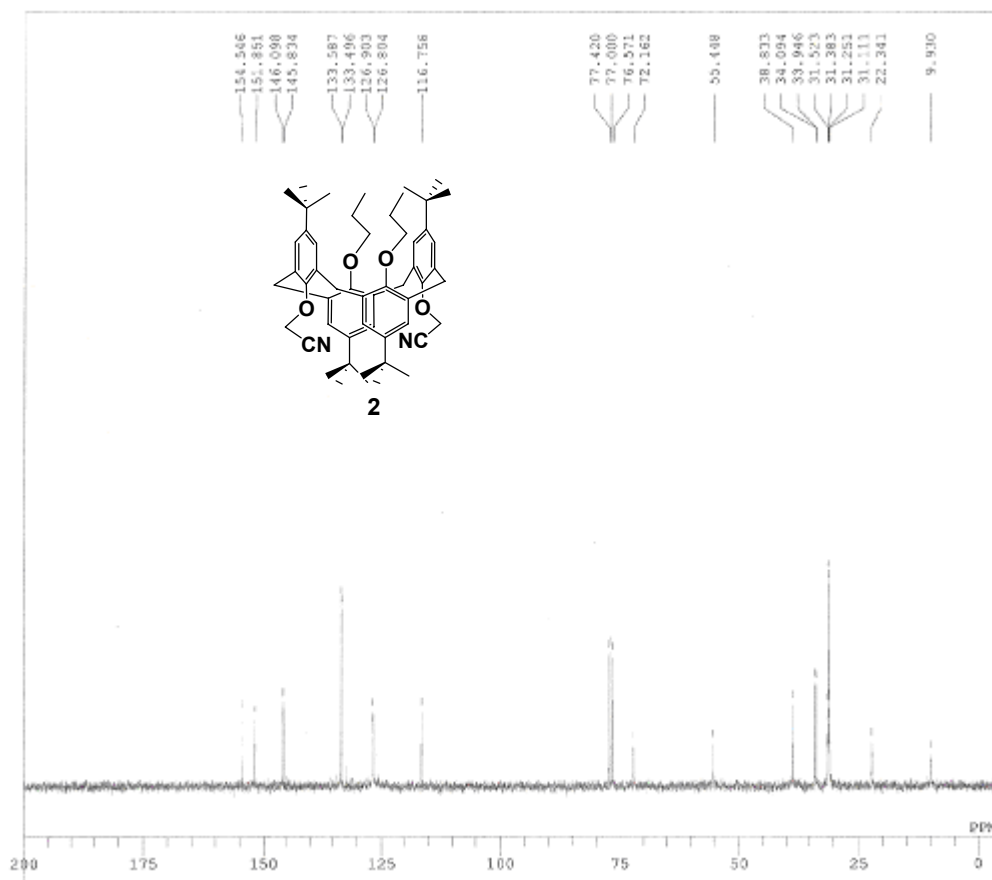
Figure S1. Job's plot with Ni^{2+} representing stoichiometry 1:2 (host: guest)

Warning! Metal pechlorates are potentially explosive and hence should be handled with care. However, we used very small quantities of these metal perchlorates and did not observe any explosion.

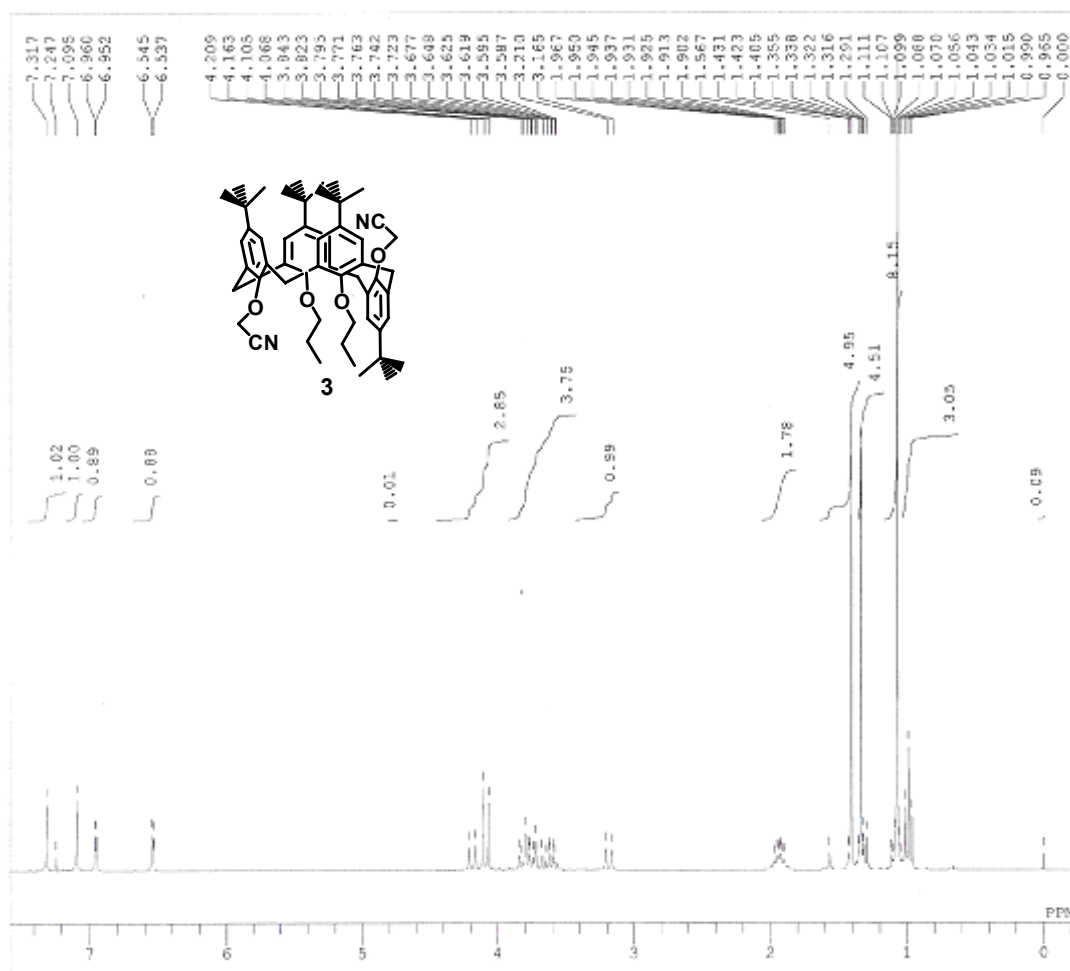
¹H NMR SPECTRUM OF 2

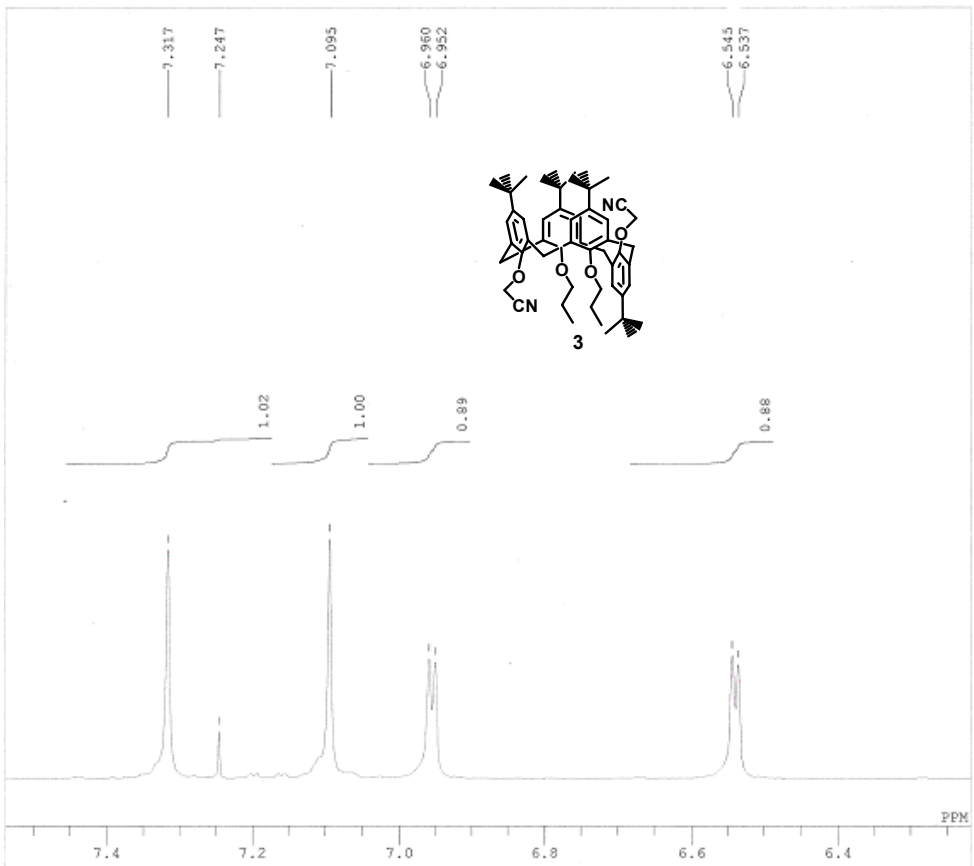


¹³C NMR SPECTRUM OF 2

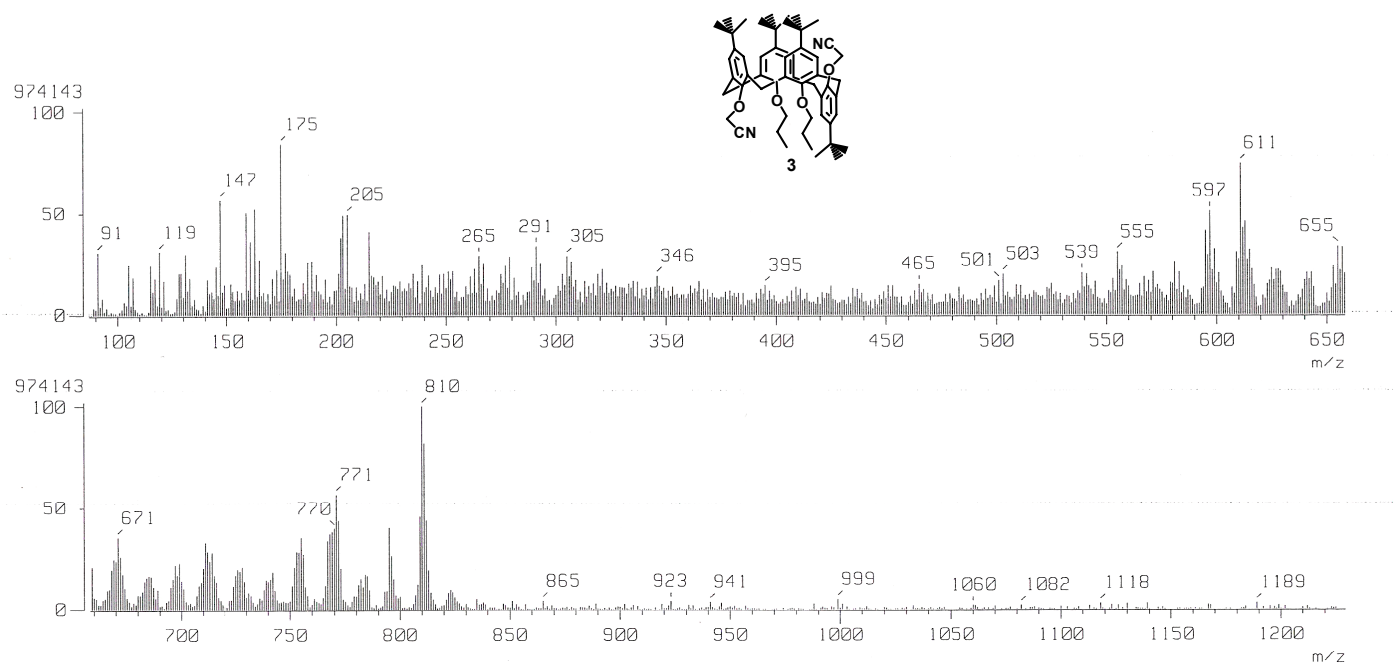


¹H NMR SPECTRUM OF 3

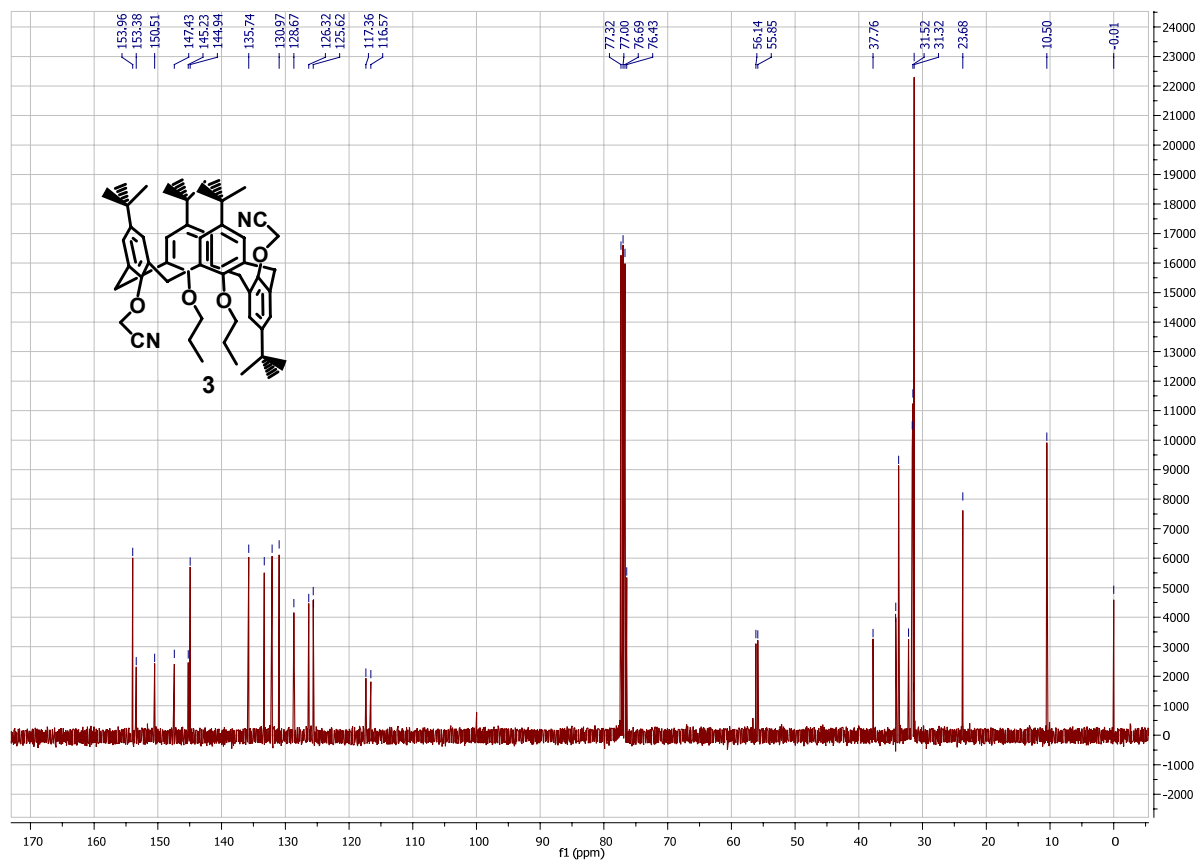




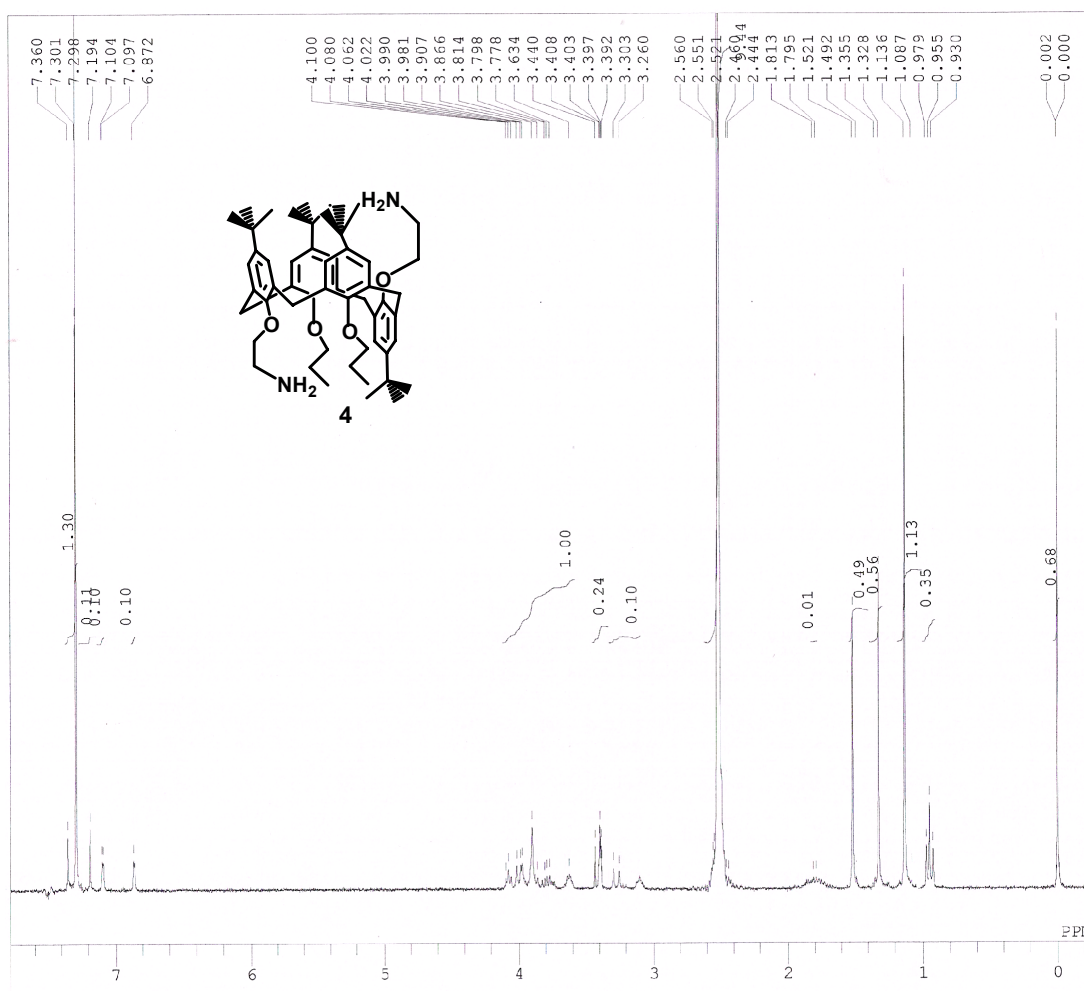
MASS SPECTRUM OF 3



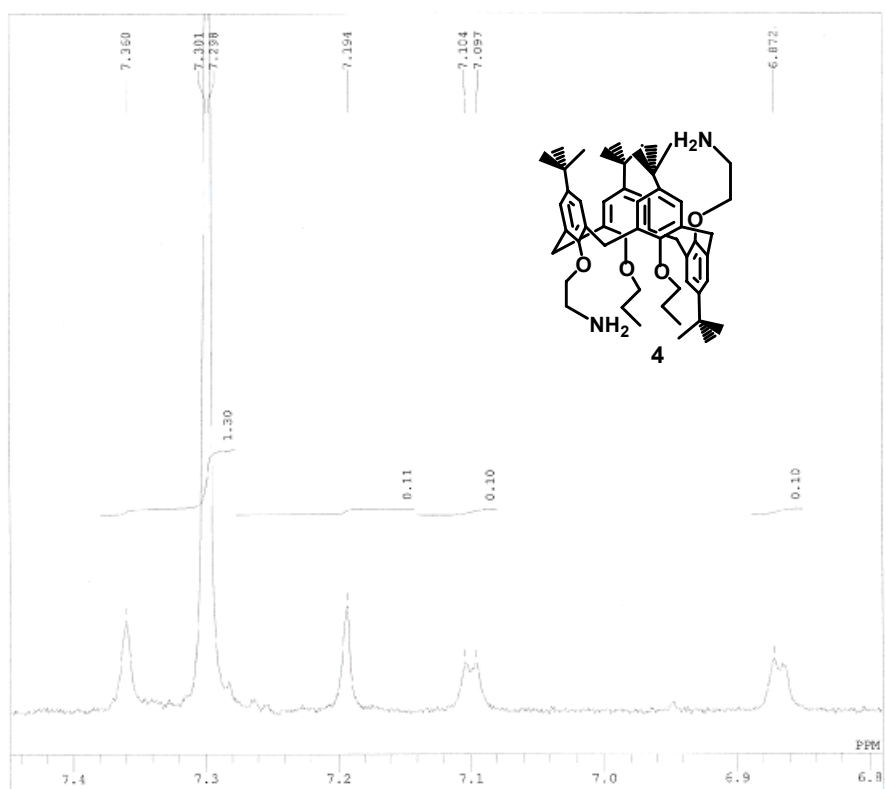
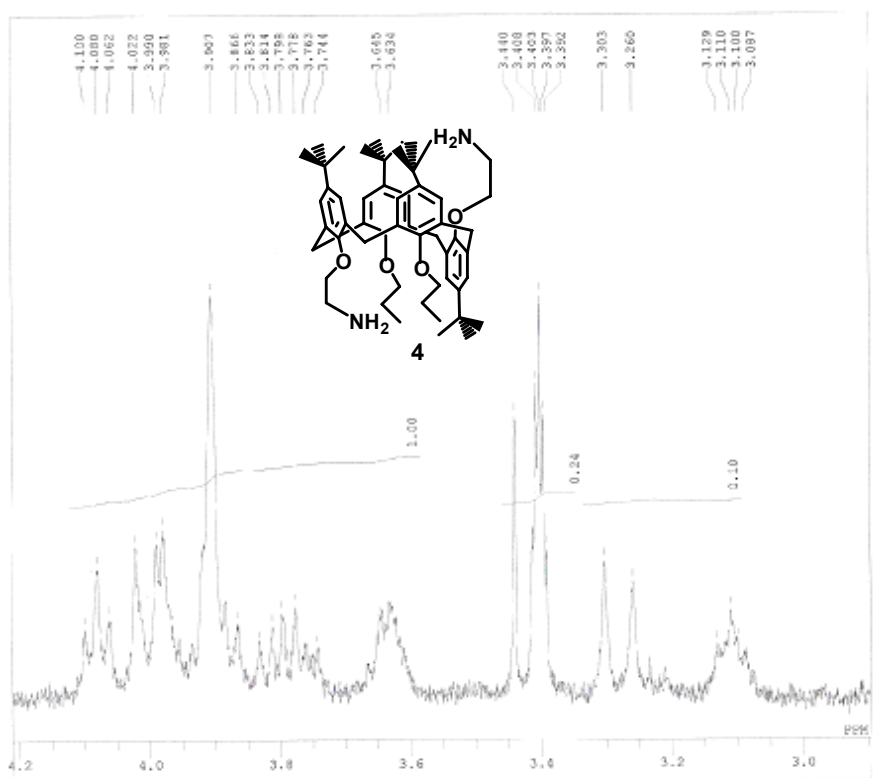
¹³C NMR SPECTRUM OF 3



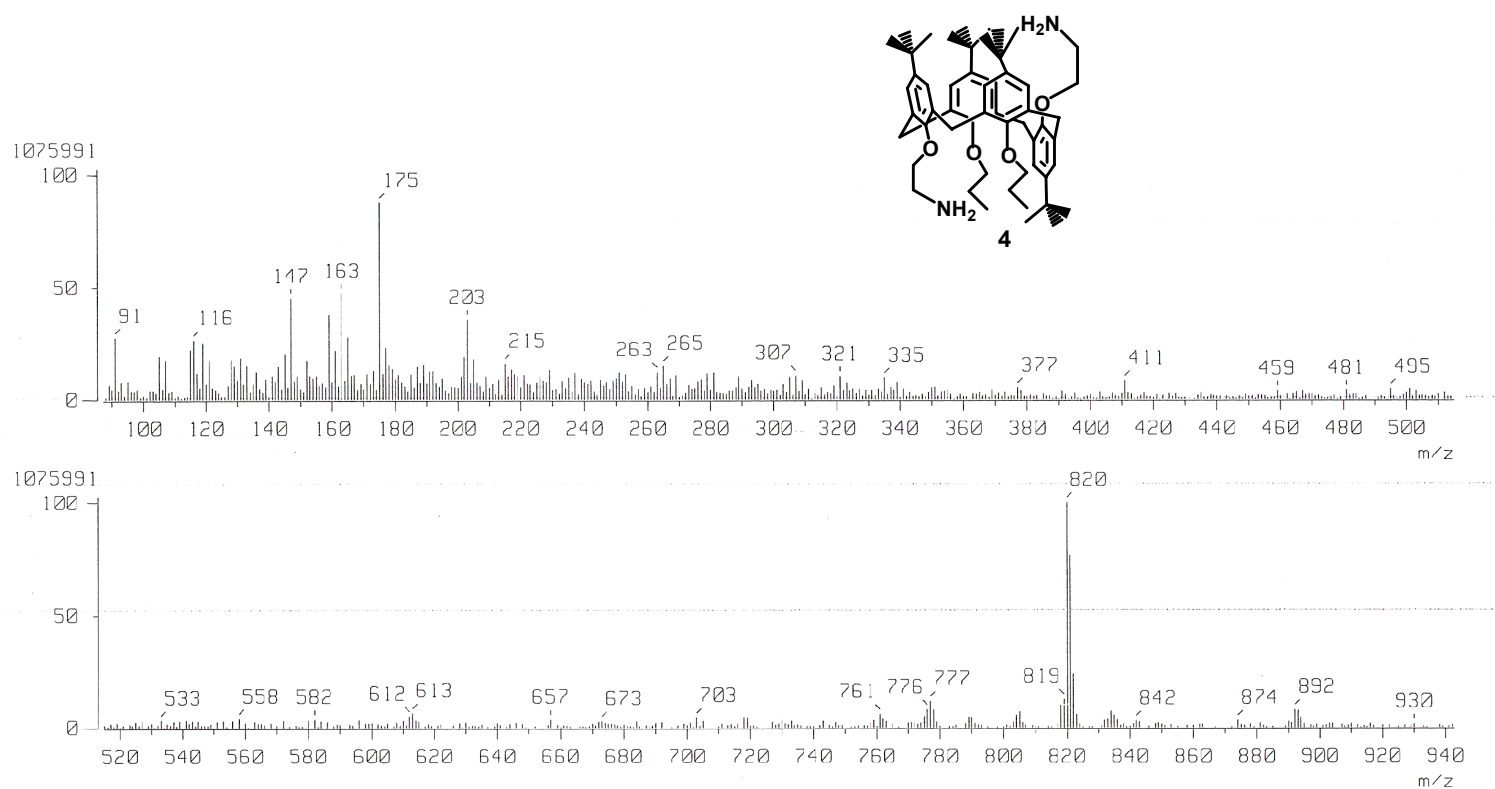
¹H NMR SPECTRUM OF 4



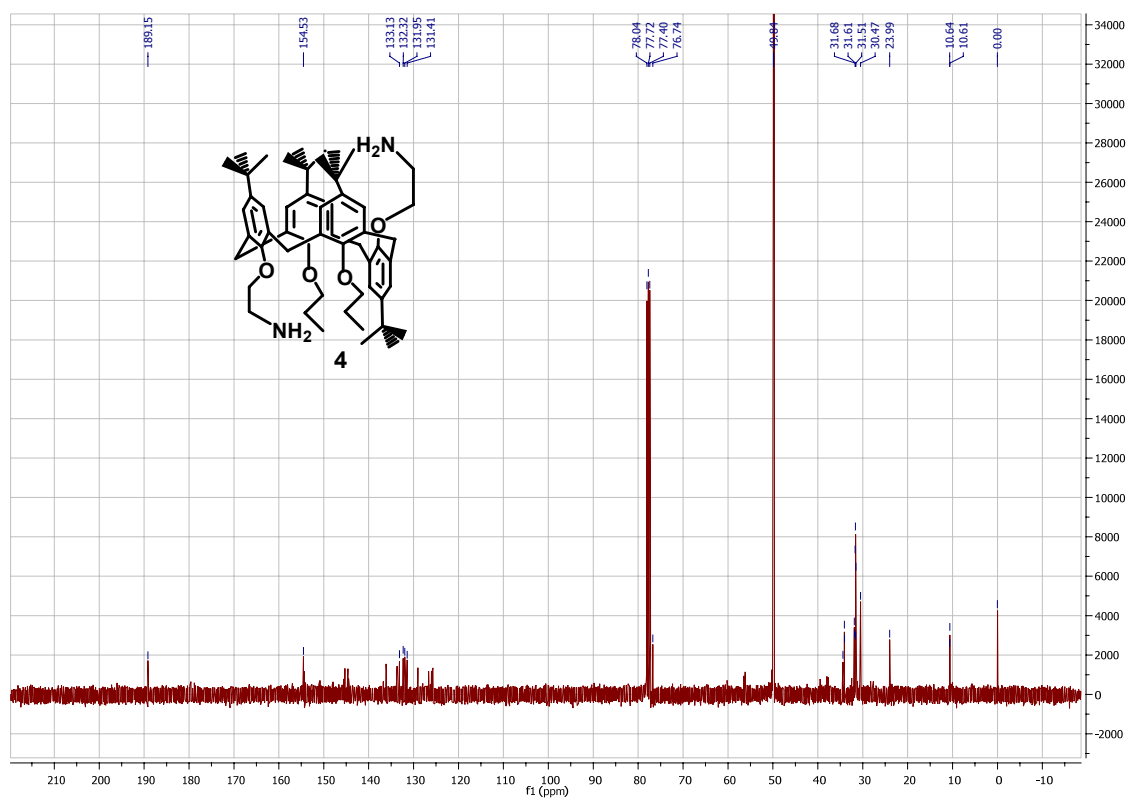
Expanded ^1H NMR SPECTRUM OF 4



MASS SPECTRUM OF 4



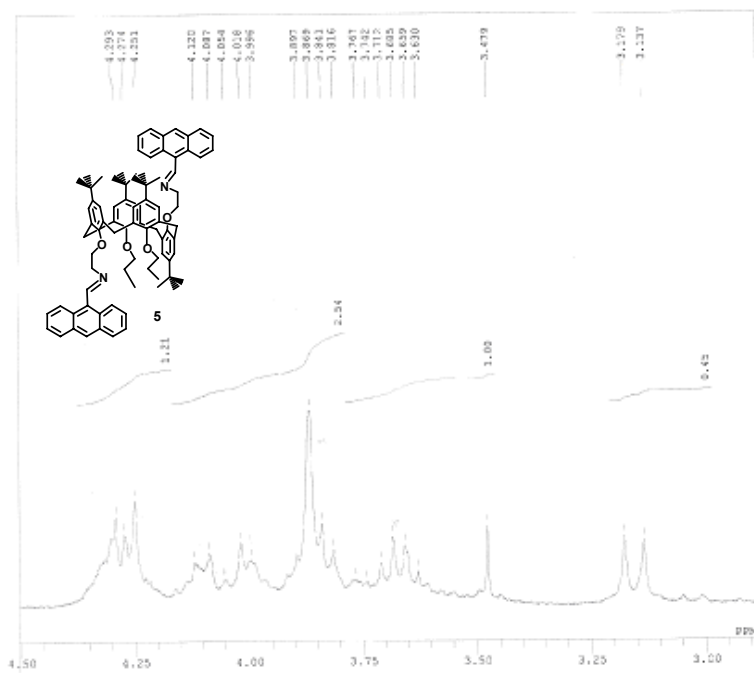
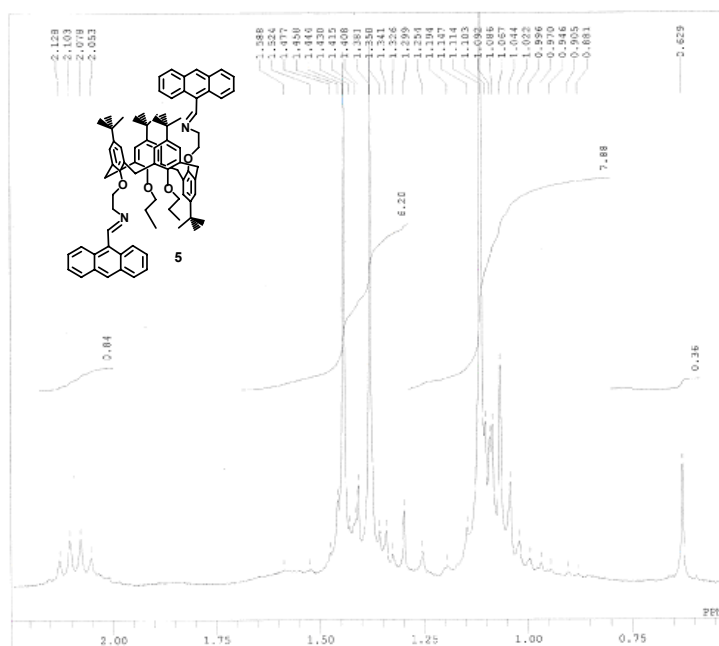
¹³C NMR SPECTRUM OF 4



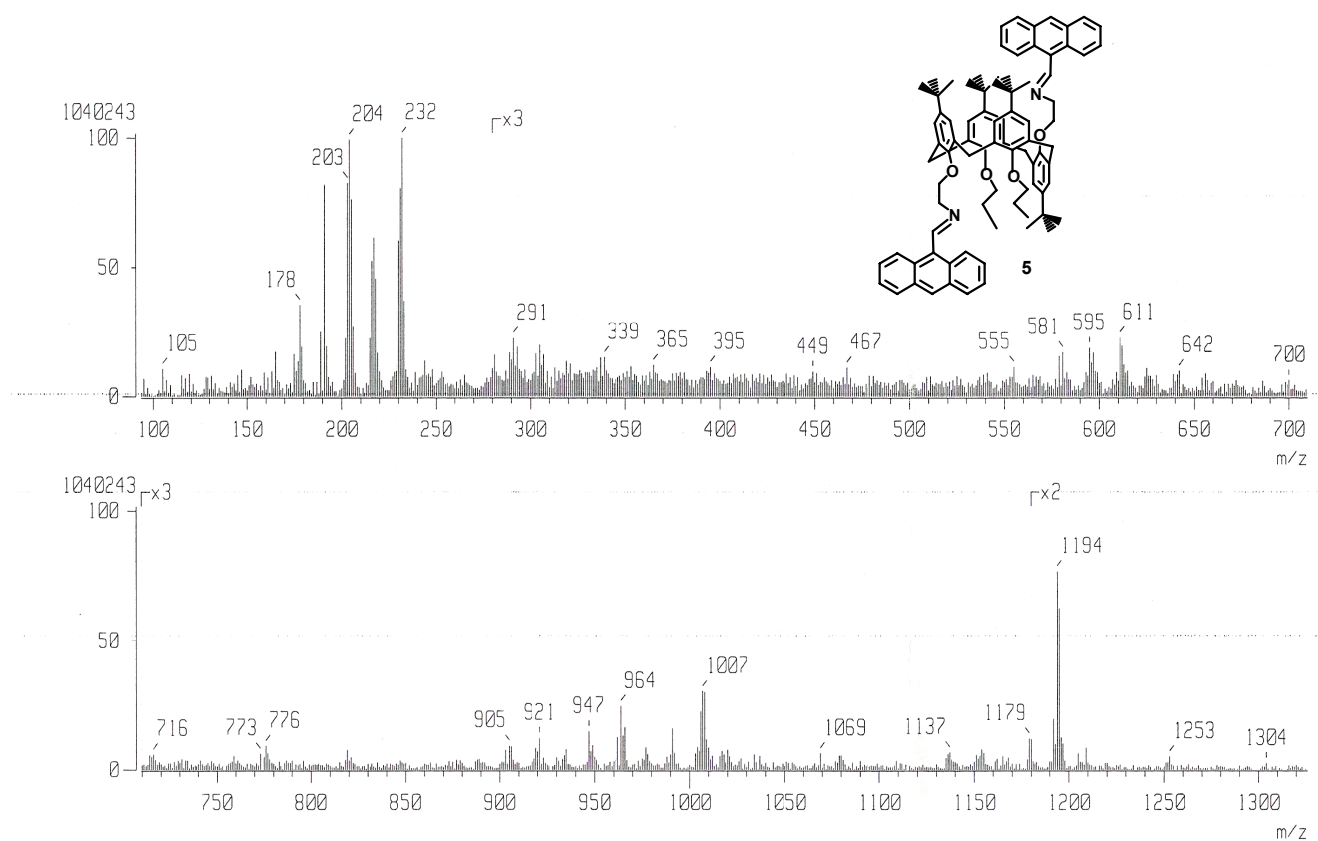
¹H NMR SPECTRUM OF 5



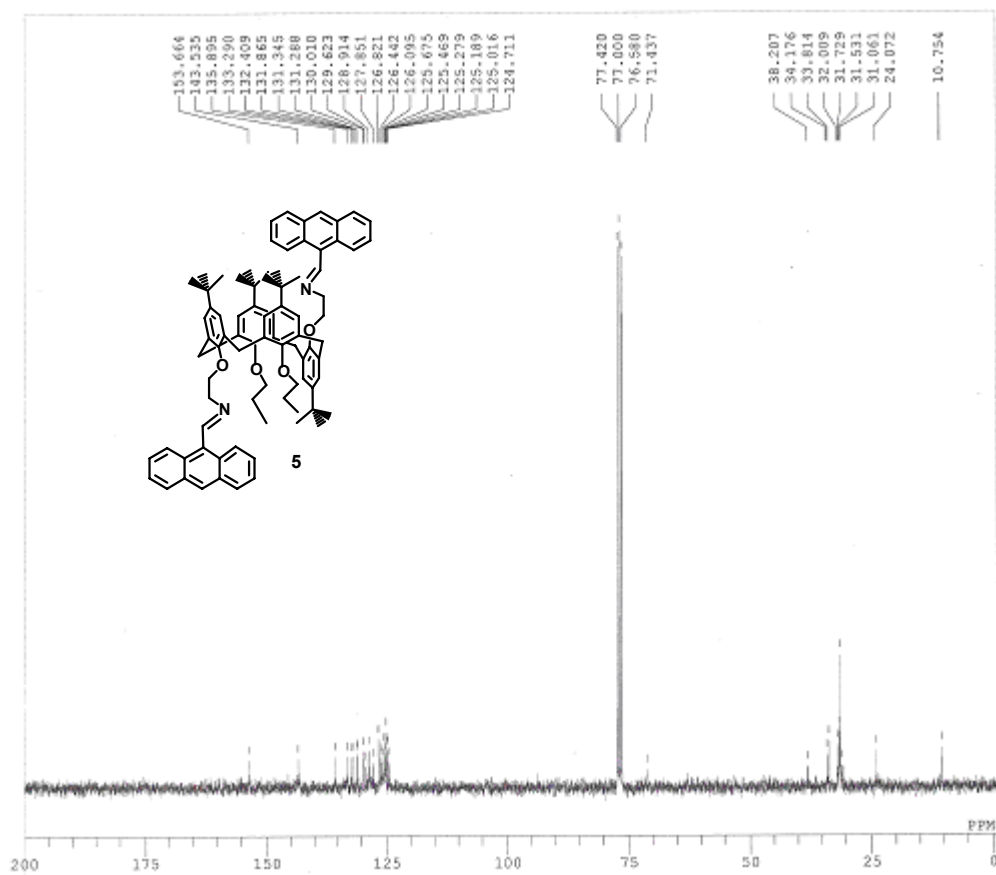
Expanded ^1H NMR SPECTRUM OF 5



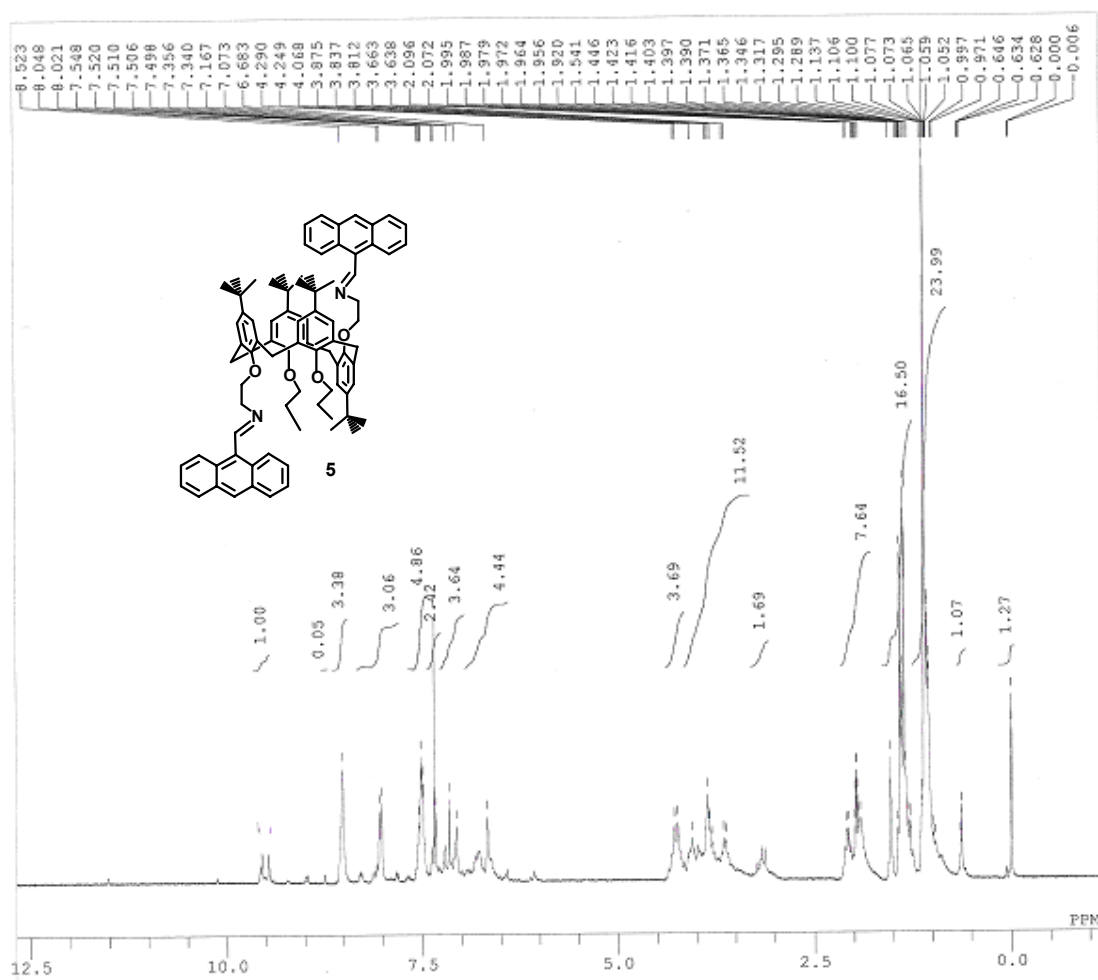
MASS SPECTRUM OF 5



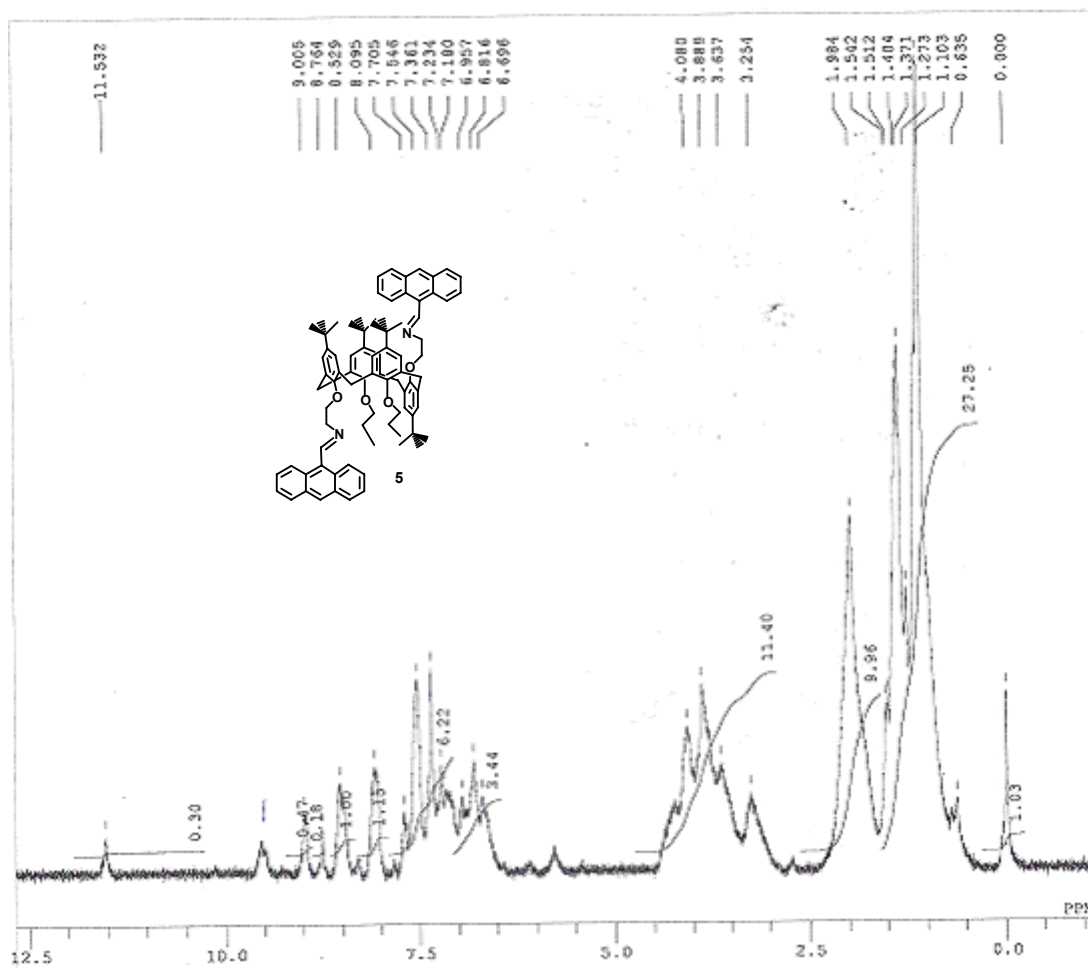
^{13}C NMR SPECTRUM OF 5



^1H NMR SPECTRUM OF 5 in $\text{CDCl}_3:\text{CD}_3\text{CN}$ (8:2)



^1H NMR SPECTRUM OF 5 + 2 equiv. Ni^{2+} in $\text{CDCl}_3:\text{CD}_3\text{CN}$ (8:2)



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