

7. Anexos

7.1. Metodología computacional

La geometría de los cationes ferrocenilo del tipo de **I** ($X = \text{Cl}, \text{Br}$) se optimizó con el funcional Becke3LYP, utilizando el conjunto de bases 6-31G*. Como referencia, también se optimizó la geometría del vinilferroceno (**1**).

En todos los casos, se caracterizaron las estructuras localizadas como mínimos de energía mediante el cálculo de las frecuencias vibracionales armónicas (valores reales) a 298.15 K y 1.0 atm. La contribución electrostática del disolvente (diclorometano) se tuvo en cuenta mediante el Modelo Continuo Polarizado (PCM) según lo implementando en el paquete de programas Gaussian. Los cálculos descritos en el presente trabajo se llevaron a cabo con el paquete de programas Gaussian09, y las coordenadas cartesianas y energías absolutas de los compuestos optimizados se encuentran en las siguientes tablas.

Vinylferrocene	I (X=Cl)
C,0,1.7497608494,-0.86326089,-1.2065955142	C,0,-2.1697698335,-1.2862830055,1.0507352462
C,0,0.9784093186,-1.7725030594,-0.4200925231	C,0,-1.1486399708,-2.0627909647,0.4396375422
C,0,2.4710412103,-0.0114527232,-0.3151894975	C,0,-2.8802887266,-0.619345414,0.0113683359
C,0,2.1444452918,-0.3935603714,1.021809384	C,0,-2.2958977143,-0.9875278019,-1.2390451246
C,0,1.2207762914,-1.4817438857,0.9571157155	C,0,-1.2128205612,-1.868900264,-0.9794460119
H,0,1.7721930478,-0.8180069787,-2.28789069	Fe,0,-0.8990643427,-0.0403793443,-0.0449359324
H,0,0.3074592772,-2.5322177035,-0.7999600561	C,0,-0.2866980606,1.5234671224,1.1463822909
H,0,3.1355253844,0.7933323459,-0.602693003	C,0,0.7748563547,0.9131110062,0.3475788063
H,0,2.5206770494,0.0692432133,1.9252159597	C,0,-1.2347370525,2.0420590396,0.2511329612
H,0,0.7709176862,-1.9857321656,1.8028228242	C,0,-0.7873863744,1.8102930658,-1.0901310743
Fe,0,0.4496956096,0.1659354371,0.0060427661	C,0,0.4484406825,1.1441569778,-1.0594751332
C,0,-0.9055873229,1.1216892608,-1.1931045341	C,0,1.2075561451,-0.3555119623,0.7497888927
C,0,-1.59768124,0.3280610478,-0.2146988929	C,0,2.1233473575,-1.2329750302,-0.0455896858
C,0,-0.0913469062,2.0748363215,-0.5139978015	Cl,0,3.8322574081,-0.9421133318,0.5349328411
C,0,-0.2620152843,1.8755570948,0.8901612911	H,0,-2.3592909085,-1.2035303922,2.1120638367
C,0,-1.1791055092,0.7992397641,1.0763106284	H,0,-0.4385033967,-2.6892164221,0.9619864156
C,0,-2.5507201752,-0.7409050452,-0.5228284642	H,0,-3.7047951038,0.0672222935,0.1467074174
C,0,-3.3870511206,-1.3276962098,0.3441505792	H,0,-2.5984997485,-0.6215954332,-2.2110069648
H,0,-0.9954327046,1.0081981476,-2.2664348298	H,0,-0.566555958,-2.3235567863,-1.7176600131
H,0,0.5547712951,2.8075948158,-0.9799125135	H,0,-0.3461506591,1.5096854723,2.2259651495
H,0,0.2361619435,2.4275628193,1.6768643839	H,0,-2.174866624,2.5040267636,0.5215715519
H,0,-1.4983199066,0.3987278514,2.029794766	H,0,-1.3402022562,2.0707883487,-1.9827713647
H,0,-2.5701292761,-1.0546859142,-1.5666271363	H,0,1.0215518262,0.8192665707,-1.9159835422
H,0,-3.4279889719,-1.0438525292,1.3929706227	H,0,1.1516420493,-0.5894199709,1.8098172621
H,0,-4.0648608371,-2.1141836434,0.0259395354	H,0,2.1167092622,-1.0239095873,-1.1131759701
HF=-1728.1067901	H,0,1.9284462057,-2.2908499499,0.1261862673
	HF=-2188.1303838

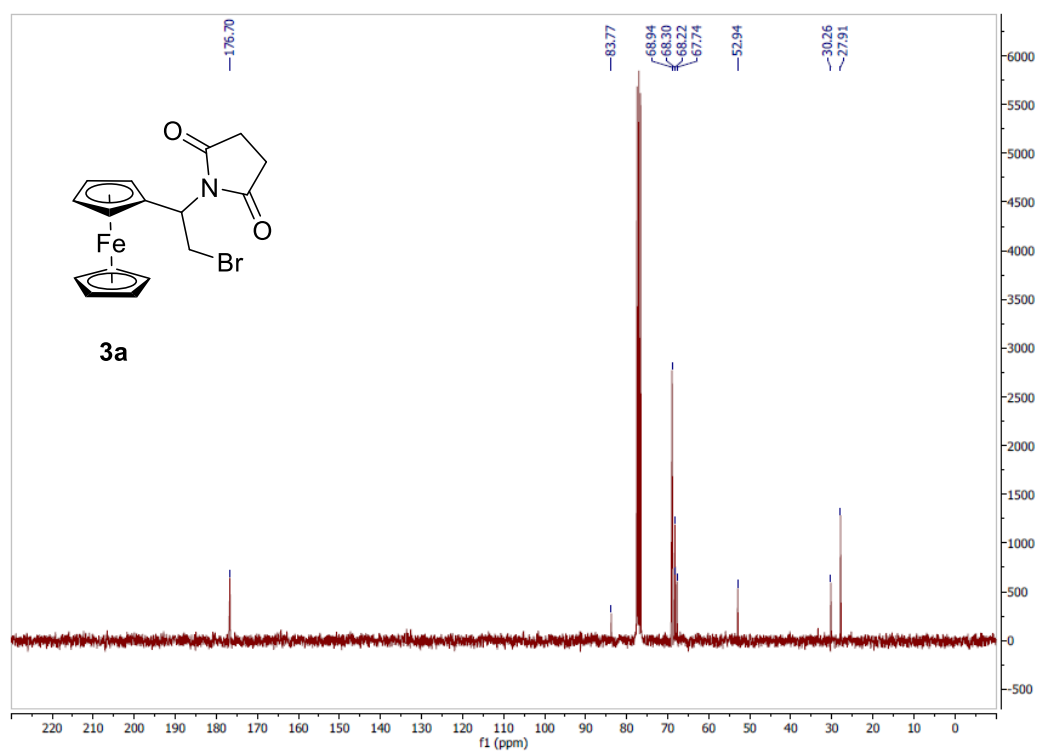
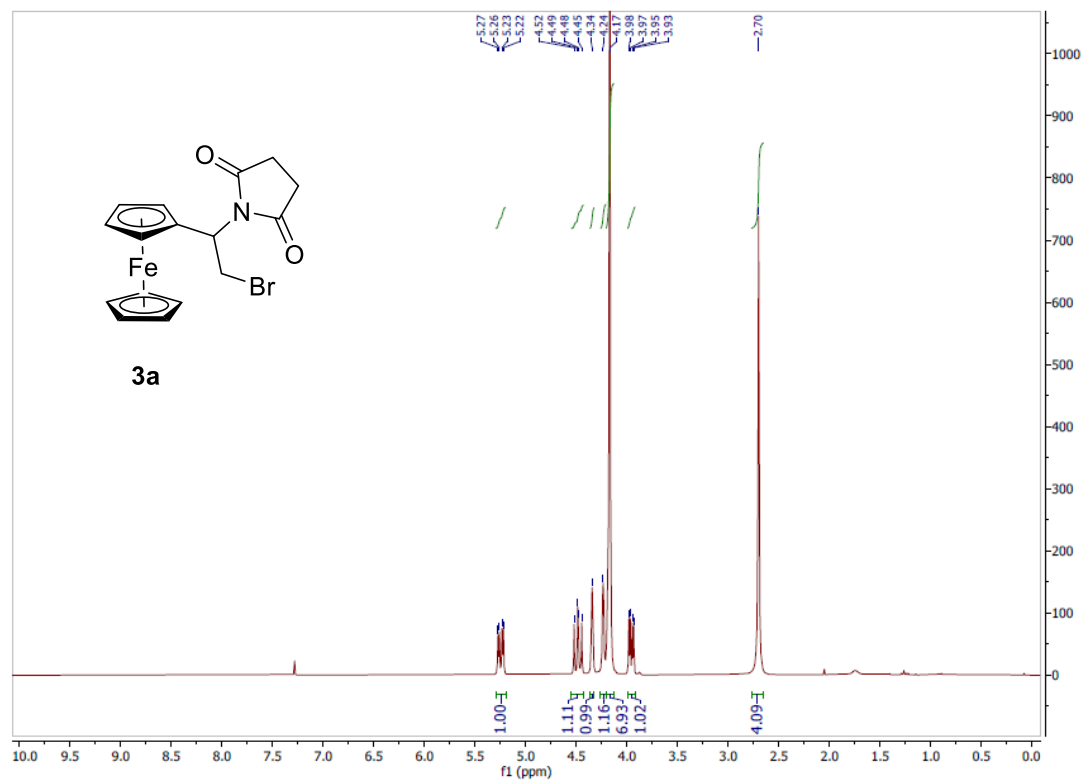
I (X=Br)

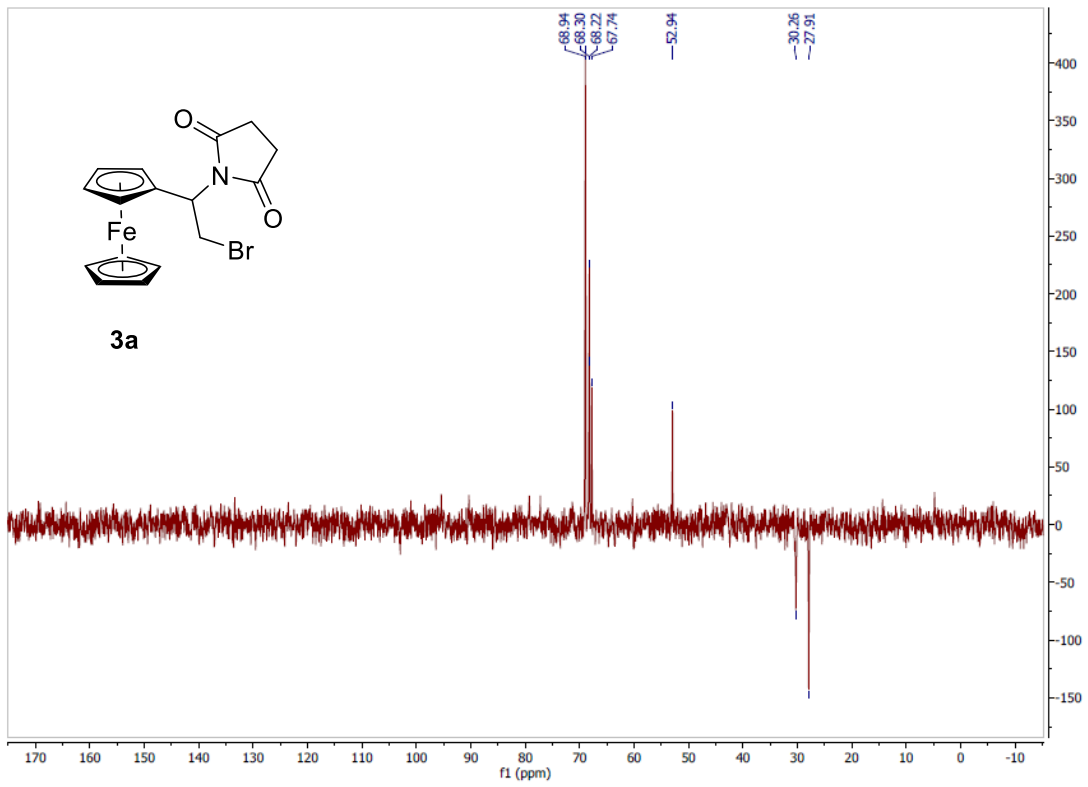
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C,0,2.244704953,-1.019575567,1.0490649758
C,0,1.0395648888,-1.7643175022,0.9439895384
Fe,0,0.8454354204,0.0675680207,-0.0148884761
C,0,0.2836063417,1.6636161155,-1.1859152218
C,0,-0.7433689399,1.2041183618,-0.2529429066
C,0,1.3819688536,2.086562412,-0.4211580779
C,0,1.0678397122,1.9397100828,0.9687336413
C,0,-0.2321000585,1.4236790756,1.0995005232
C,0,-1.3740388672,-0.0070804192,-0.5610842492
C,0,-2.2783068271,-0.7503852317,0.3602184744
Br,0,-4.1427889516,-0.1769428753,-0.0542104101
H,0,1.8948774852,-1.3162385808,-2.2778848806
H,0,-0.0478869043,-2.5239628389,-0.8672043954
H,0,3.6021830964,-0.17970666,-0.5223995698
H,0,2.7000008143,-0.6734764556,1.9672739527
H,0,0.4318297182,-2.1175717336,1.7656755672
H,0,0.2166451493,1.6195300948,-2.2642583638
H,0,2.3317221043,2.4272411676,-0.8113337101
H,0,1.7456091932,2.1524524918,1.7845965853
H,0,-0.736362897,1.1878769537,2.0256675174
H,0,-1.4631549072,-0.2704985922,-1.6117823866
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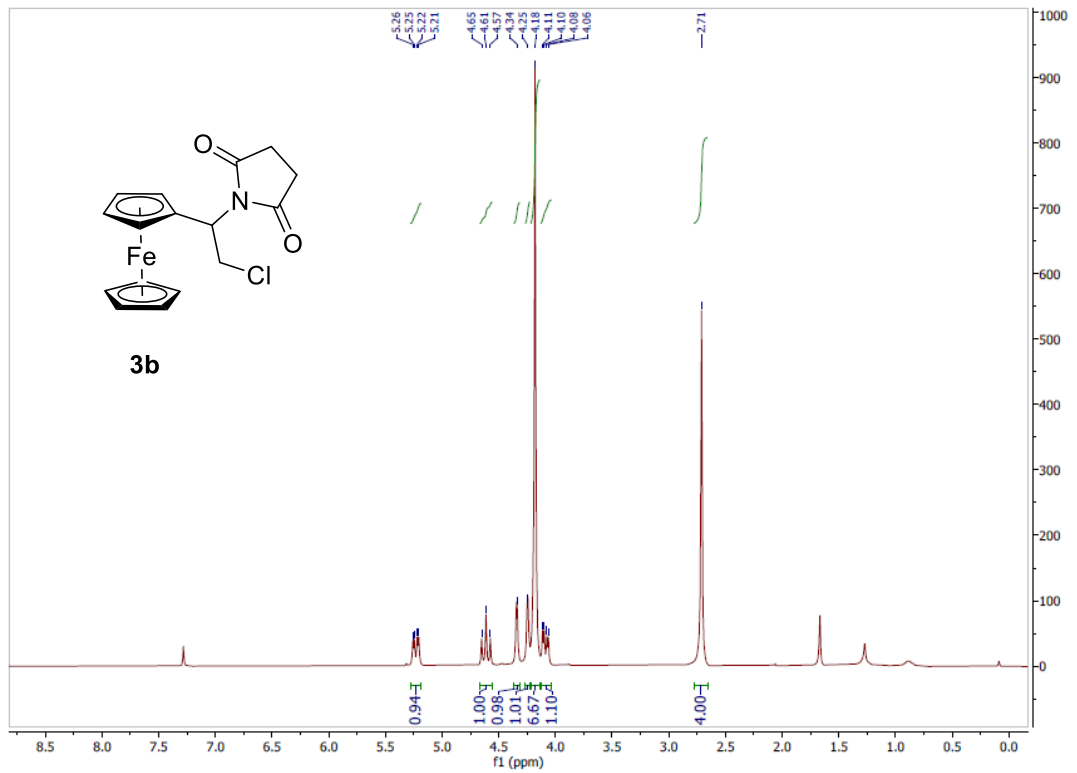
7.2. Caracterización mediante Espectroscopía de Resonancia Magnética Nuclear

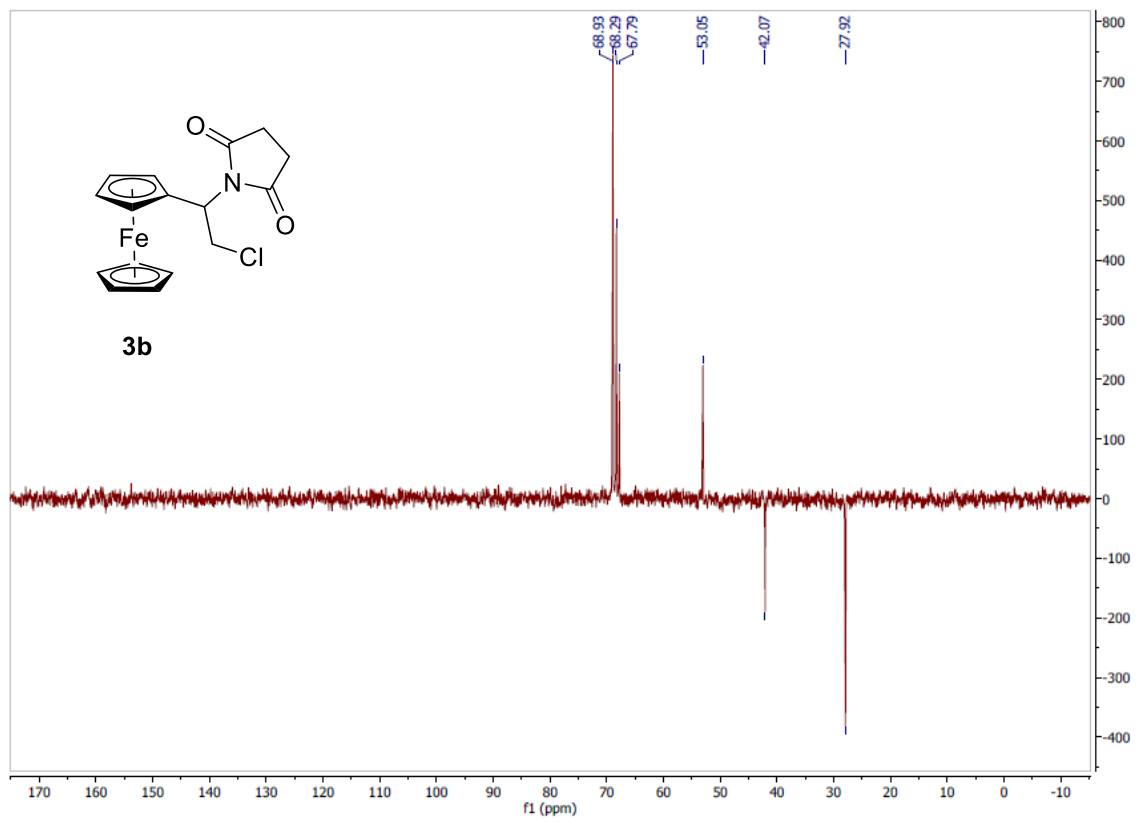
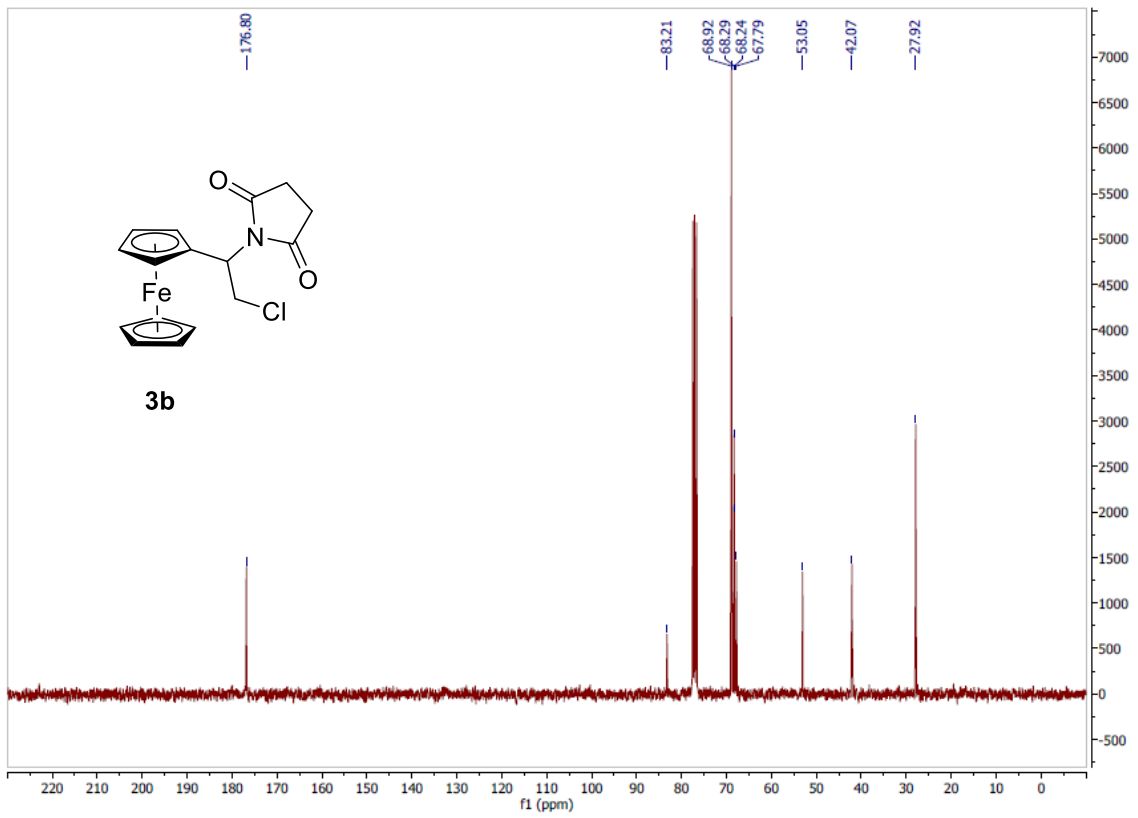
N-(2-bromo-1-ferroceniletíl)succinimida (3a)



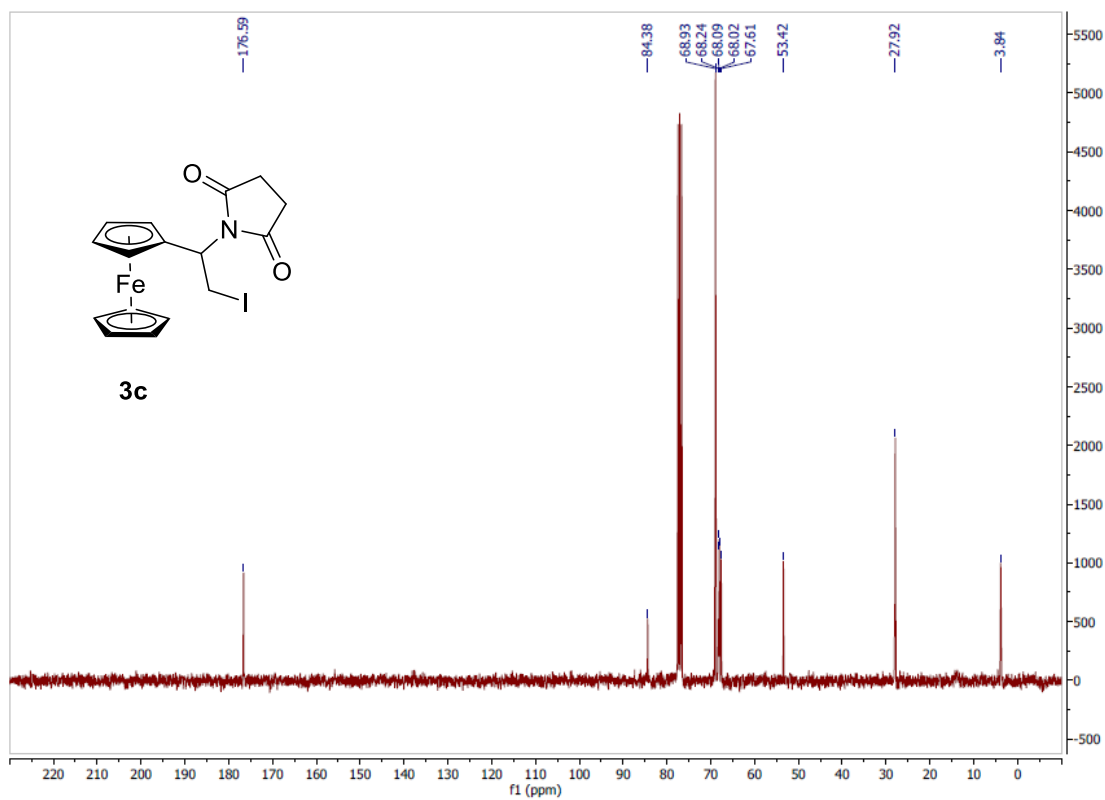
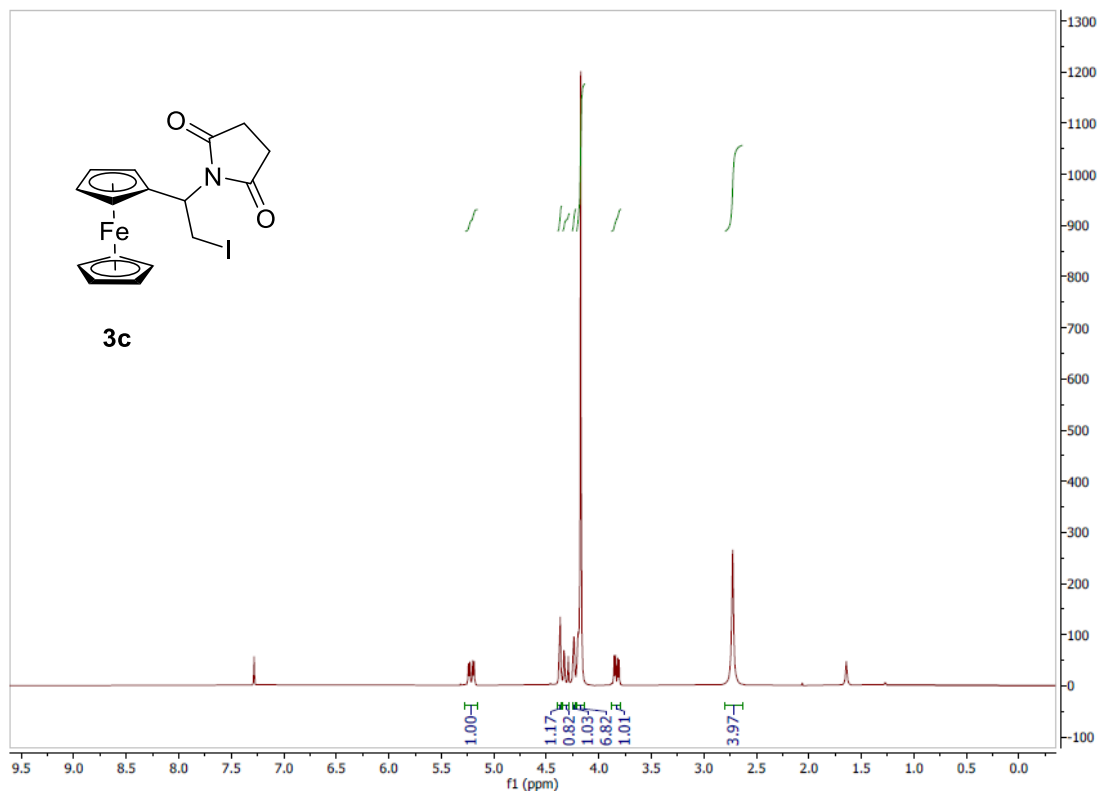


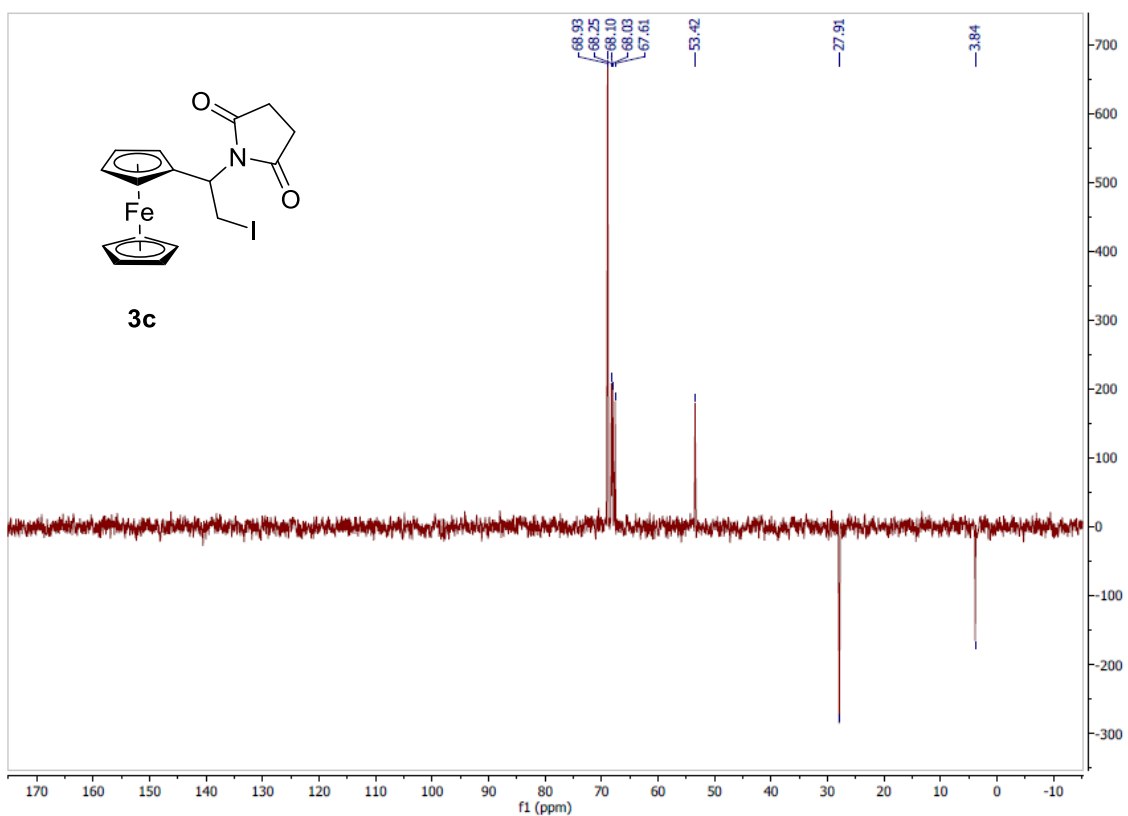
N-(2-cloro-1-ferroceniletil)succinimida (3b)



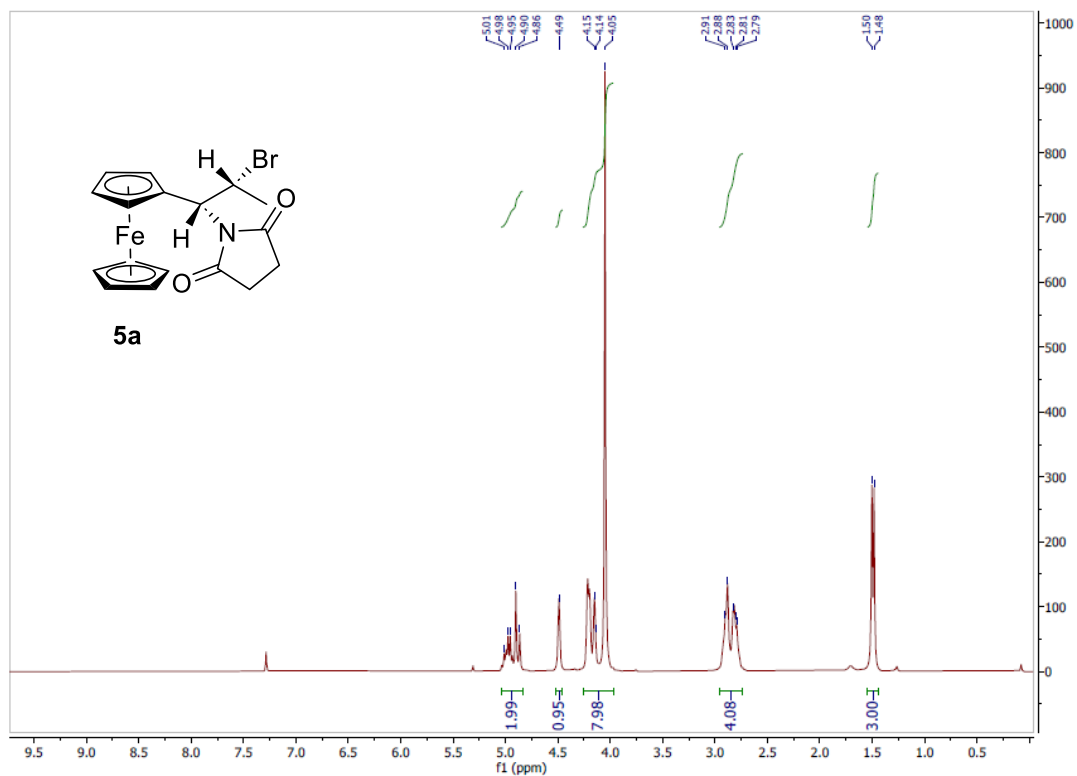


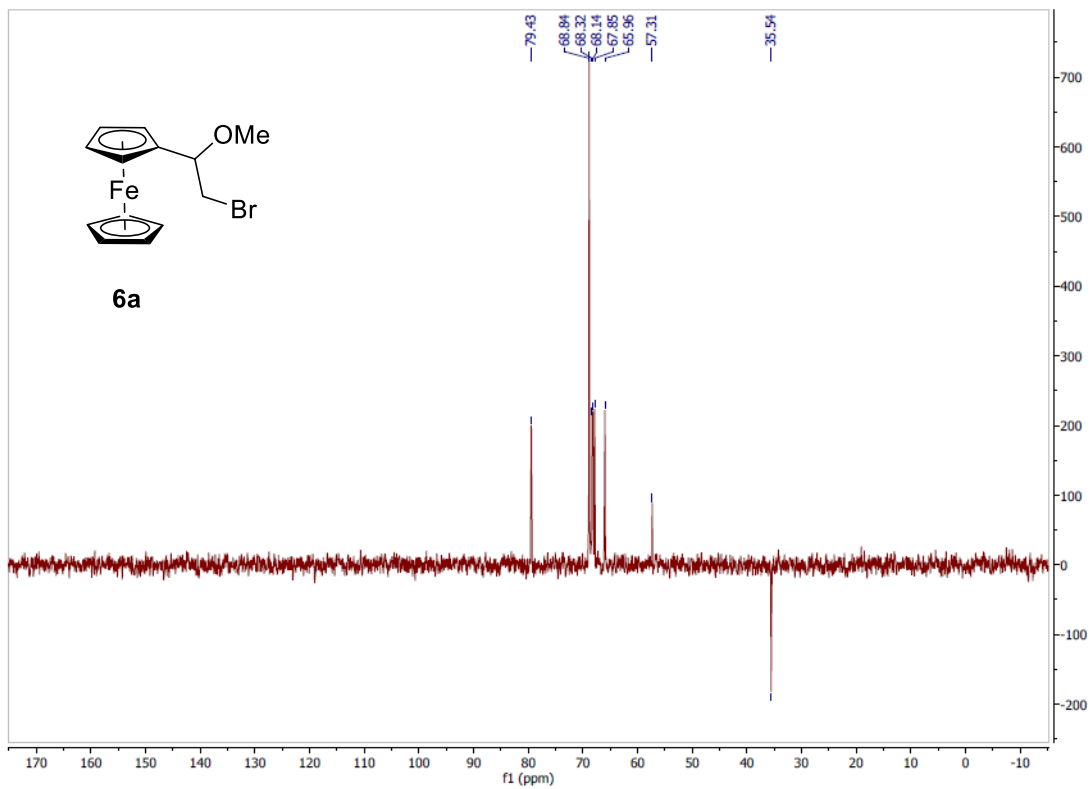
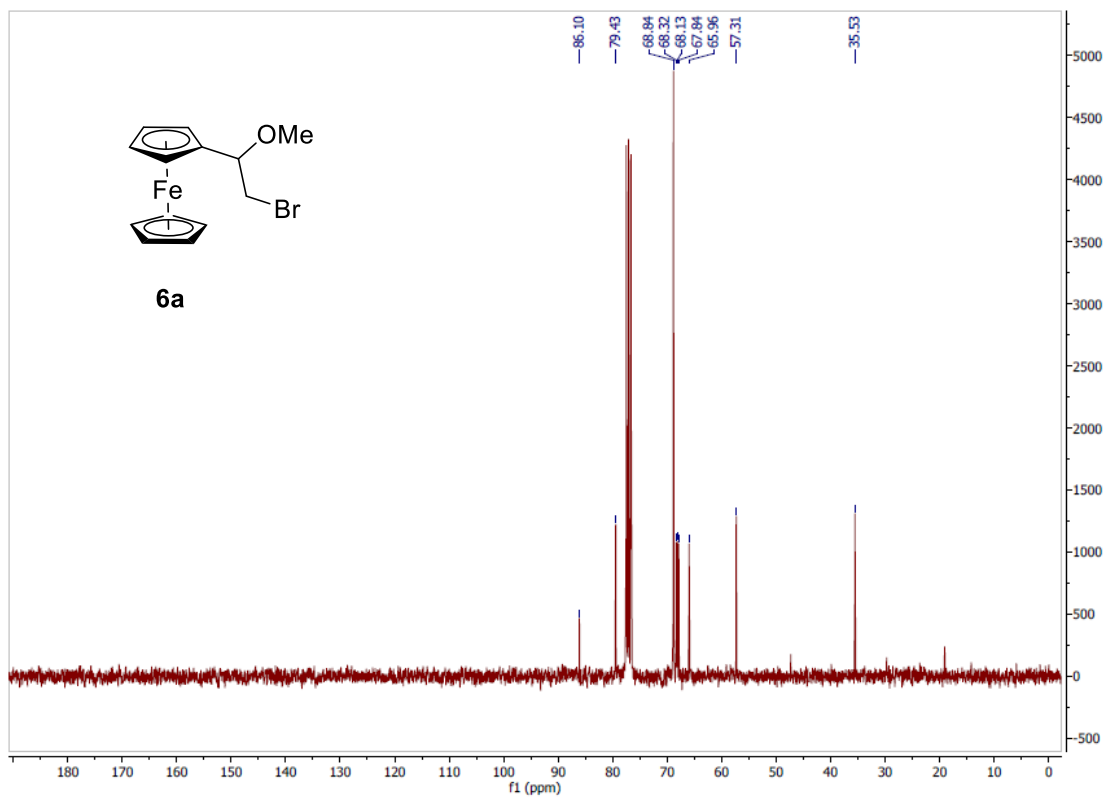
N-(1-ferrocenyl-2-iodoethyl)succinimida (3c)



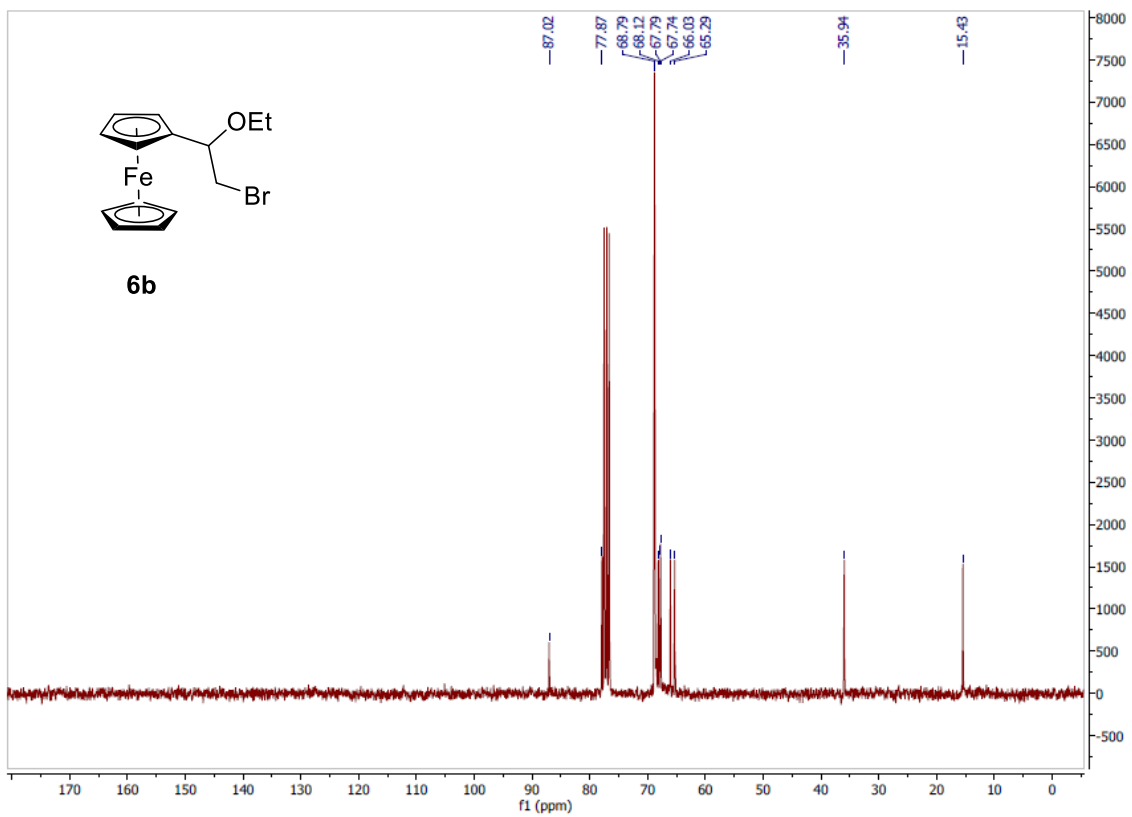
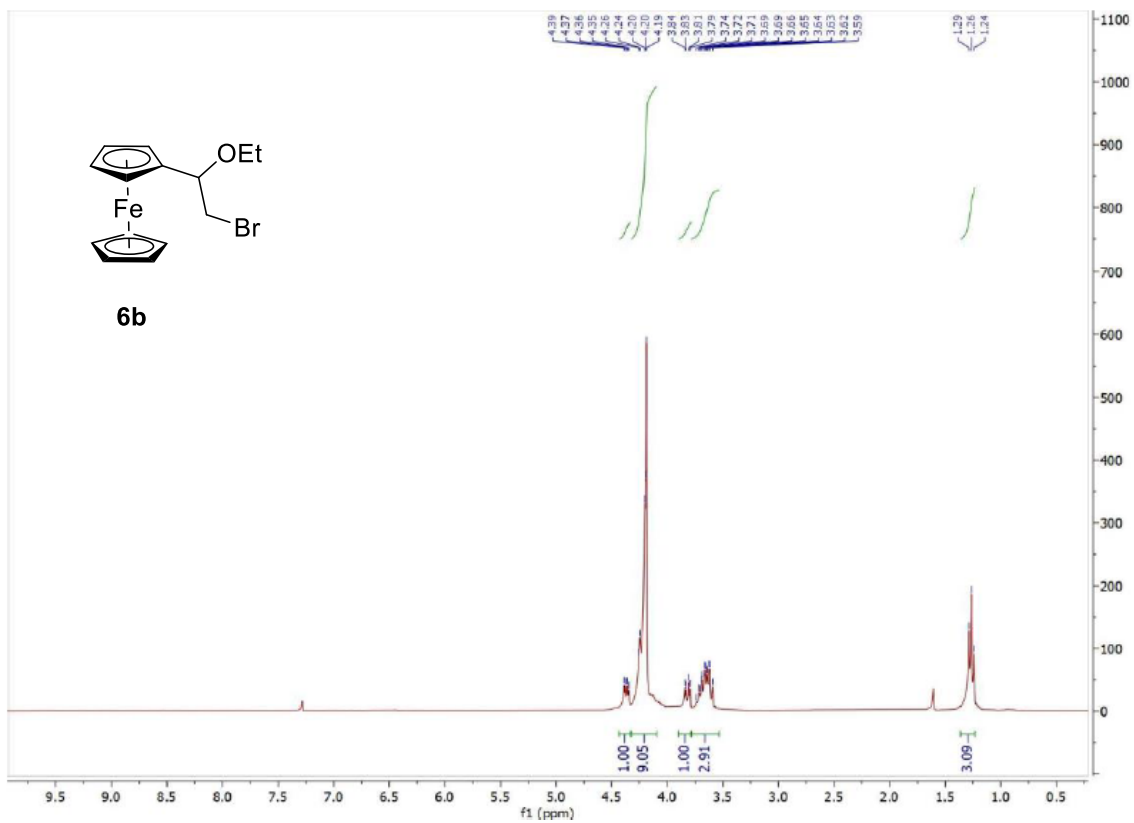


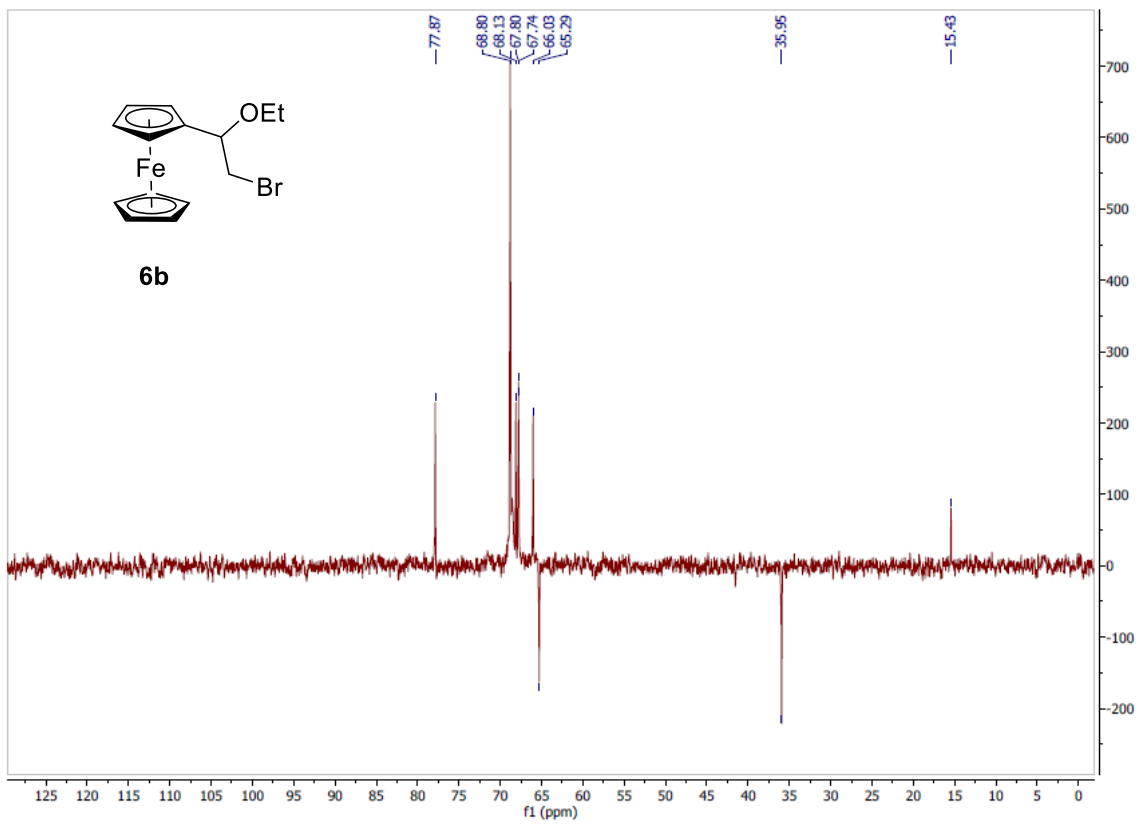
N-(2-bromo-1-ferrocenylpropyl)succinimida (5a)



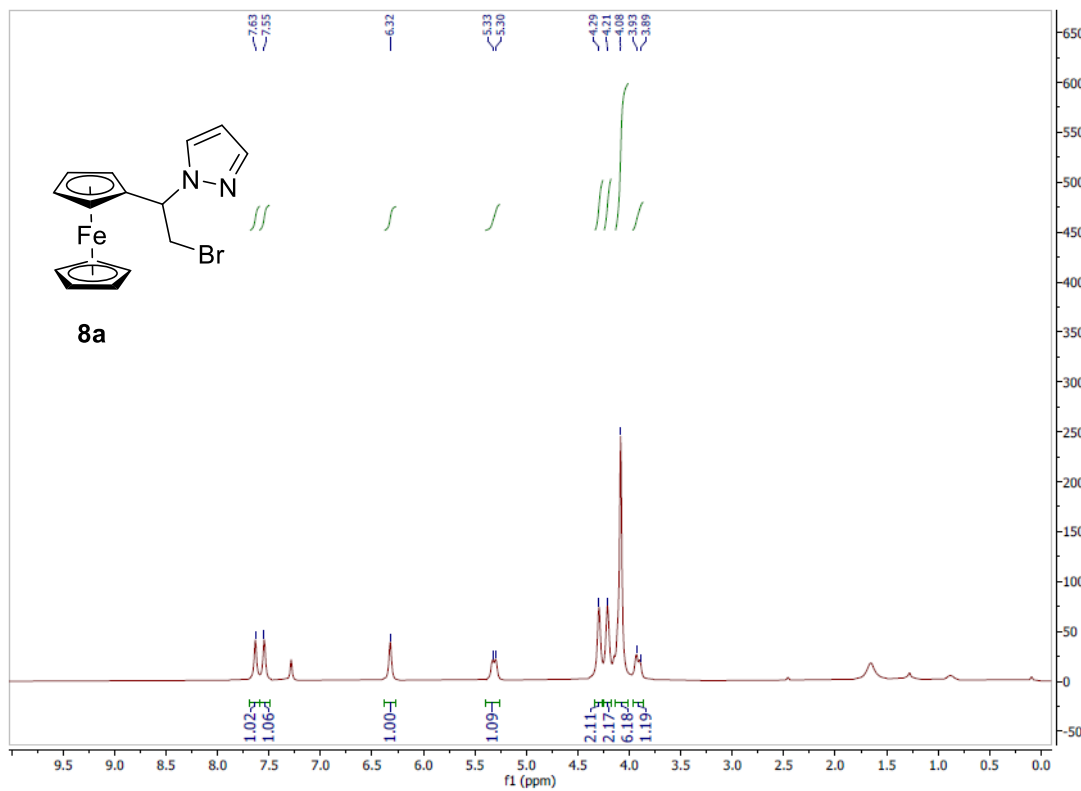


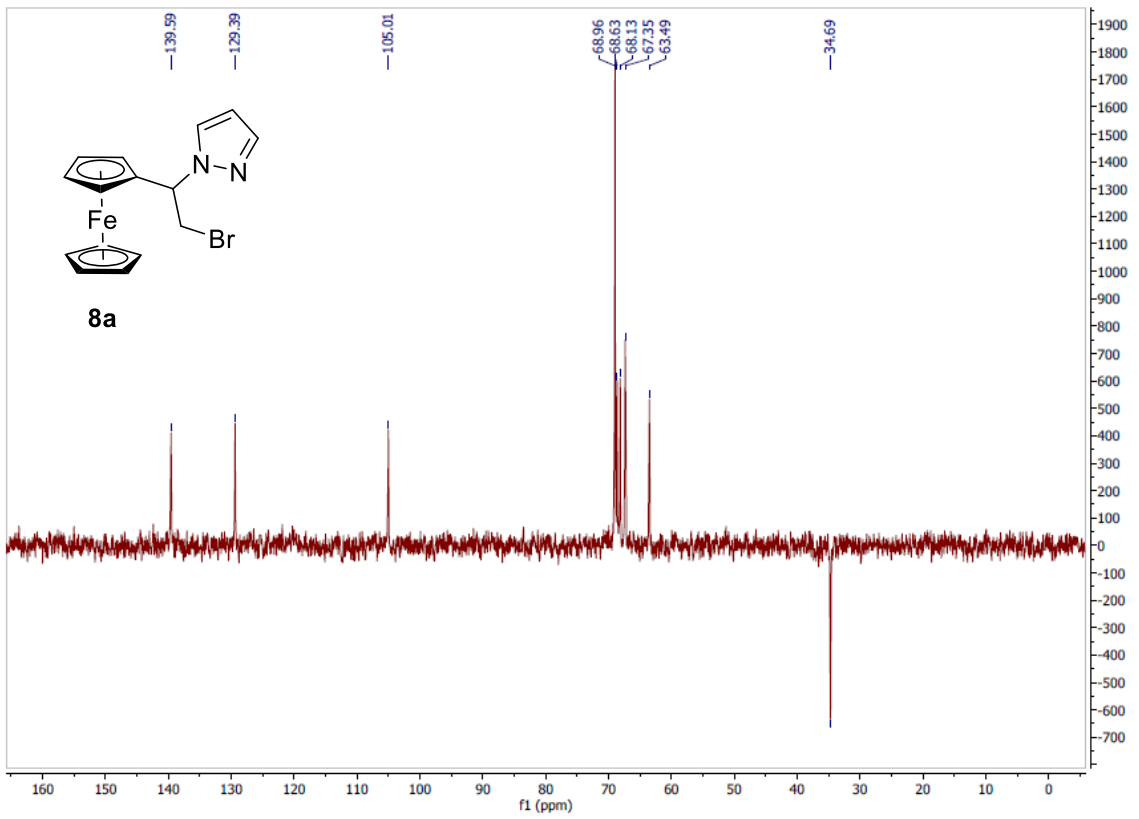
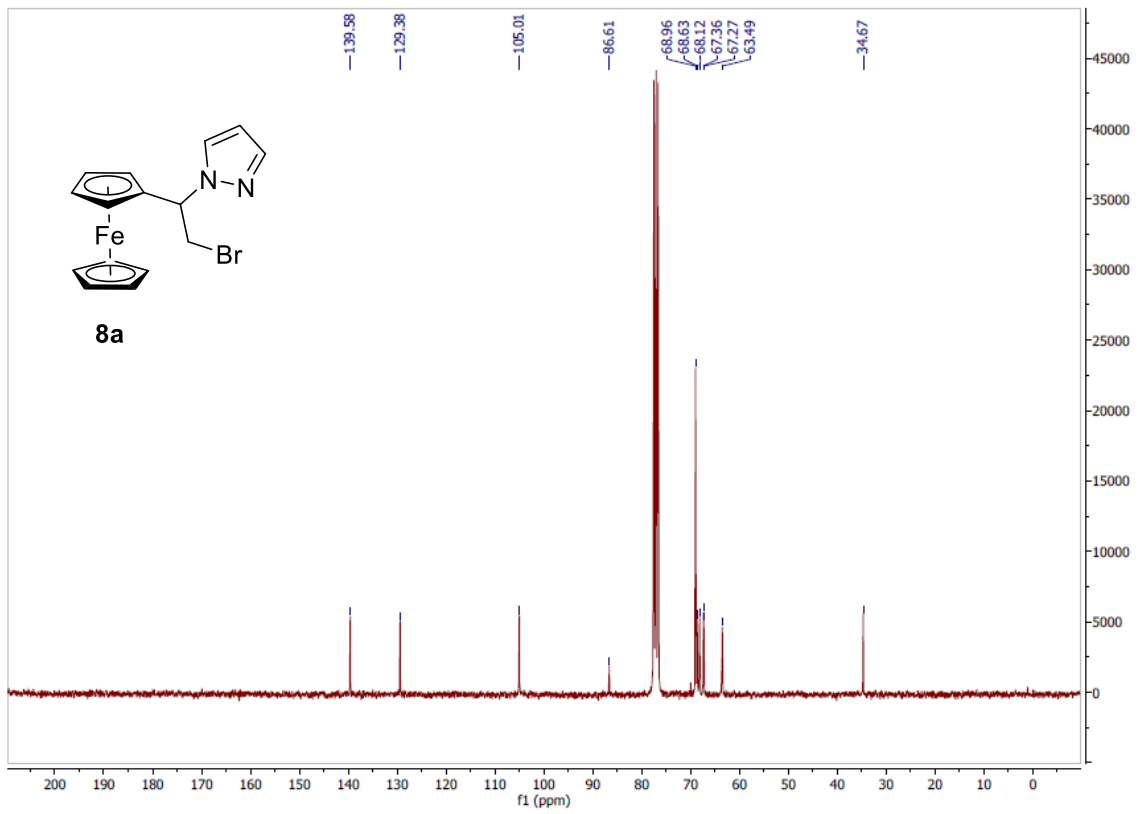
(2-bromo-1-etoetil)ferroceno (6b)



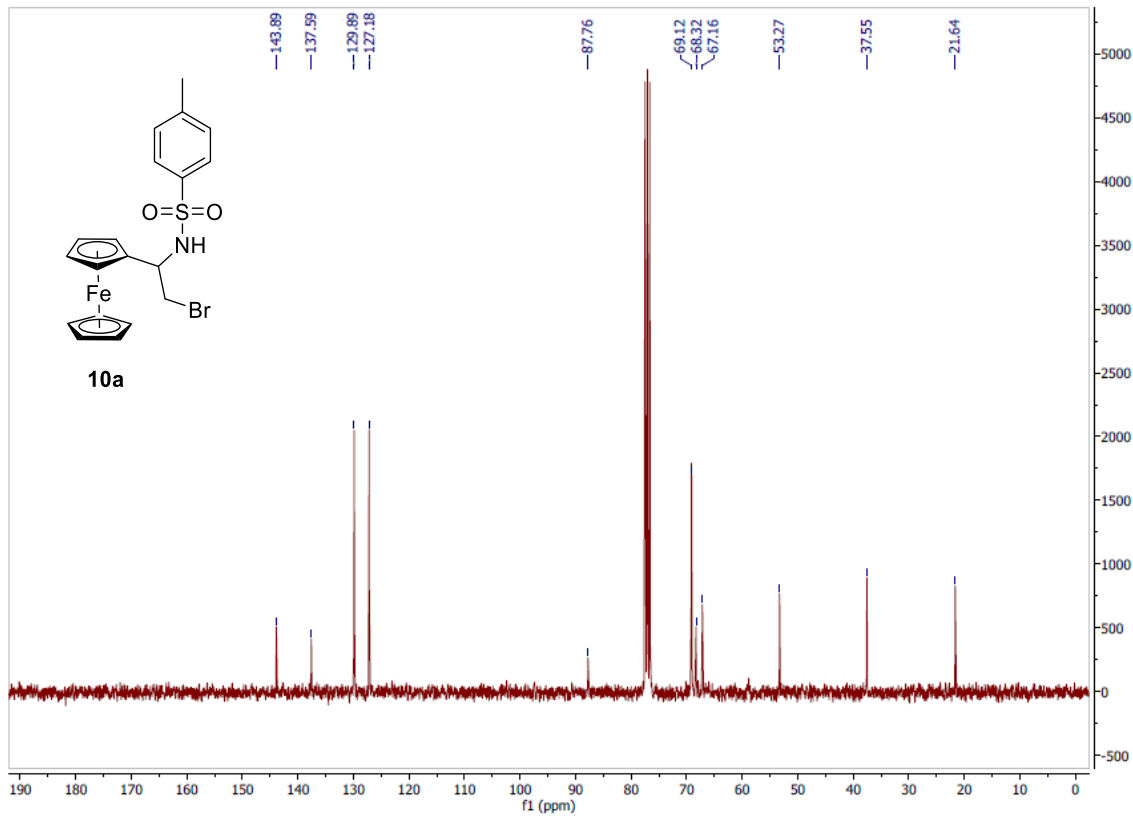
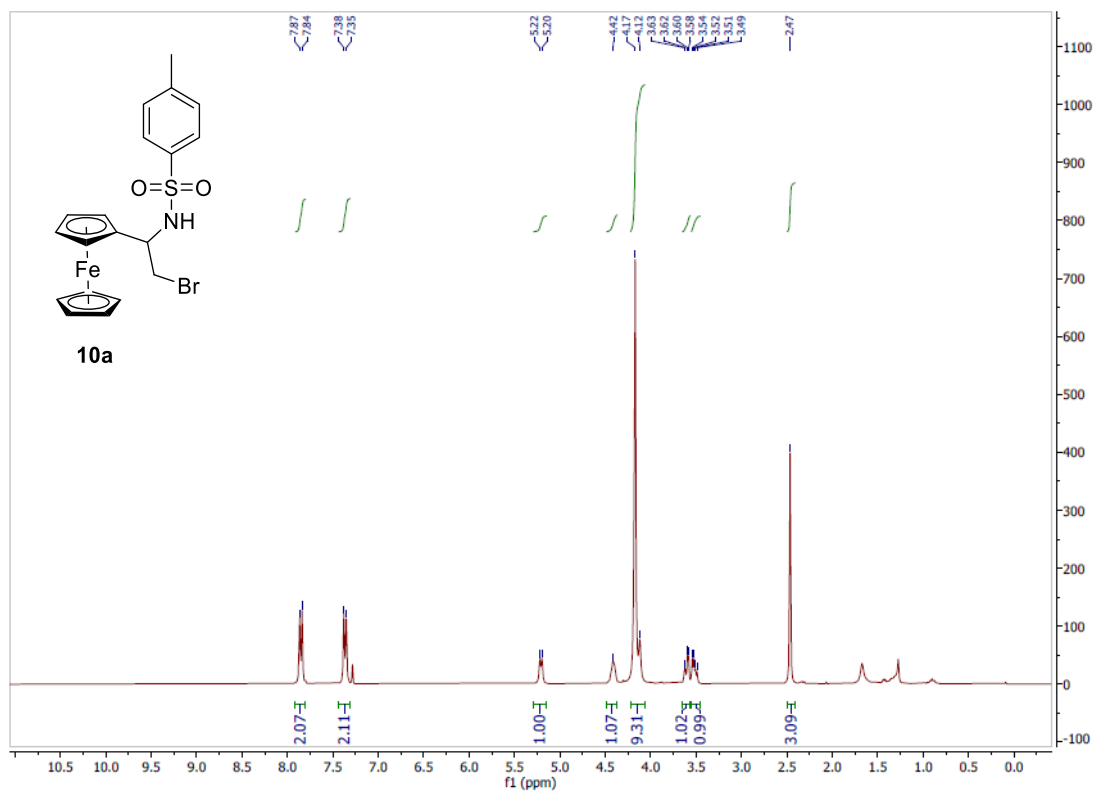


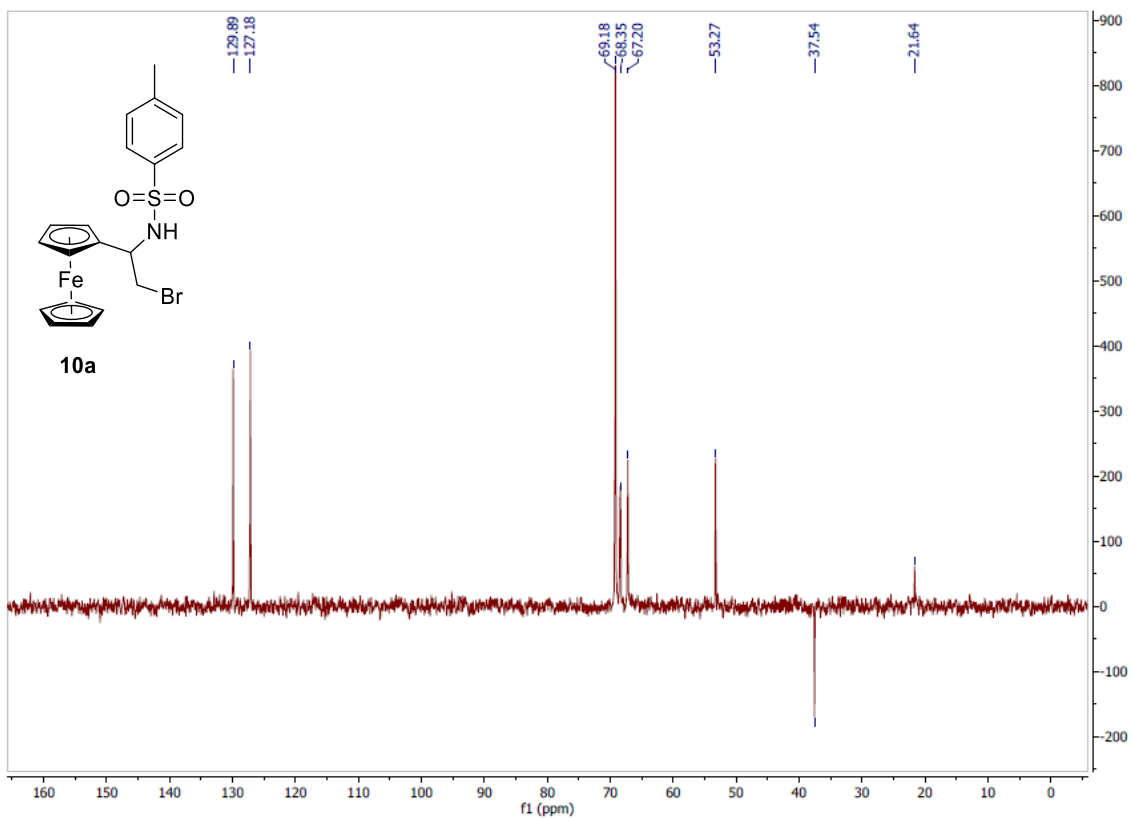
1-(2-bromo-1-ferrocenylethyl)-1H-pirazol (8a)



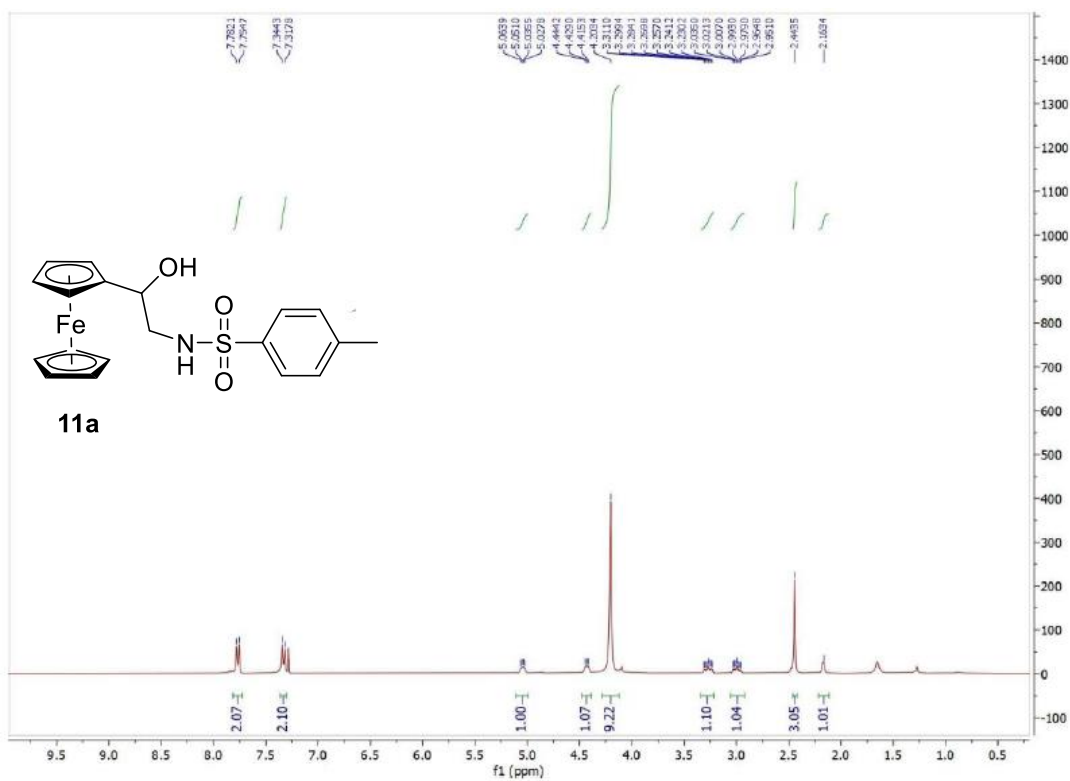


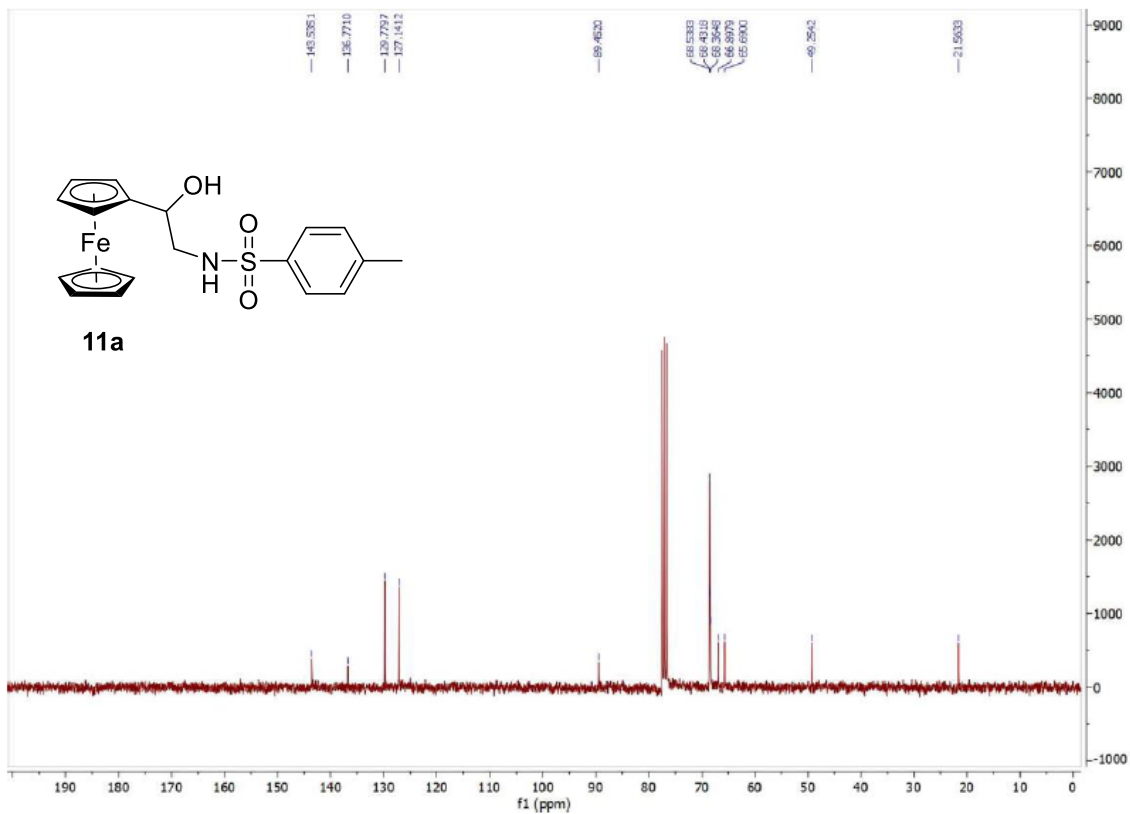
N-(2-bromo-1-ferrocenyletil)-4-metilbenzenosulfonamida (10a)



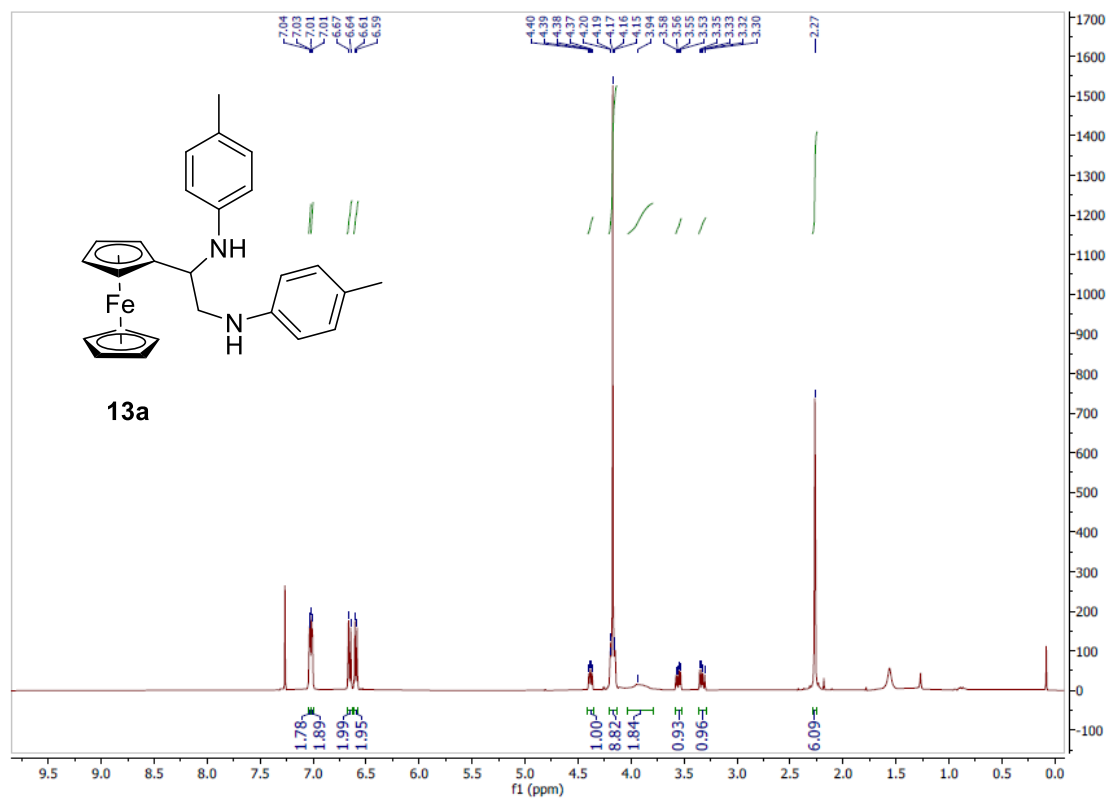


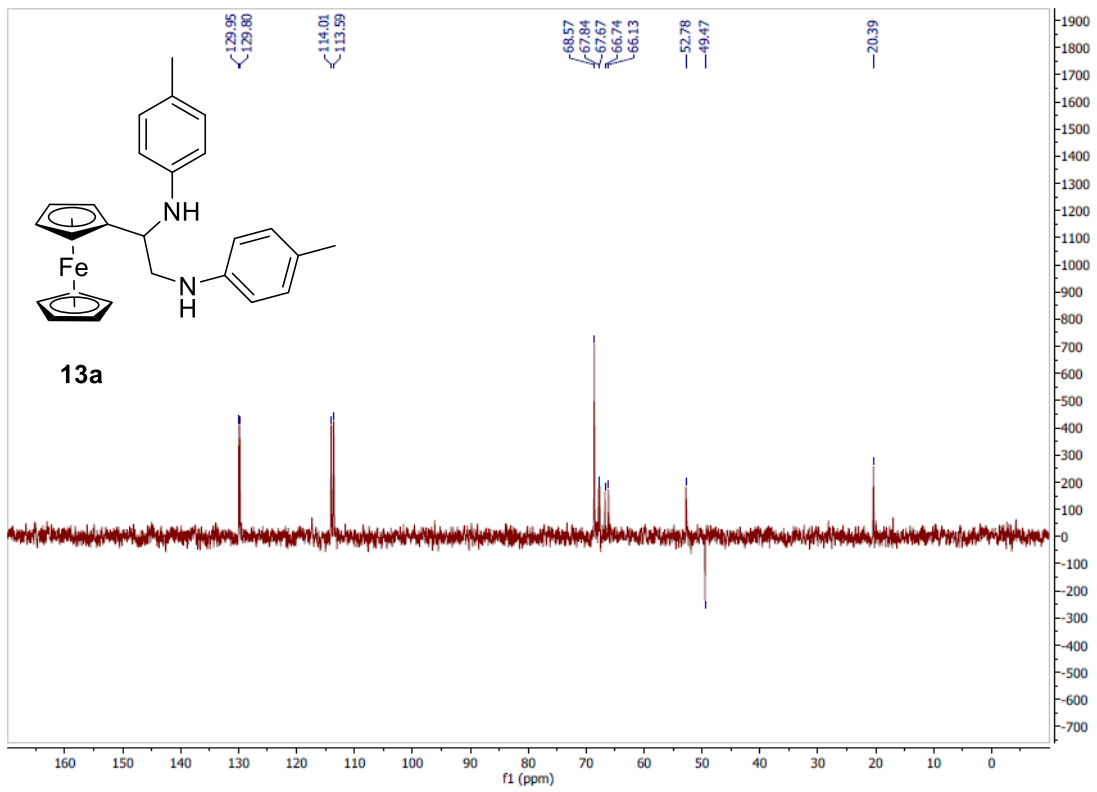
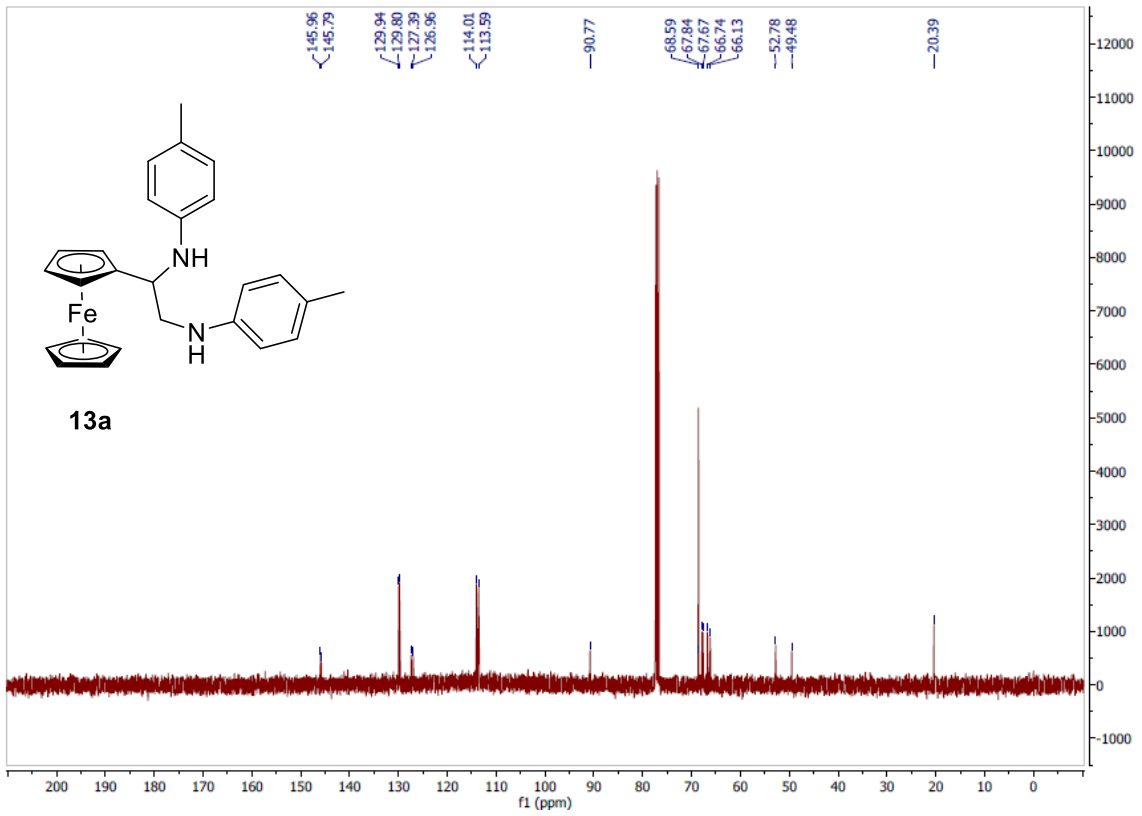
N-(2-ferrocenil-2-hidroxietyl)-4-metilbenenosulfonamida (11a)



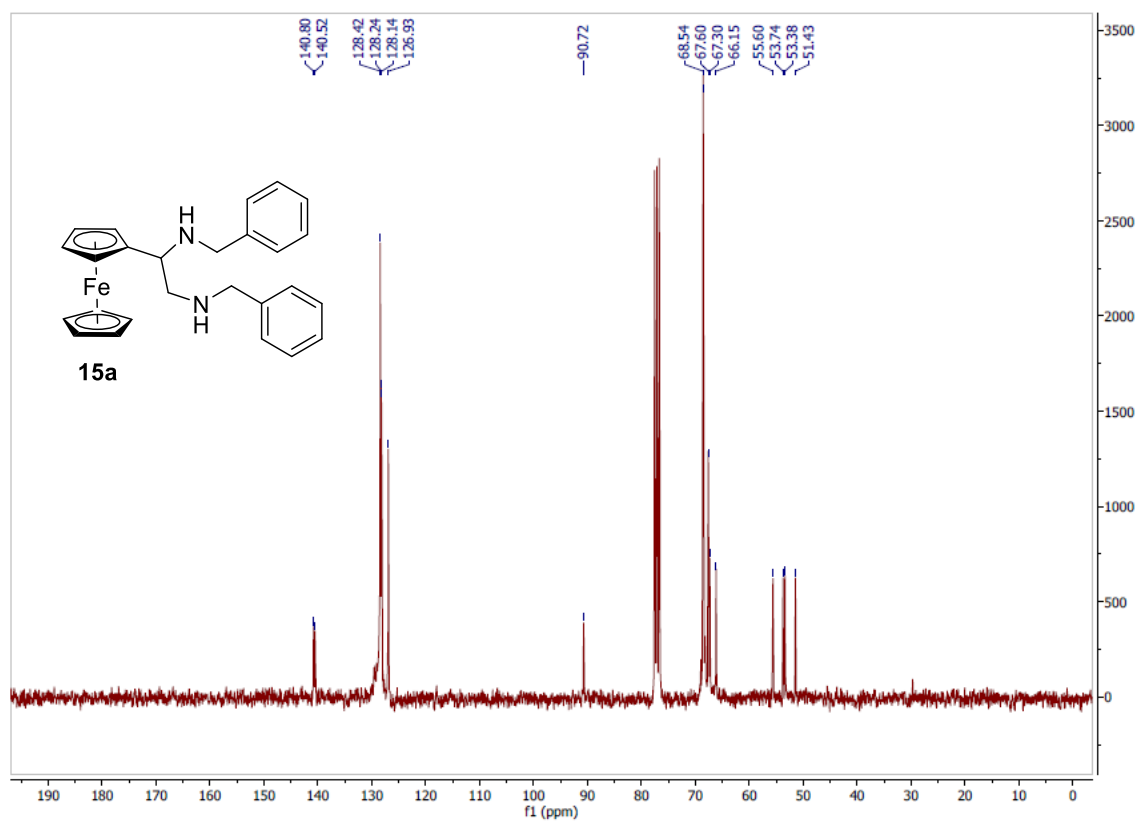
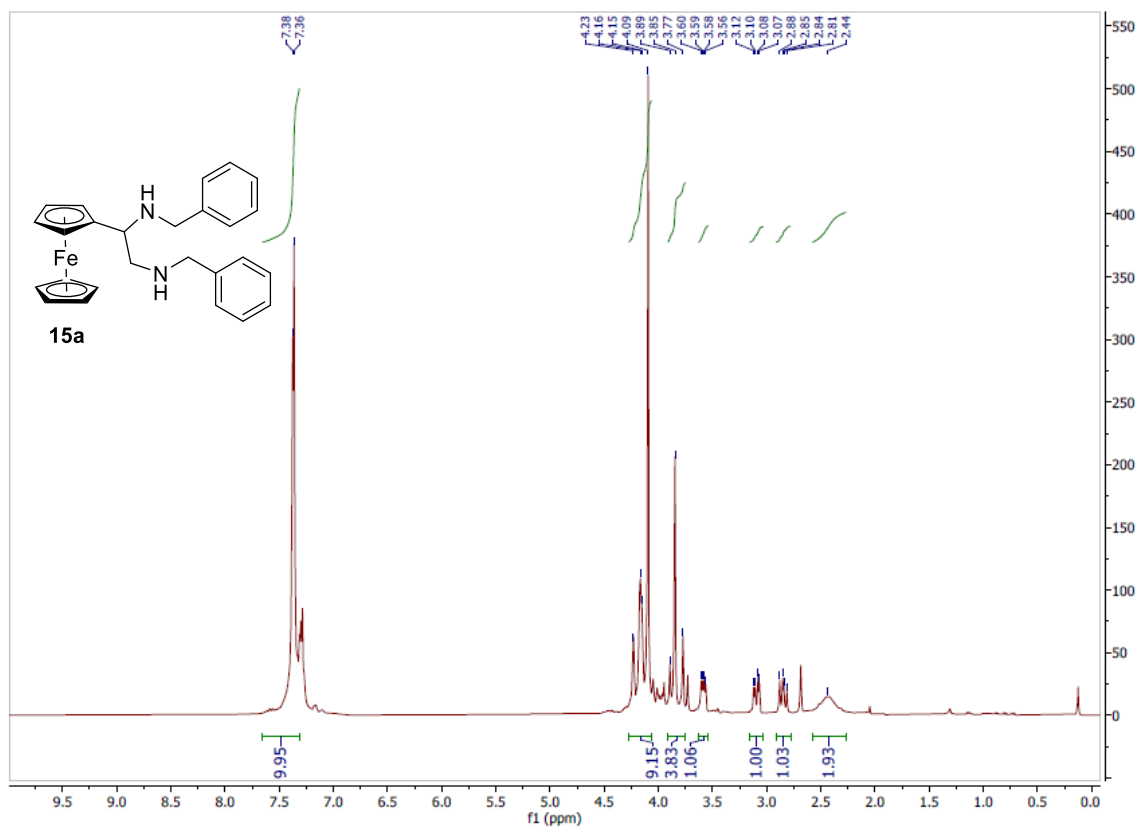


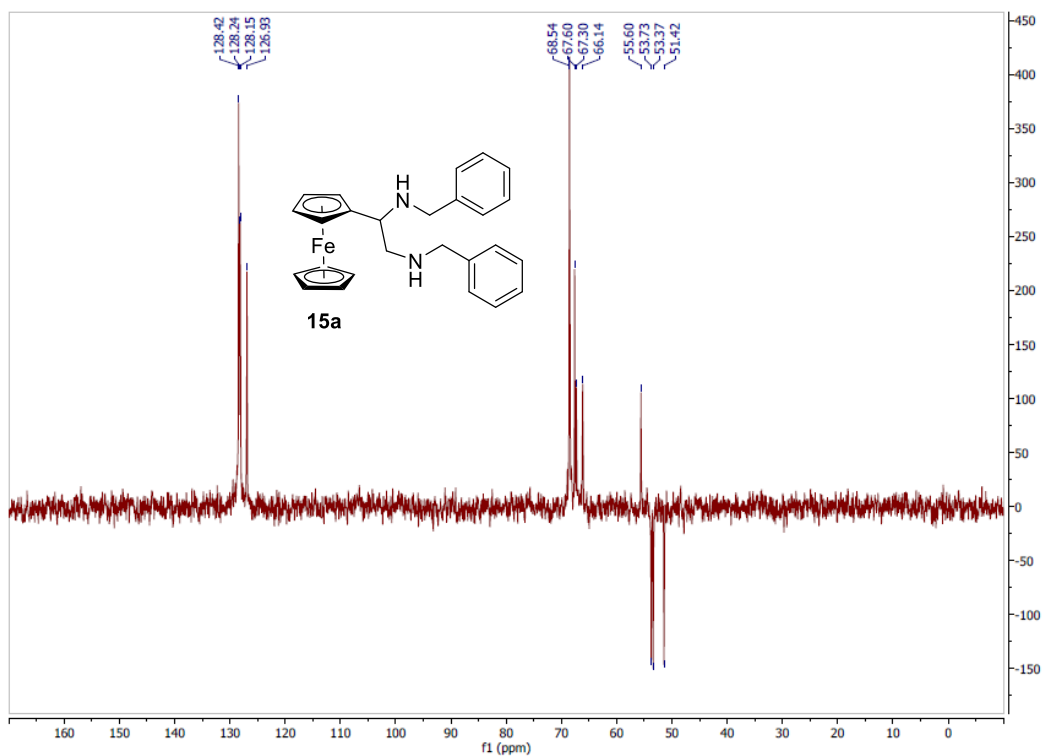
(N,N'-1,2-di(*p*-metilanilina)etilferroceno (13a)



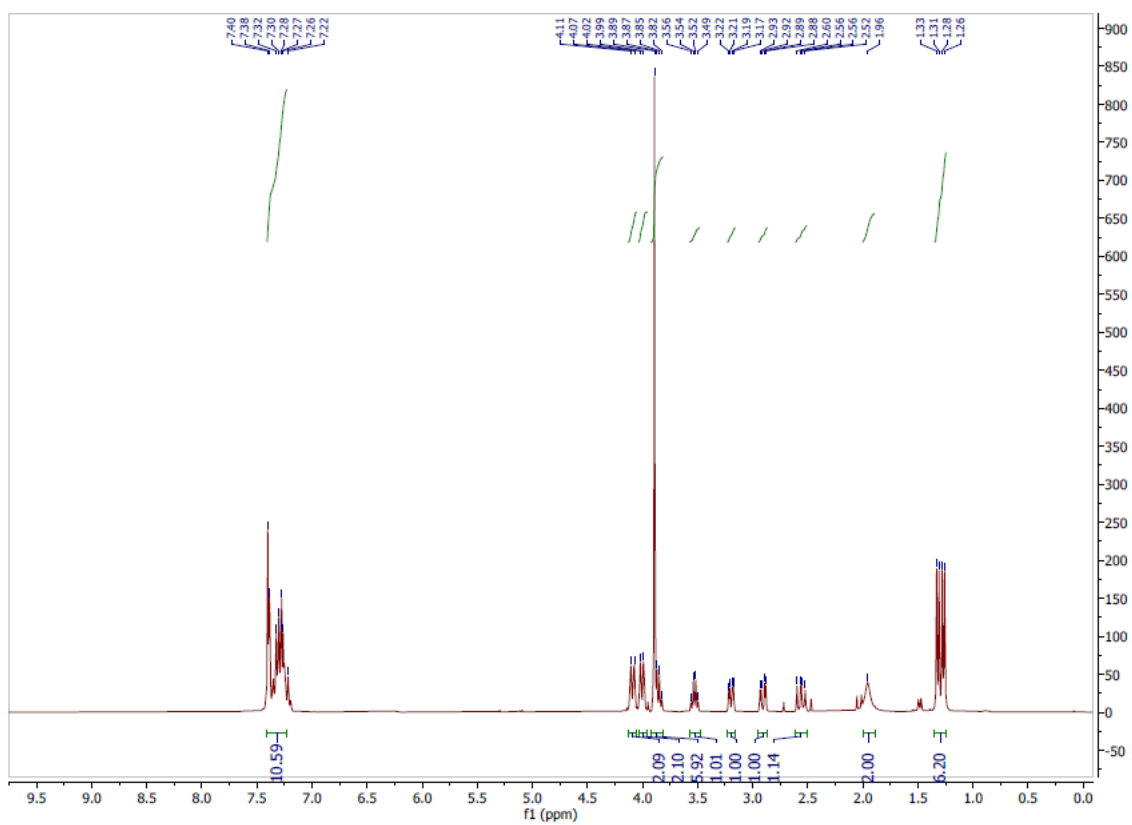


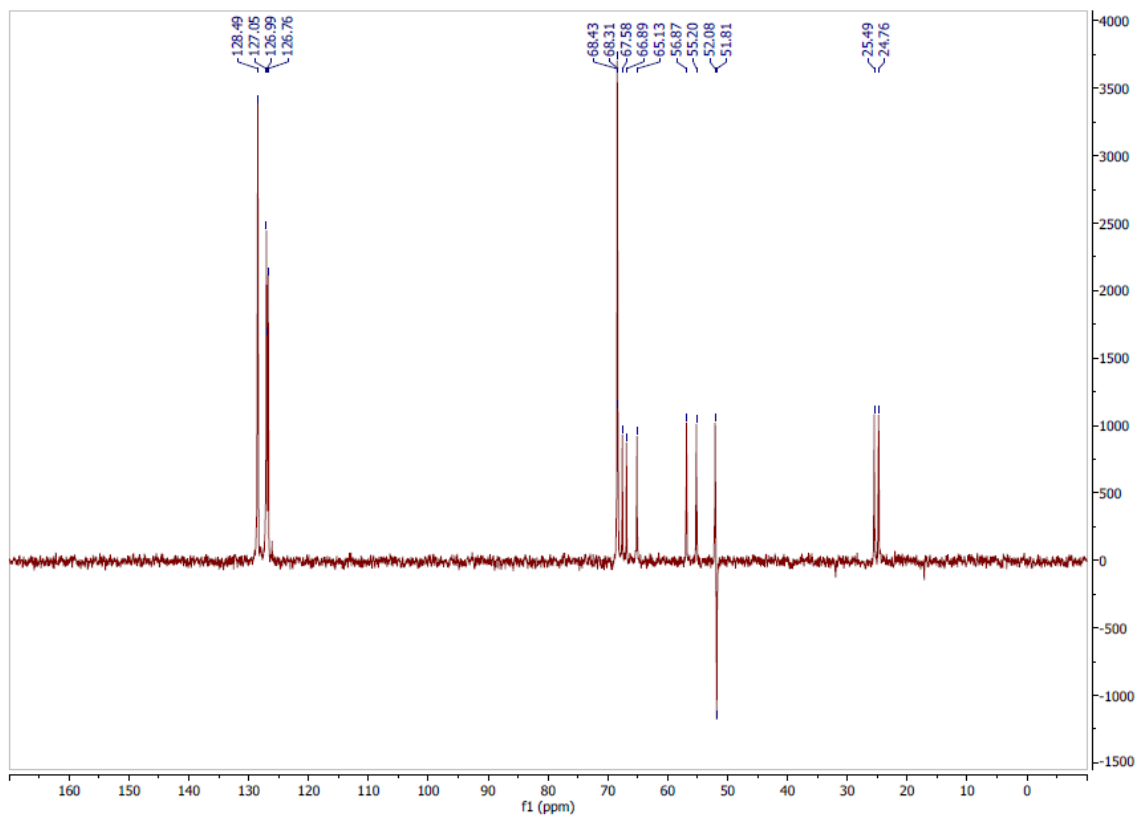
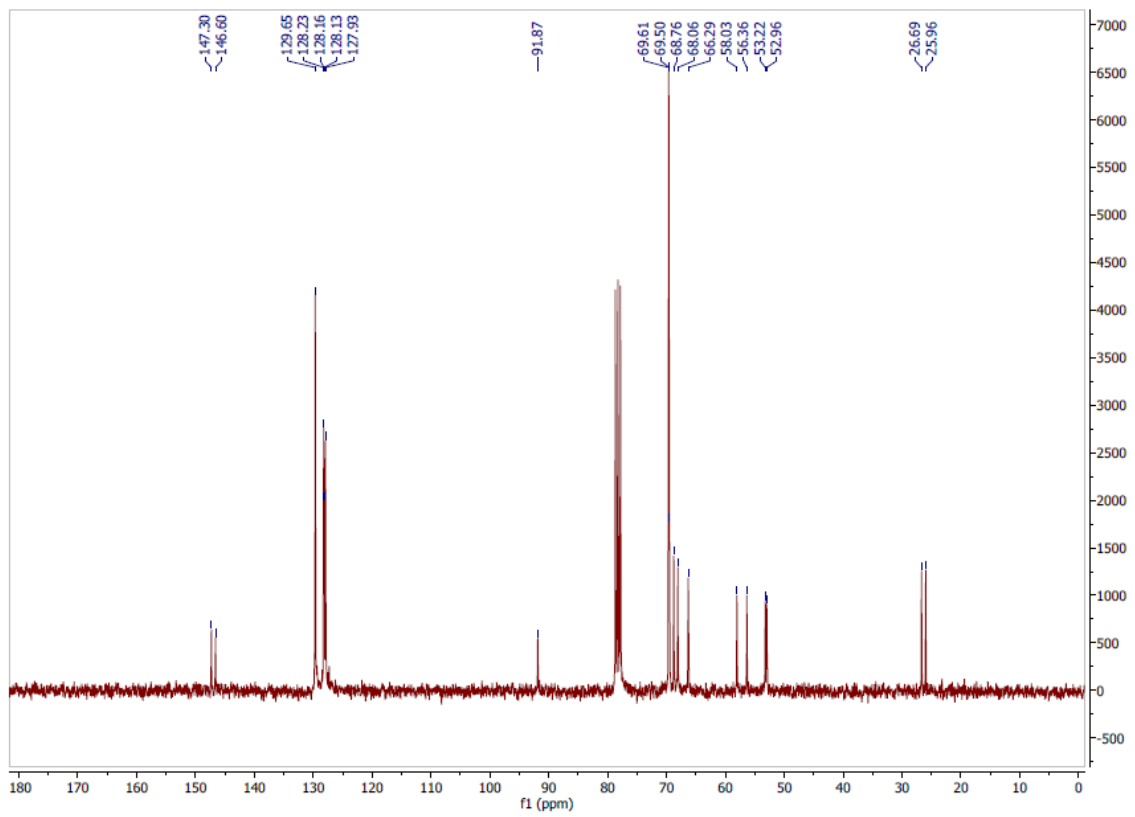
(N,N'-1,2-di(bencilamina)etil)ferroceno (15a)





(N,N'-1,2-di(1-feniletilamina)etil)ferroceno (17a y 17b) (Fracción 1)





(N,N'-1,2-di(1-feniletamina)etil)ferroceno (17a y 17b) (Fracción 2)

