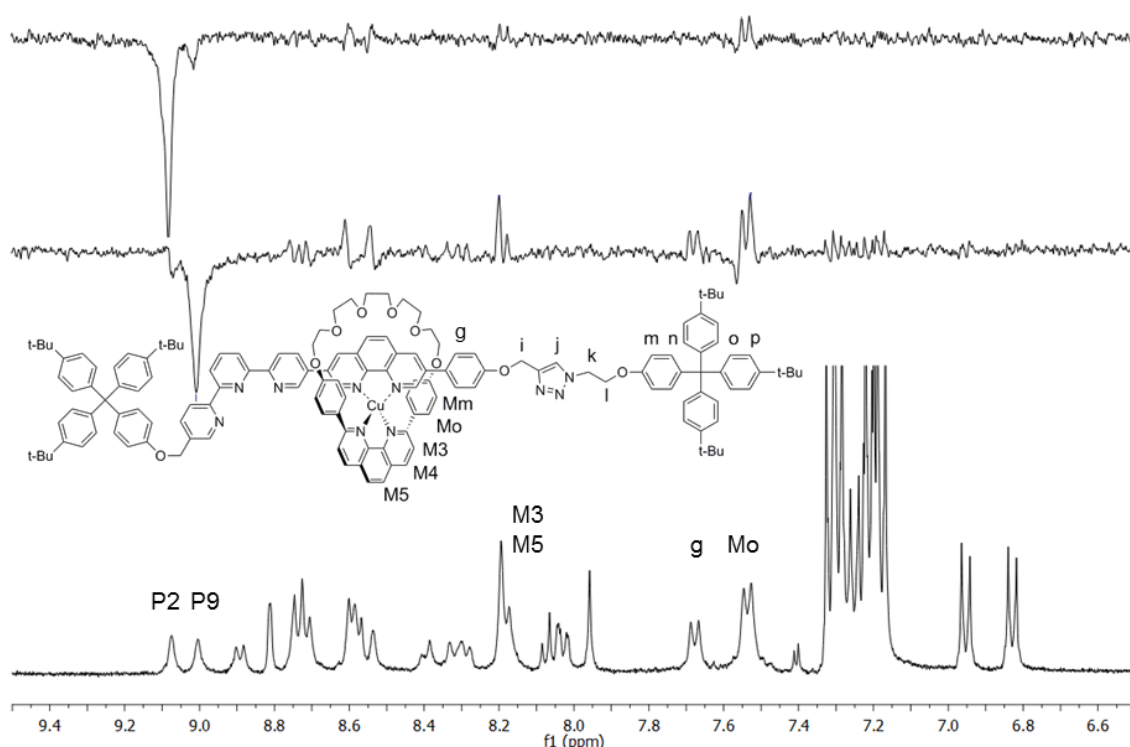


Supporting information

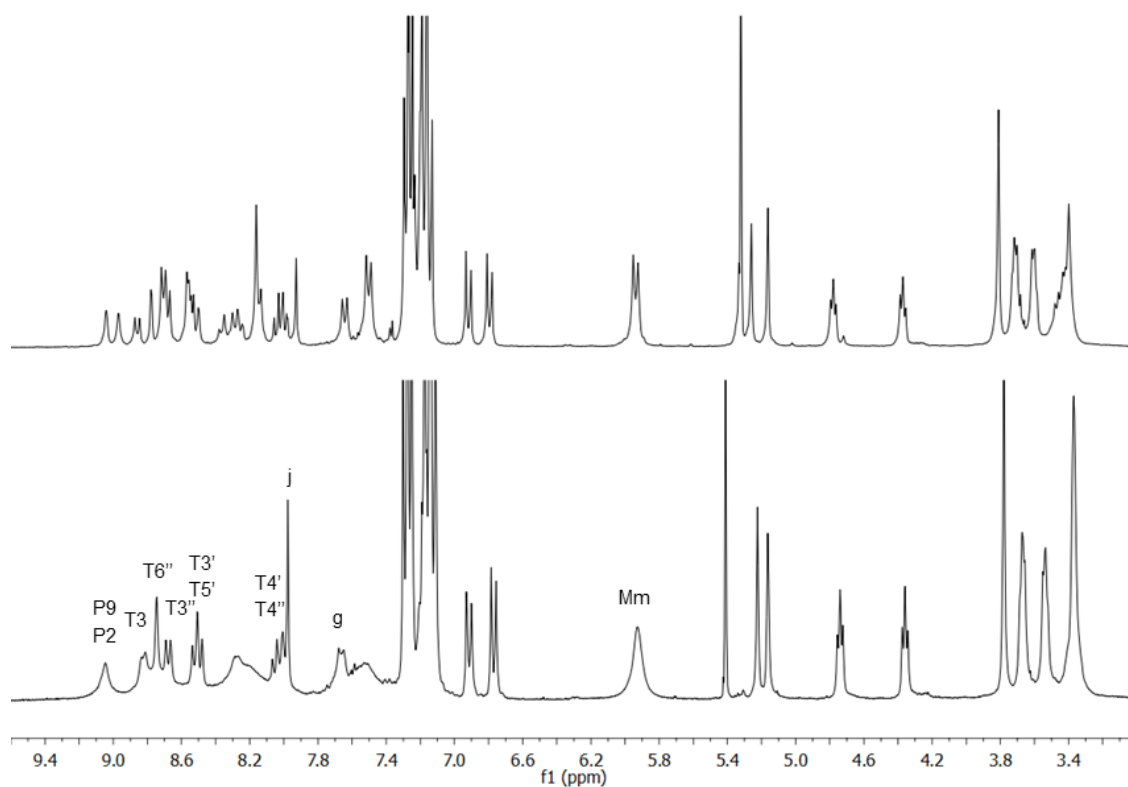
**Fast redox-triggered shuttling motions in a copper rotaxane
based on a directly bonded phenanthroline/terpyridine
conjugate**

Eugenio Coronado, Pablo Gaviña, Julia Ponce and Sergio Tatay**



S.I. Figure 1 1D NOE experiments with **1**(PF₆) carried out in CD₂Cl₂.

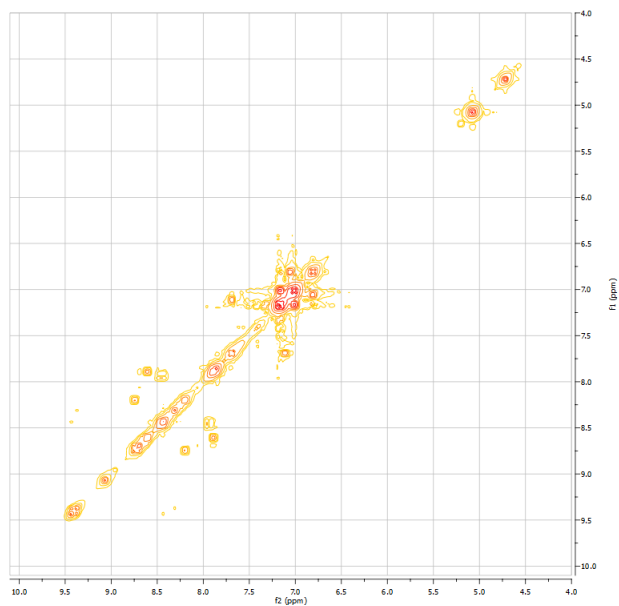
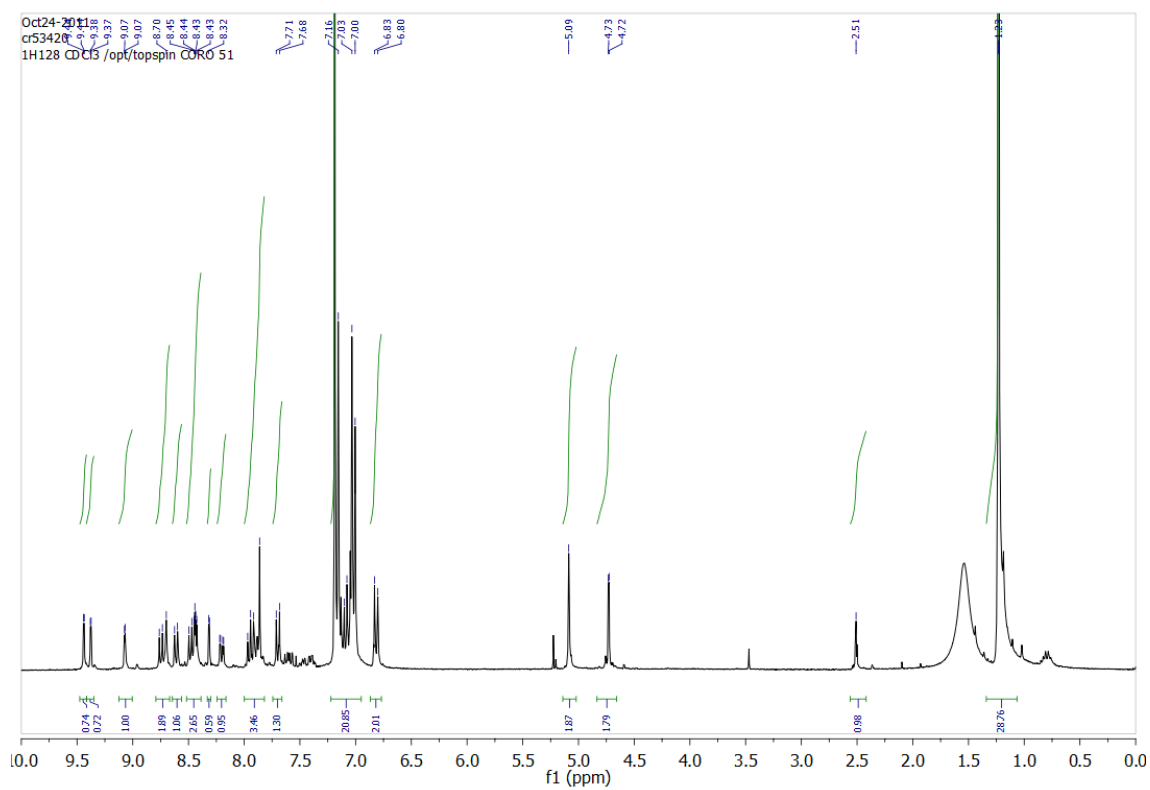
The identity of P2 and P9 protons was confirmed by NOE experiments (see S.I. Figure 1). Irradiation of the proton at $\delta = 9.04$ ppm generates a NOE effect at protons Mo (7.50 ppm), whereas the irradiation of the peak at 8.97 ppm results in a NOE effect at protons g and Mo. Since they both lay close to Mo, these protons correspond to P2 and P9, being P9 the proton at 8.97 ppm, due to its proximity to g, and P2 the one appearing at 9.04 ppm.



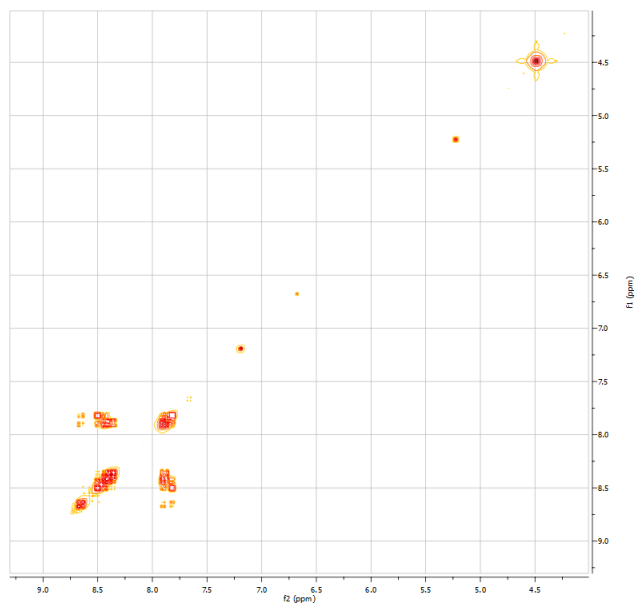
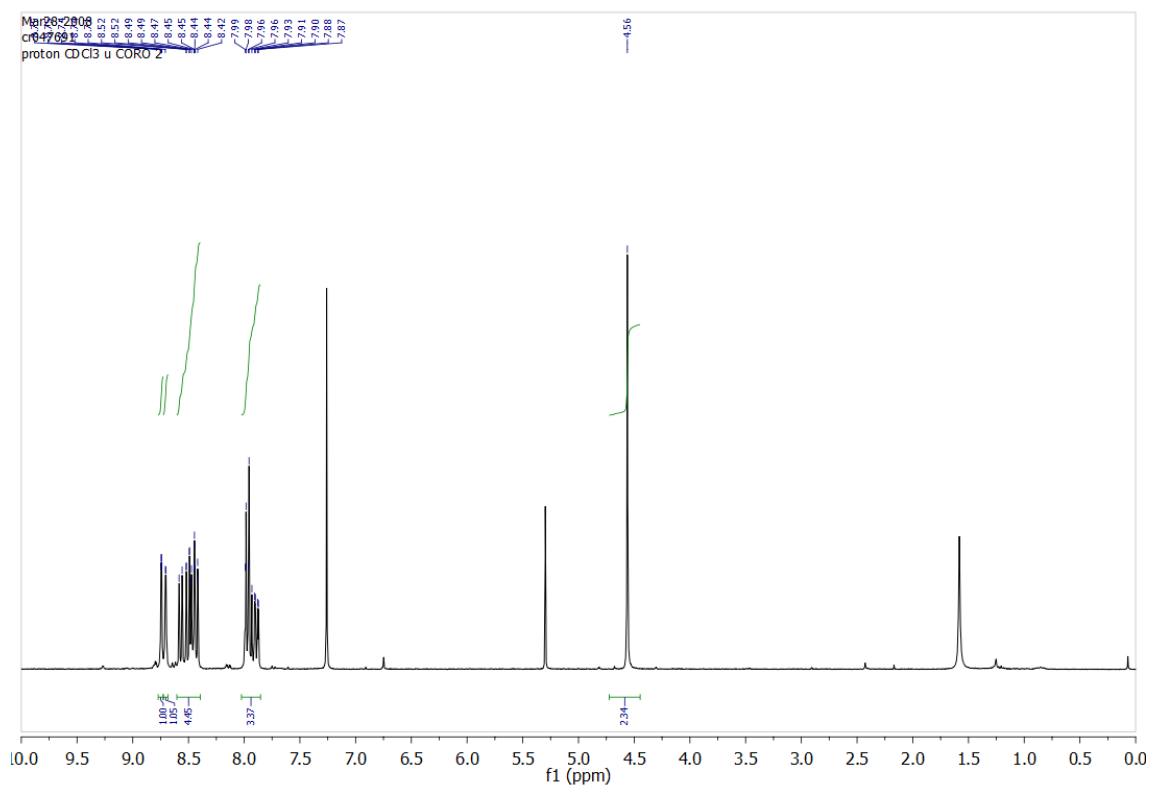
S.I. Figure 2 ^1H NMR spectra of rotaxane **1**(PF₆) in CD₂Cl₂ (up) and 1:9 CD₂Cl₂ / CD₃CN mixture.

¹H NMR (300 MHz)

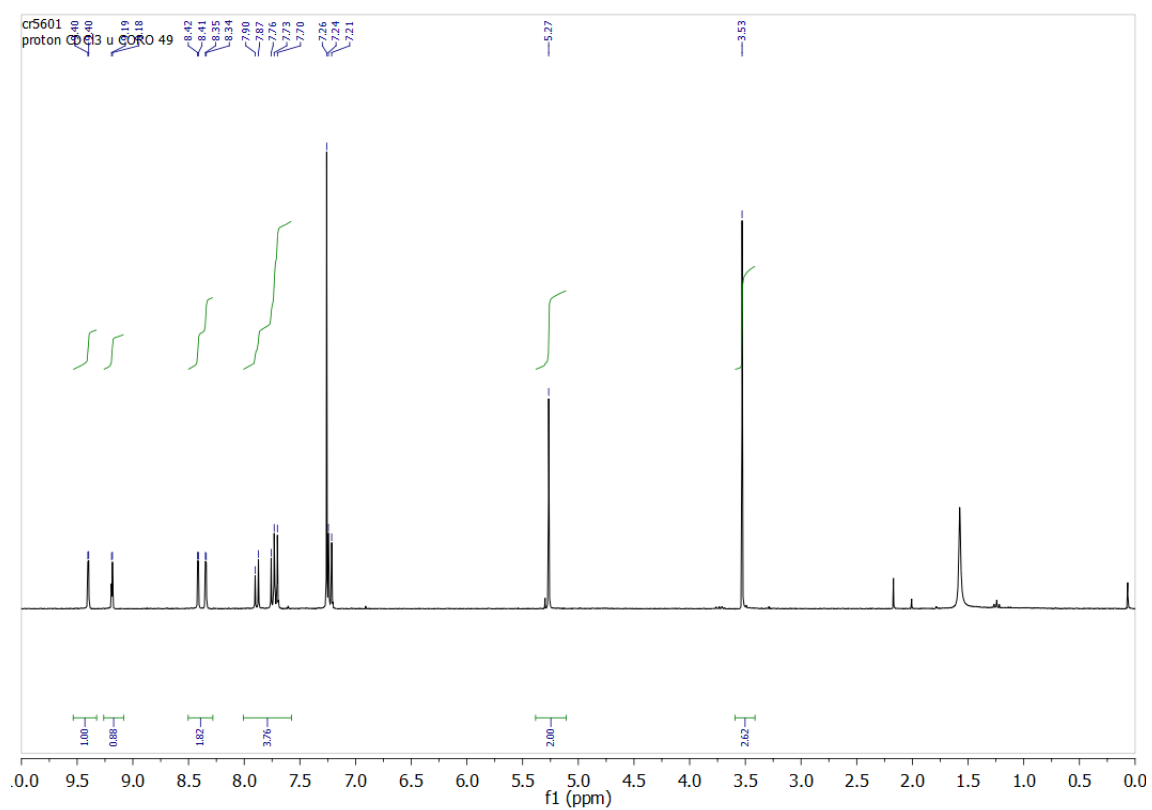
Compound 2:



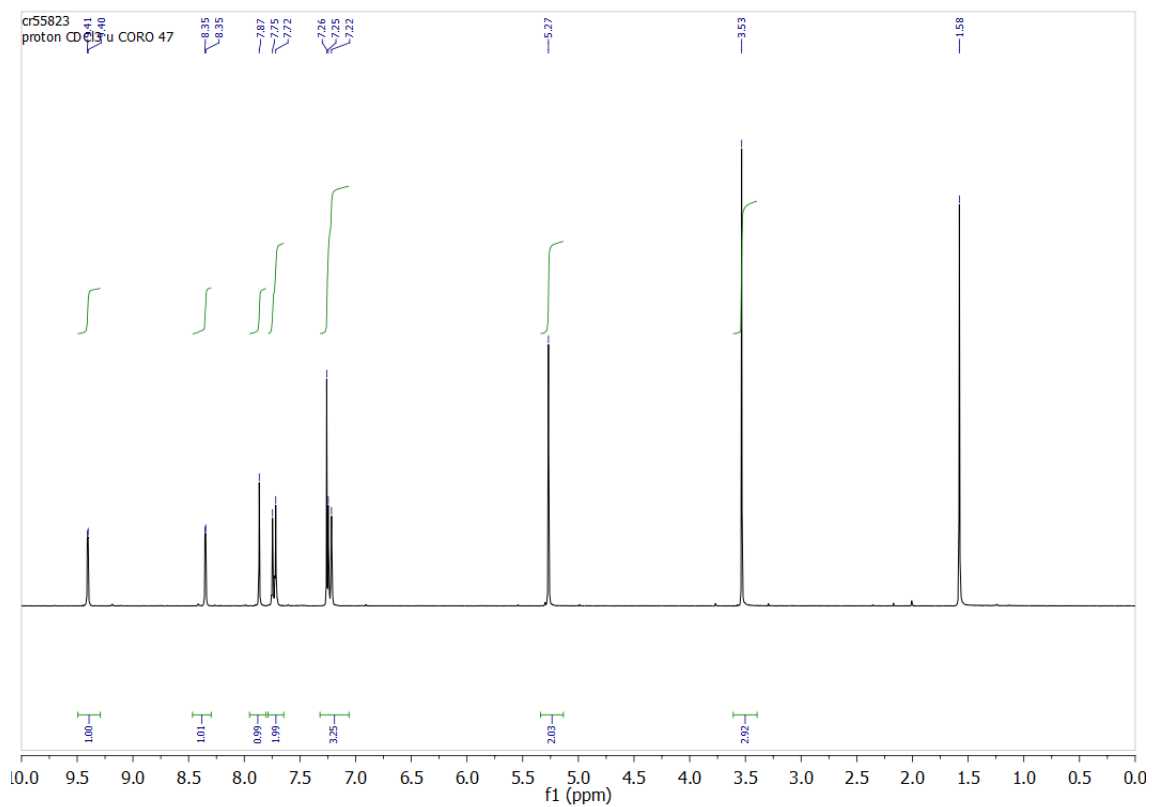
Compound 4:



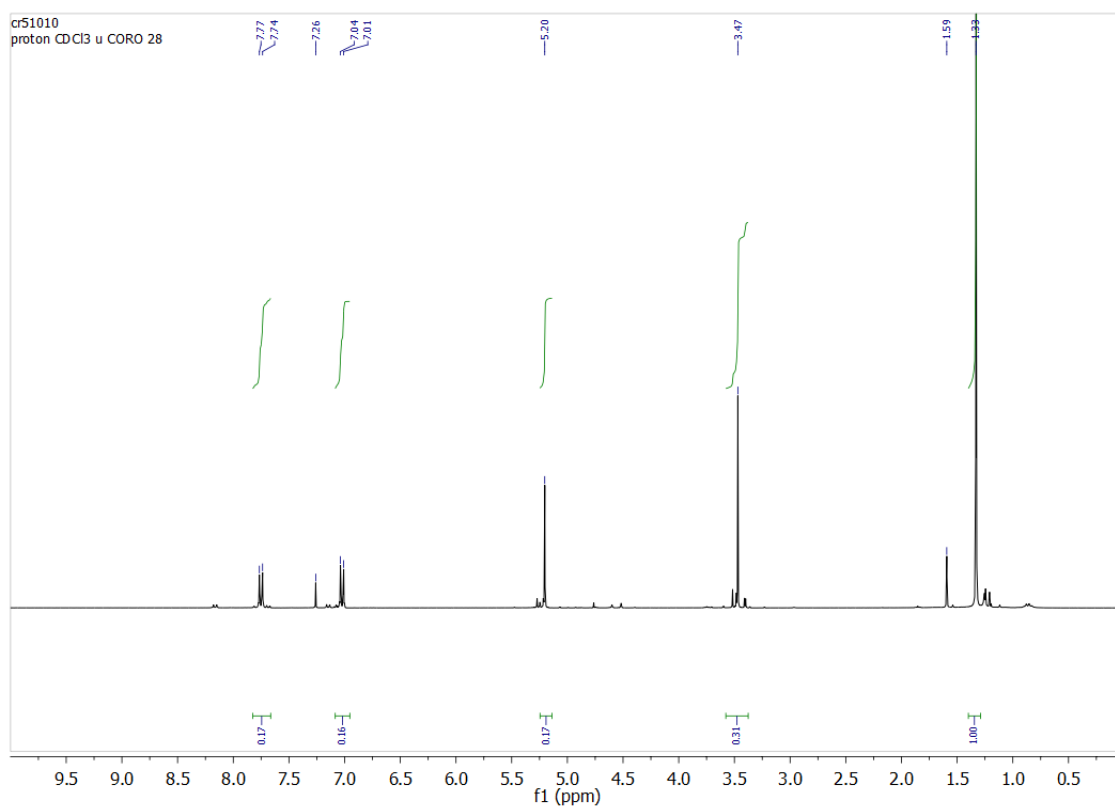
Compound 5:



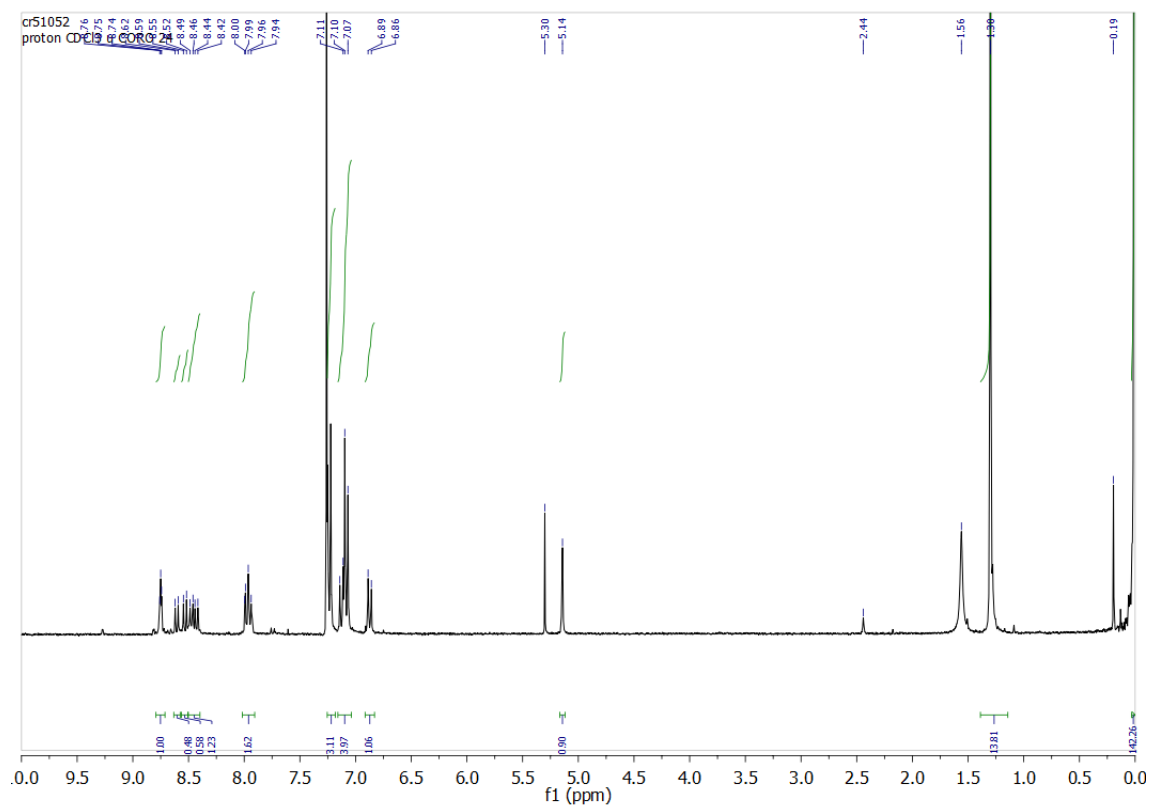
Disubstituted:



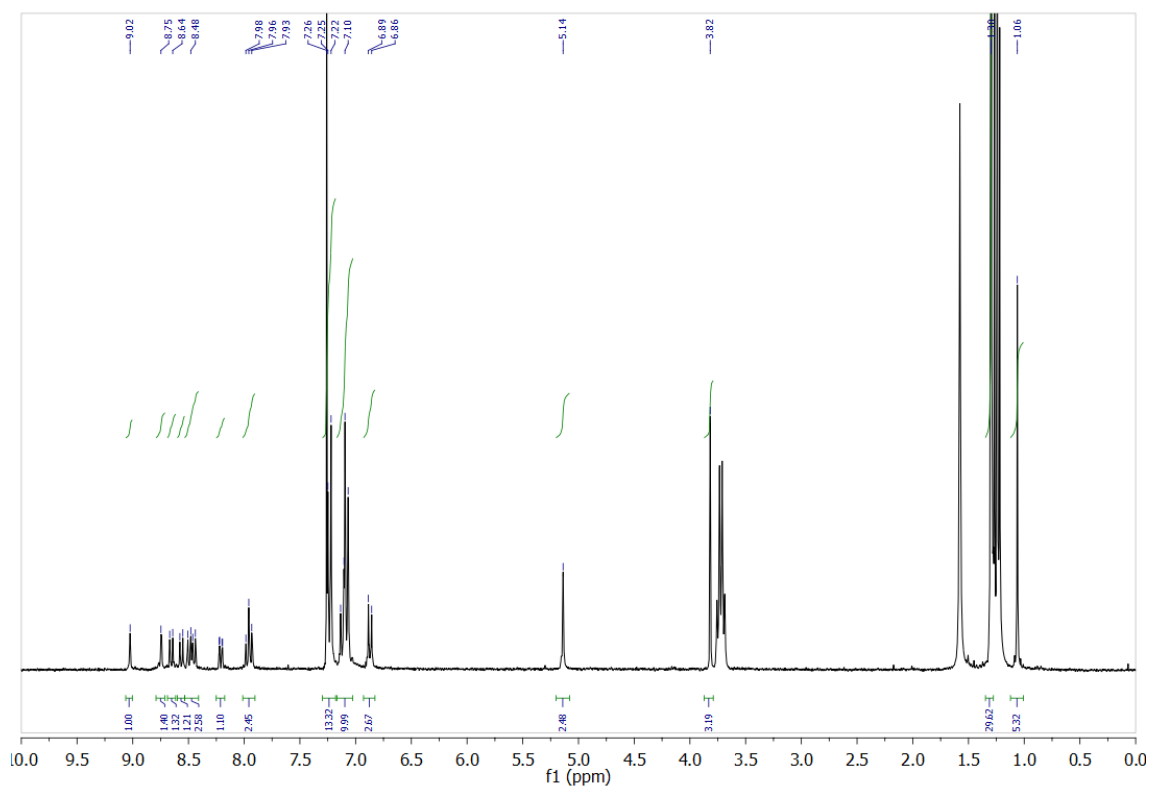
Compound 9:



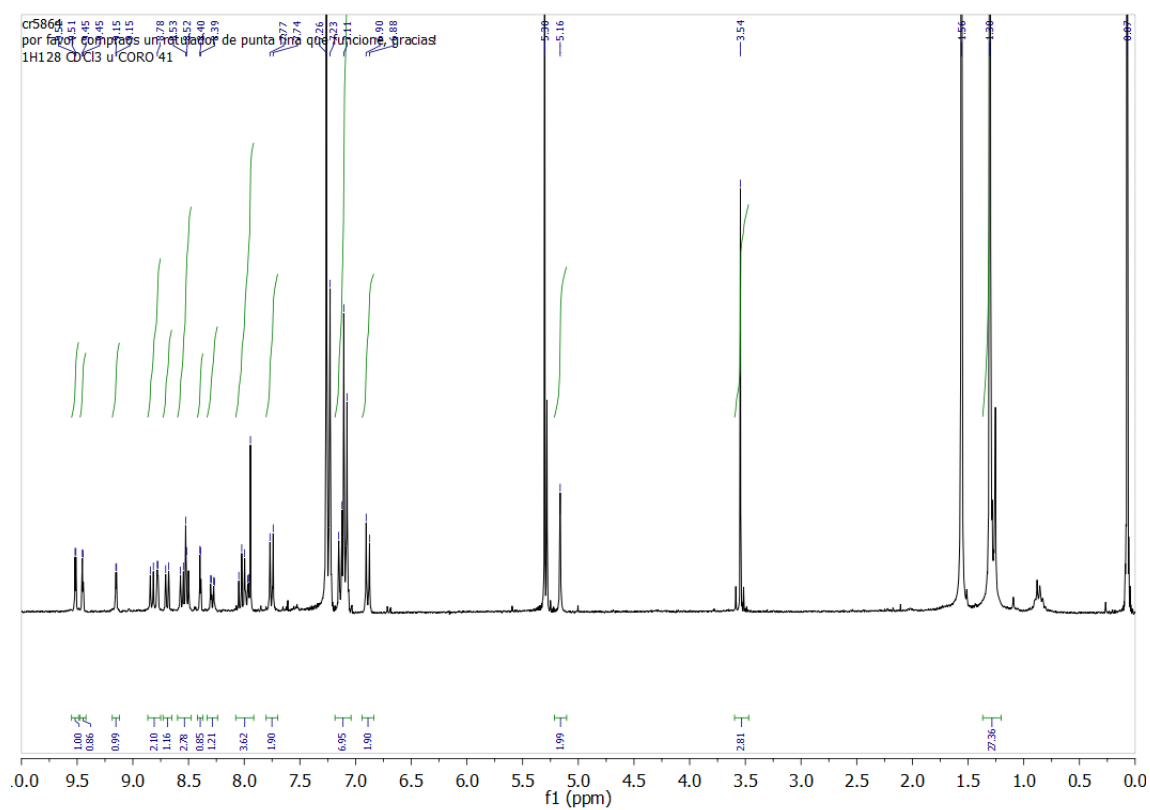
Compound 11:

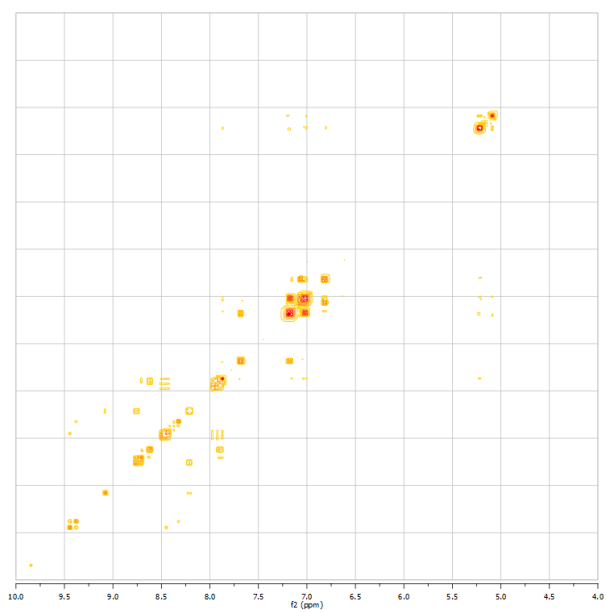


Compound 12:

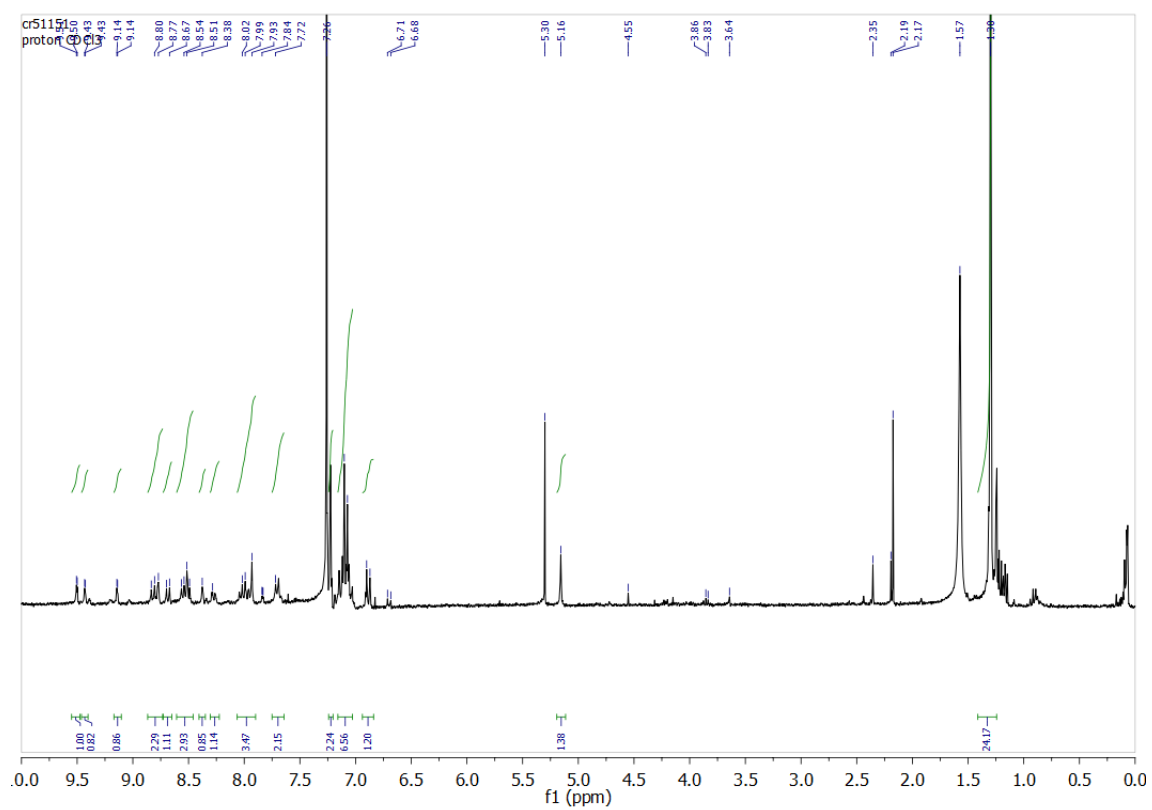


Compound 13:

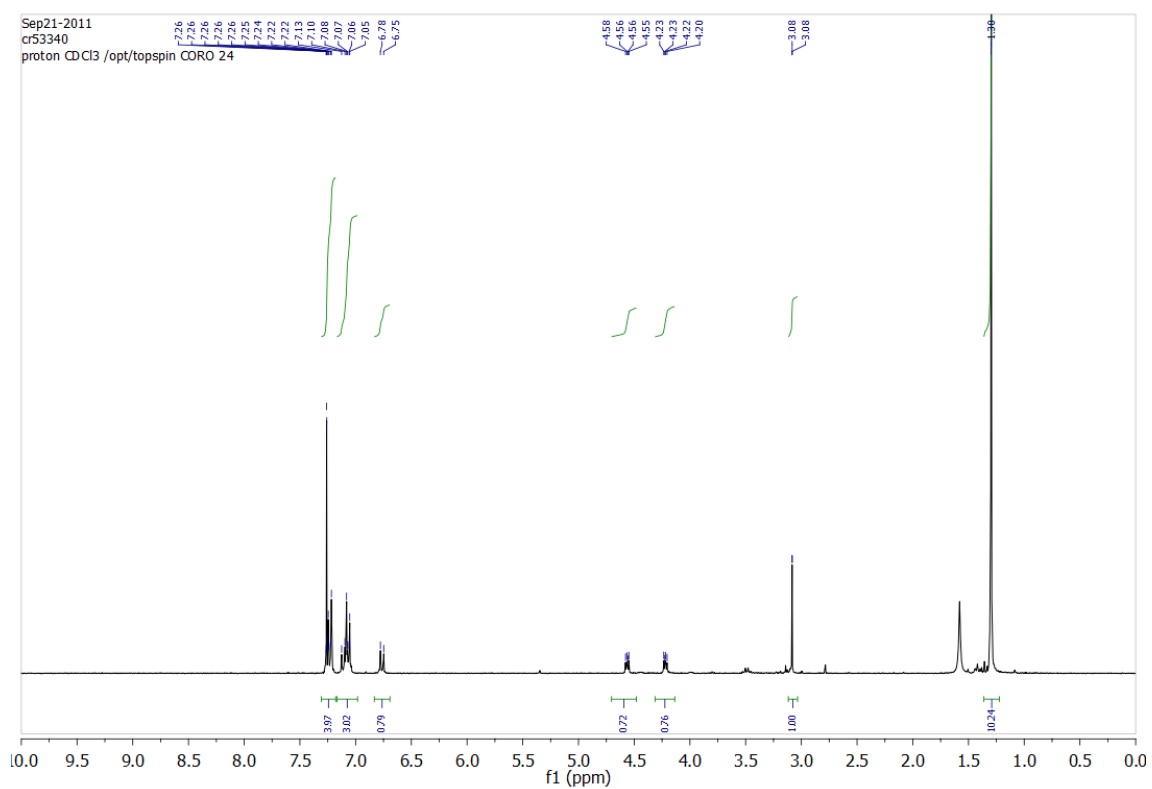




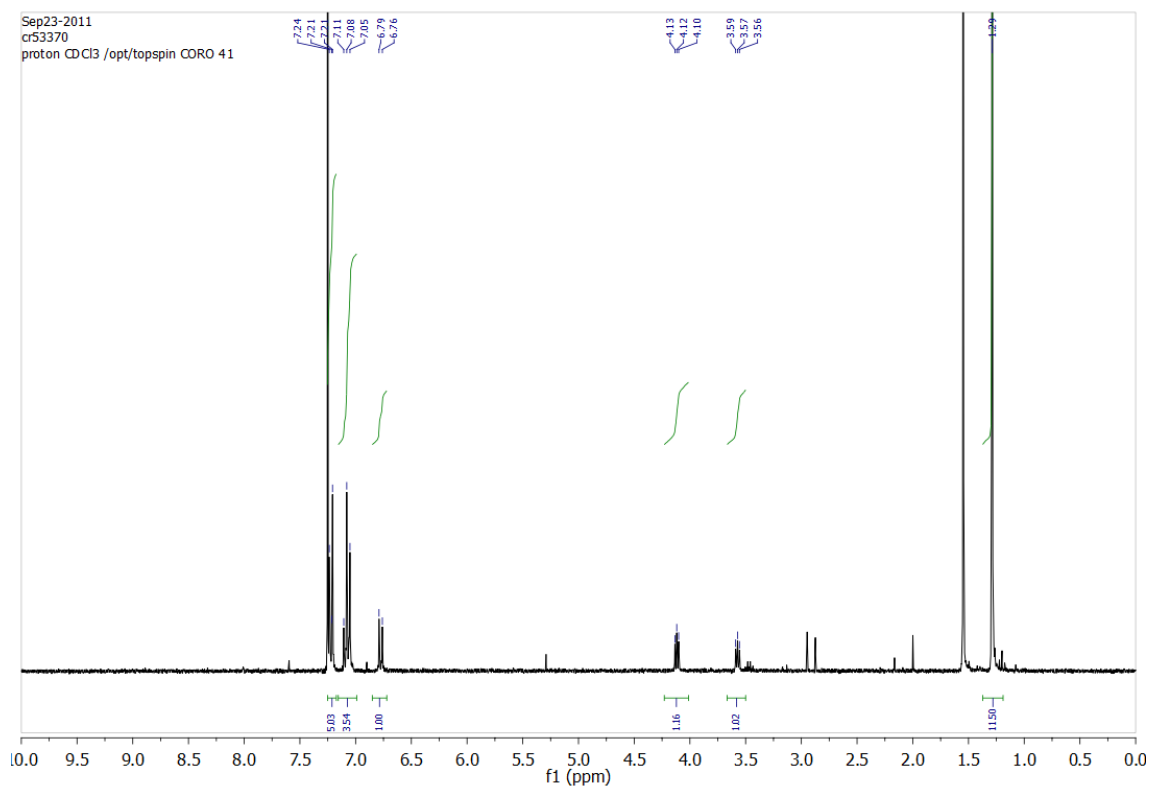
Compound 14:



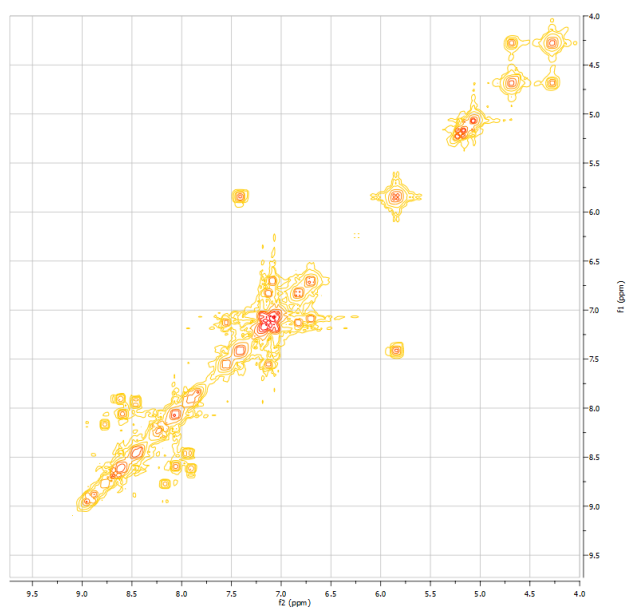
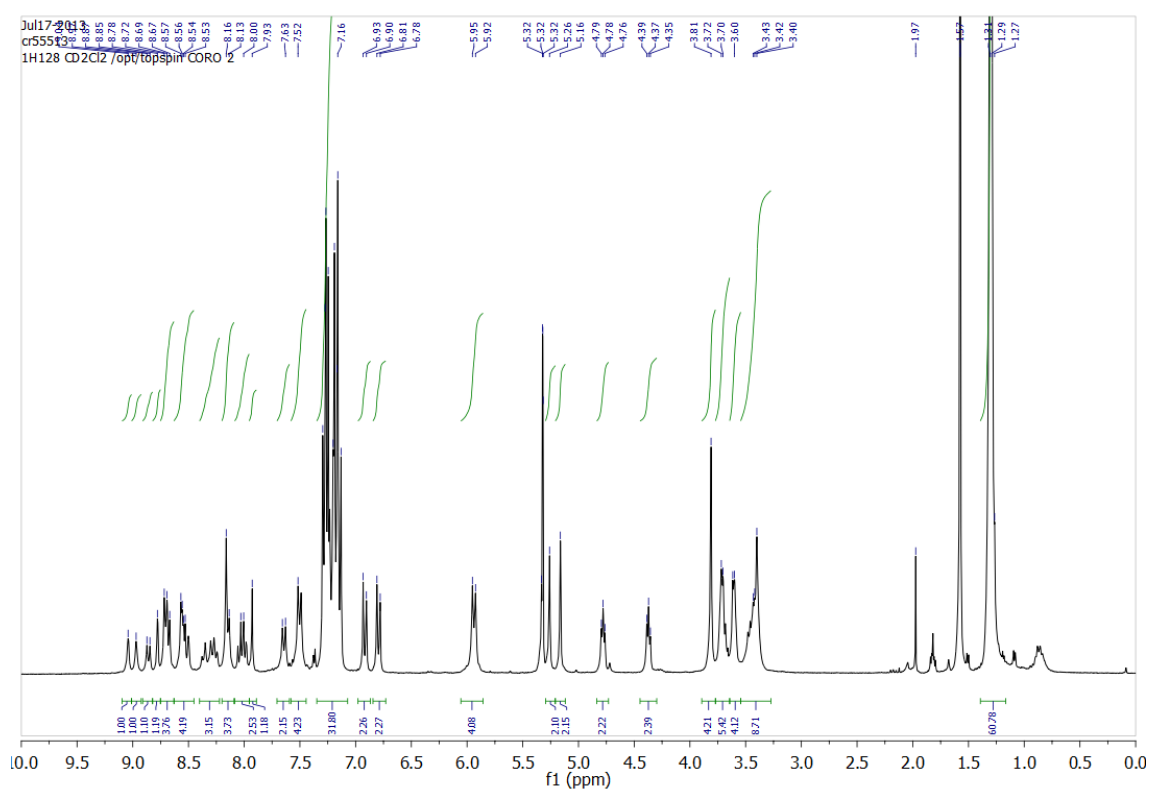
Compound 15:



Compound 16:

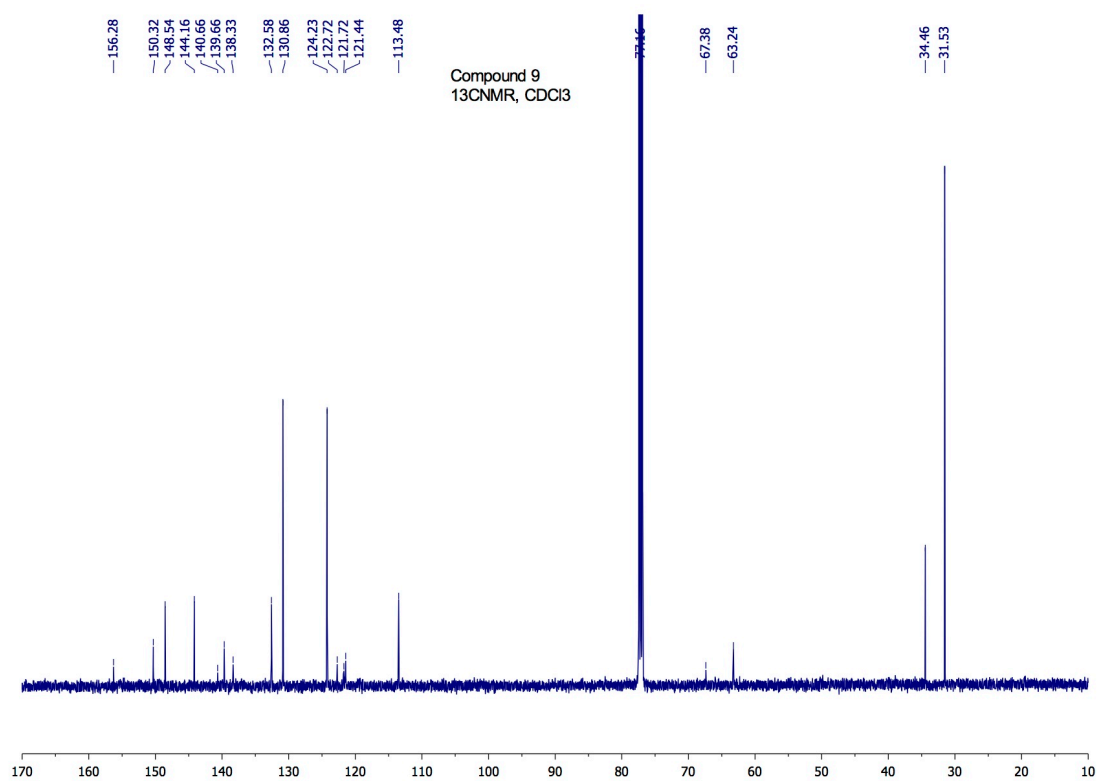


Rotaxane 1(PF₆):

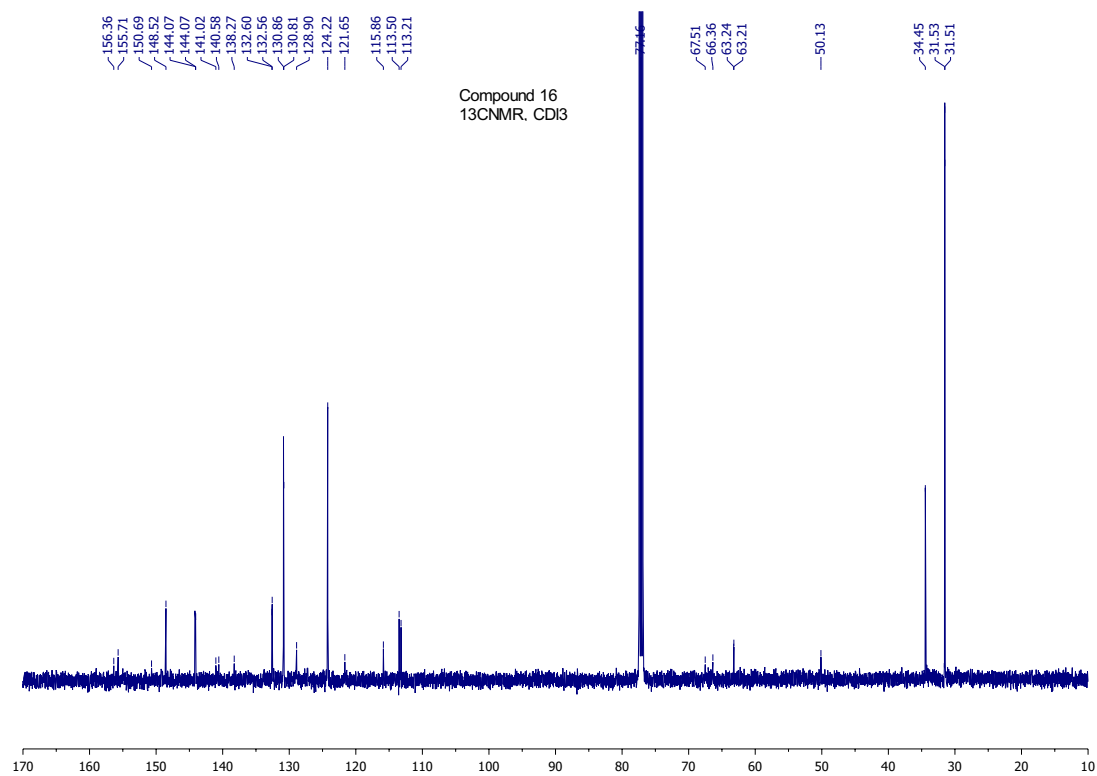


^{13}C NMR (126 MHz)

Compound 9:



Compound 16:



Rotaxane 1(PF₆):

