Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information for

Vinyl sulfone-based ferrocenylation reagents: Applications in conjugation and bioconjugation

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Universidad de Granada, E-18071-Granada, Spain

1. Voltammograms of different compounds

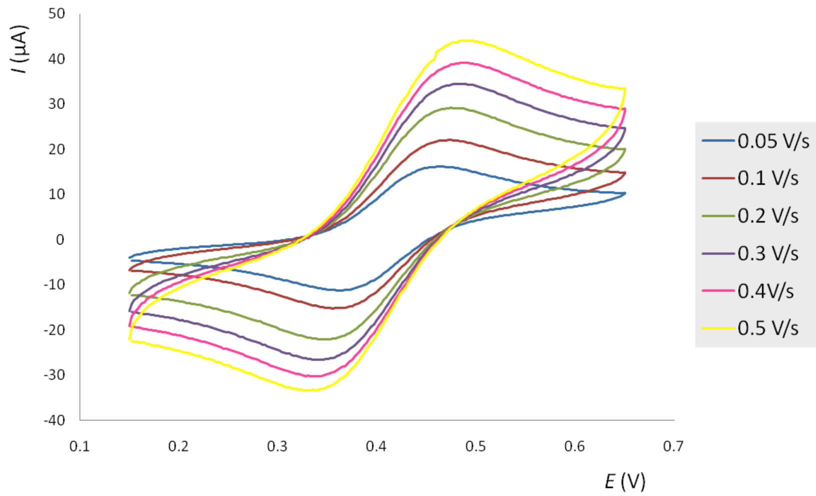


Figure S1. Cyclic voltammetry curves (5 scans) of the ferrocene derivative **2** (0.2 mM) in 50mM $NaClO_4$ acetonitrile solution at 25ºC and different sweep rates (from 0.05 to 0.5 V/s).

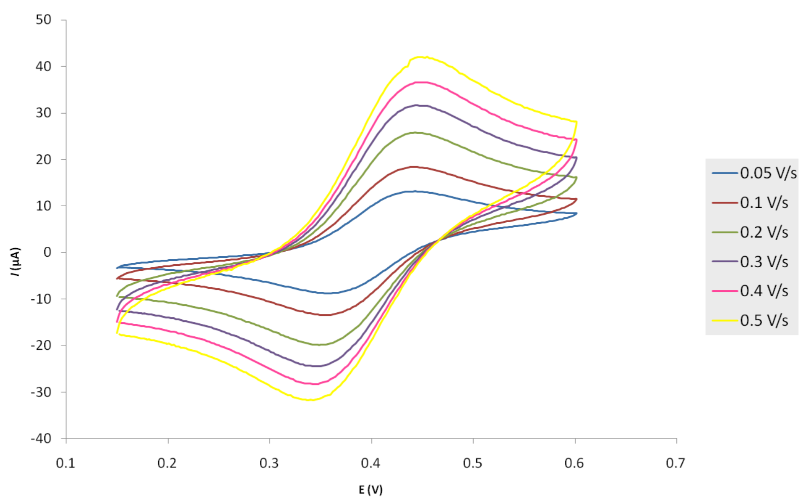


Figure S2. Cyclic voltammetry curves (5 scans) of the ferrocene derivative **5** (0.2 mM) in 50mM $NaClO_4$ acetonitrile solution at 25ºC and different sweep rates (from 0.05 to 0.5 V/s).

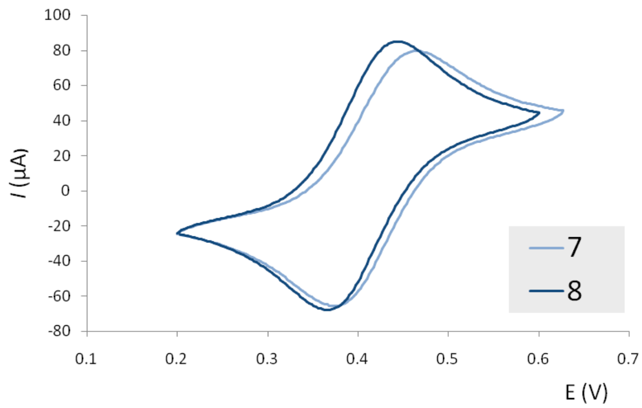


Figure S3. Cyclic voltammetry curves (5 scans; sweep rate = 0.2V/s) of the ferrocene derivatives **7** and **8** (0.2 mM) in 50mM $NaClO_4$ acetonitrile solution at 25ºC.

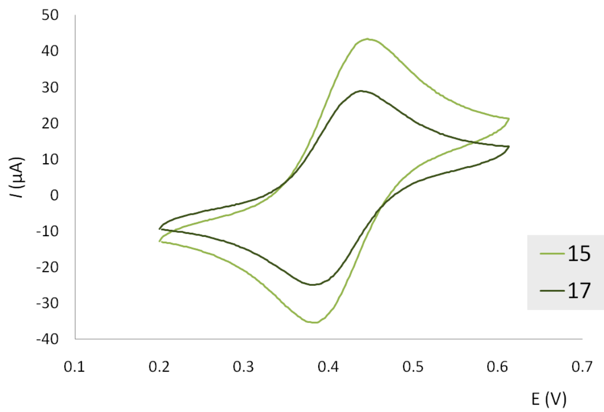


Figure S4. Cyclic voltammetry curves (5 scans; sweep rate = 0.2V/s) of the ferrocene derivatives **15** and **17** (0.2 mM) in 50mM $NaClO_4$ acetonitrile solution at 25ºC.

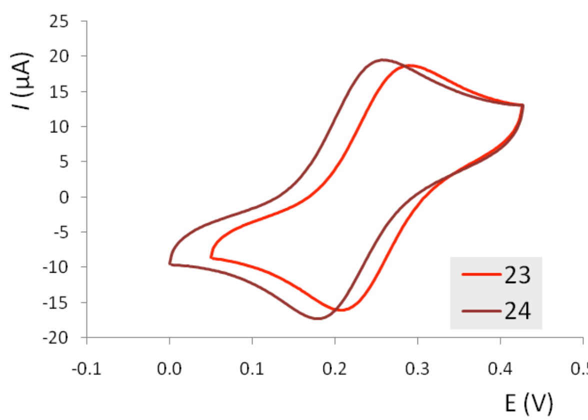


Figure S5. Cyclic voltammetry curves (5 scans; sweep rate = 0.2V/s) of the ferrocene derivatives **23** and **24** (0.2 mM) in 50mM $NaClO_4$ aqueous solution at 25ºC.

2. Diffusion coefficient D_0: plot of I_{pa} *vs* $v^{1/2}$

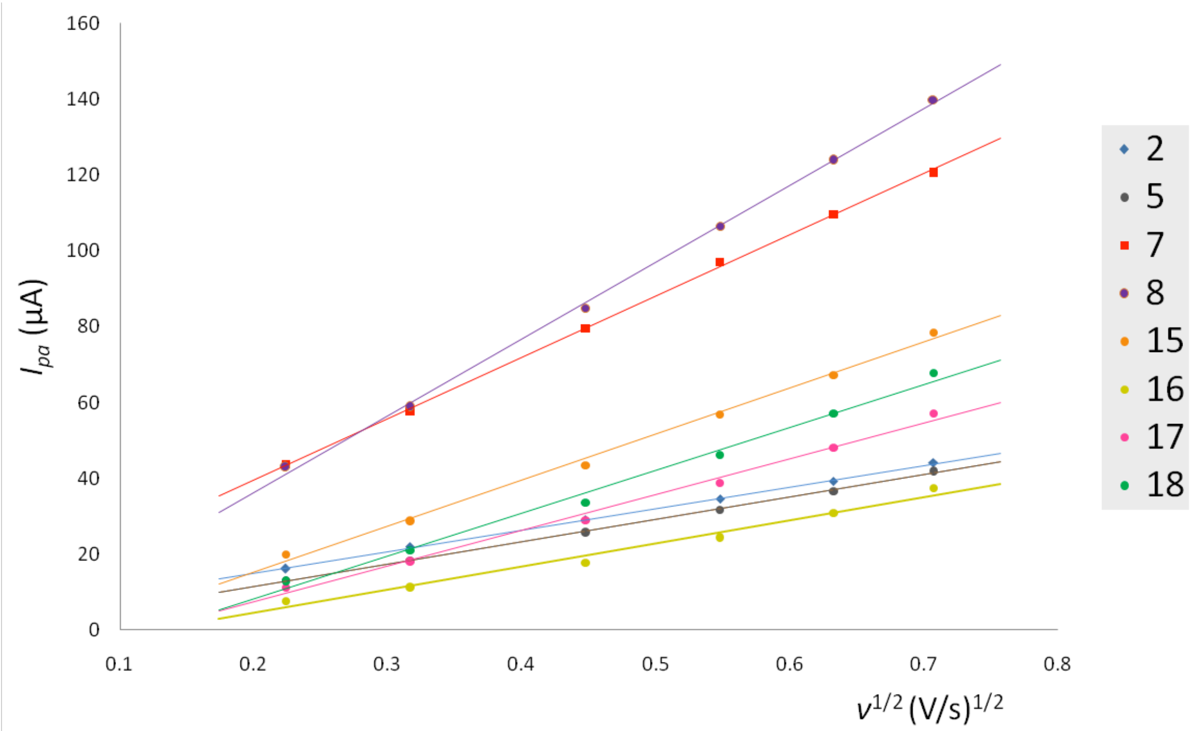
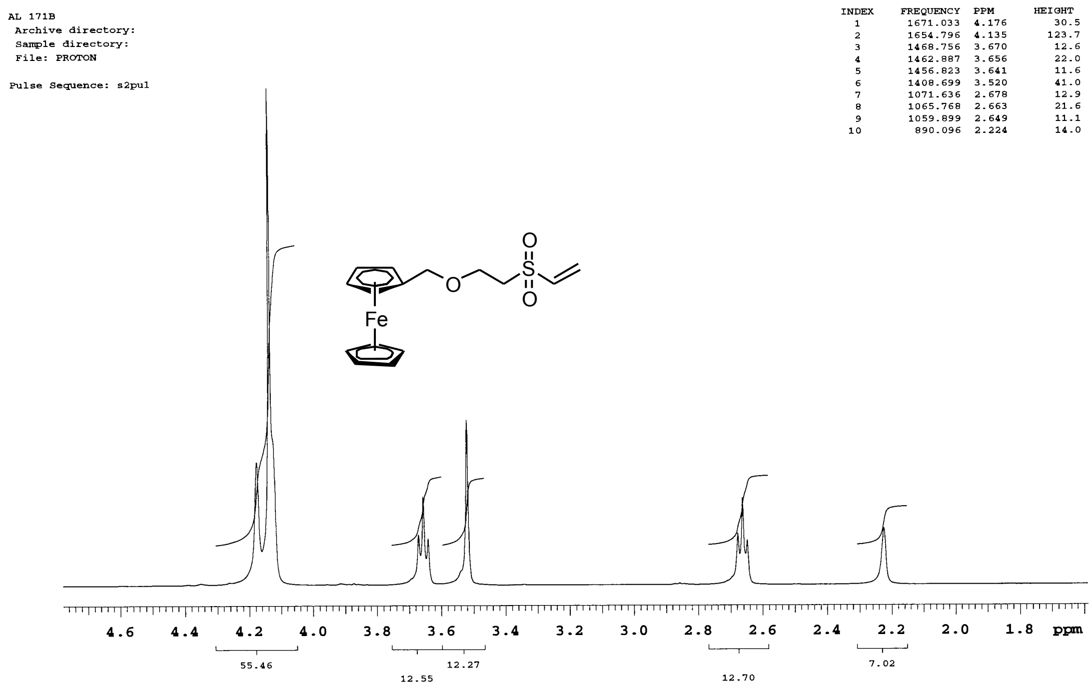


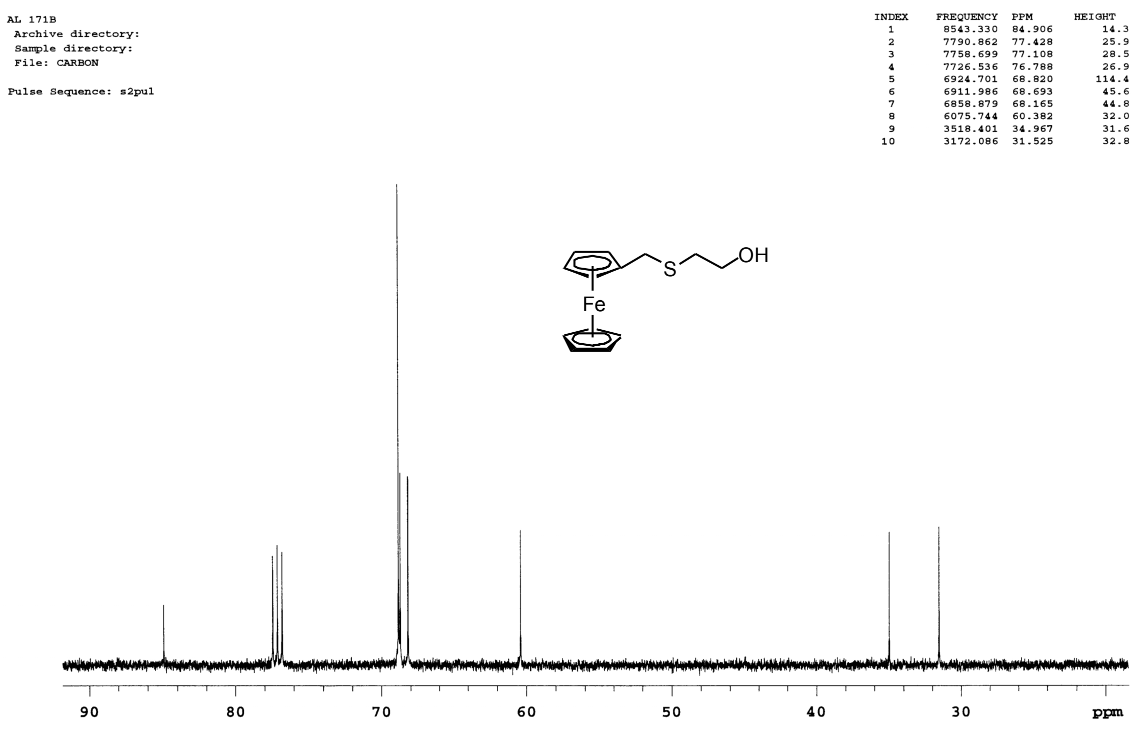
Figure S6. Representation of the anodic peak current (I_{pa}) versus square root of the sweep rate ($v^{1/2}$) for the ferrocene derivatives in acetonitrile. The diffusion coefficients were calculated by linear fitting of I_{pa} versus $v^{1/2}$ in accordance with the Randles-Sevcik equation [Eq. 1].

$$I_p = 0.4463\left(\frac{F^3}{RT}\right)^{1/2} n^{3/2} A C_0 (D_0 v)^{1/2} \qquad \text{Eq (1)}$$

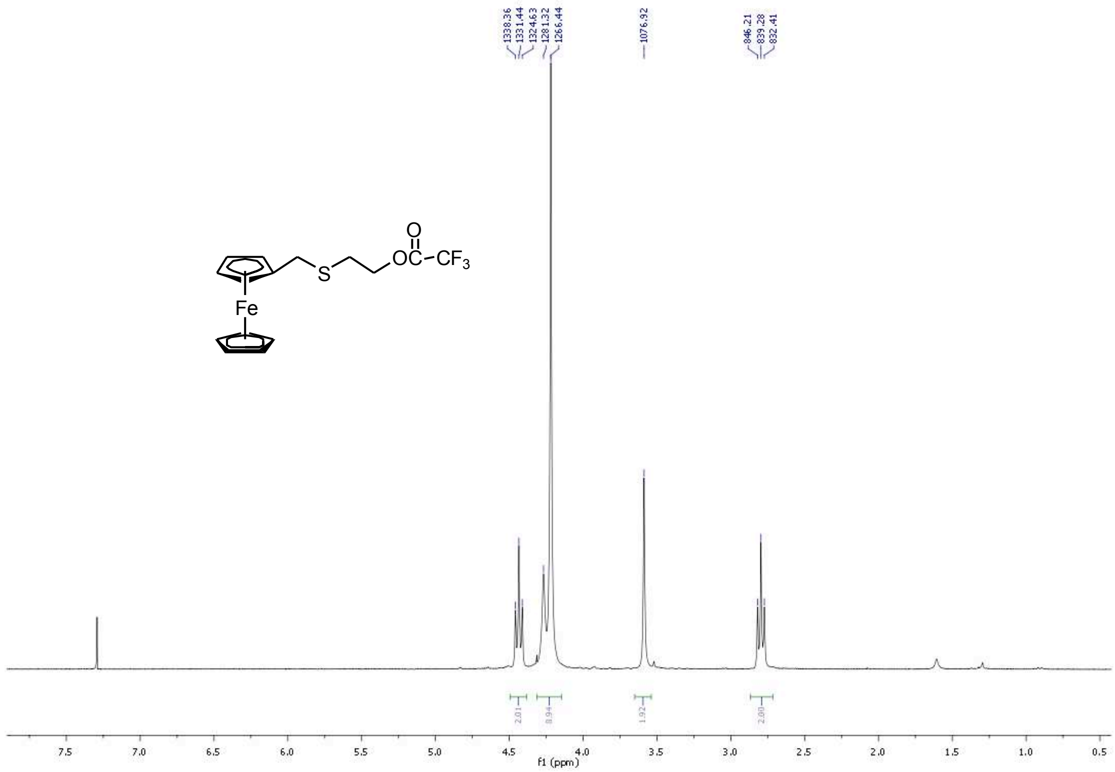
3. Copy of NMR spectra



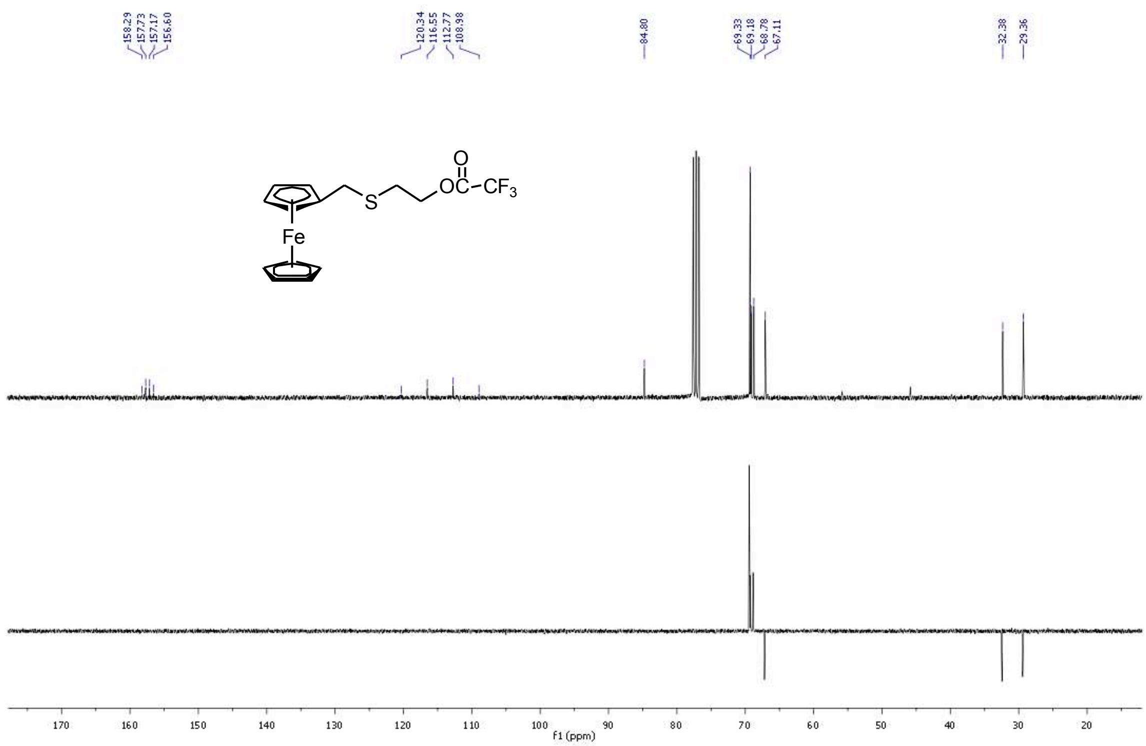
[1]H-NMR spectra of compound **3**



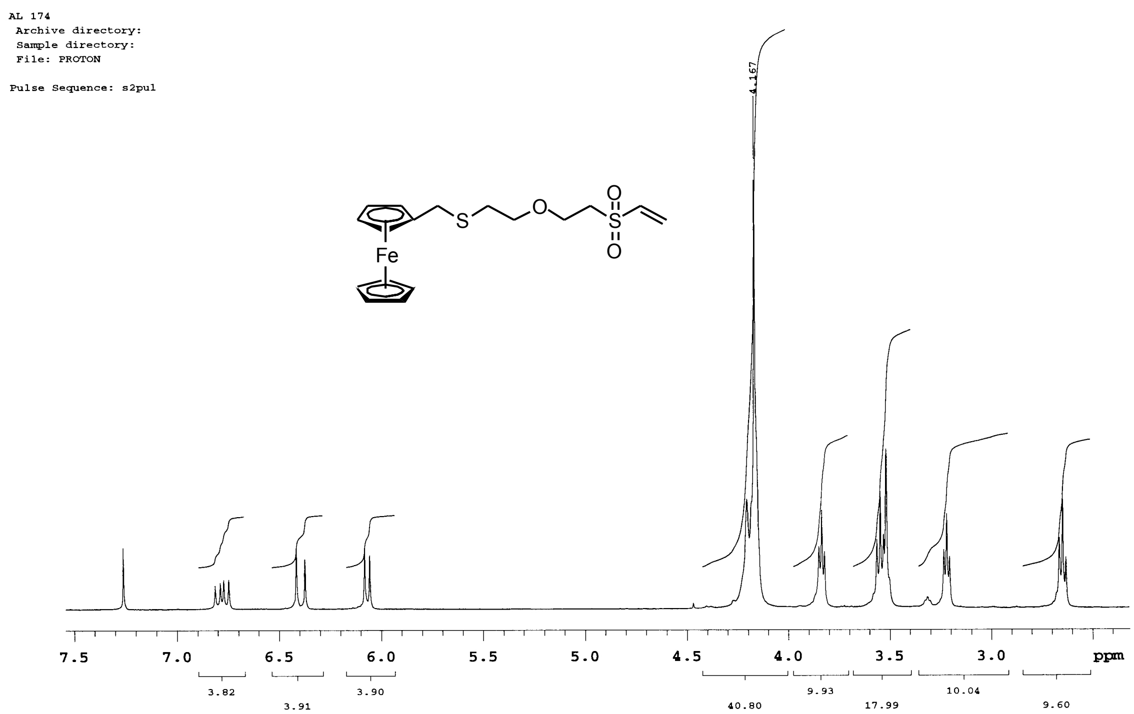
[13]C NMR spectra of compound **3**



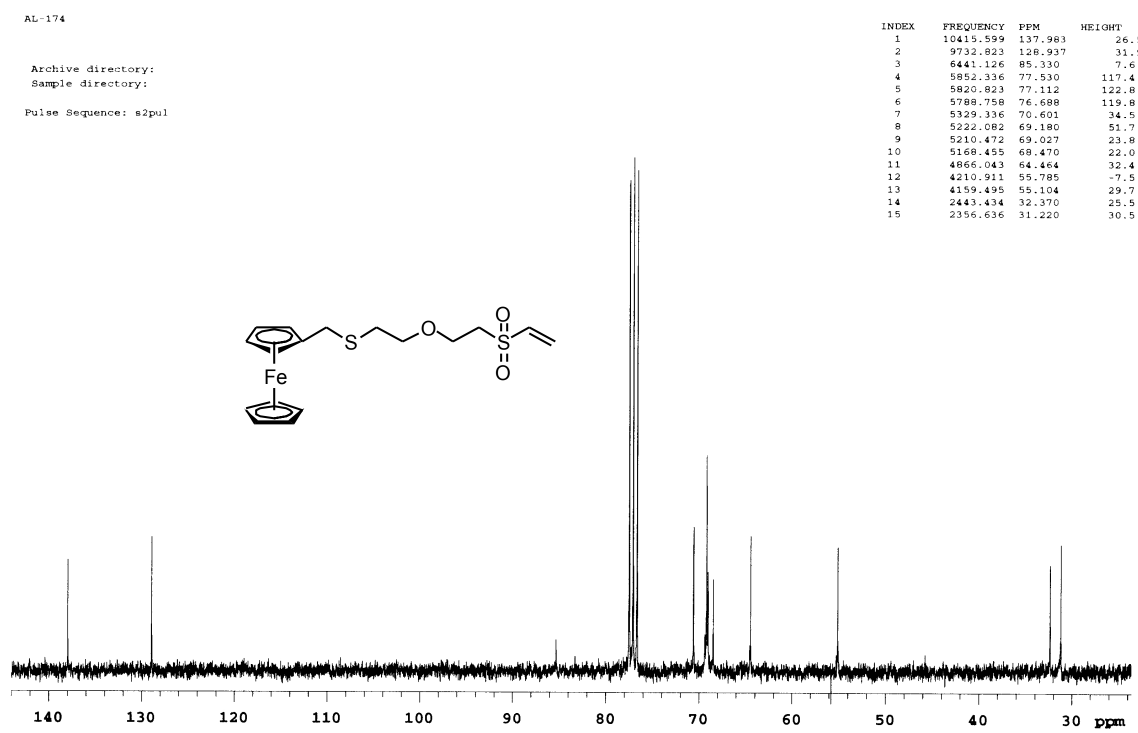
[1]H-NMR spectra of compound **4**



[13]C and DEPT-NMR spectra of compound **4**

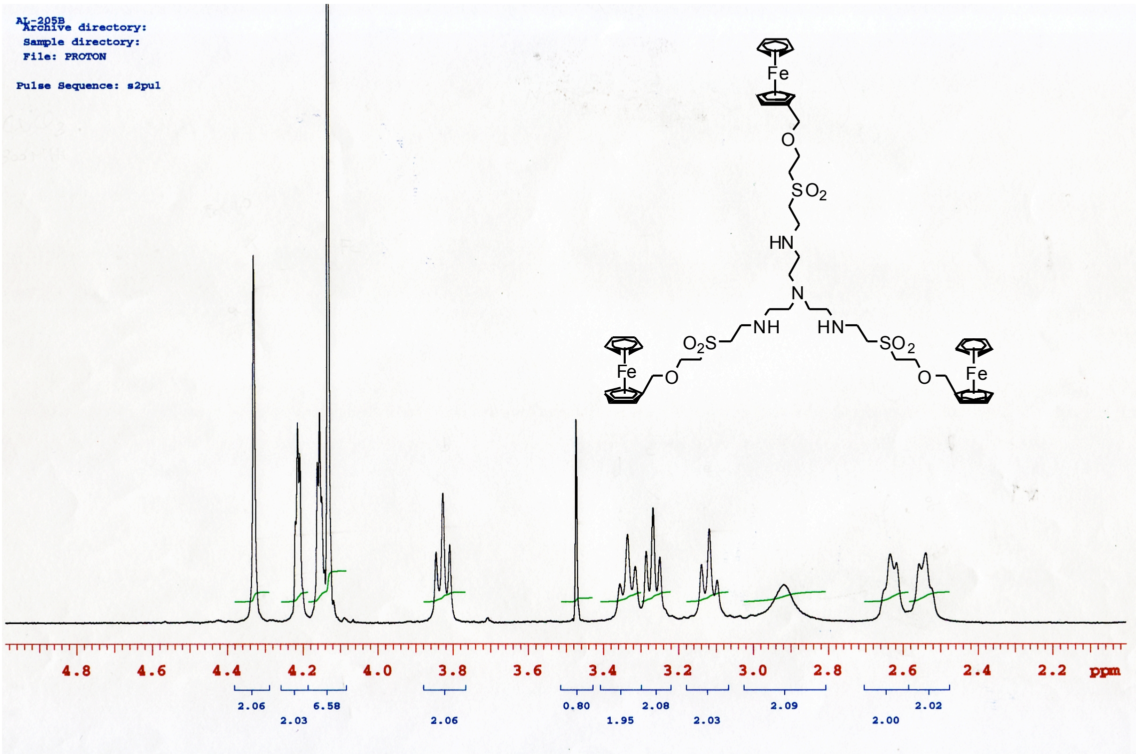


[1]H-NMR spectra of compound **5**

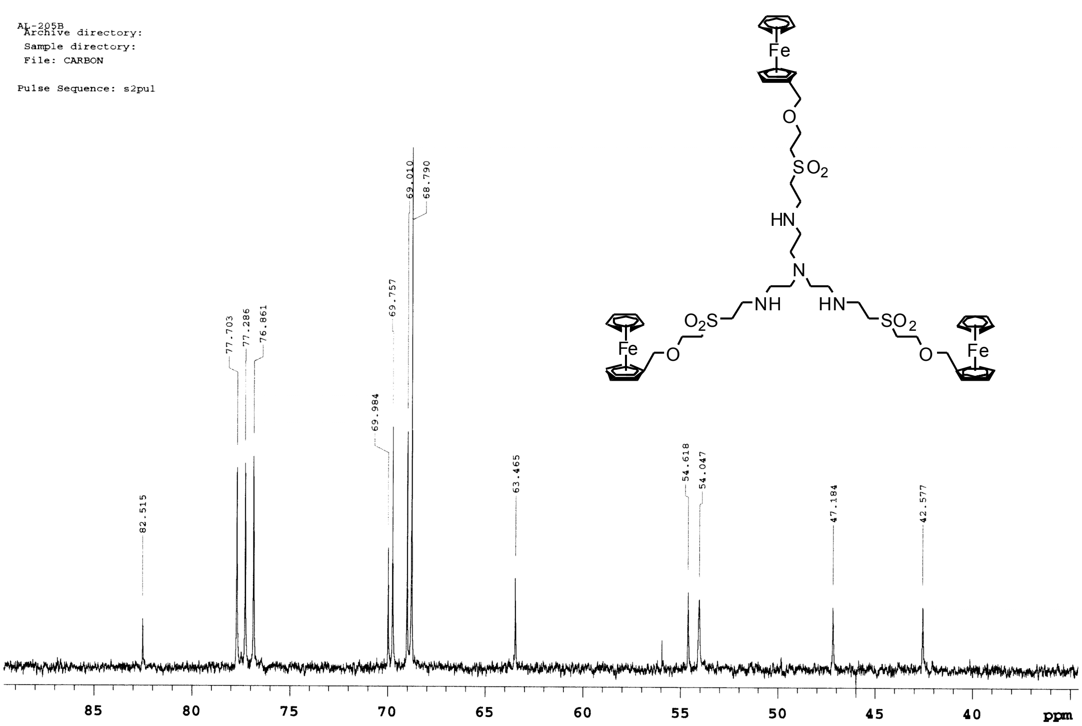


INDEX	FREQUENCY	PPM	HEIGHT
1	10415.599	137.983	26.5
2	9732.823	128.937	31.9
3	6441.126	85.330	7.6
4	5852.336	77.530	117.4
5	5820.823	77.112	122.8
6	5788.758	76.688	119.8
7	5329.336	70.601	34.5
8	5222.082	69.180	51.7
9	5210.472	69.027	23.8
10	5168.455	68.470	22.0
11	4866.043	64.464	32.4
12	4210.911	55.785	-7.5
13	4159.495	55.104	29.7
14	2443.434	32.370	25.5
15	2356.636	31.220	30.5

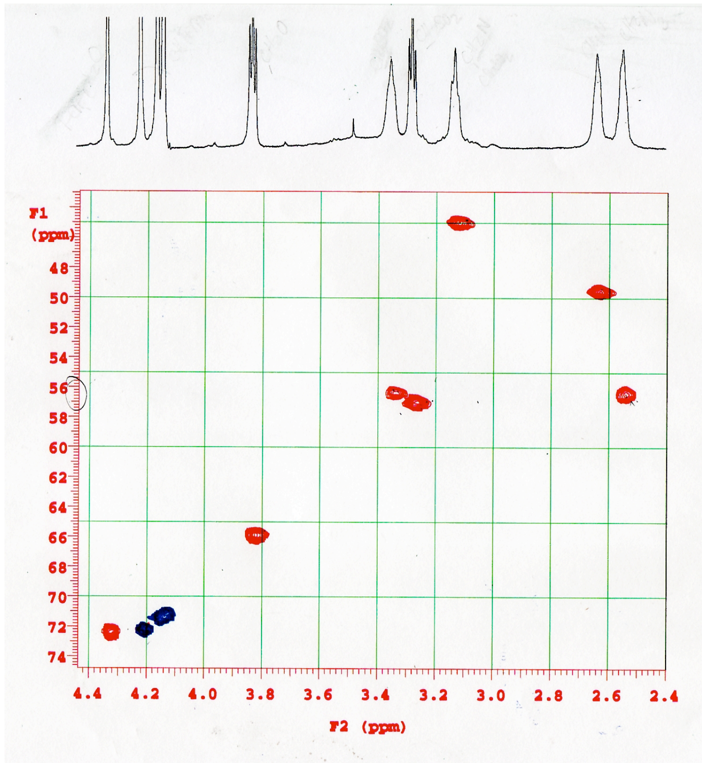
[13]C NMR spectra of compound **5**



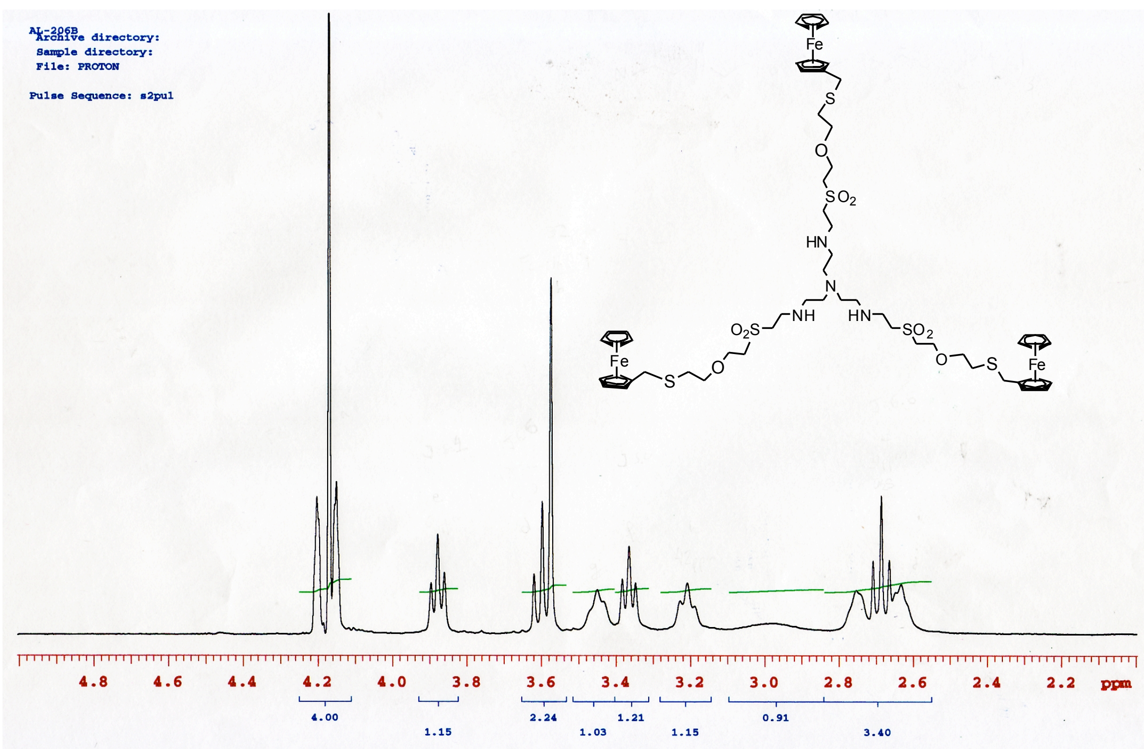
^{1}H-NMR spectra of compound **7**



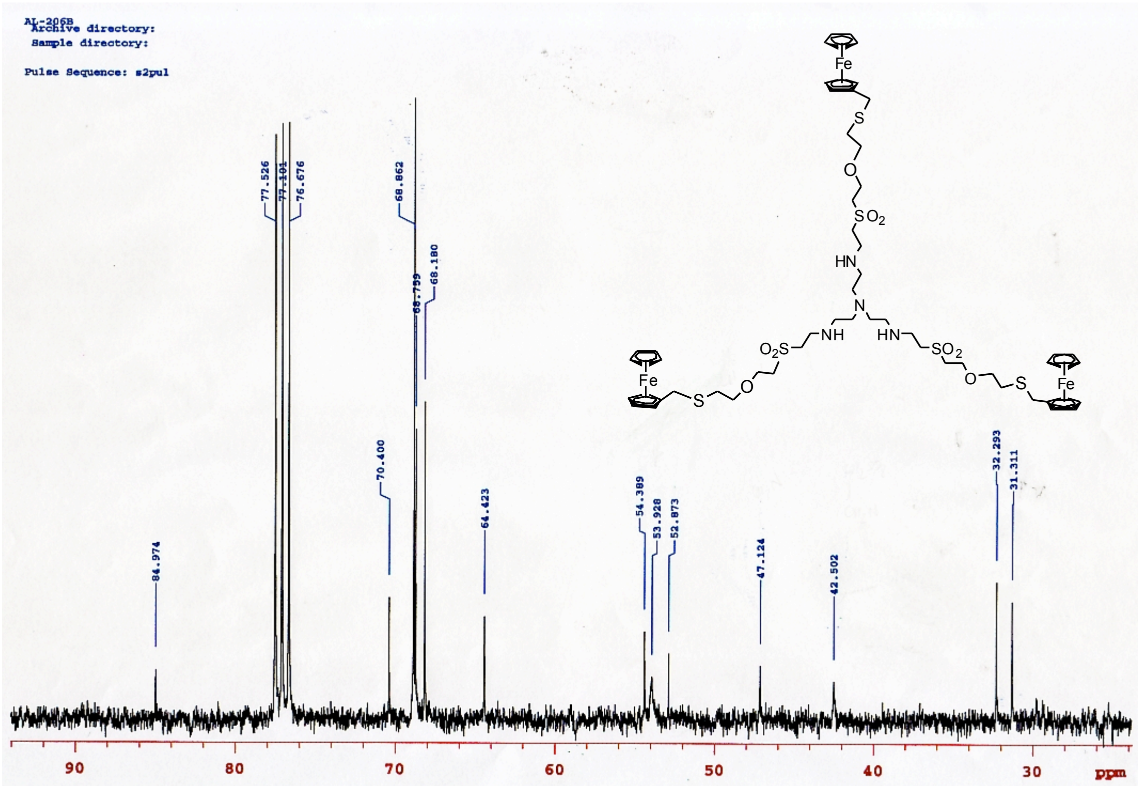
^{13}C-NMR spectra of compound **7**



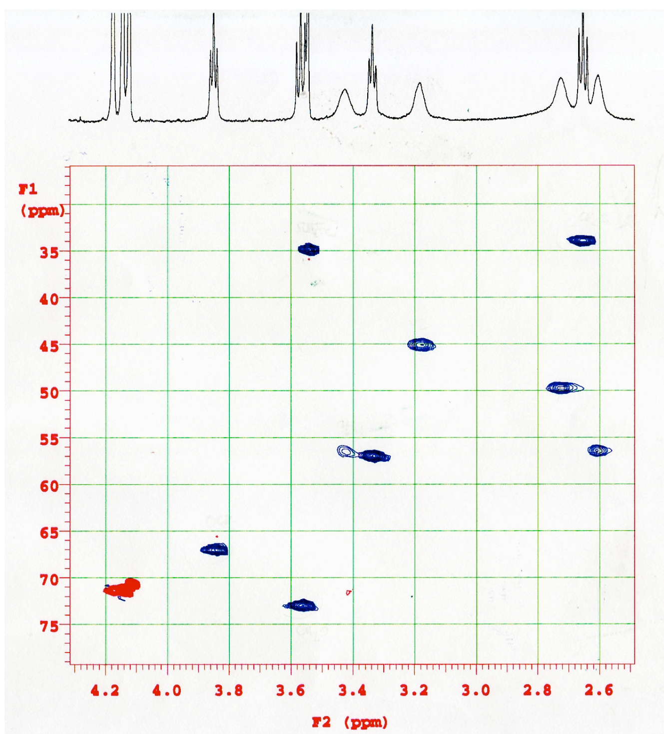
HSQC spectra of compound **7**



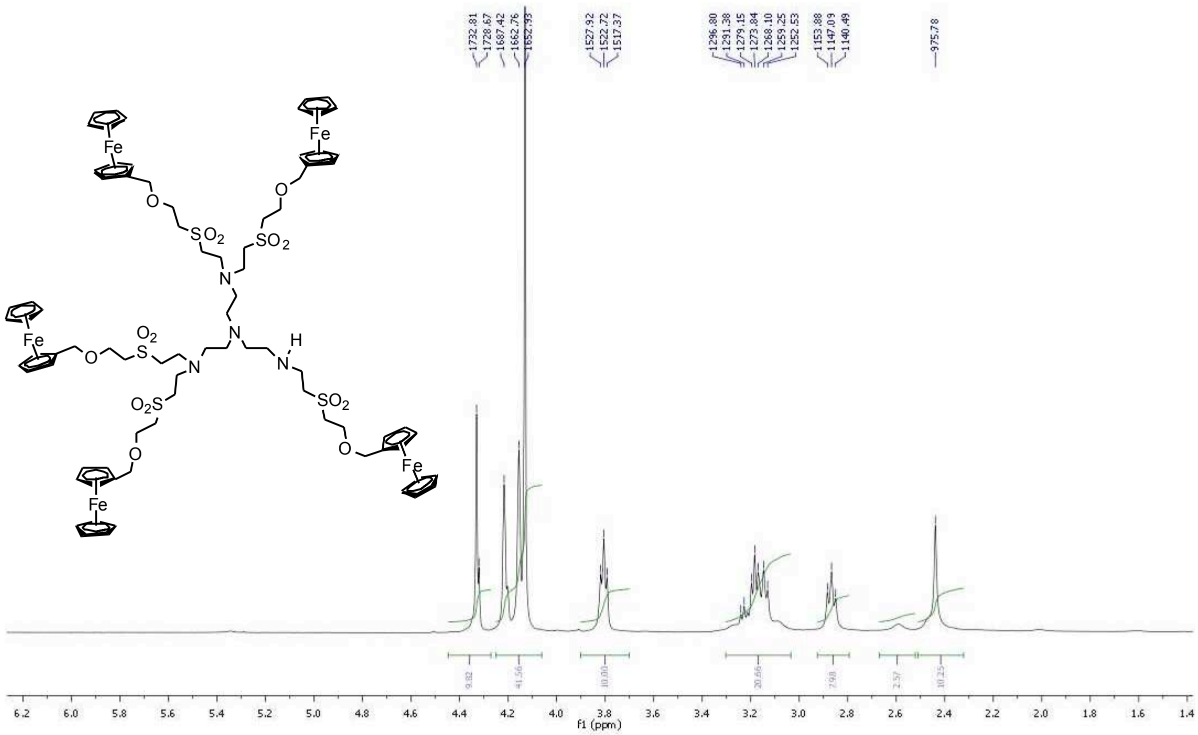
^{1}H-NMR spectra of compound **8**



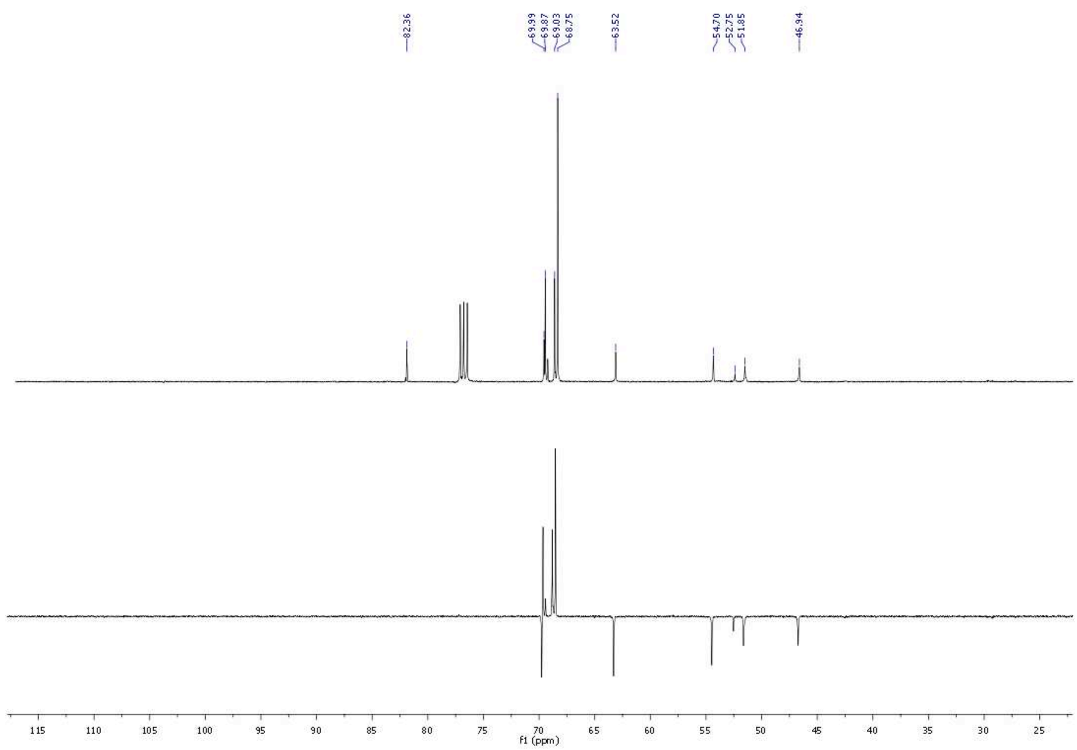
^{13}C-NMR spectra of compound **8**



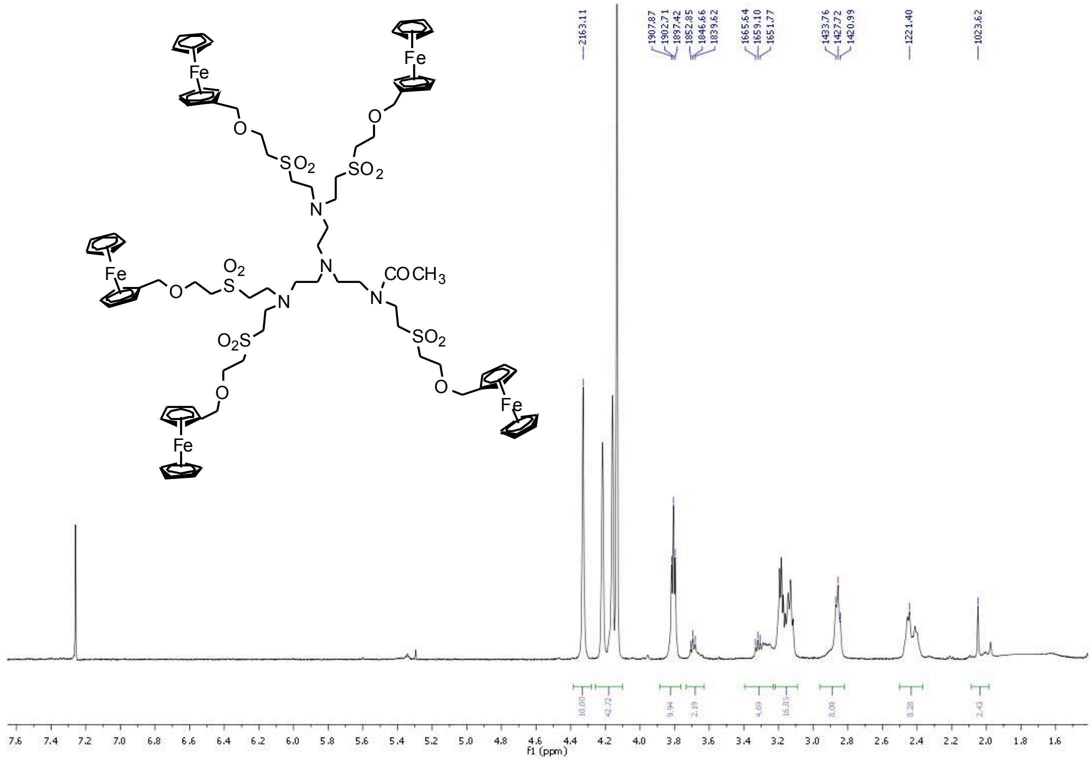
HSQC spectra of compound **8**



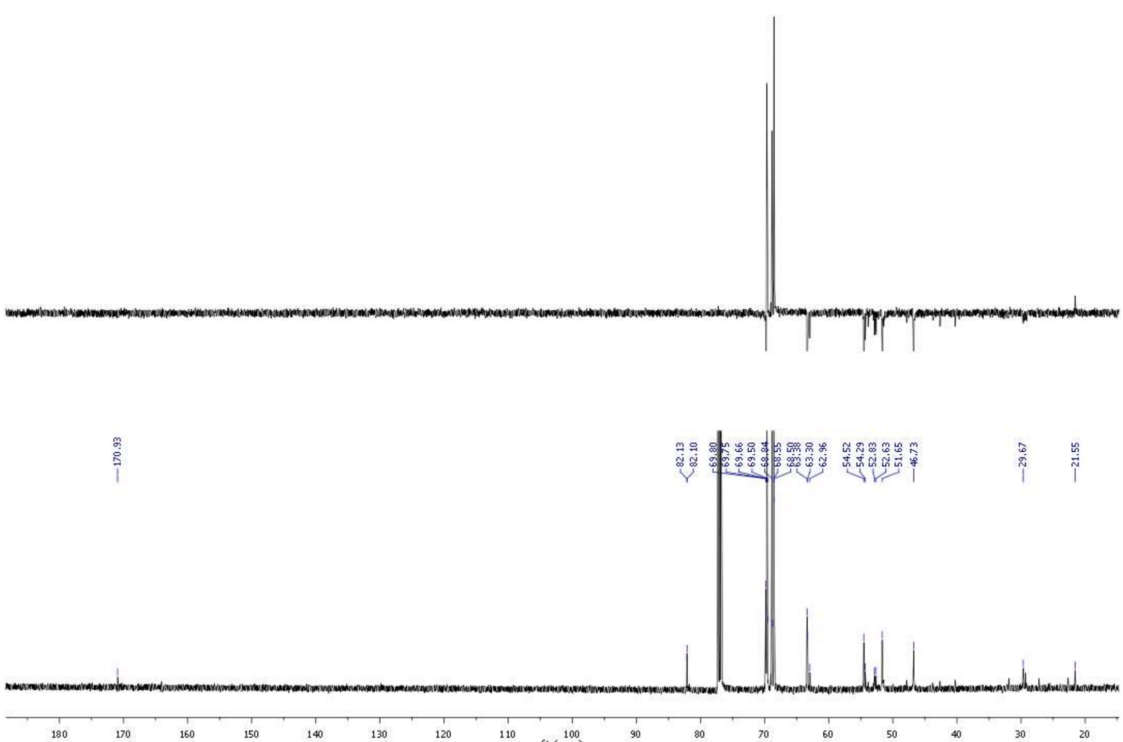
[1]H-NMR spectra of compound **9**



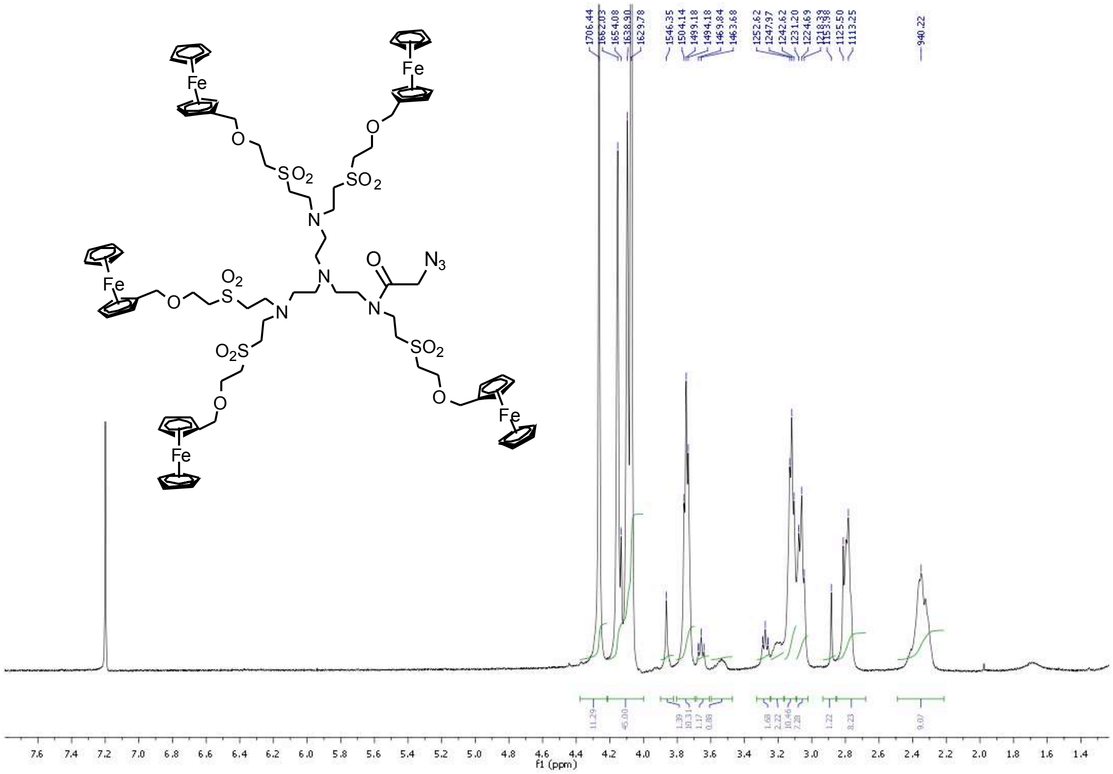
[13]C and DEPT-NMR spectra of compound **9**



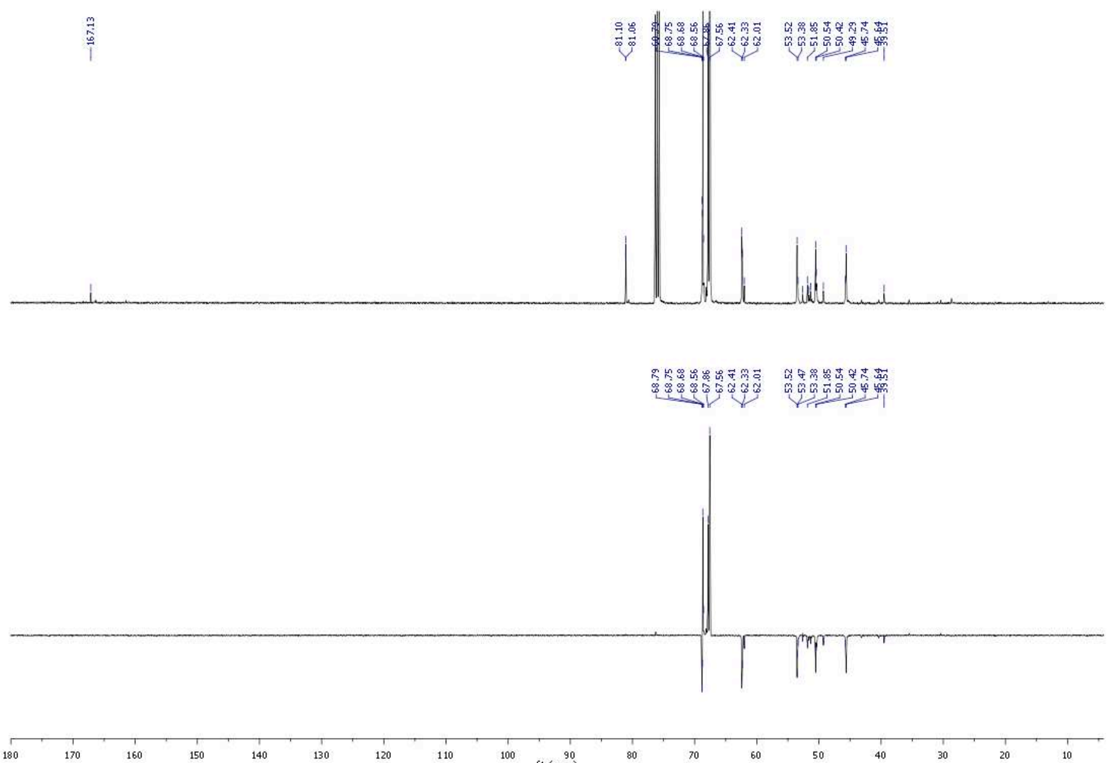
^{1}H-NMR spectra of compound **10**



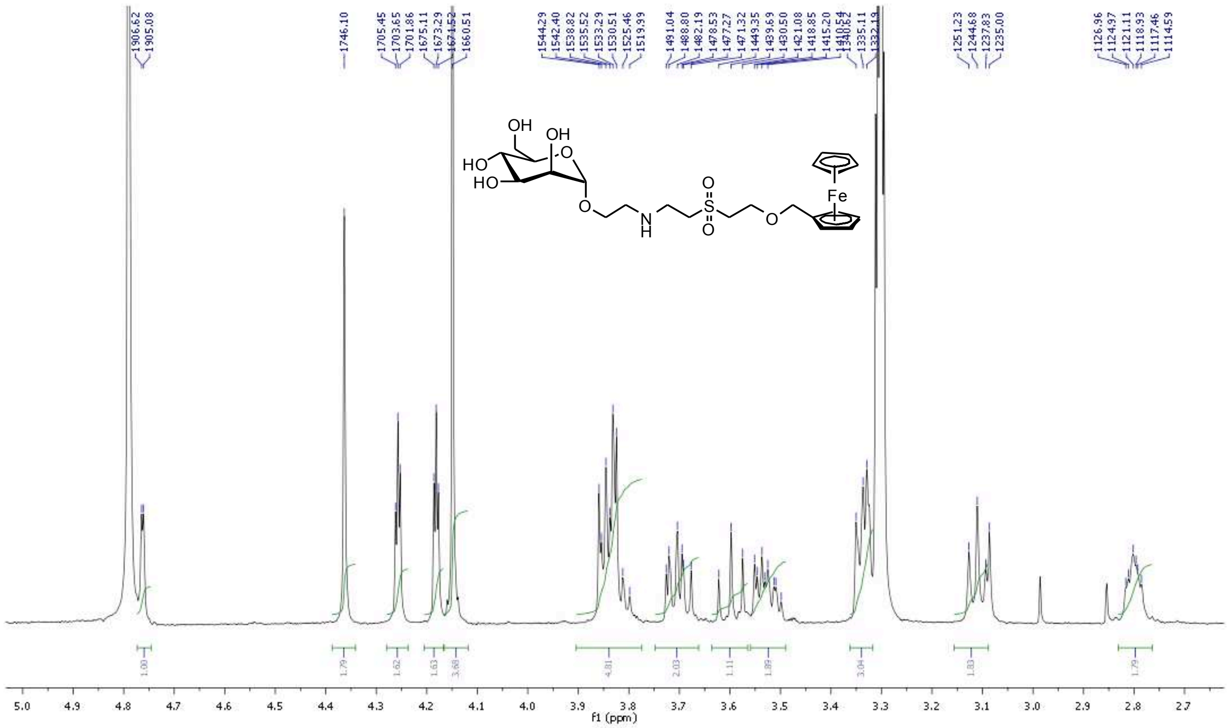
^{13}C and DEPT-NMR spectra of compound **10**



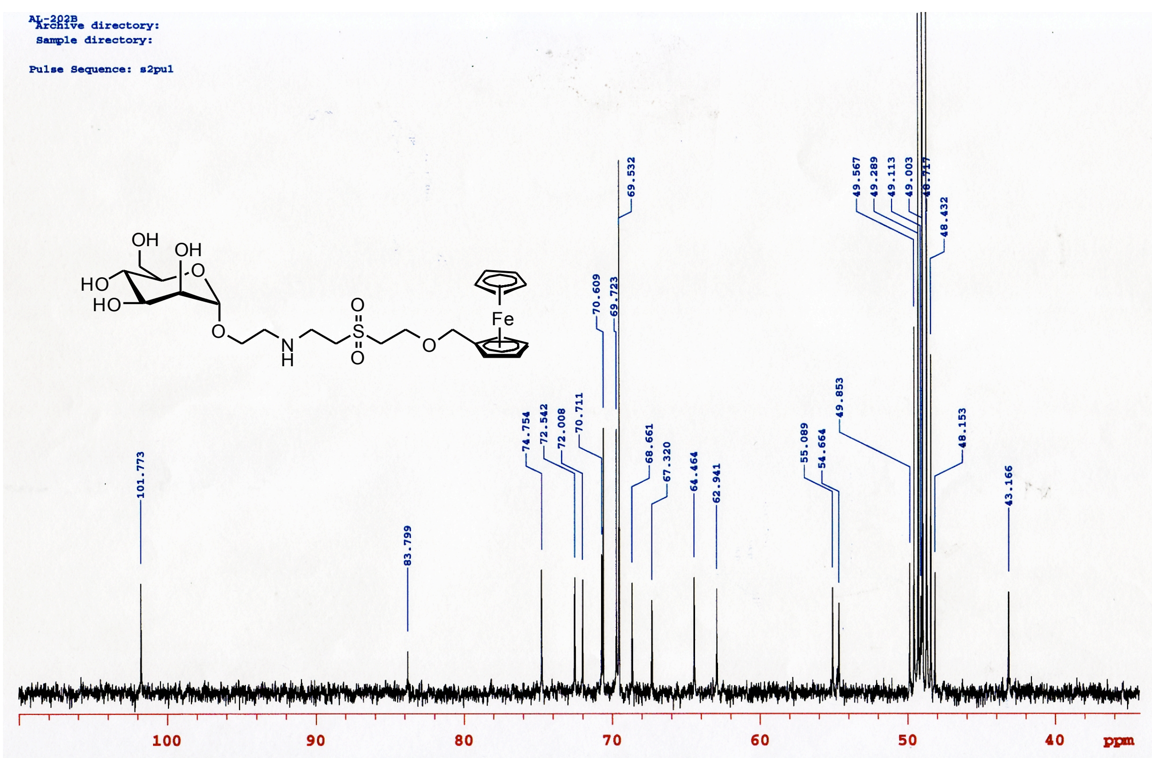
^{1}H-NMR spectra of compound **11**



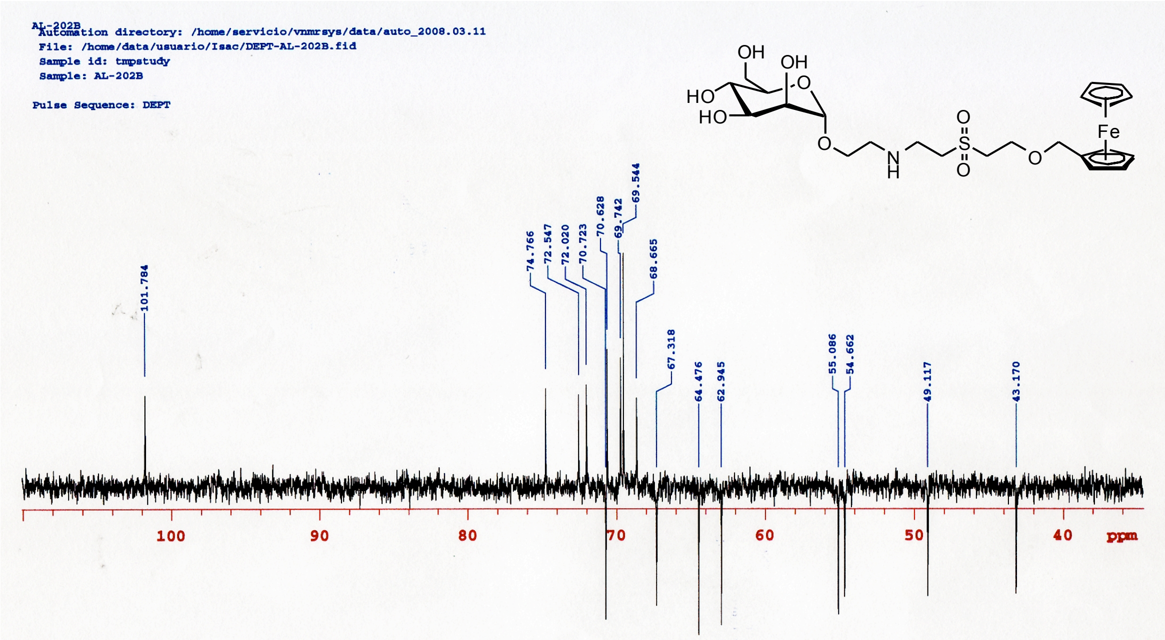
^{13}C and DEPT-NMR spectra of compound **11**



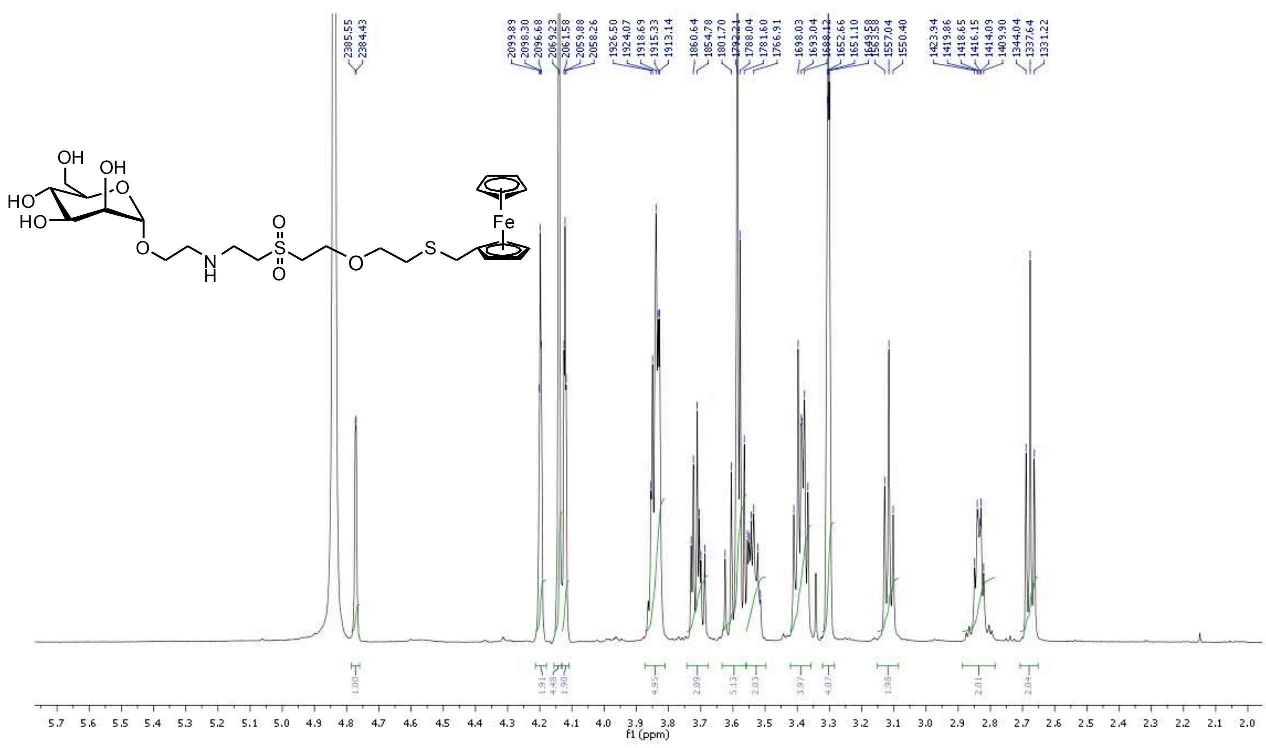
[1]H-NMR spectra of compound **15**



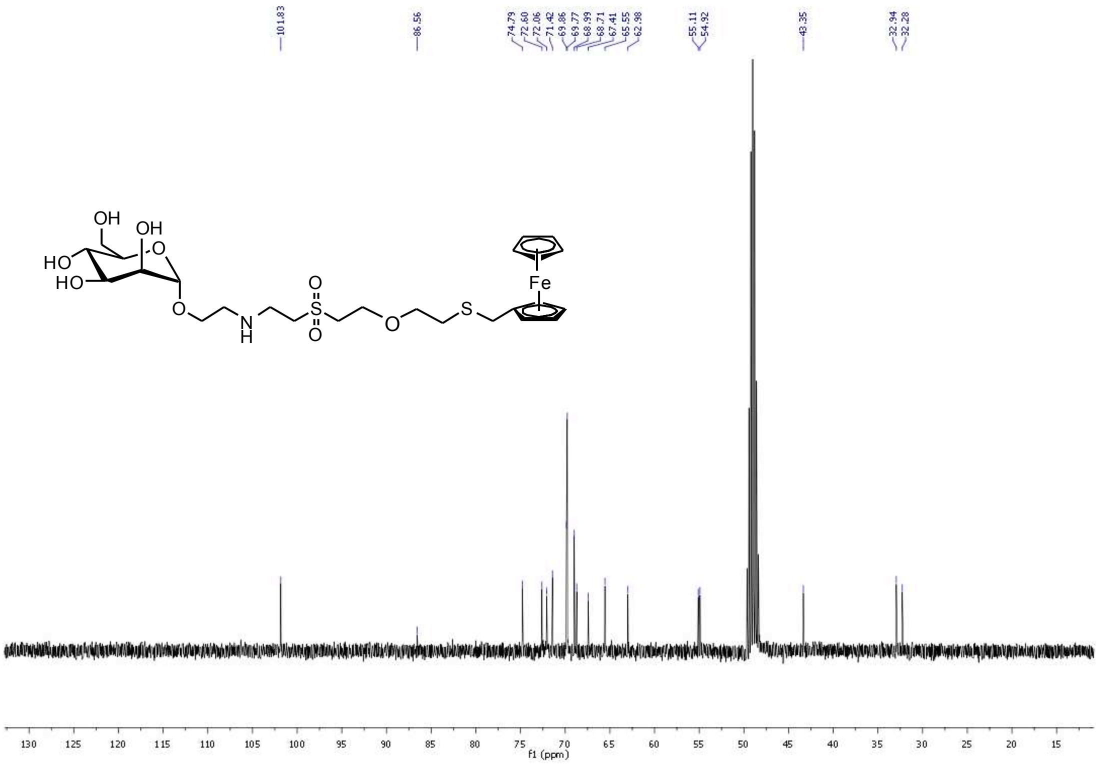
[13]C-NMR spectra of compound **15**



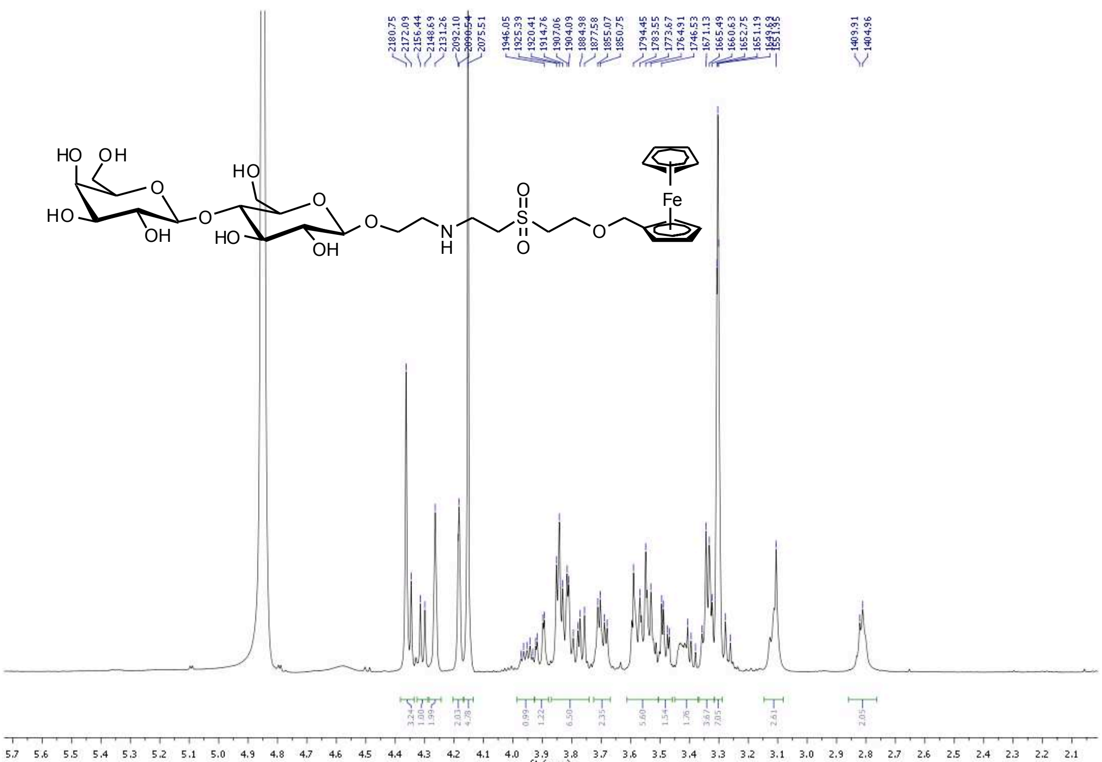
DEPT-NMR spectra of compound **15**



[1]H-NMR spectra of compound **16**



^{13}C-NMR spectra of compound **16**



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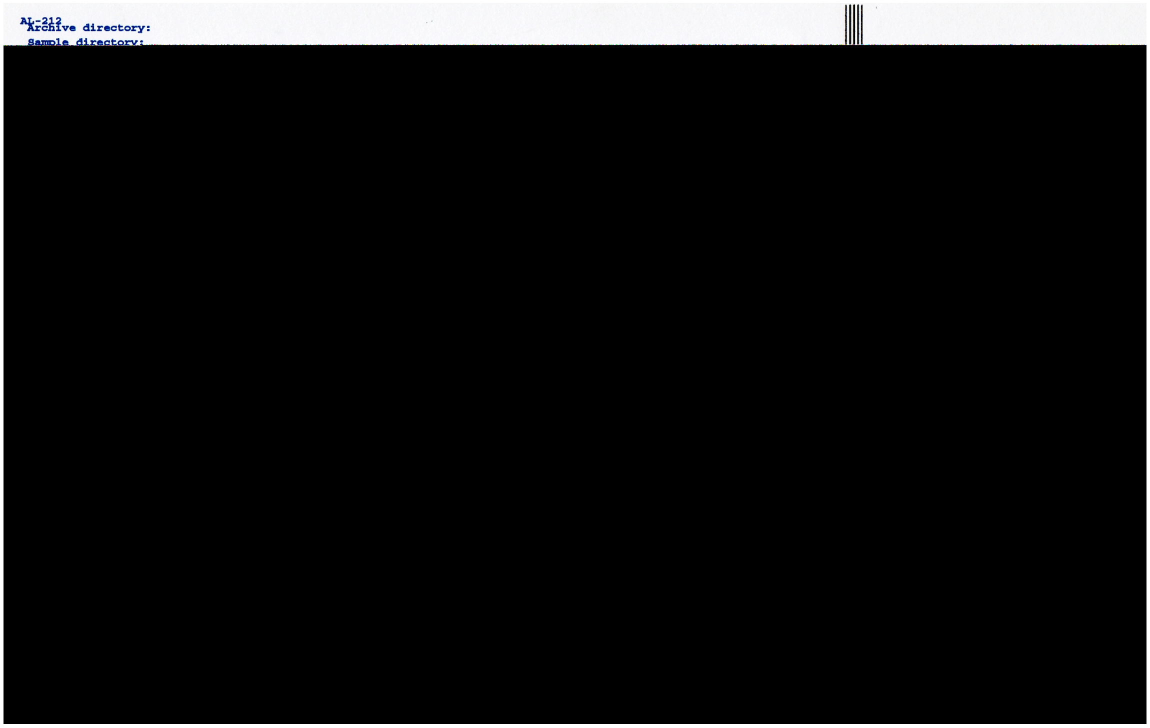
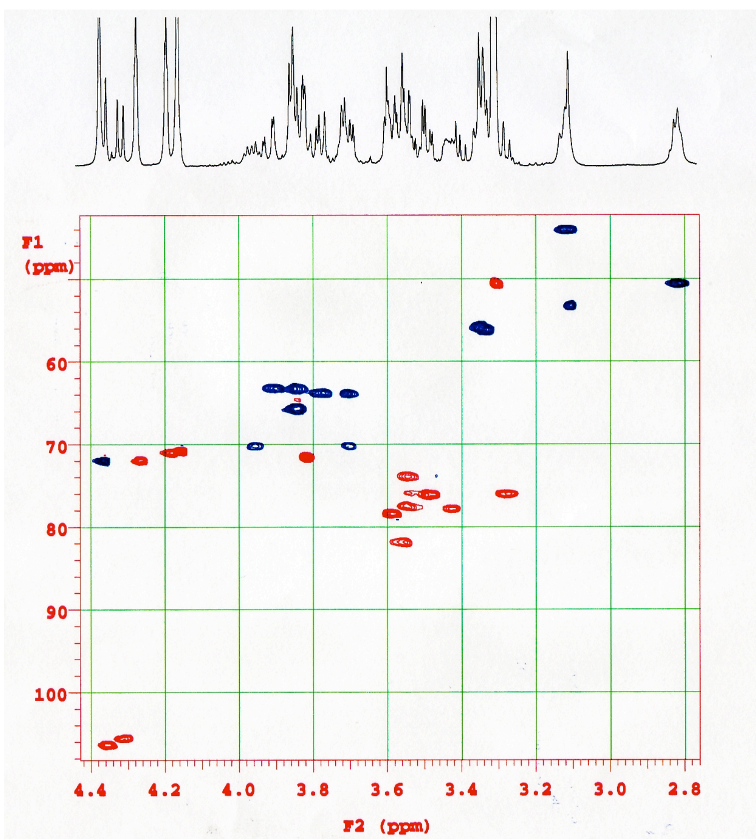
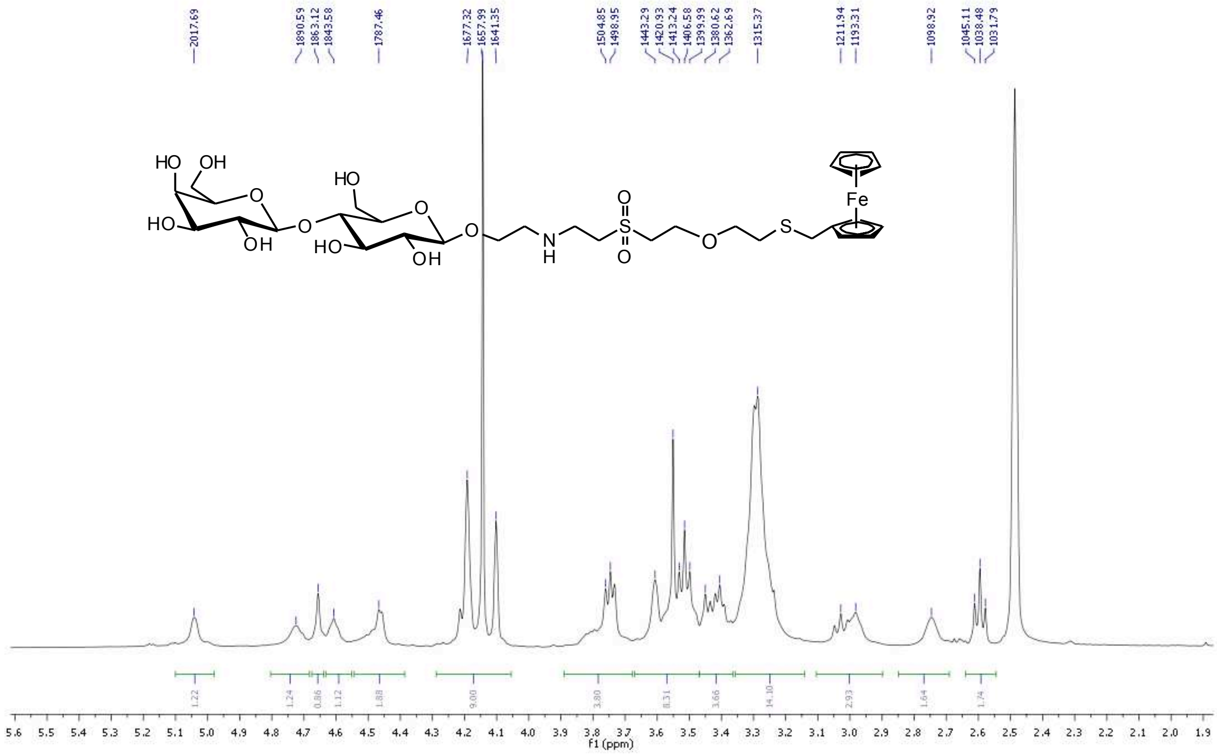


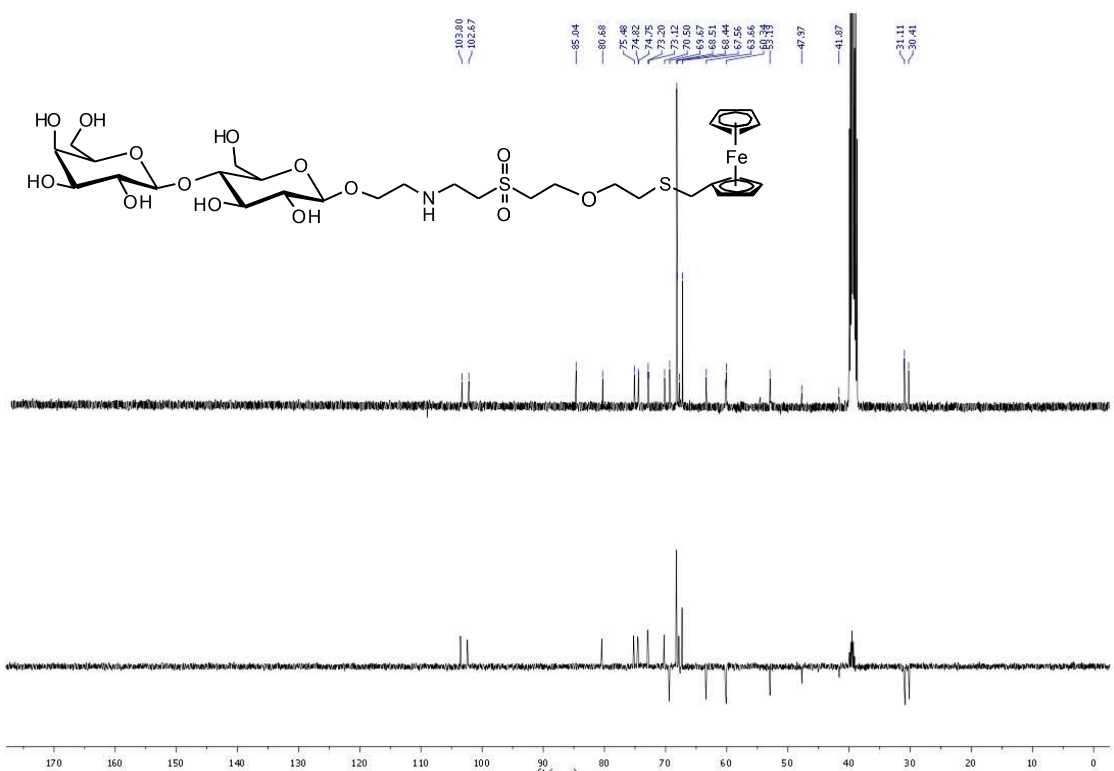
^{13}C-NMR spectra of compound **17**



HSQC spectra of compound **17**



[1]H-NMR spectra of compound **18**



[13]C and DEPT NMR spectra of compound **18**

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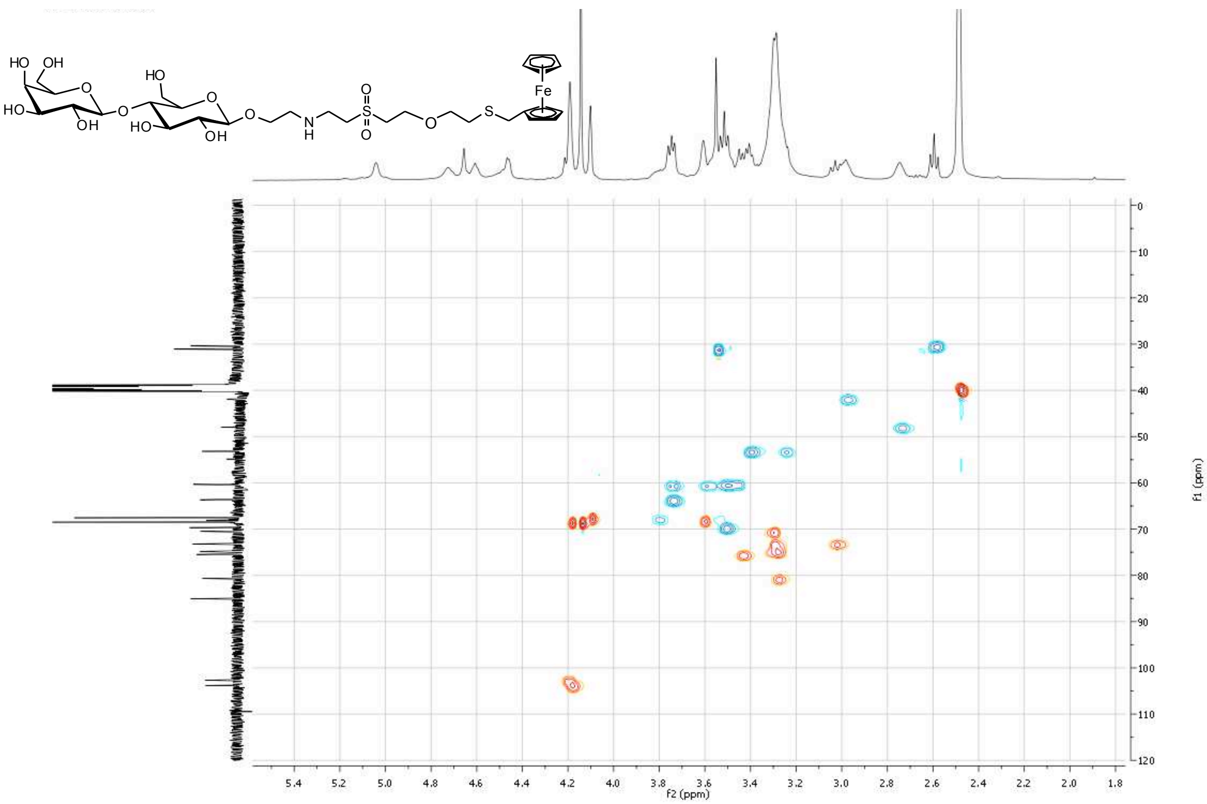
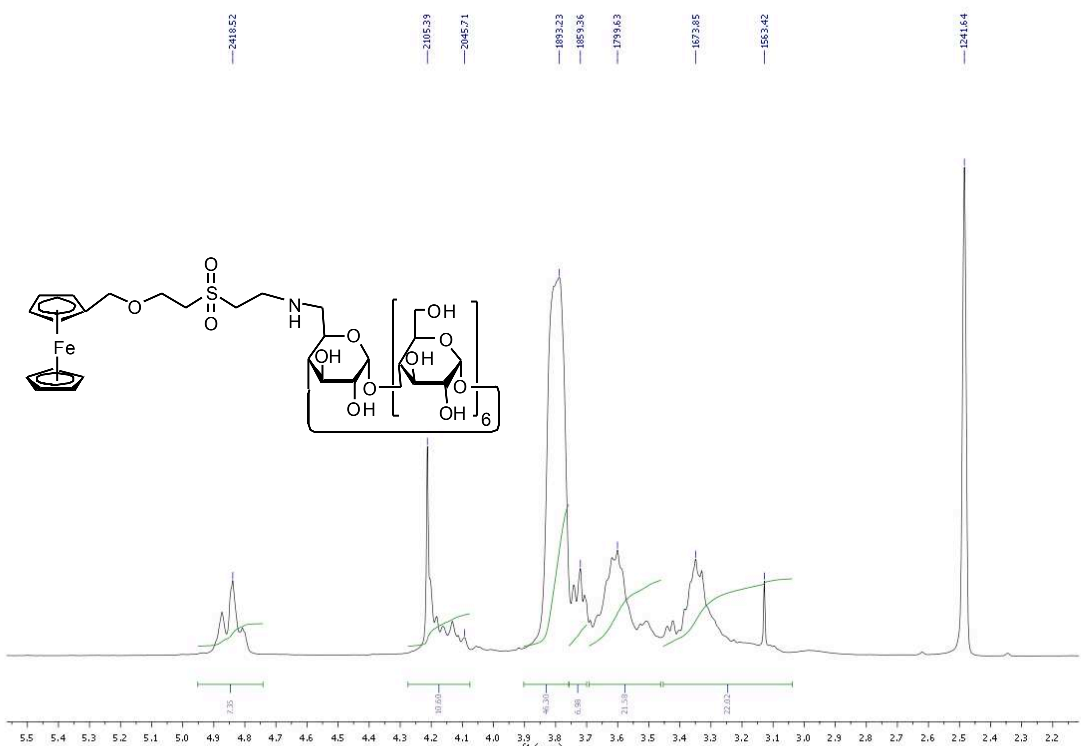
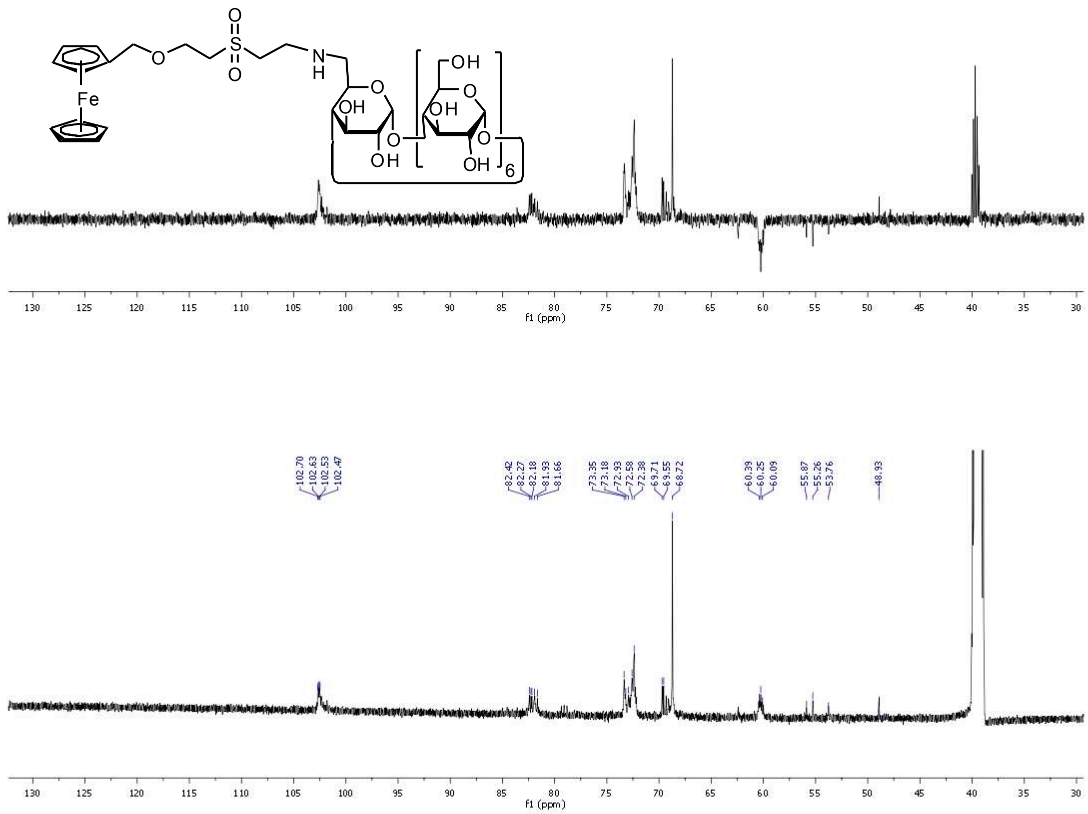


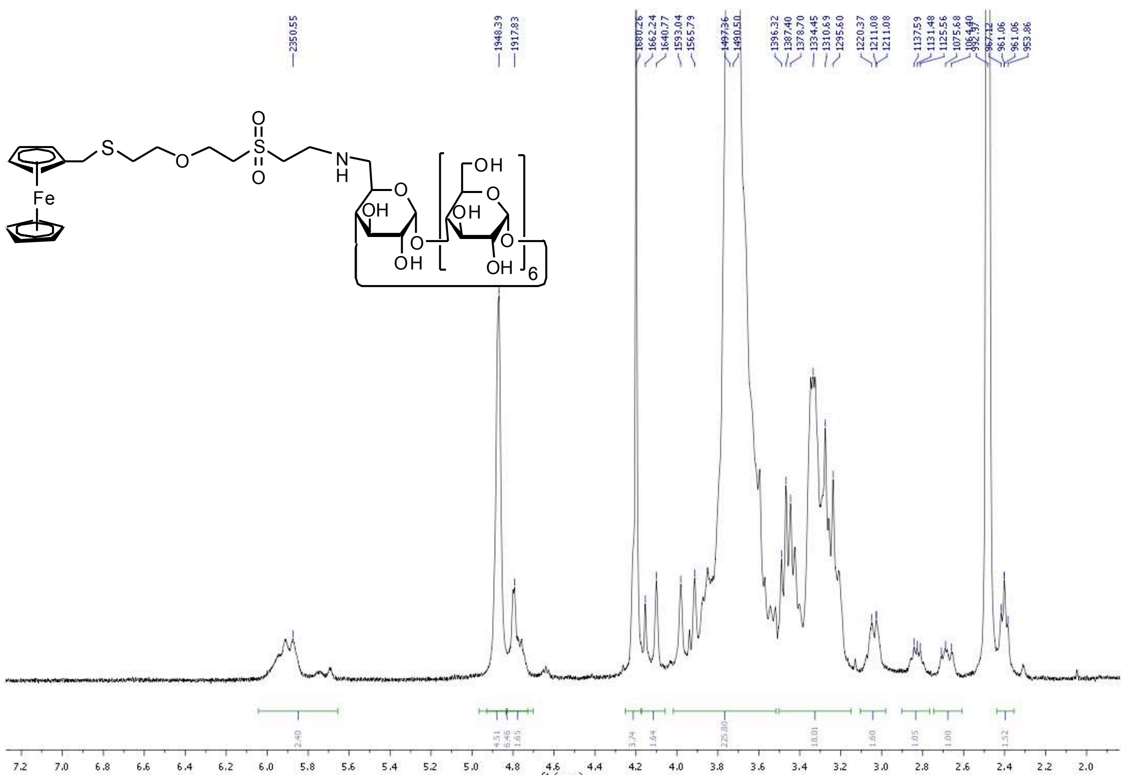
HSQC spectra of compound **18**



^{1}H-NMR spectra of compound **19**



^{13}C and DEPT-NMR spectra of compound **19**



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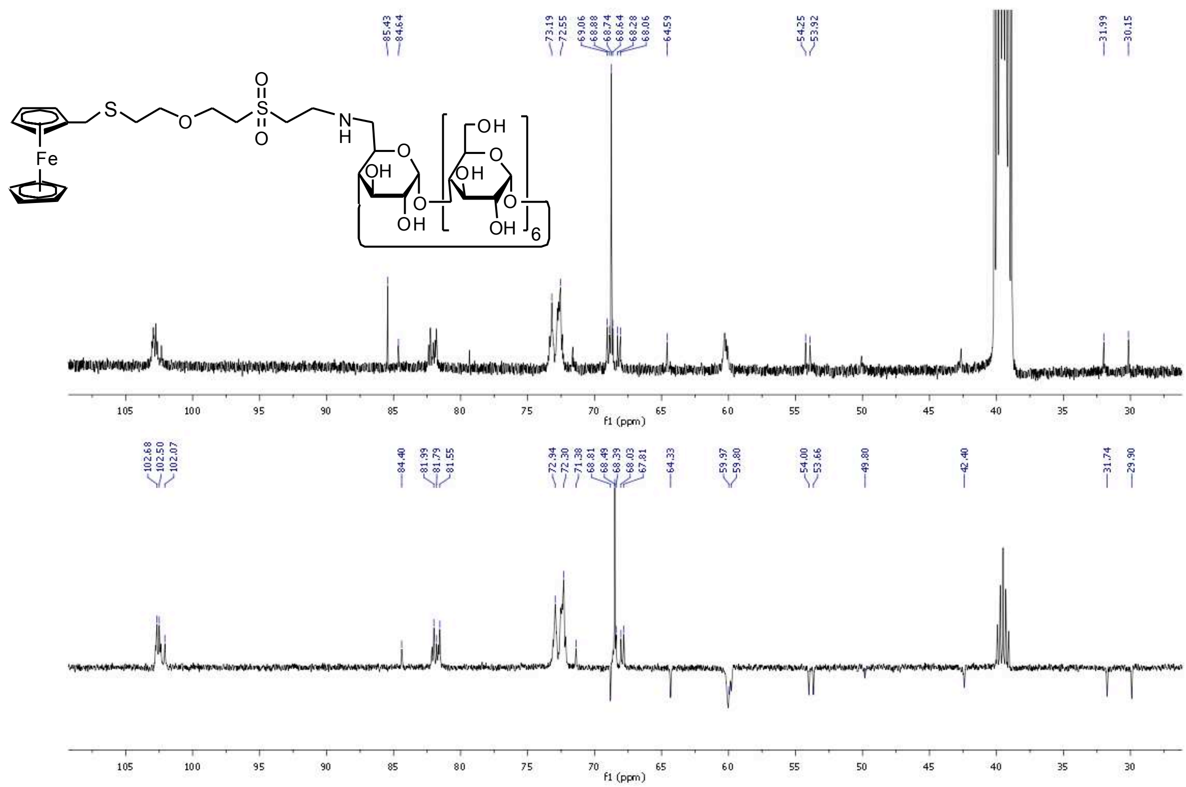
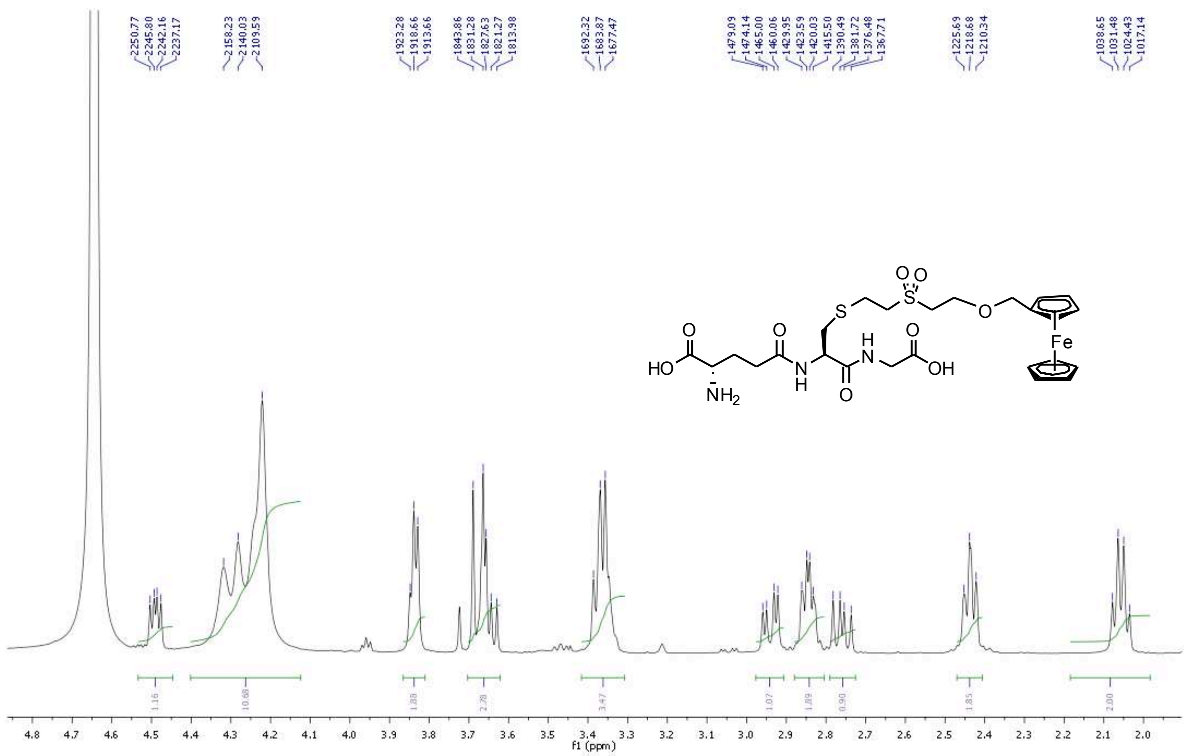
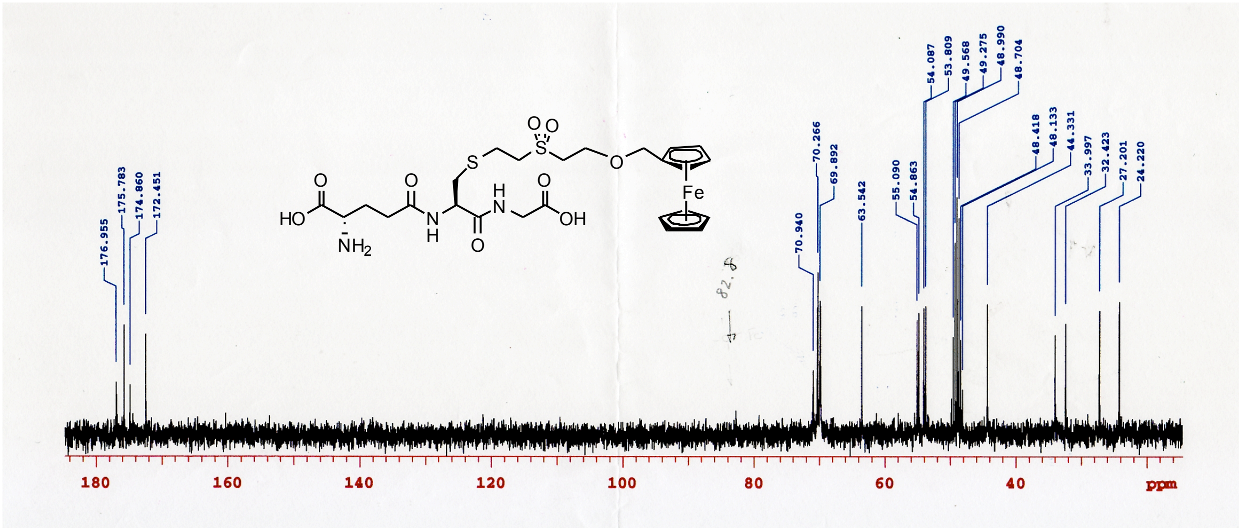


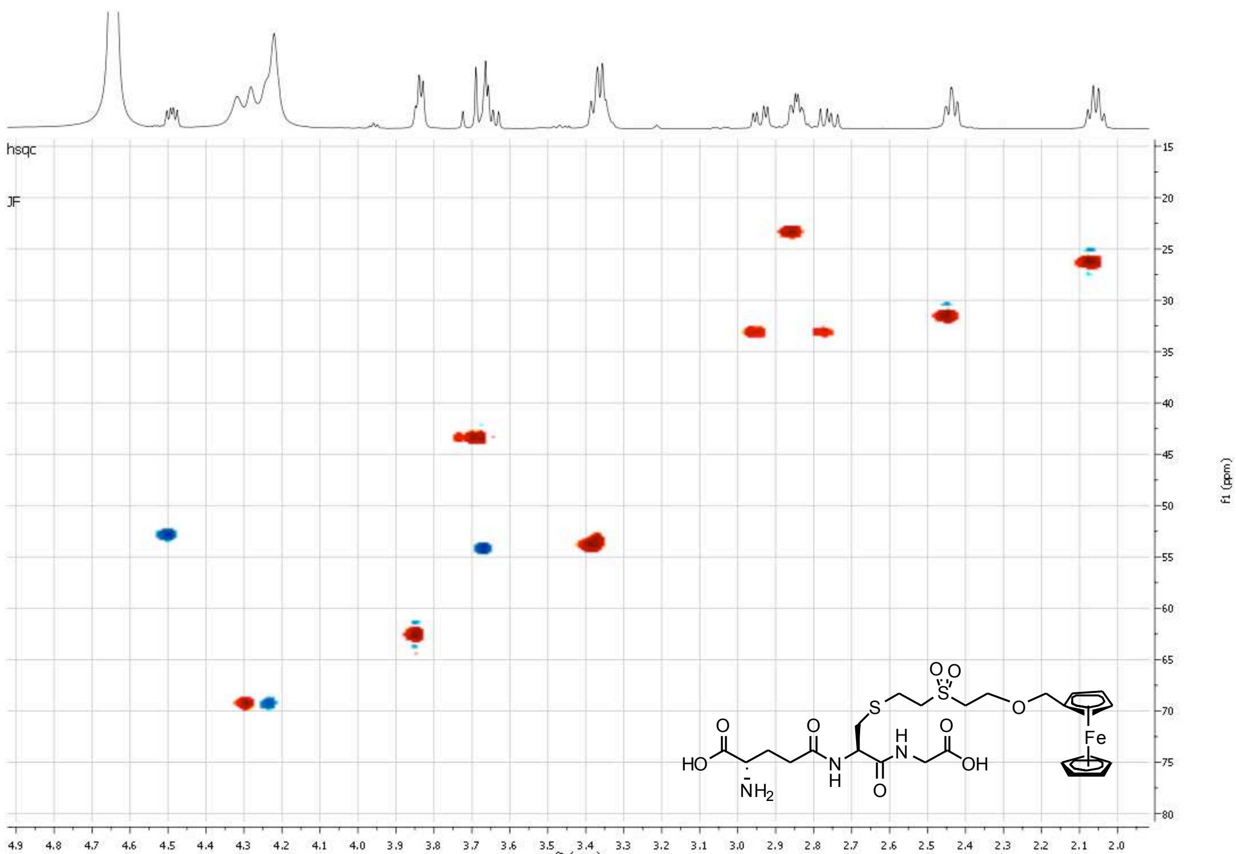
^{13}C and DEPT-NMR spectra of compound **20**



^{1}H-NMR spectra of compound **23**



^{13}C-NMR spectra of compound **23**



HSQC spectra of compound **23**

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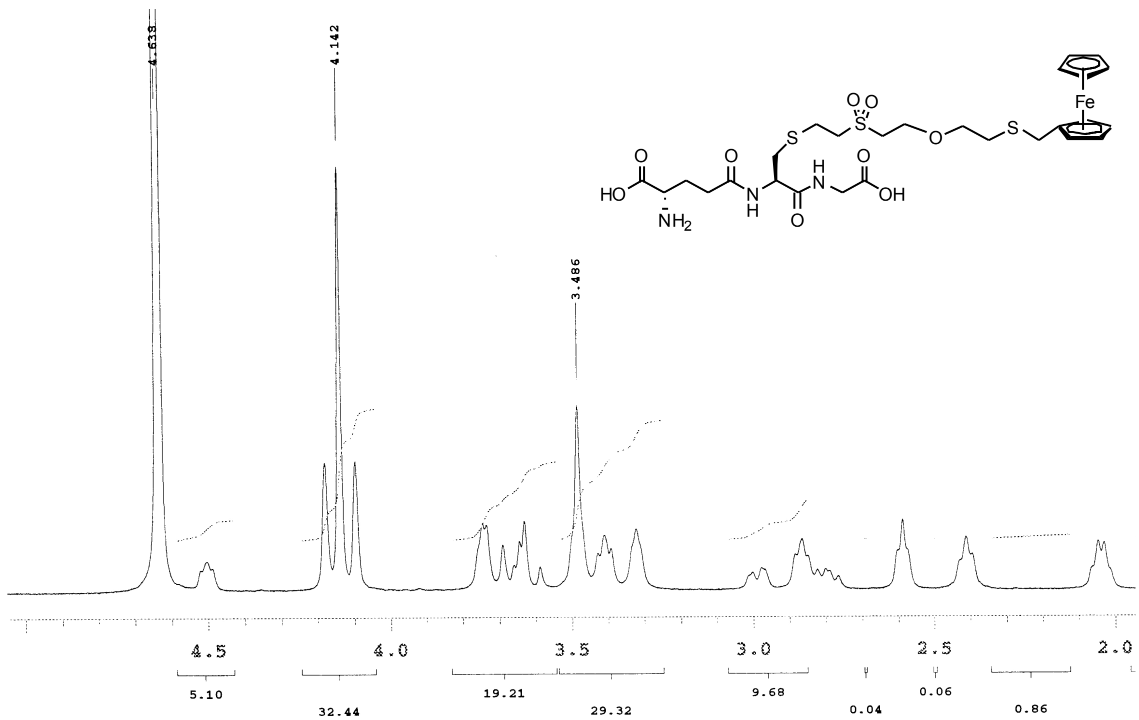

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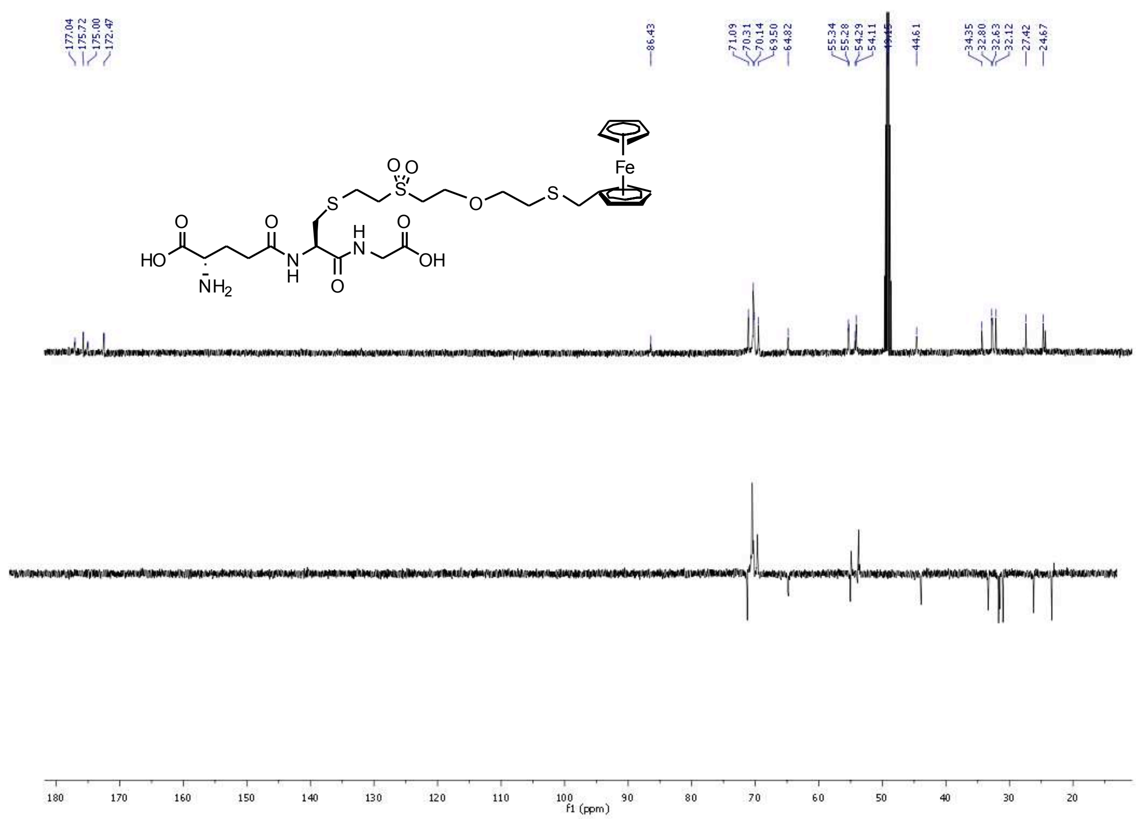
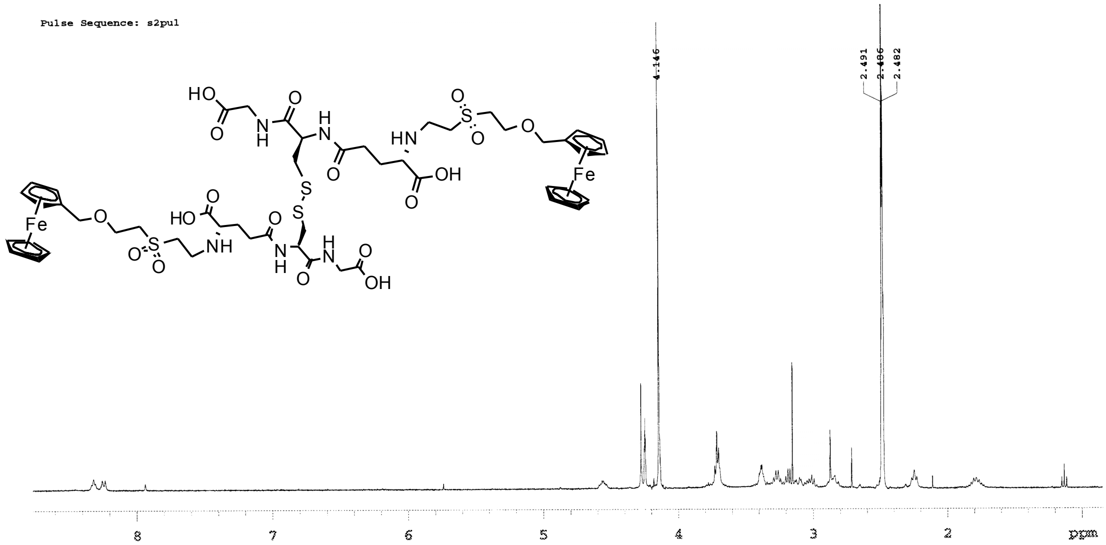
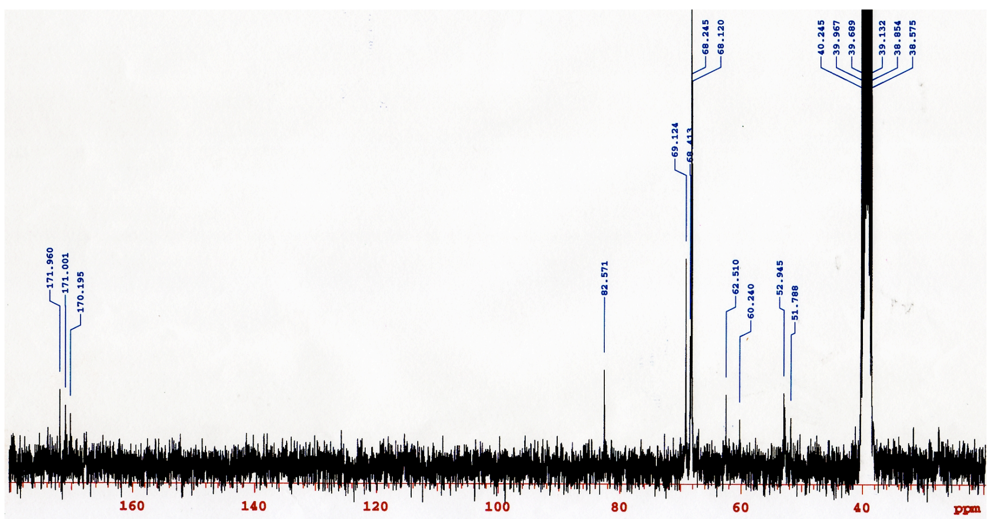
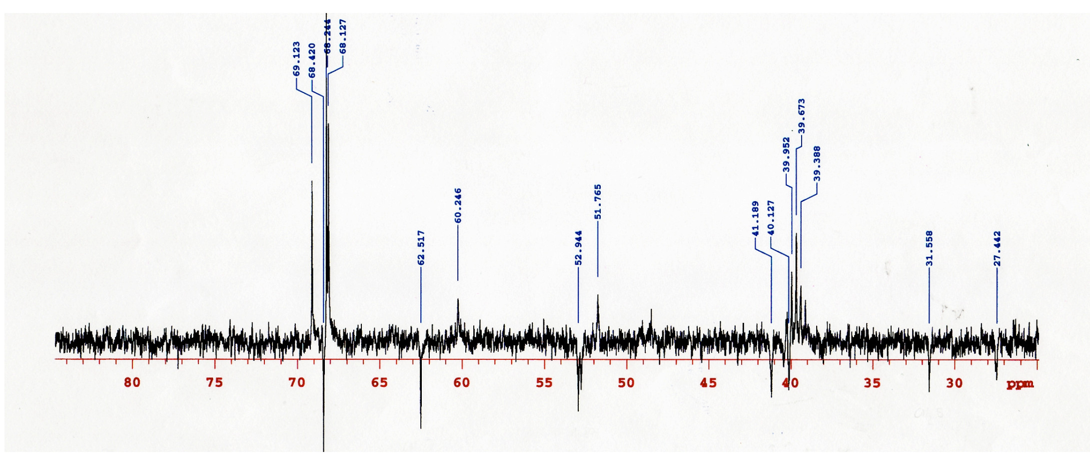


[13]C and DEPT-NMR spectra of compound **24**

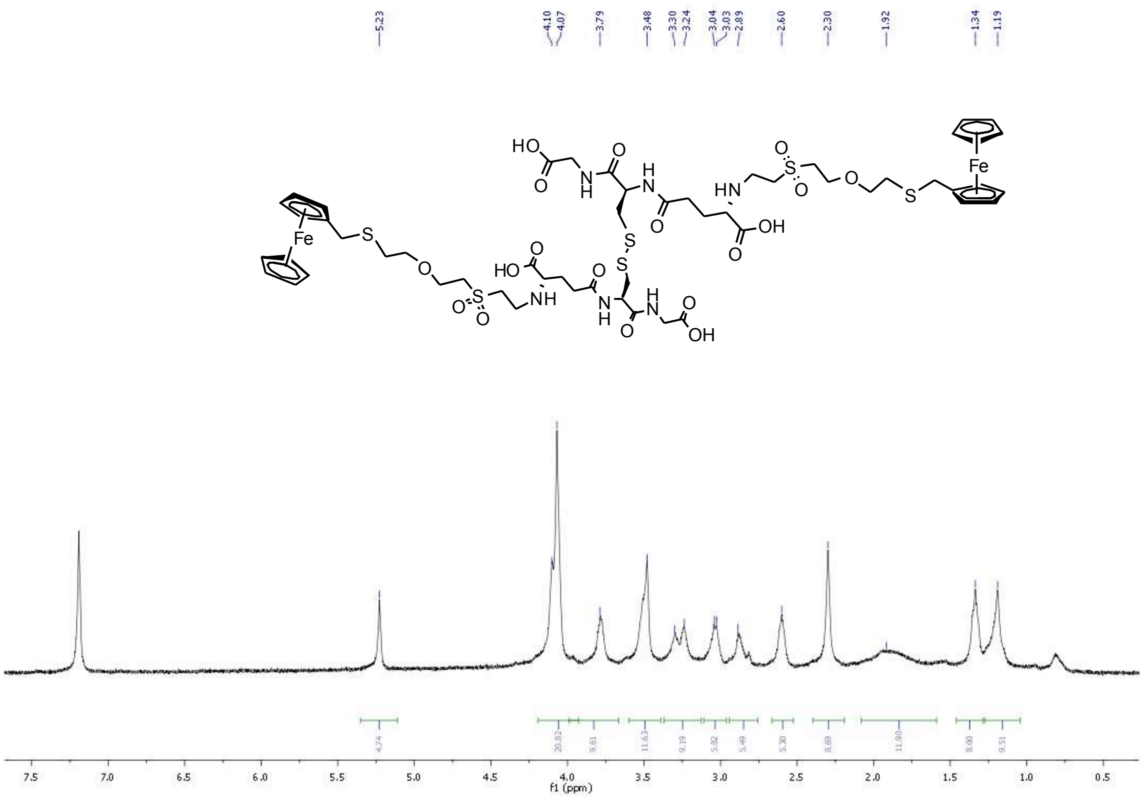


^{1}H-NMR spectra of compound **25**

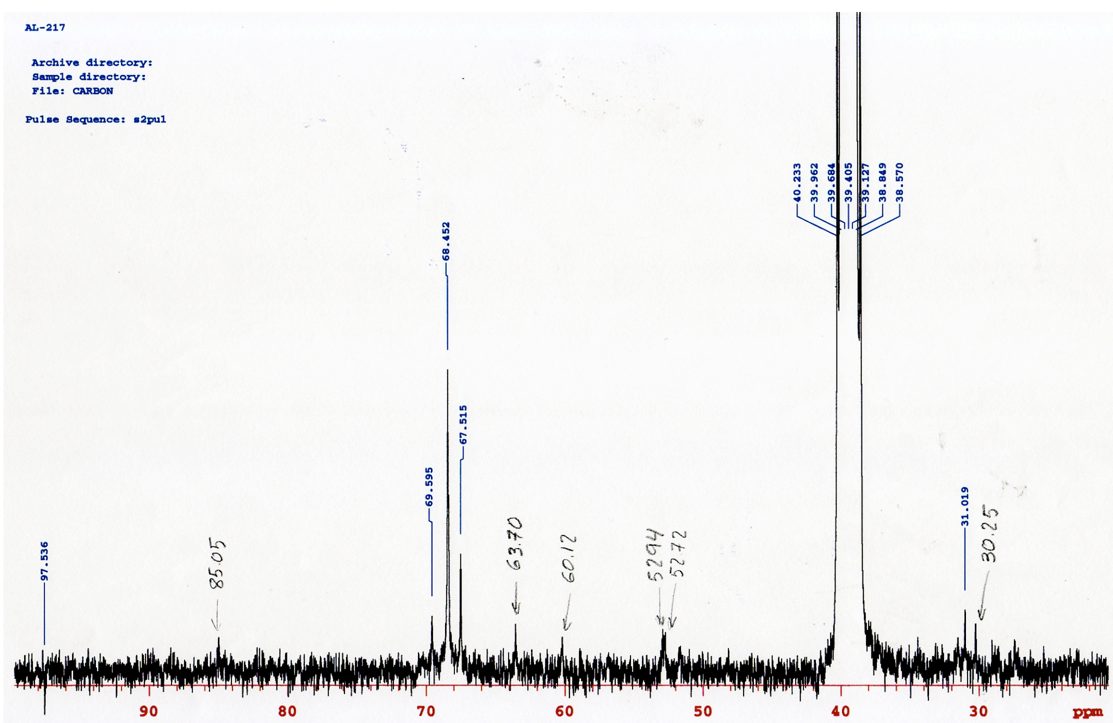




^{13}C and DEPT-NMR spectra of compound **25**



^{1}H-NMR spectra of compound **26**



^{13}C and DEPT-NMR spectra of compound **26**