

## Supporting Information

### Functionalization of 3-Iodo-*N,N*-diisopropylferrocene-carboxamide, a Pivotal Substrate to Open the Chemical Space to 1,3-Disubstituted Ferrocenes

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## TABLE OF CHEMICAL SHIFTS

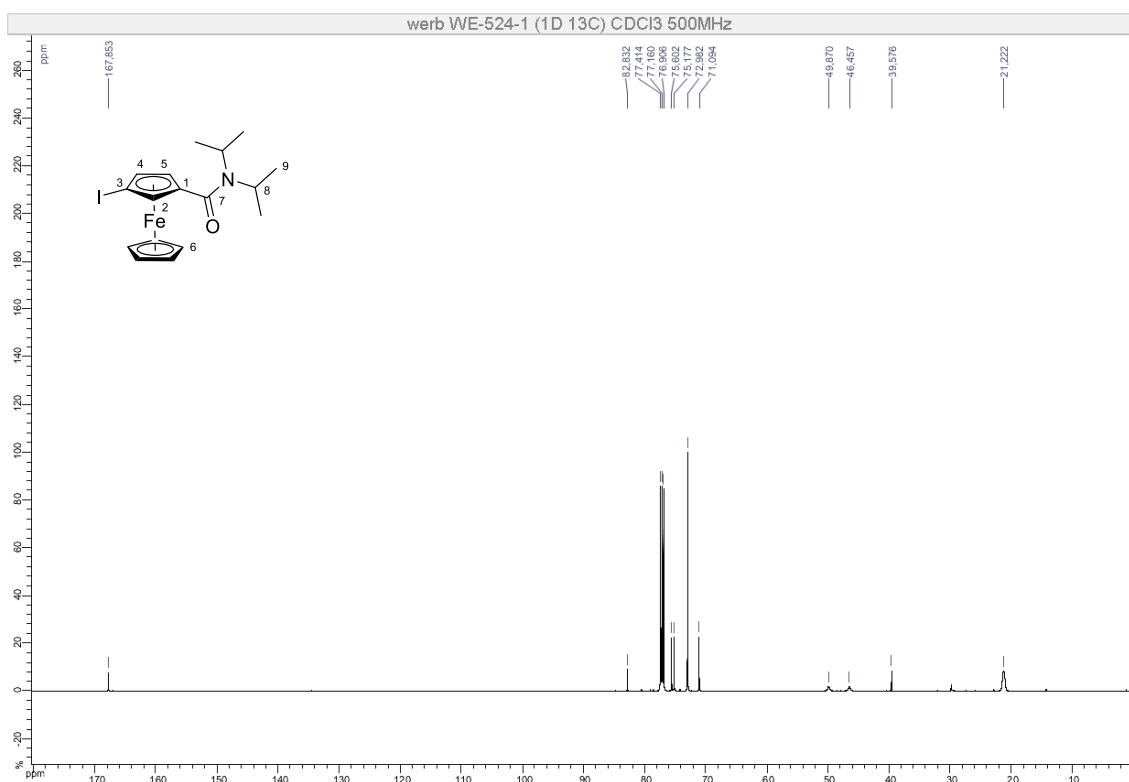
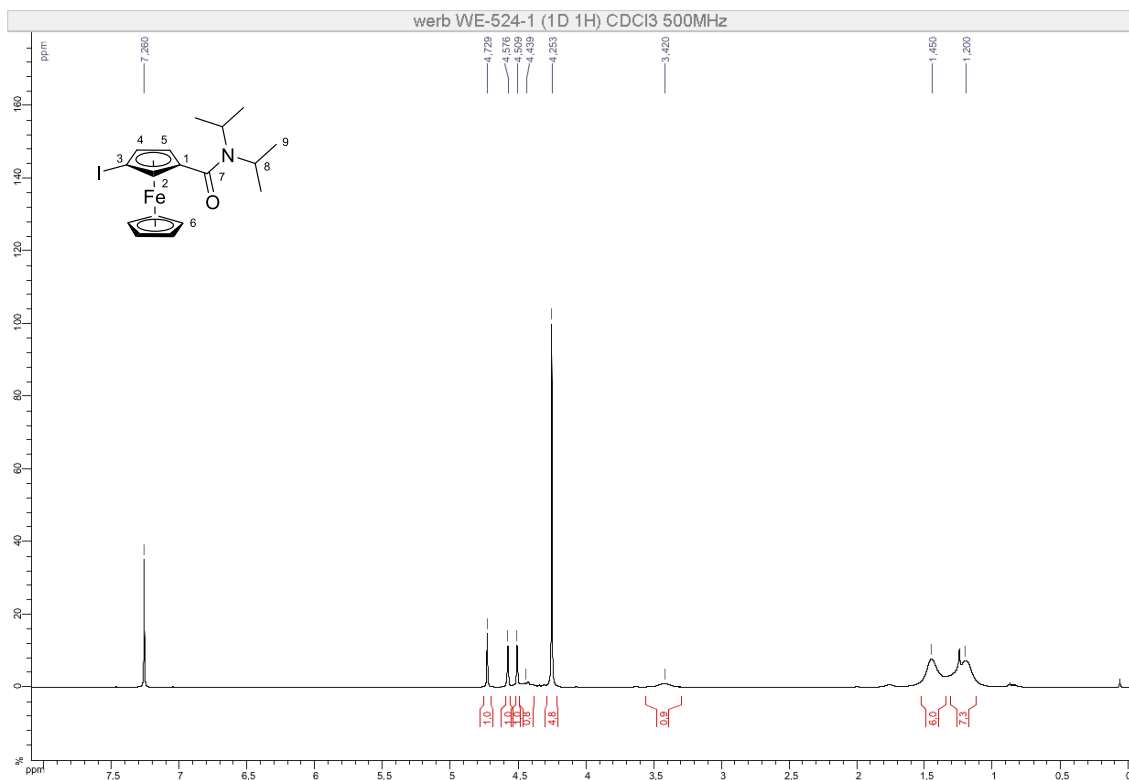
**Table S1.** Changes in chemical shifts,<sup>a</sup> relative to *N,N*-diisopropylferrocenecarboxamide, for the esters **3-10**.

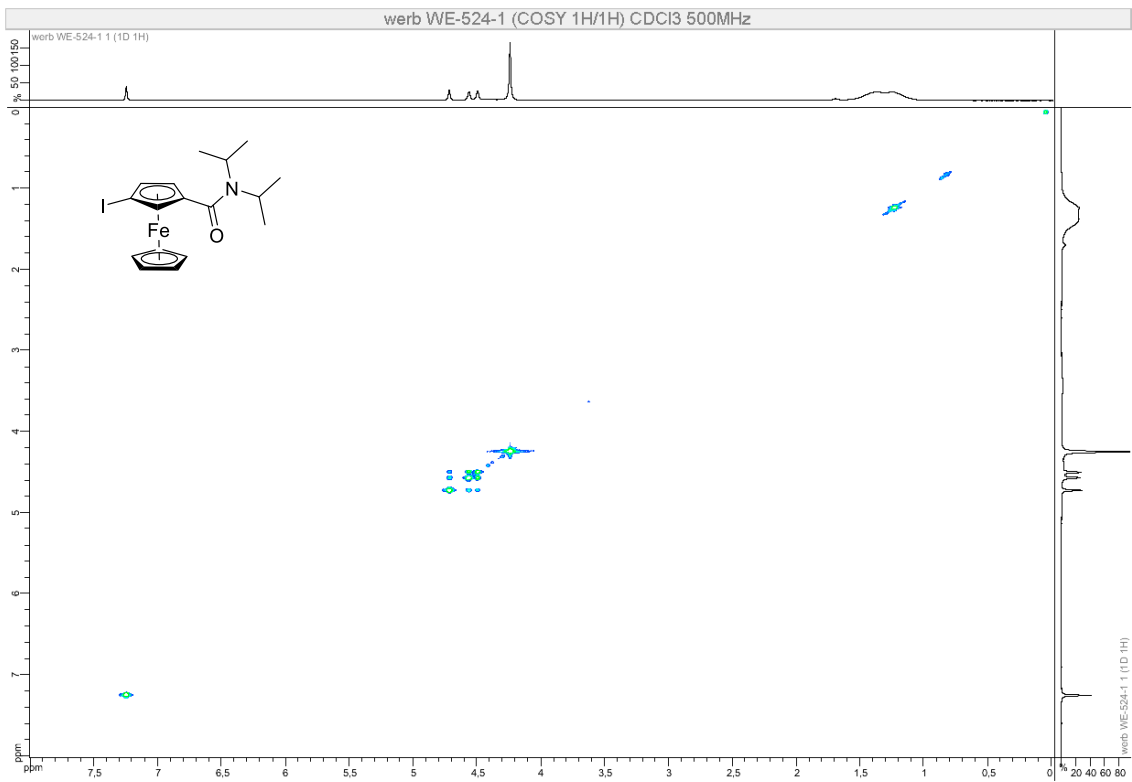
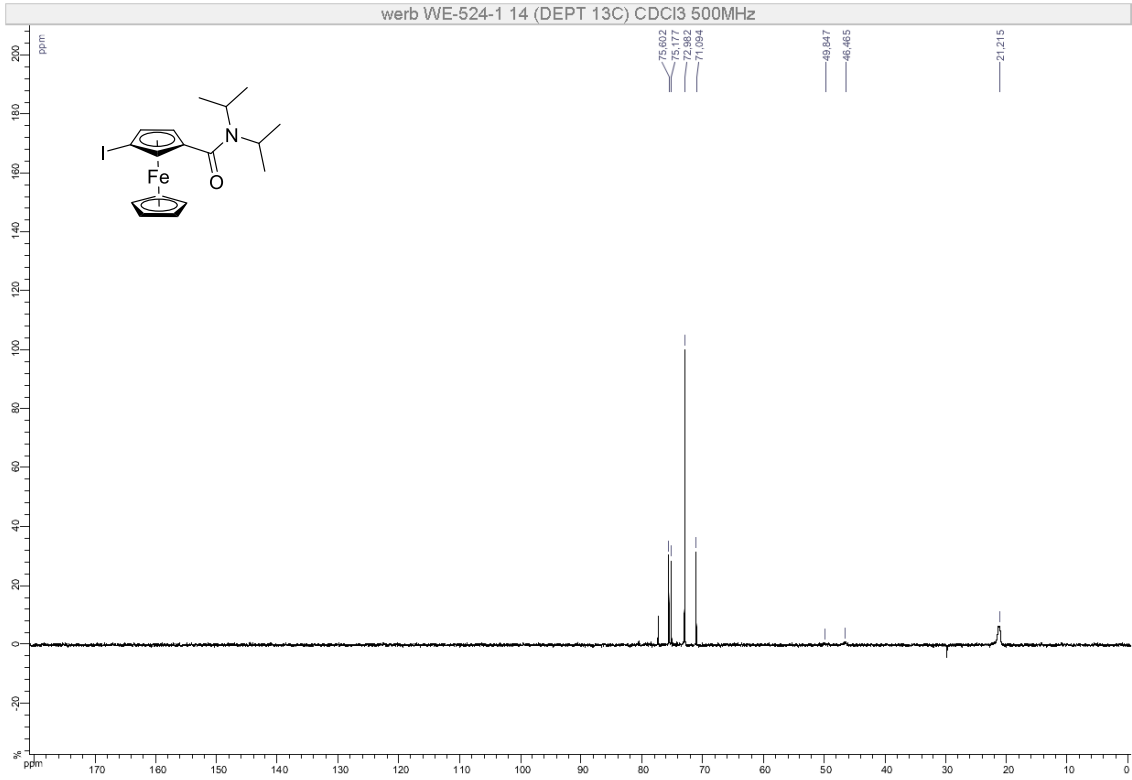
Compound	$\delta$ (ppm)									
	H2	H4	H5	Cp	C1	C2	C3	C4	C5	Cp
3	0.26	0.30	-0.13	0.06	-5.2	-7.5	46.5	-7.0	-4.5	1.5
4	0.25	0.31	-0.13	0.05	-5.4	-7.6	46.7	-7.0	-4.5	1.4
5	0.36	0.41	-0.08	0.08	5.3	-7.6	46.7	-7.0	-4.4	1.5
6	0.34	0.38	-0.14	0.01	-4.8	-7.6	46.9	-7.1	-4.3	1.6
7	0.40	0.45	-0.06	0.10	-5.0	-7.7	46.8	-7.1	-4.3	1.6
8	0.30	0.35	-0.15	0.00	-5.0	-7.5	46.8	-7.0	-4.3	1.5
9	0.36	0.43	-0.19	0.01	-5.2	-7.7	46.9	-7.1	-4.4	1.5
10	0.36	0.39	-0.10	nd	-5.3	-7.4	46.9	-7.0	-4.6	nd

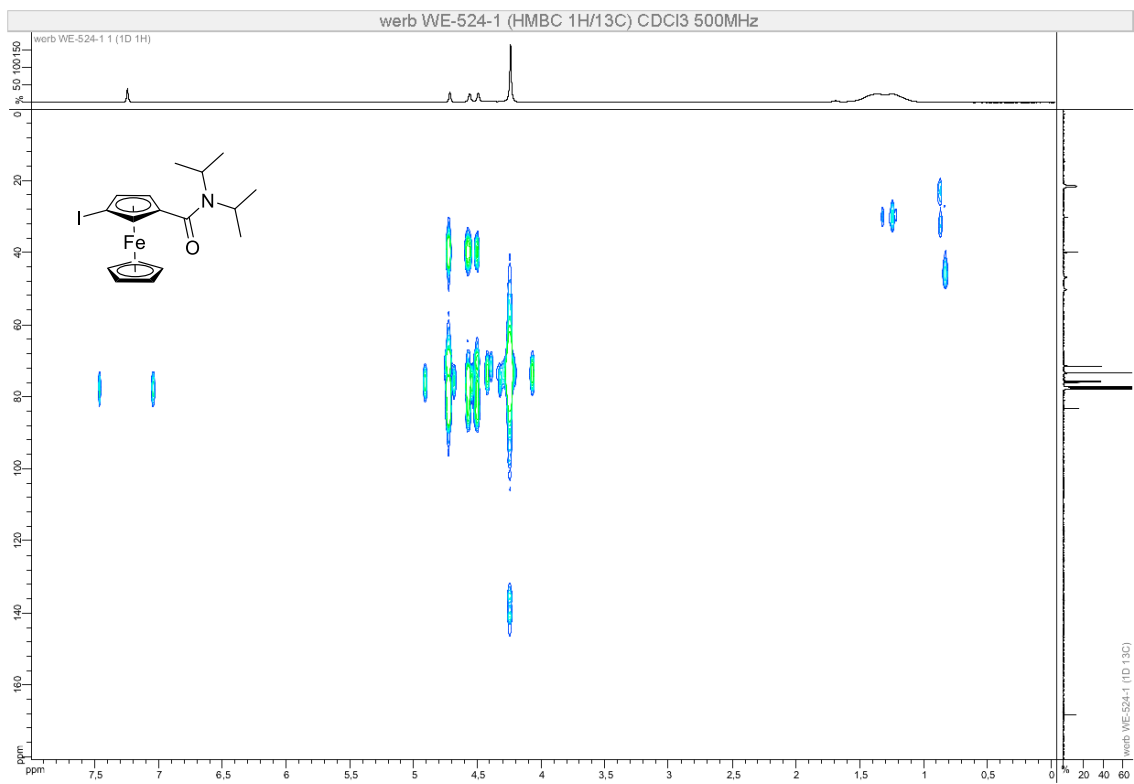
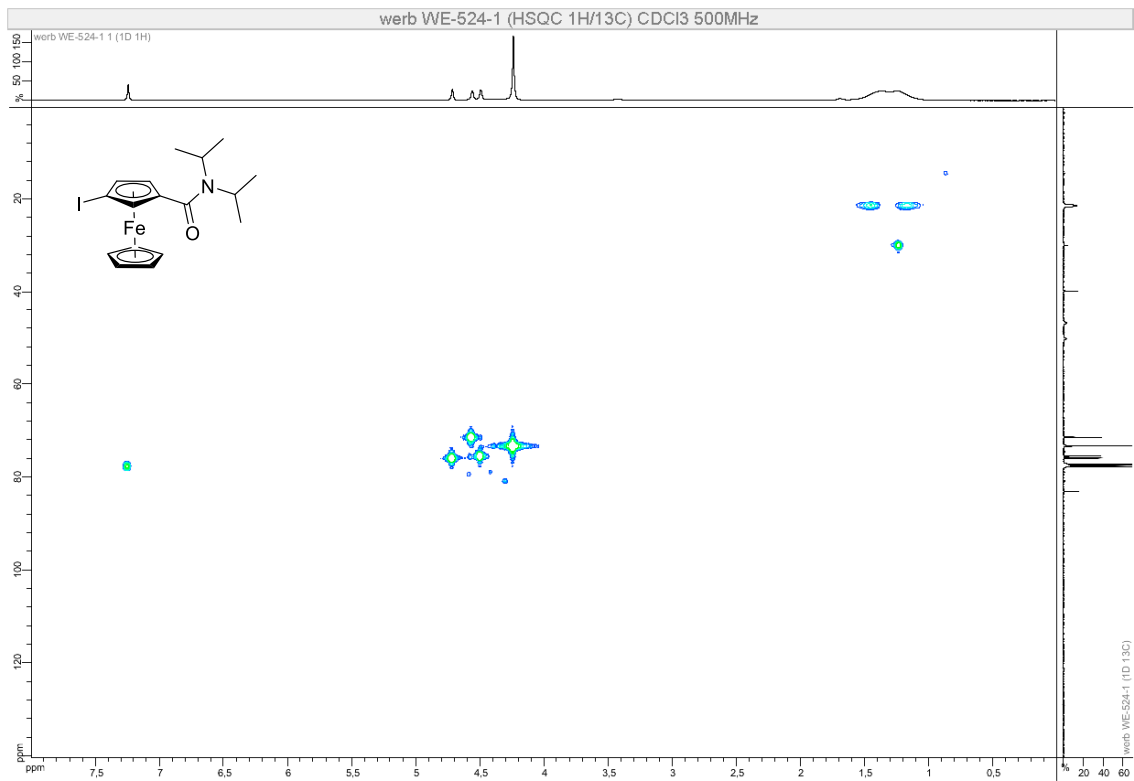
<sup>a</sup> Spectra recorded in CDCl<sub>3</sub>. nd: not determined.

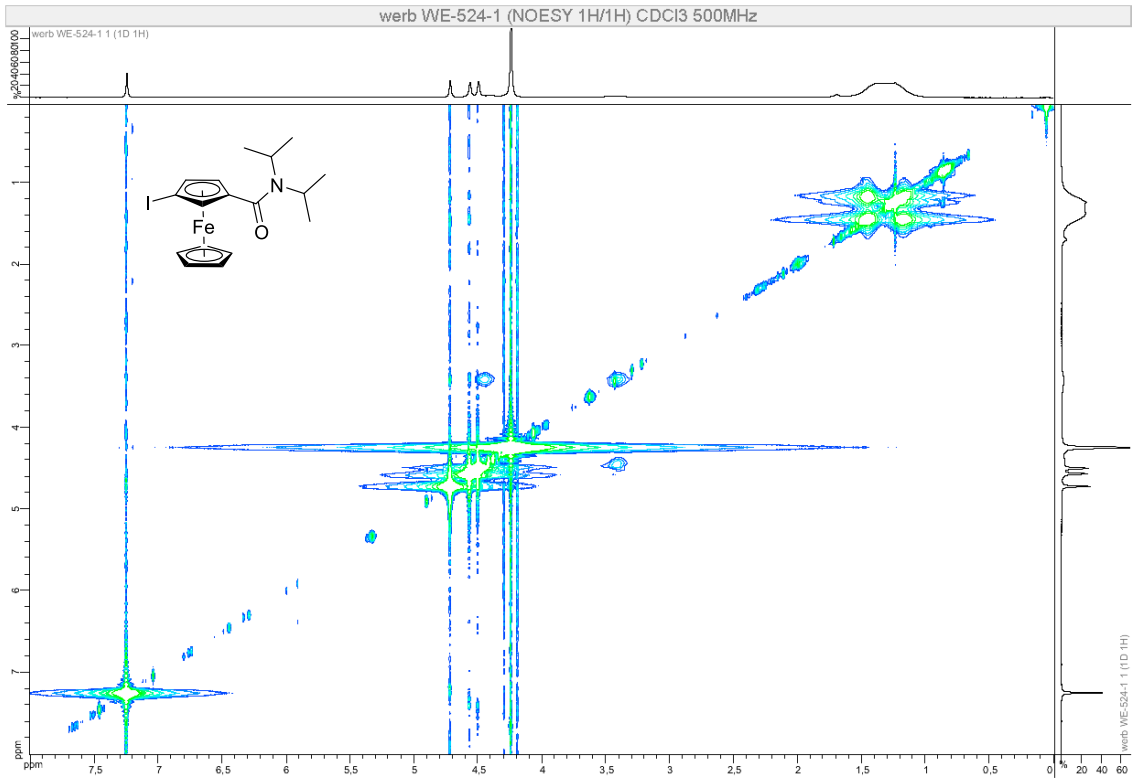
# NMR Spectra

## 3-Iodo-N,N-diisopropylferrocenecarboxamide (1)

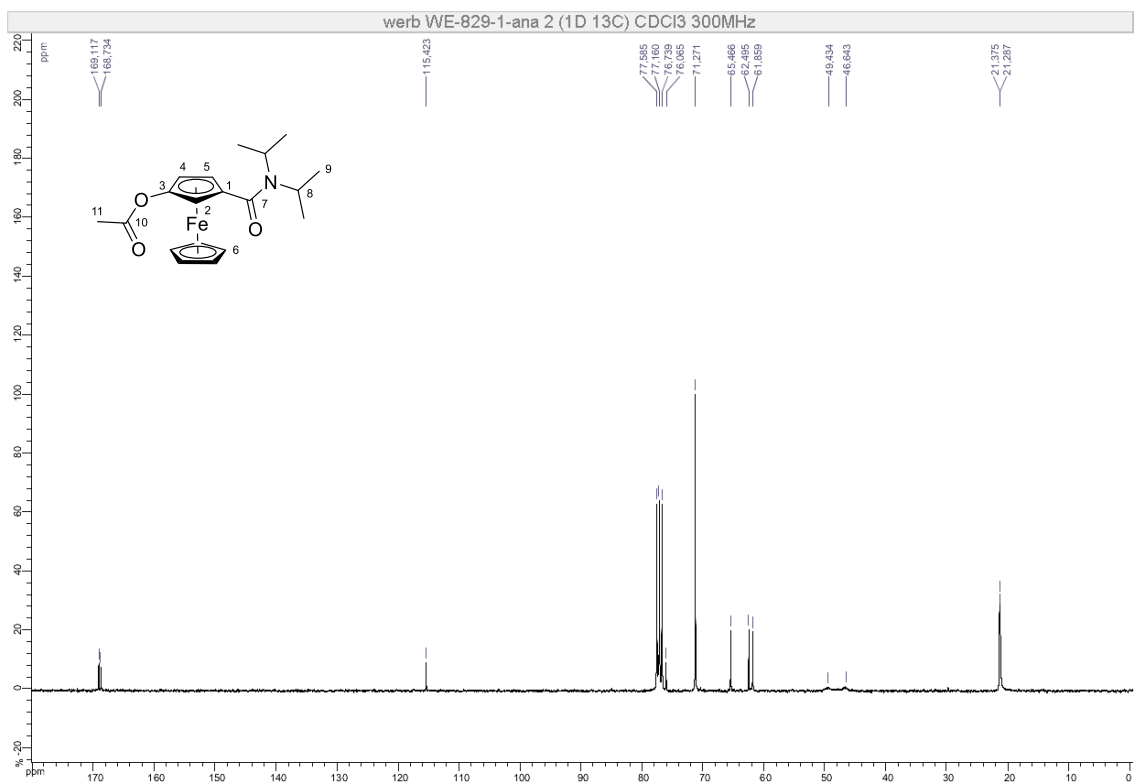
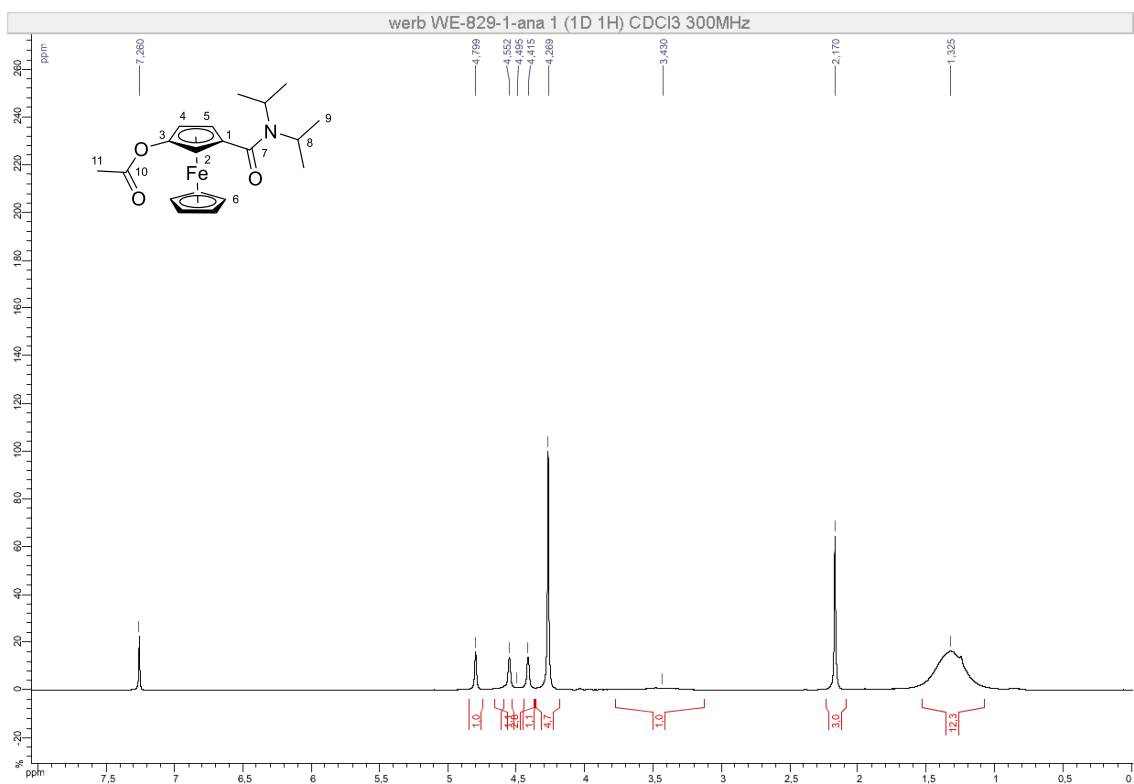


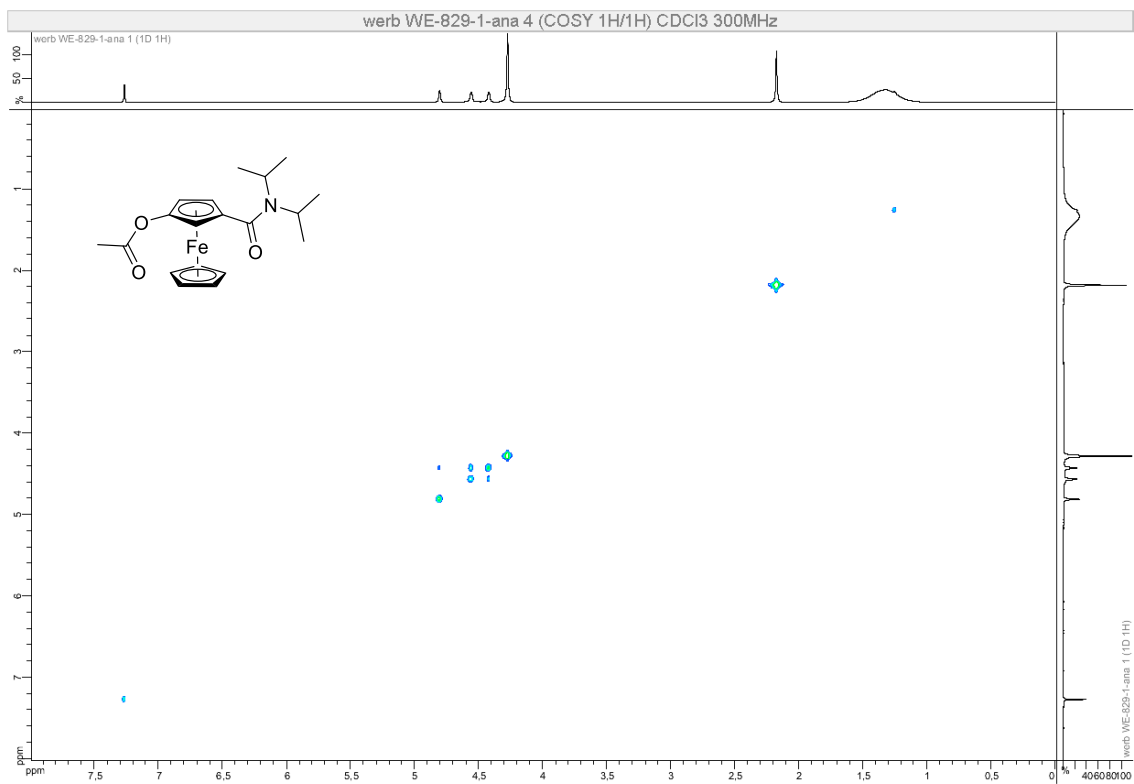
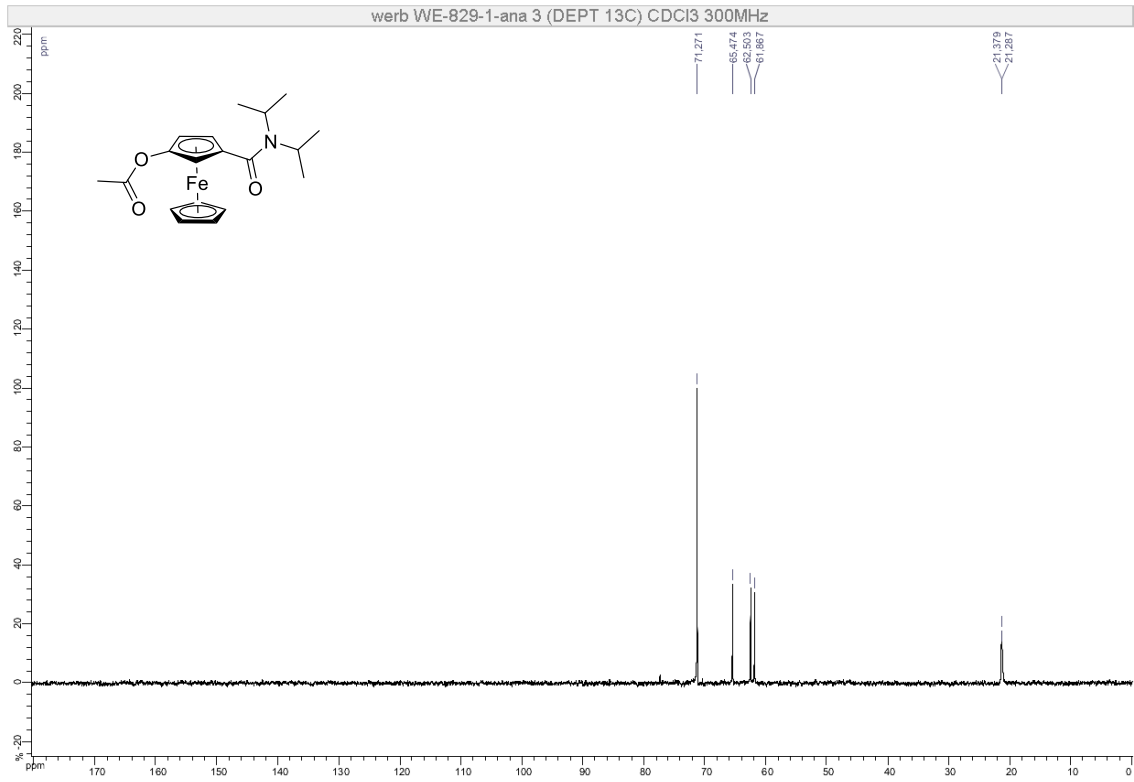




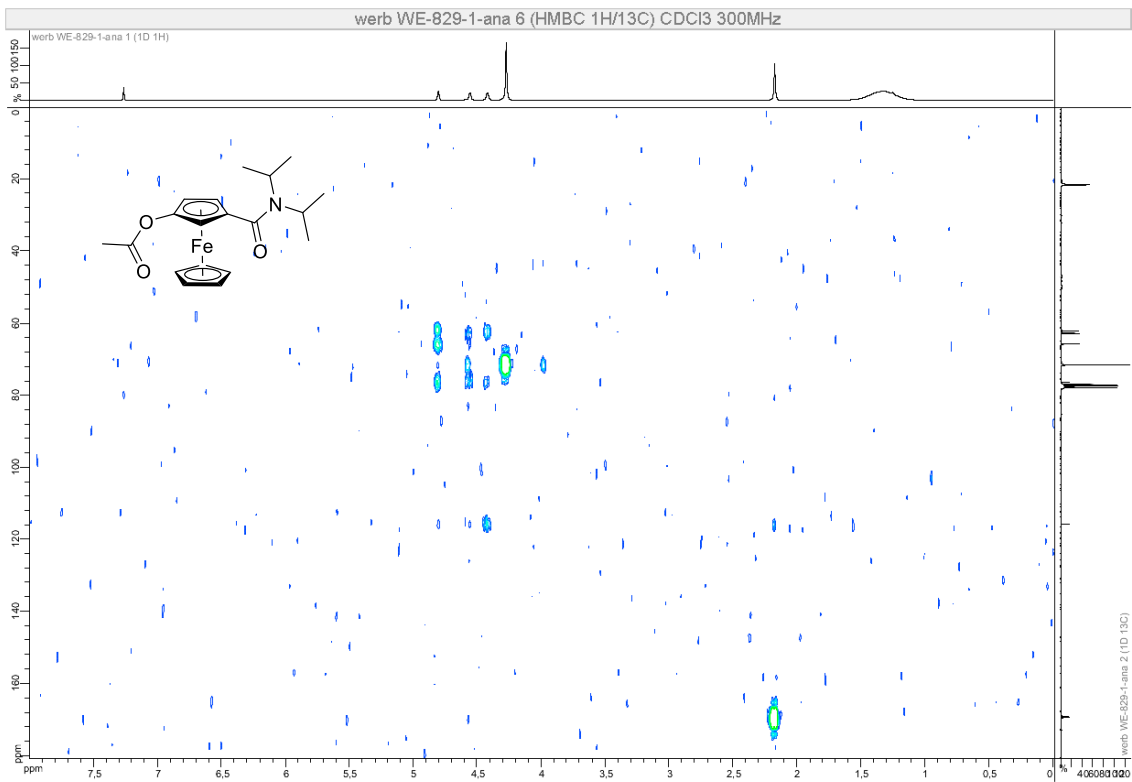
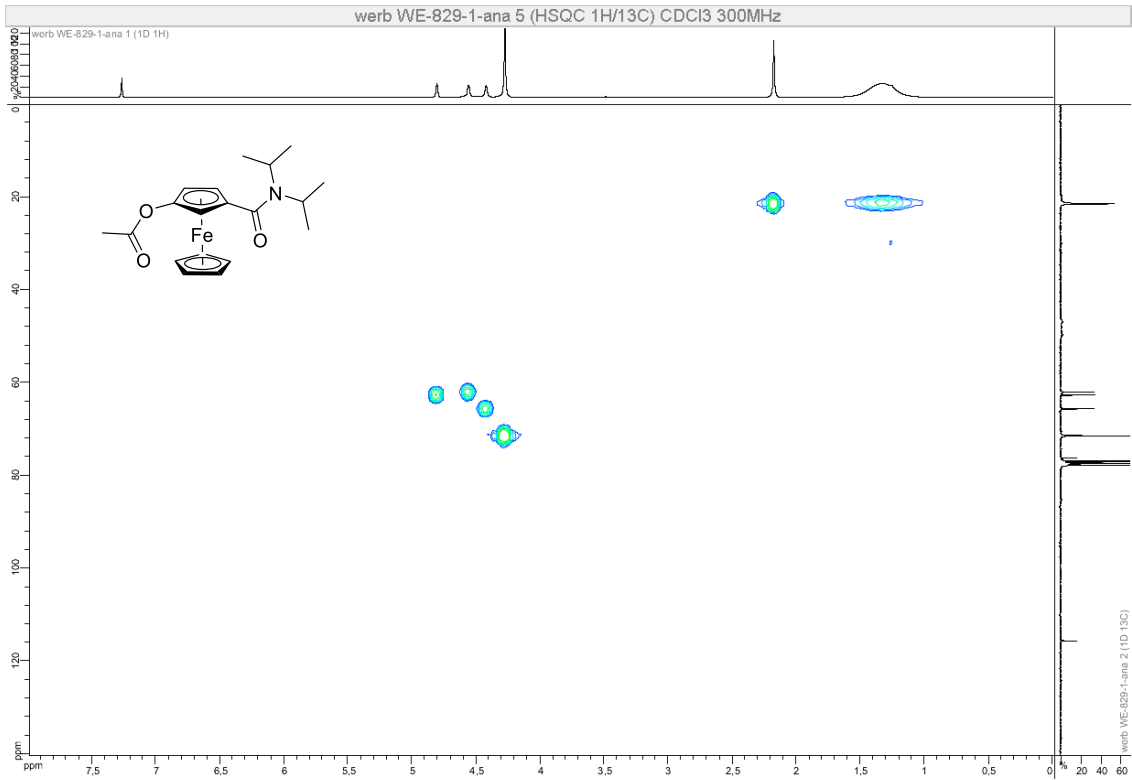


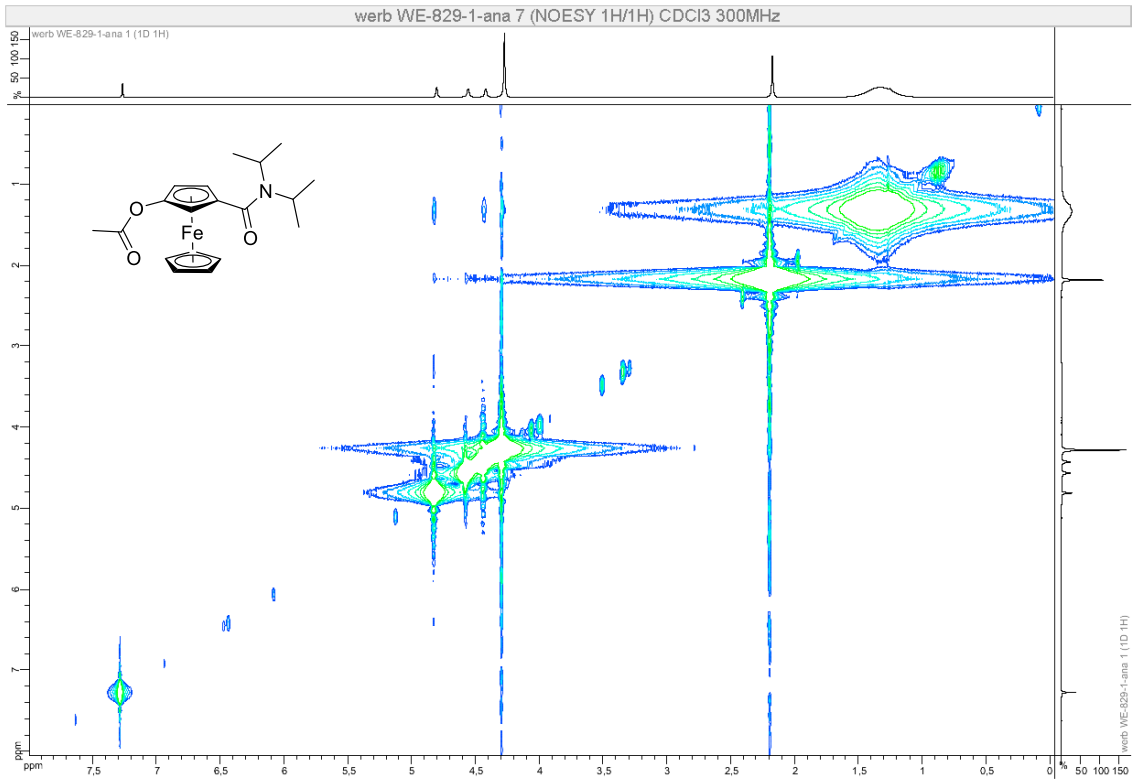
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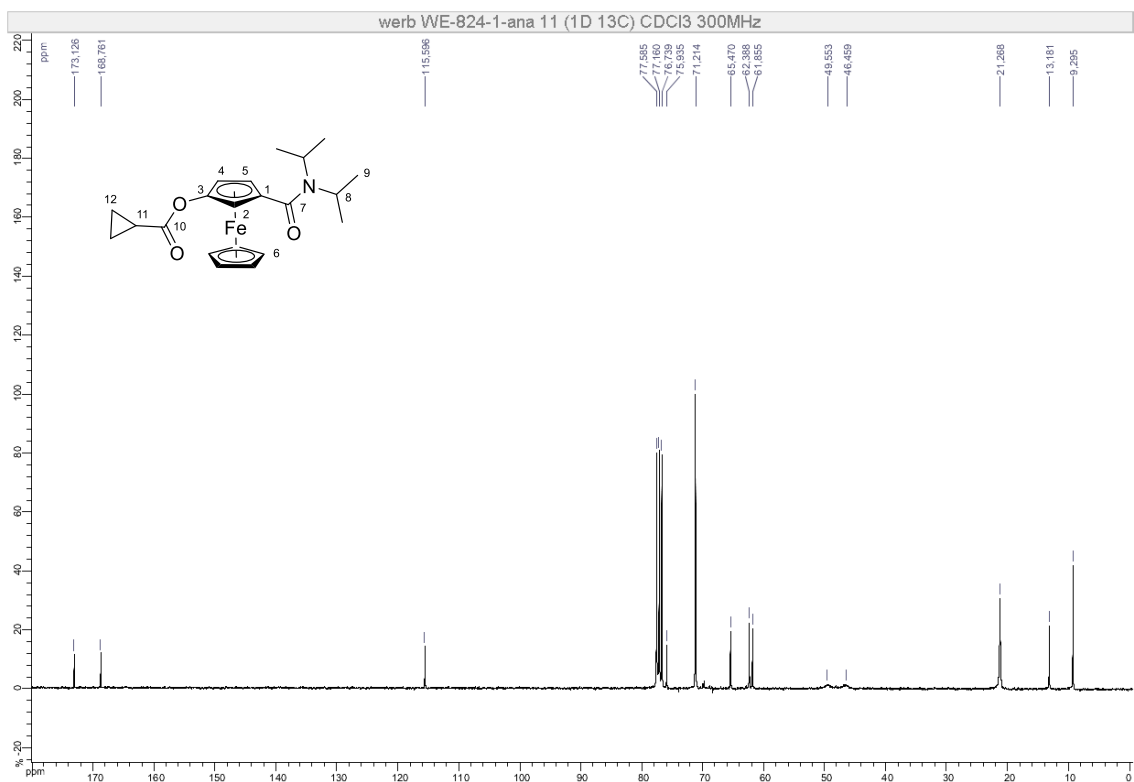
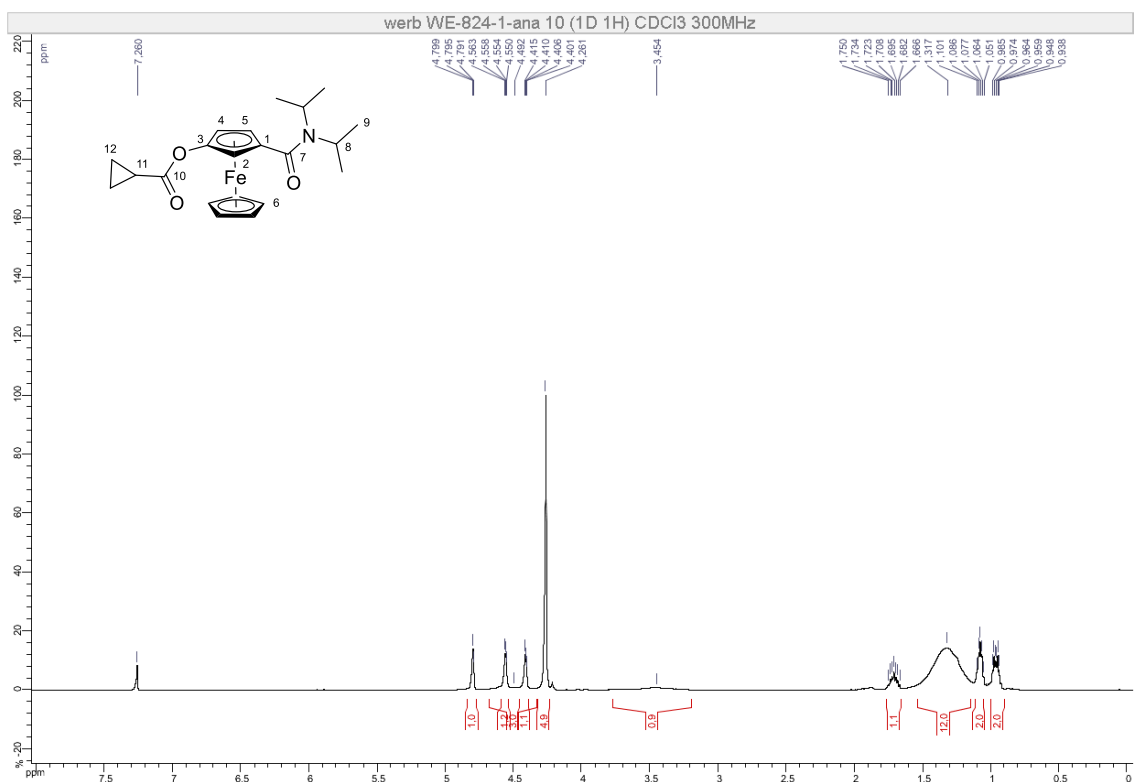


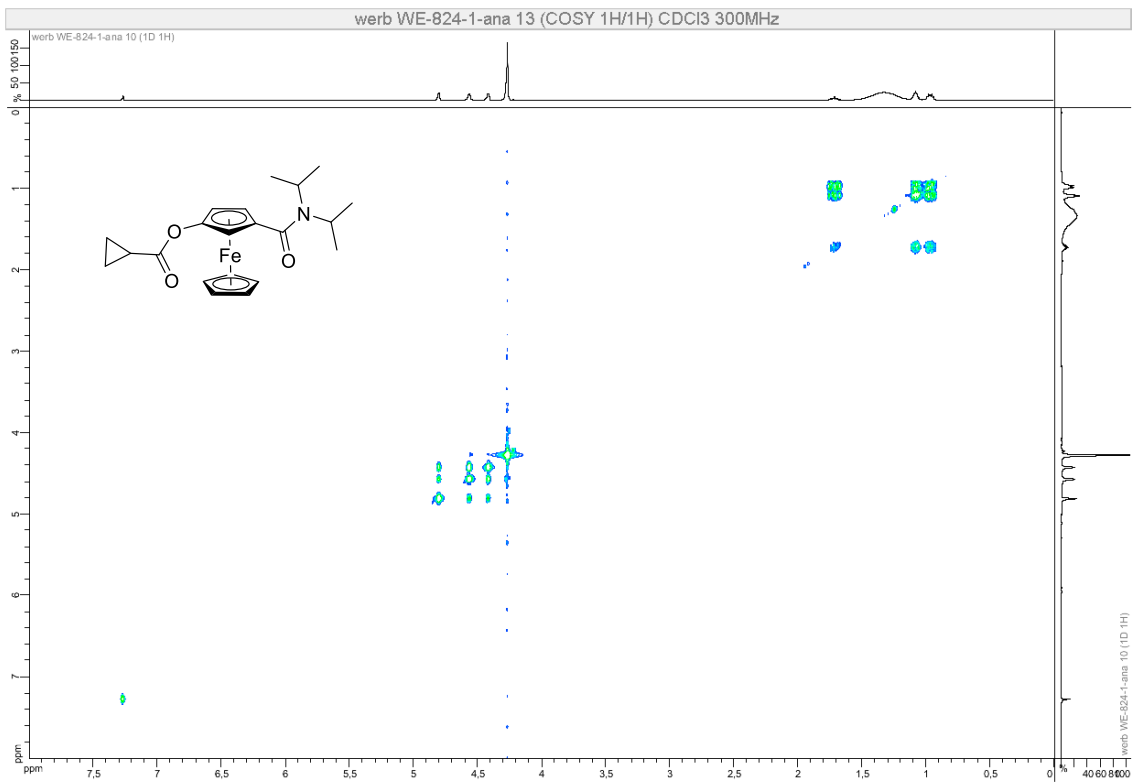
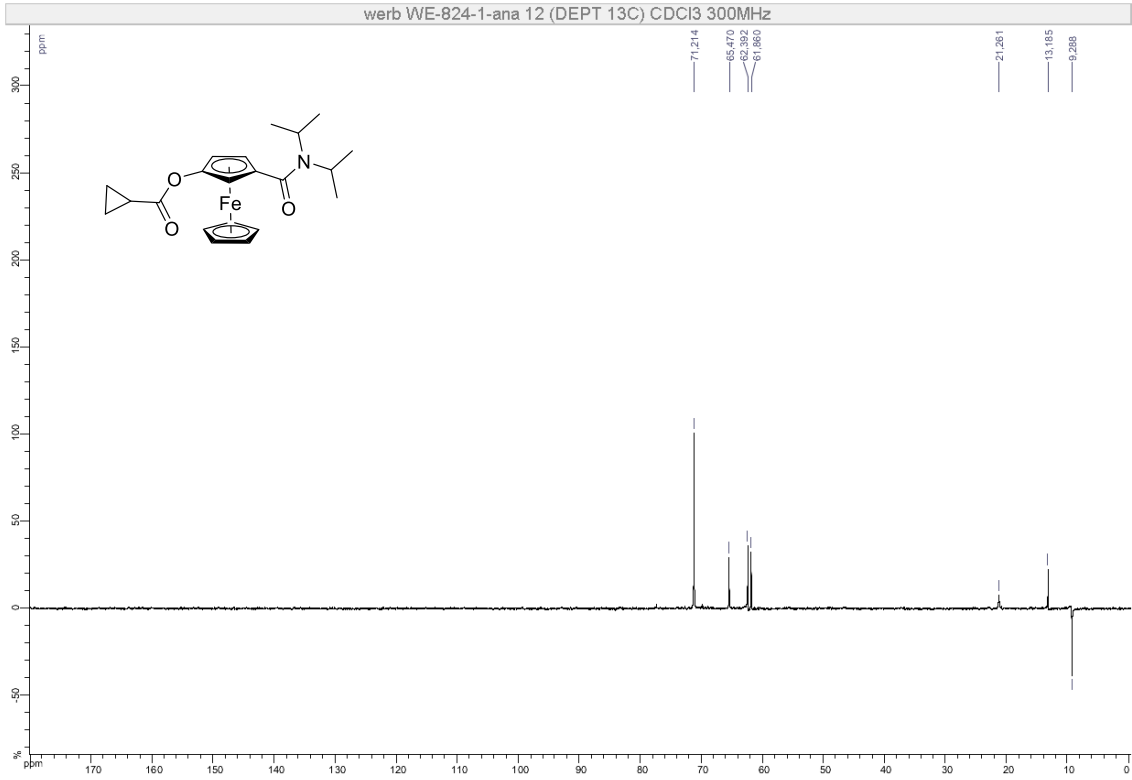


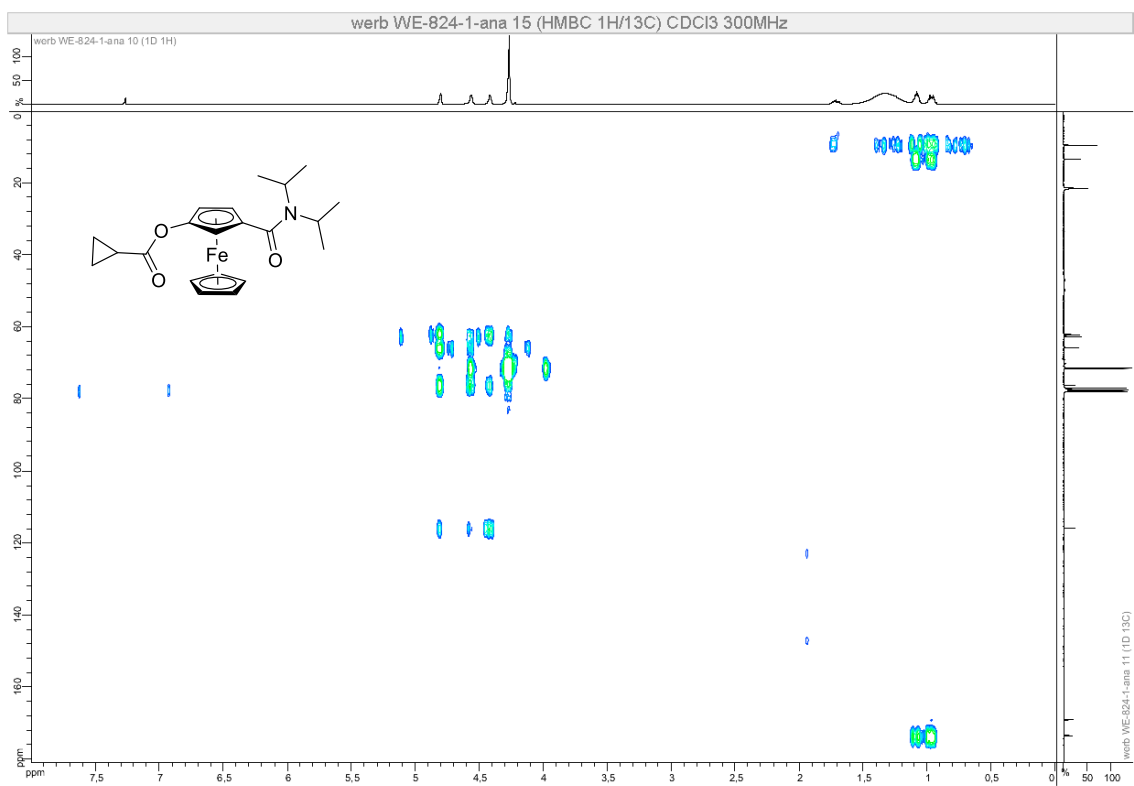
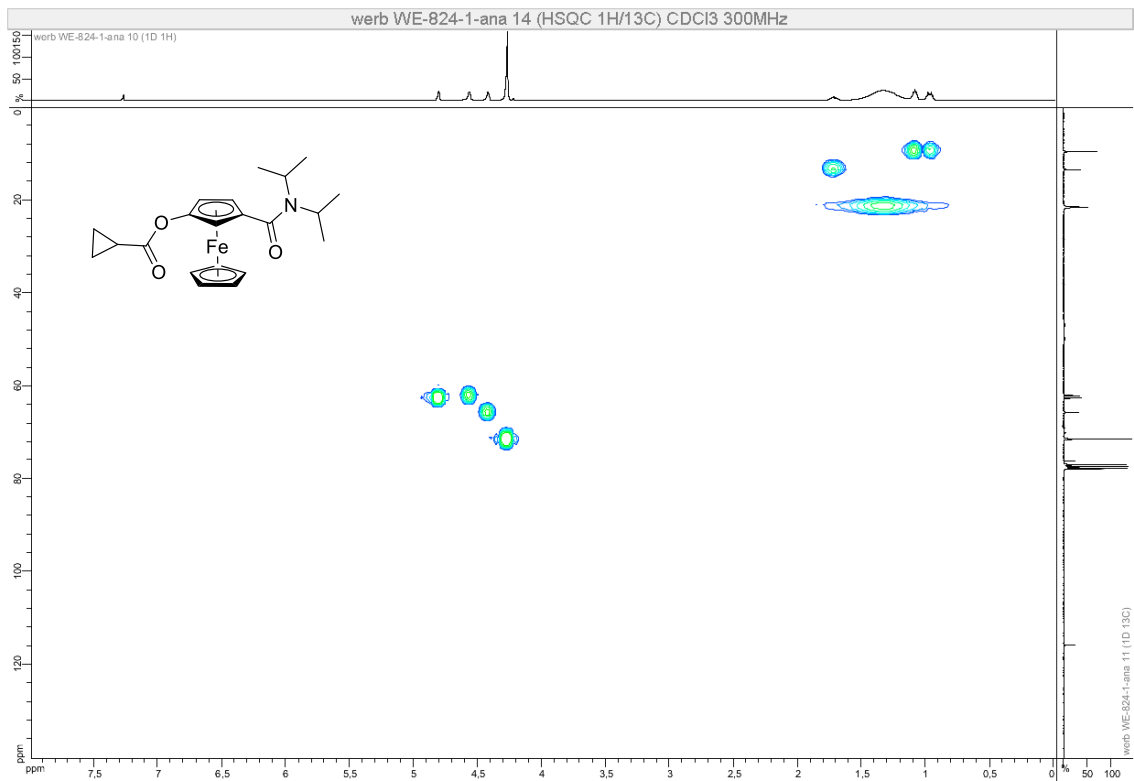


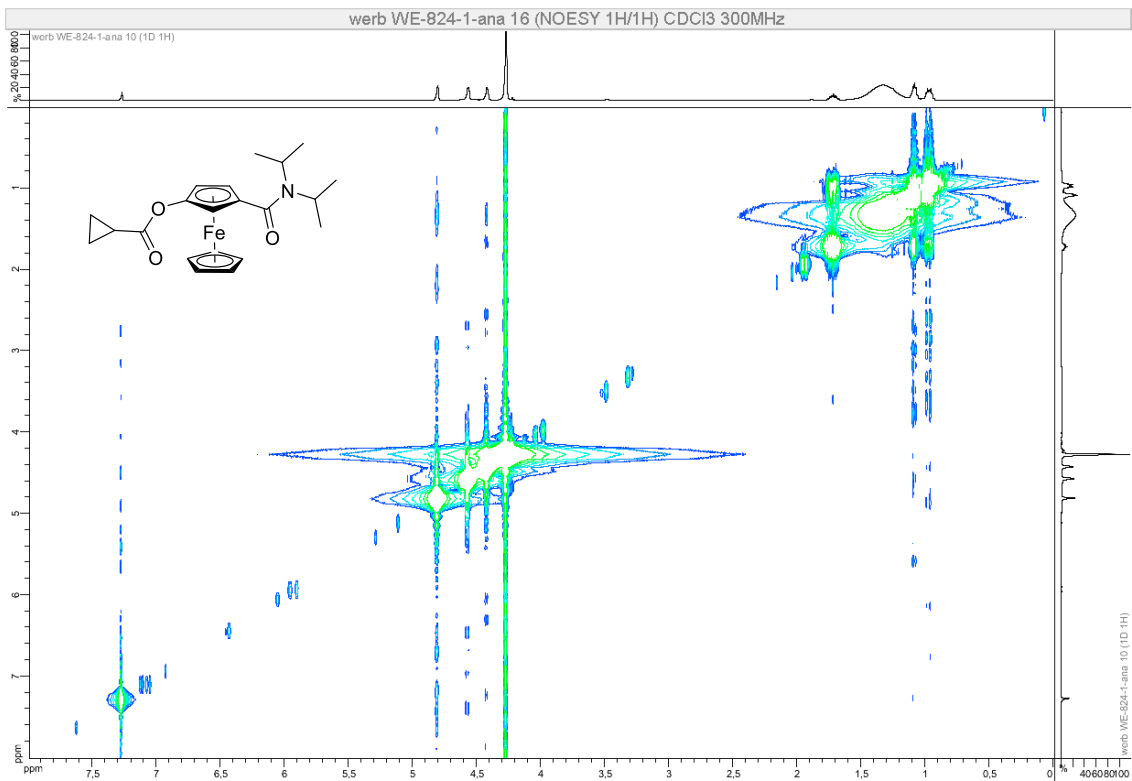


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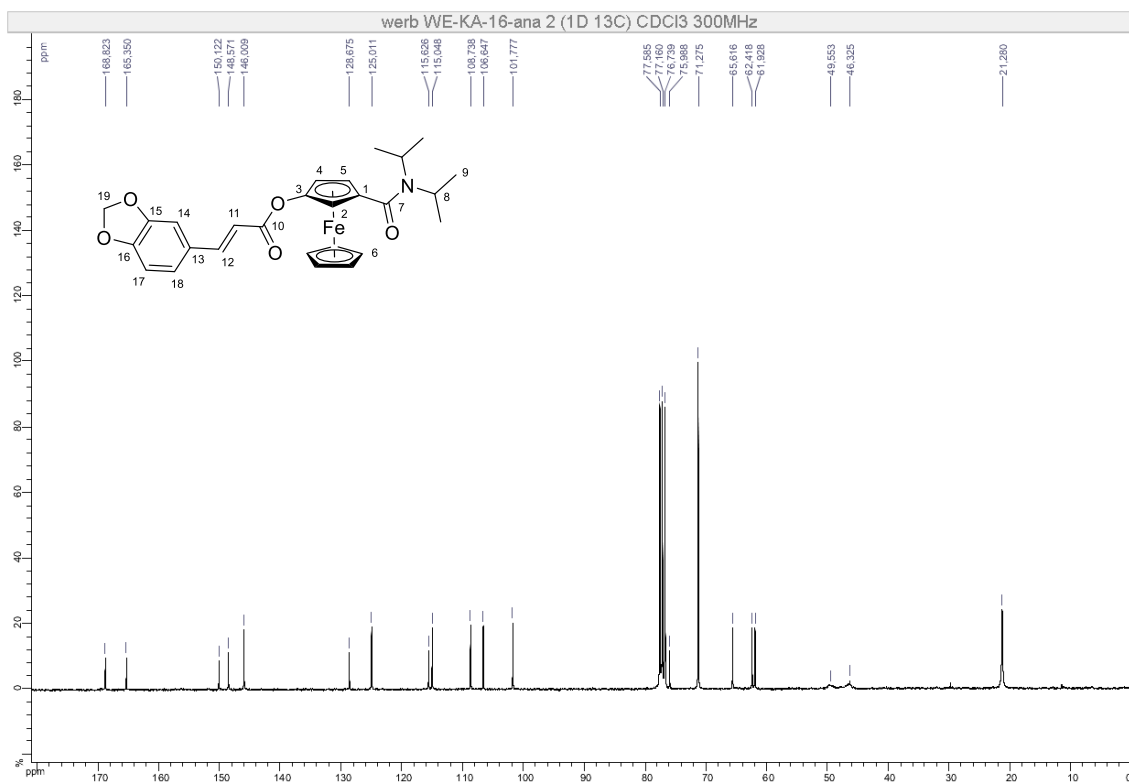
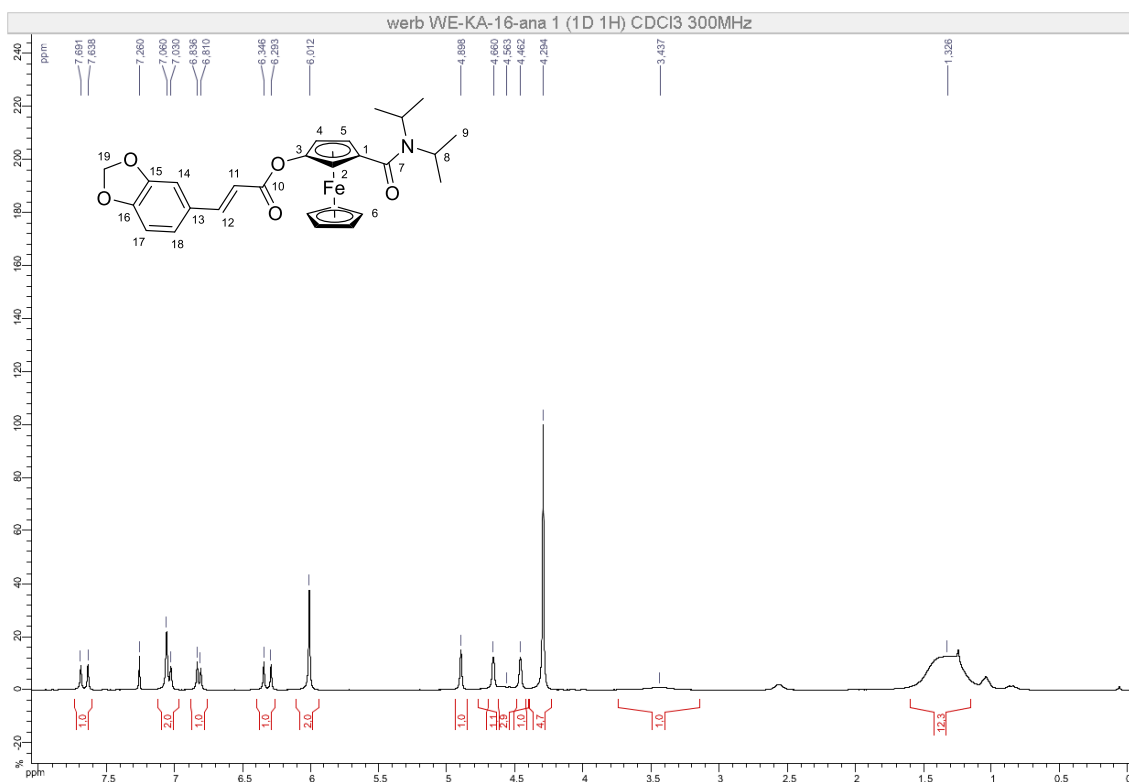


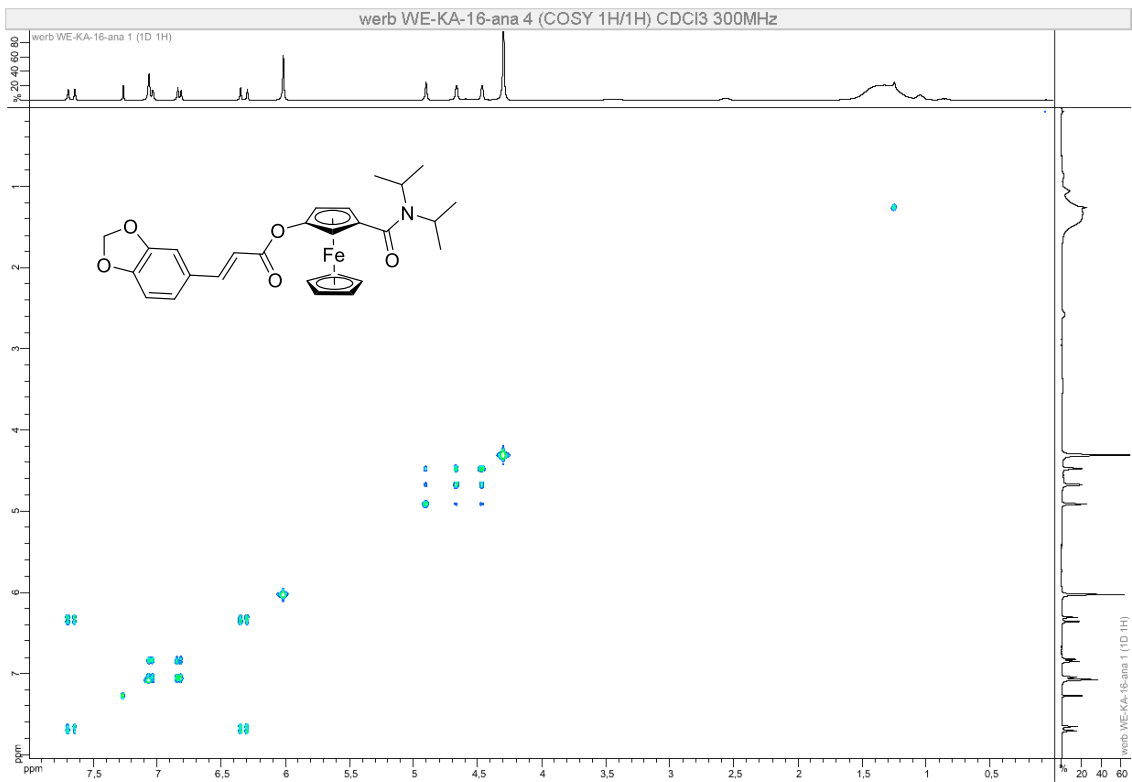
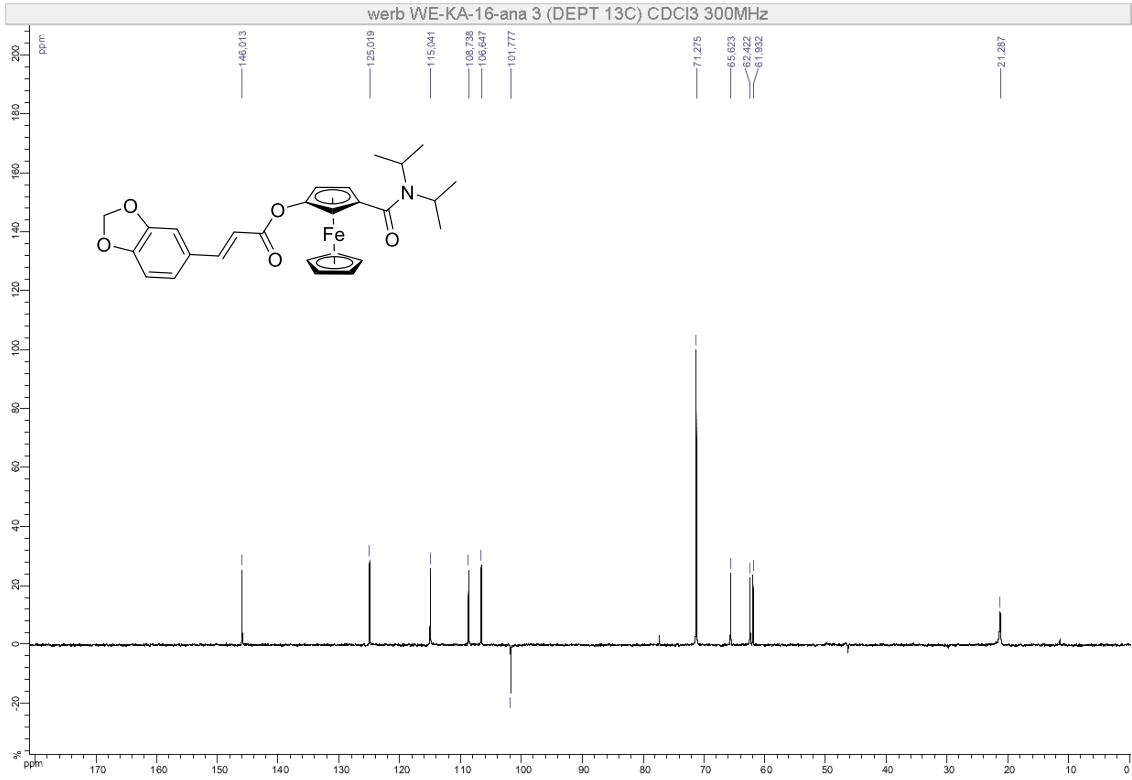




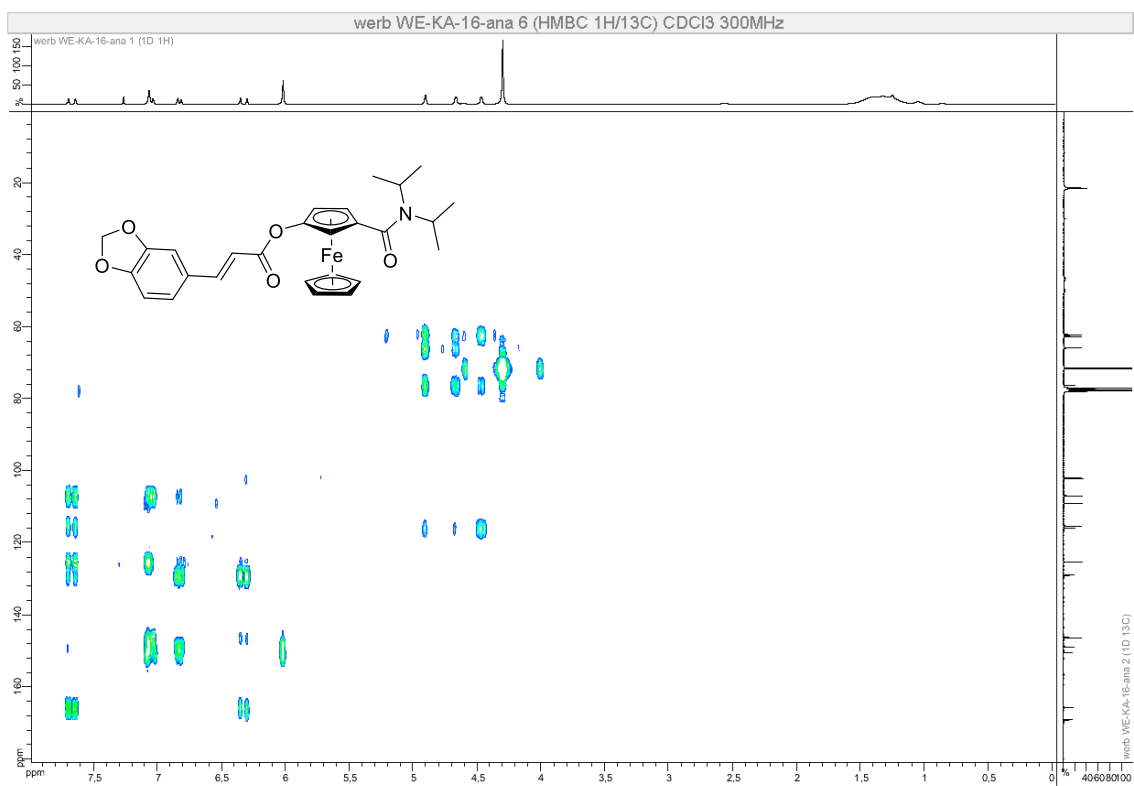
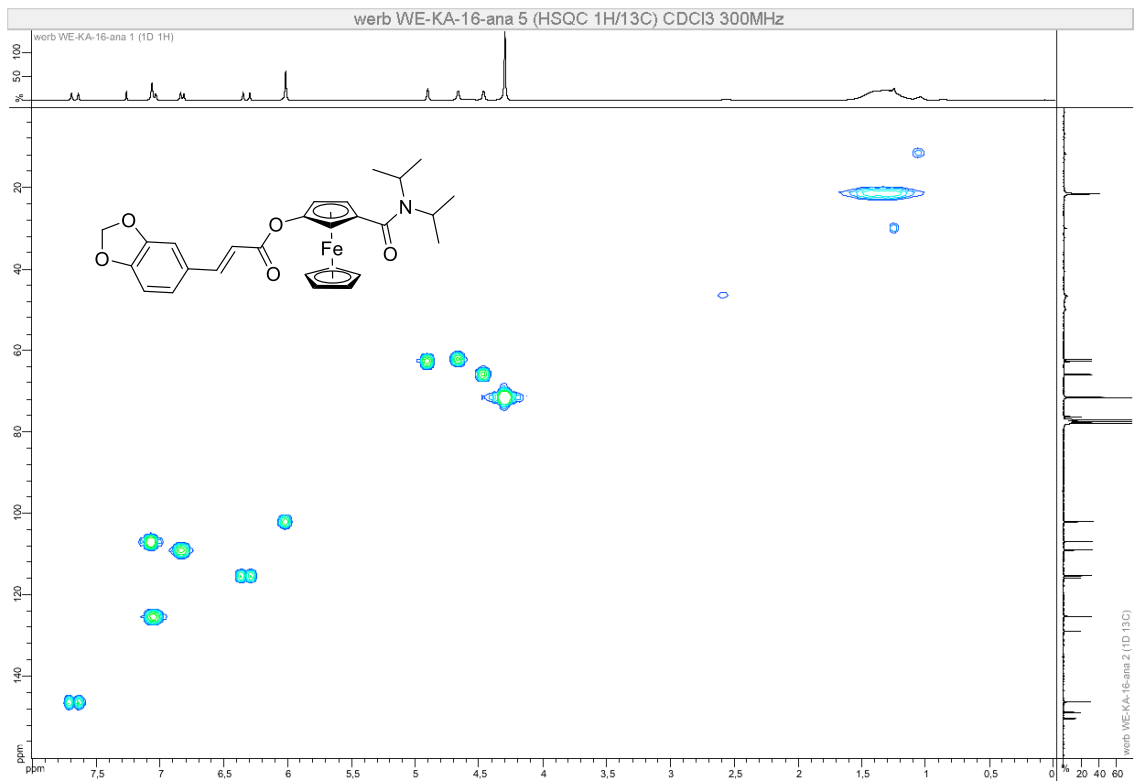


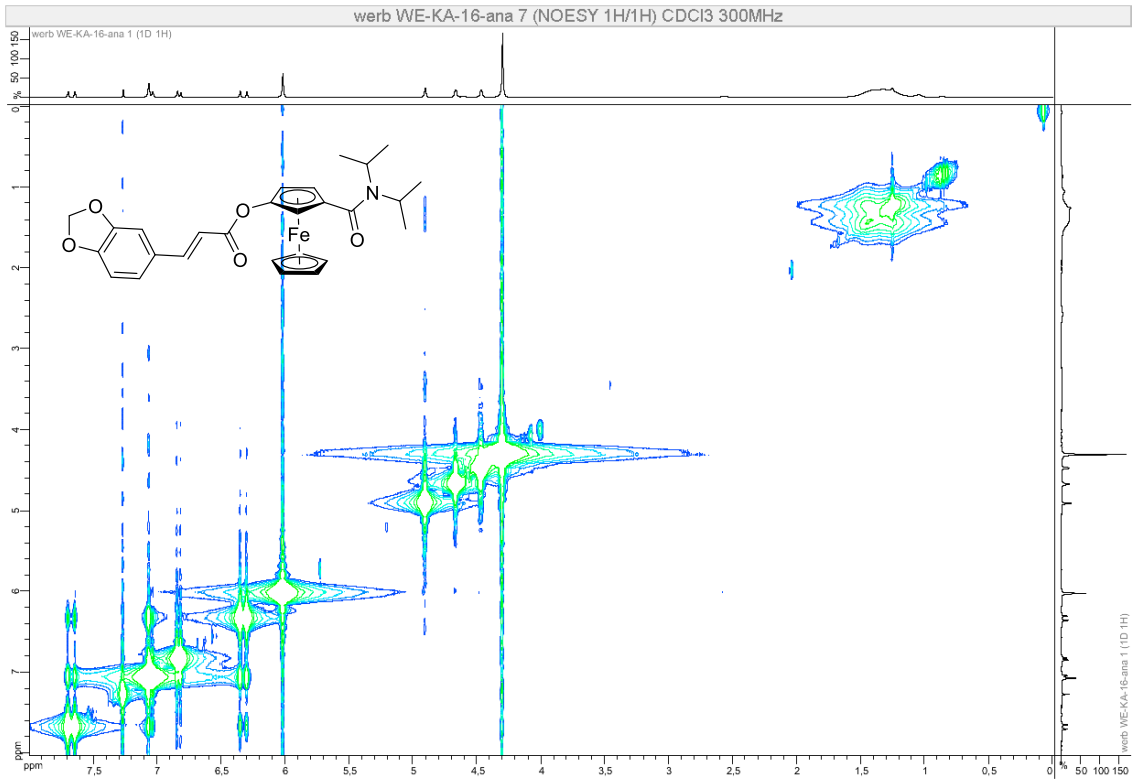
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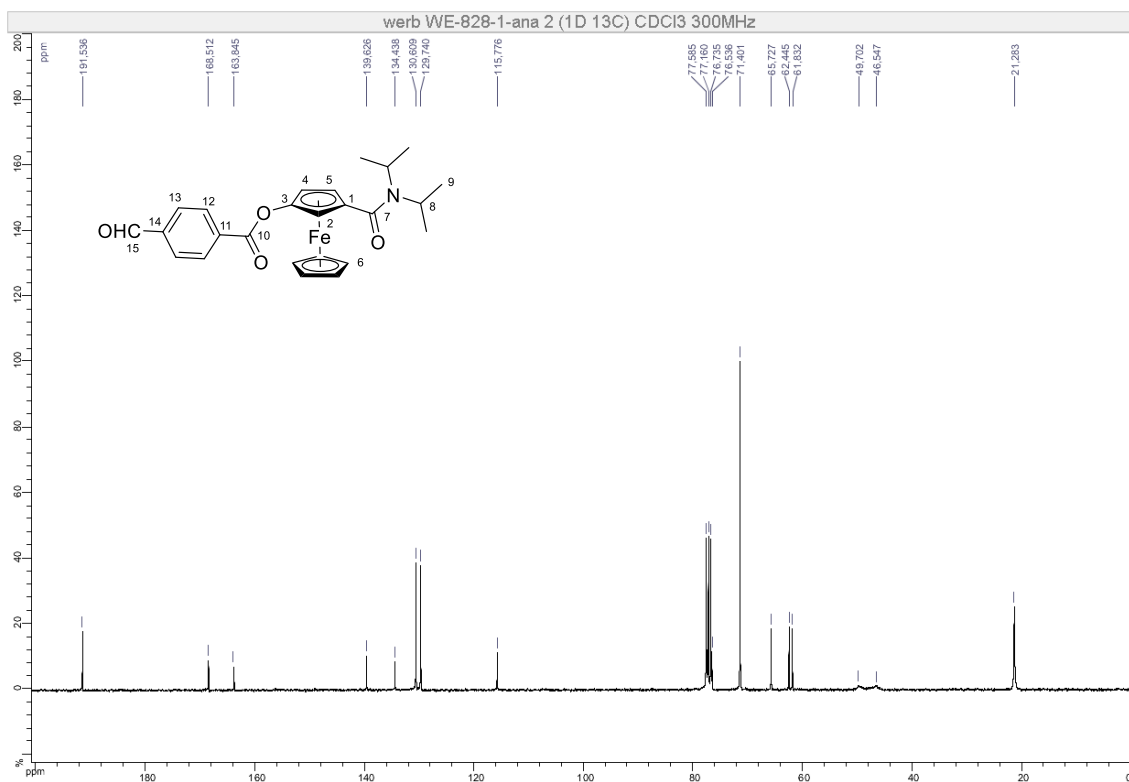
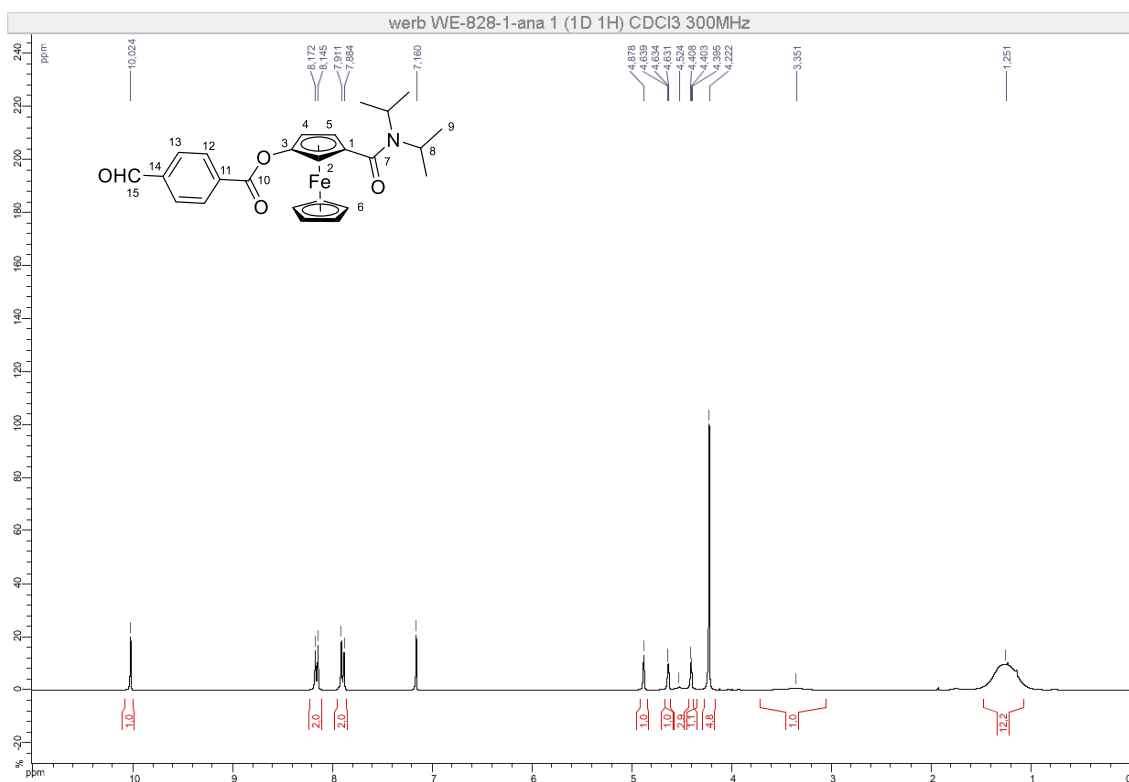


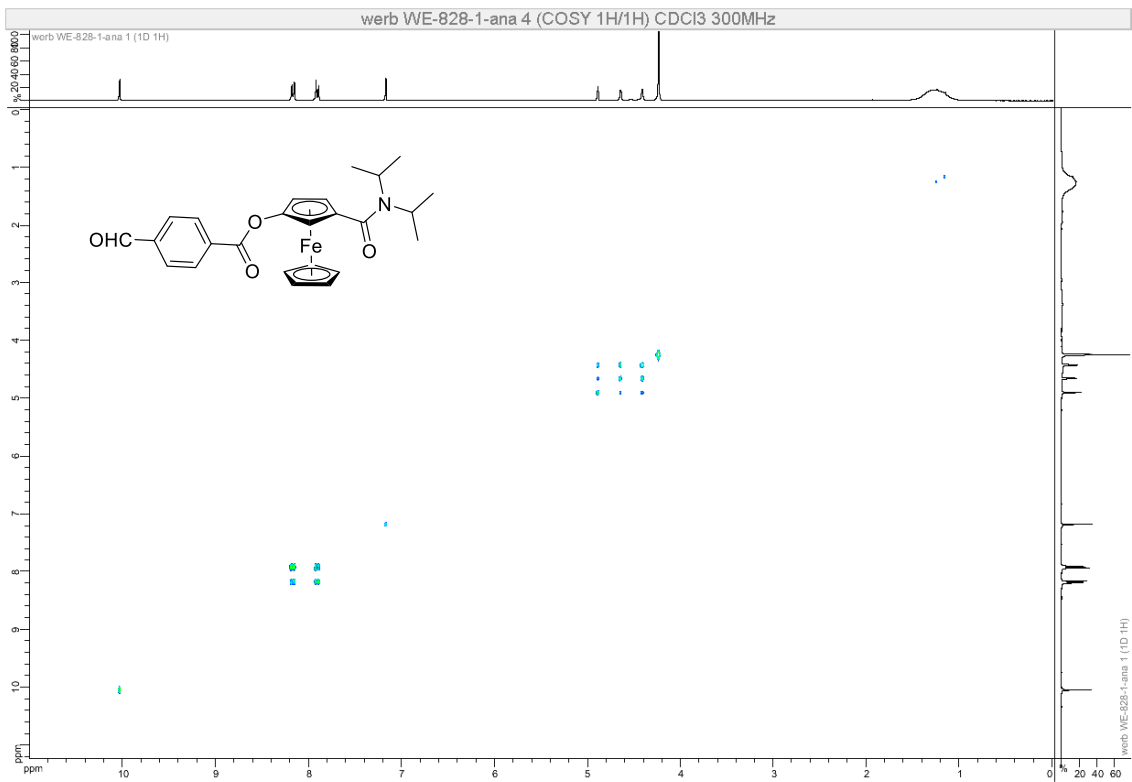
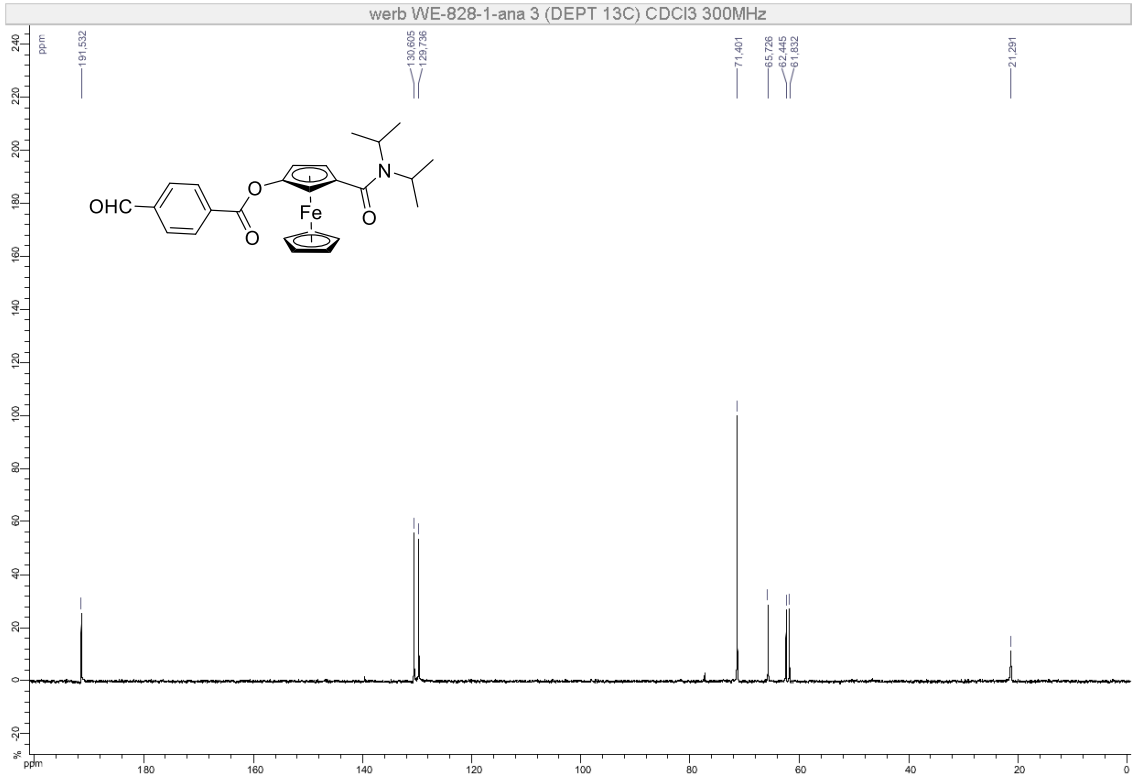


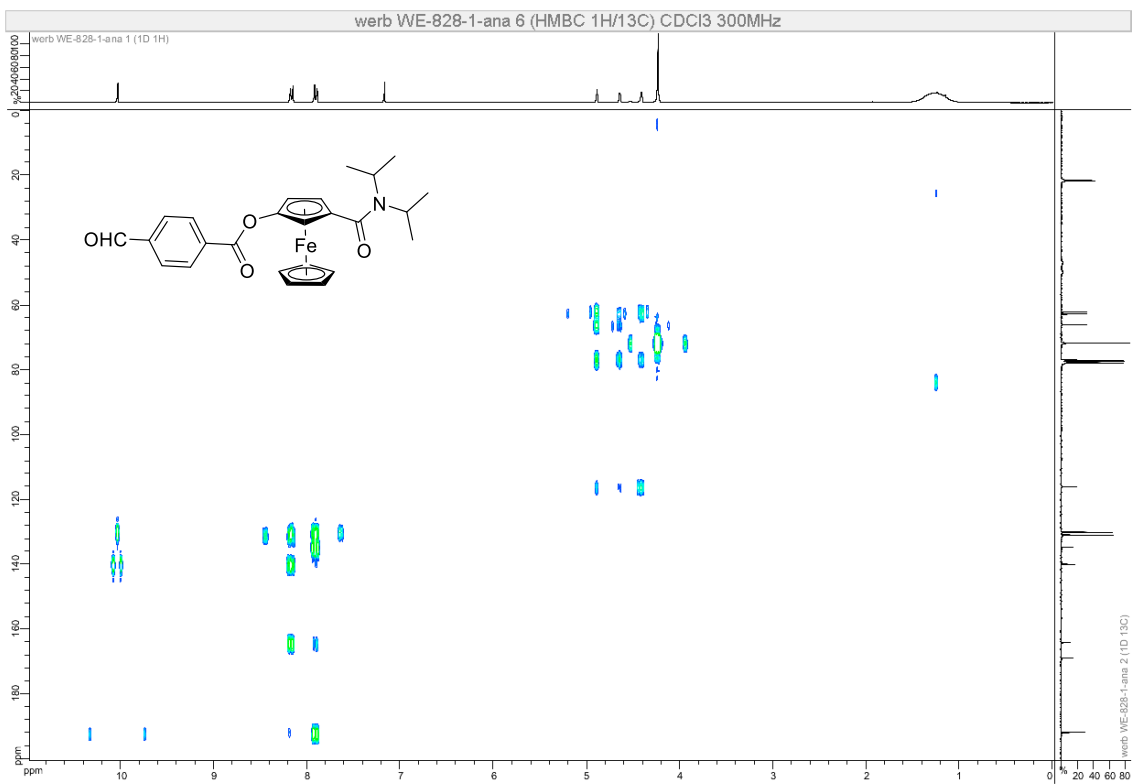
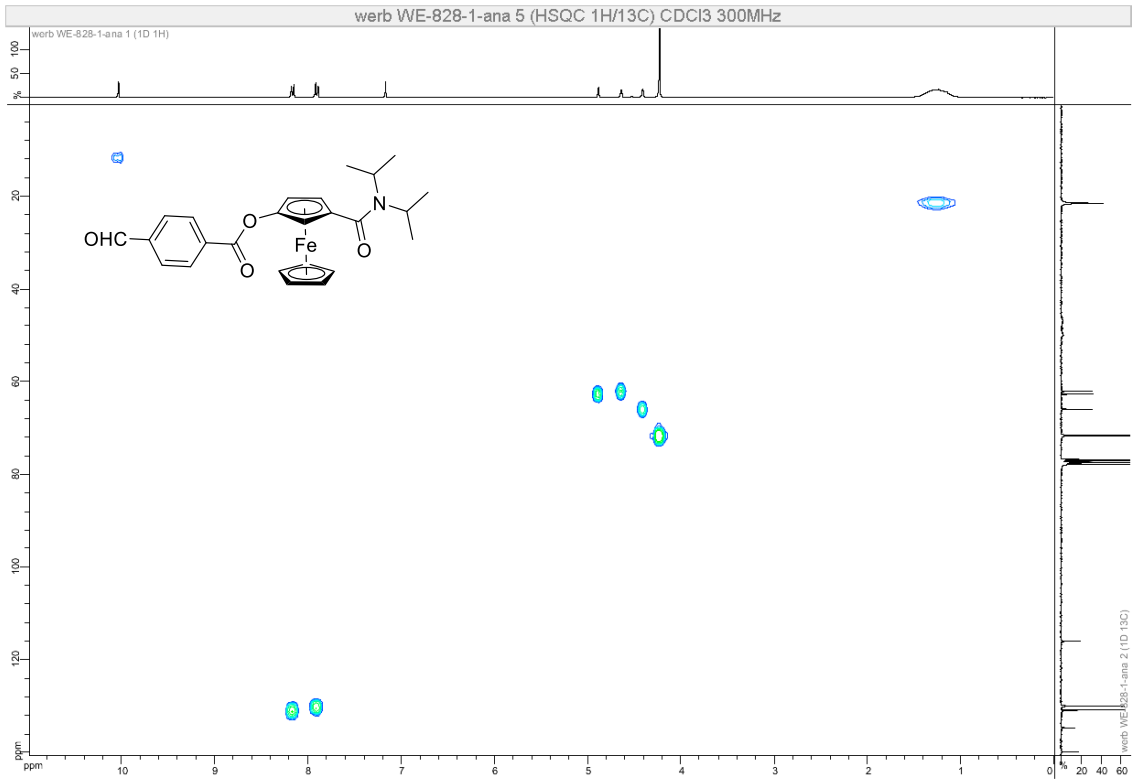




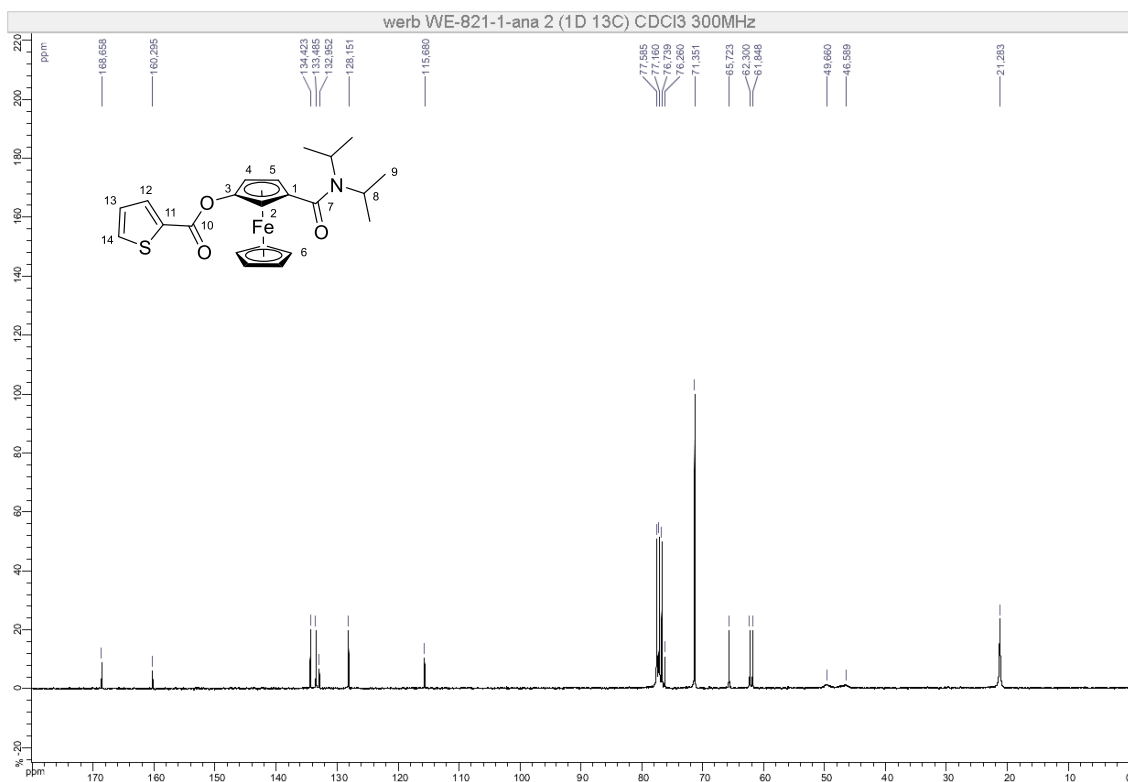
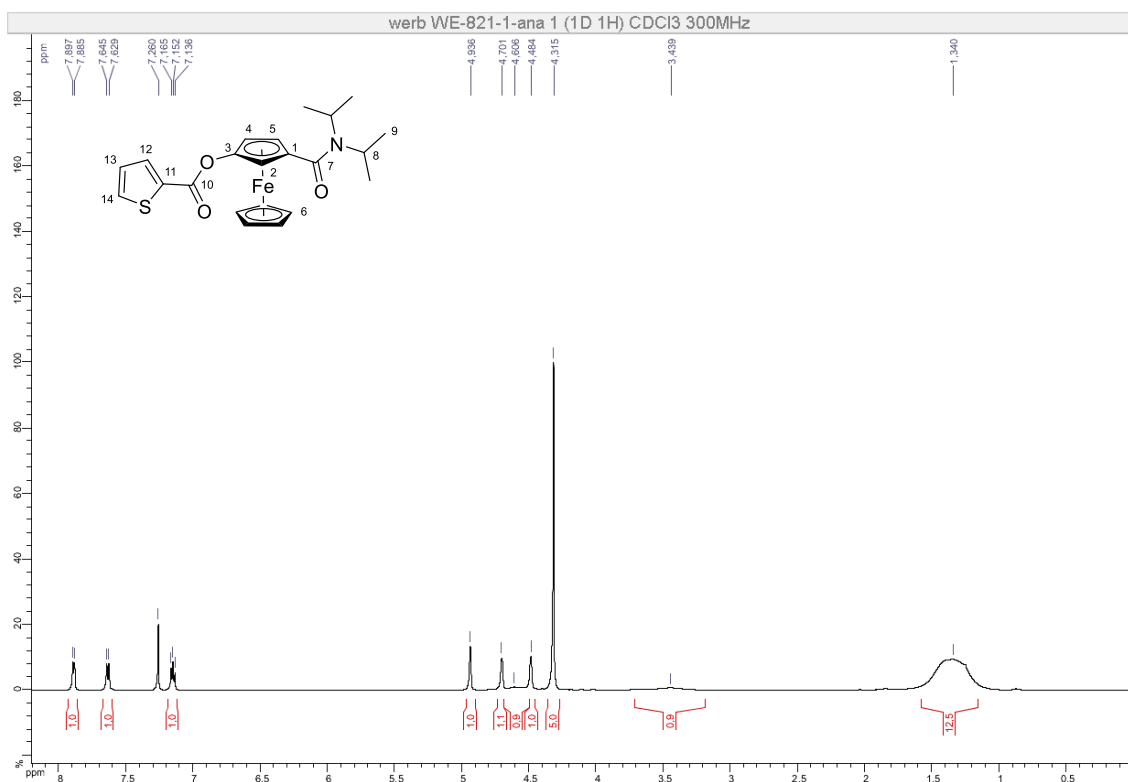
**3-(4-Formylbenzoyl)-N,N-diisopropylferrocenecarboxamide (6)**

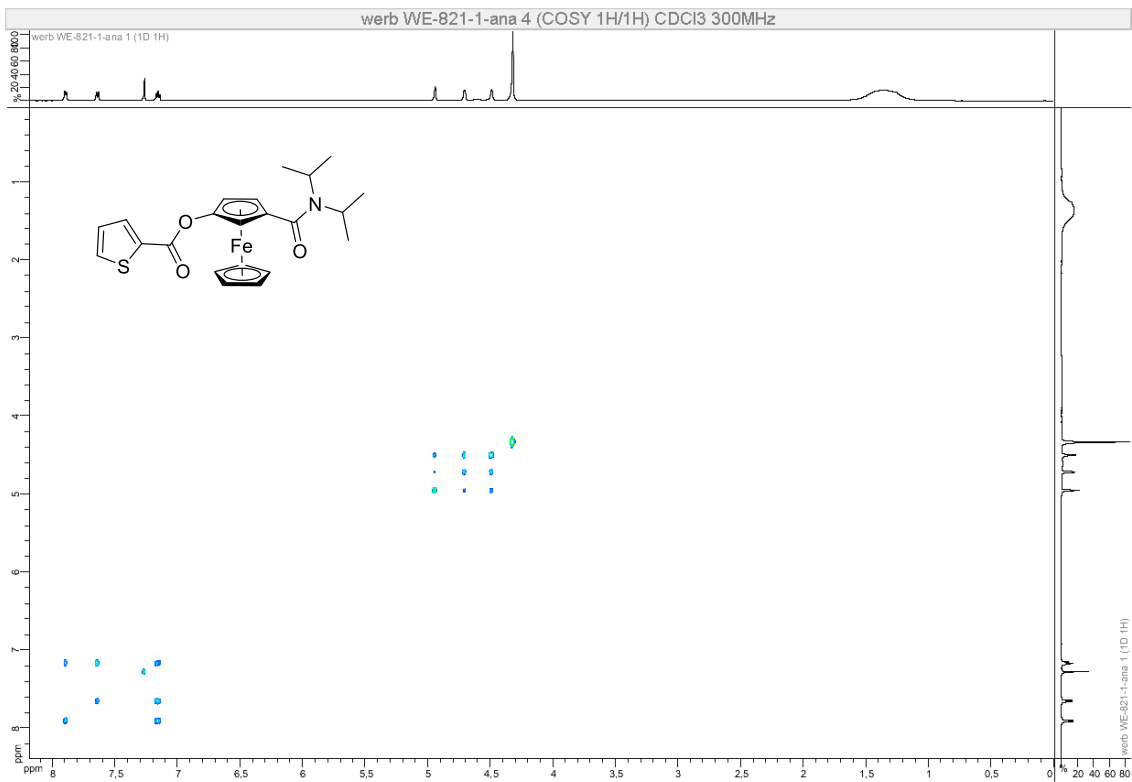
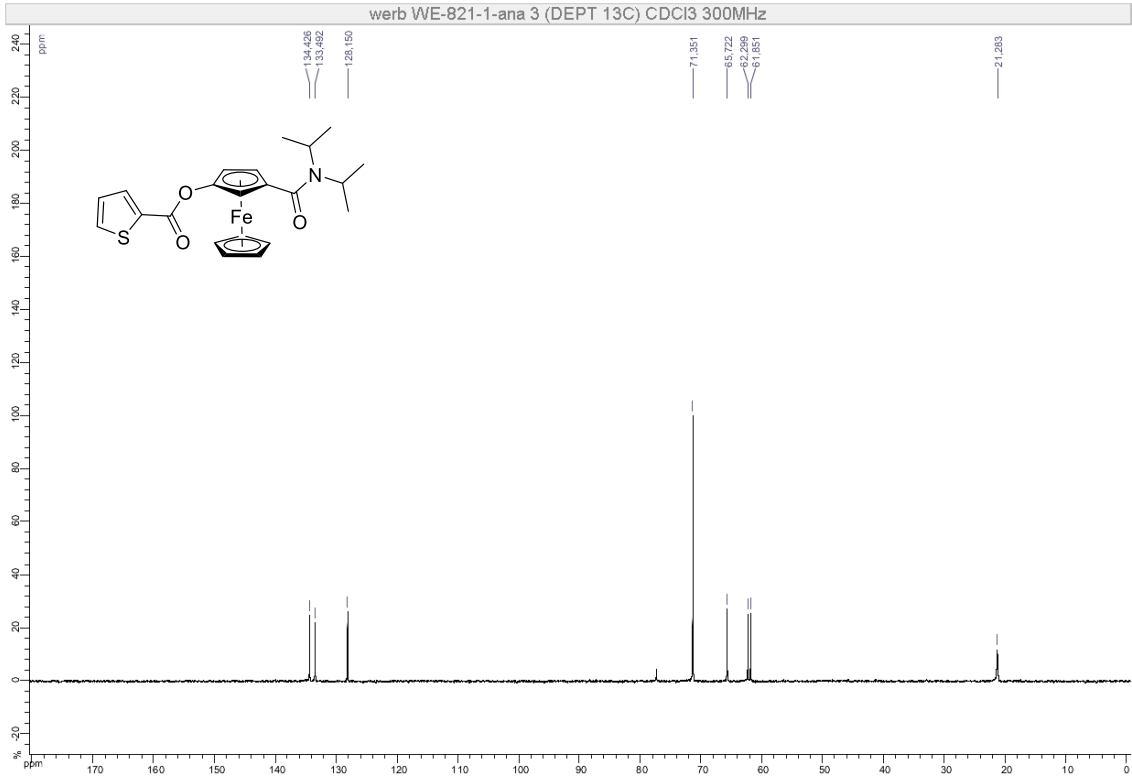


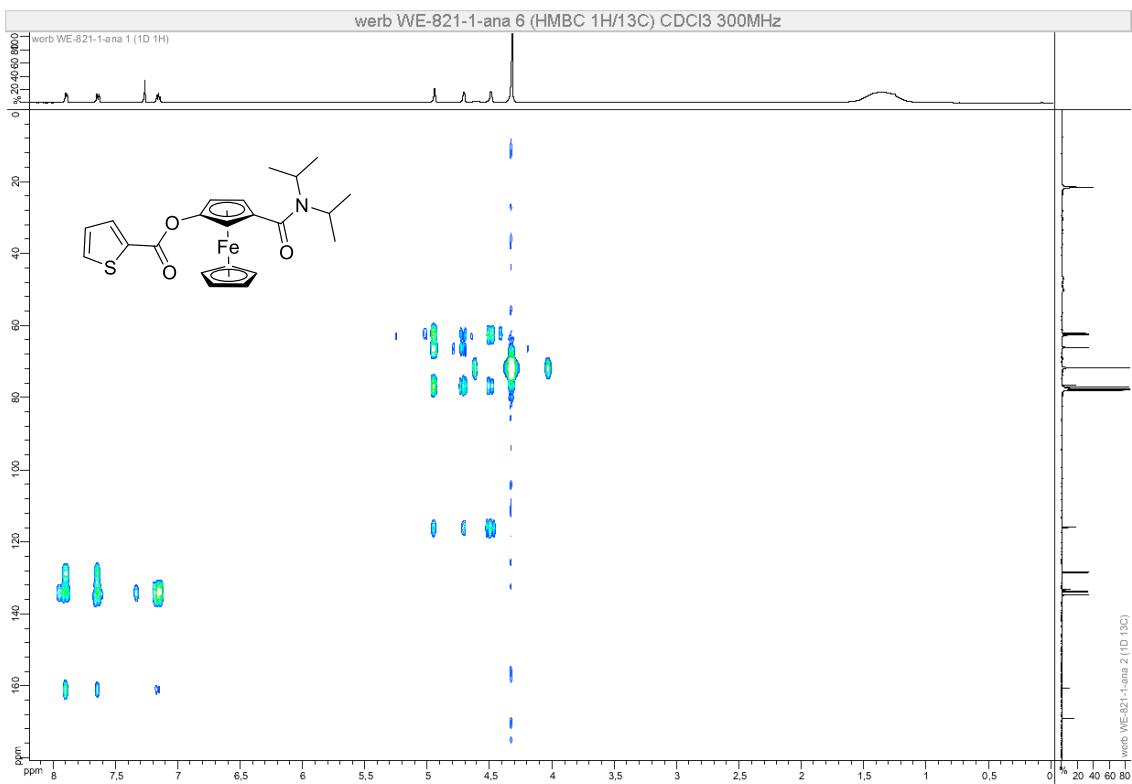
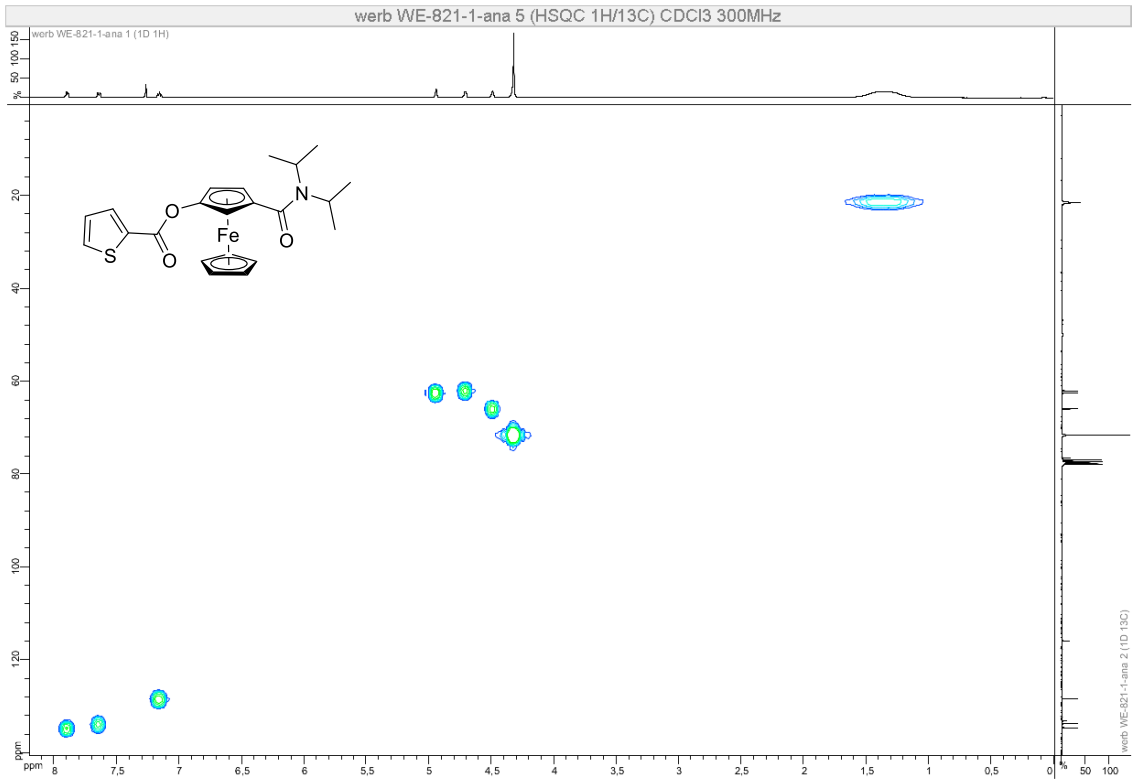




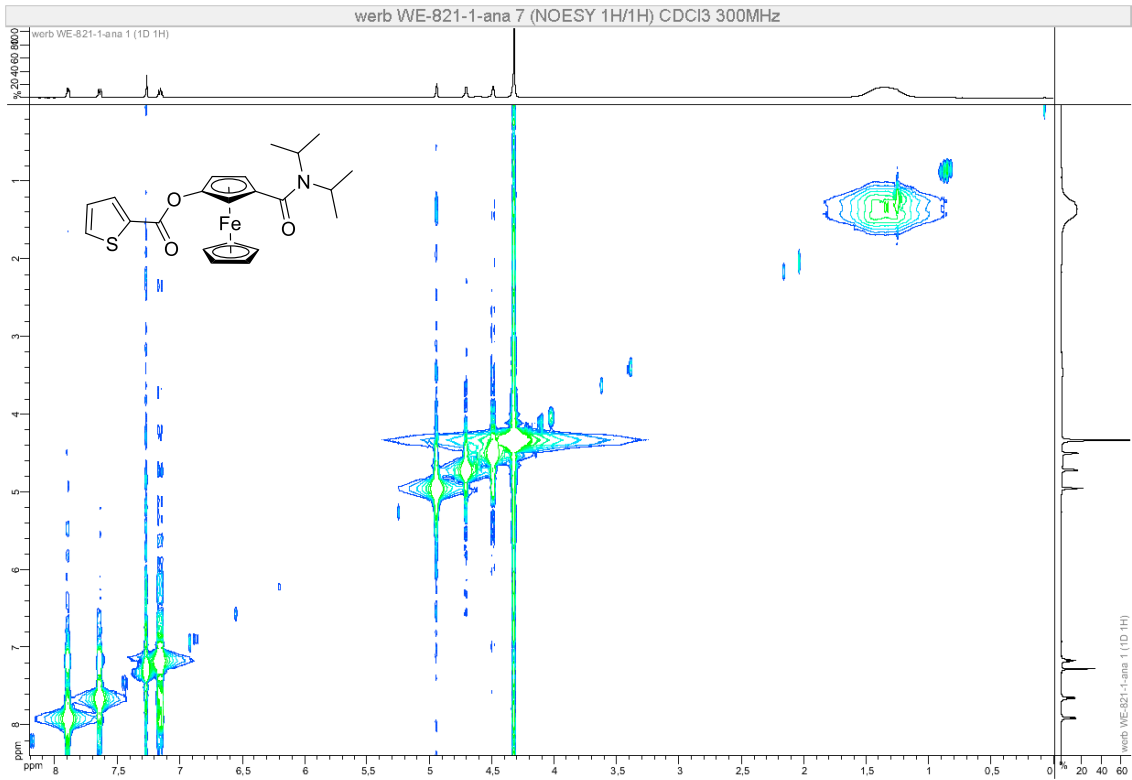
***N,N*-Diisopropyl-3-(2-thiophenyl)ferrocenecarboxamide (7)**



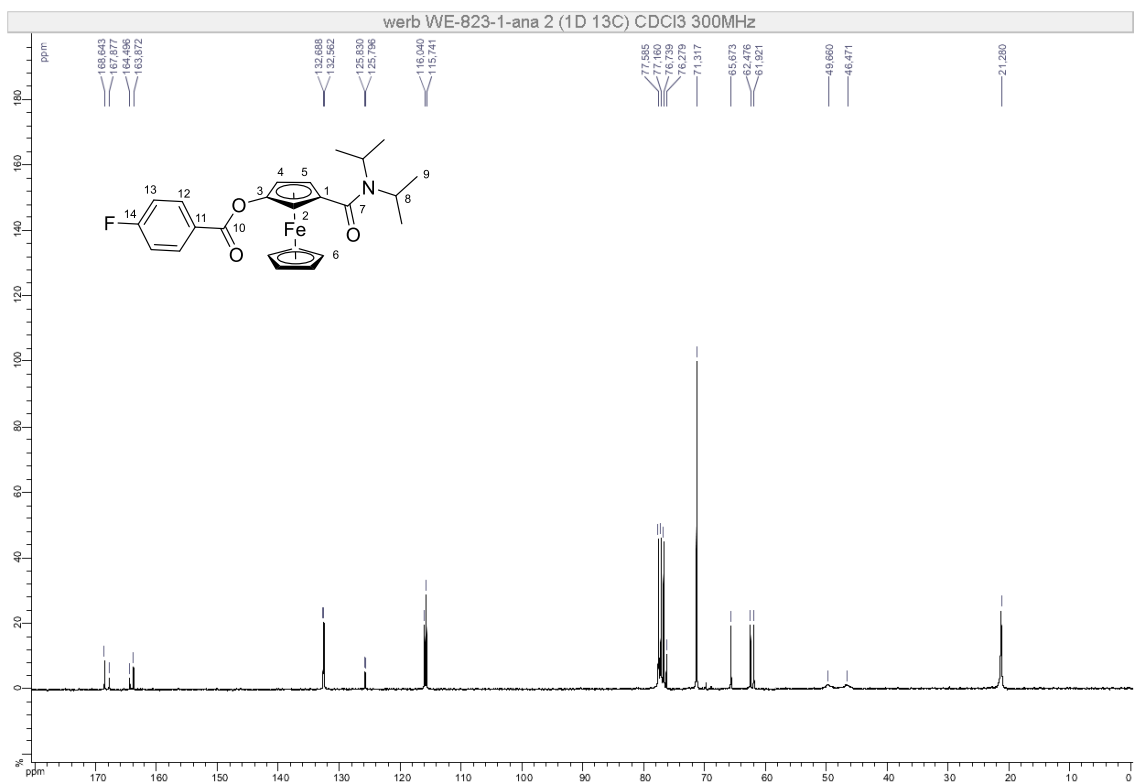
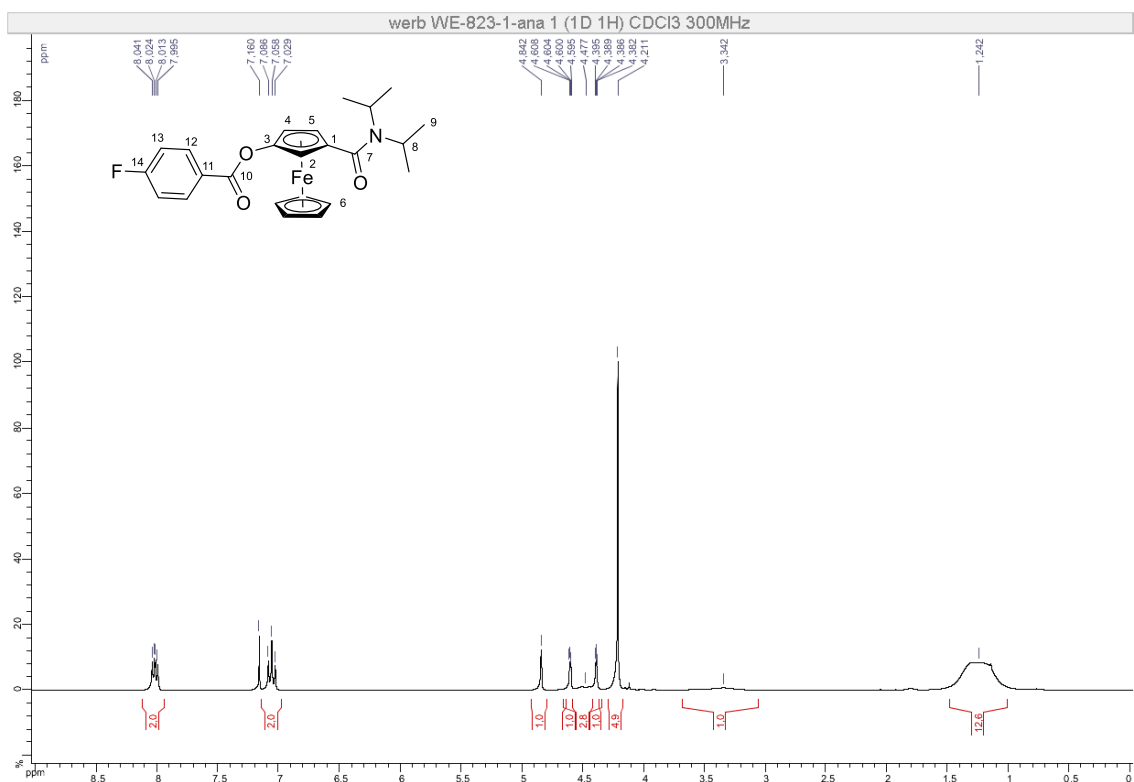


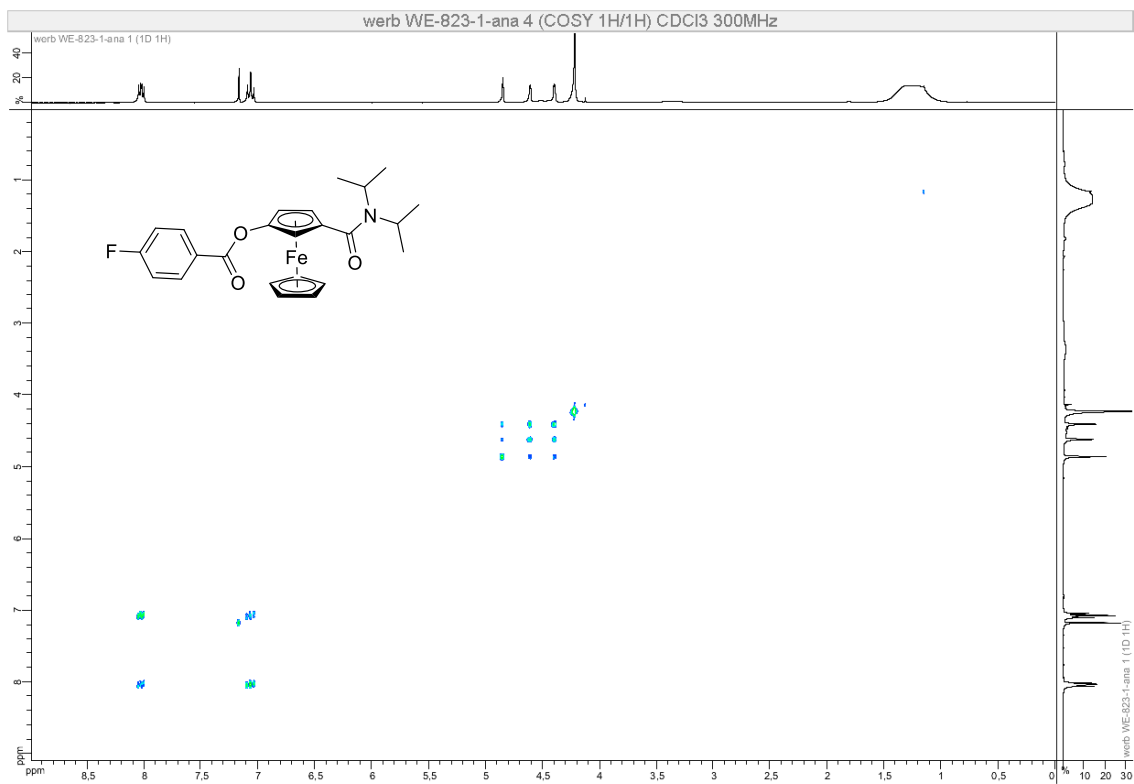
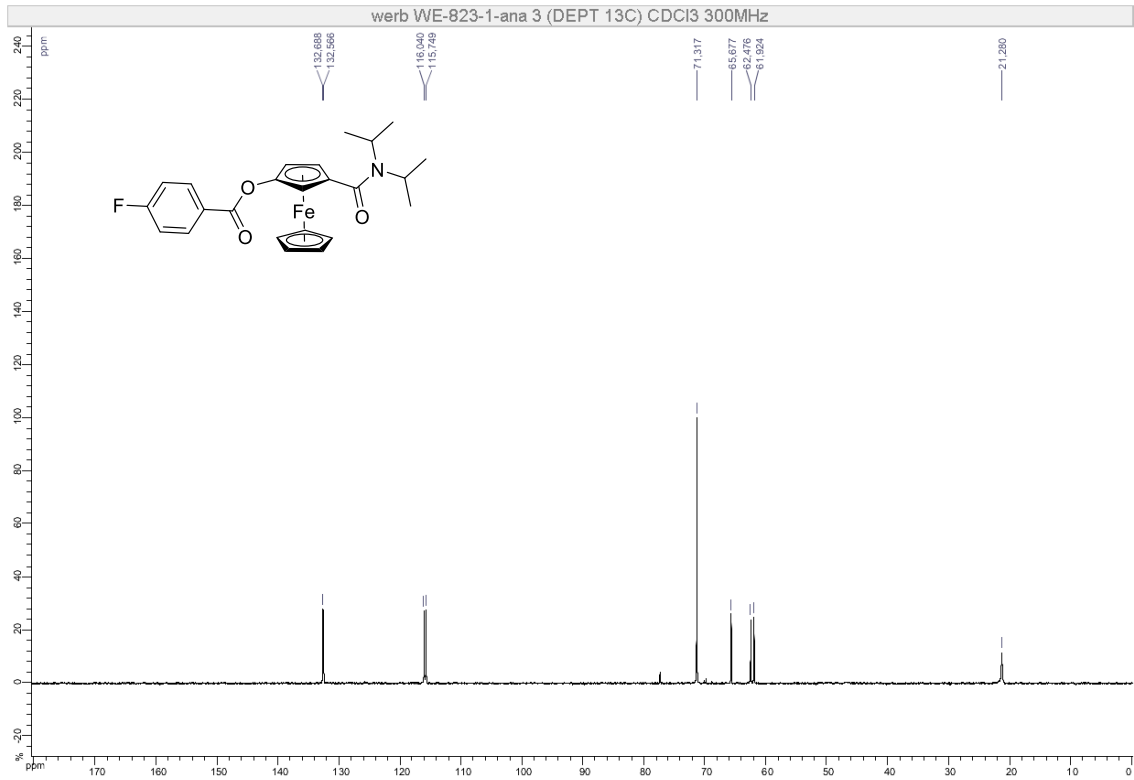


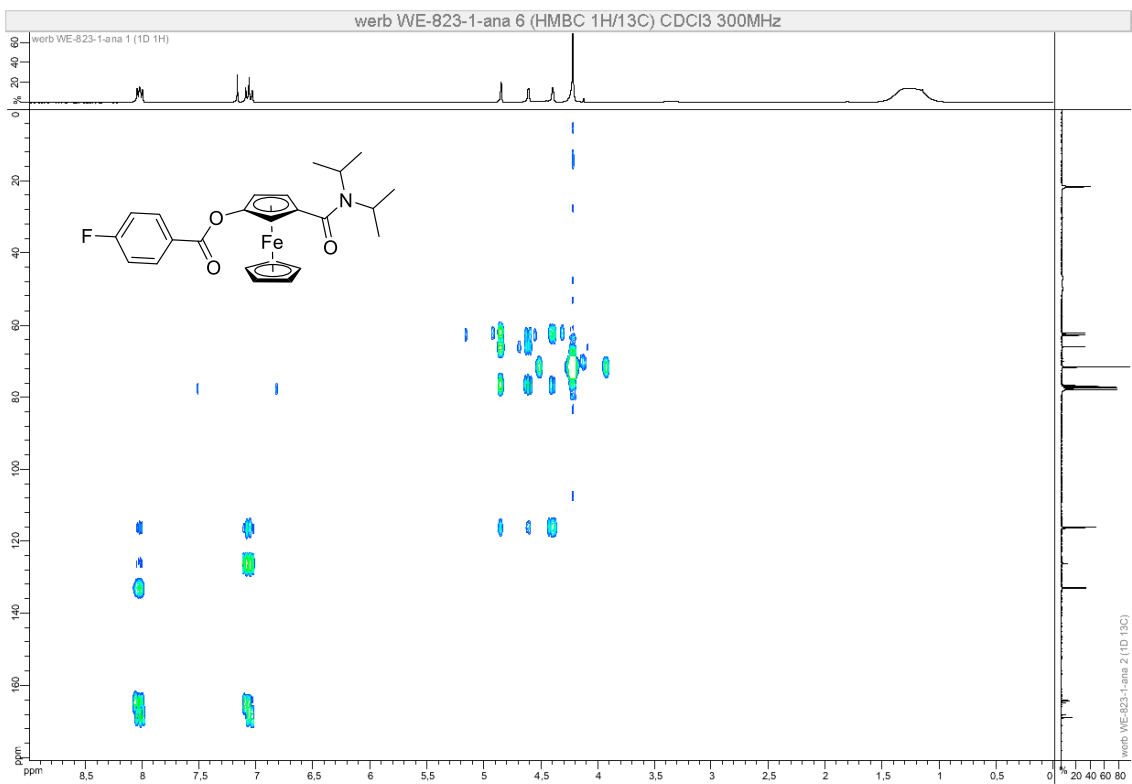
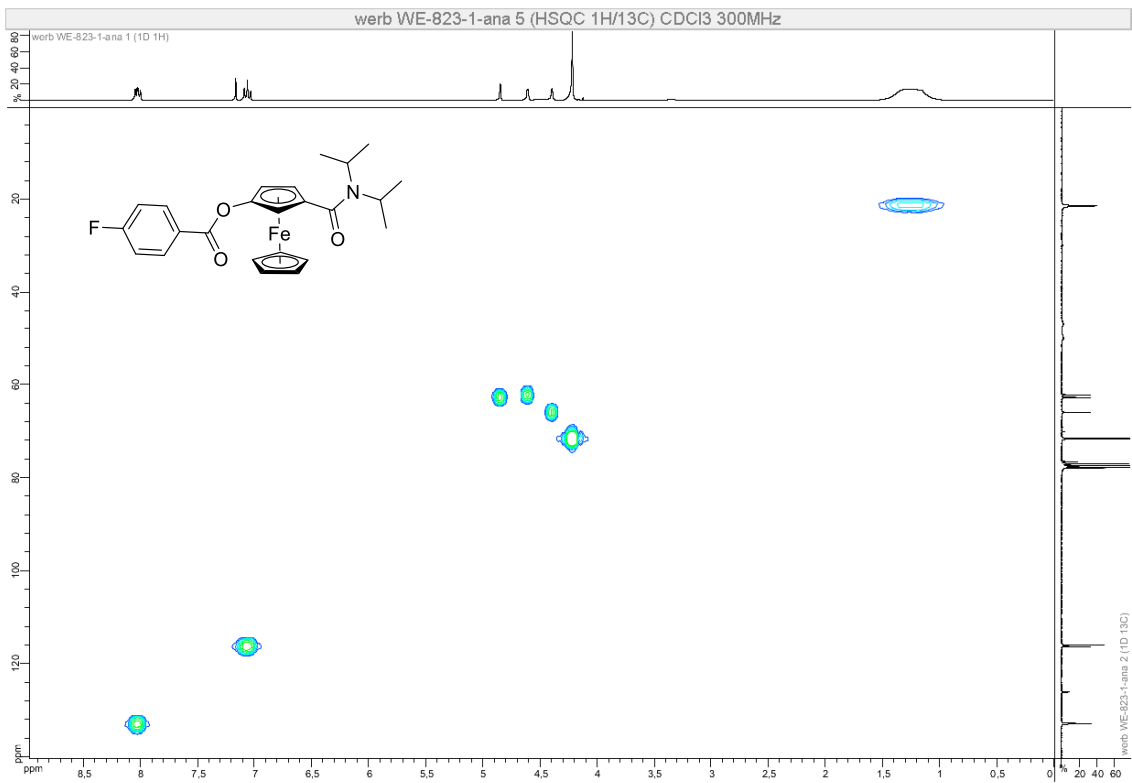


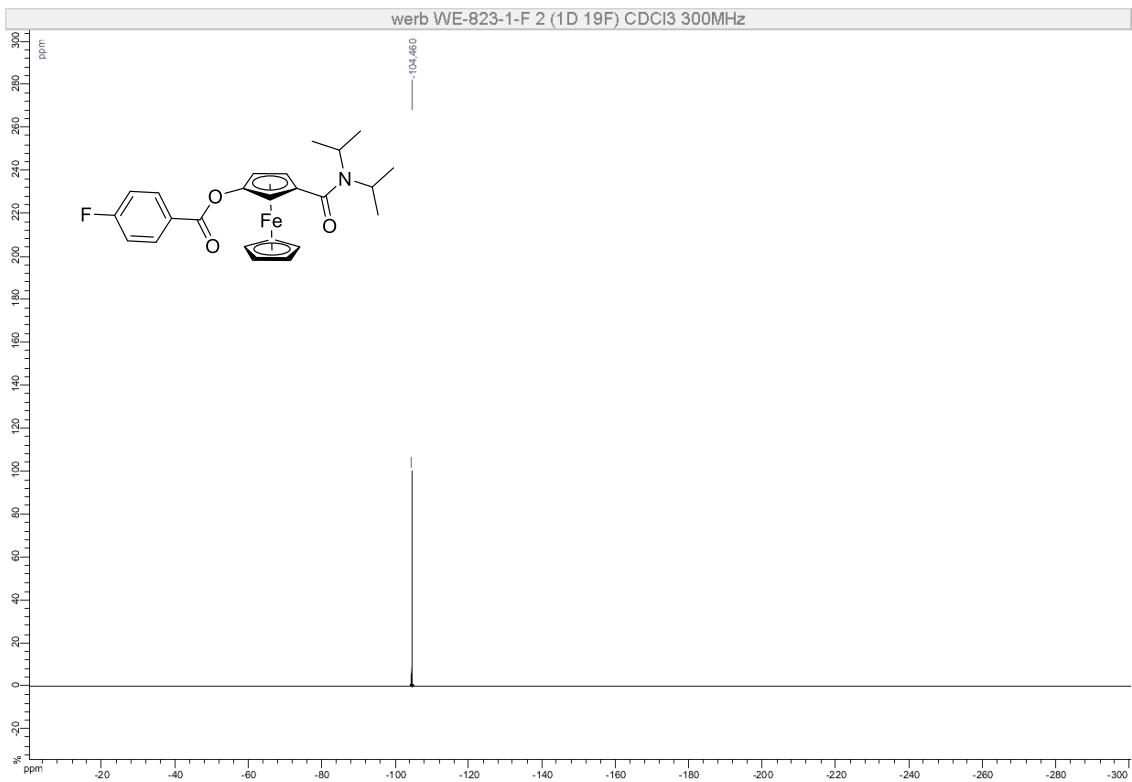
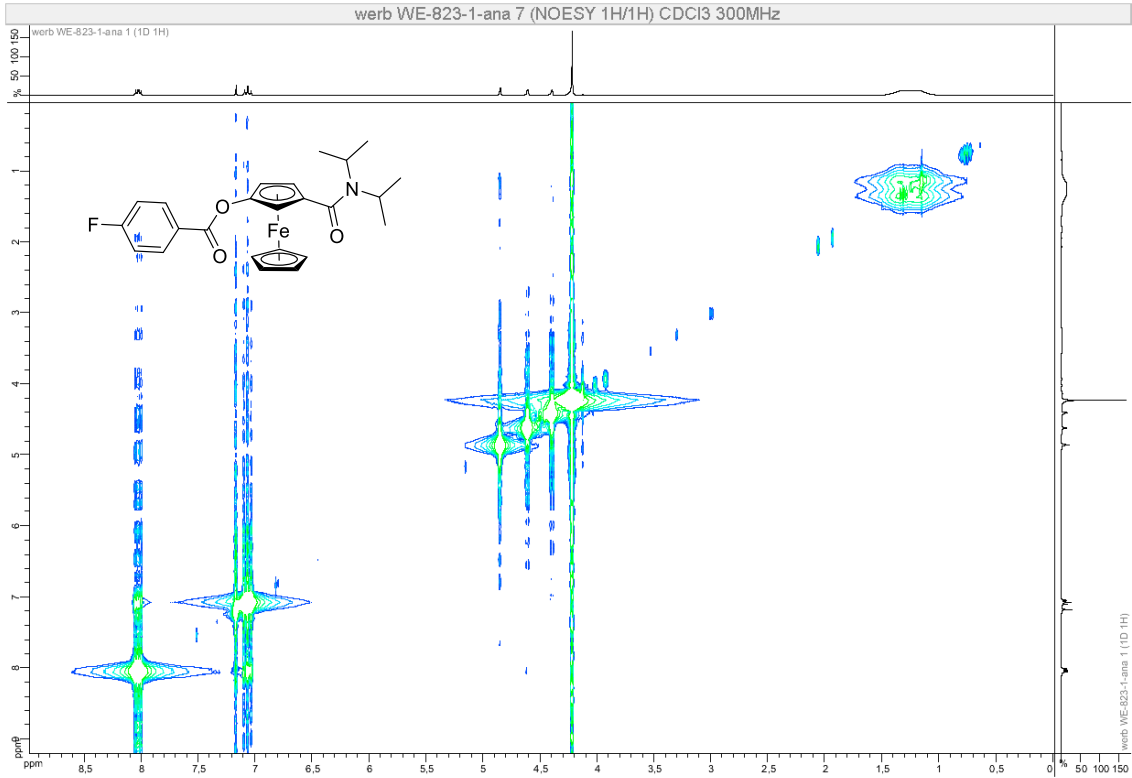


**3-(4-Fluorobenzoyl)-N,N-diisopropylferrocenecarboxamide (8)**

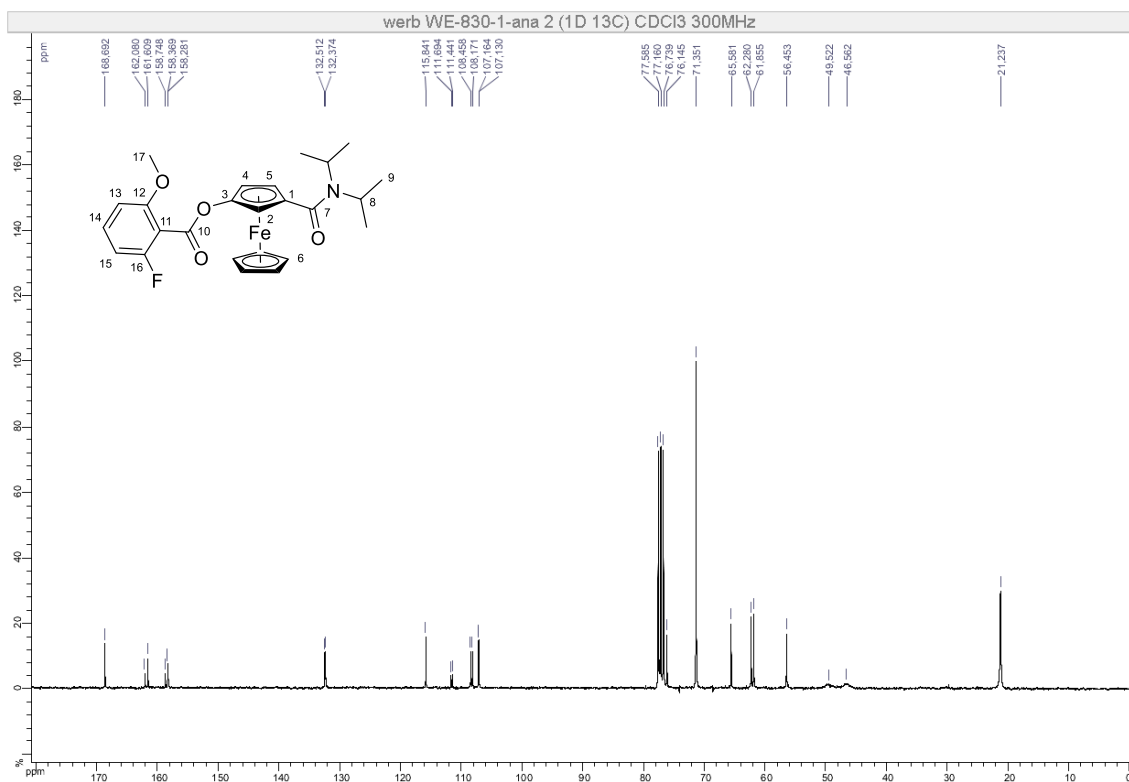
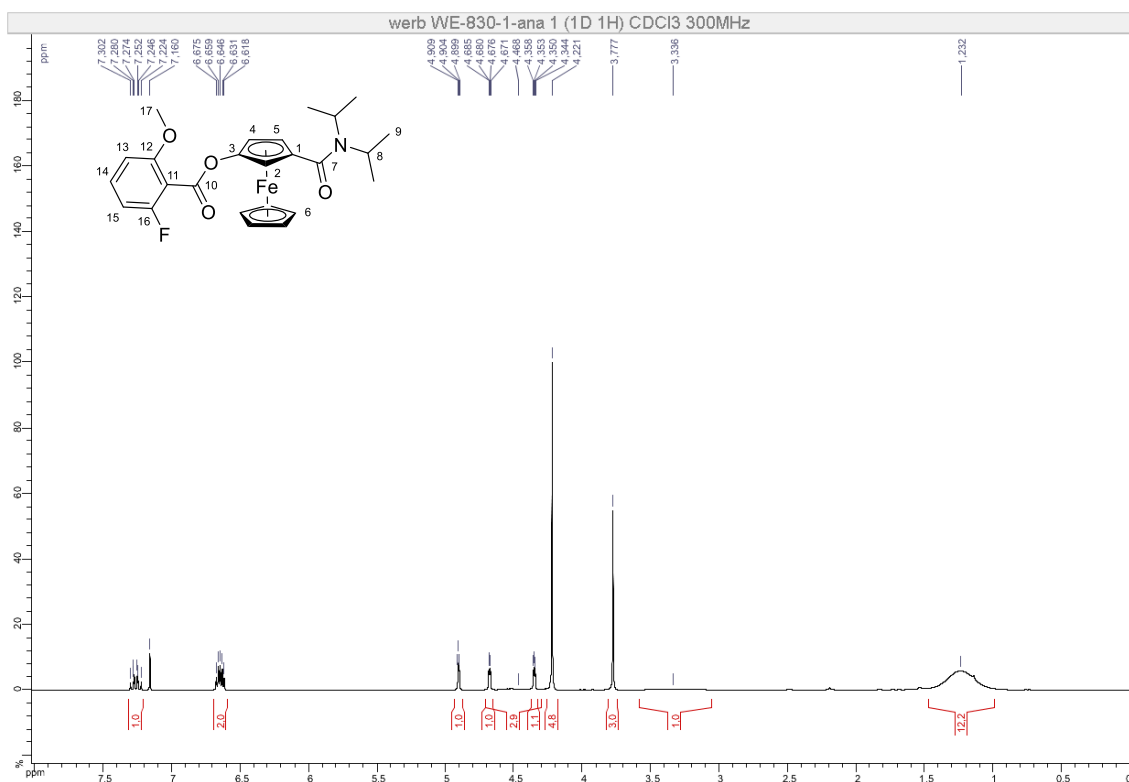


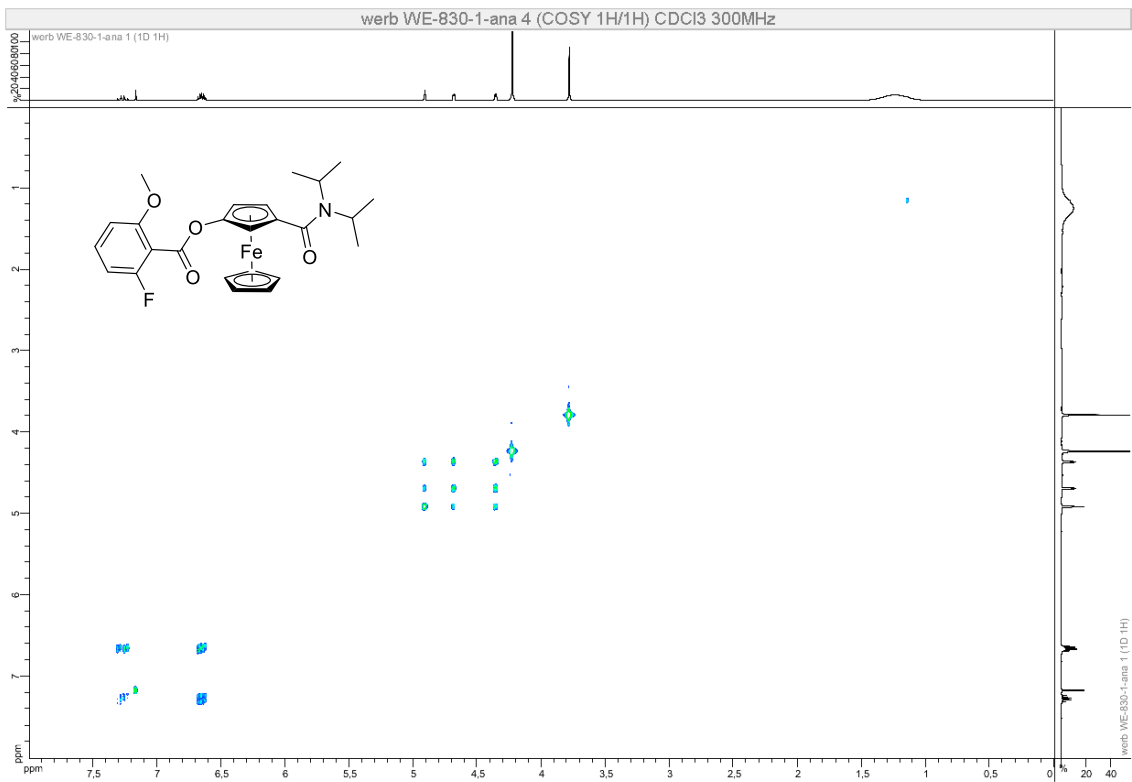
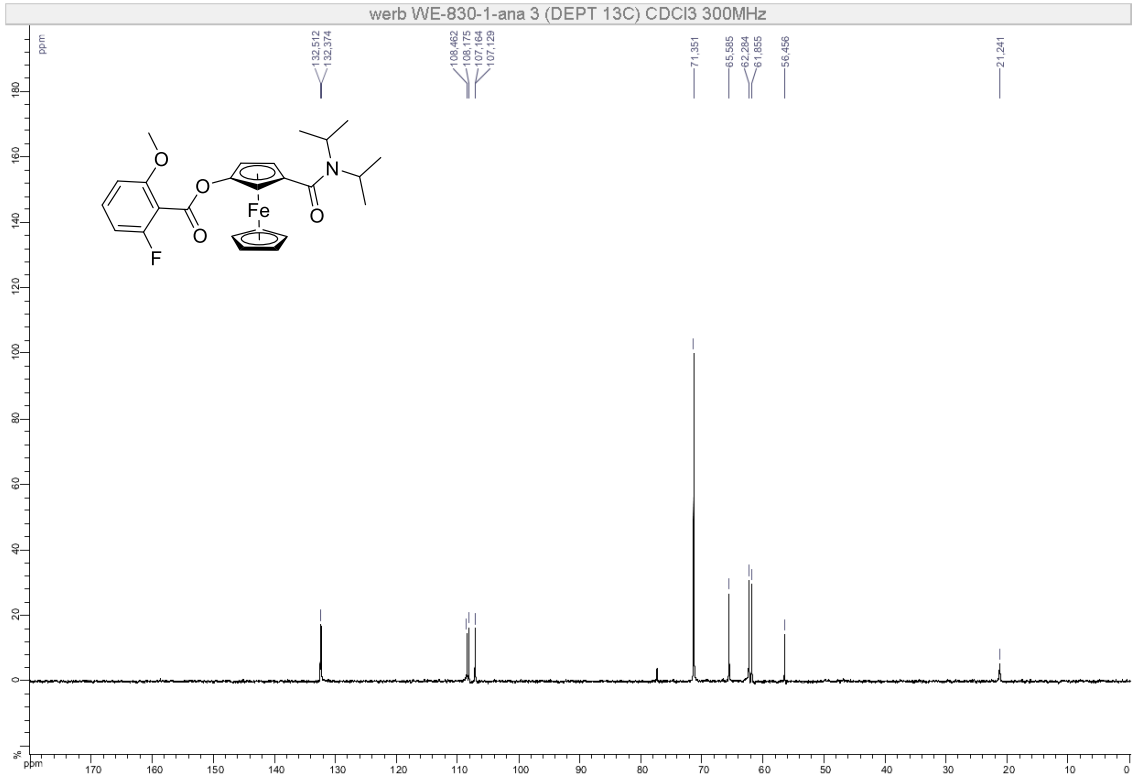


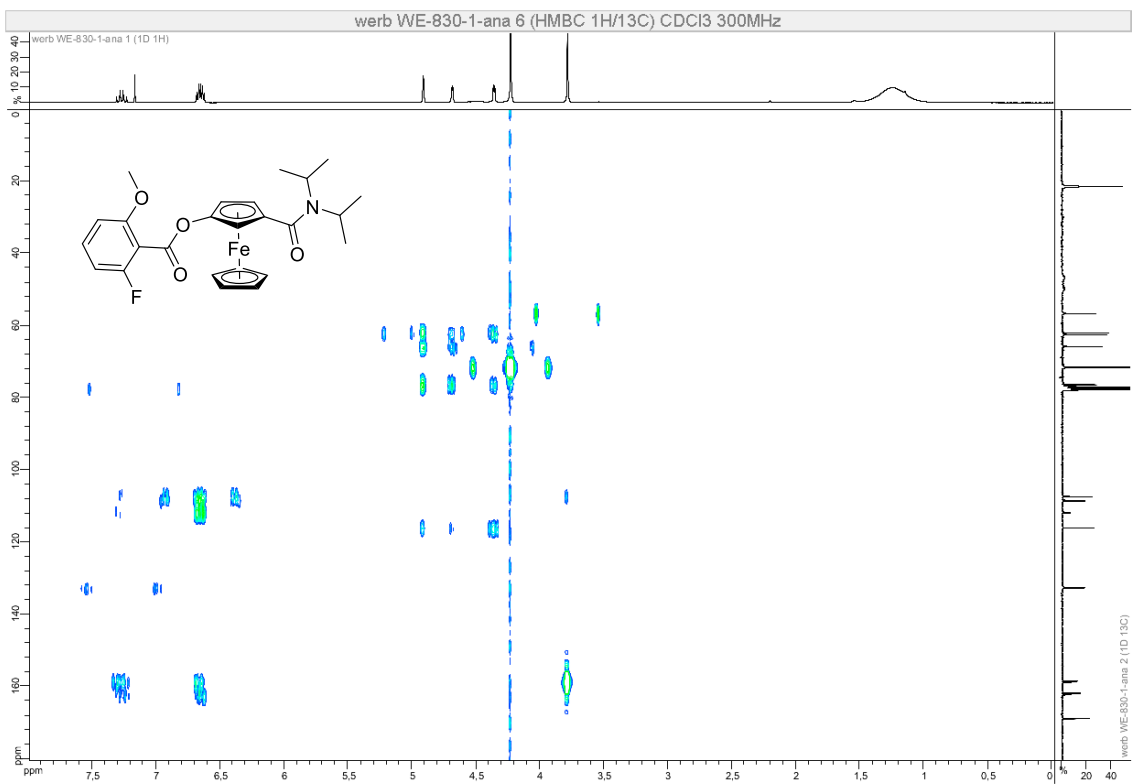
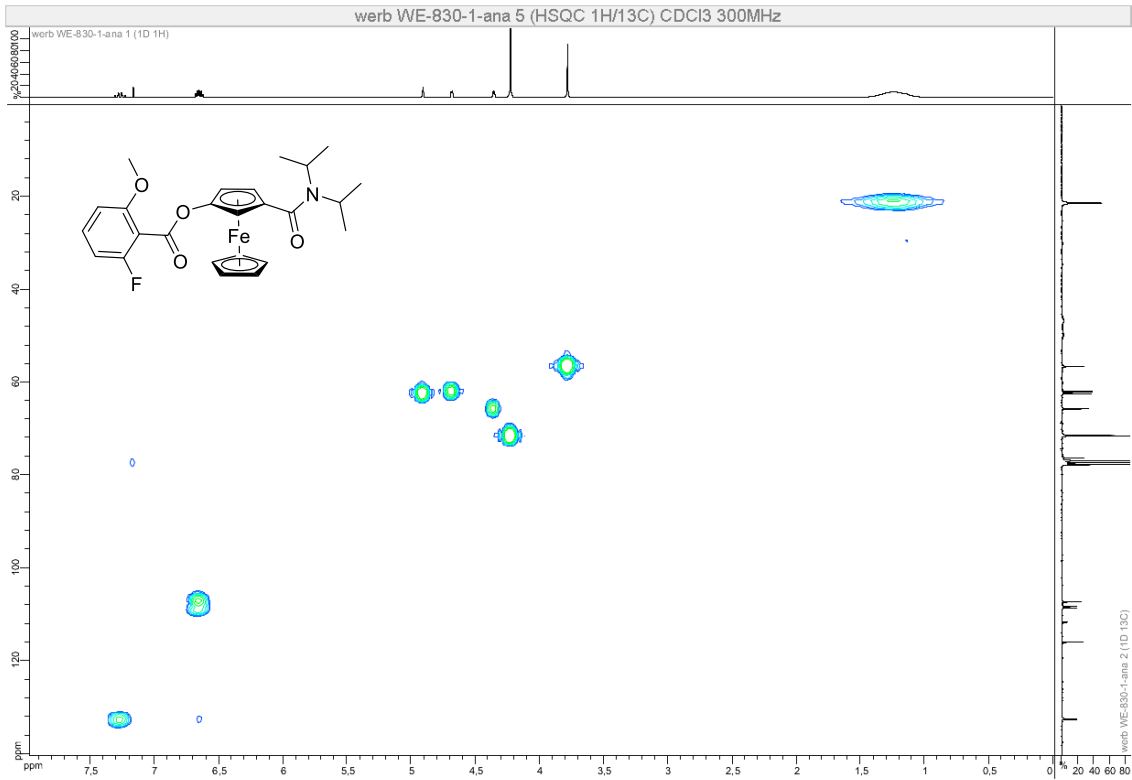




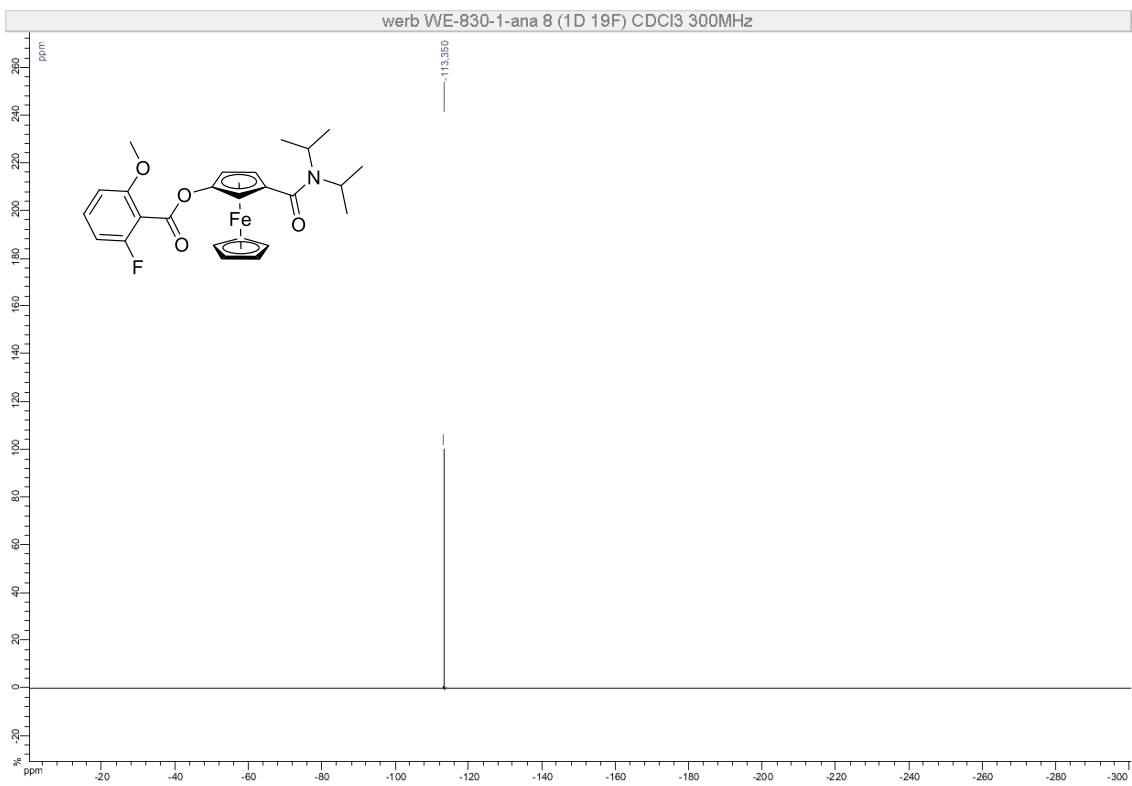
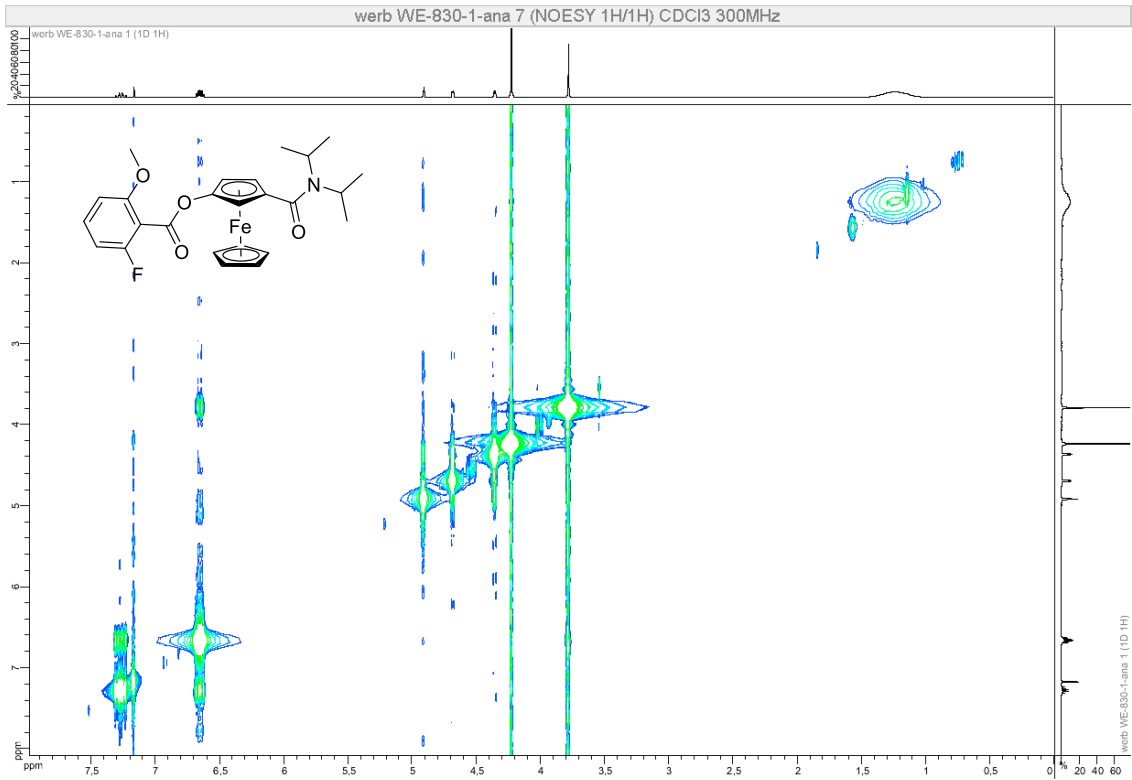
**3-(2-Fluoro-6-methoxybenzoyl)-N,N-diisopropylferrocene-carboxamide (9)**



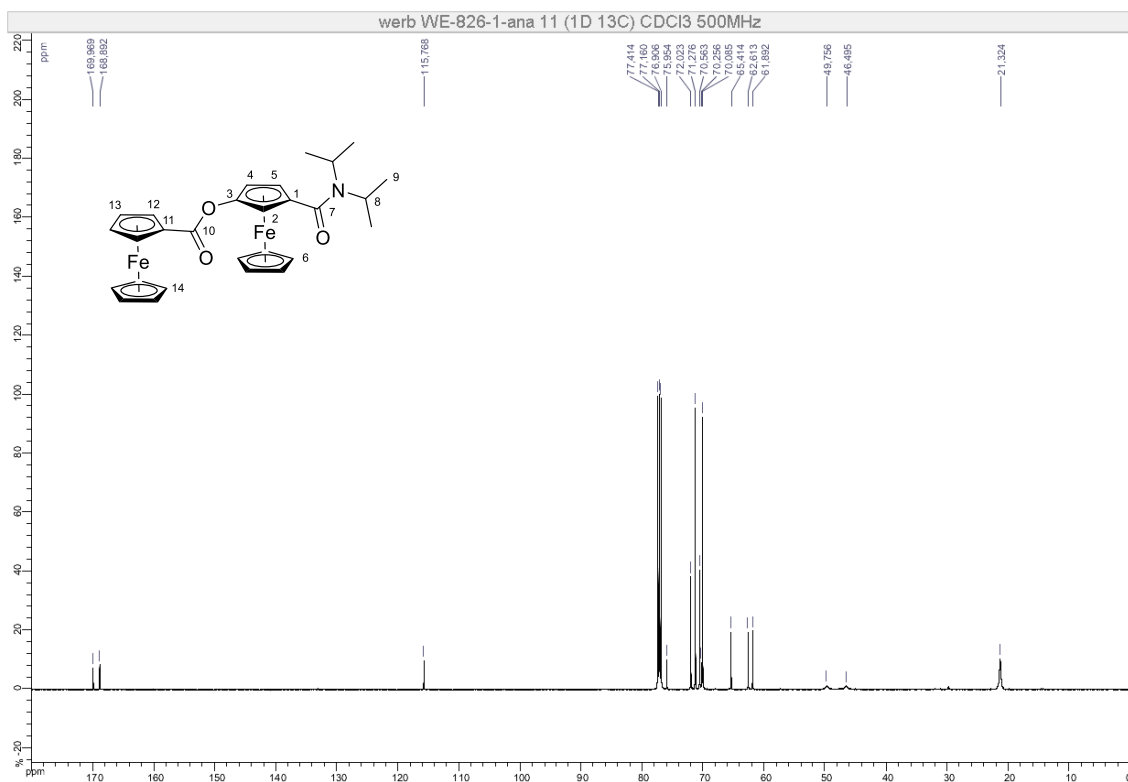
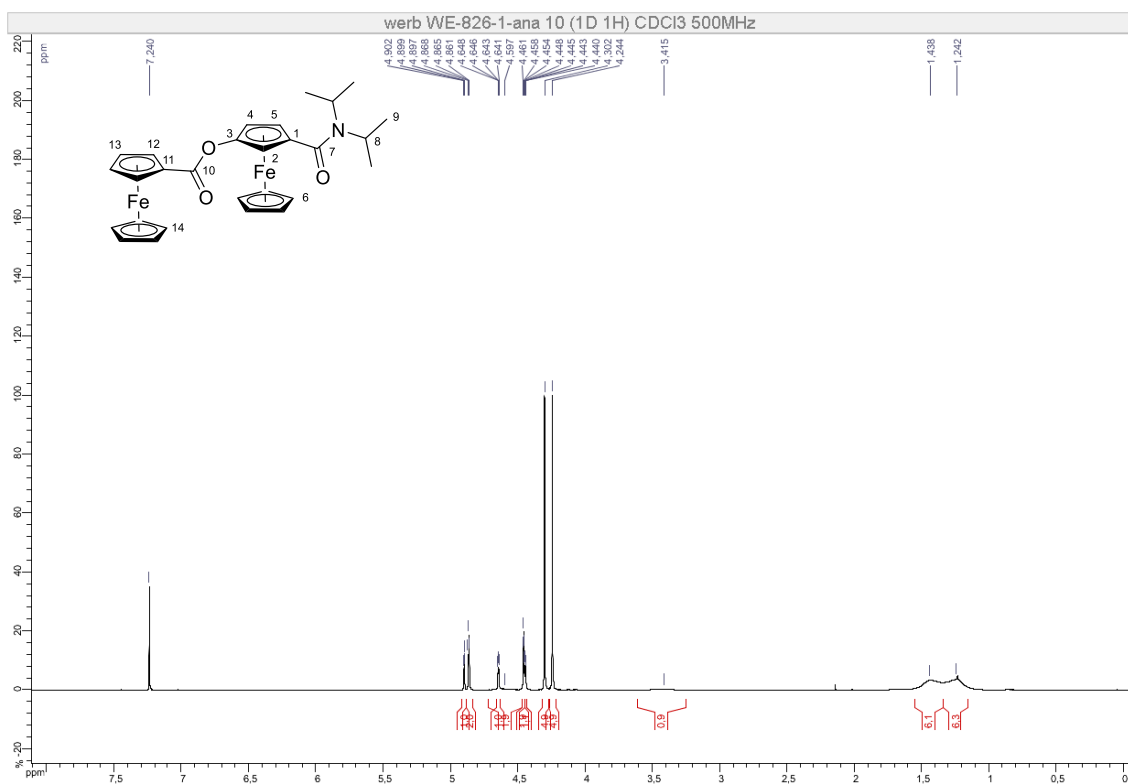


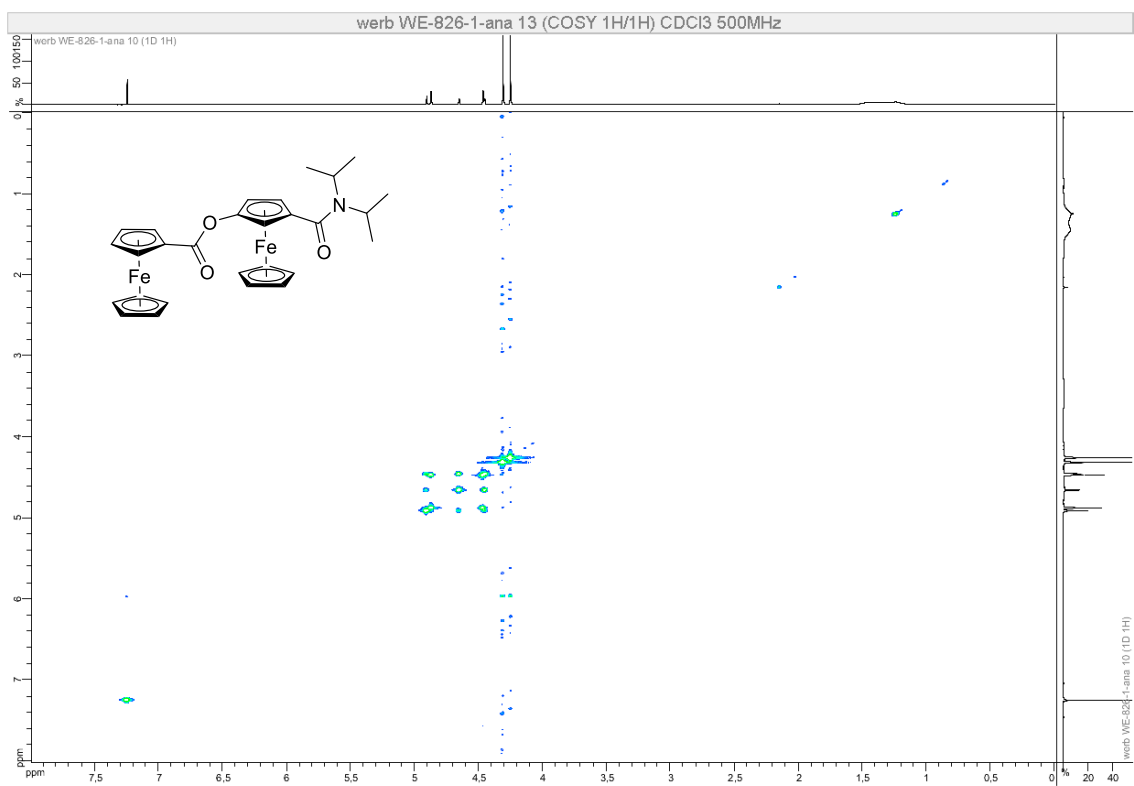
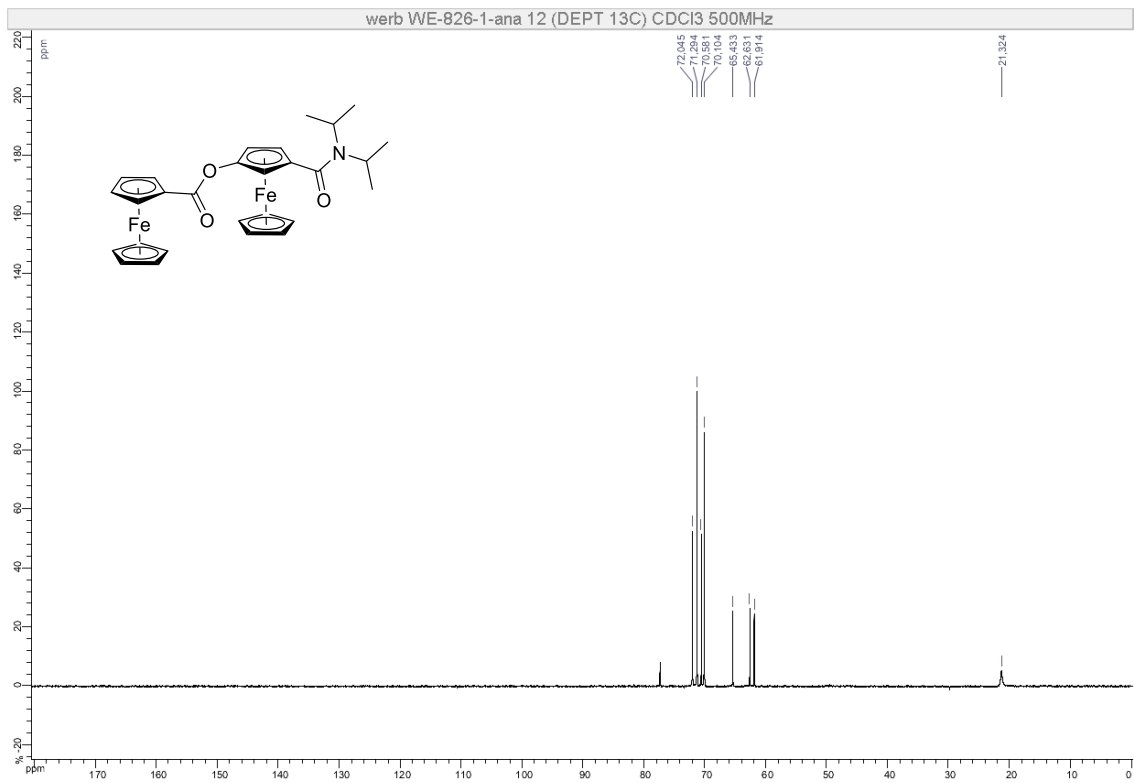


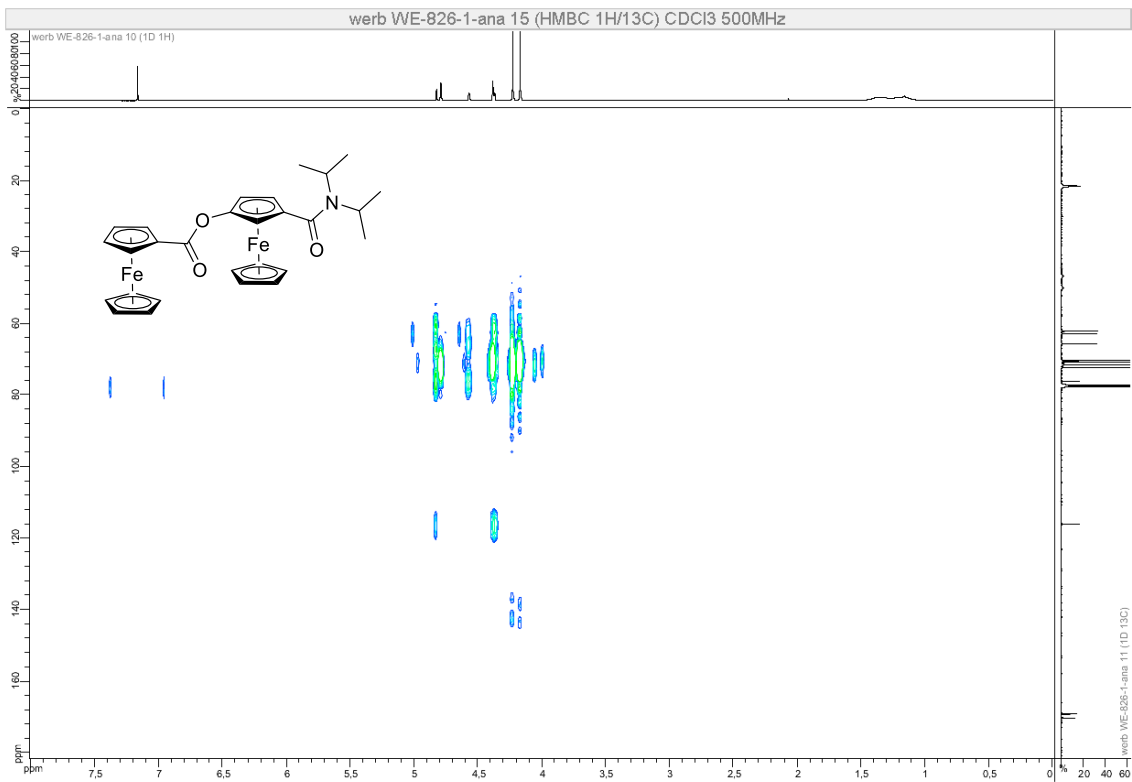
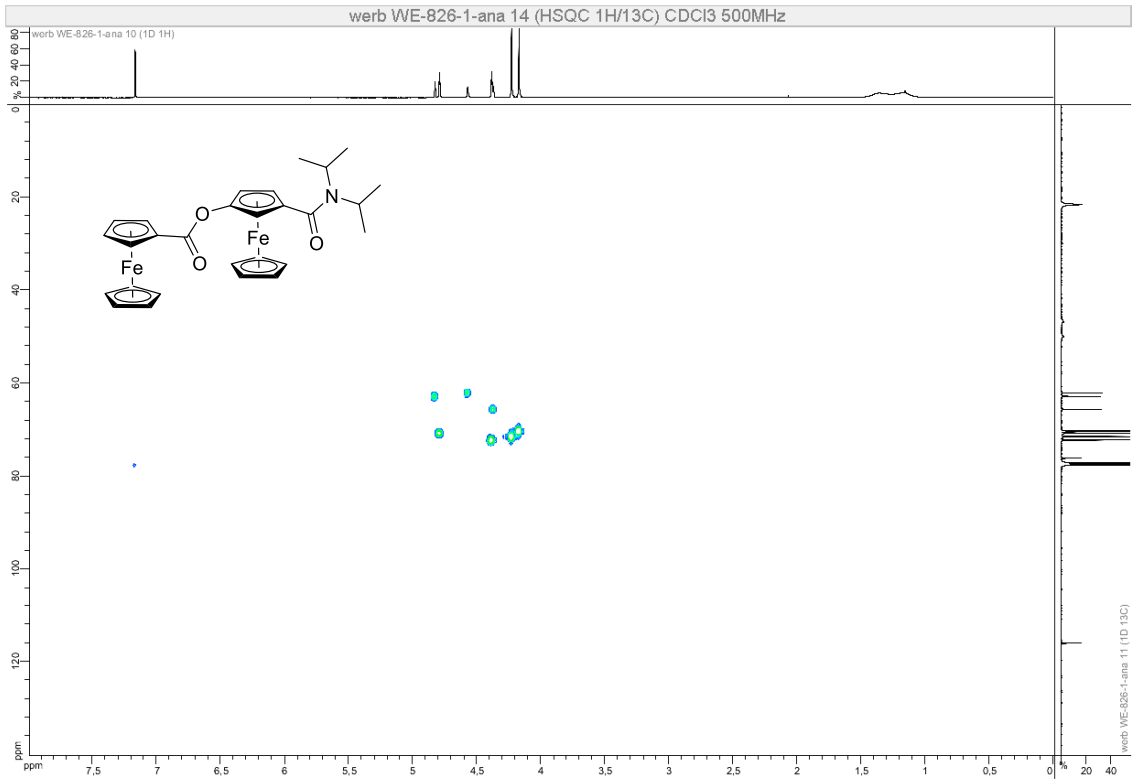


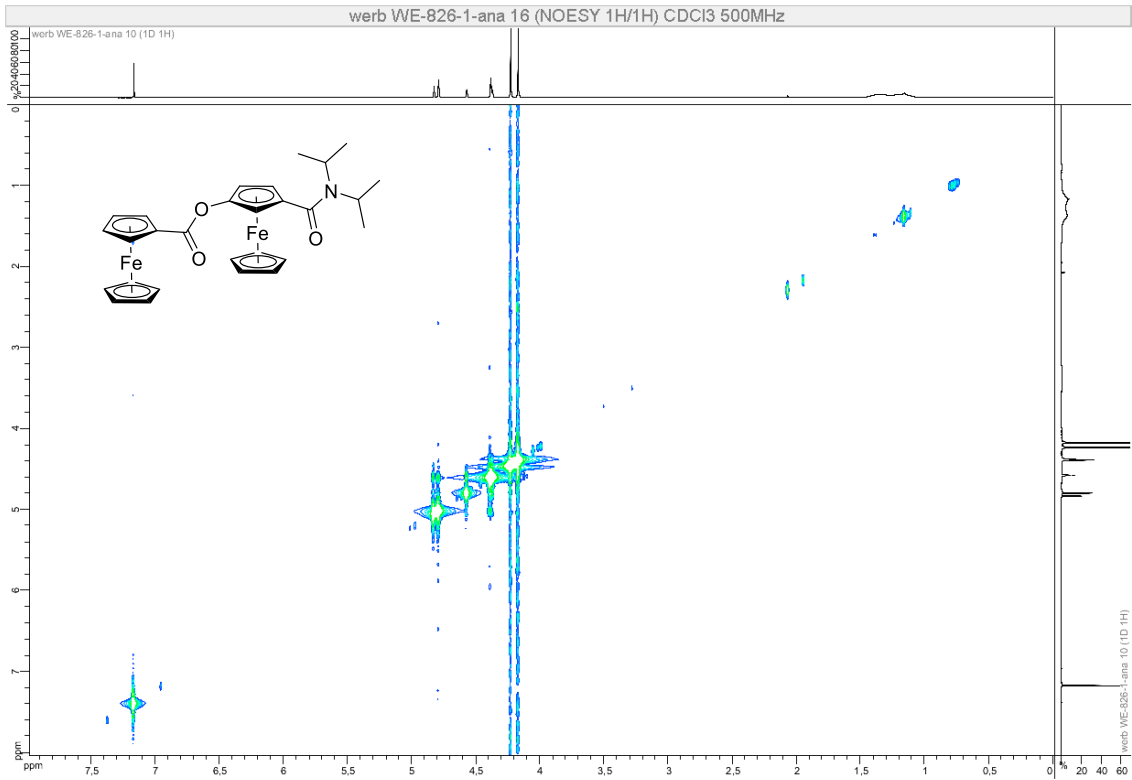


**3-(Ferrocenoyl)-N,N-diisopropylferrocenecarboxamide (10)**

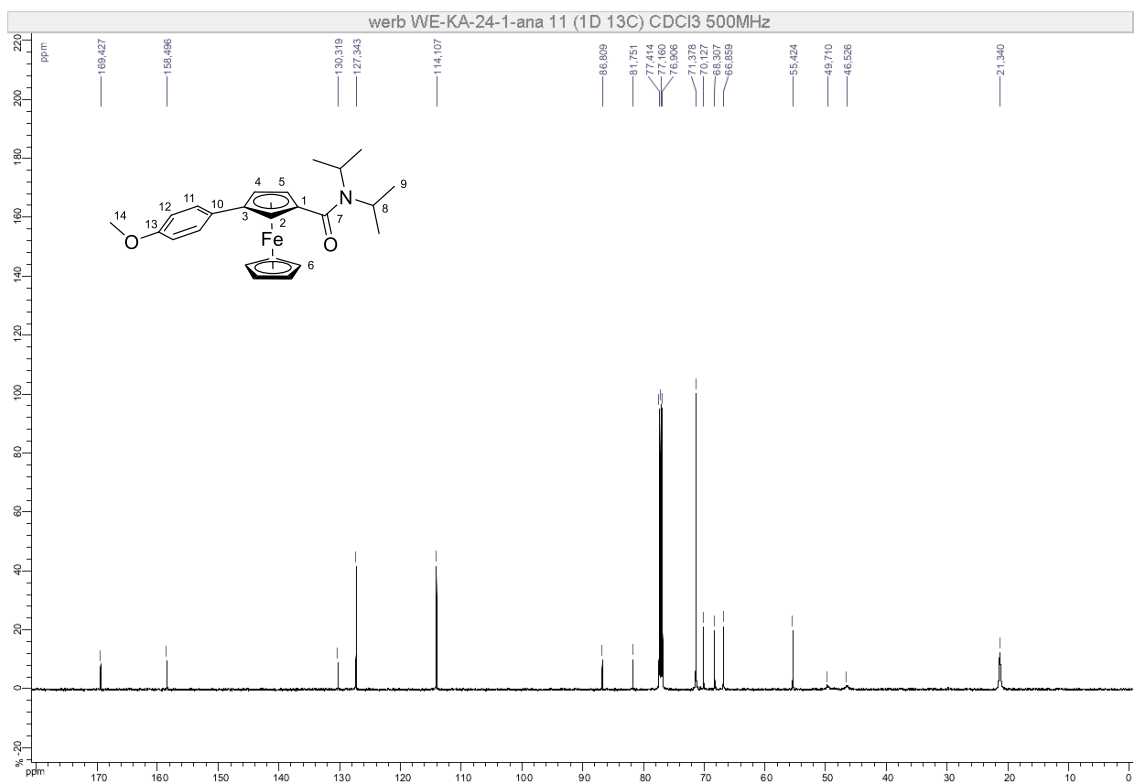
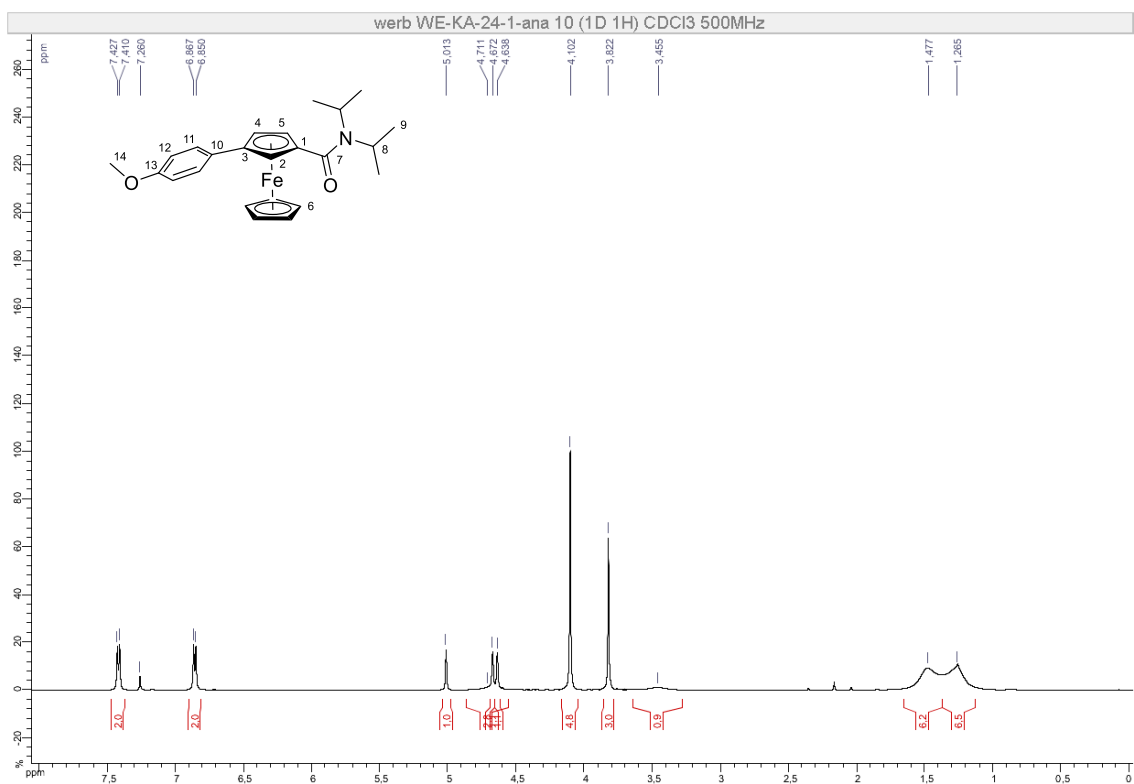


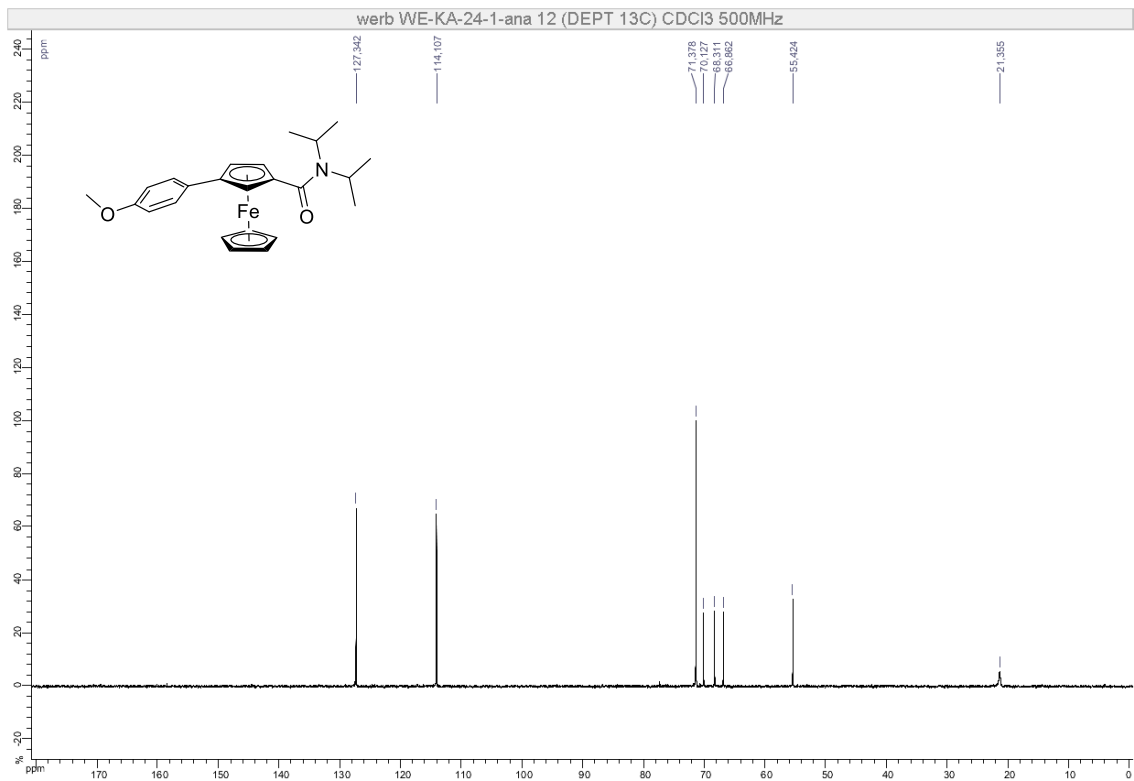




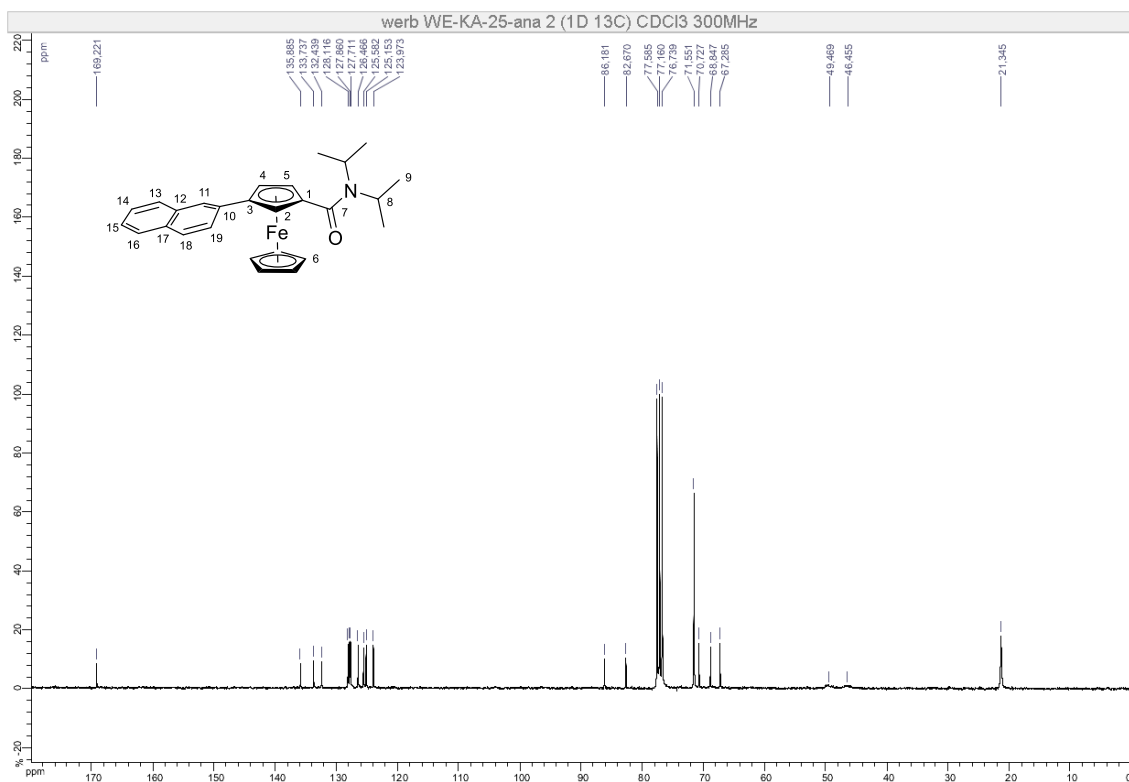
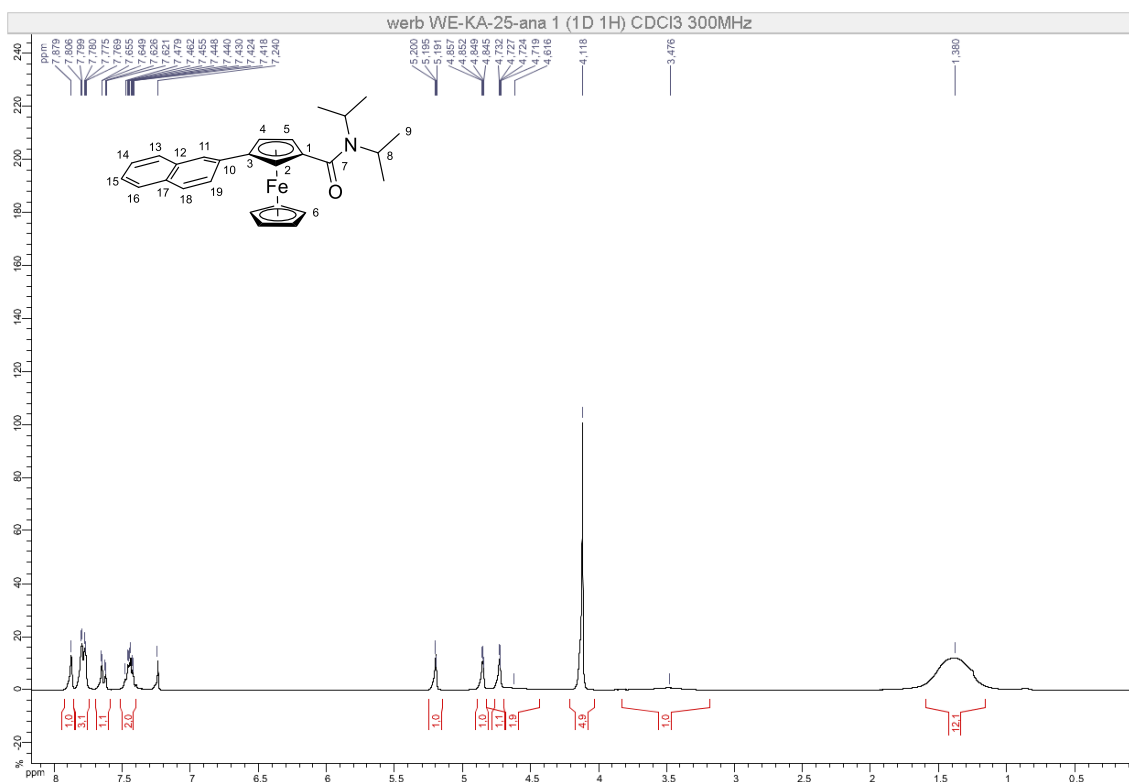


***N,N*-Diisopropyl-3-(4-methoxyphenyl)ferrocenecarboxamide (11)**

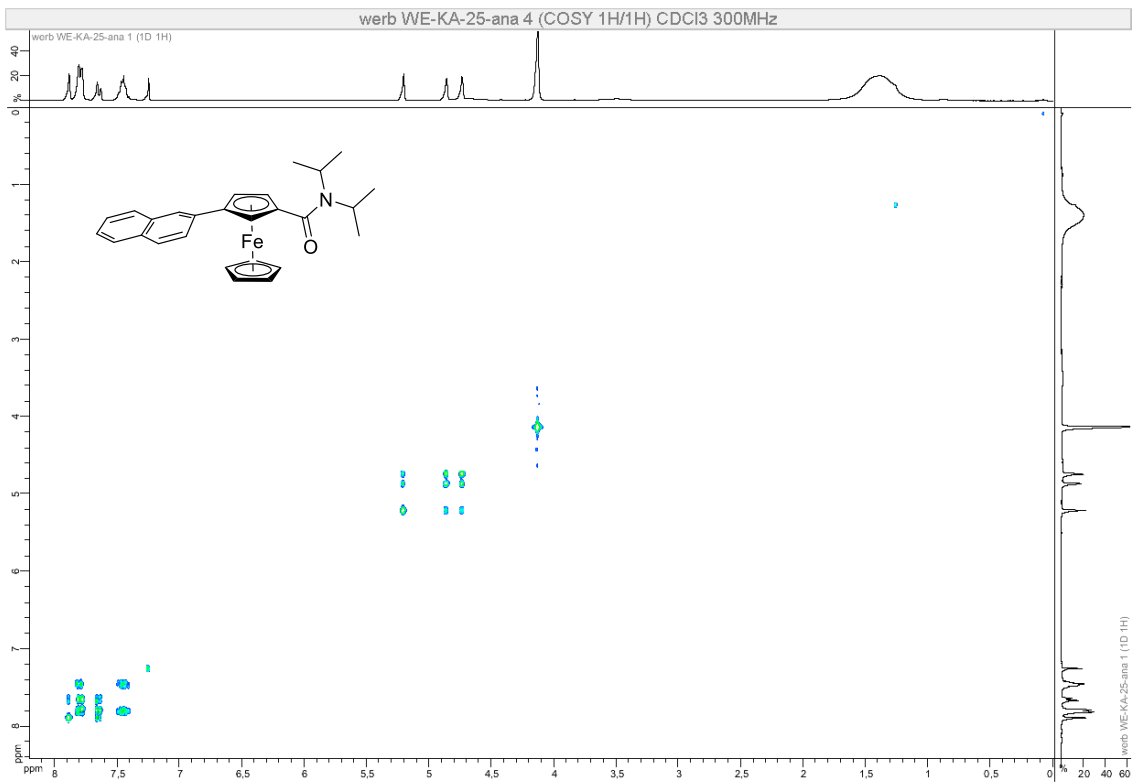
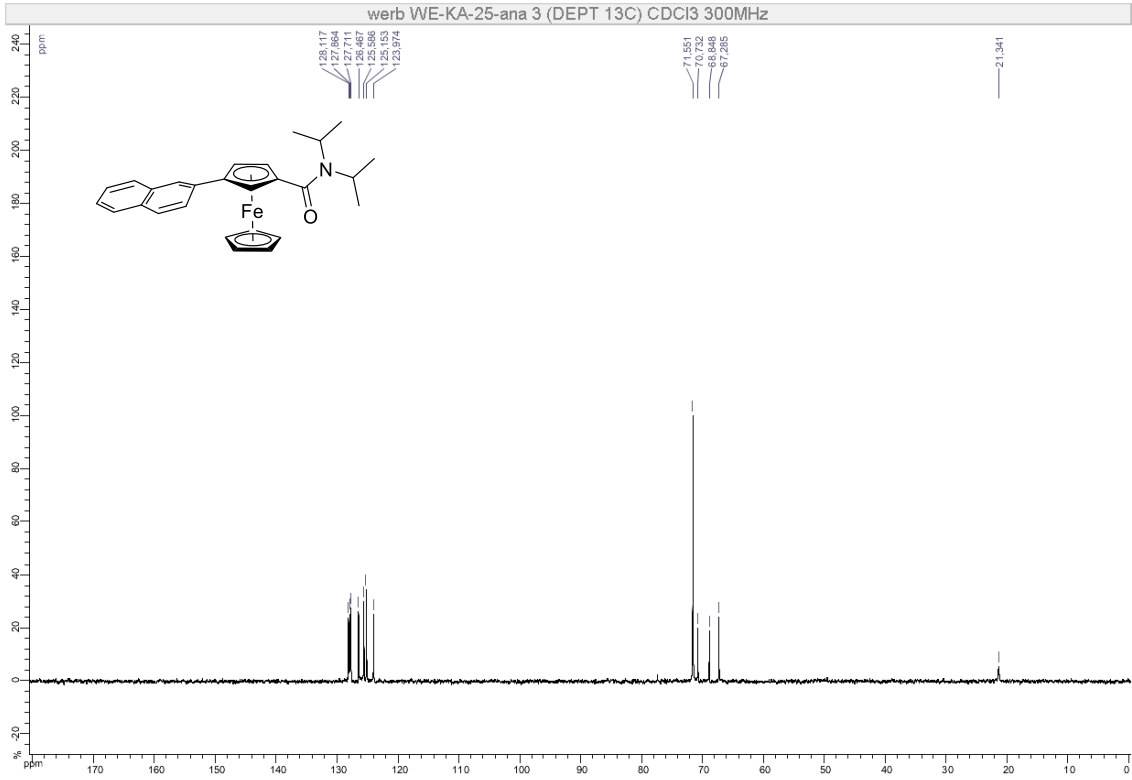


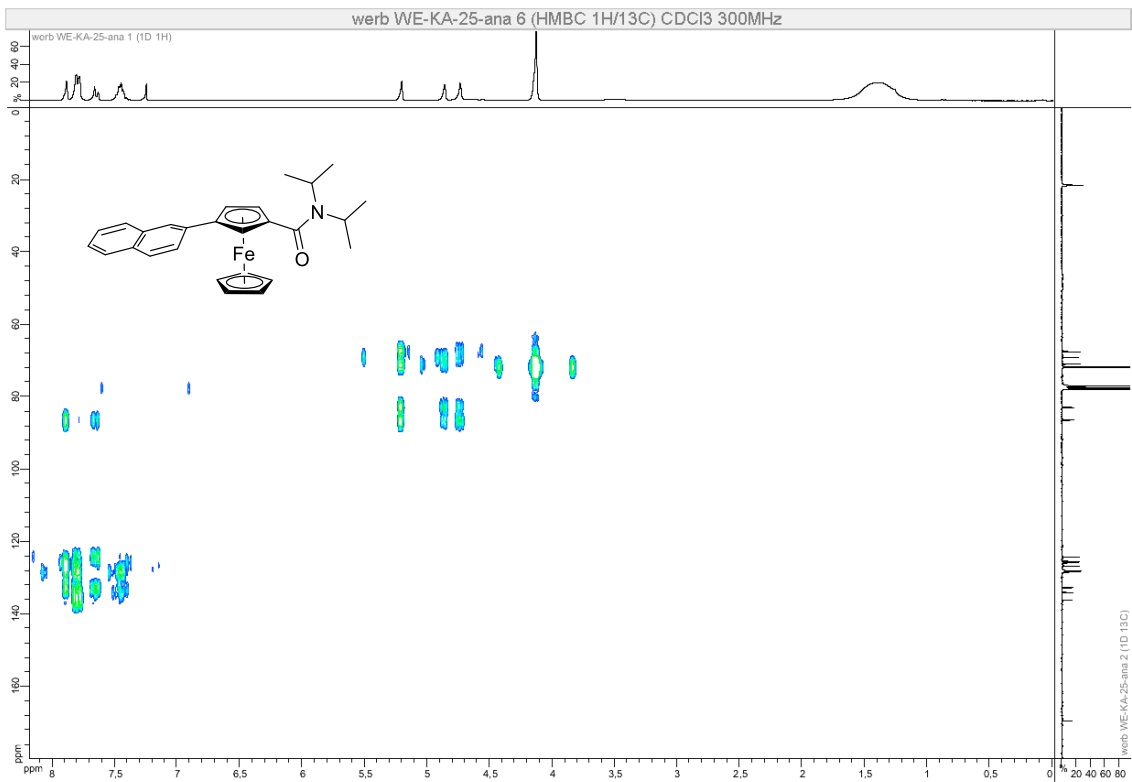
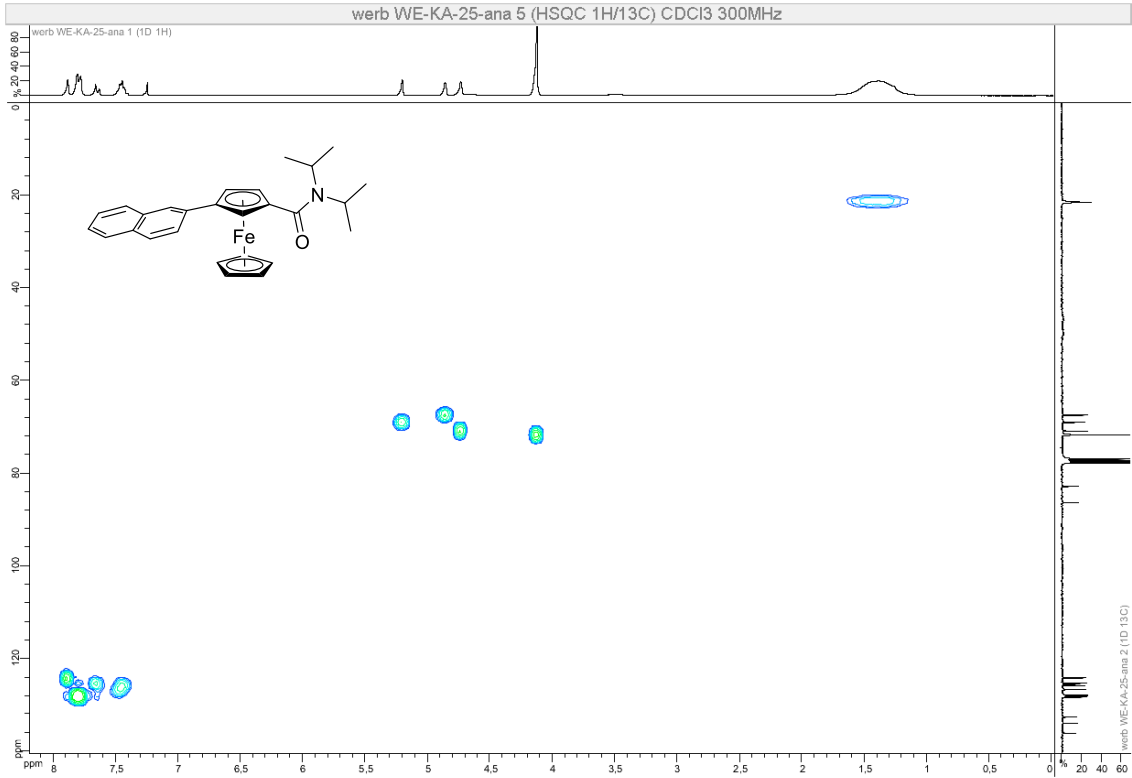


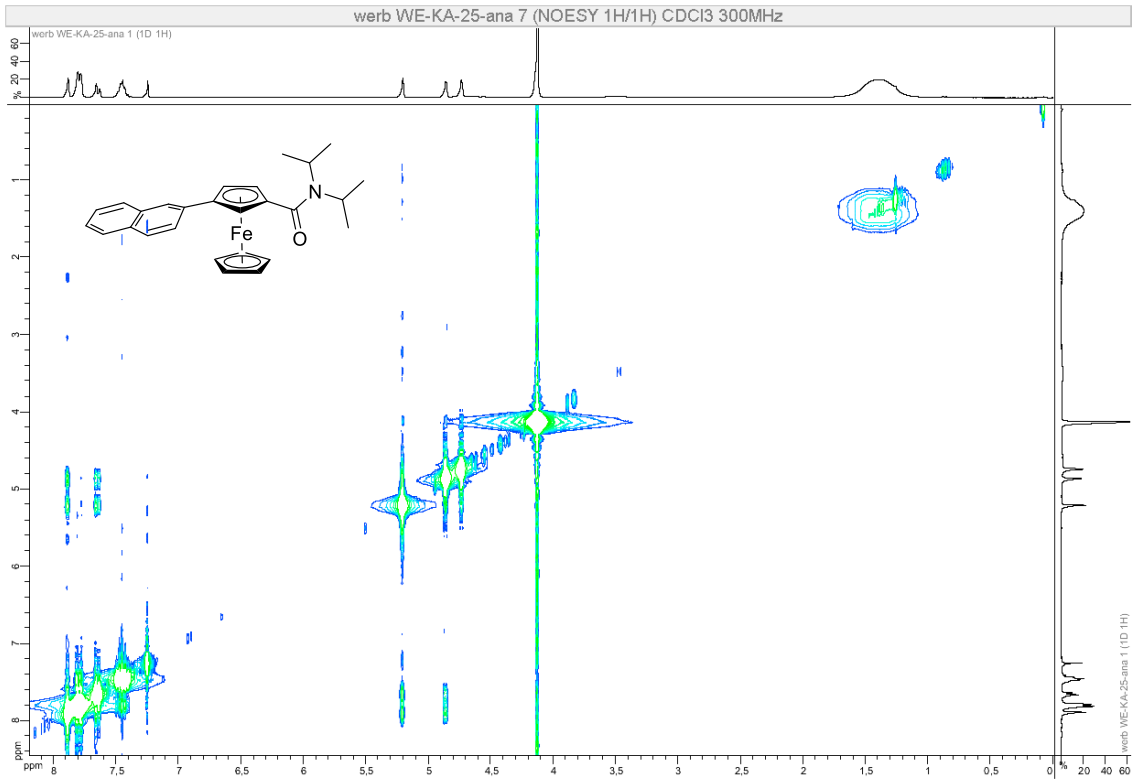
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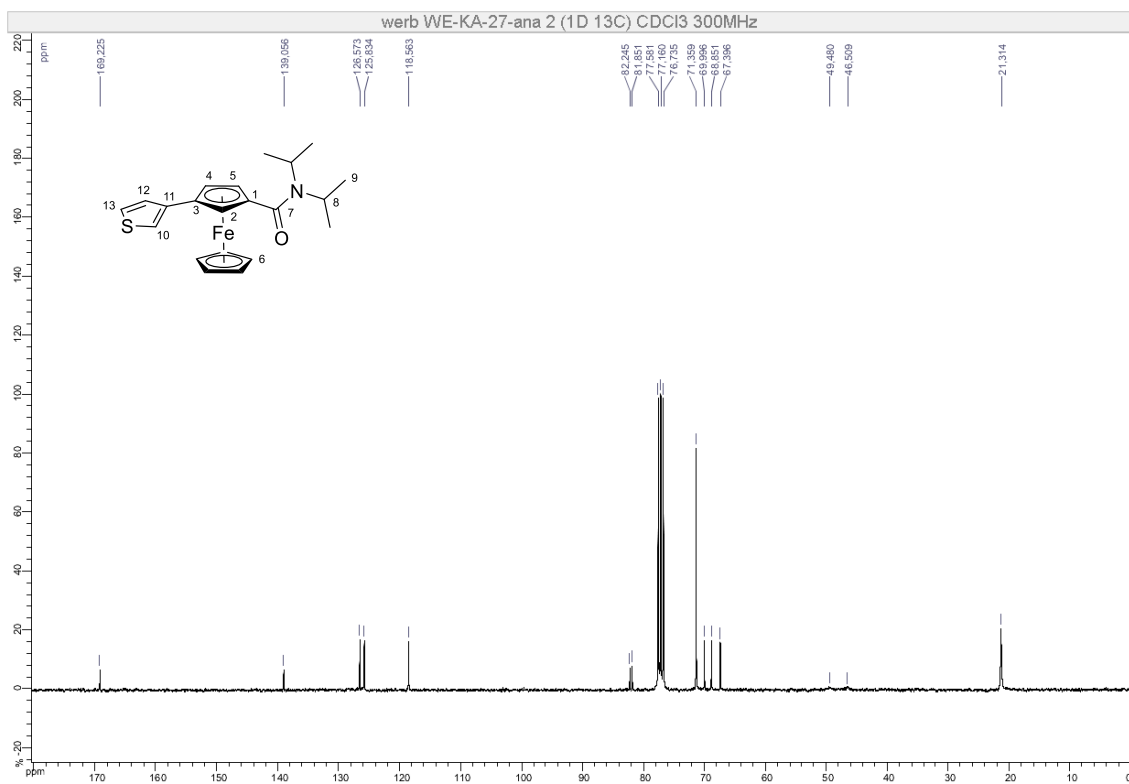
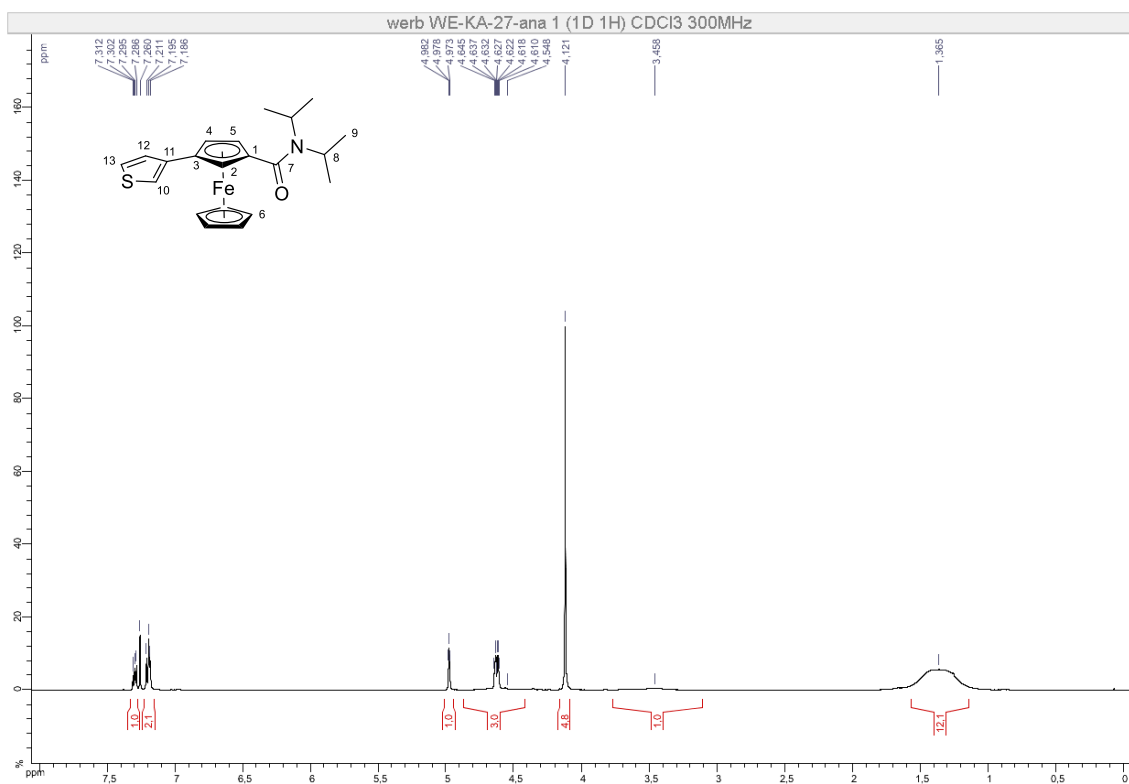


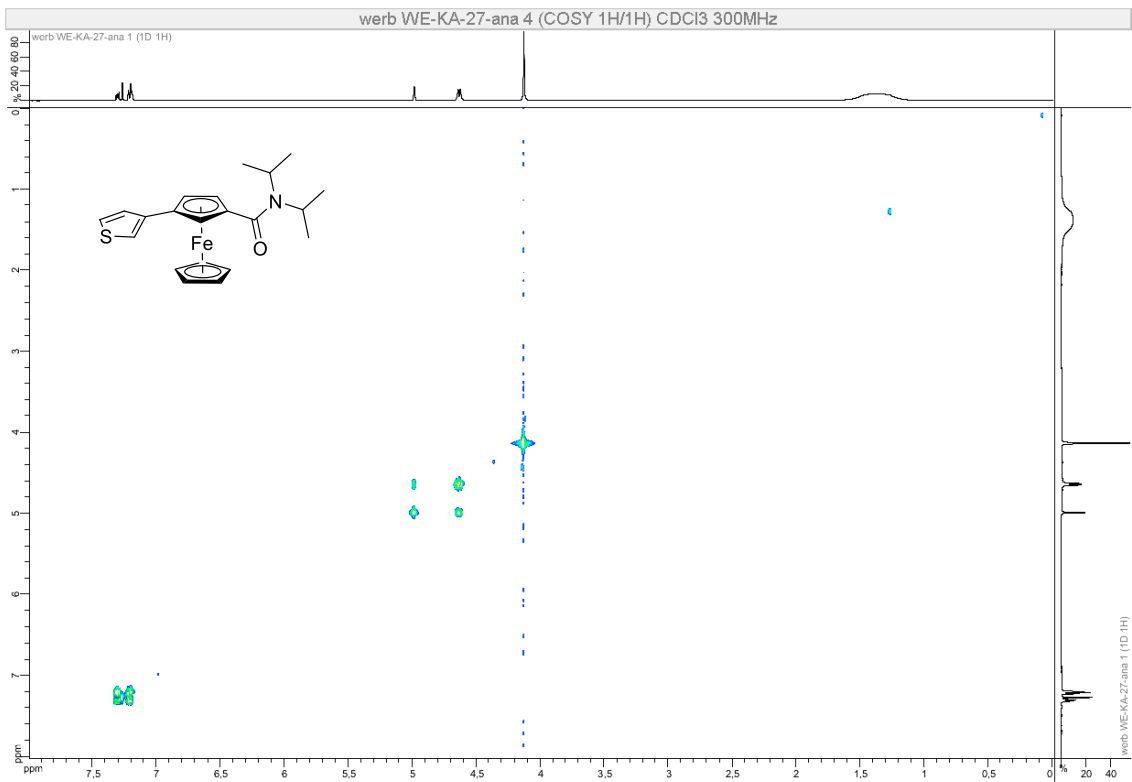
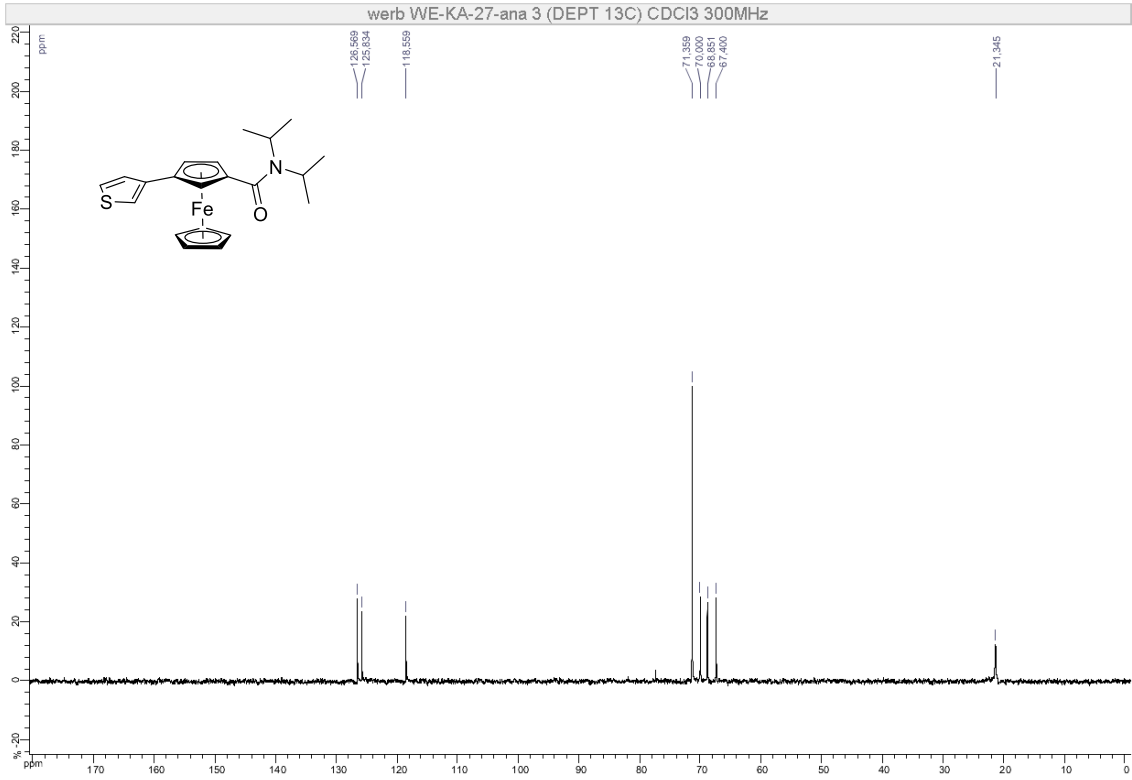


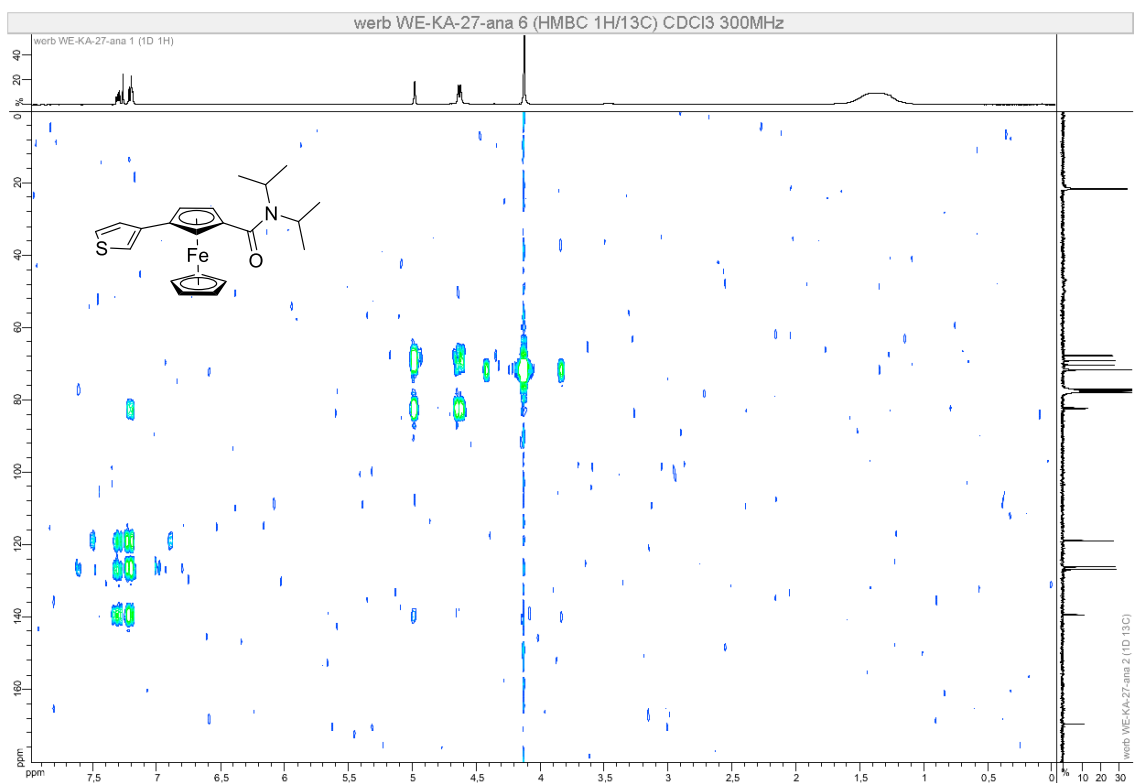
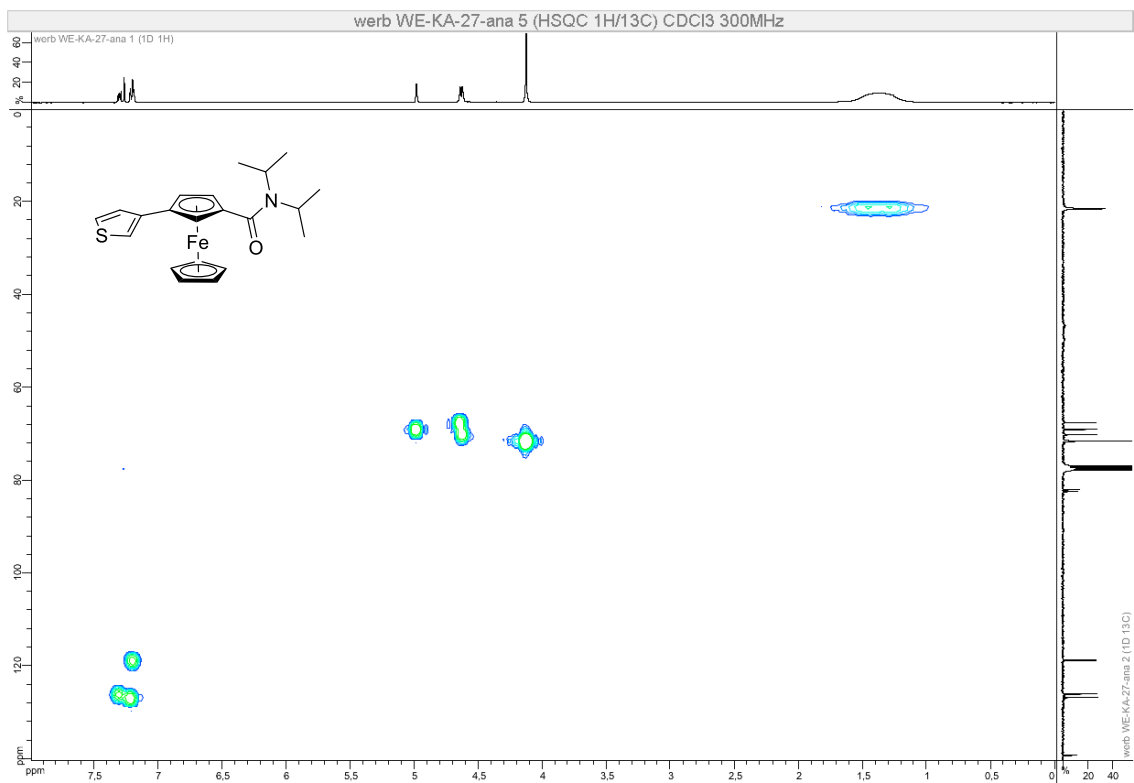


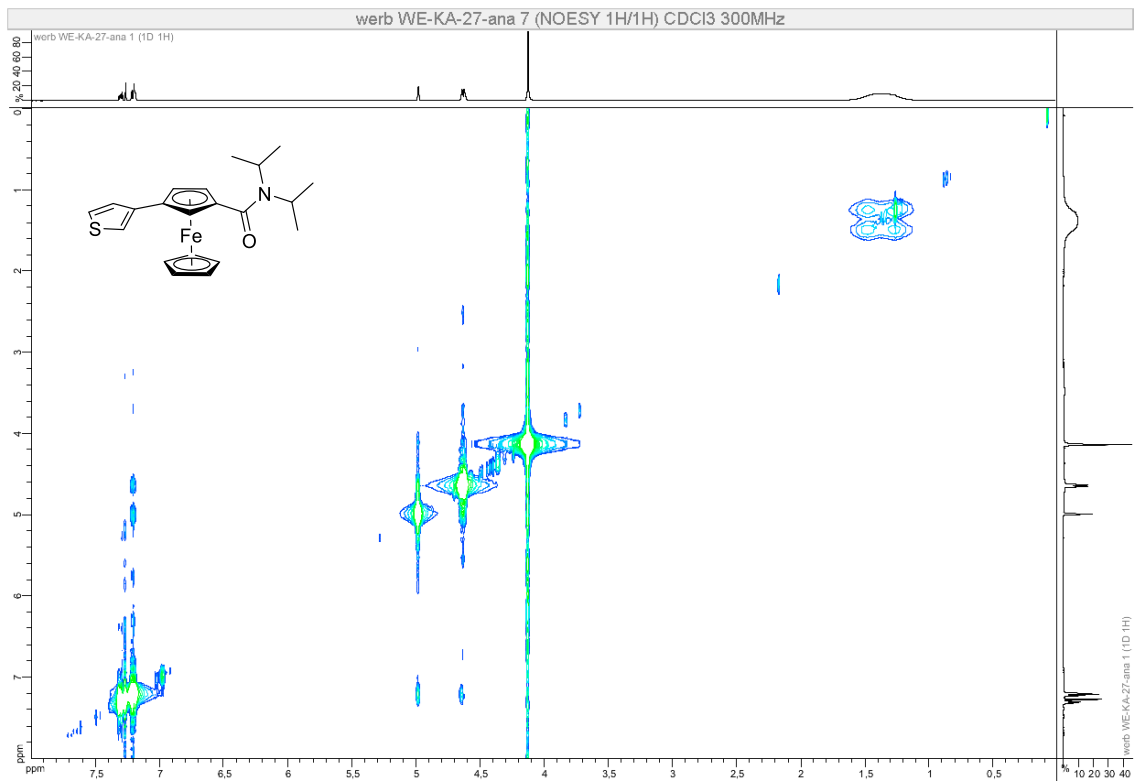


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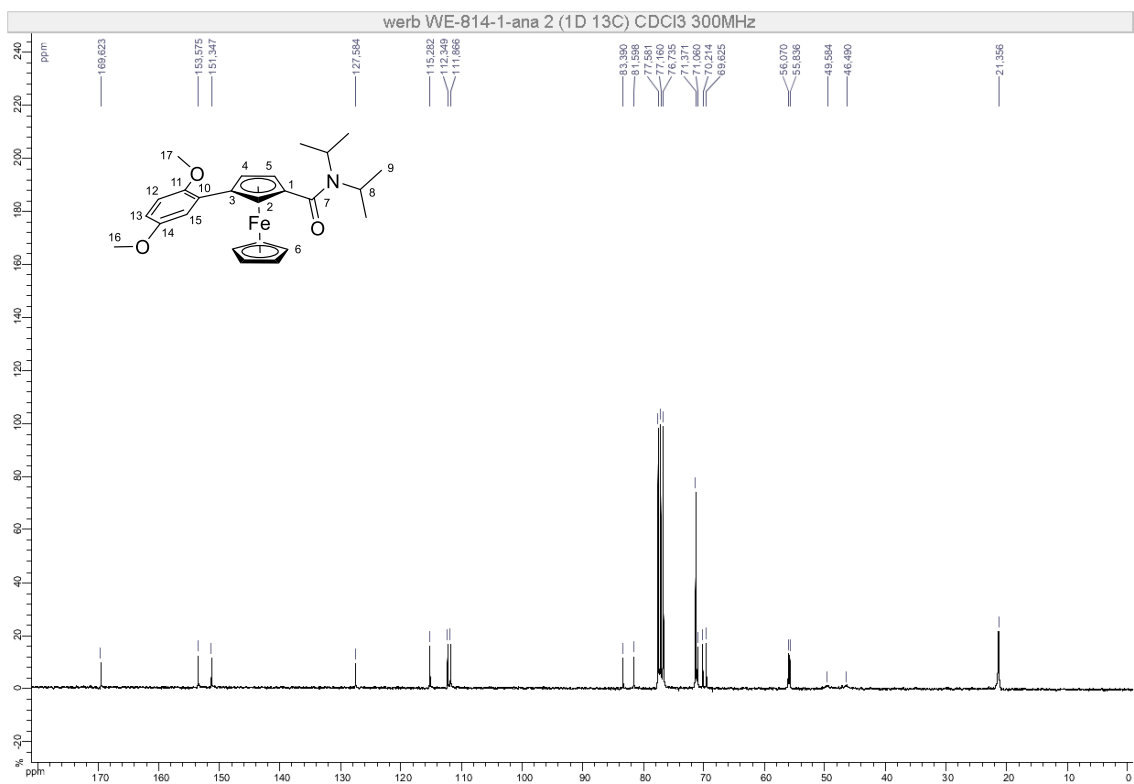
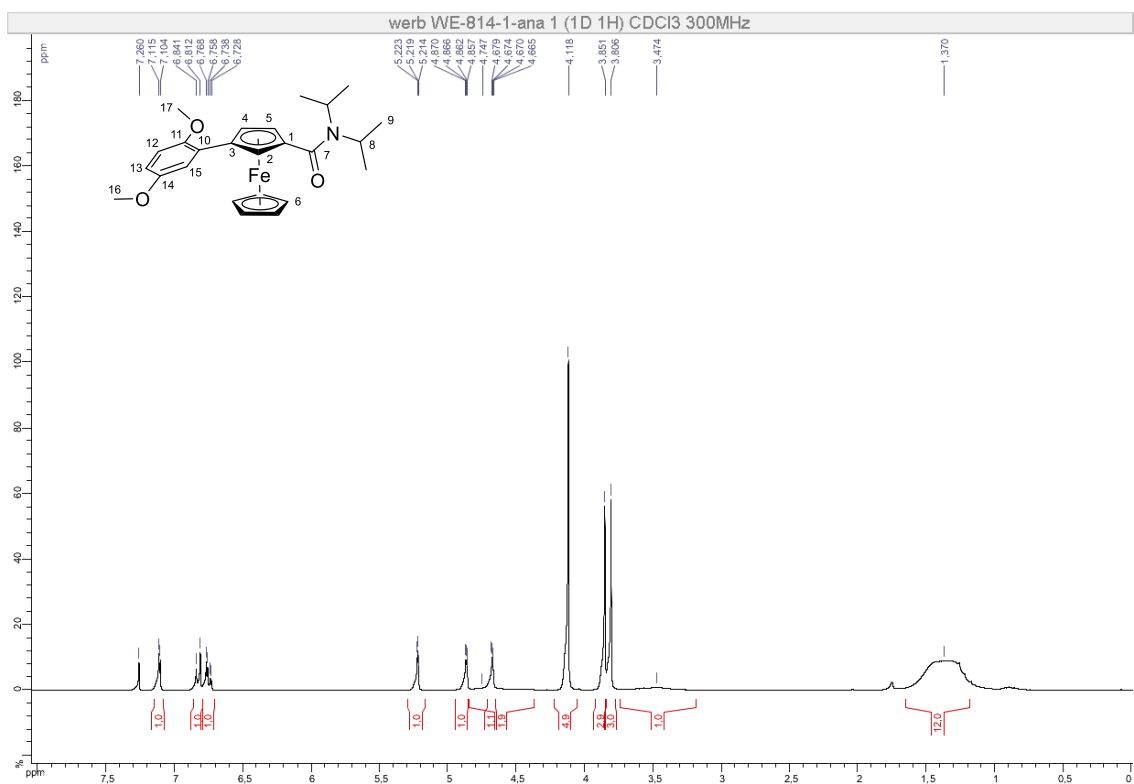




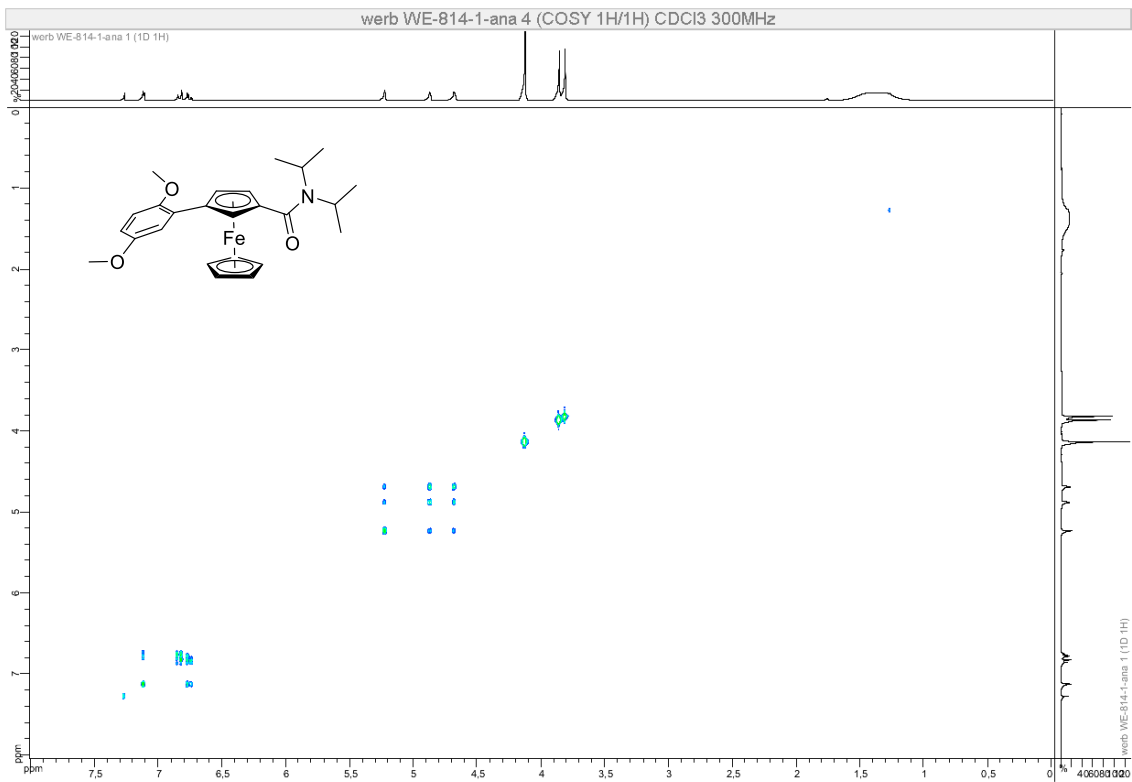
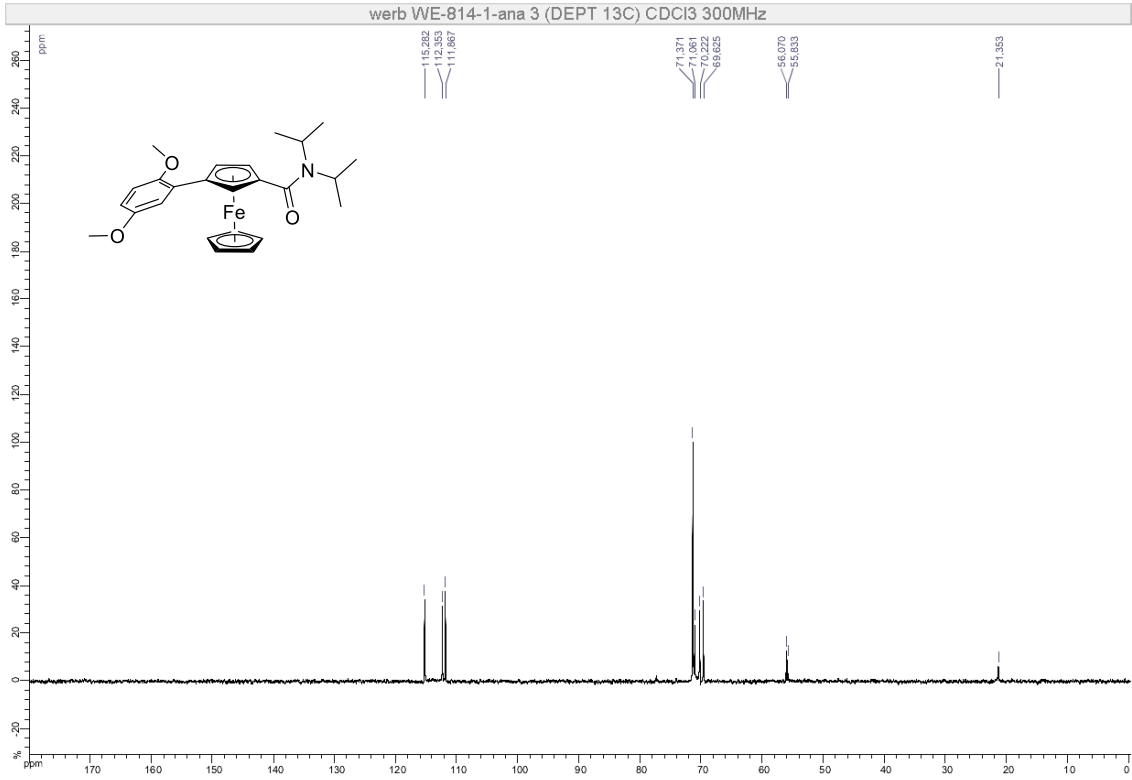


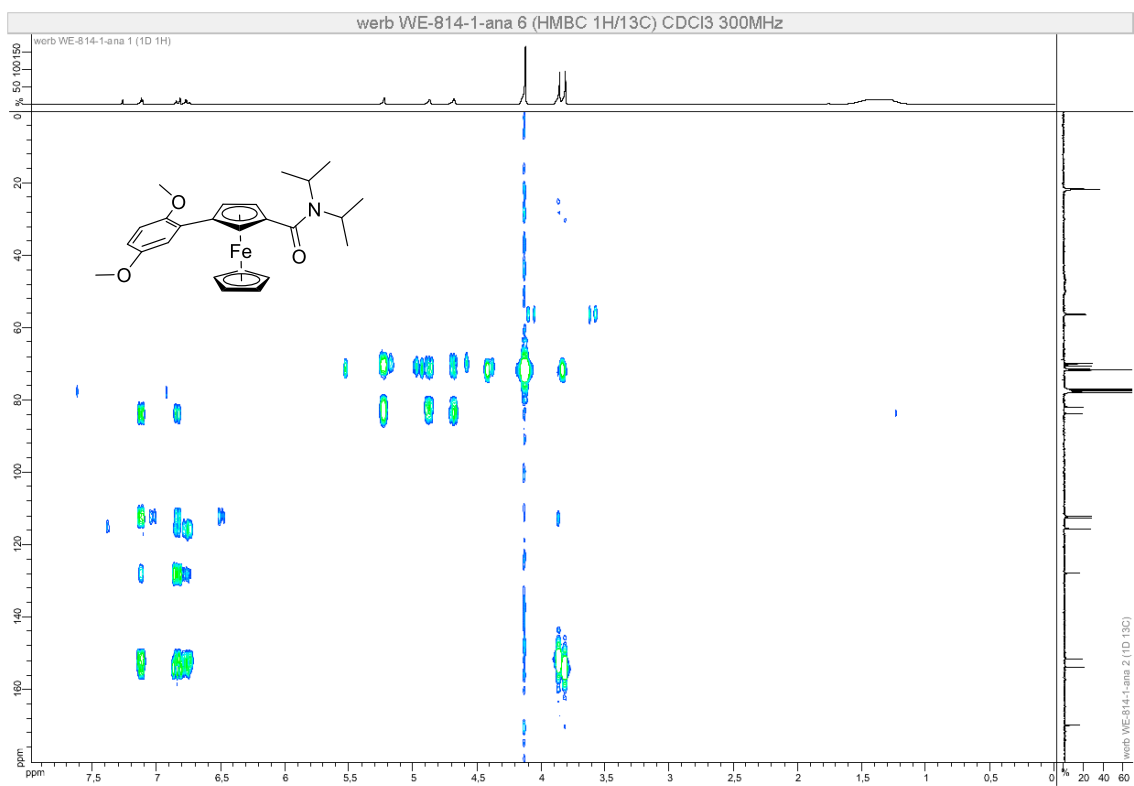
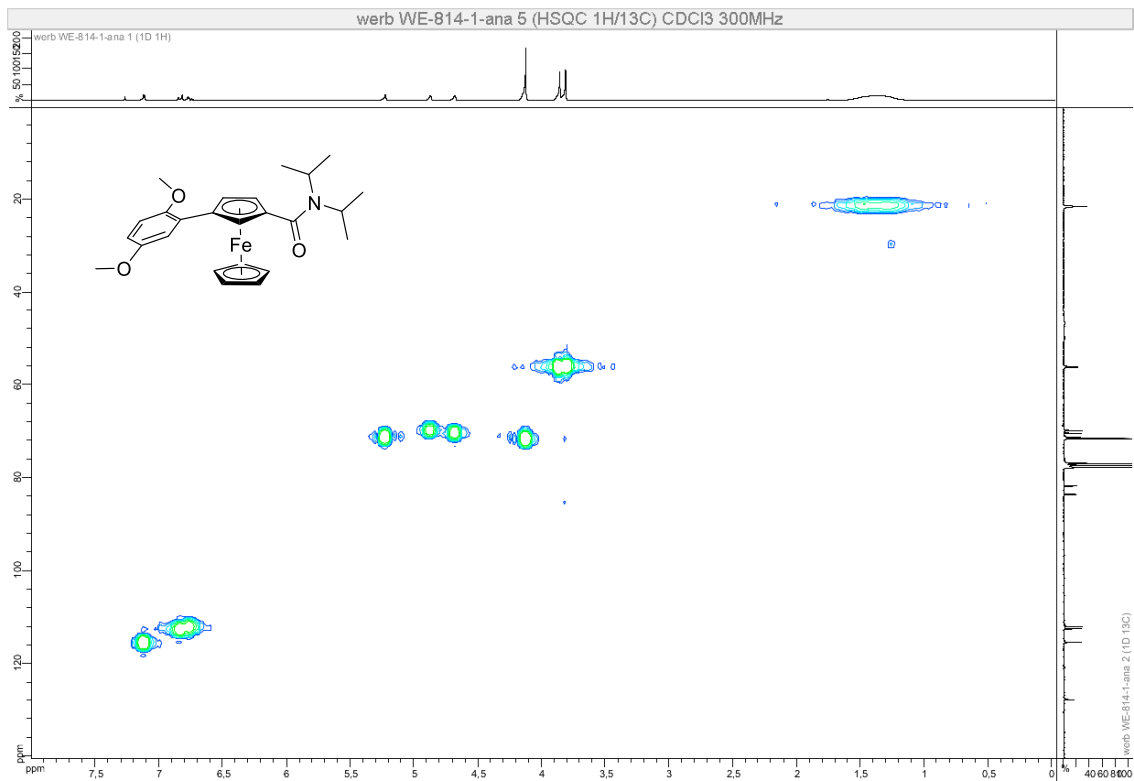


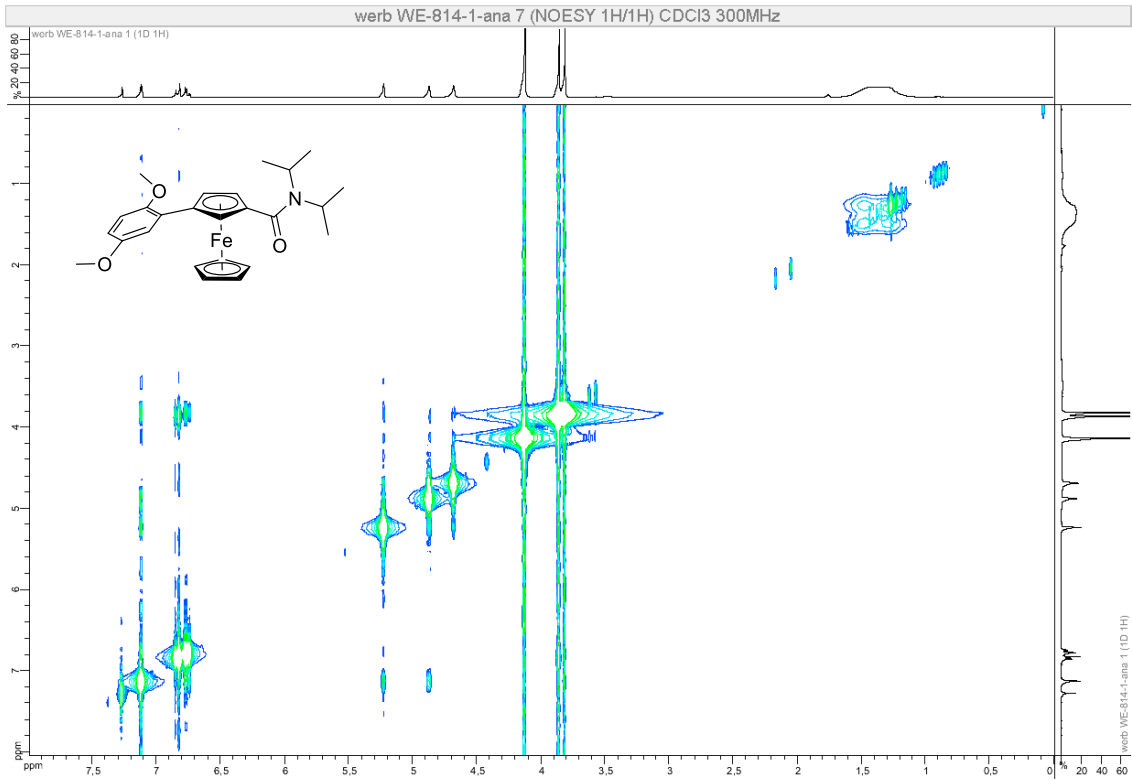
**3-(2,5-Dimethoxyphenyl)-N,N-diisopropylferrocenecarboxamide (14)**



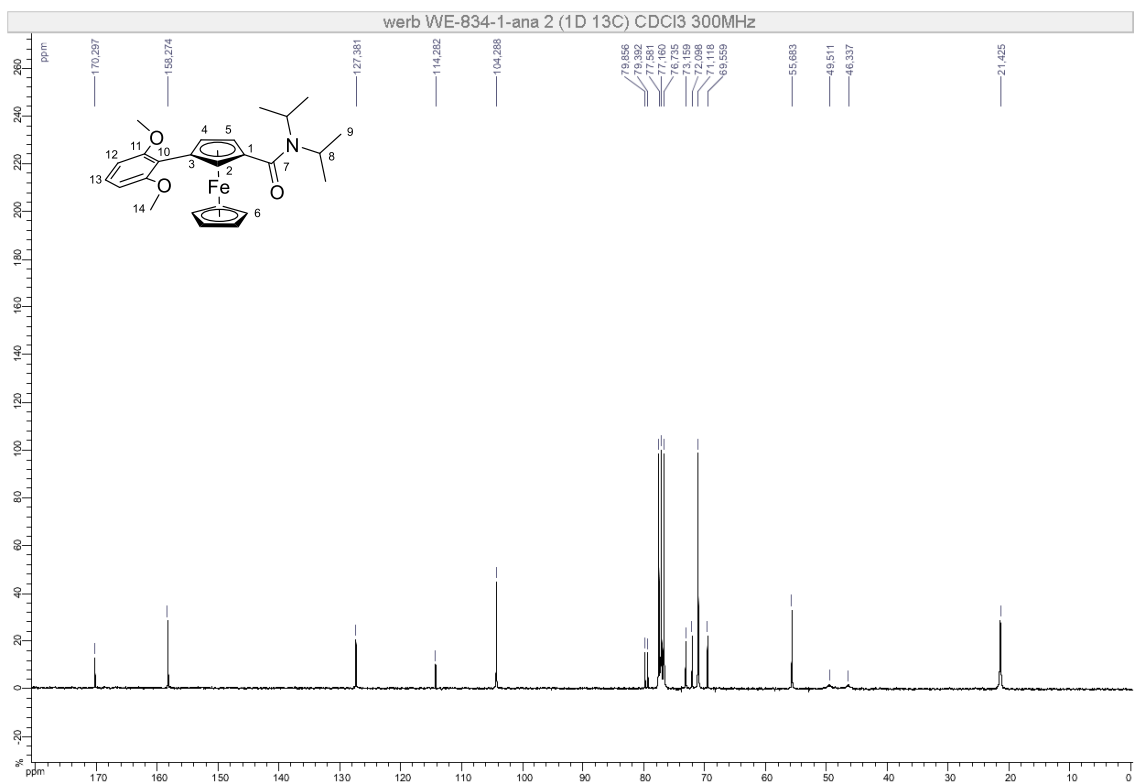
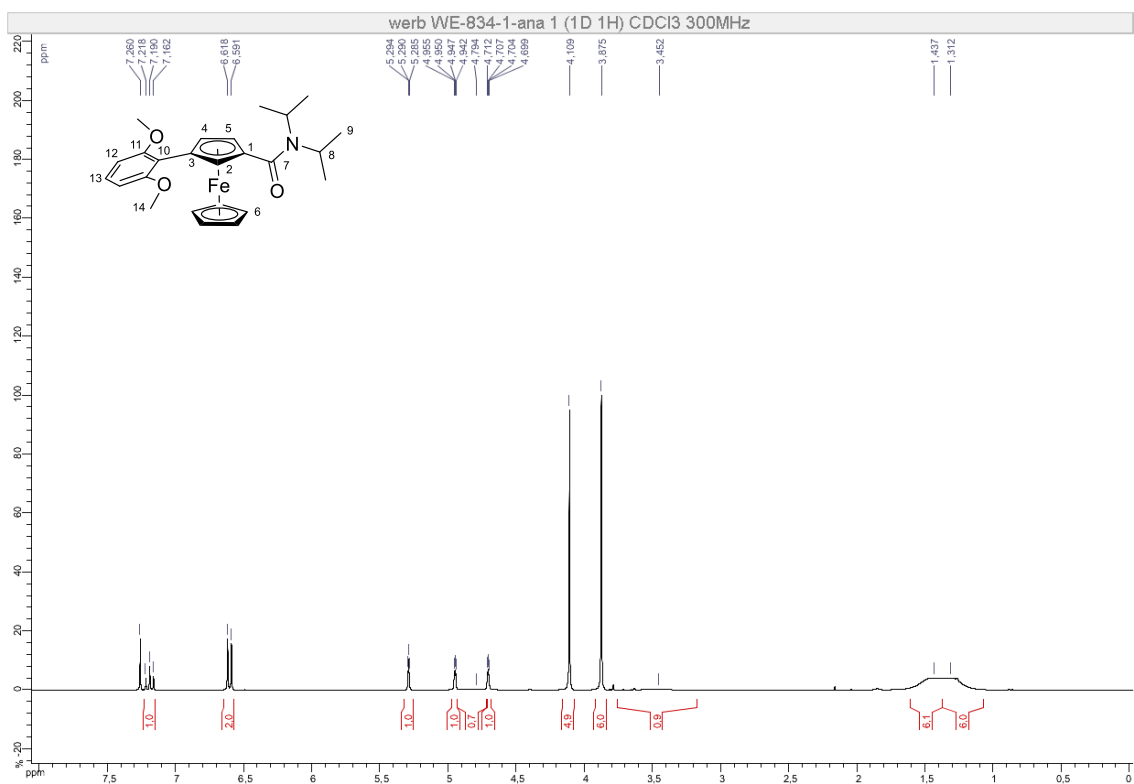


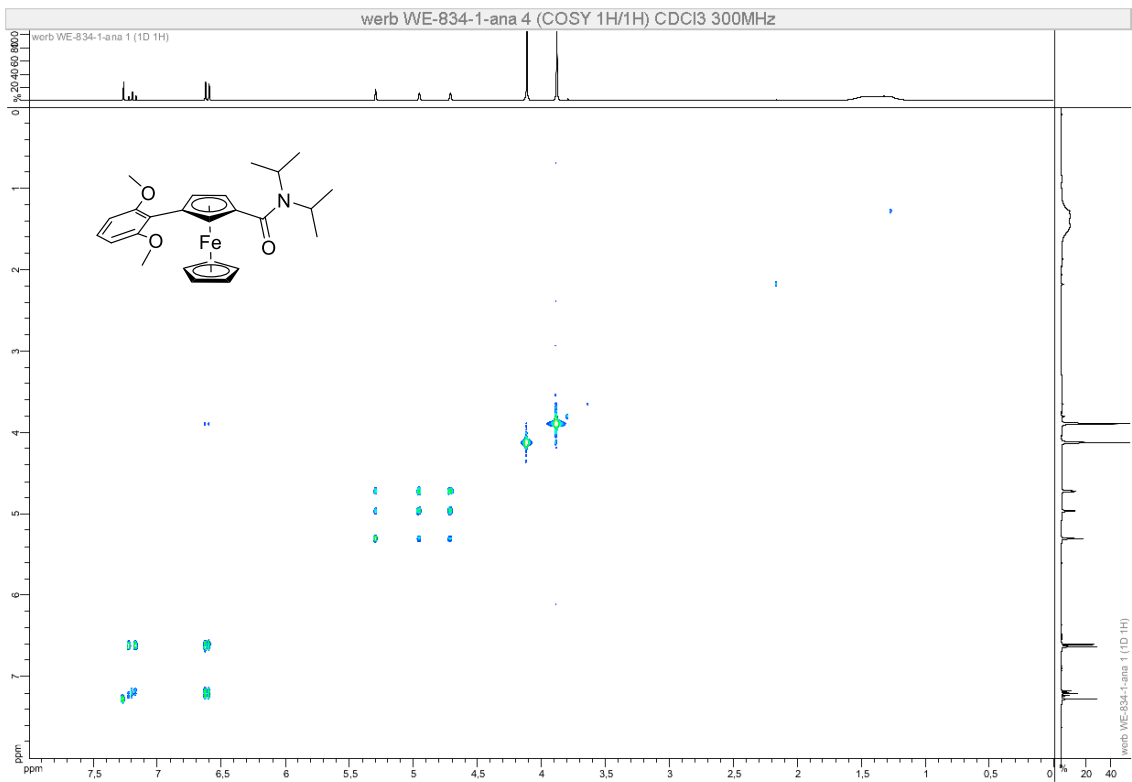
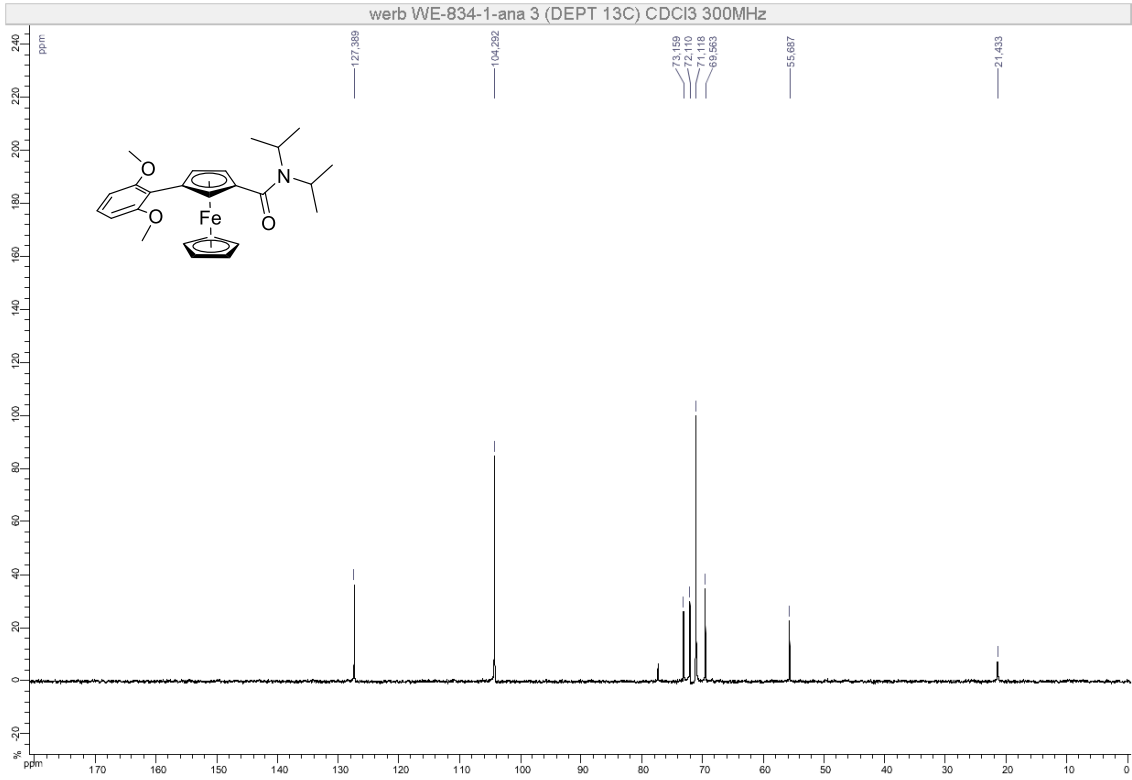


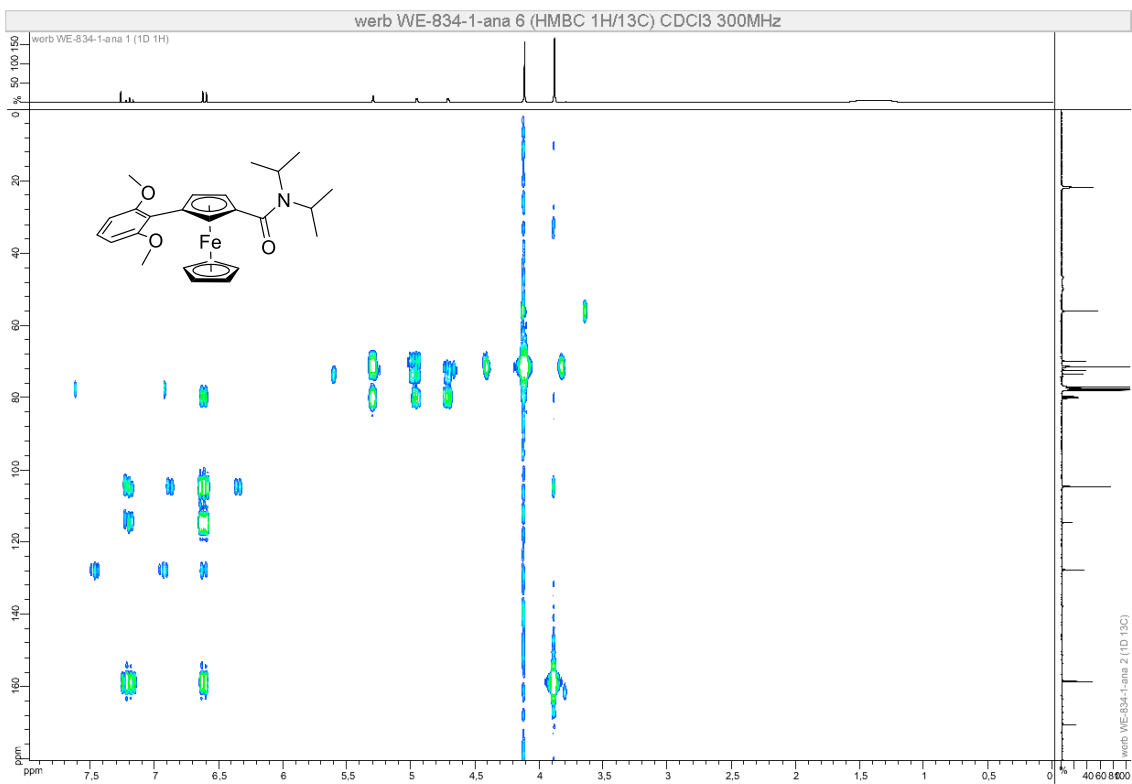
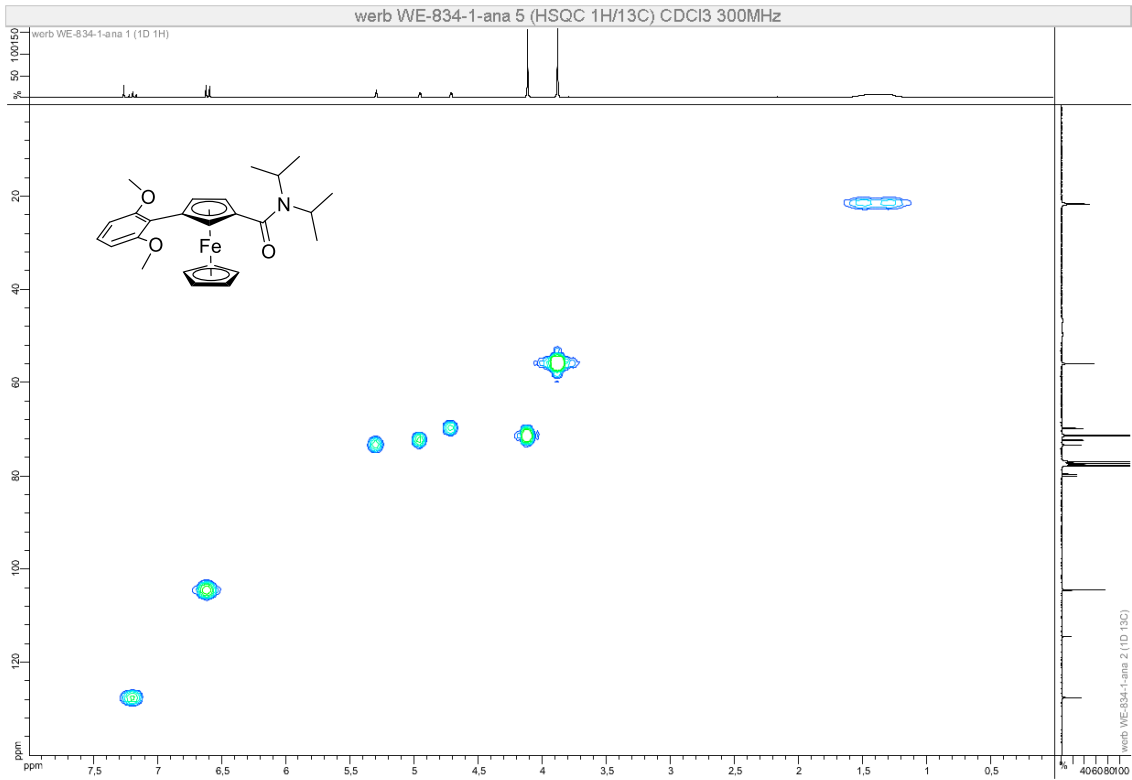


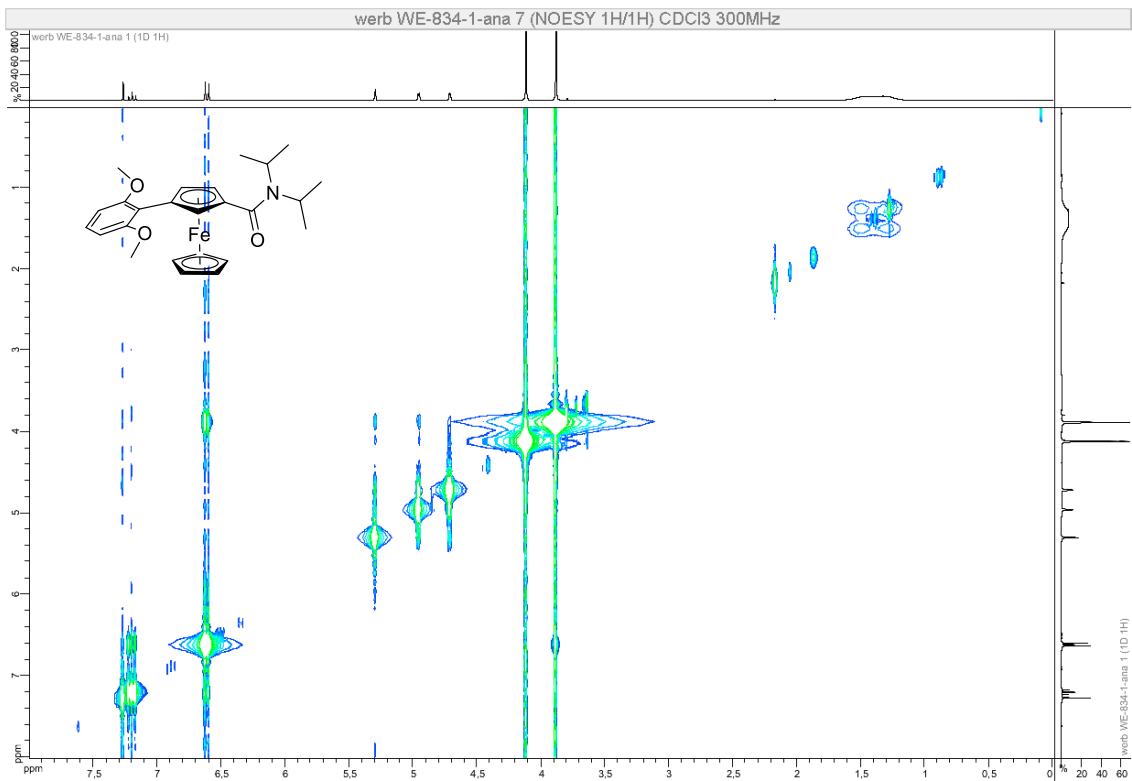


**3-(2,6-Dimethoxyphenyl)-N,N-diisopropylferrocenecarboxamide (15)**

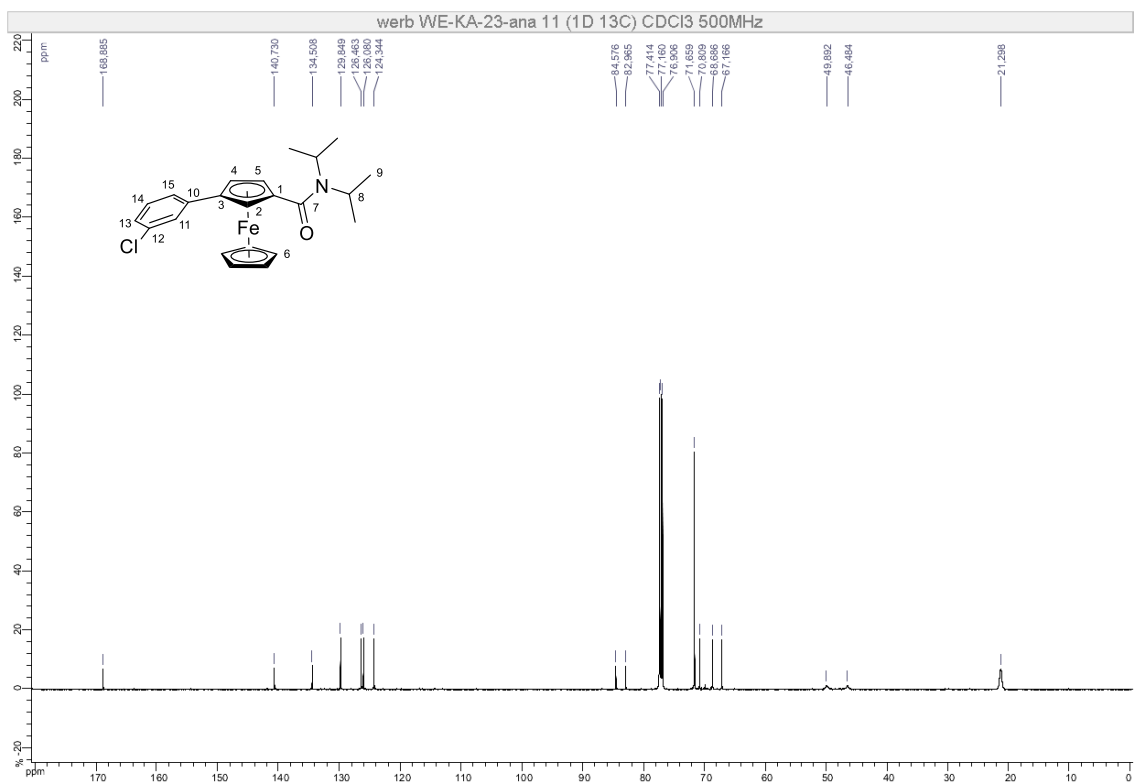
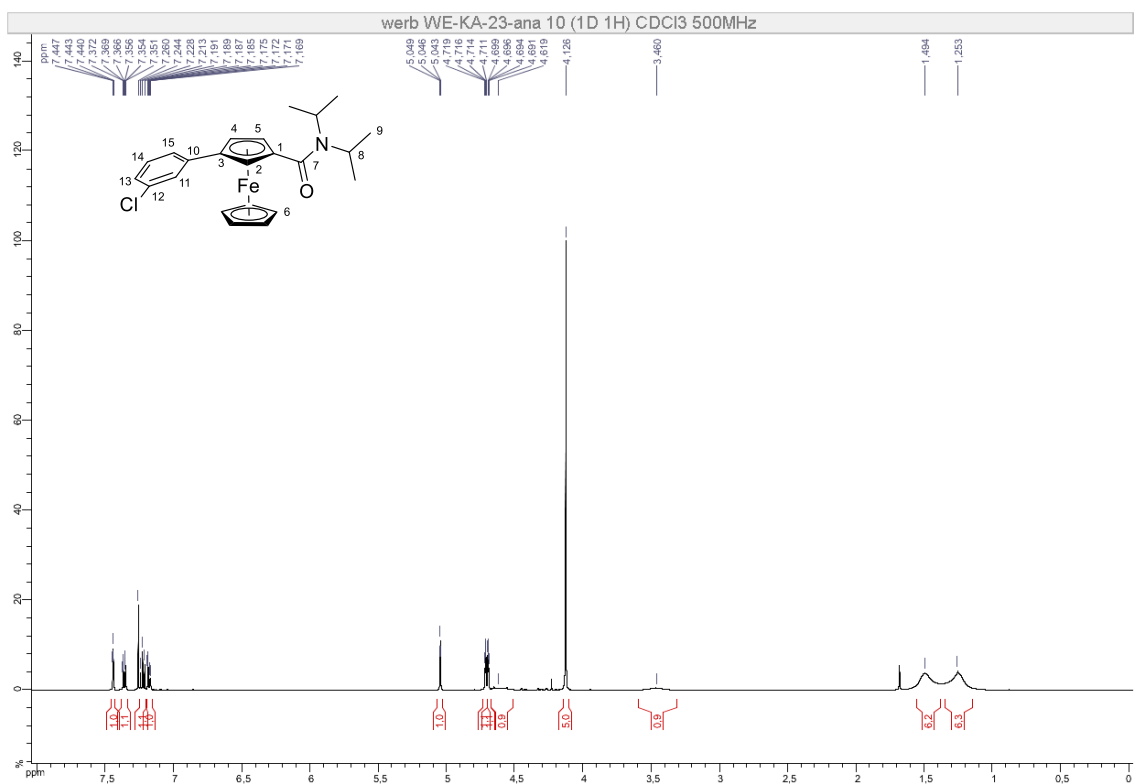




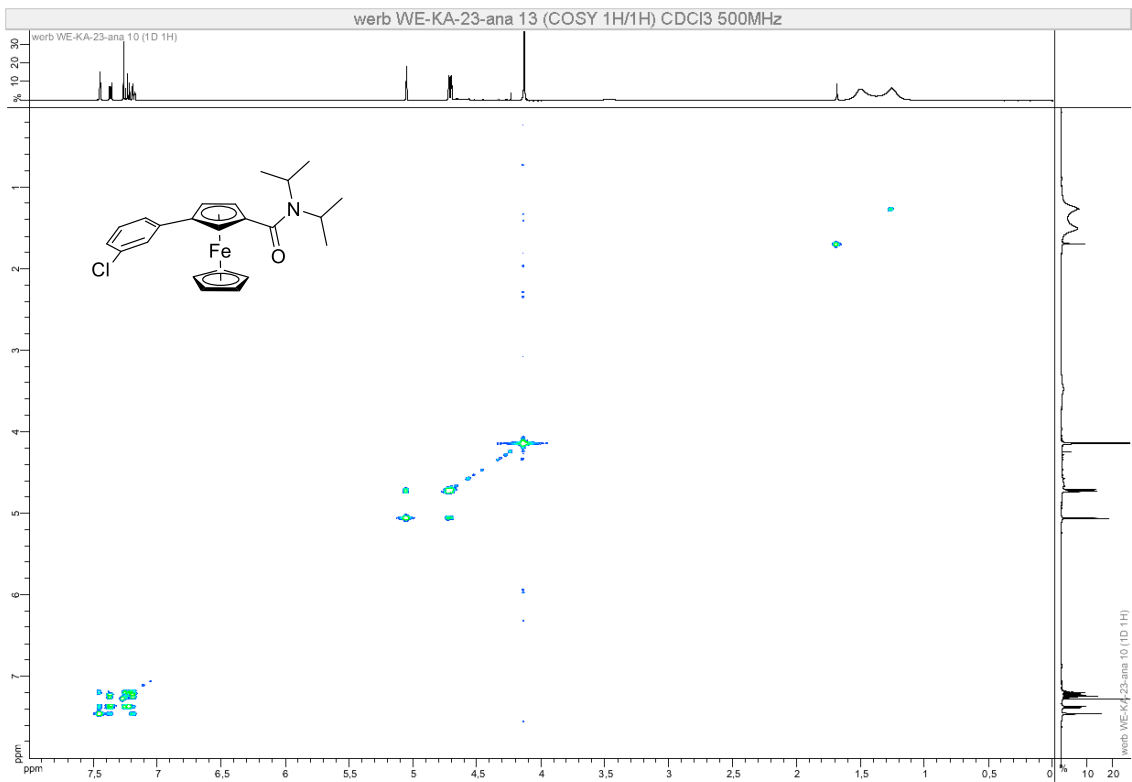
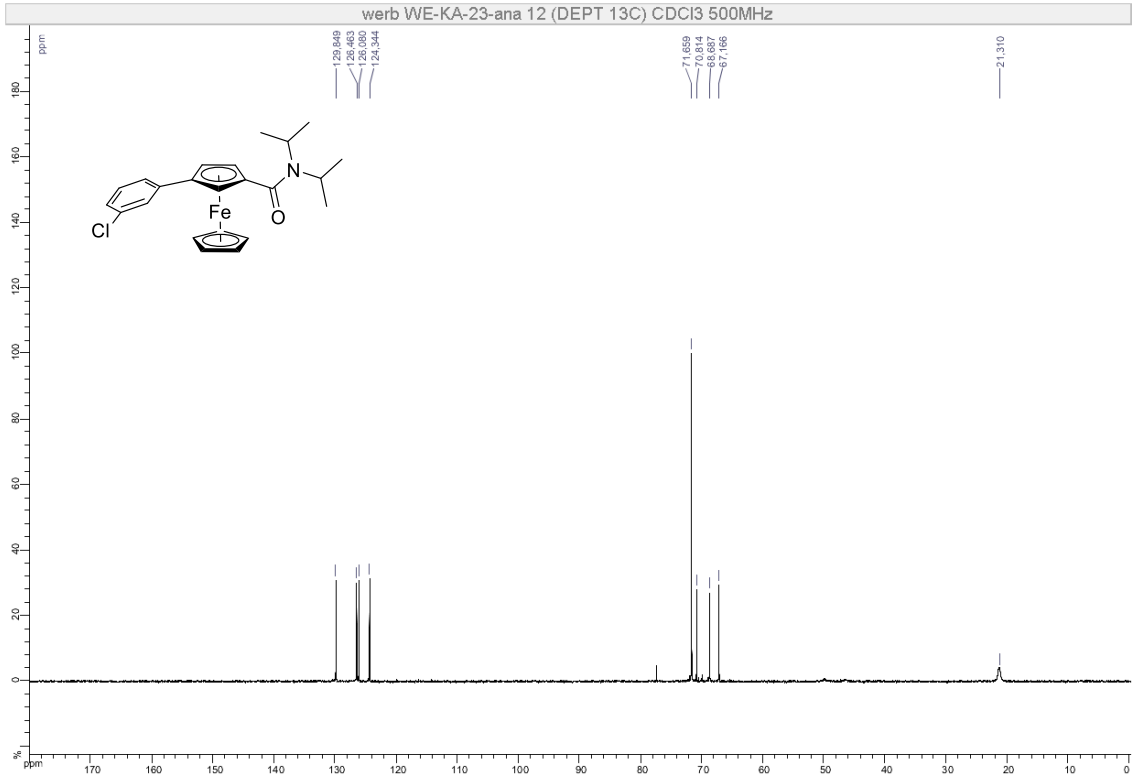


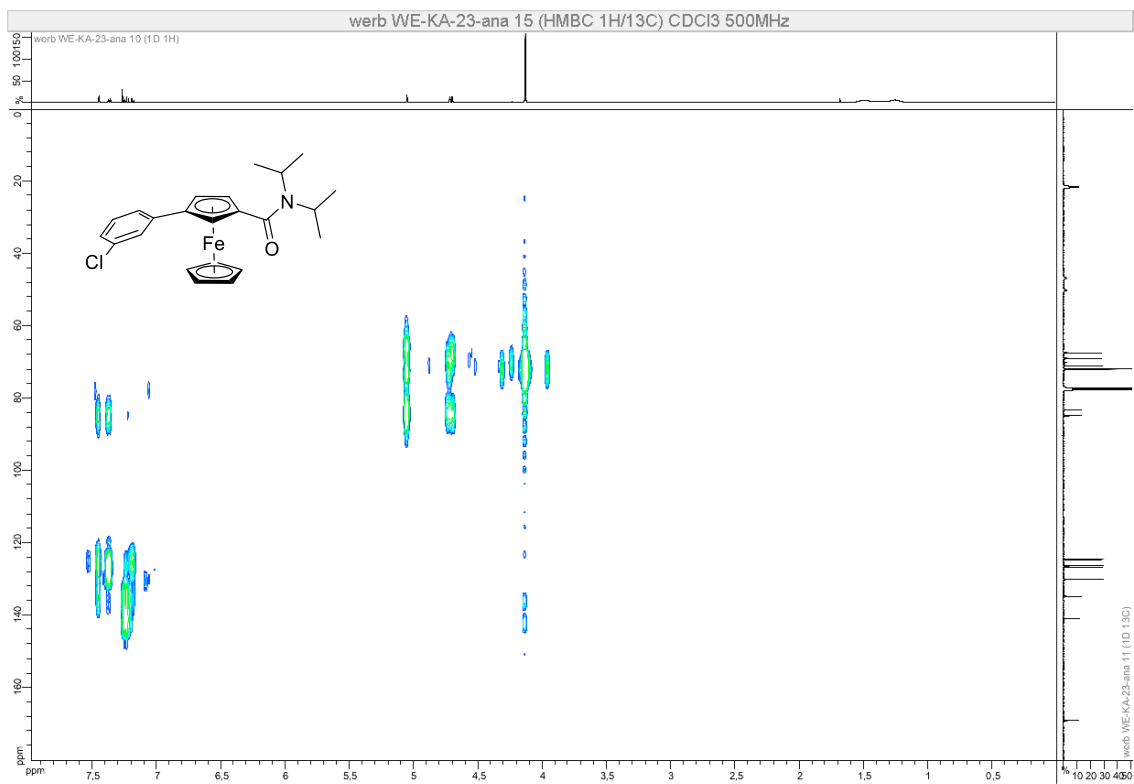
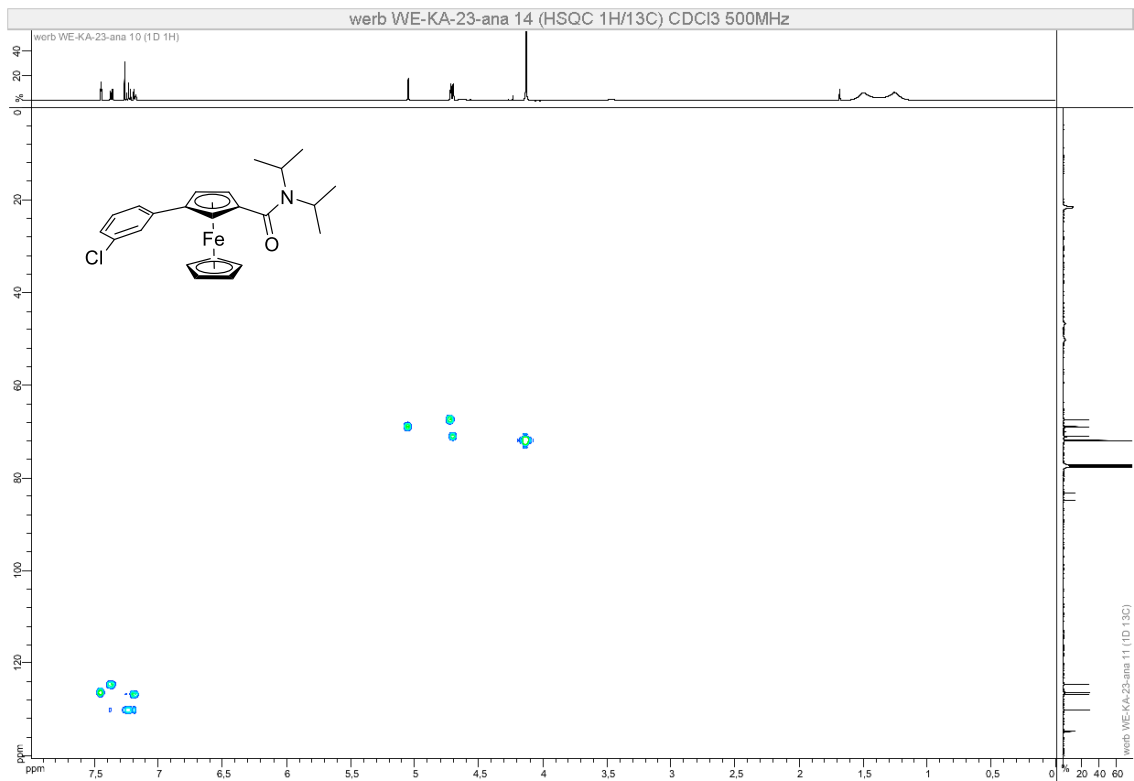


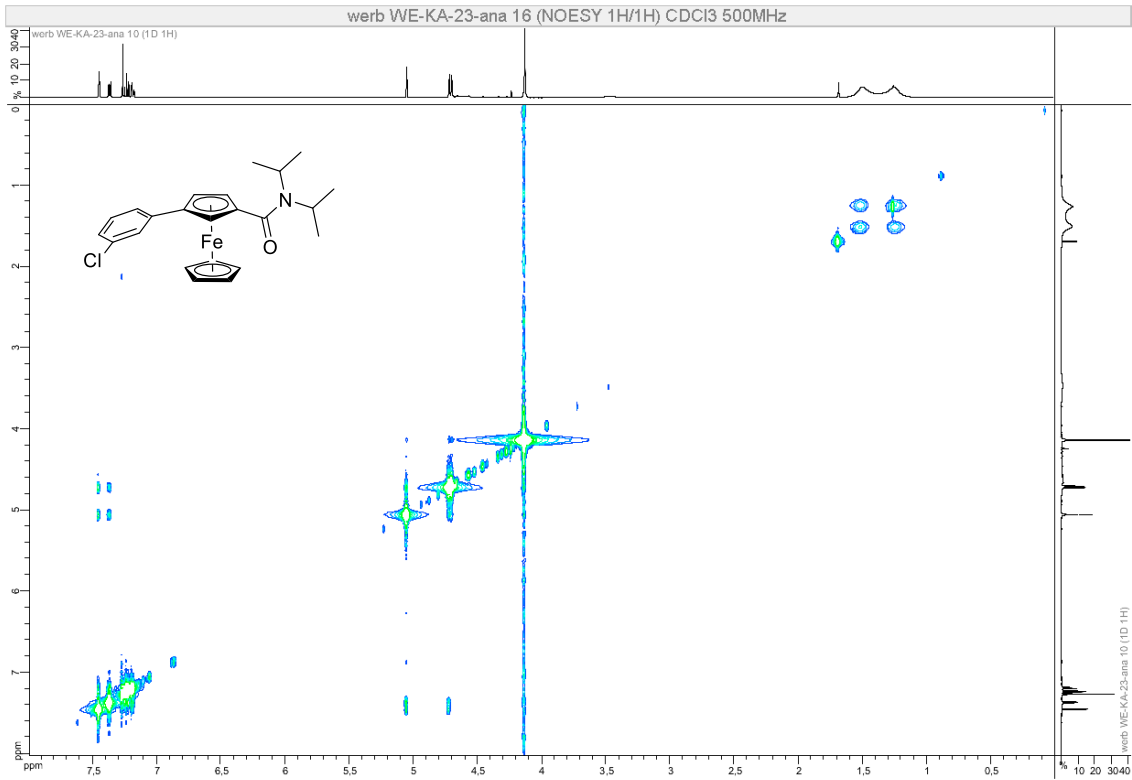
**3-(3-Chlorophenyl)-N,N-diisopropylferrocenecarboxamide (16)**



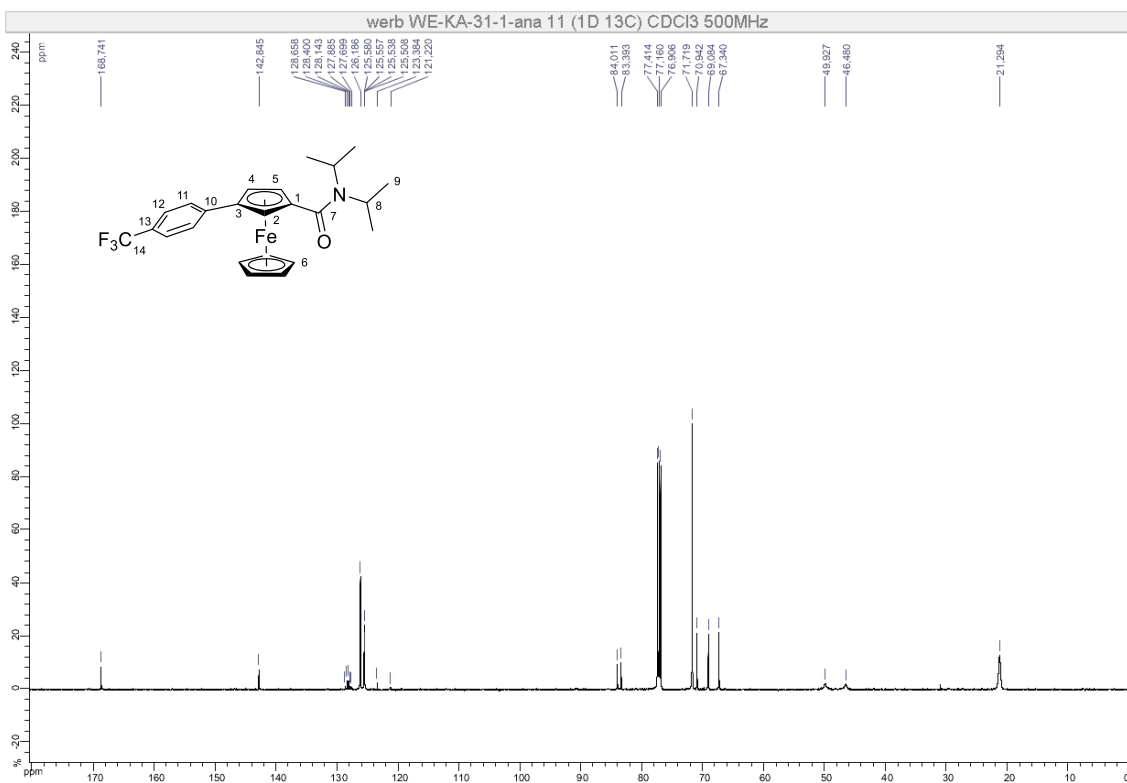
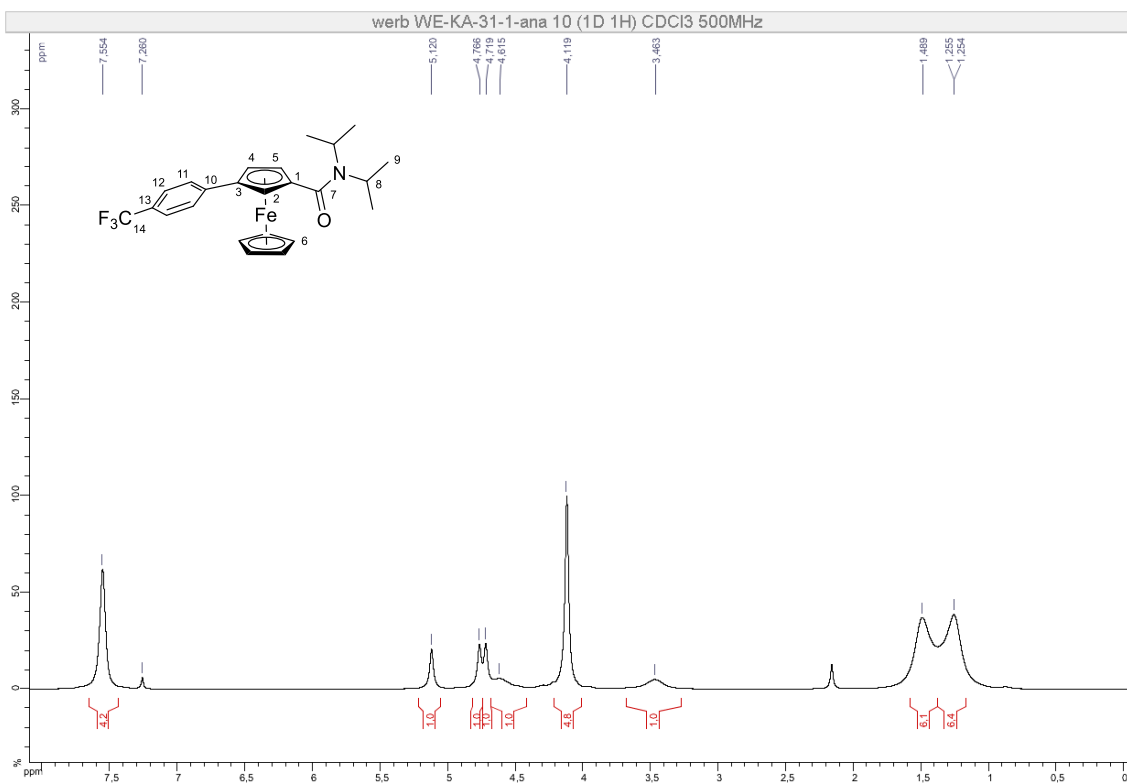


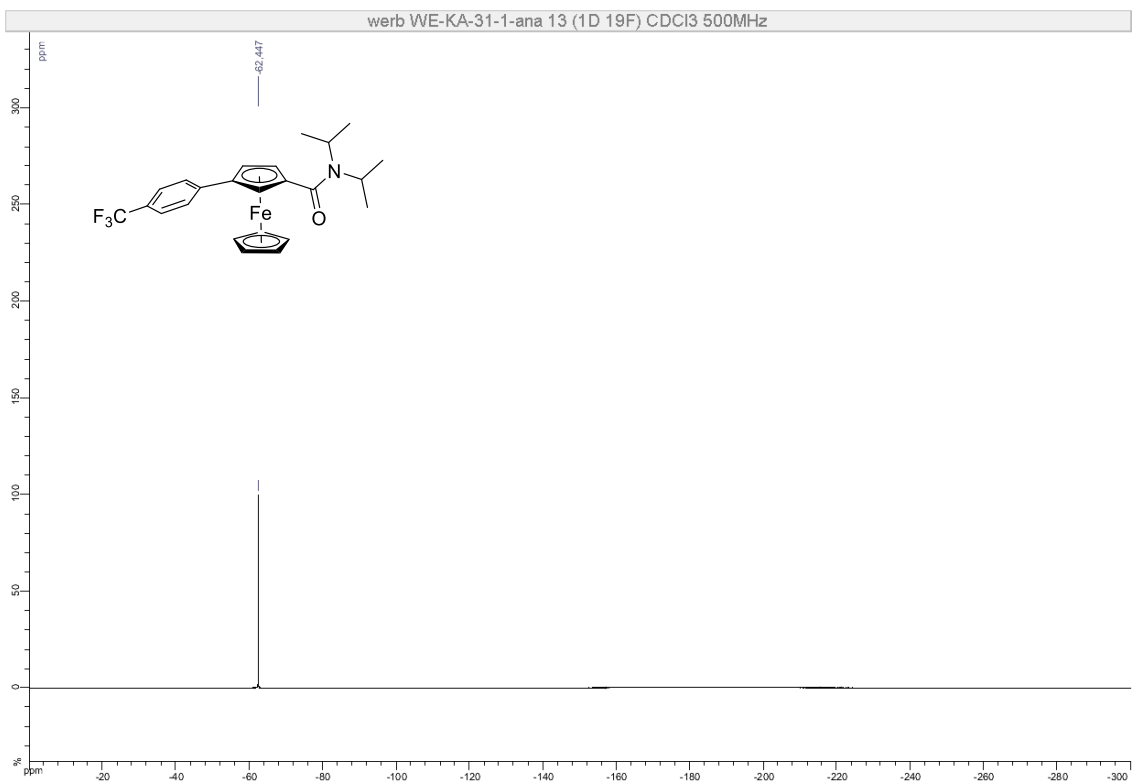
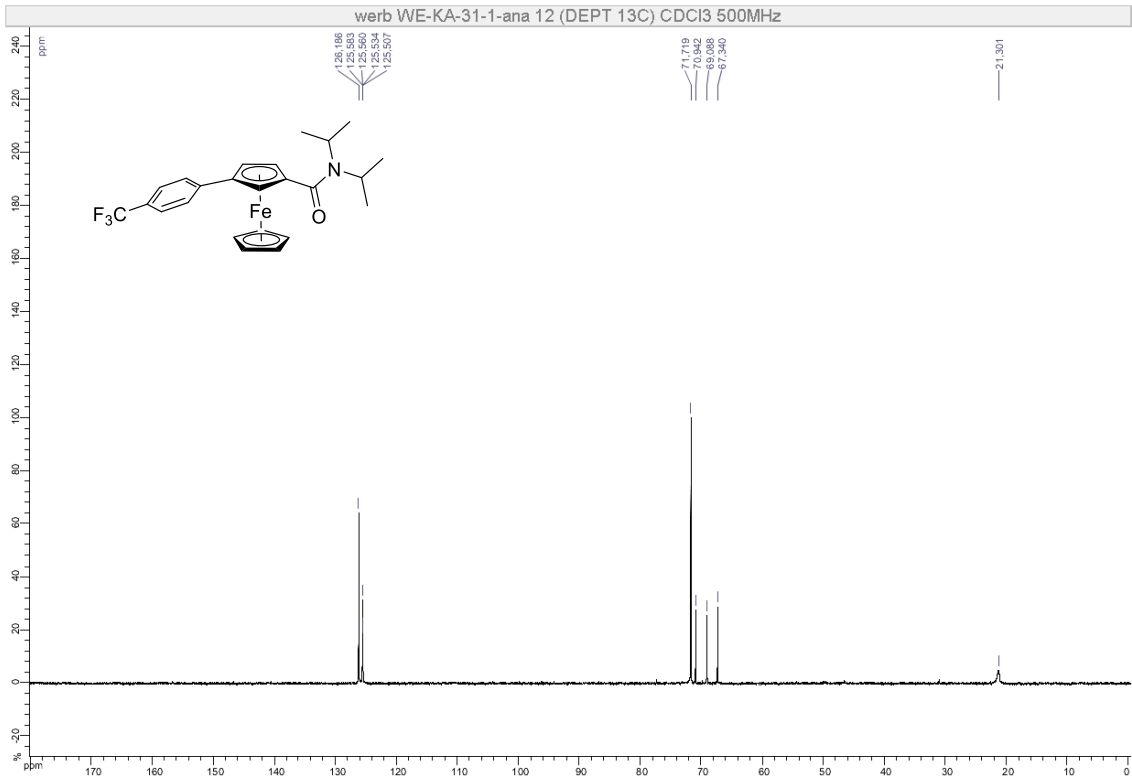




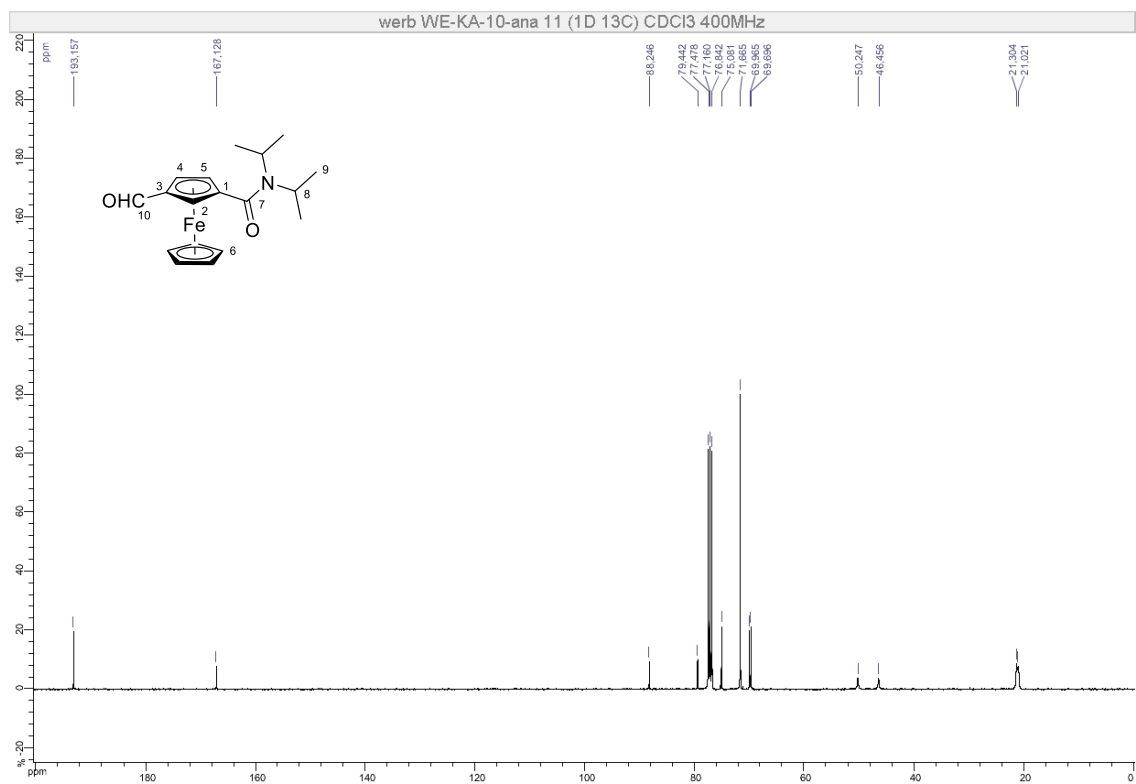
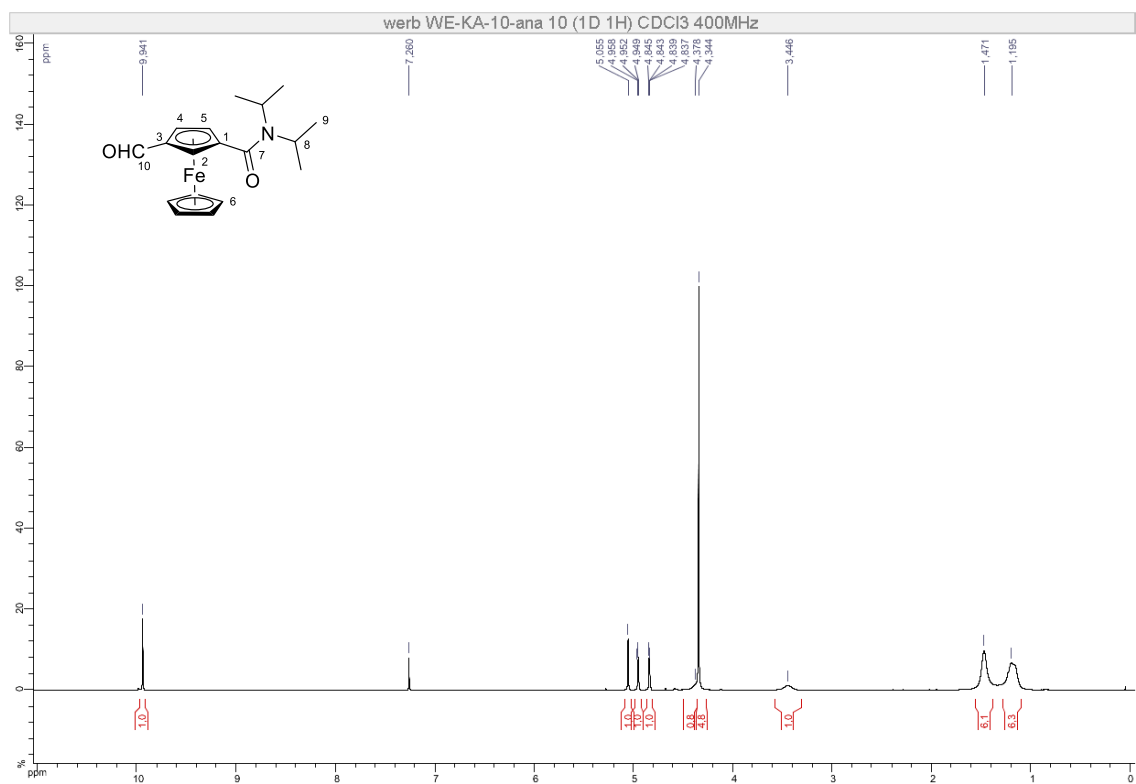


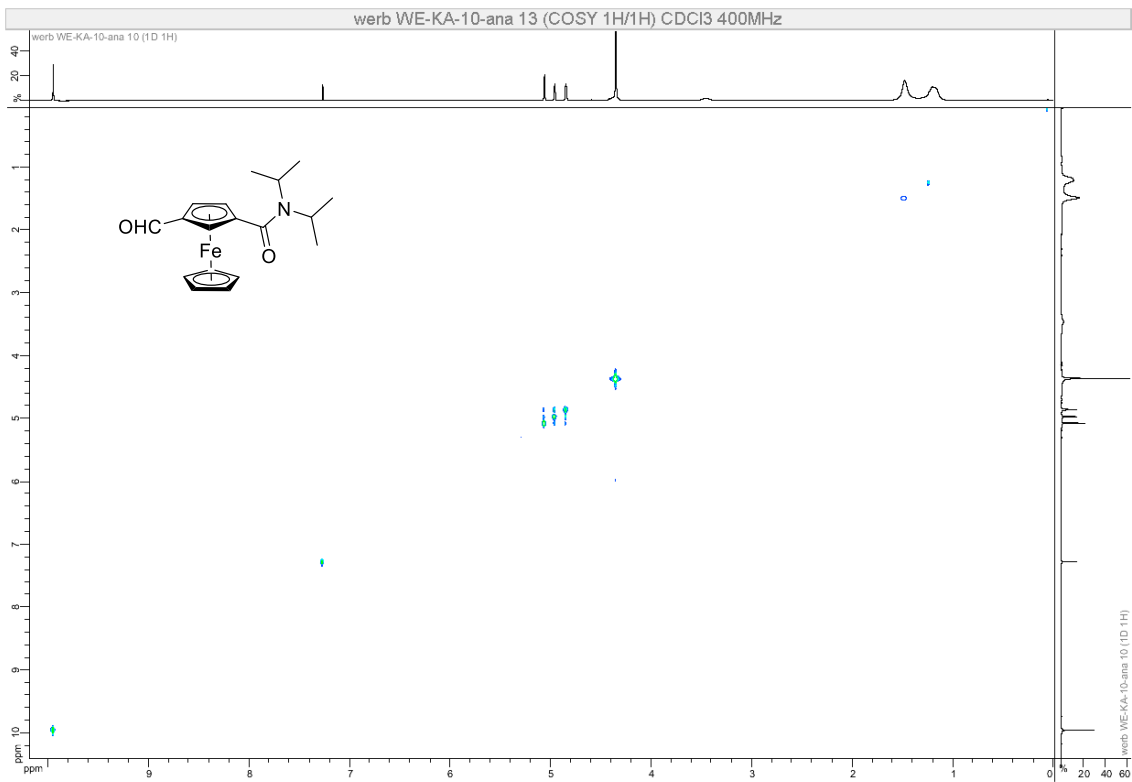
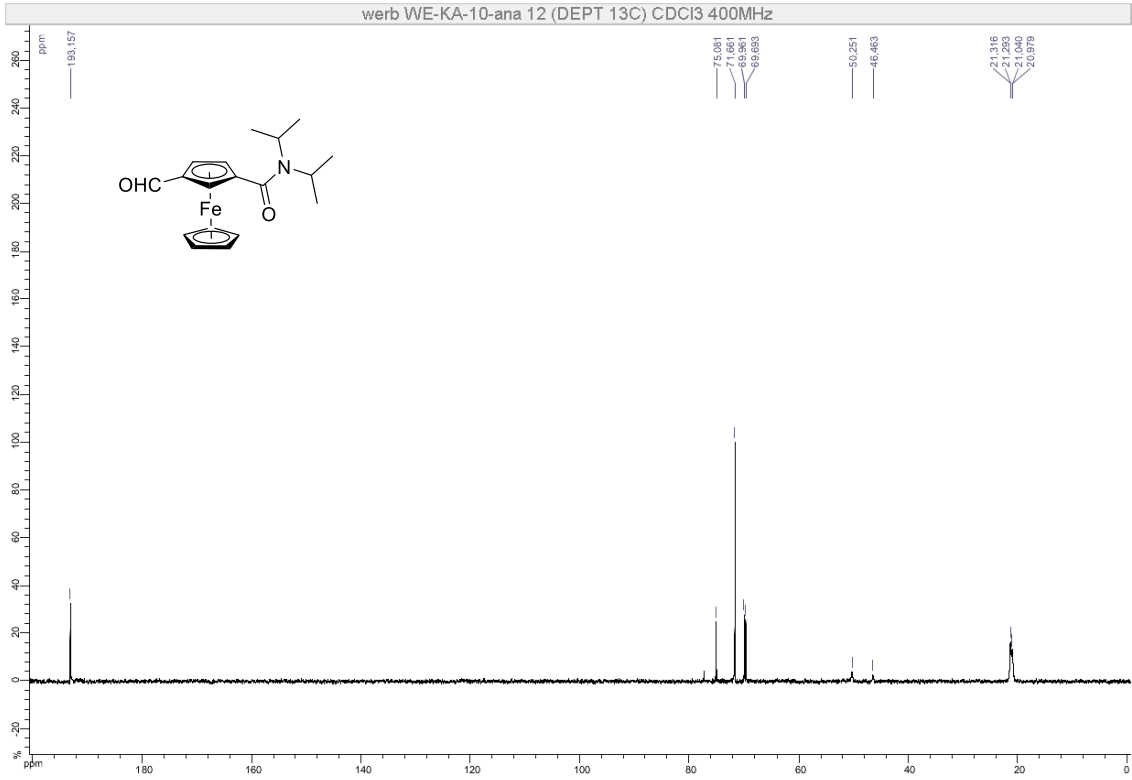
**N,N-Diisopropyl-3-(4-trifluoromethylphenyl)ferrocenecarboxamide (17)**

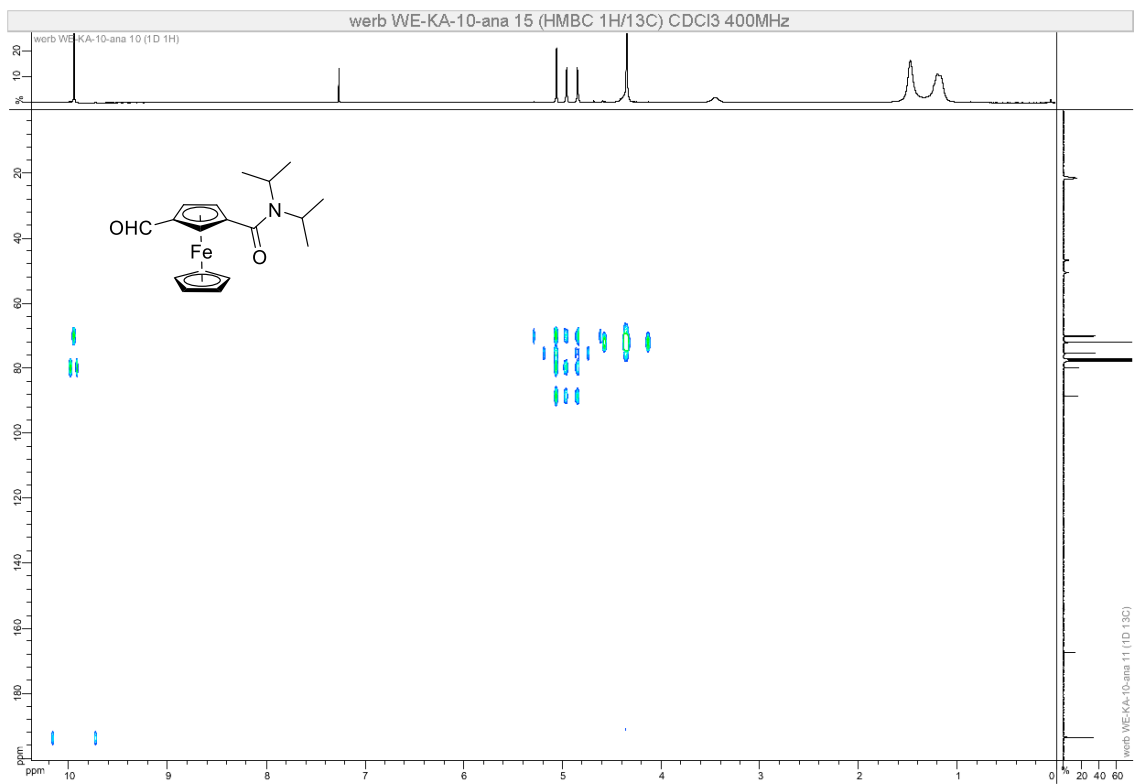
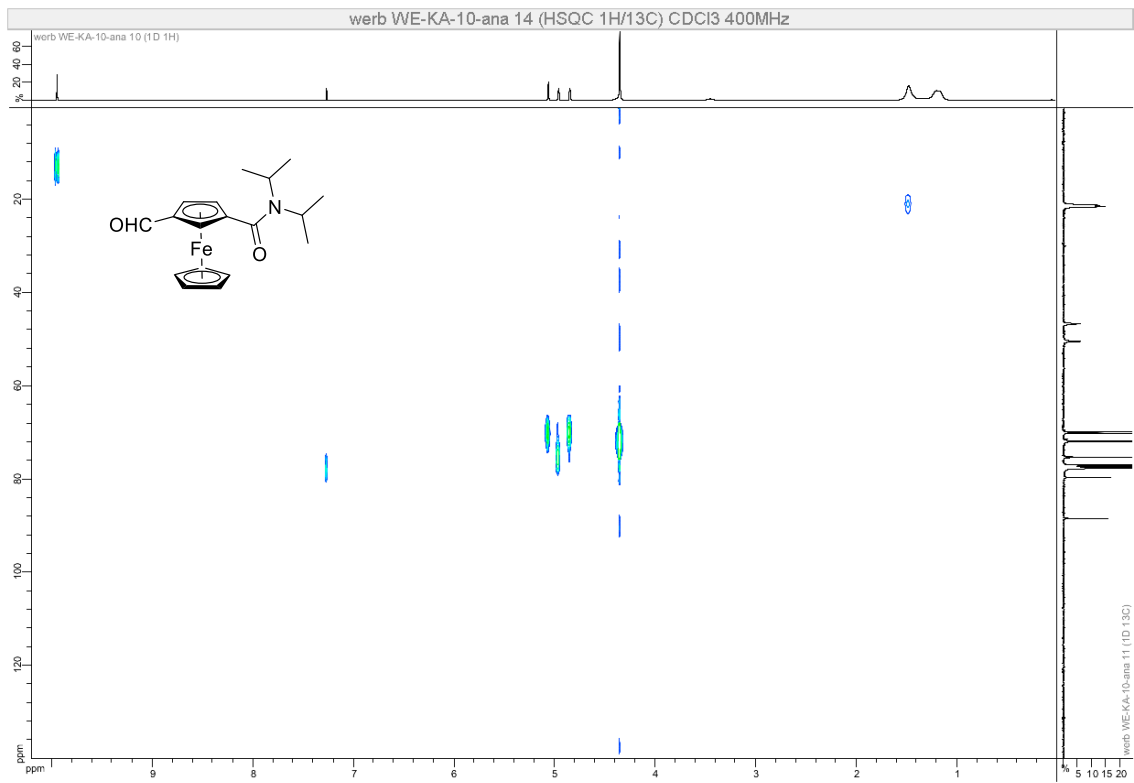




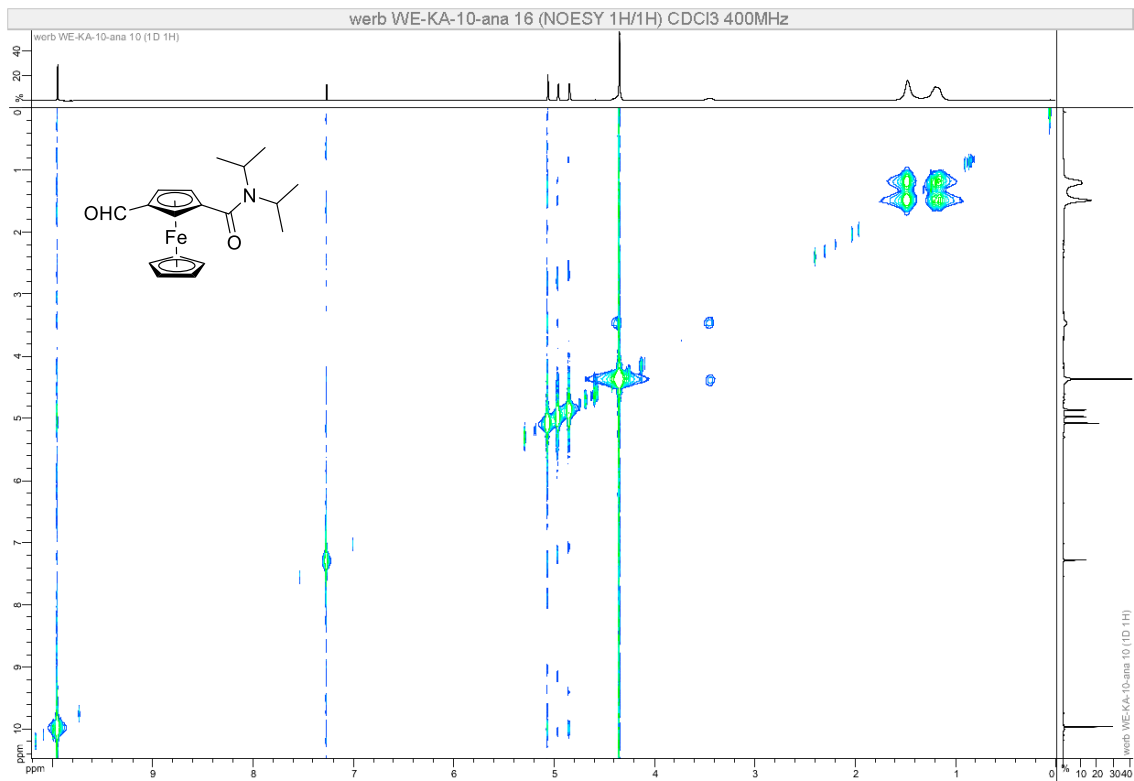
### 3-Formyl-N,N-diisopropylferrocenecarboxamide (18)



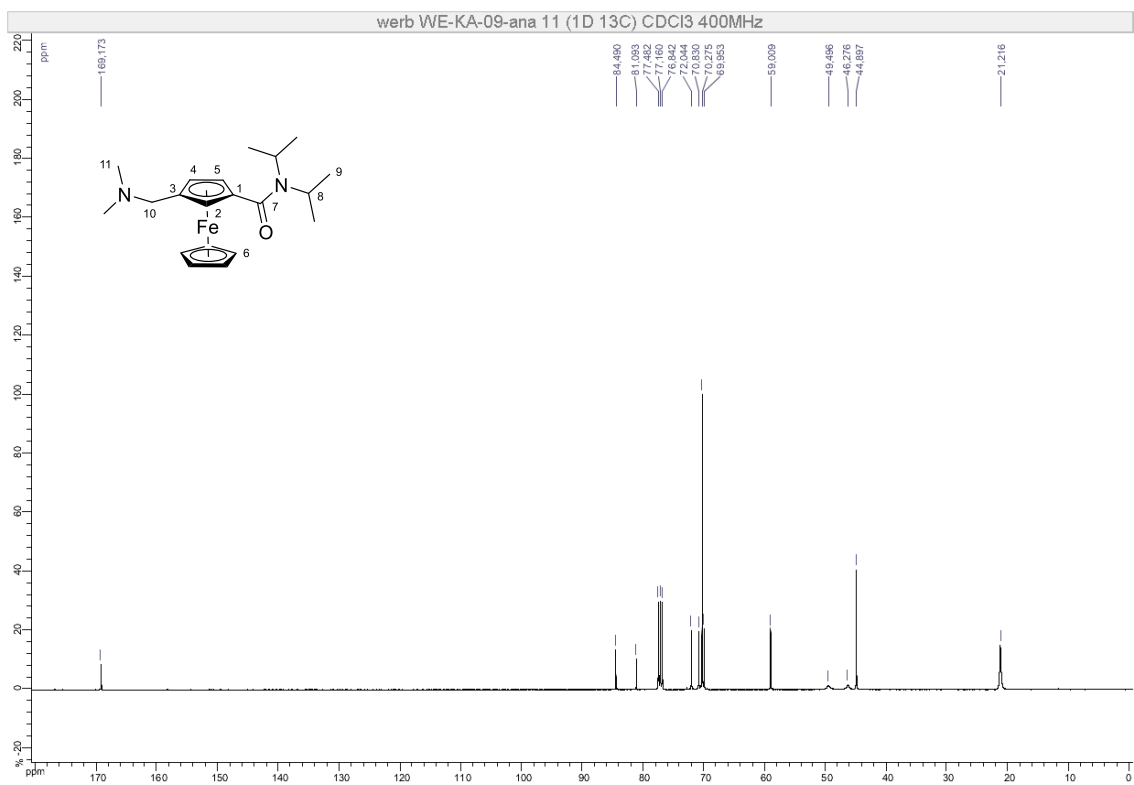
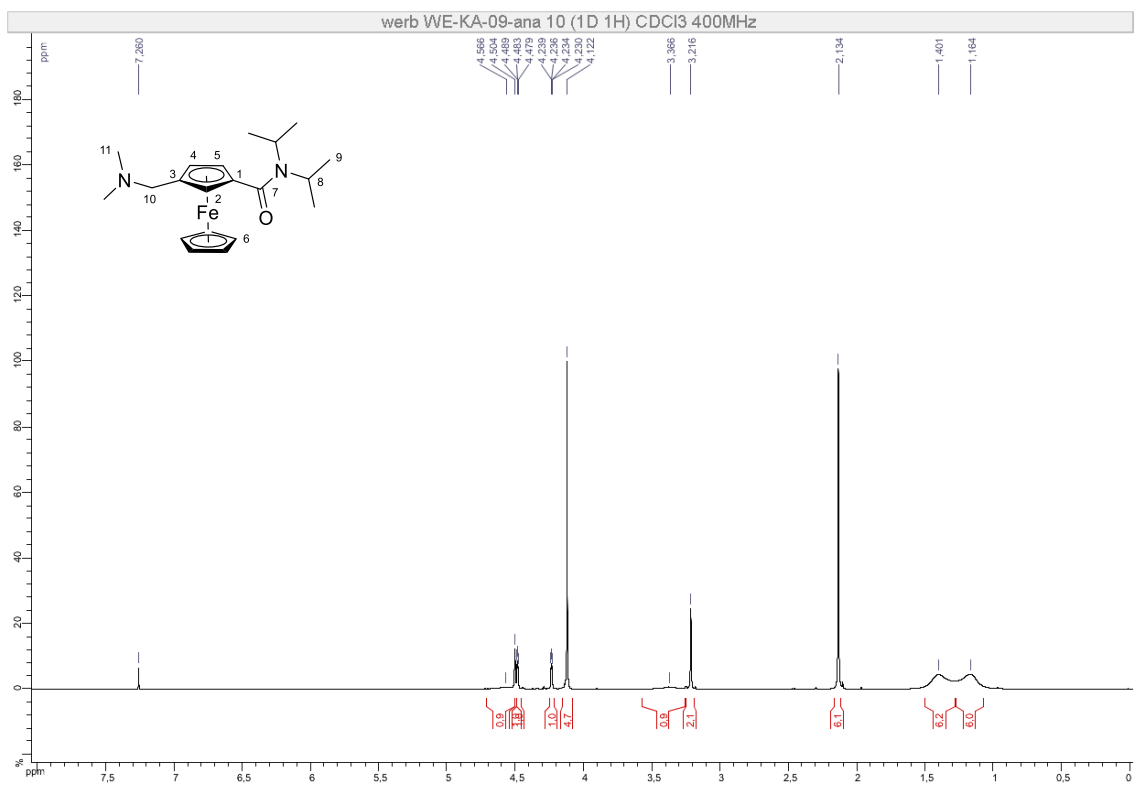


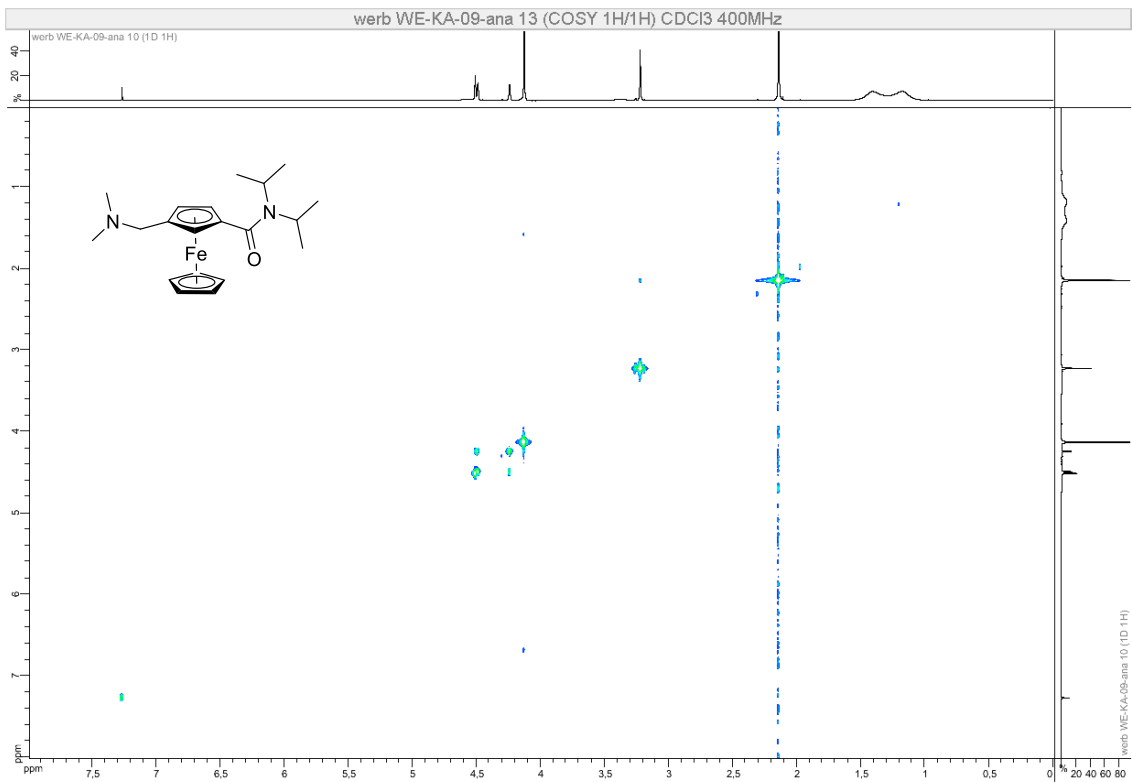
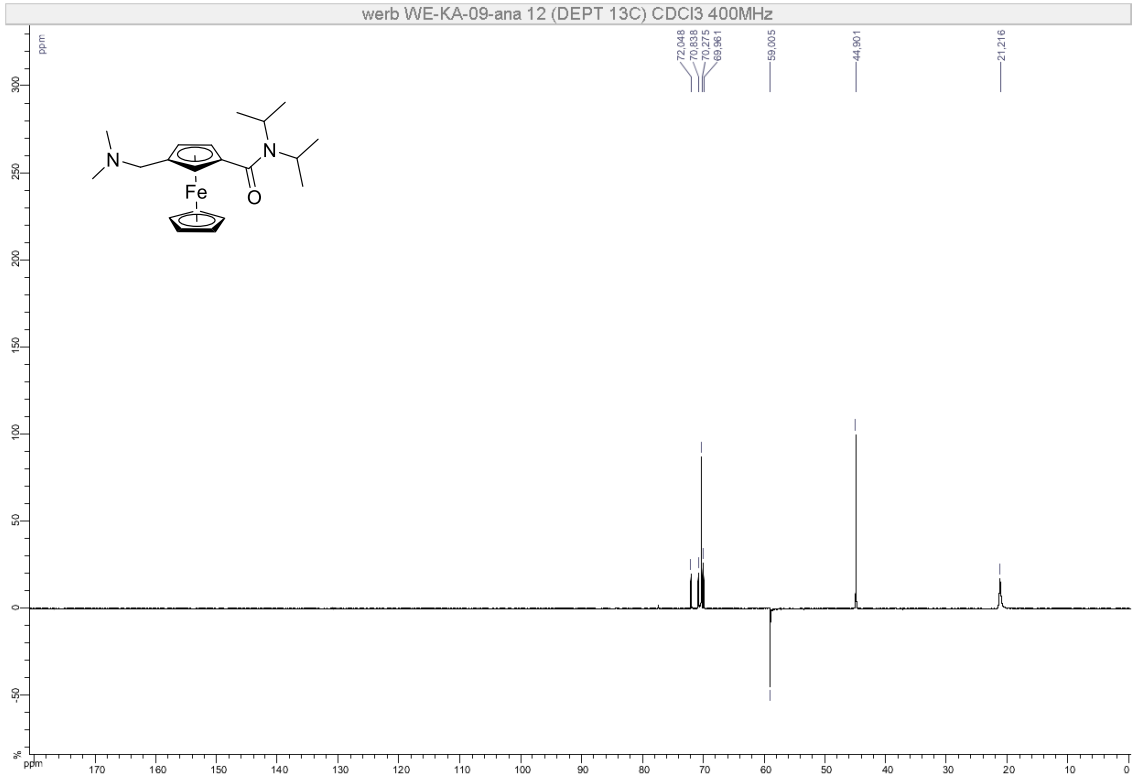


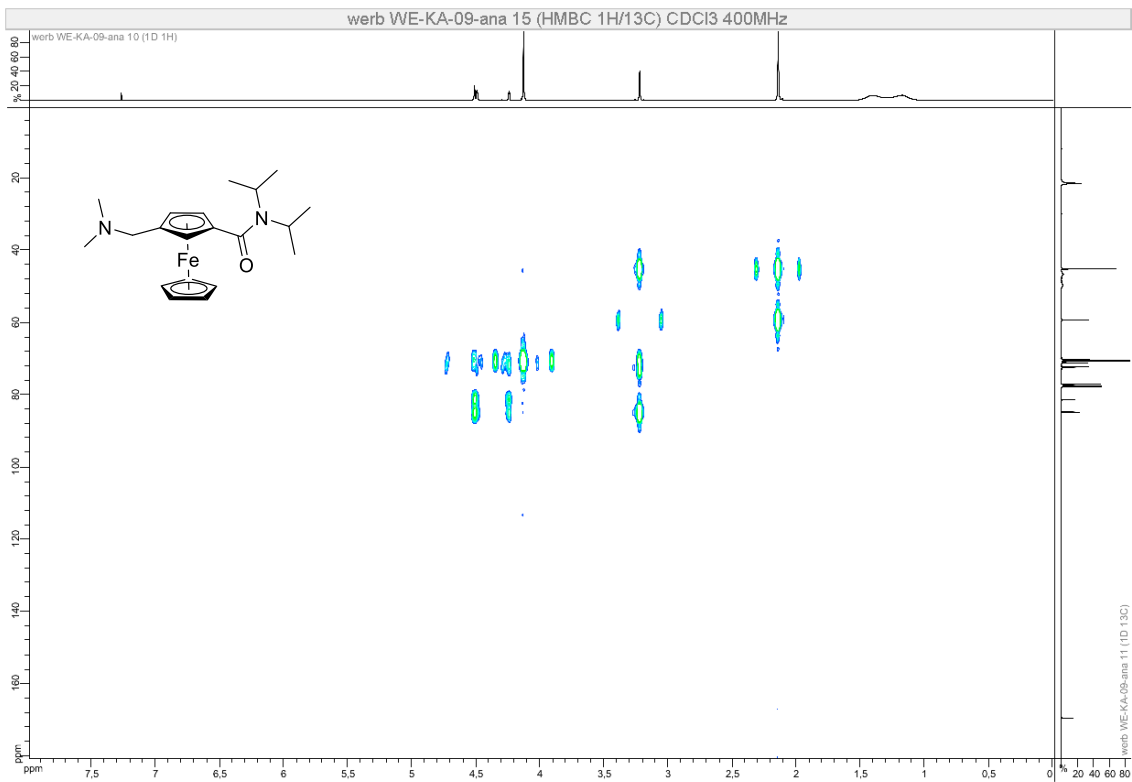
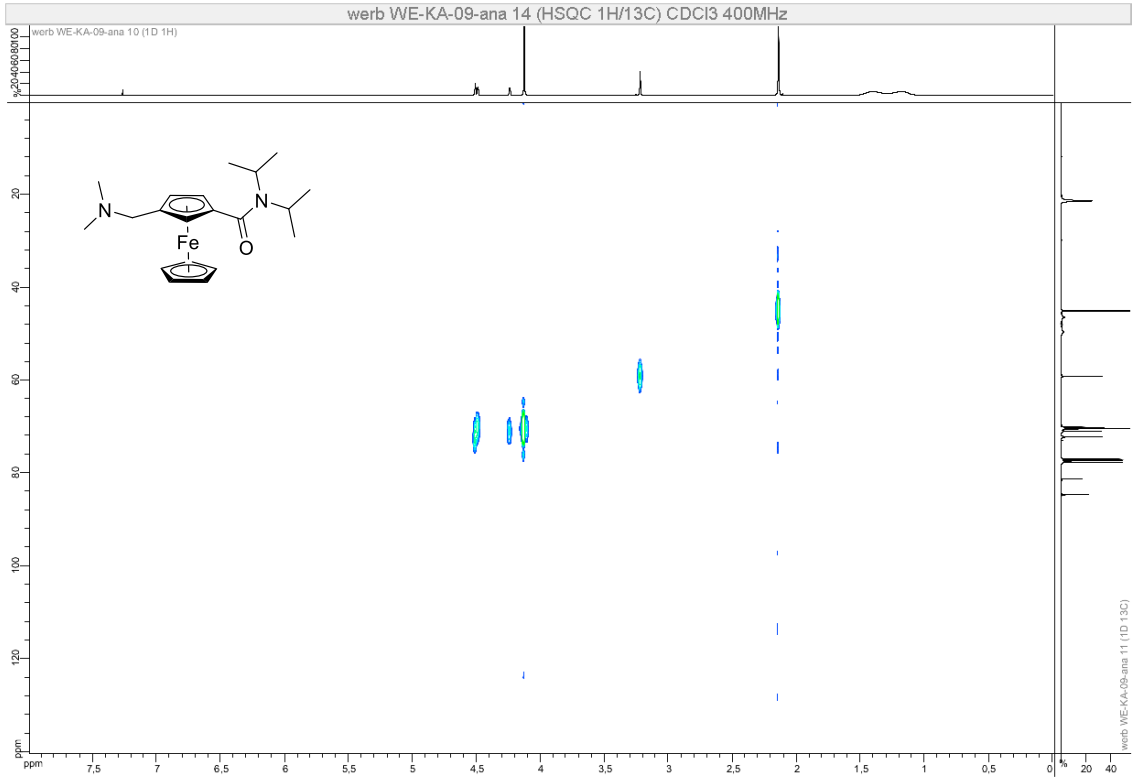


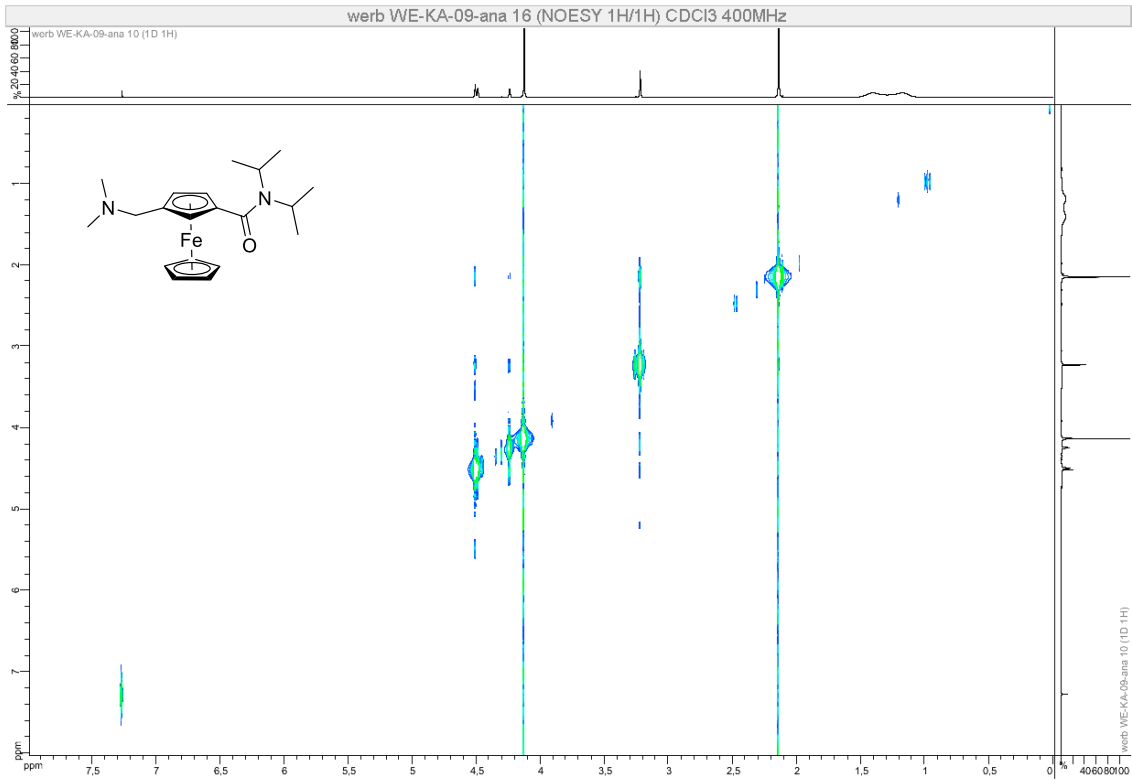


**3-(*N,N*-Dimethylaminomethyl)-*N,N*-diisopropylferrocenecarboxamide (19)**

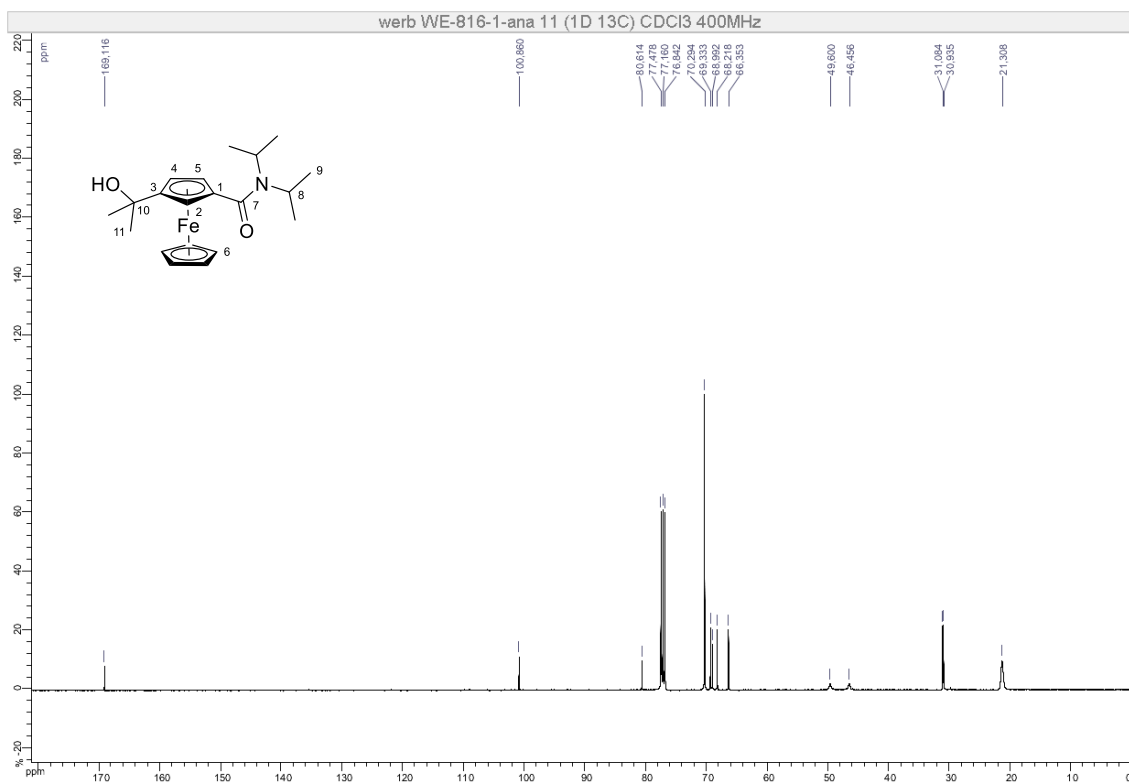
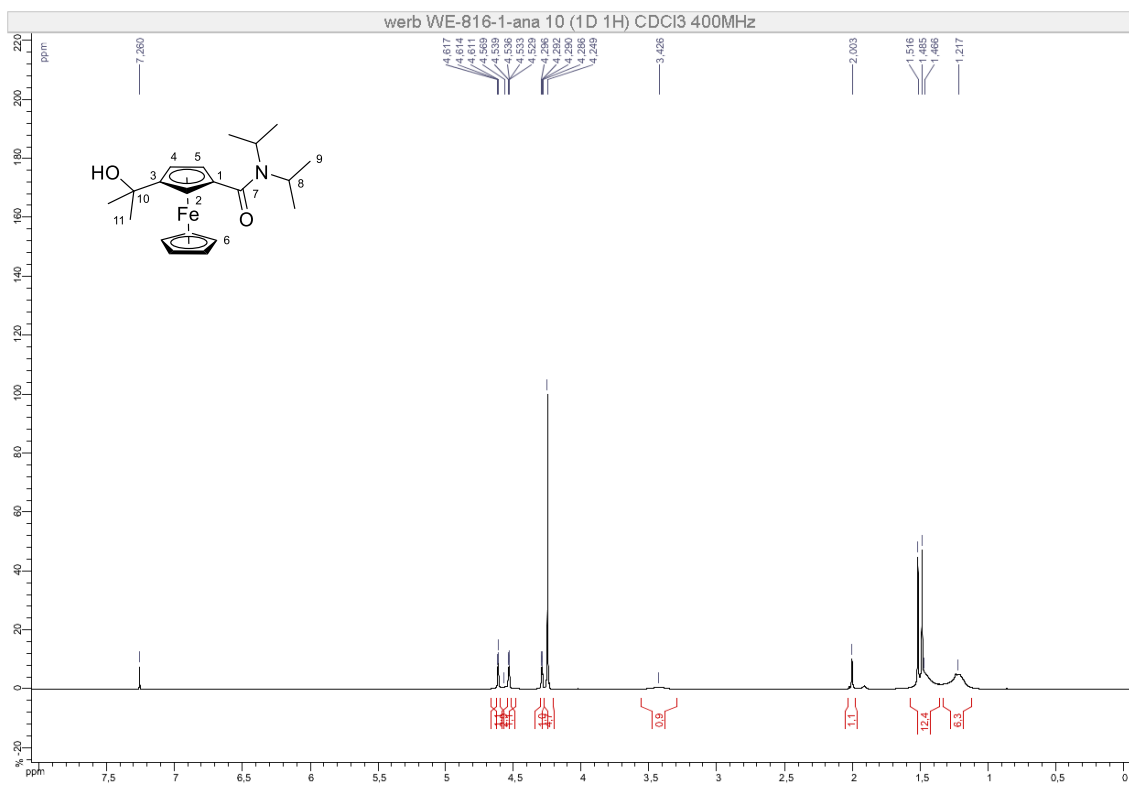


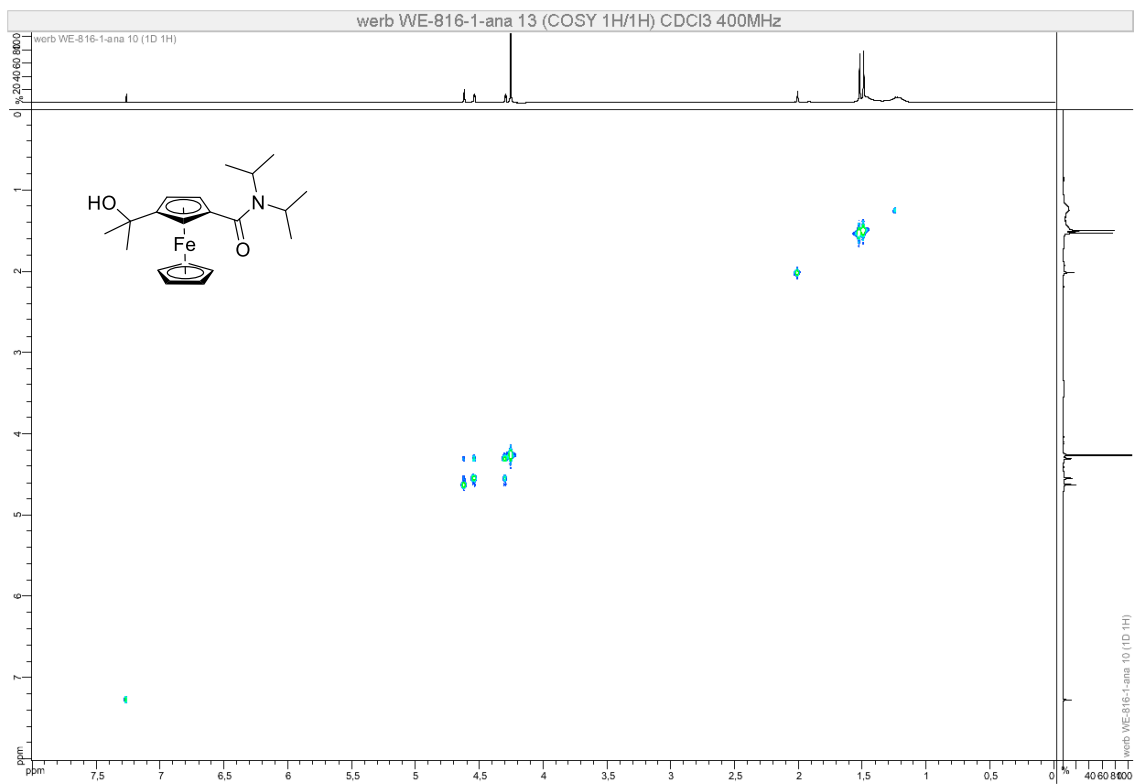
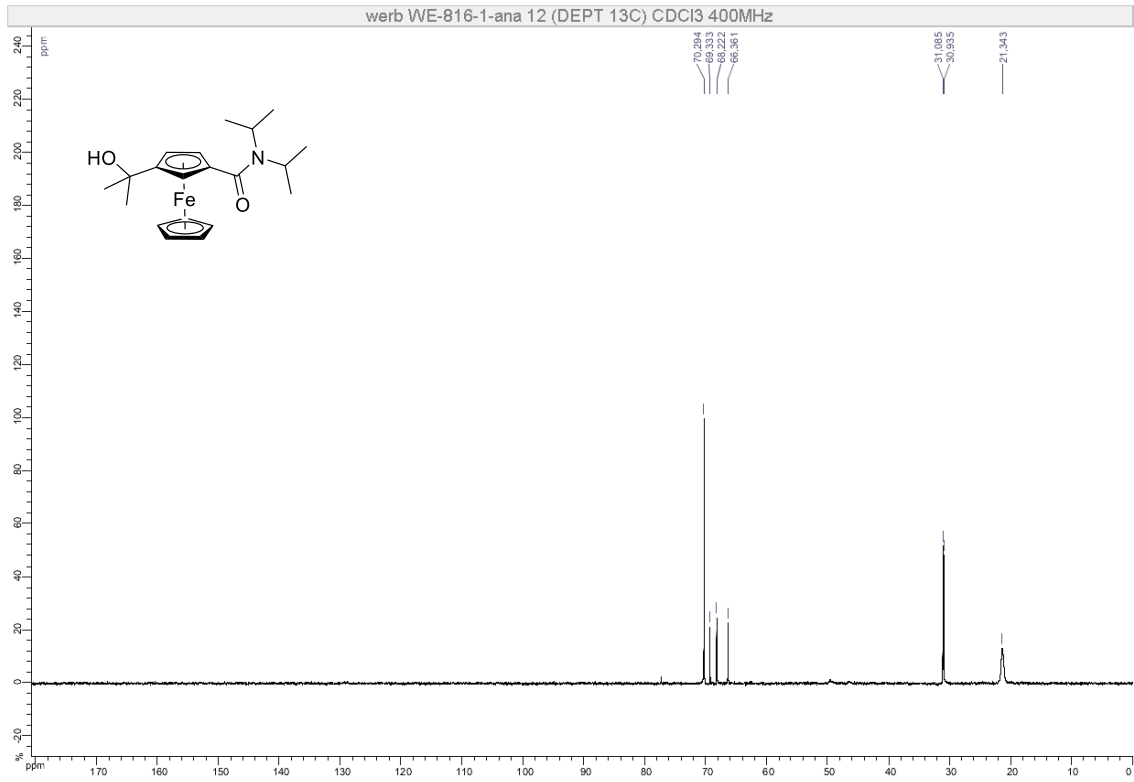


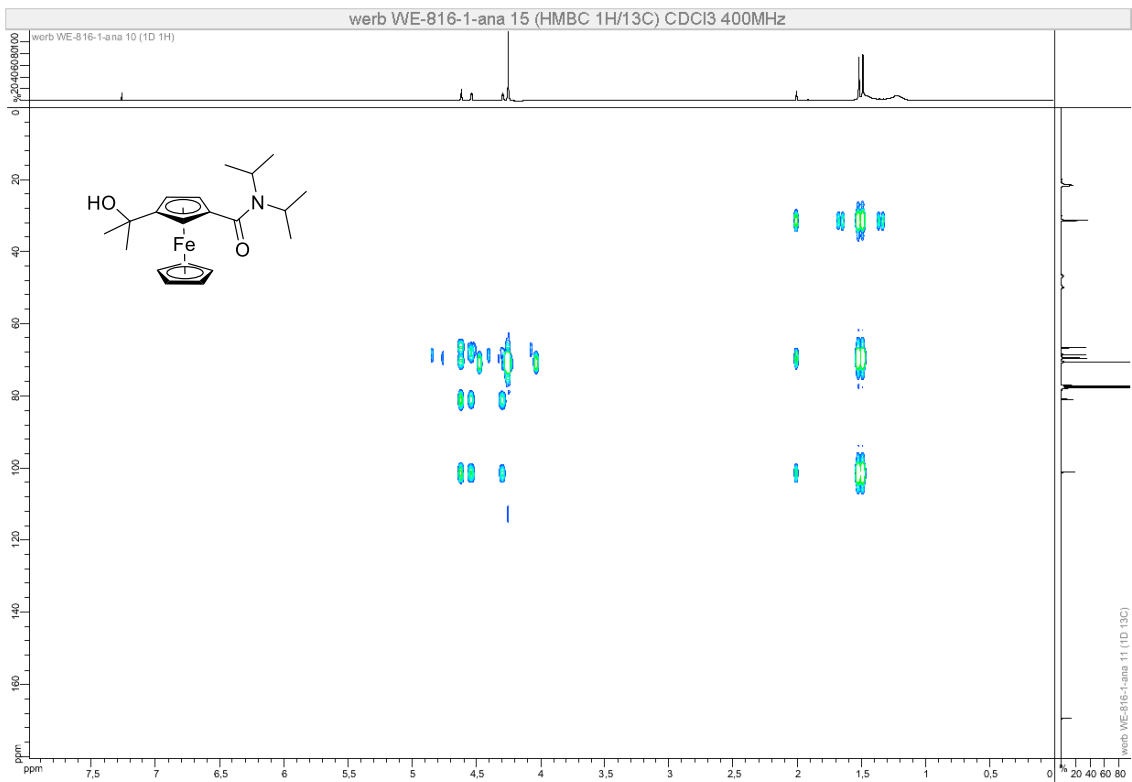
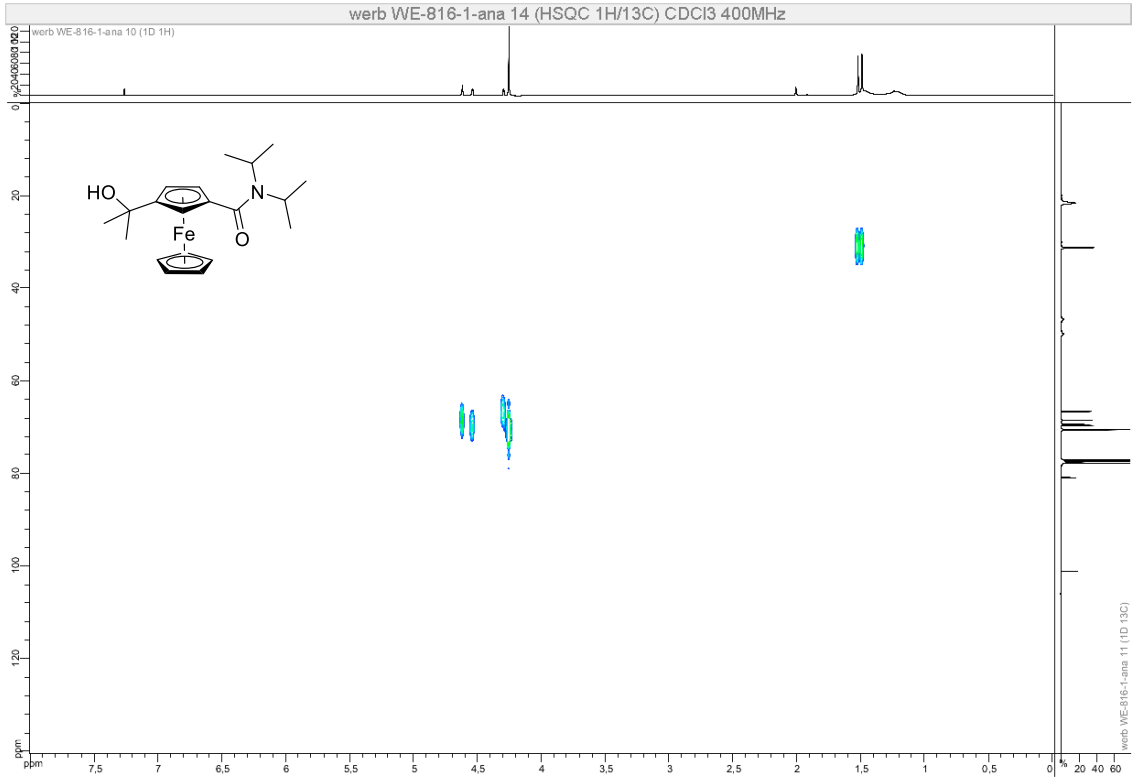




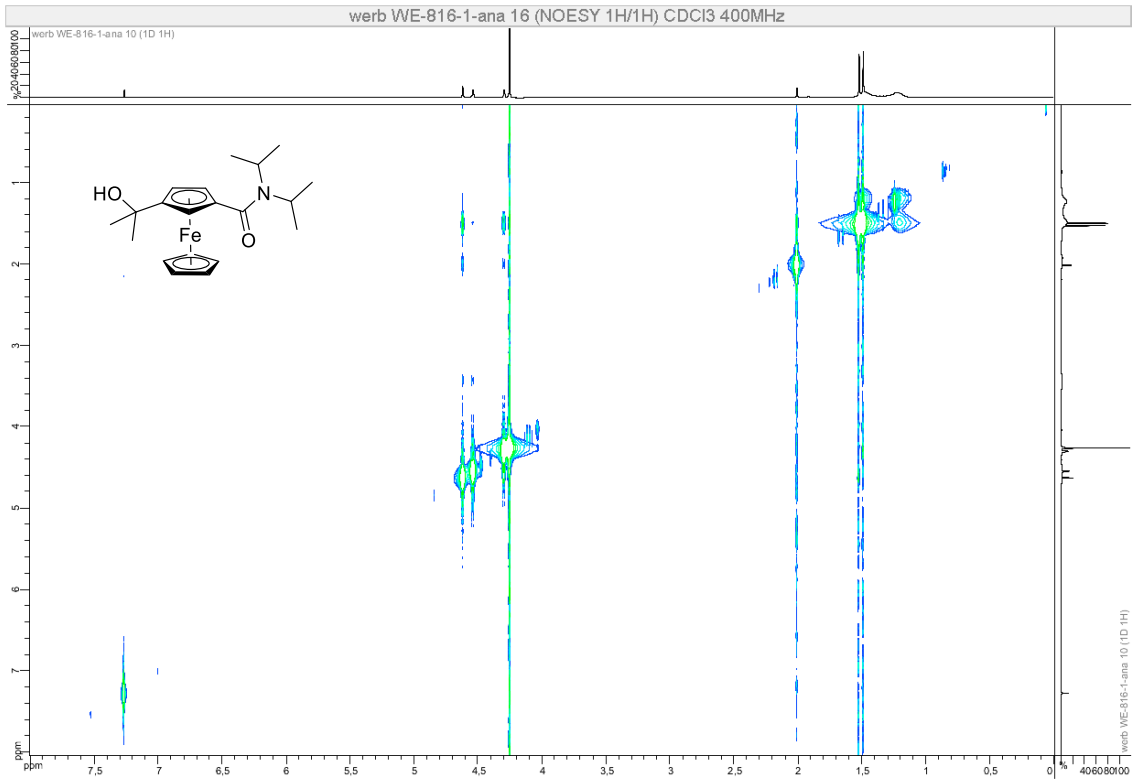
**3-(Hydroxydimethylmethyl)-N,N-diisopropylferrocenecarboxamide (20)**



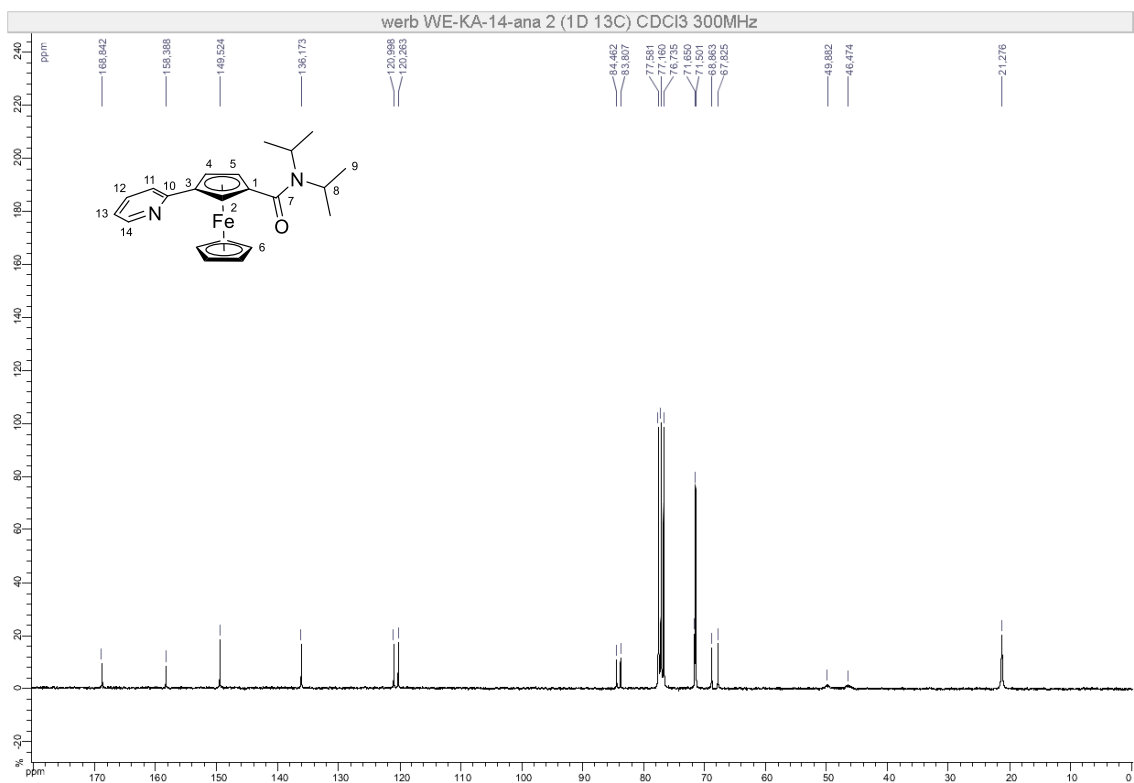
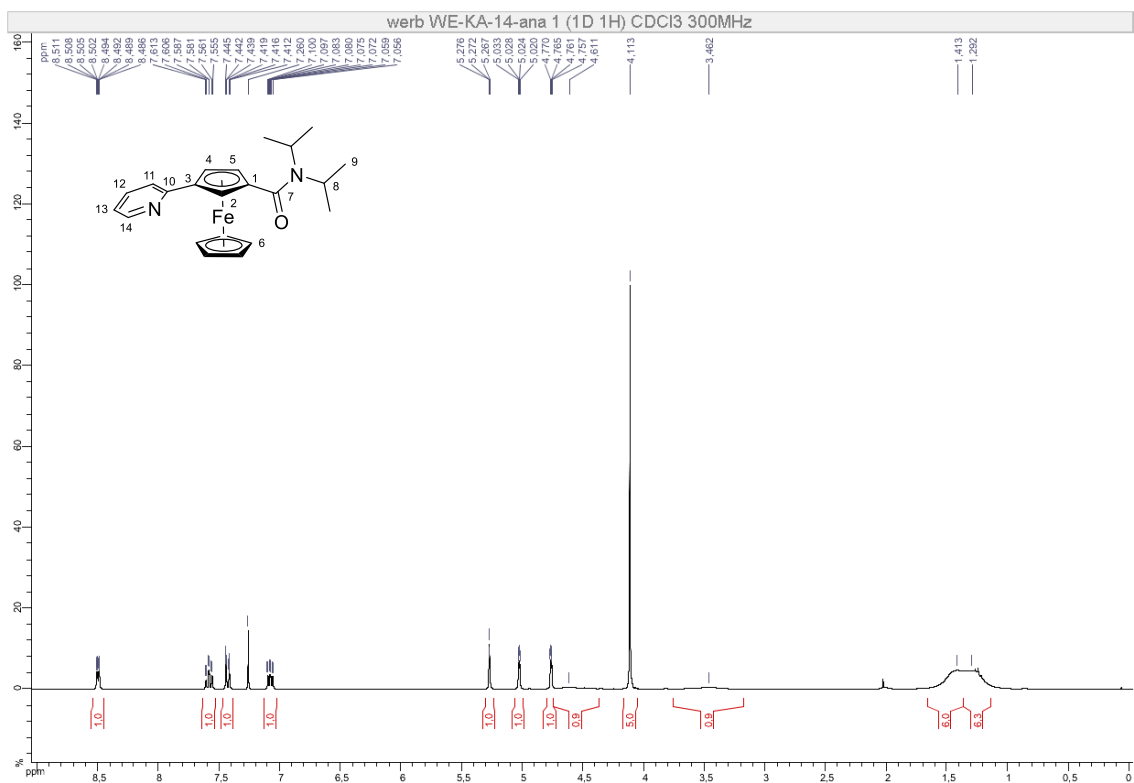


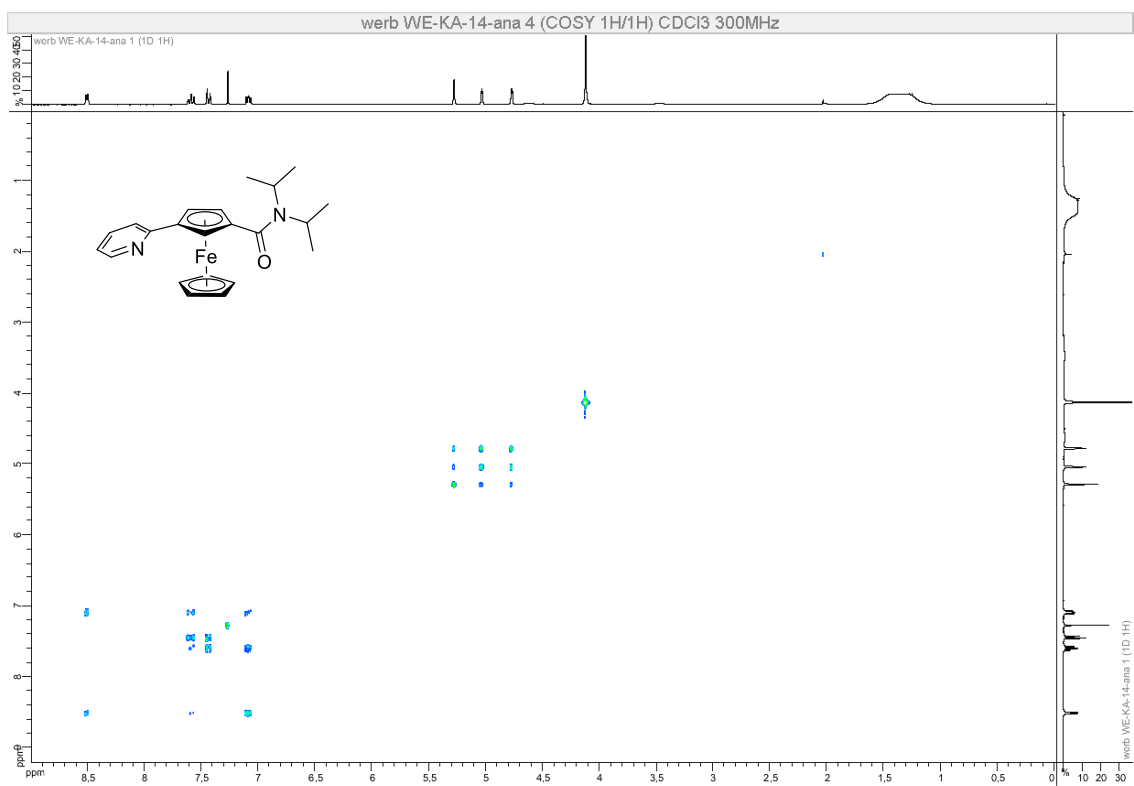
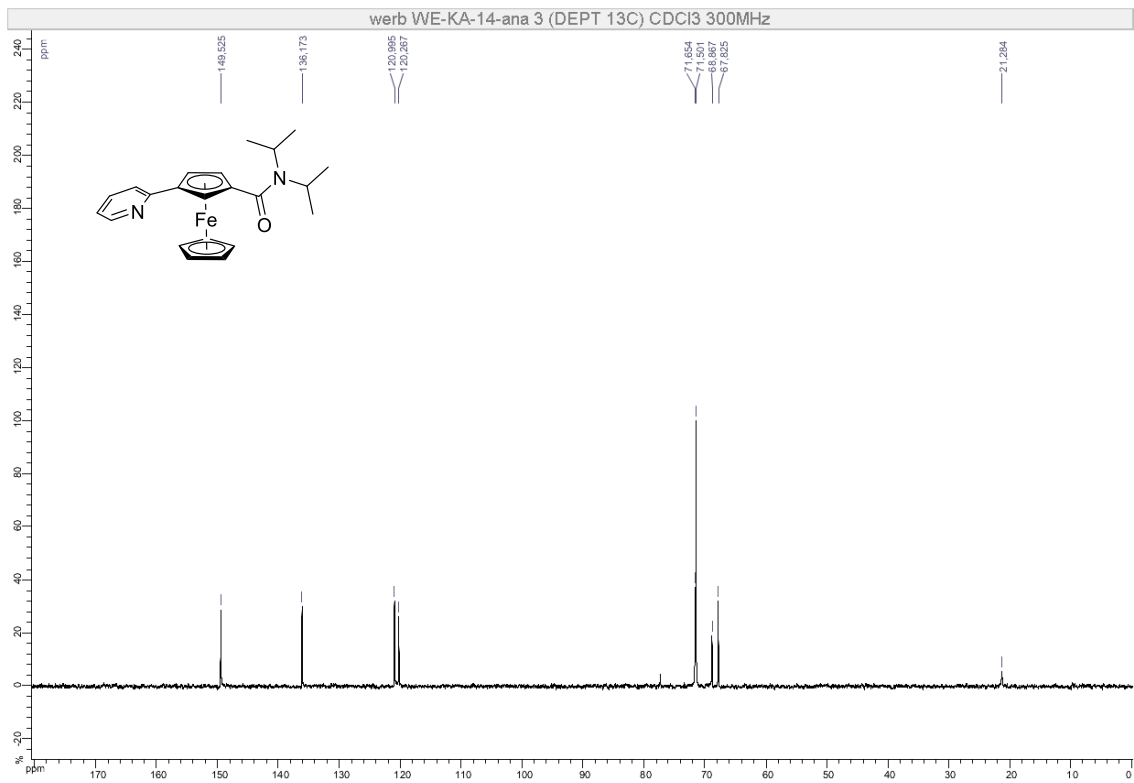


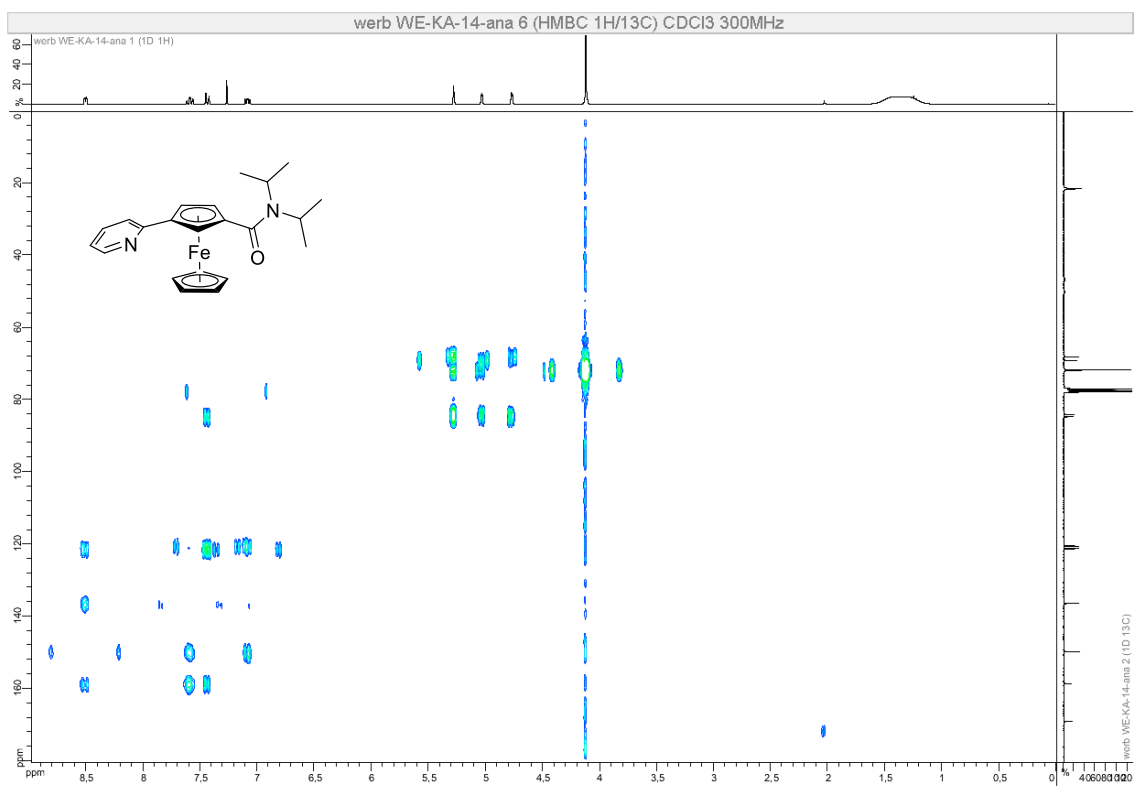
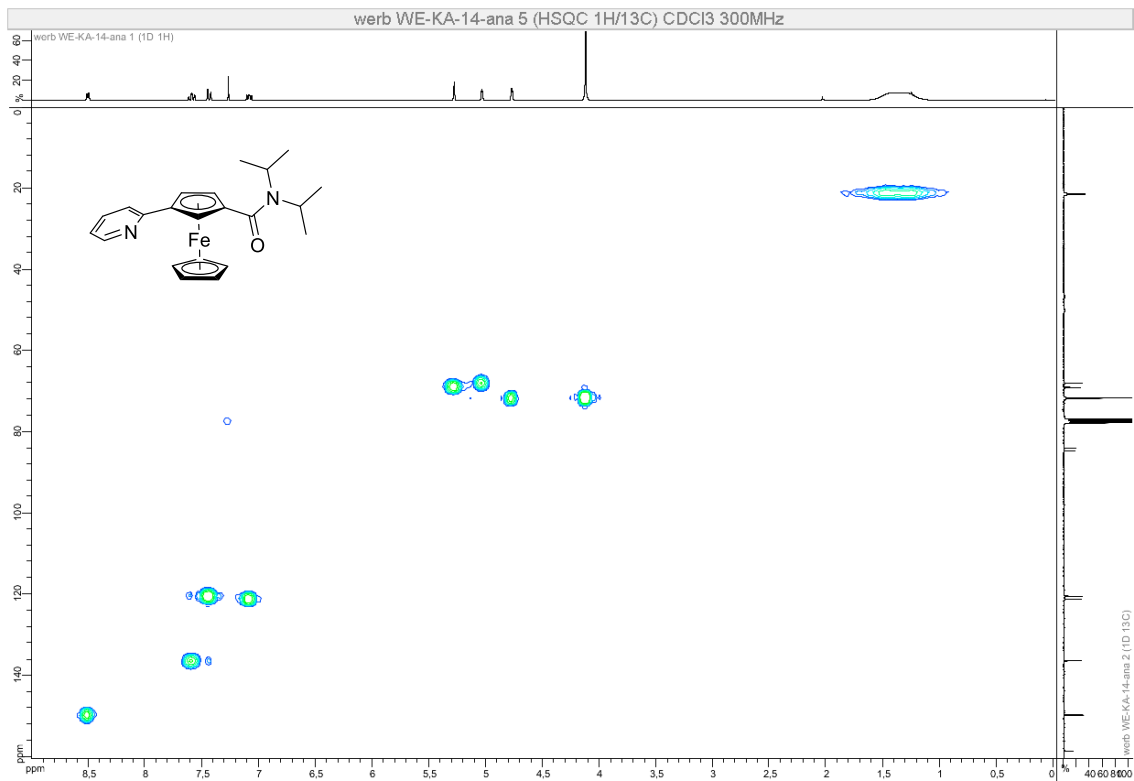


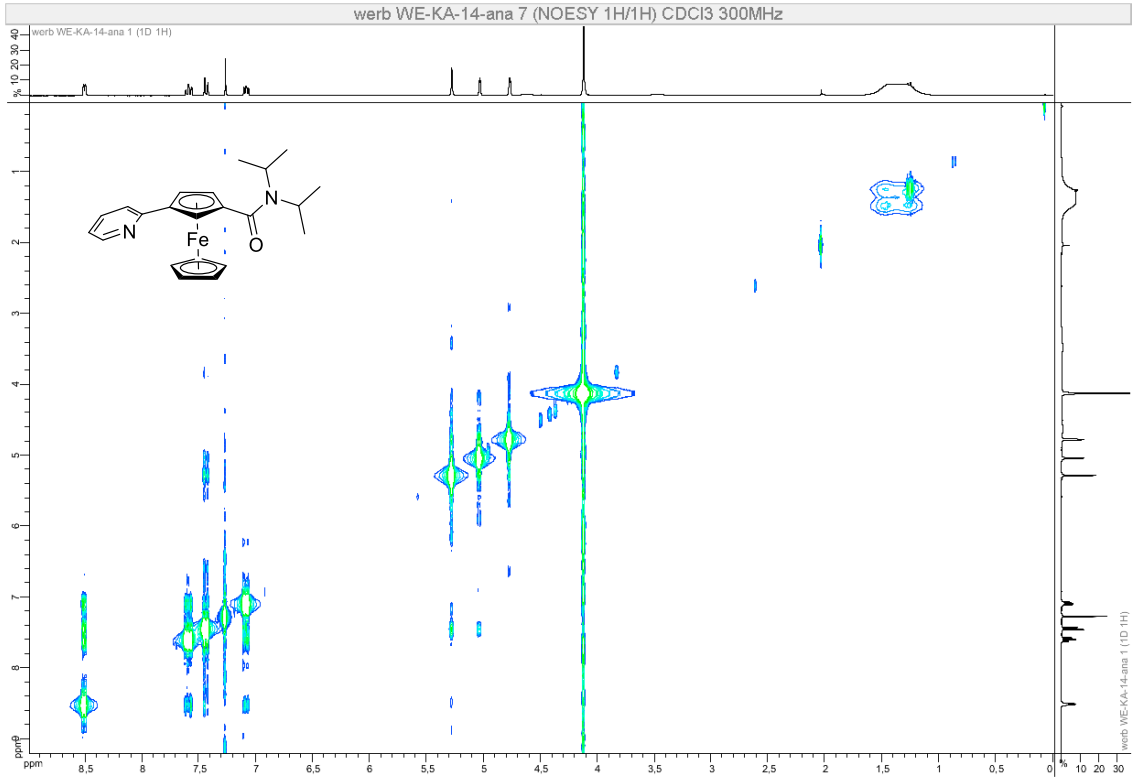


***N,N*-Diisopropyl-3-(2-pyridinyl)ferrocenecarboxamide (21)**

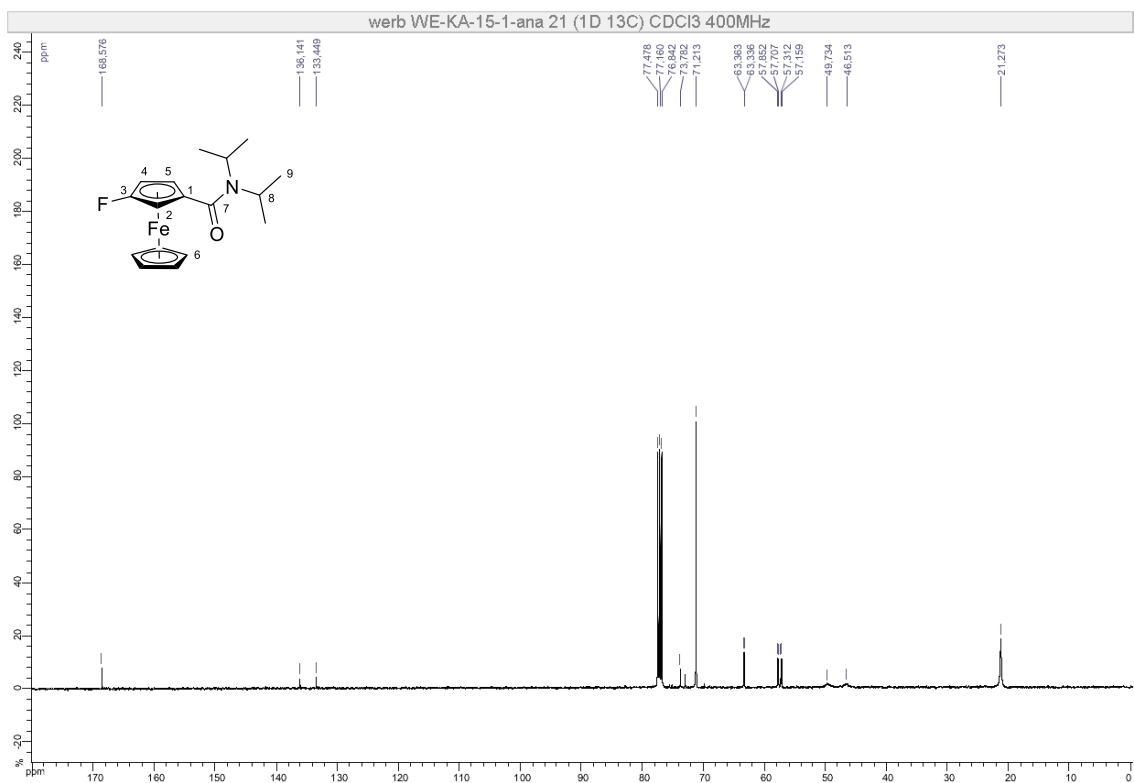
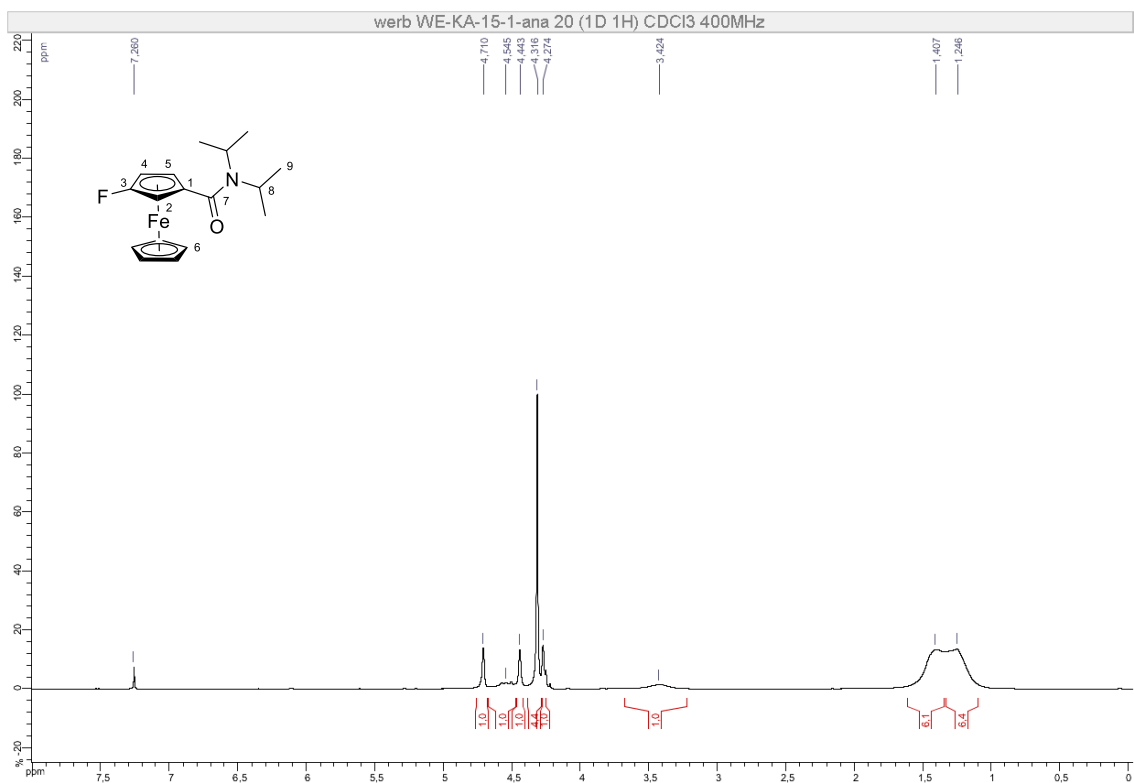


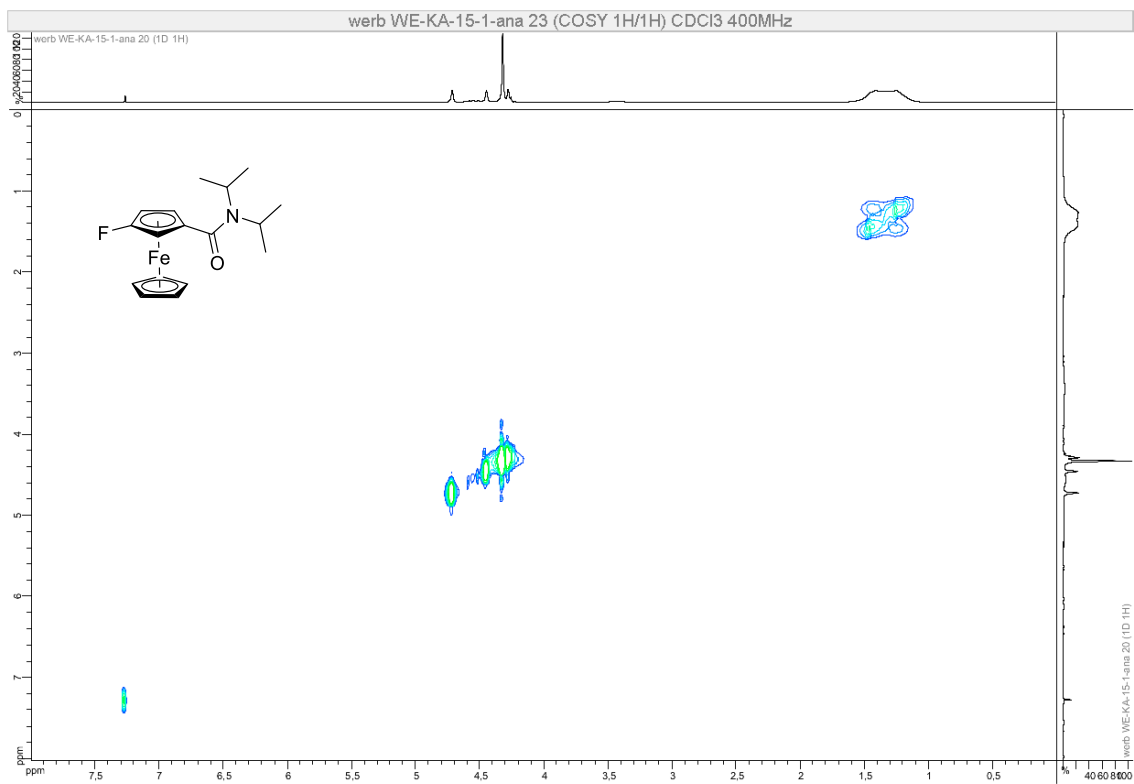
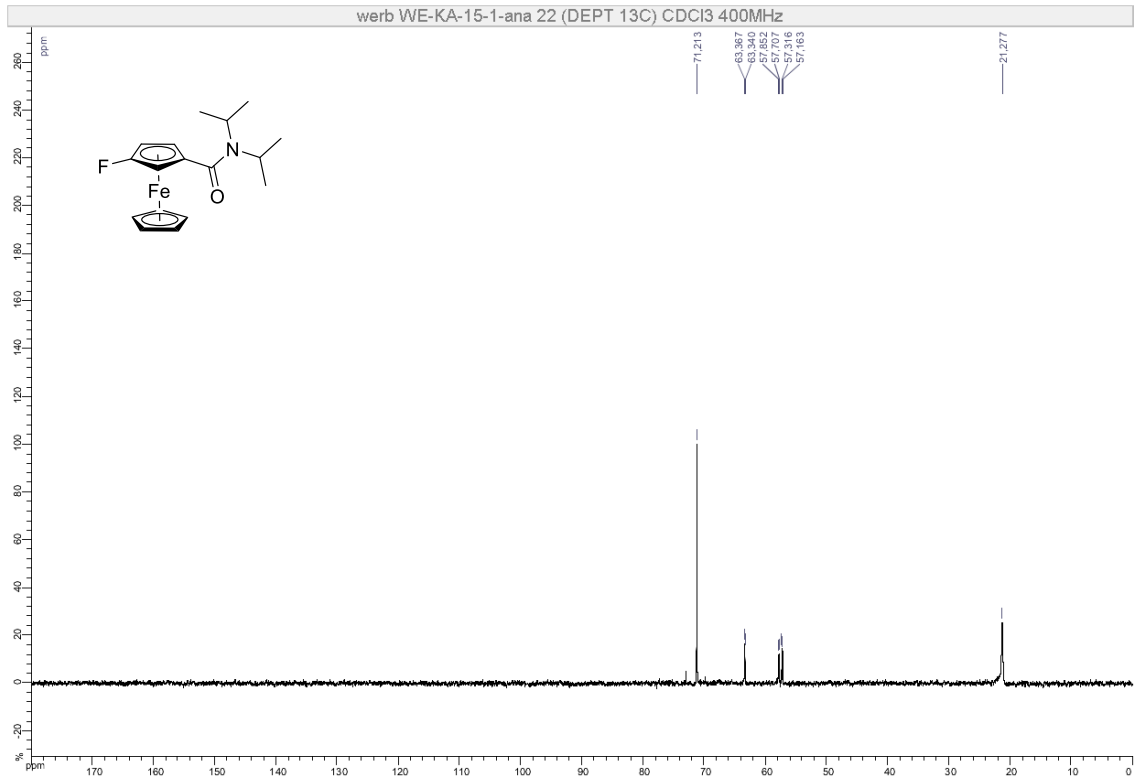


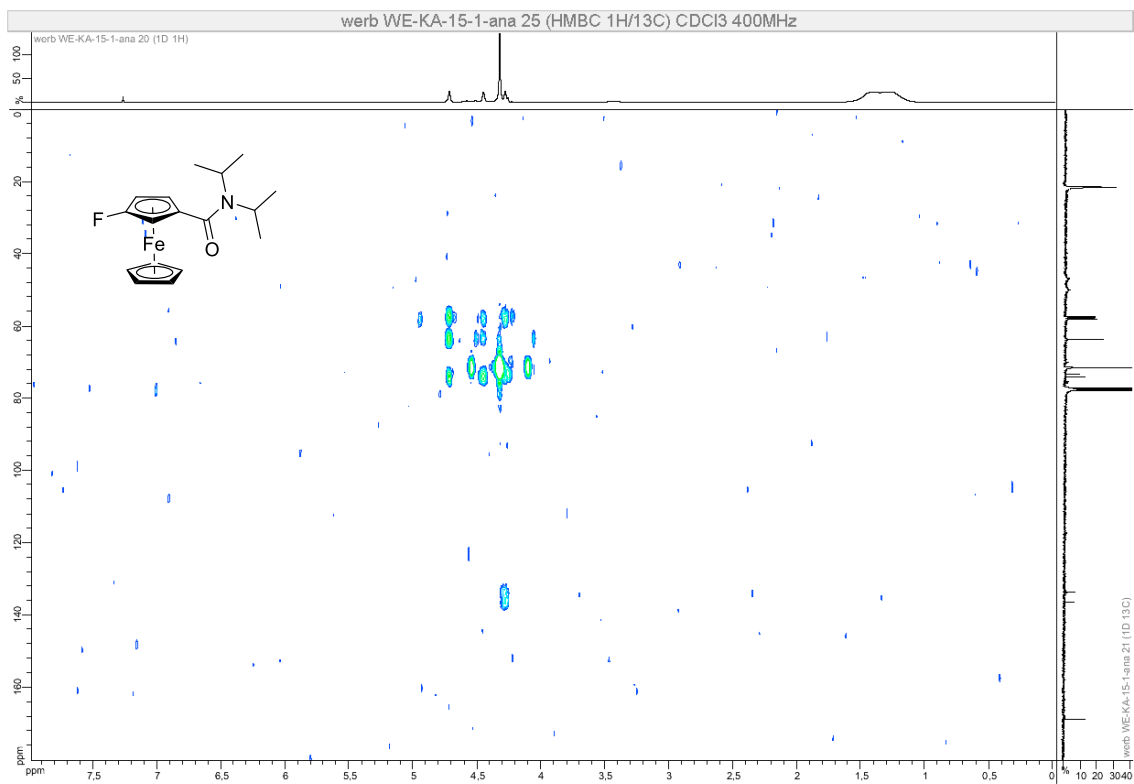
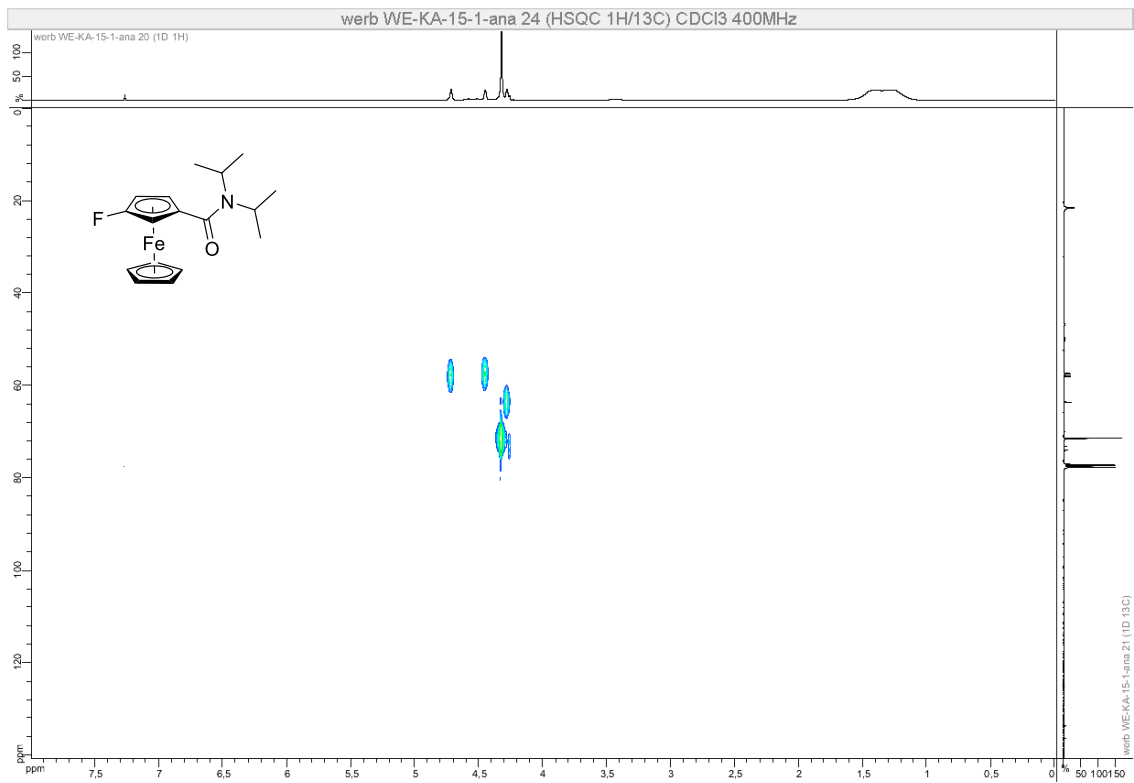




### 3-Fluoro-N,N-diisopropylferrocenecarboxamide (22)

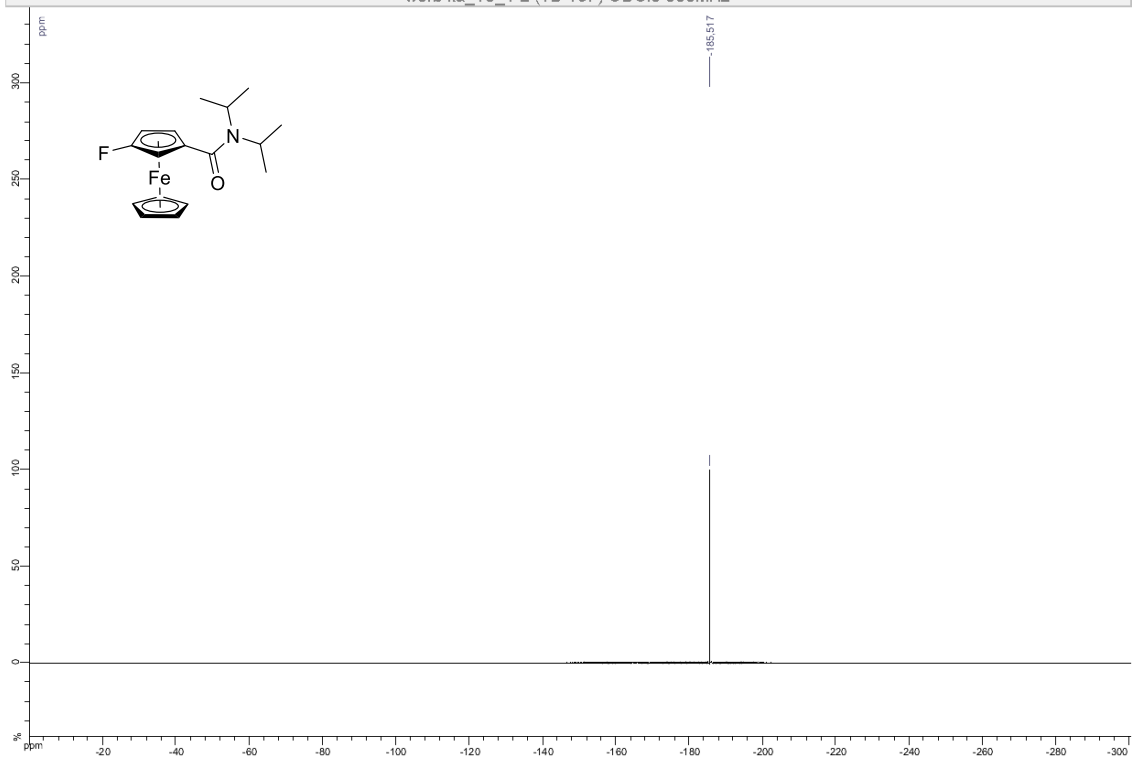




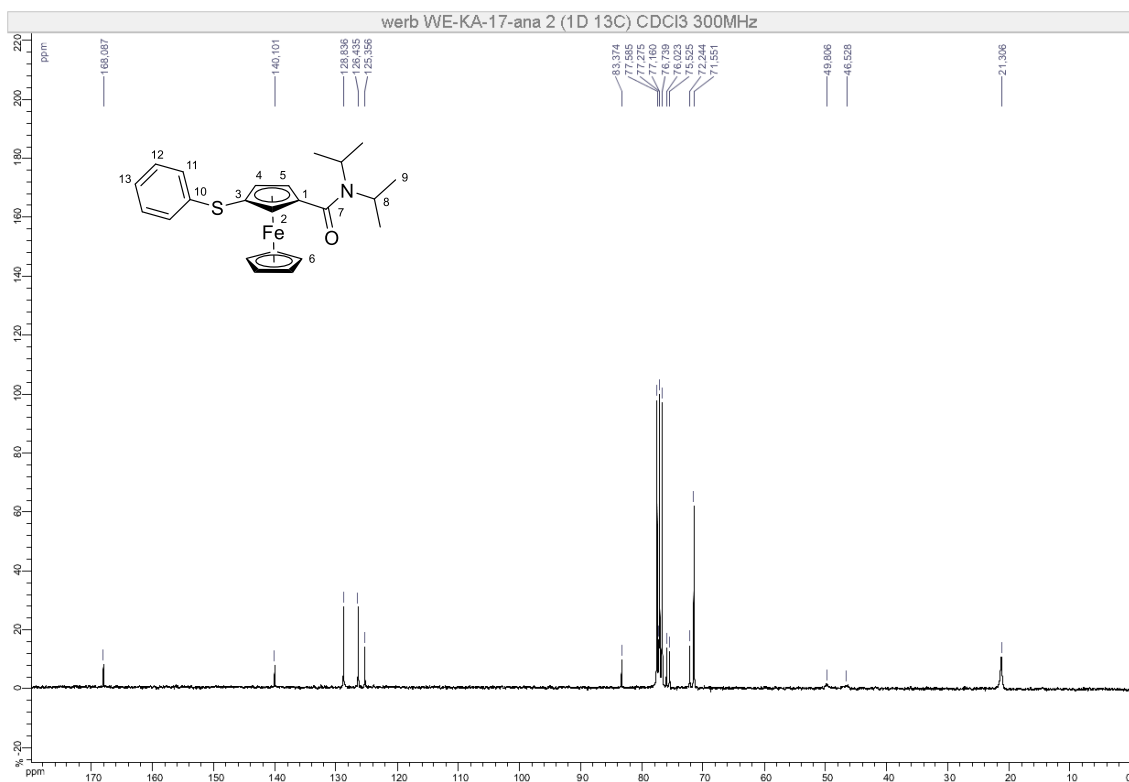
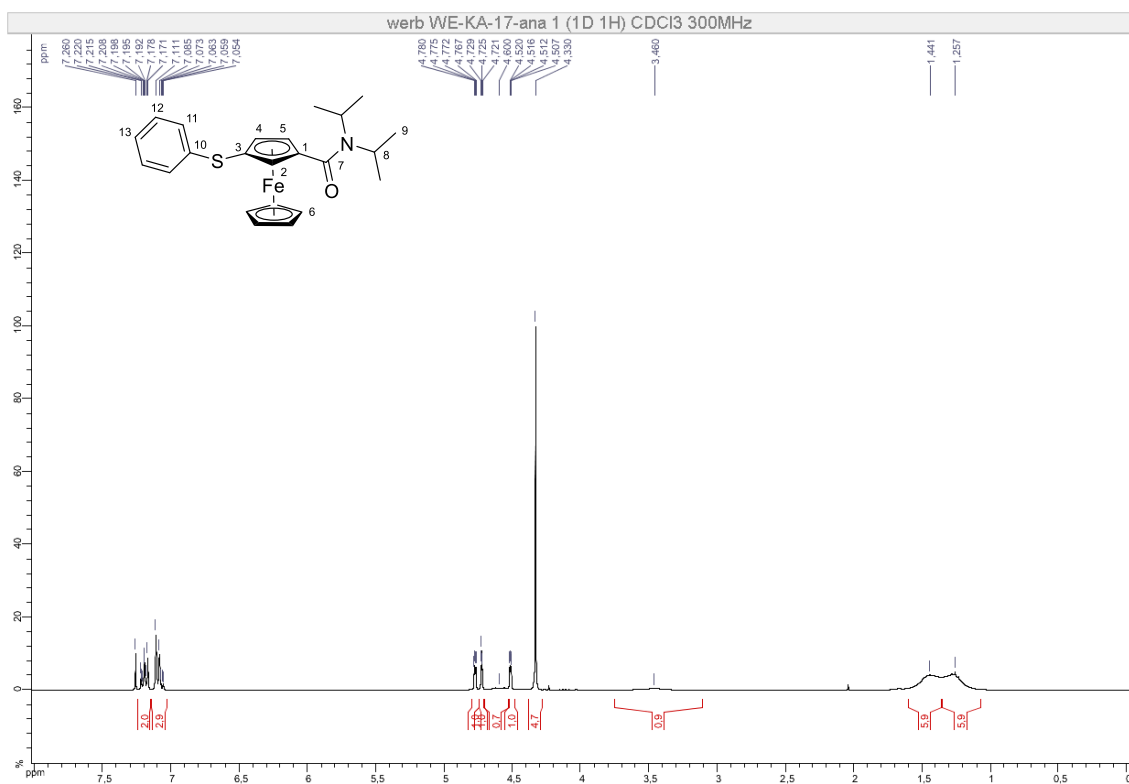


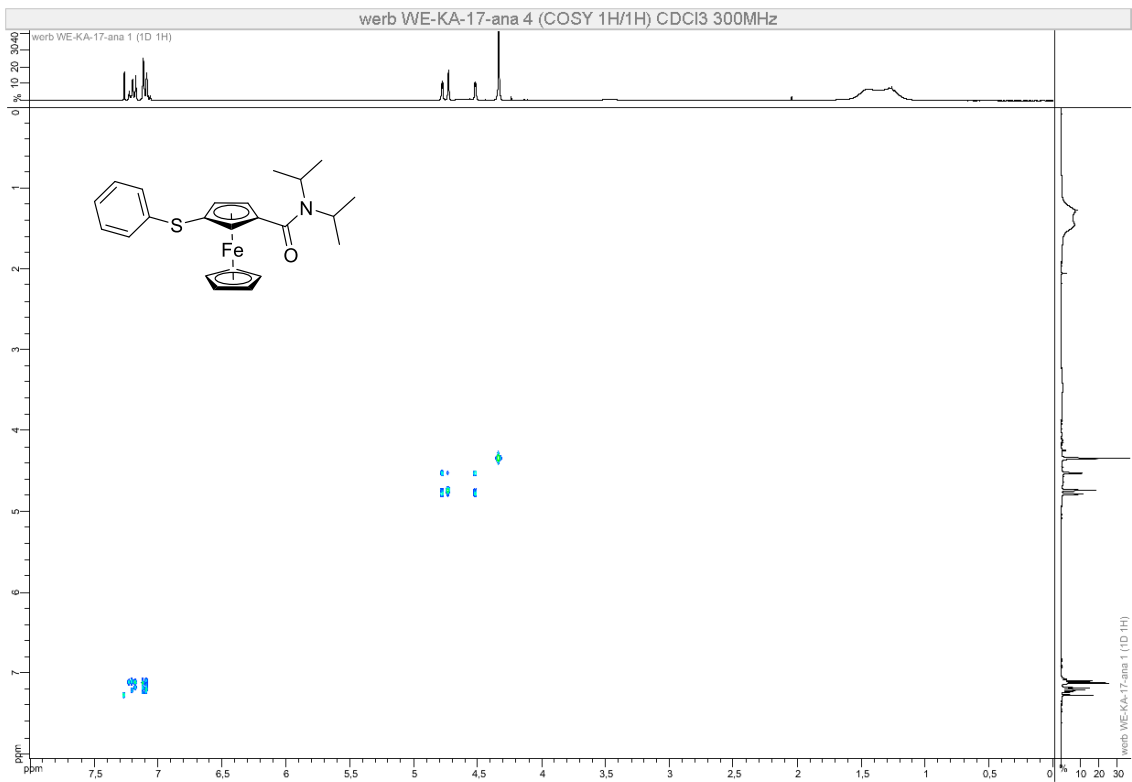
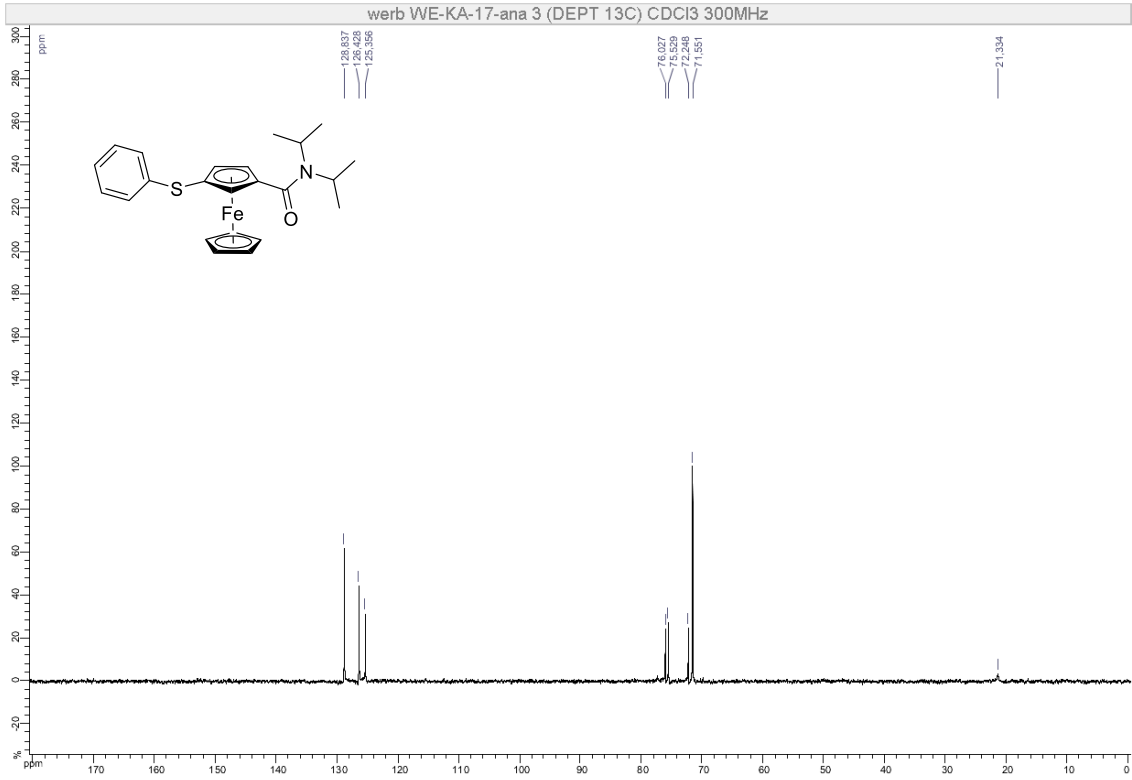


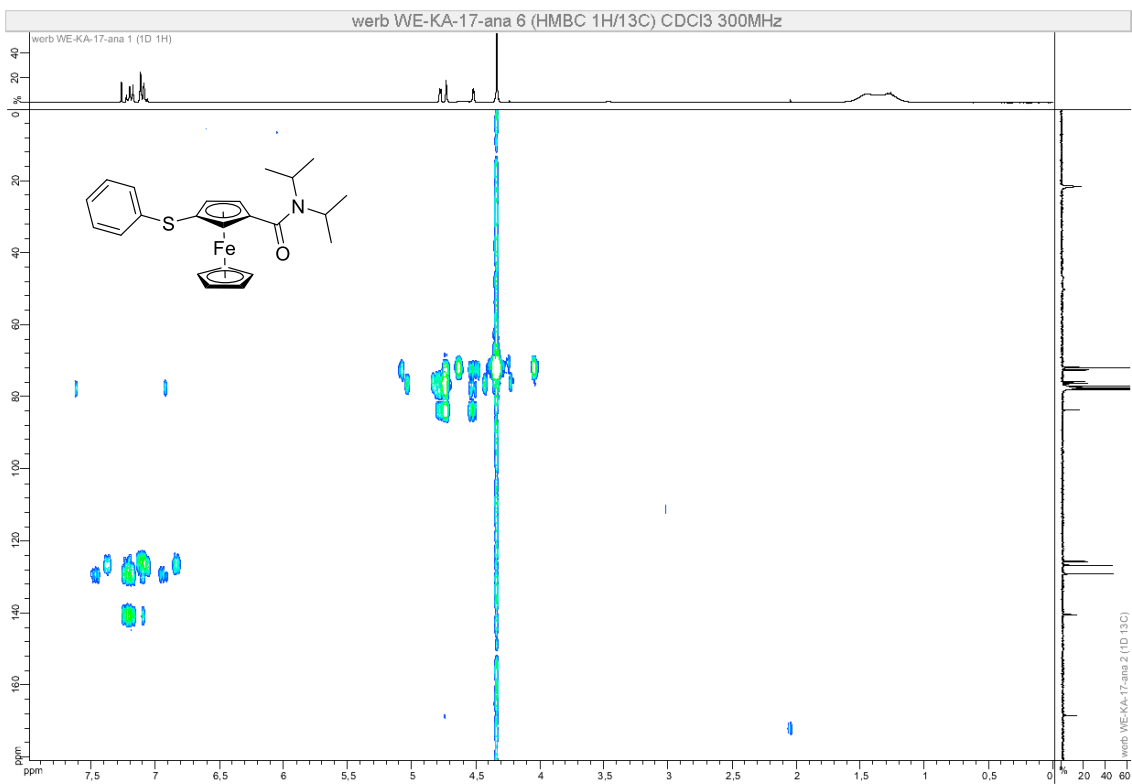
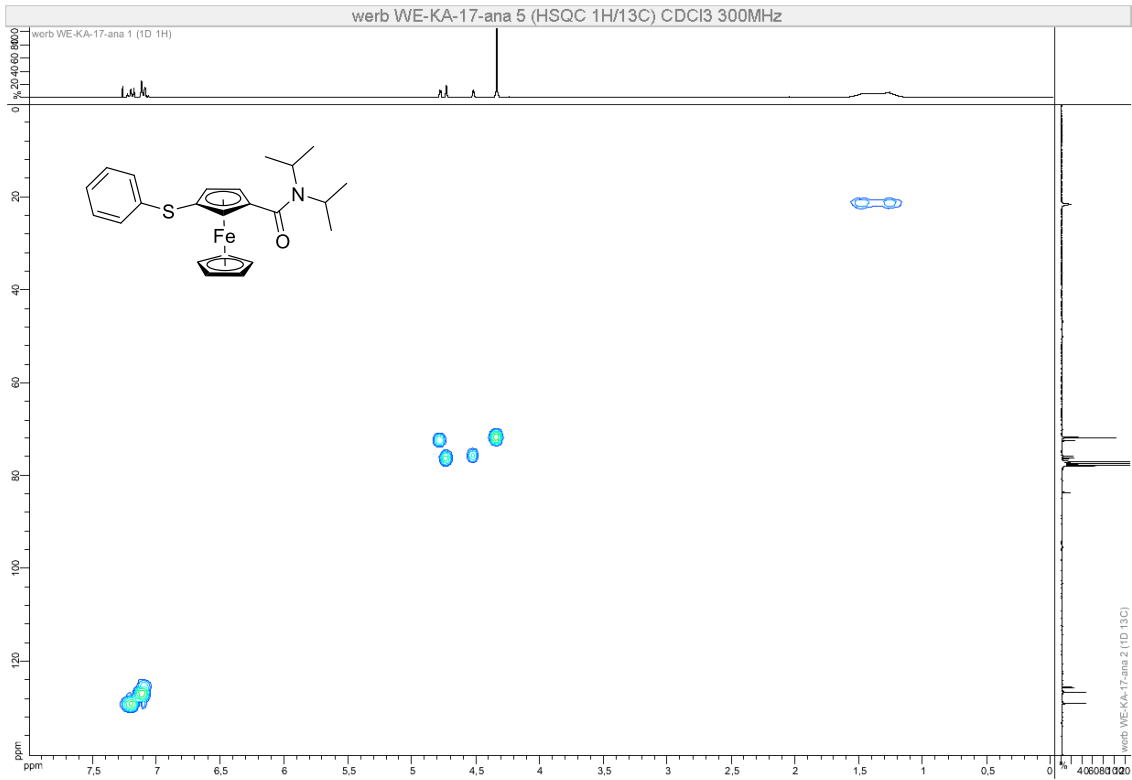
werb ka\_15\_1 2 (1D 19F) CDCl3 300MHz

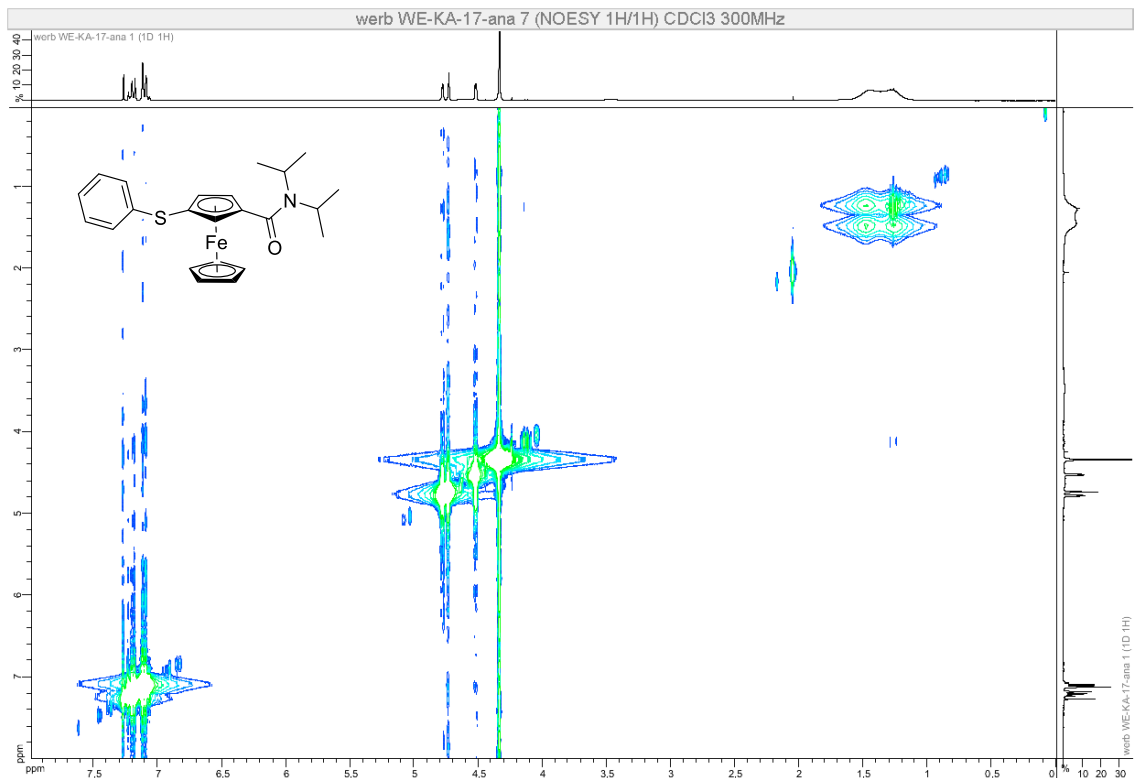


***N,N*-Diisopropyl-3-(phenylthio)ferrocenecarboxamide (23)**

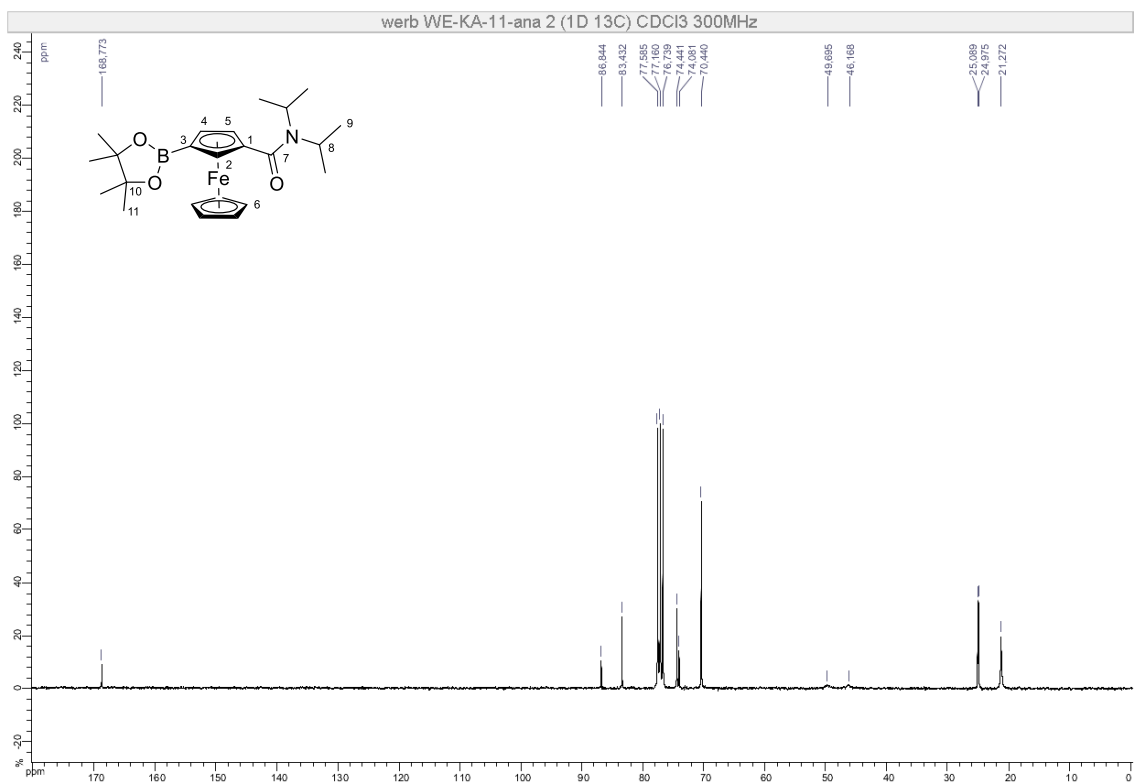
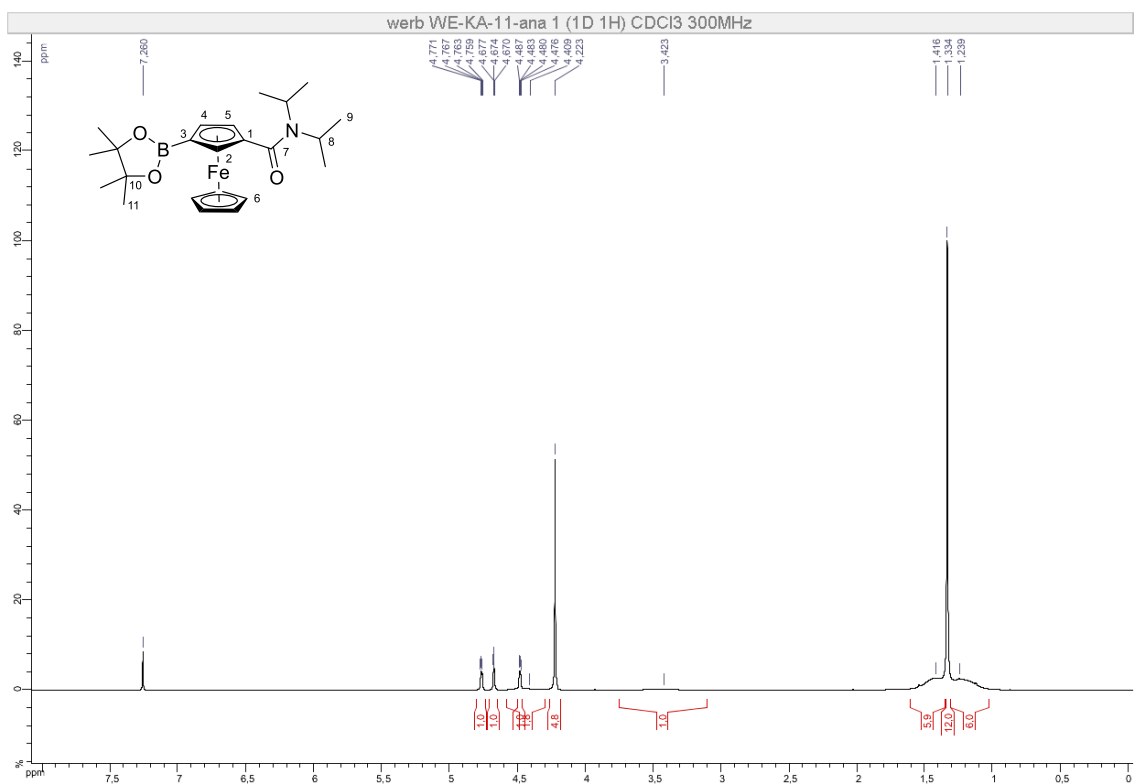


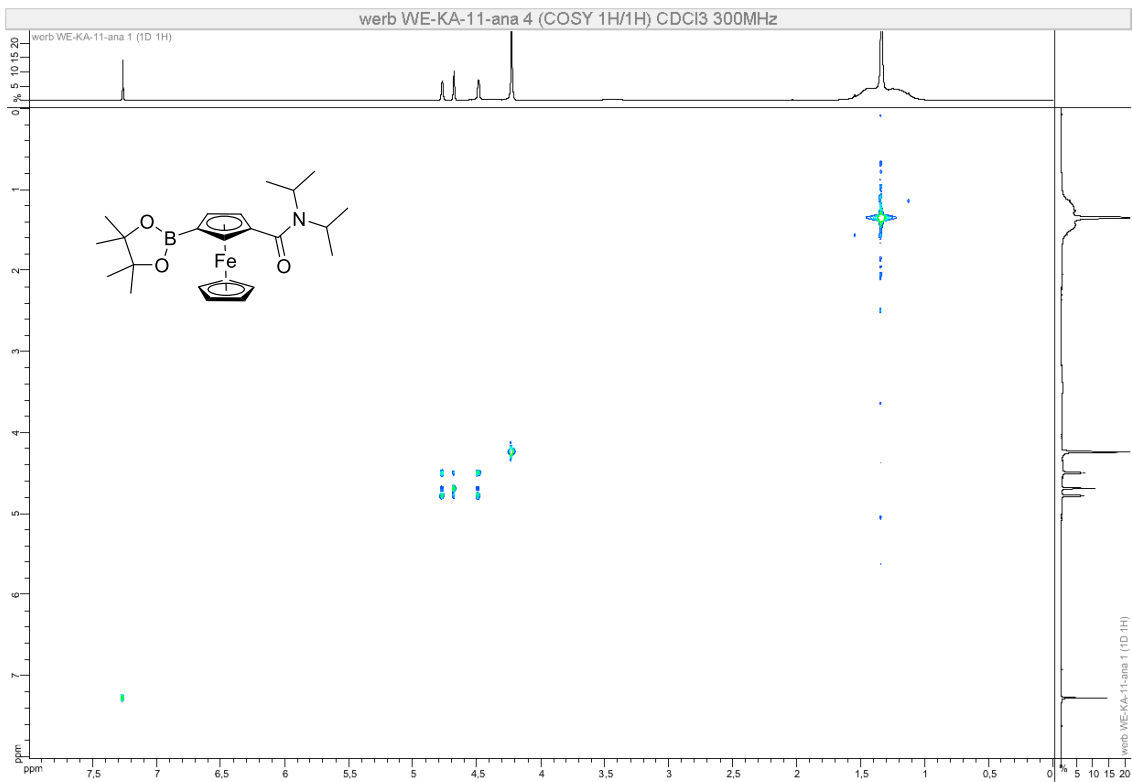
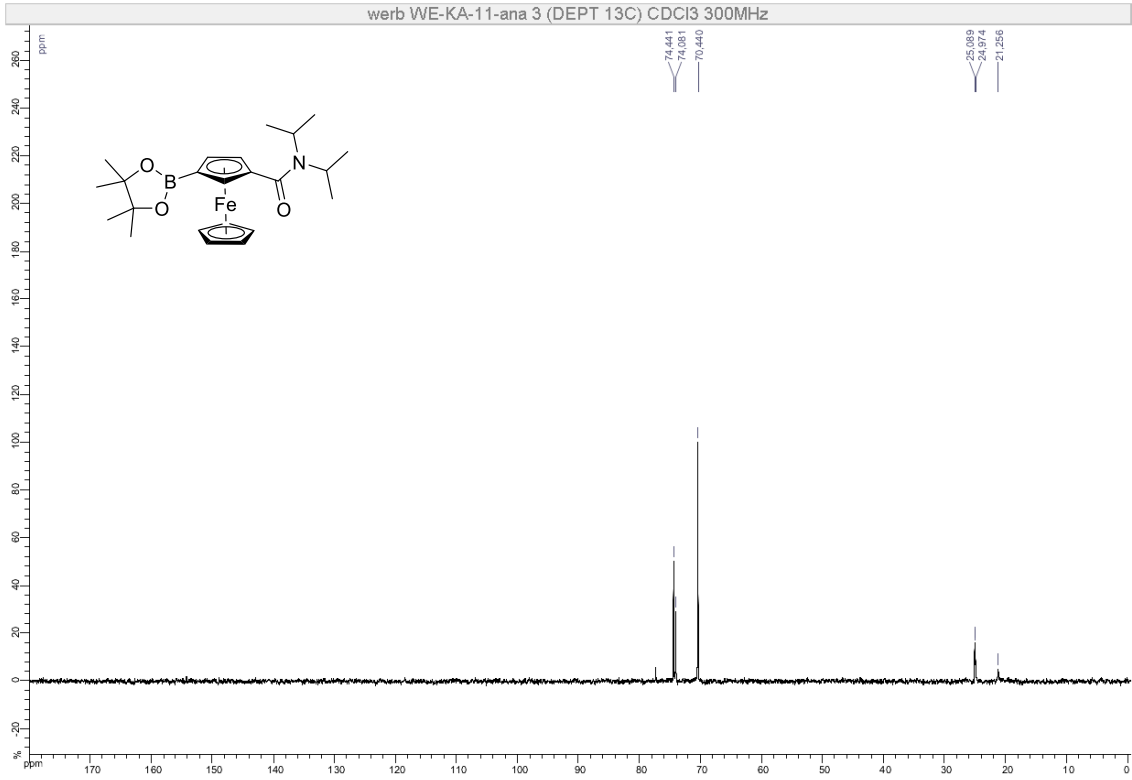


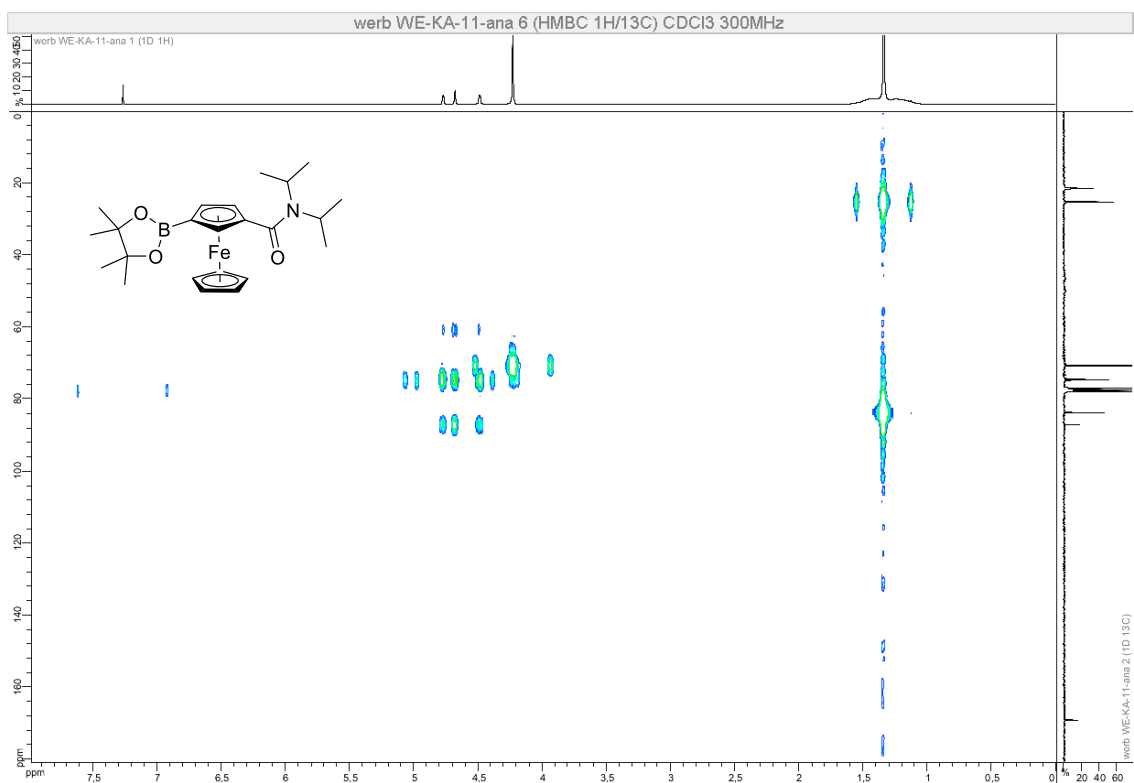
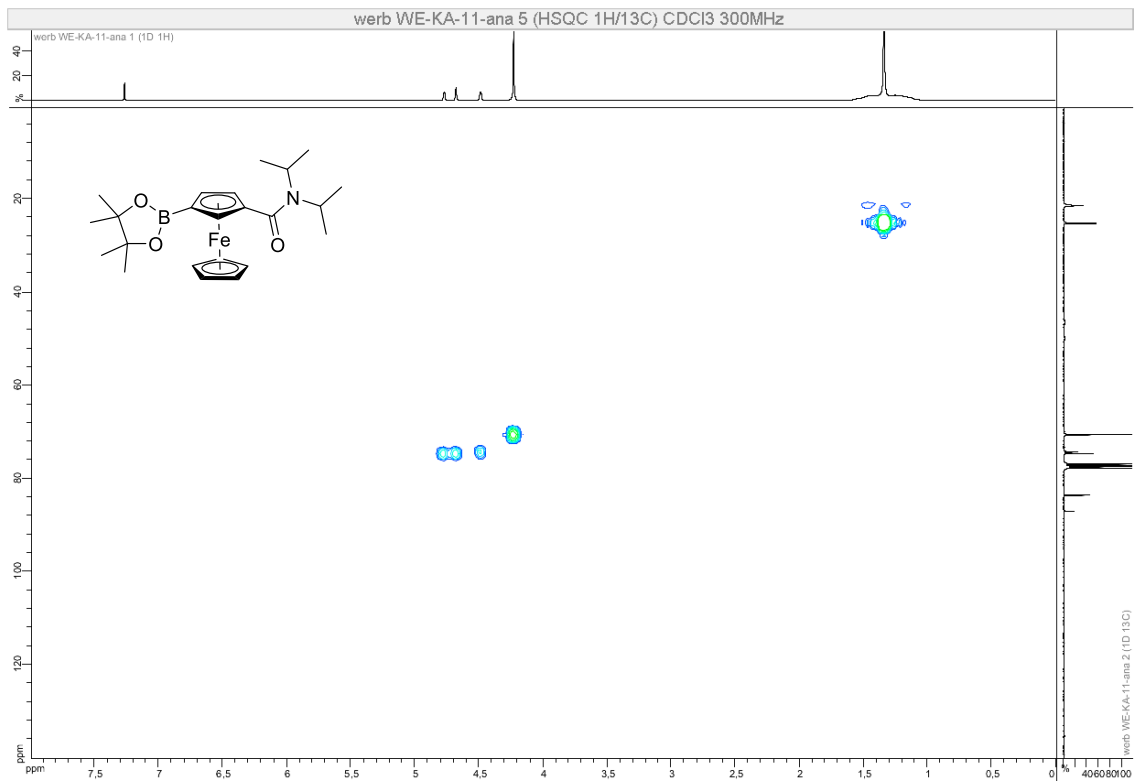




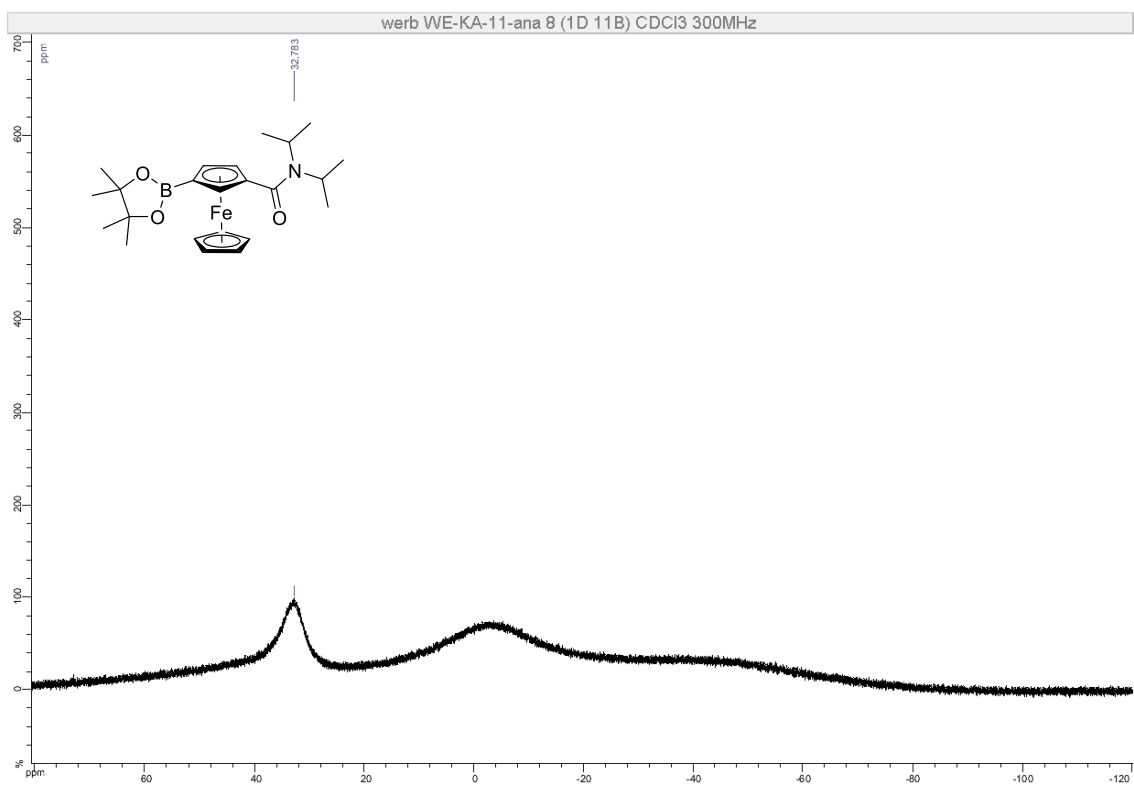
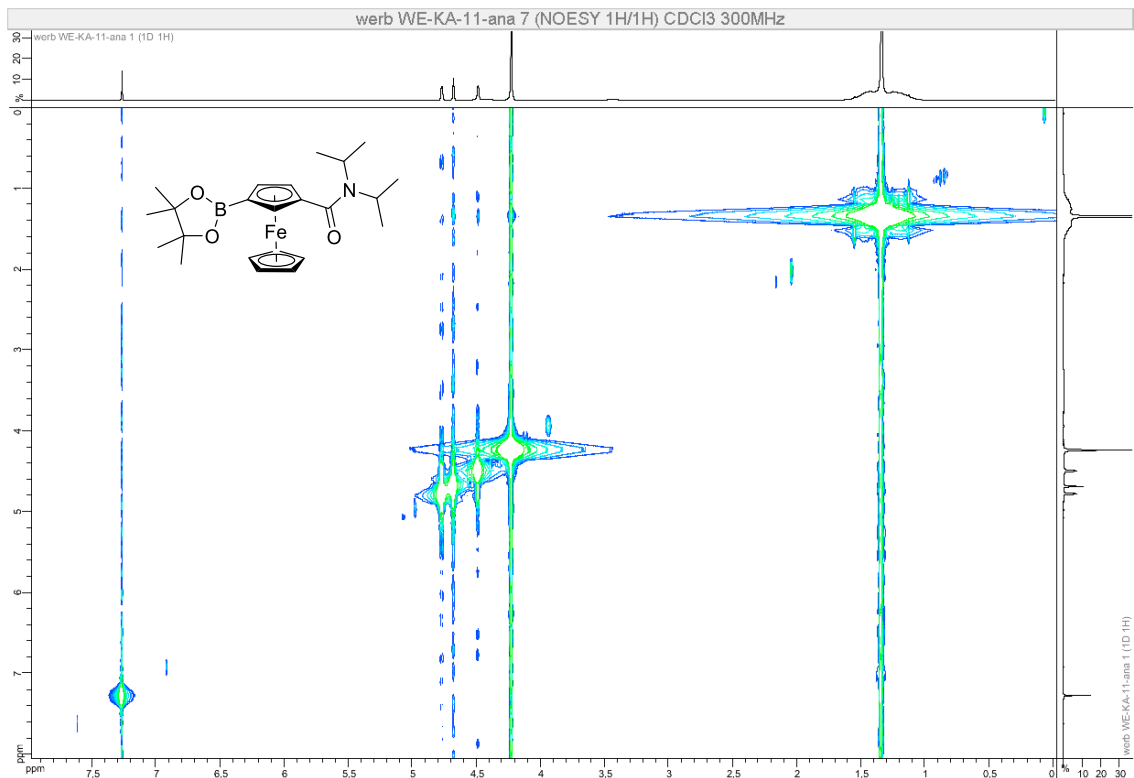
***N,N*-Diisopropyl-3-(pinacolboryl)ferrocenecarboxamide (24)**



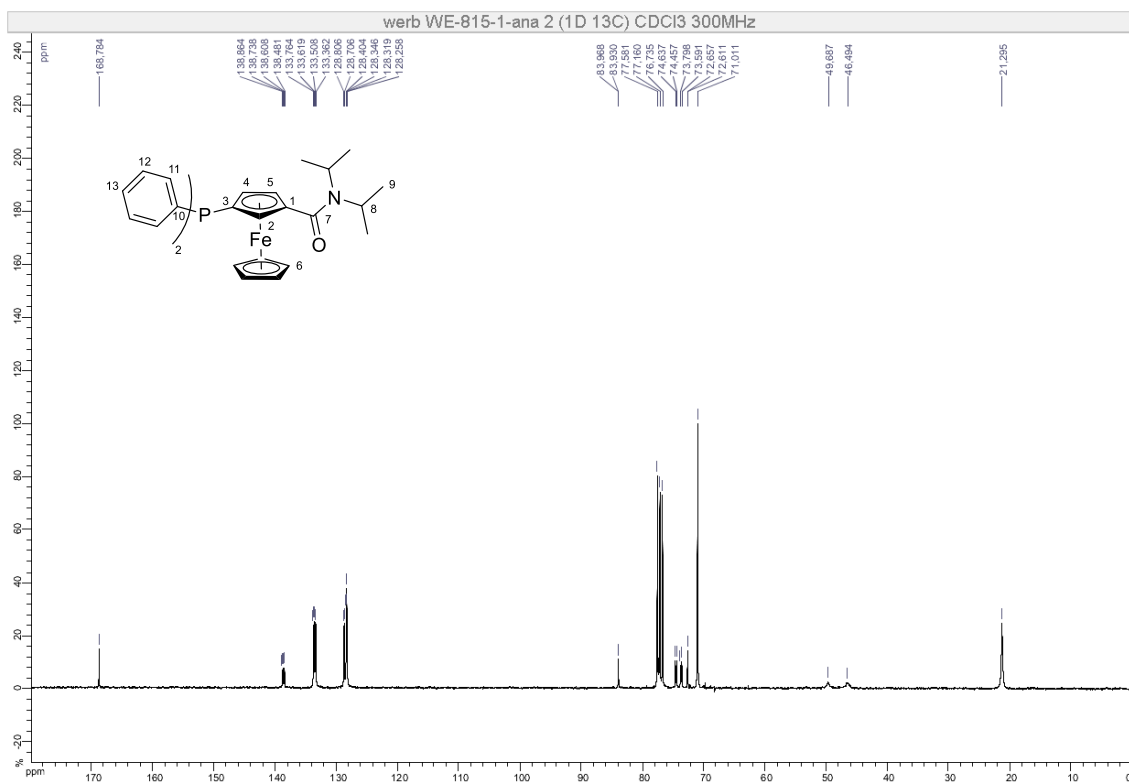
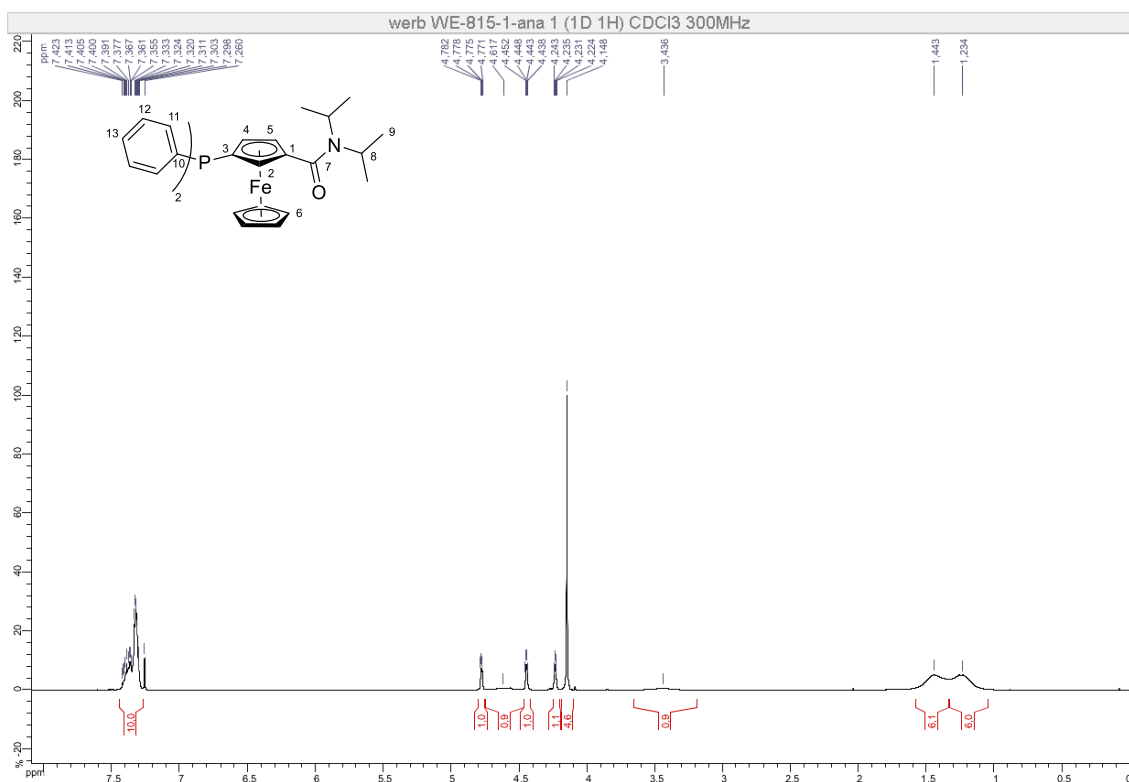


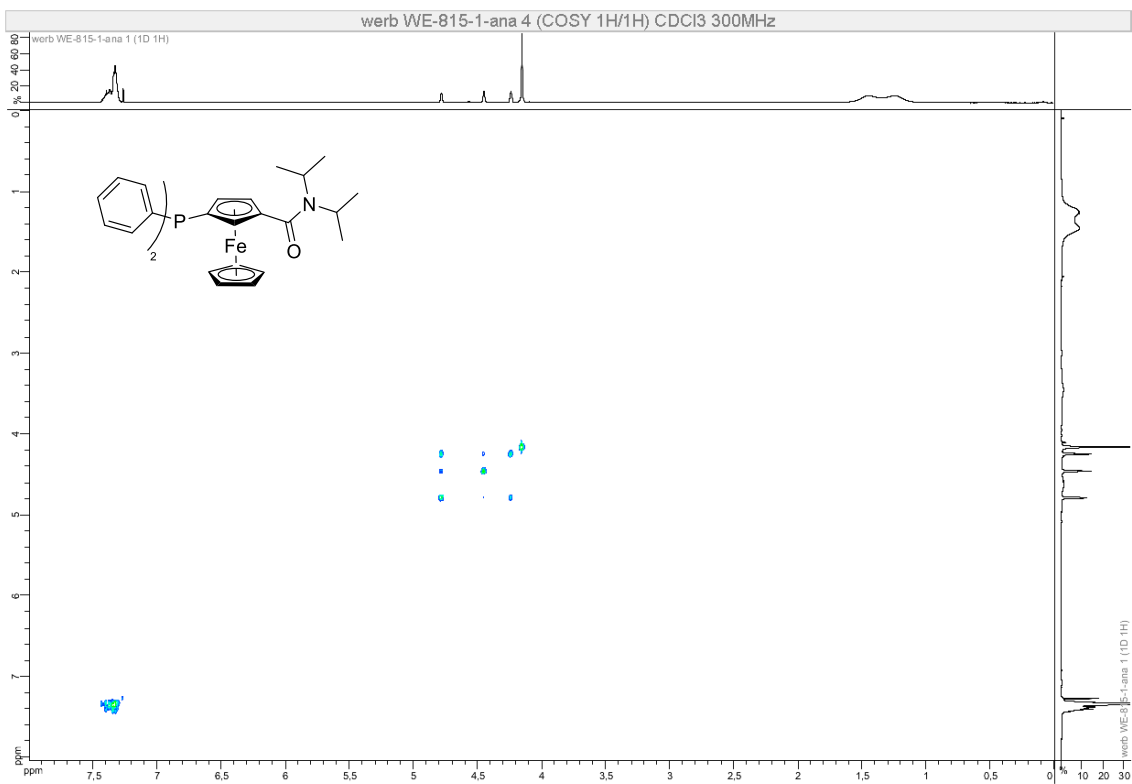
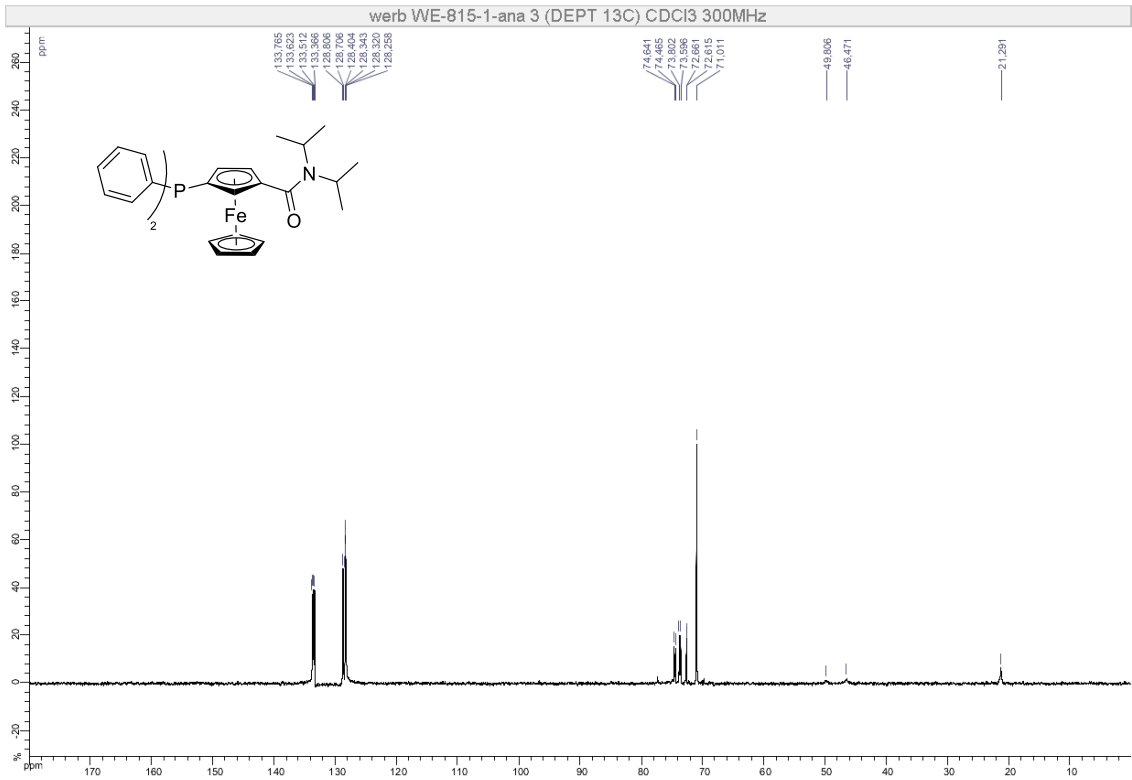


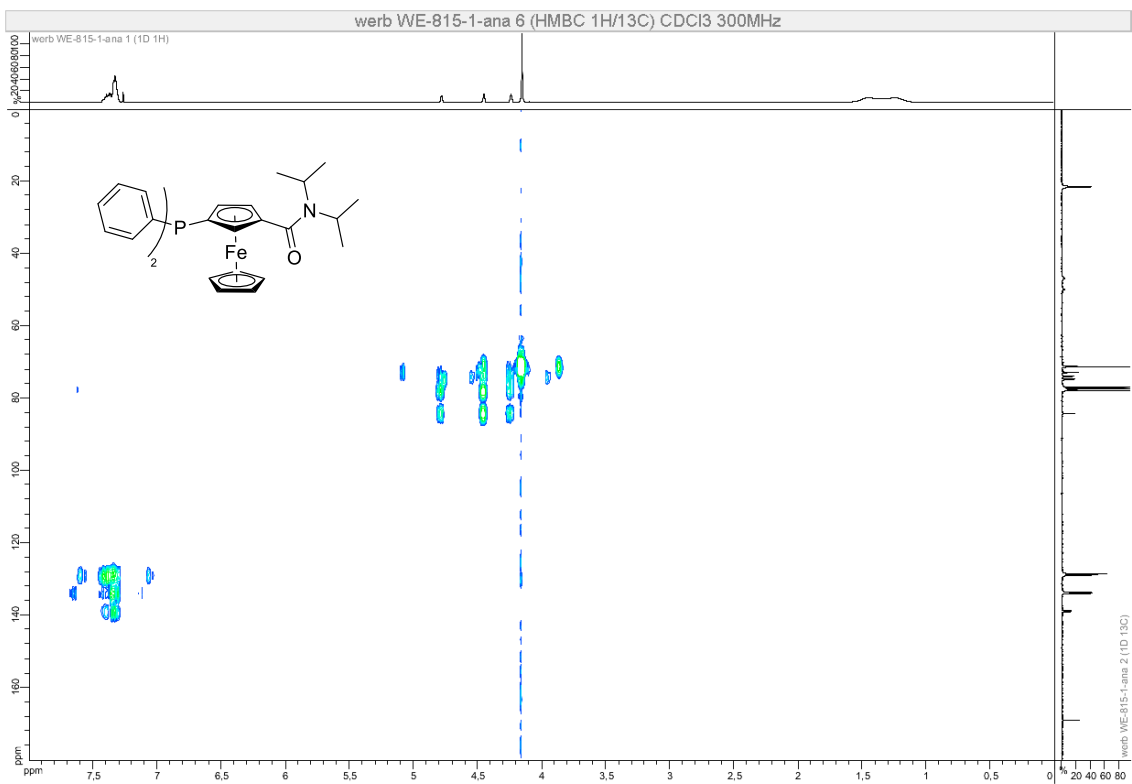
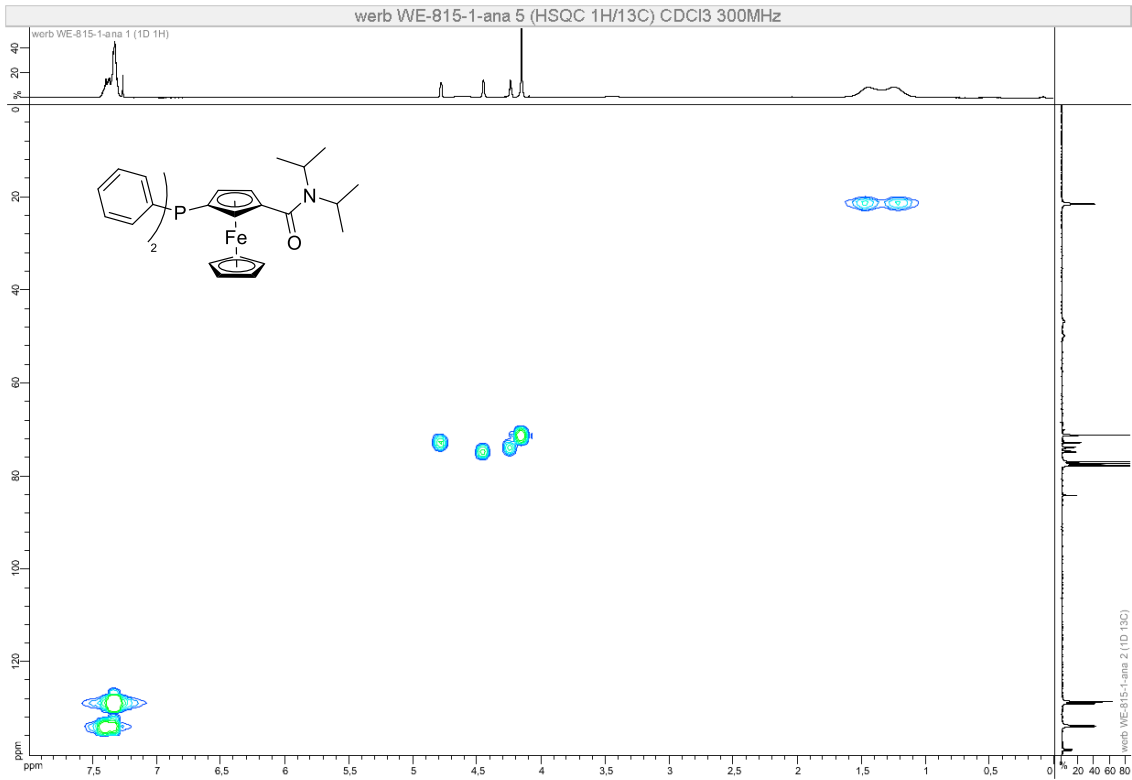


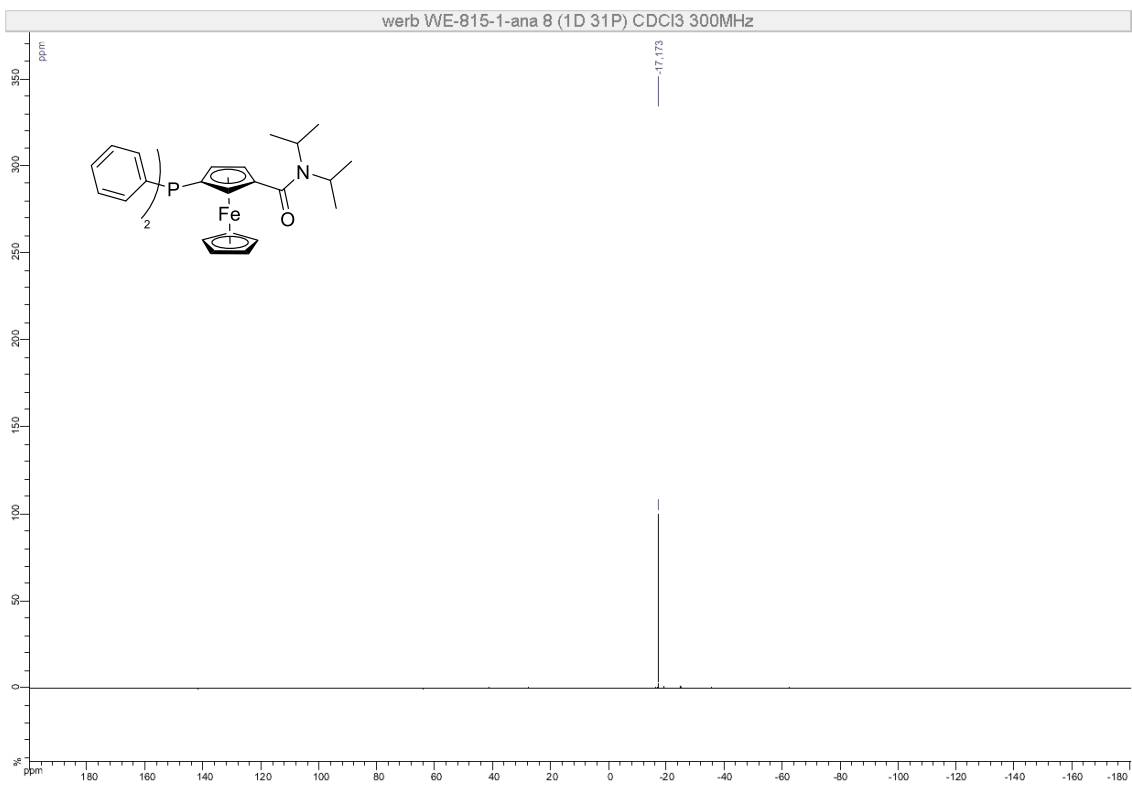
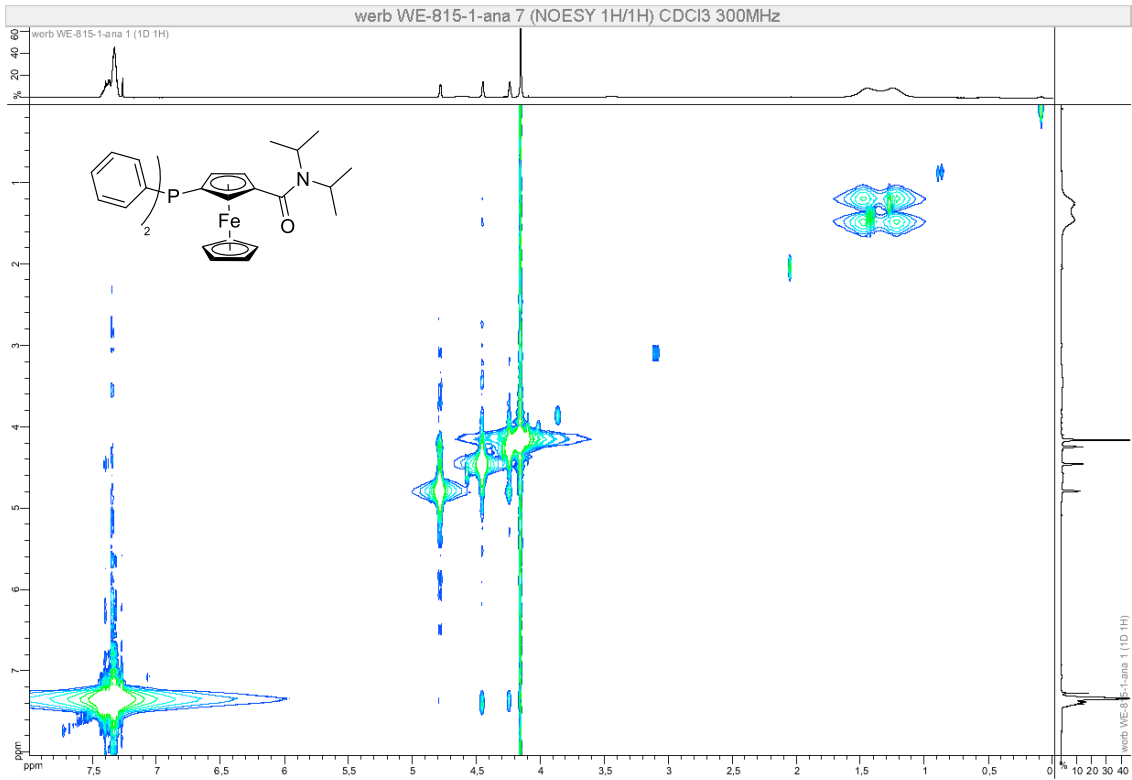


***N,N*-Diisopropyl-3-(diphenylphosphino)ferrocenecarboxamide (25)**

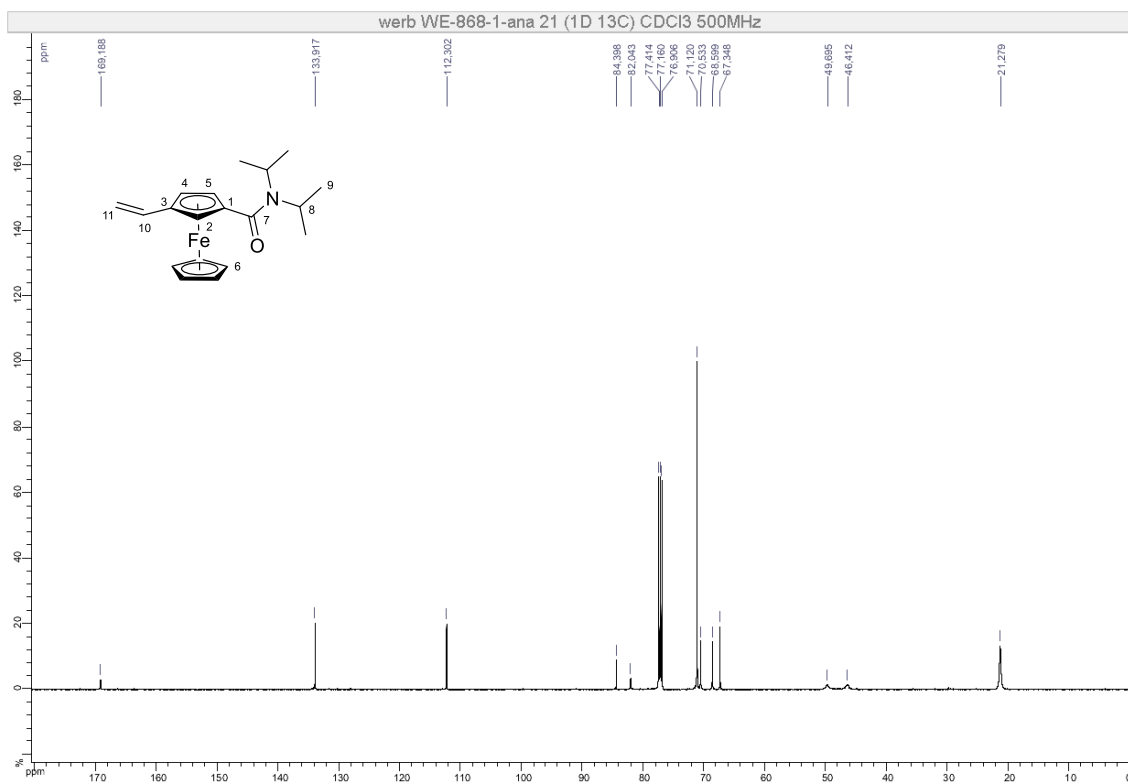
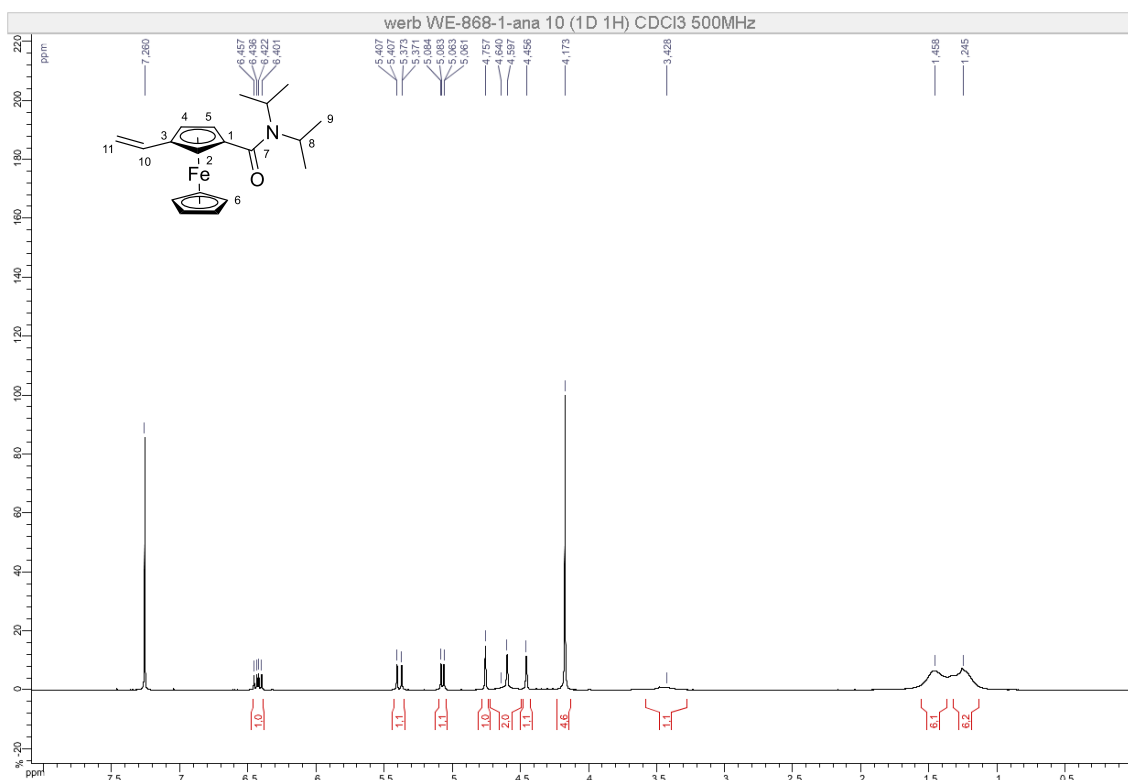


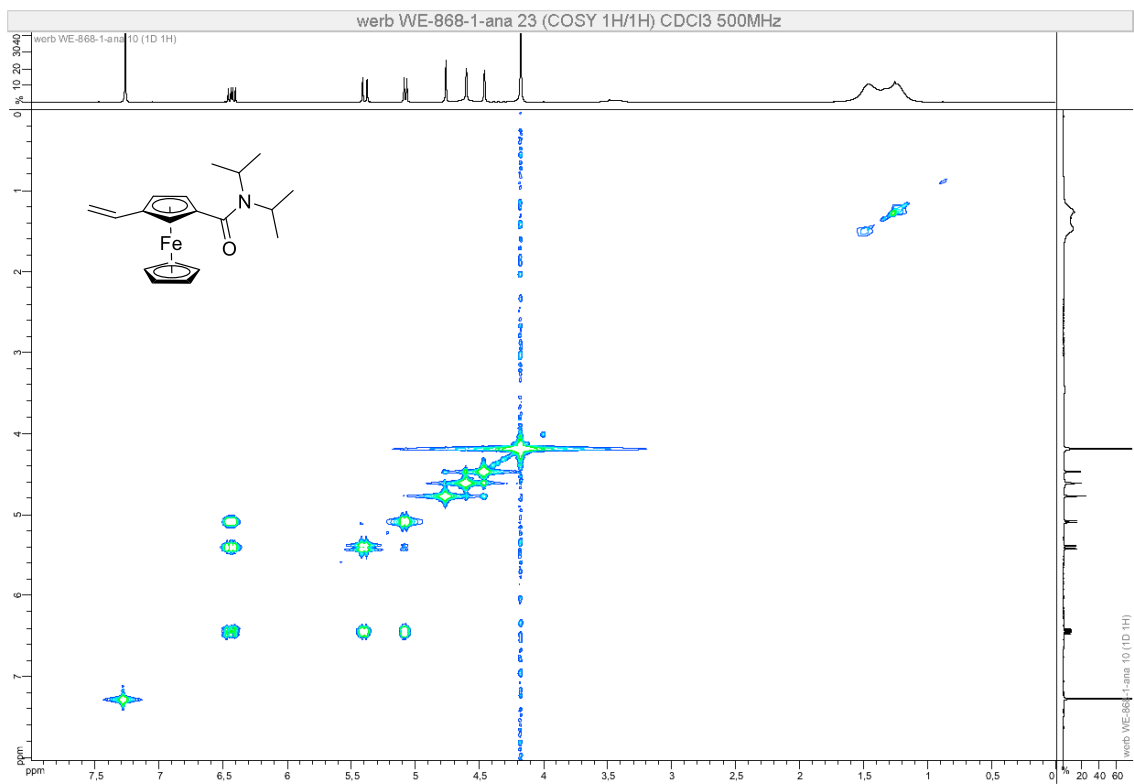
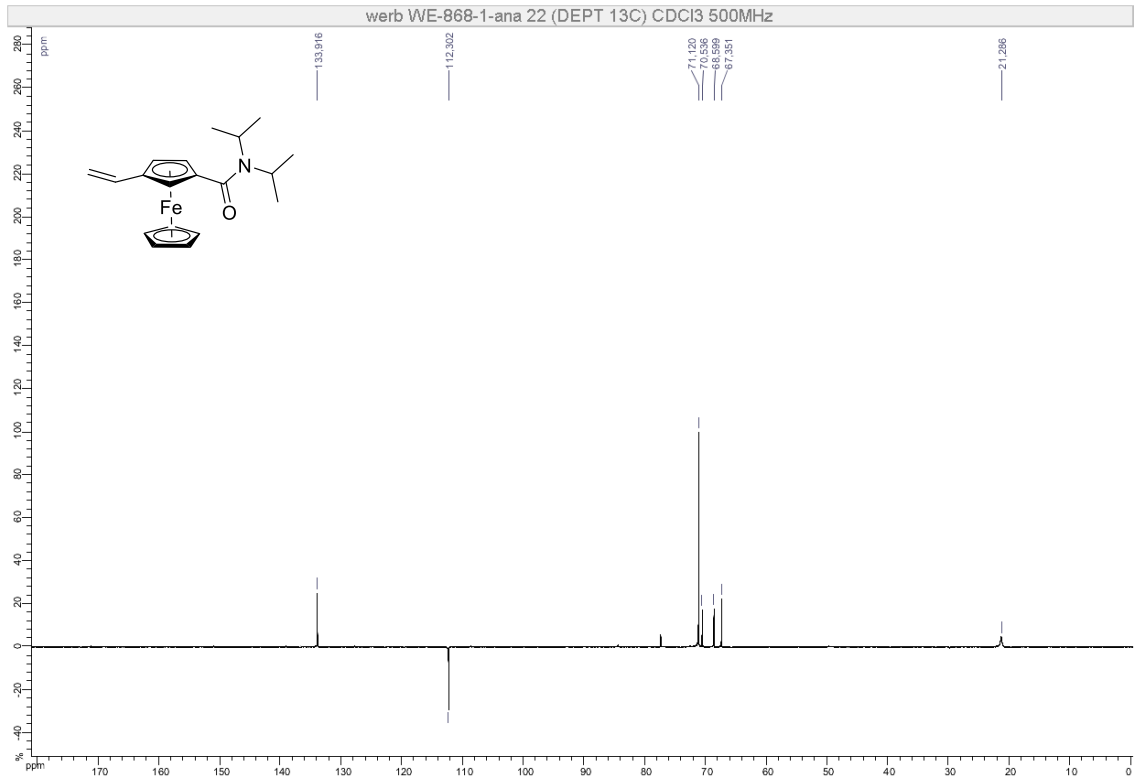


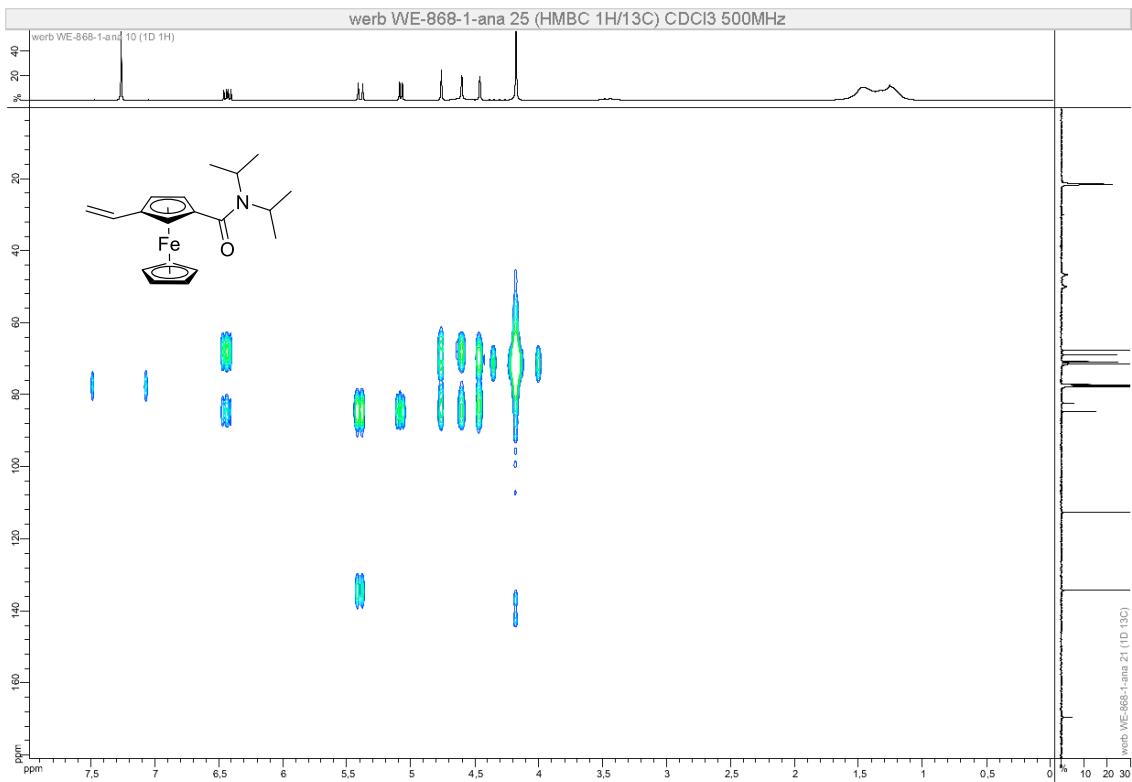
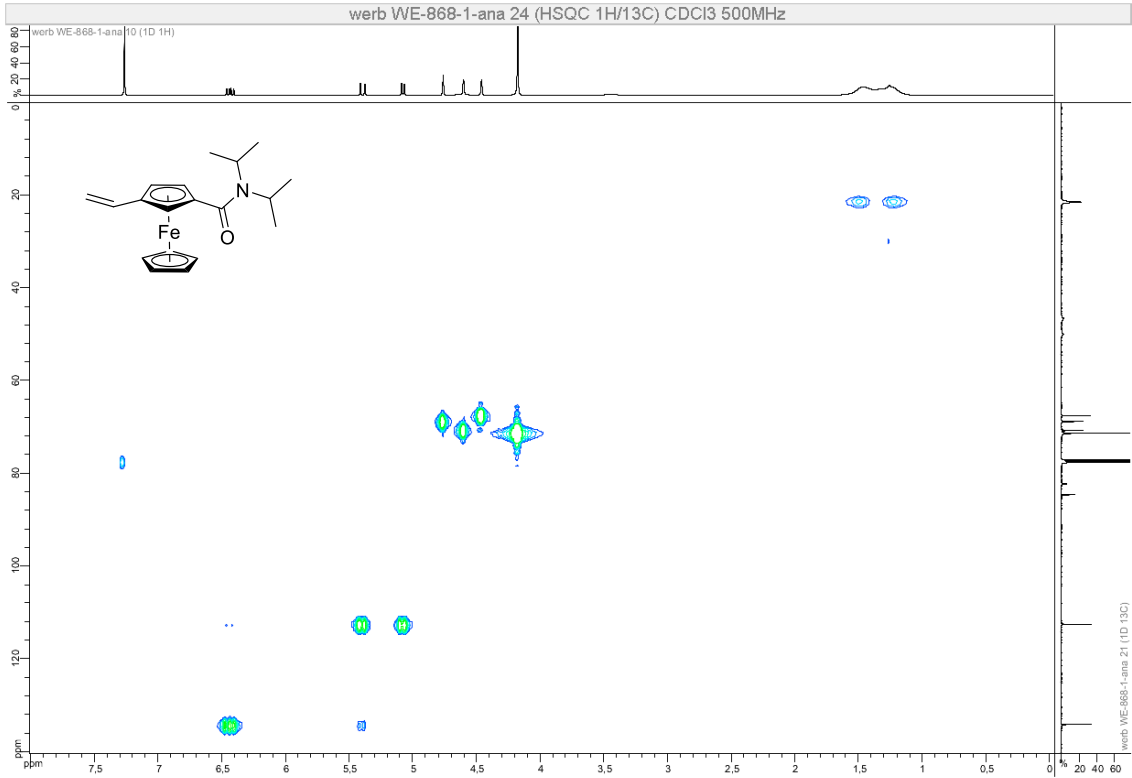




***N,N*-Diisopropyl-3-vinylferrocenecarboxamide (26)**

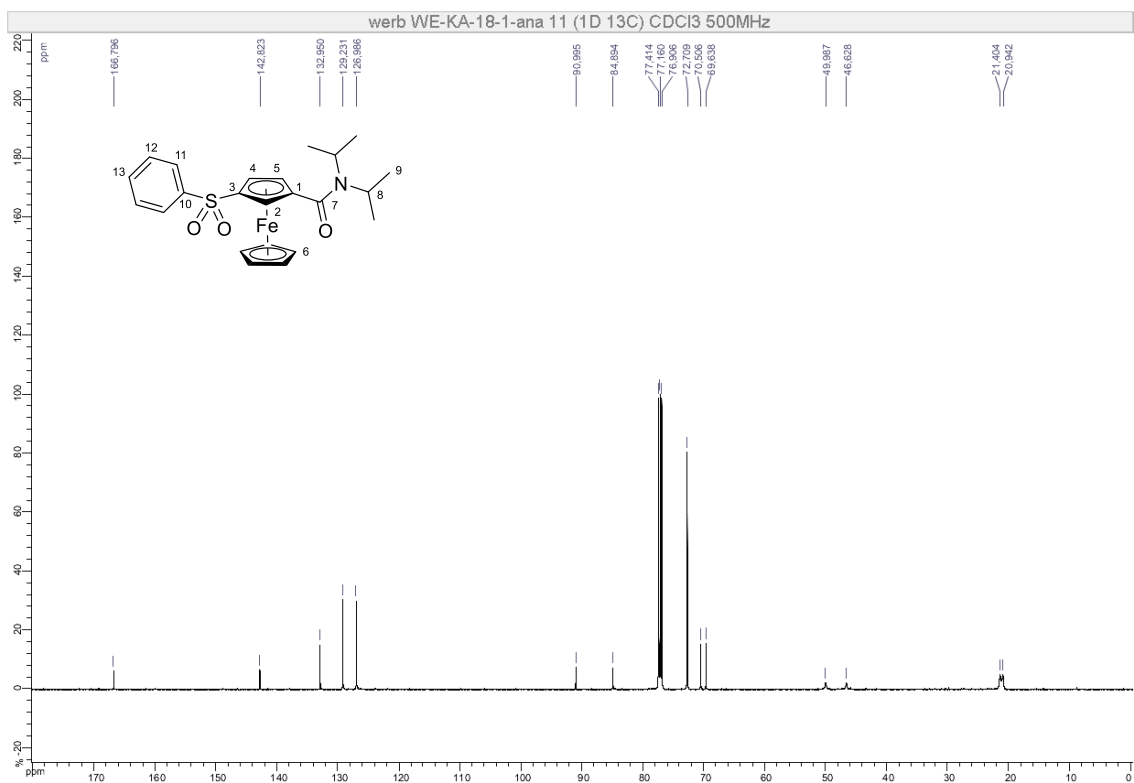
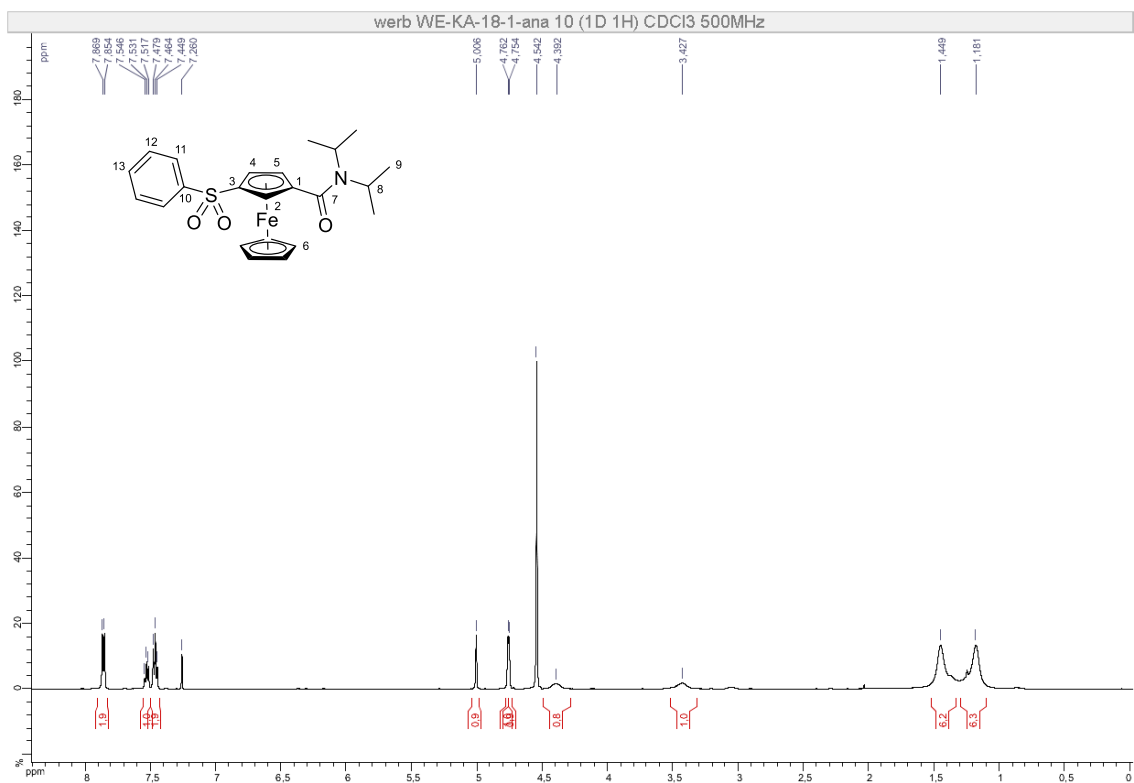


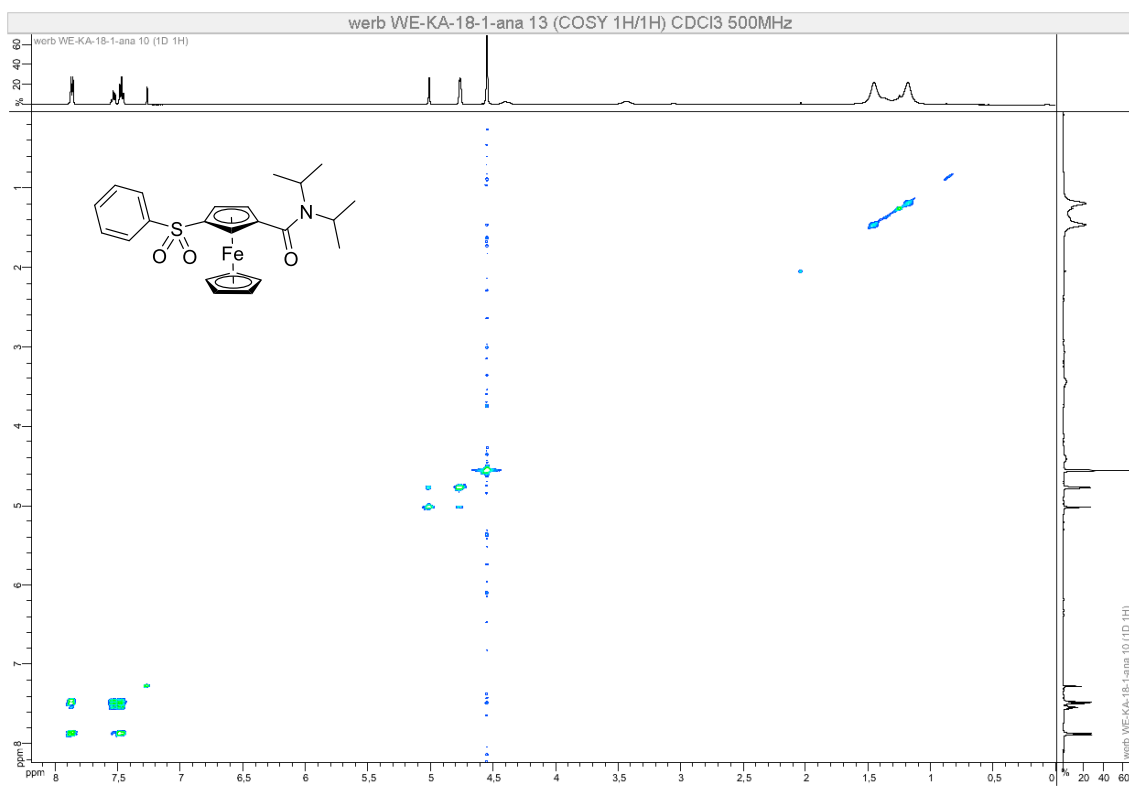
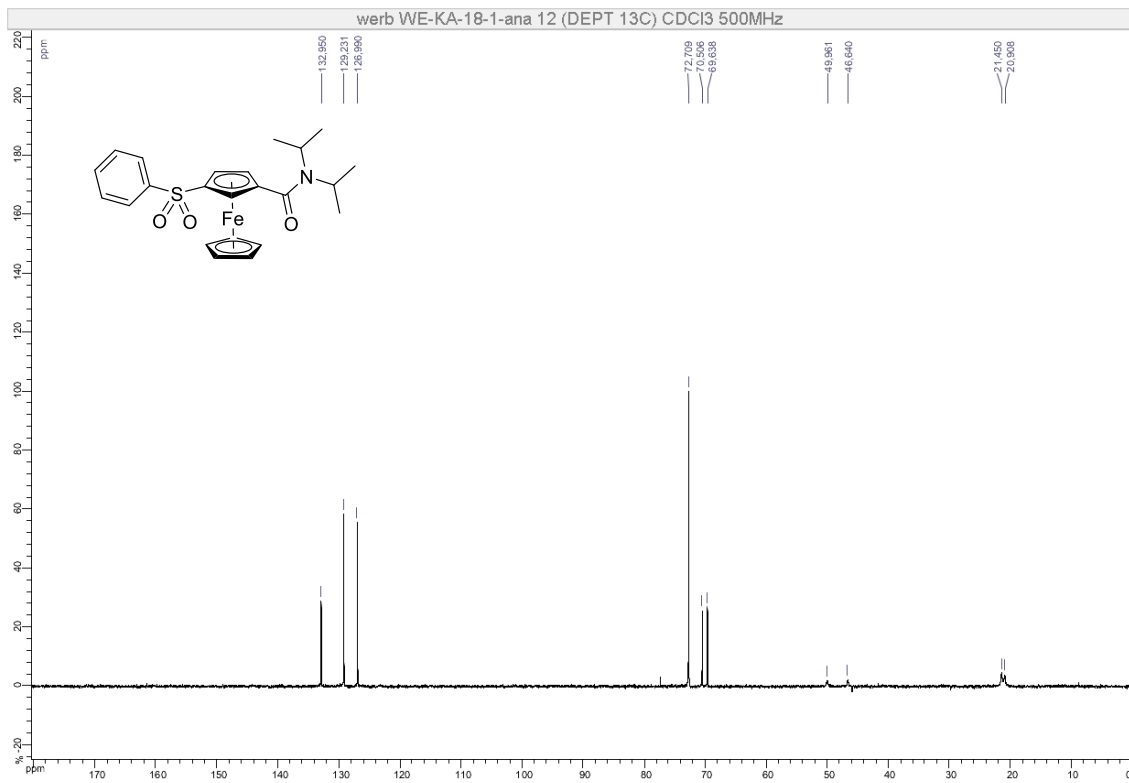


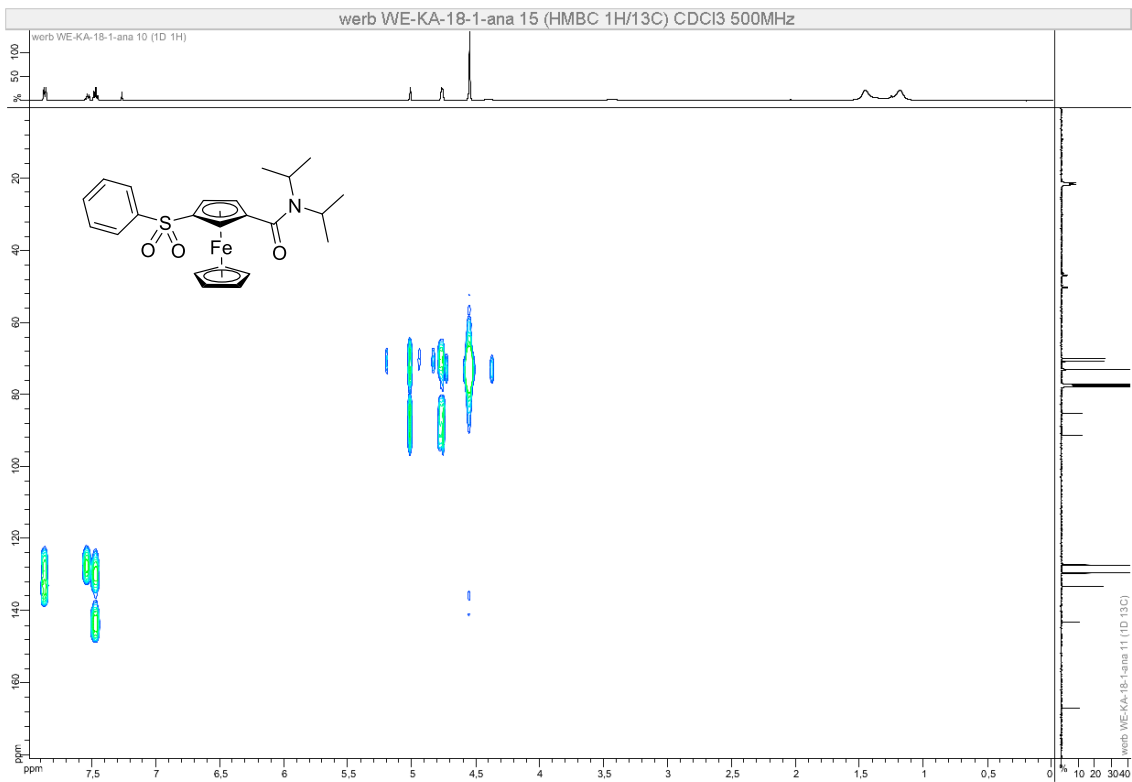
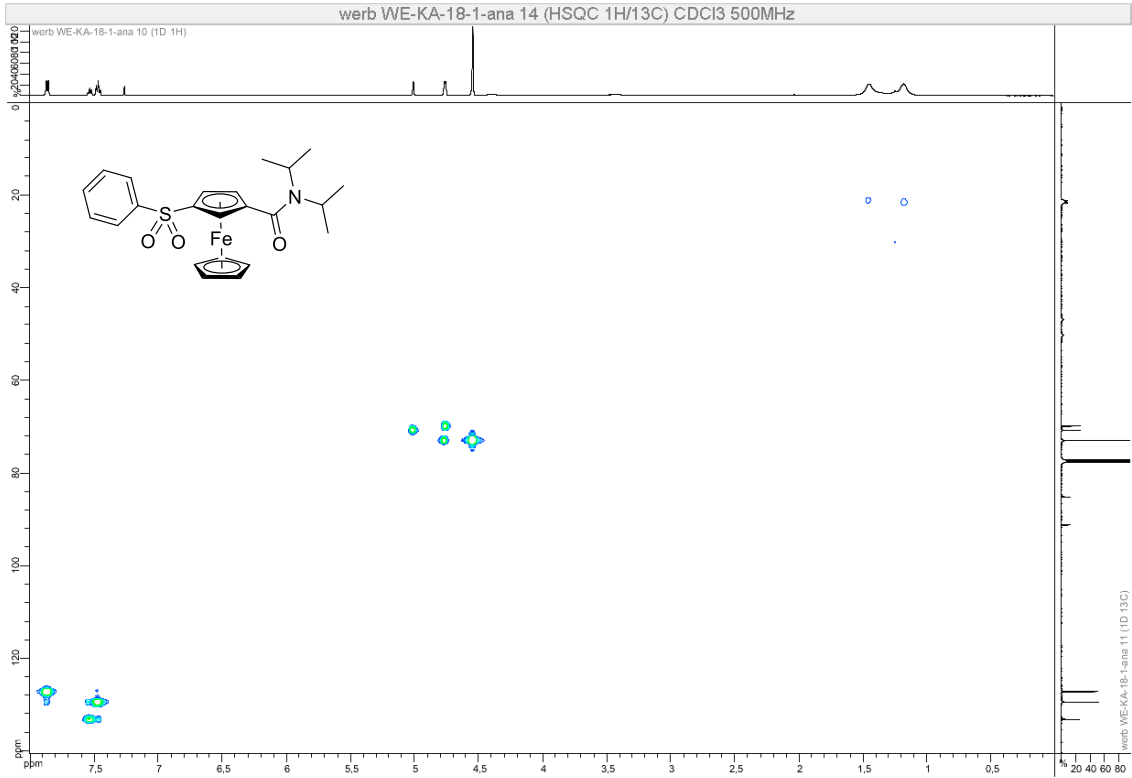


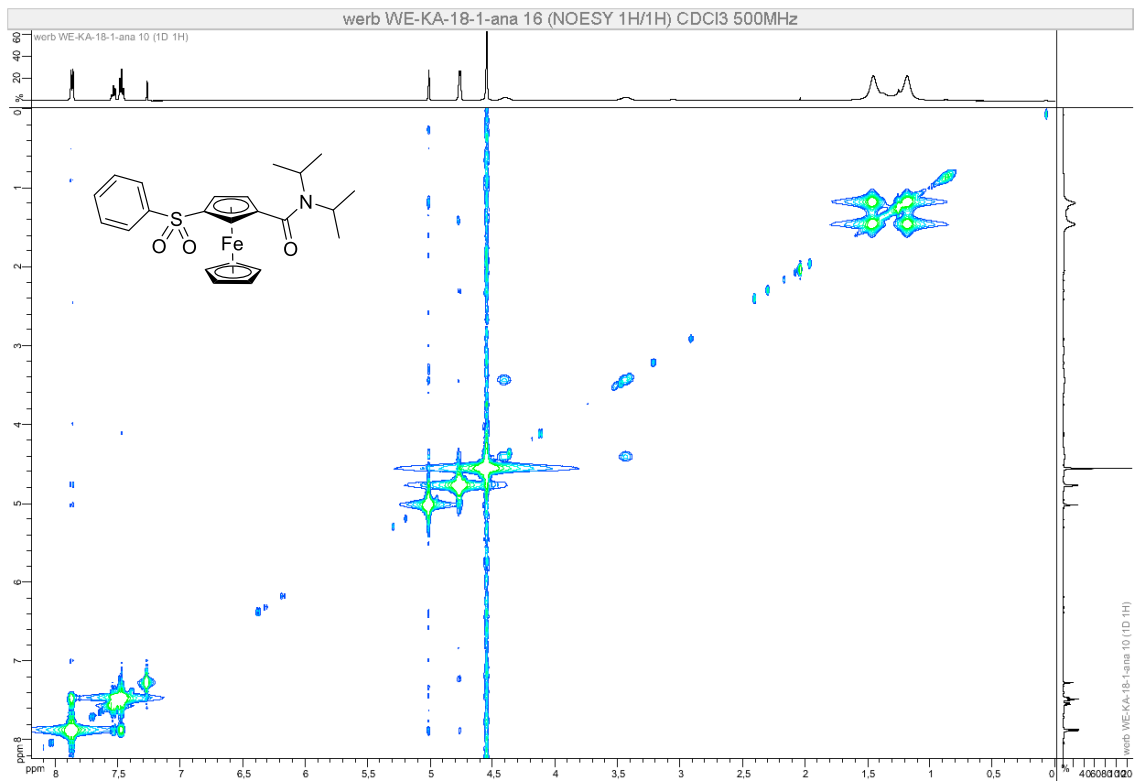


**N,N-Diisopropyl-3-(phenylsulfonyl)ferrocenecarboxamide (27)**

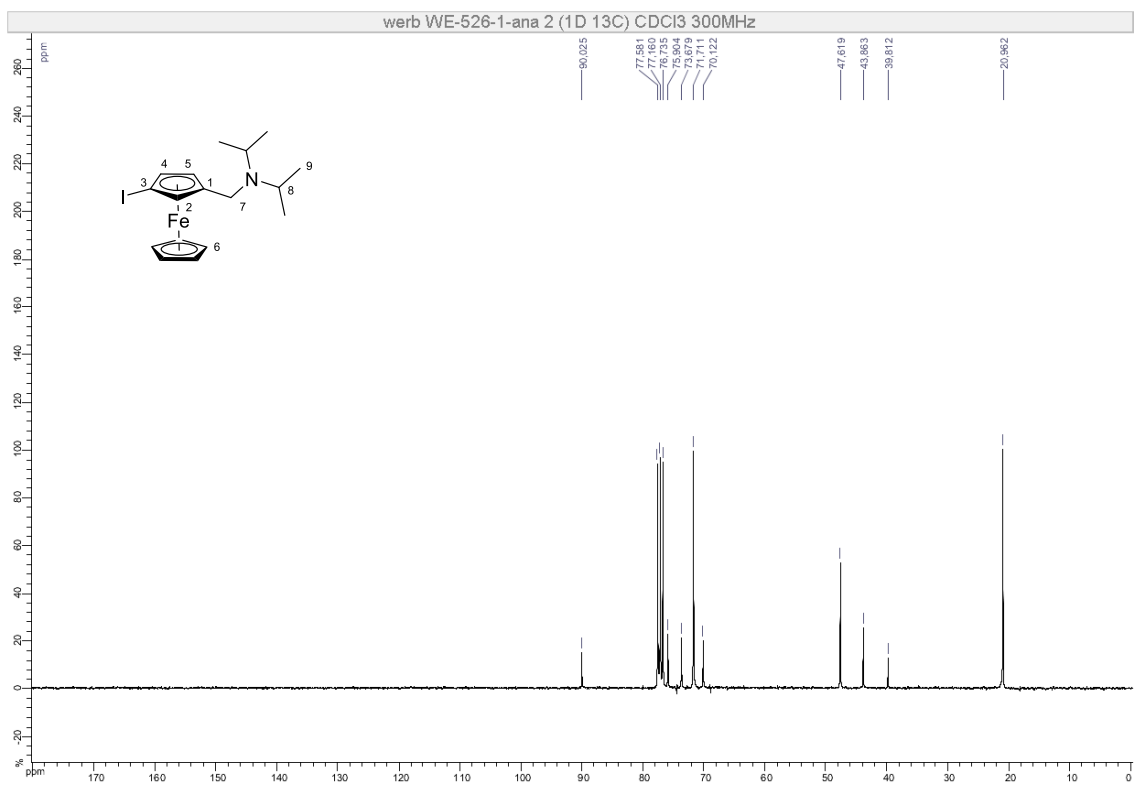
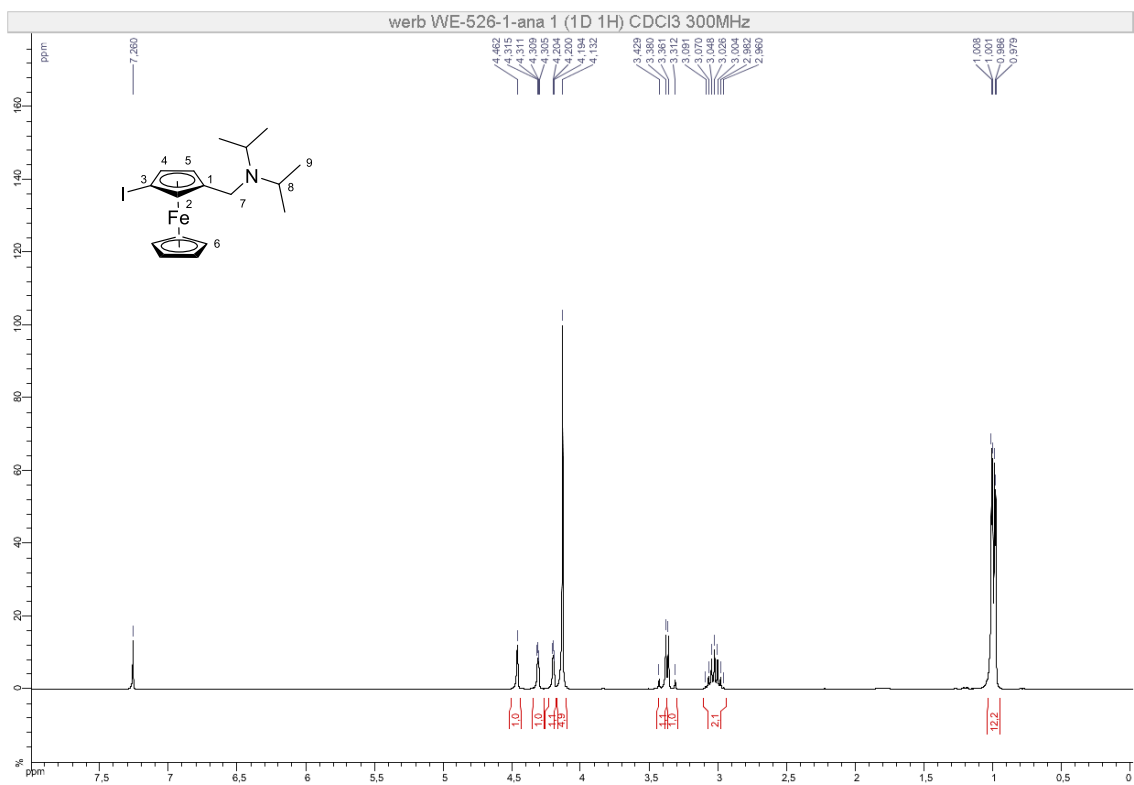


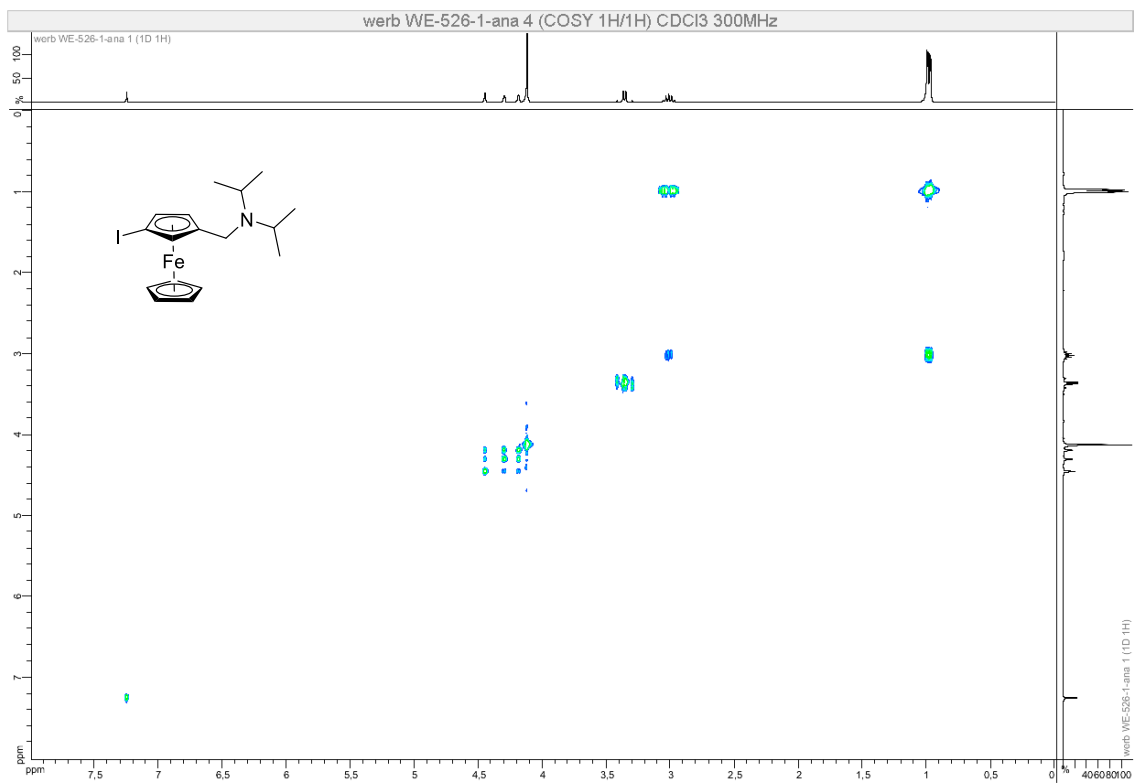
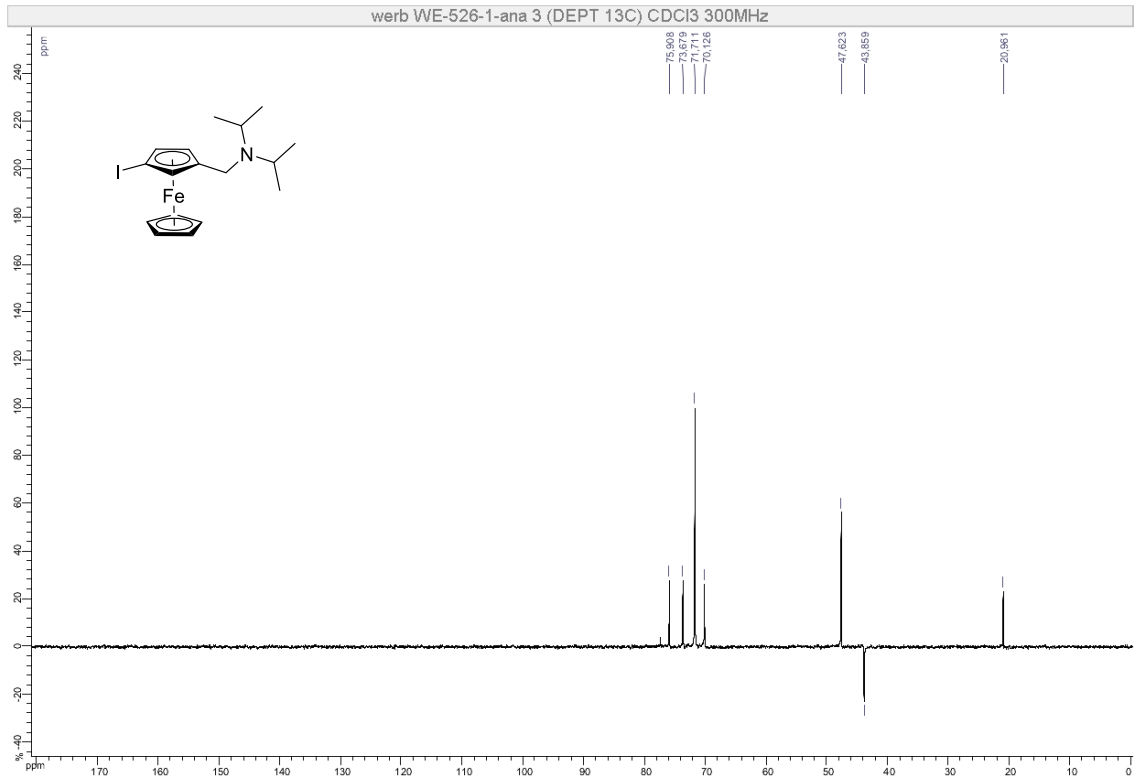


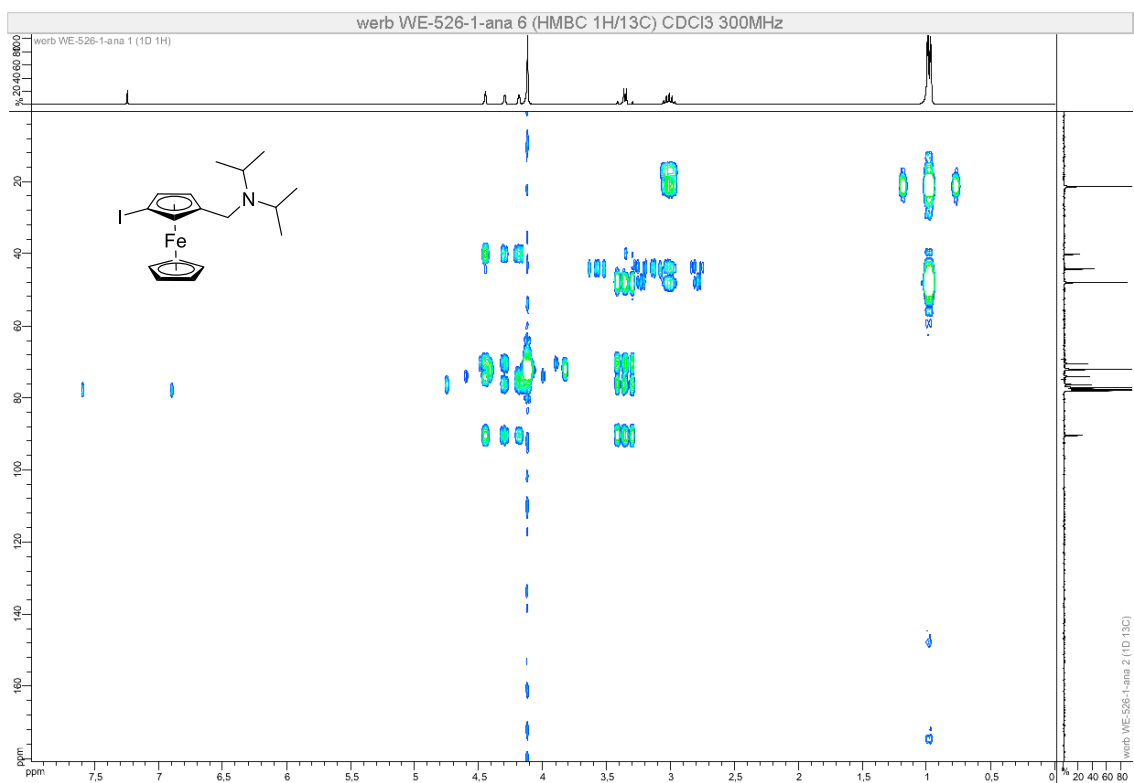
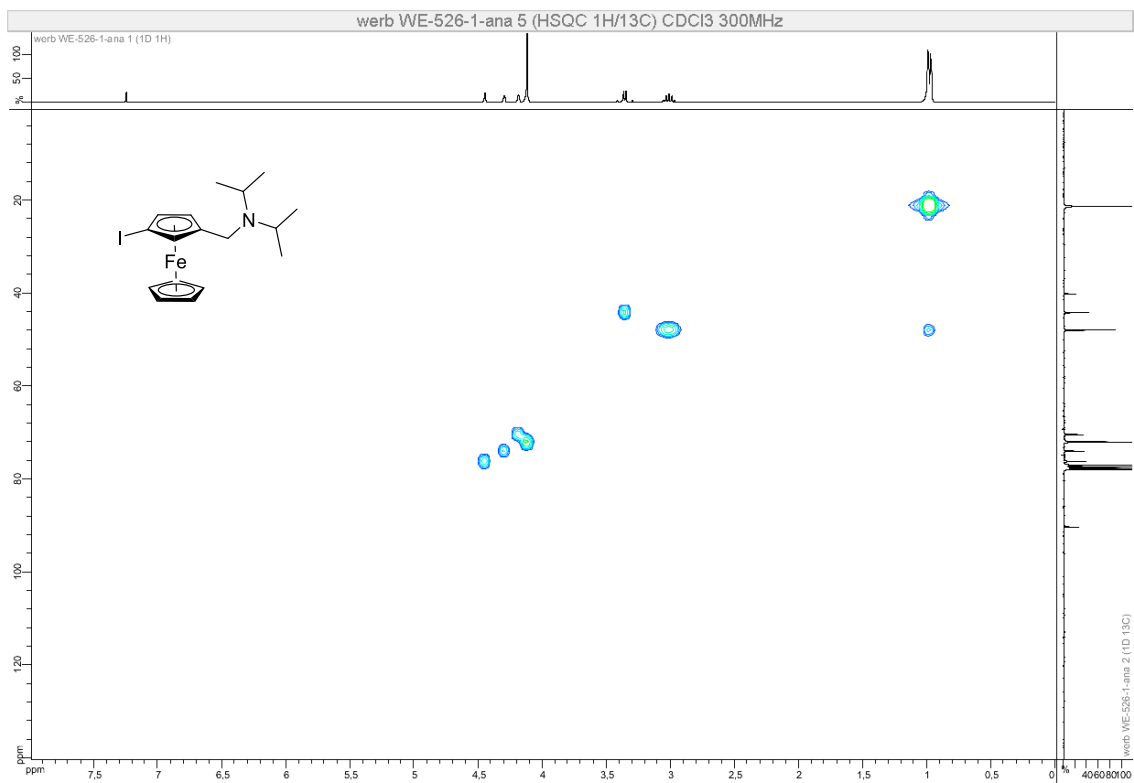


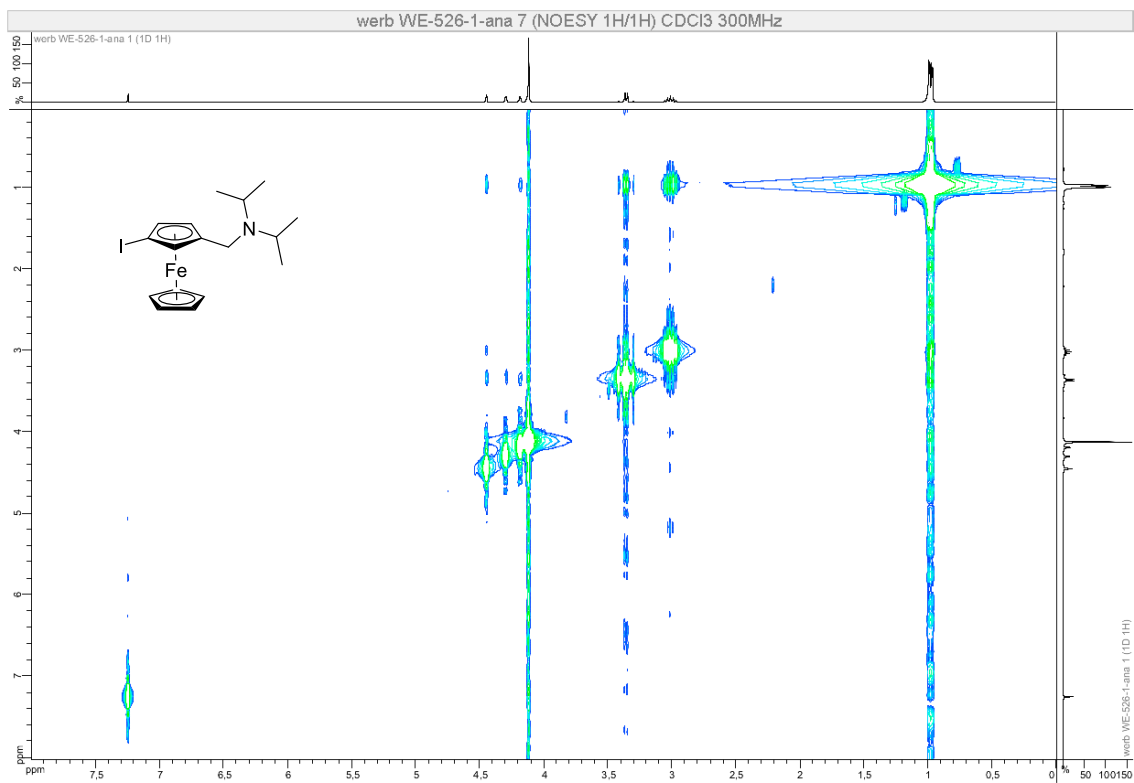


**1-(N,N-Diisopropylaminomethyl)-3-iodoferrocene (28)**



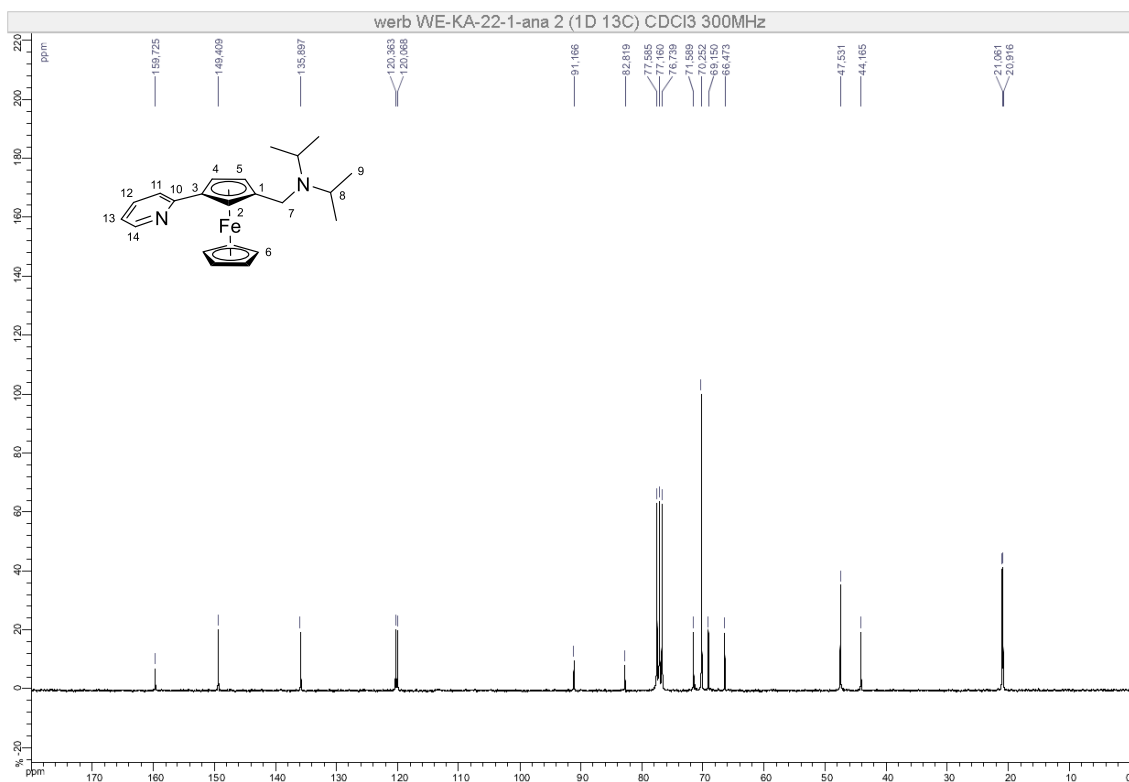
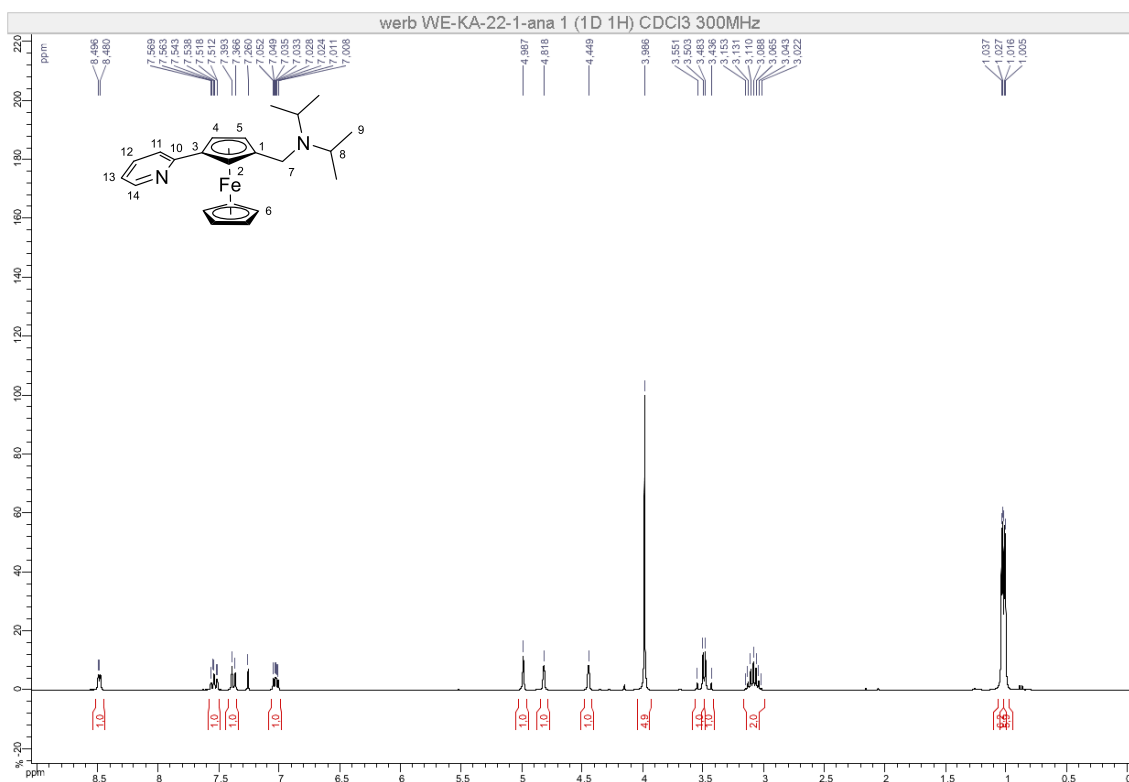


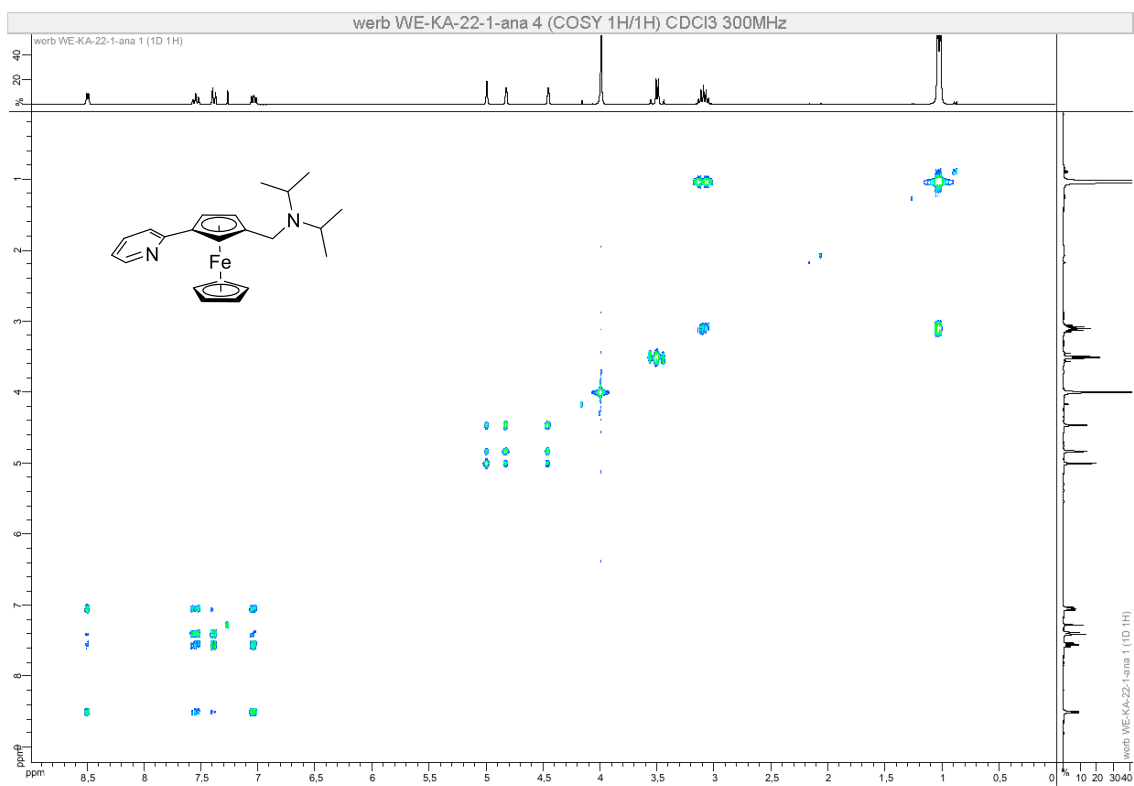
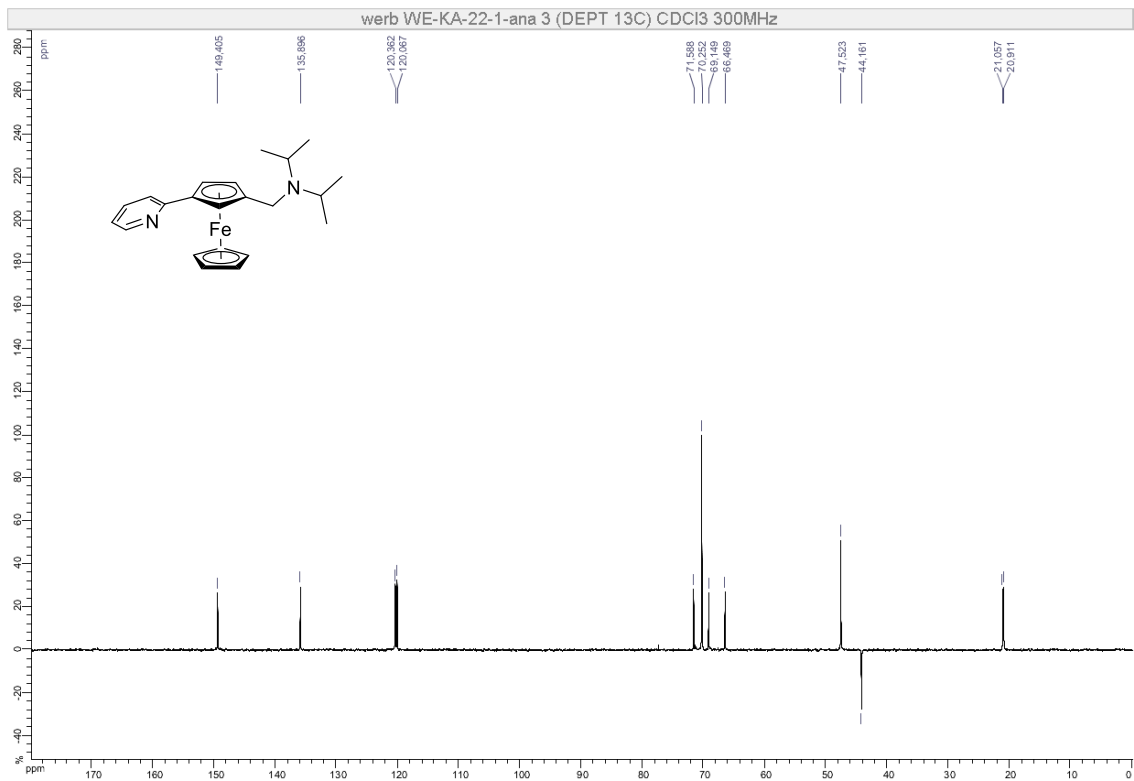


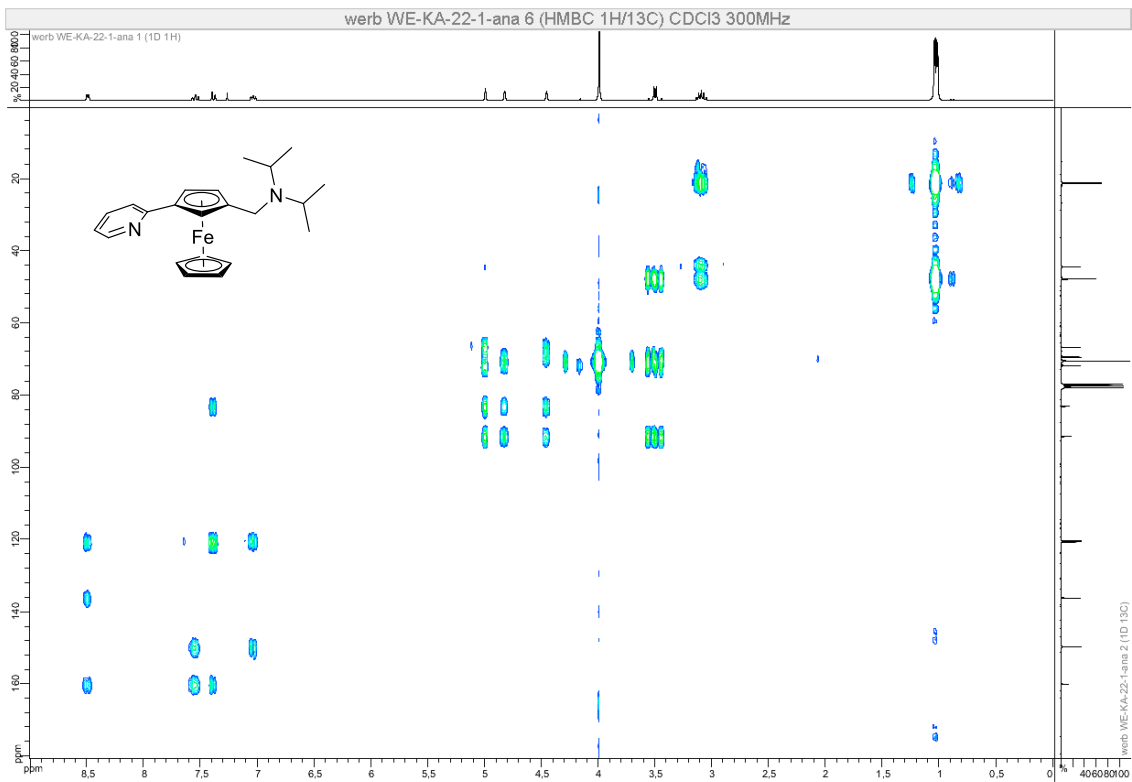
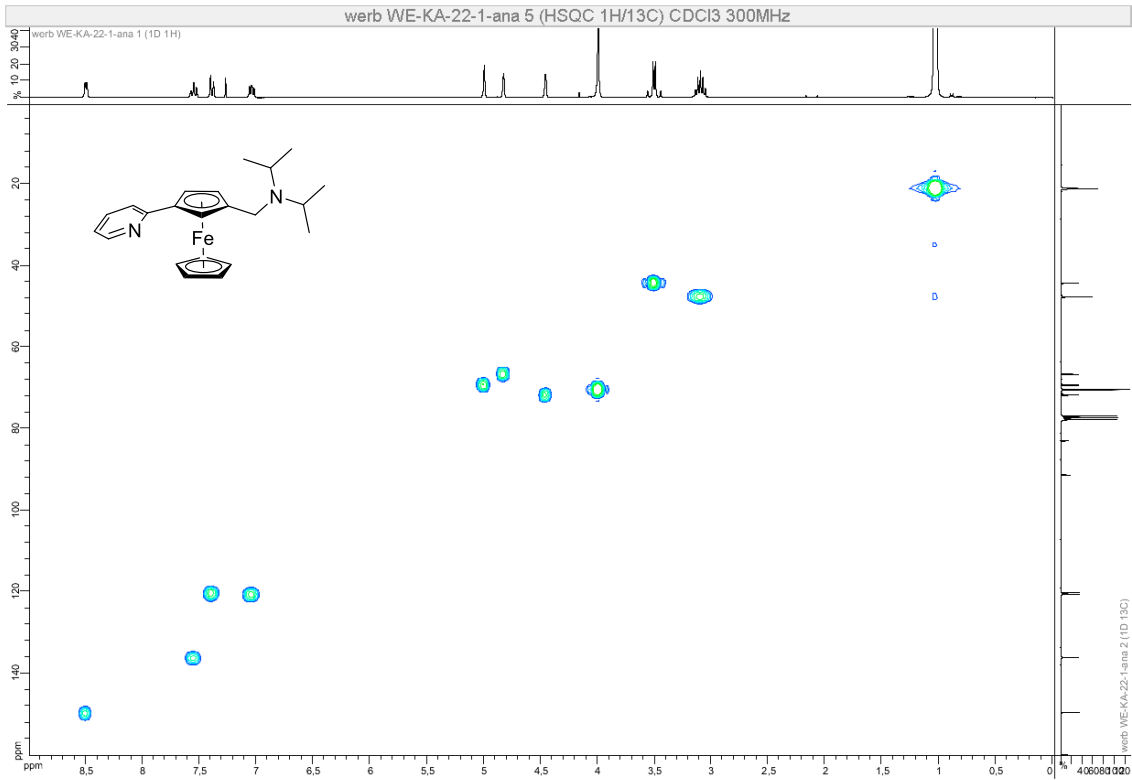


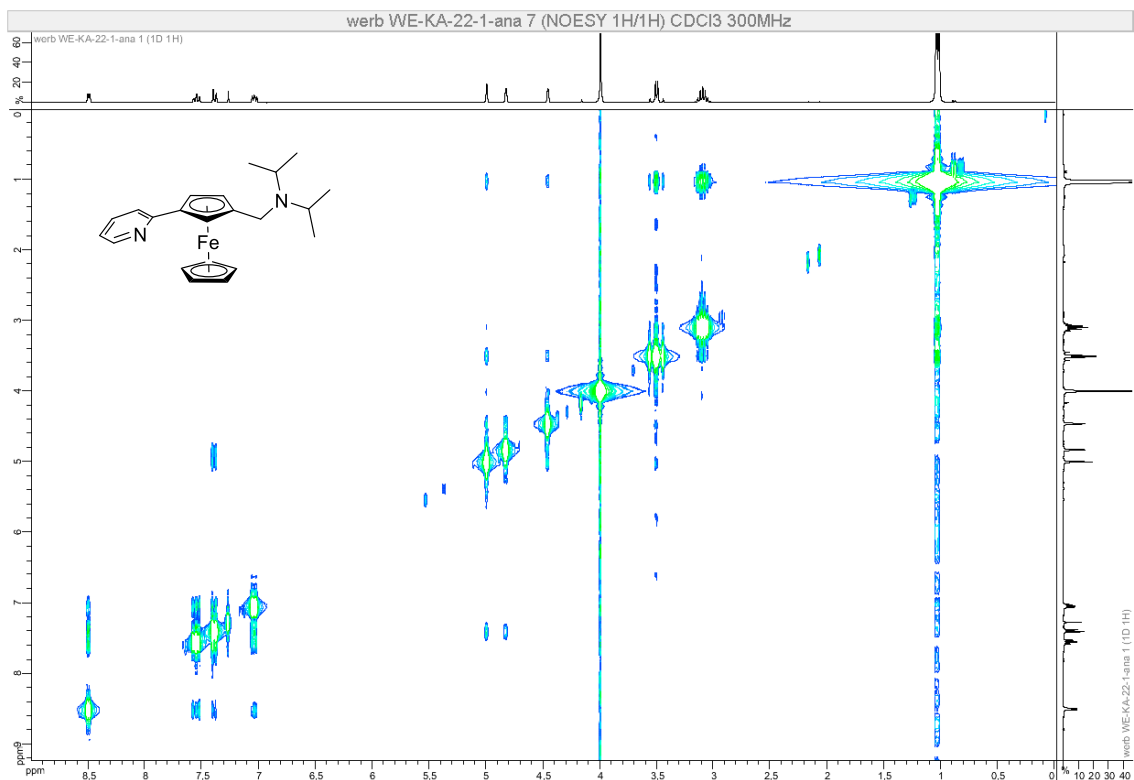


***1-(N,N-Diisopropylaminomethyl)-3-(2-pyridinyl)ferrocene (29)***

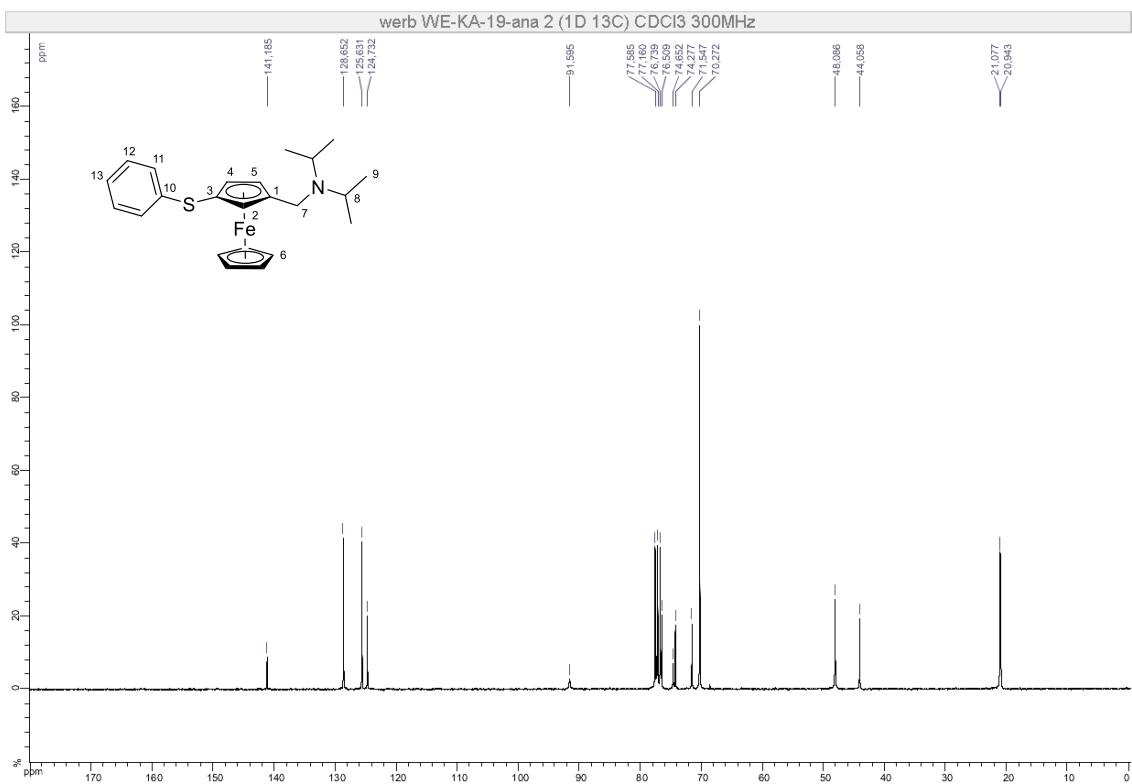
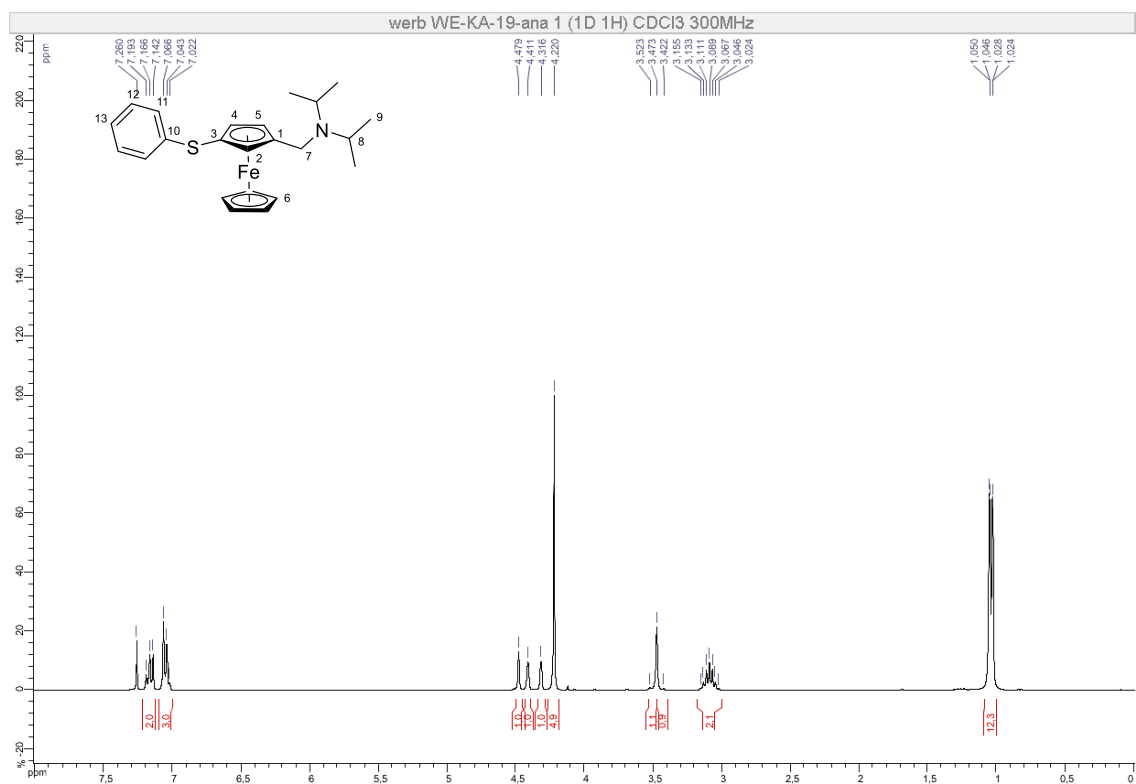


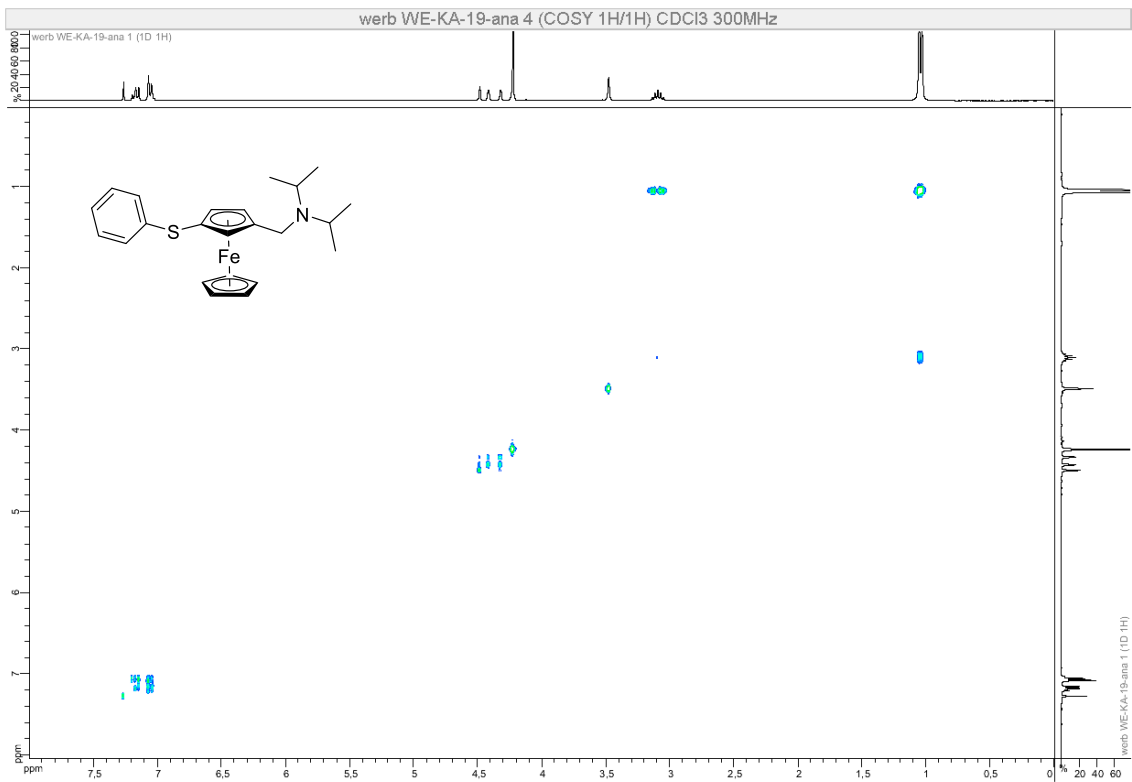
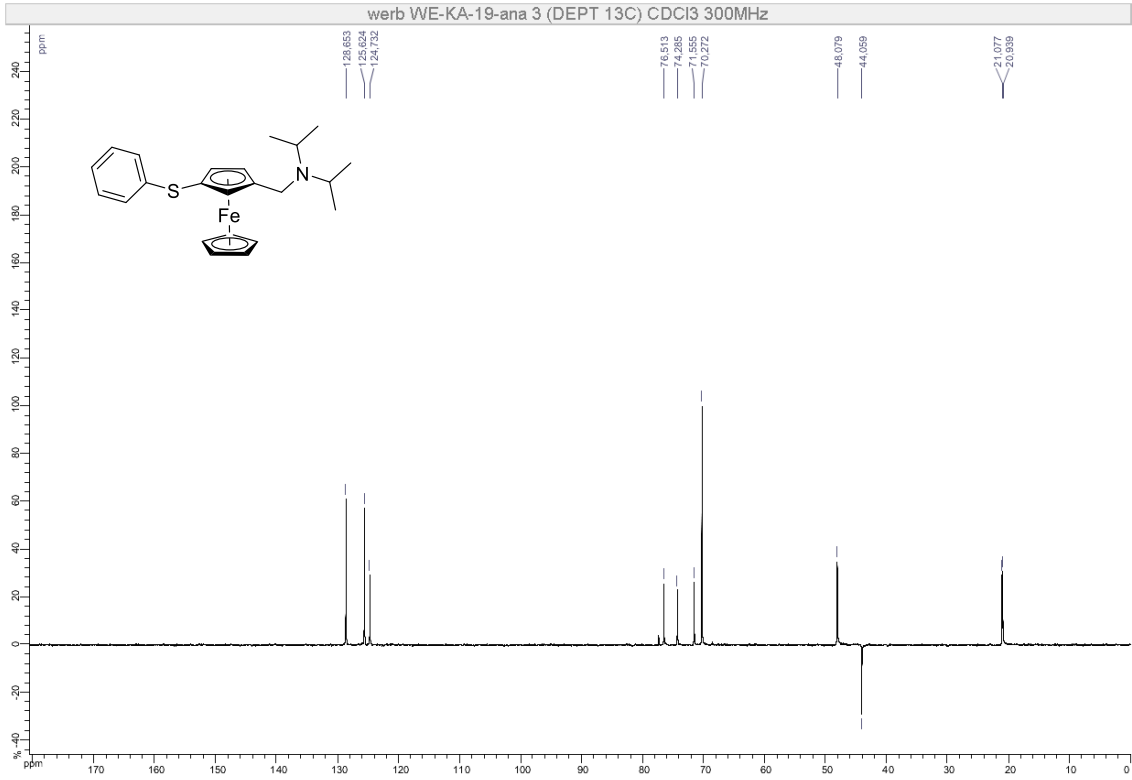


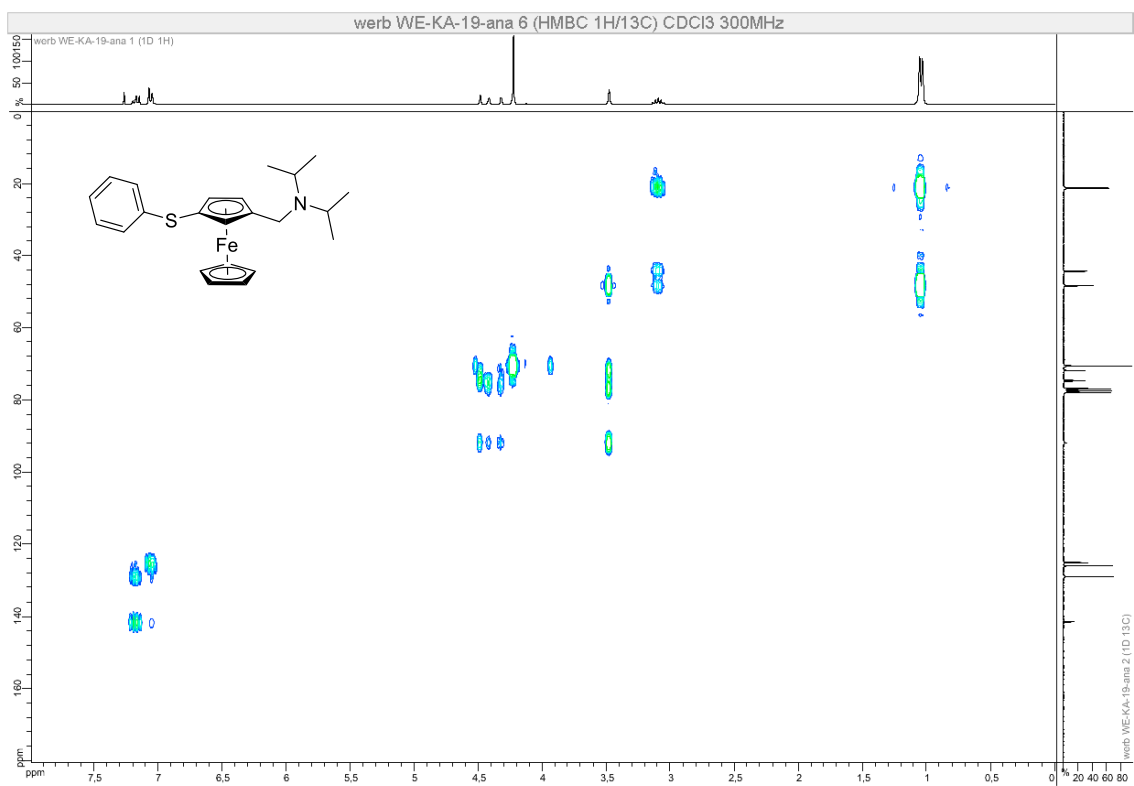
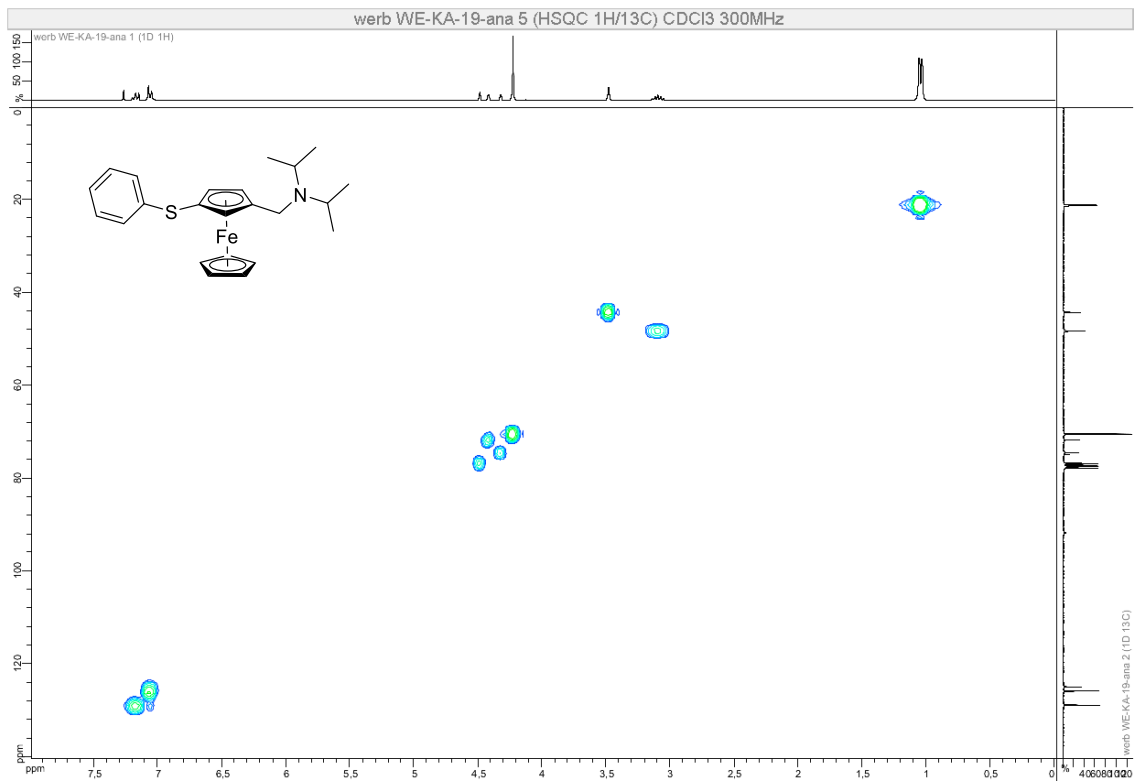




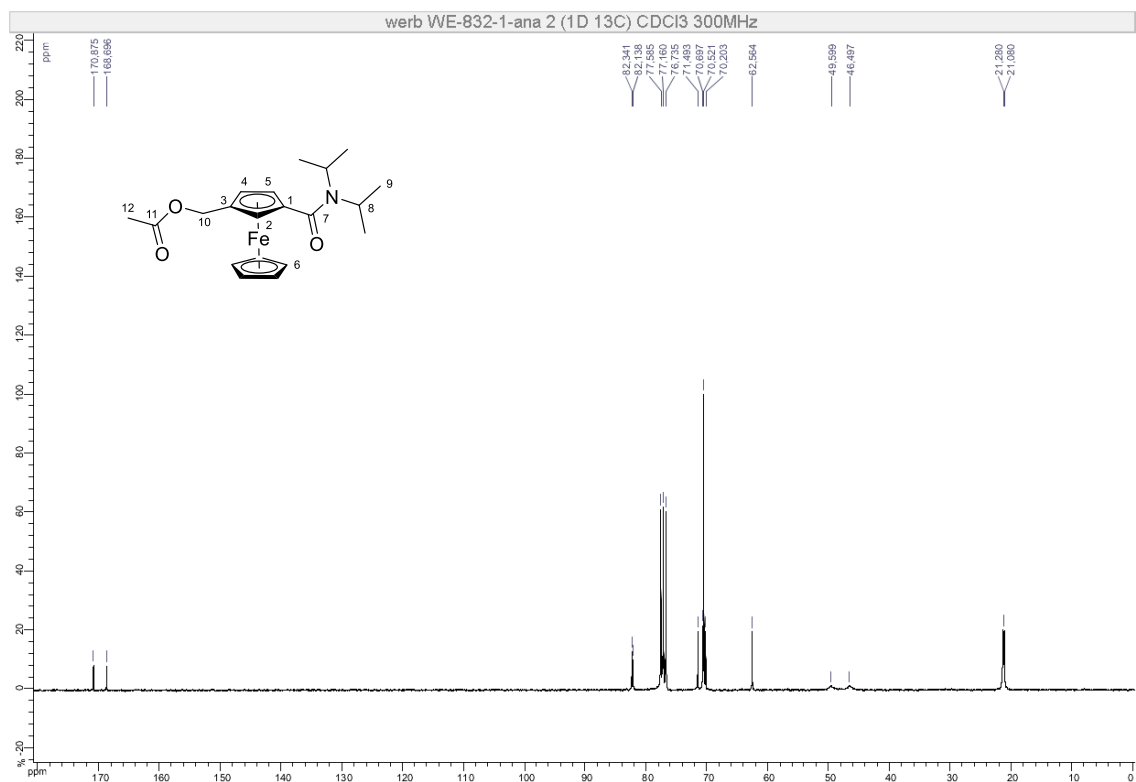
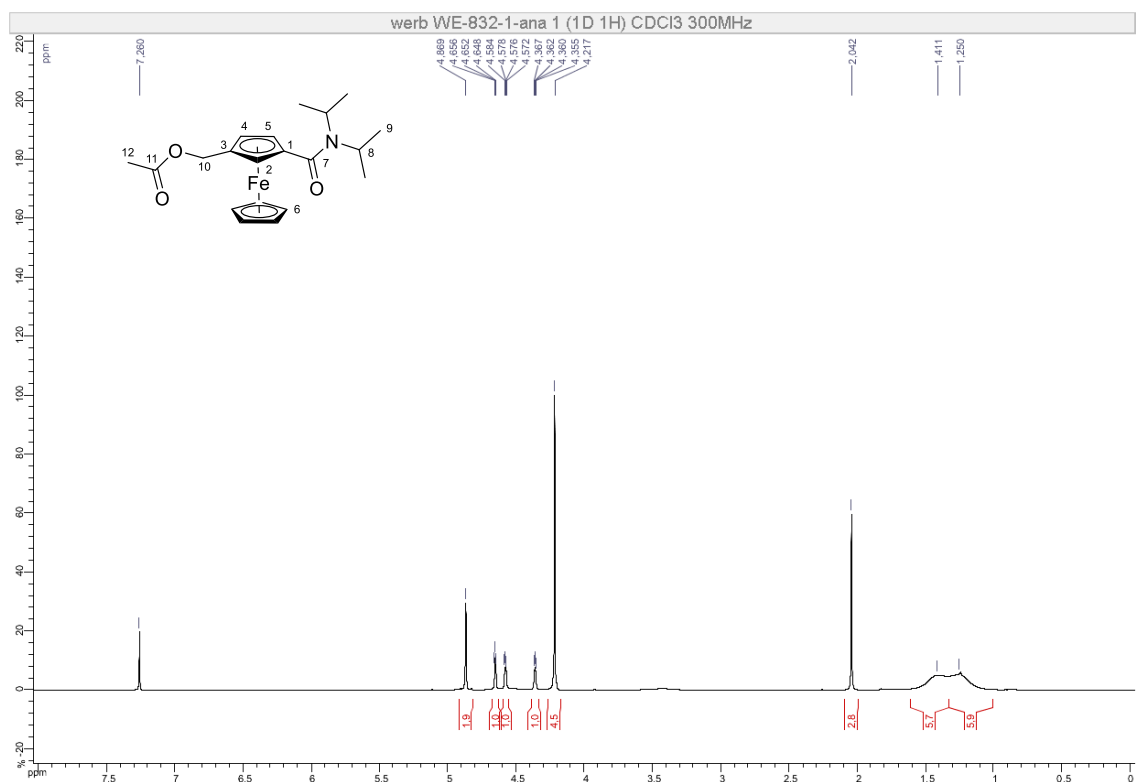
***1-(N,N-Diisopropylaminomethyl)-3-(phenylthio)ferrocene (30)***



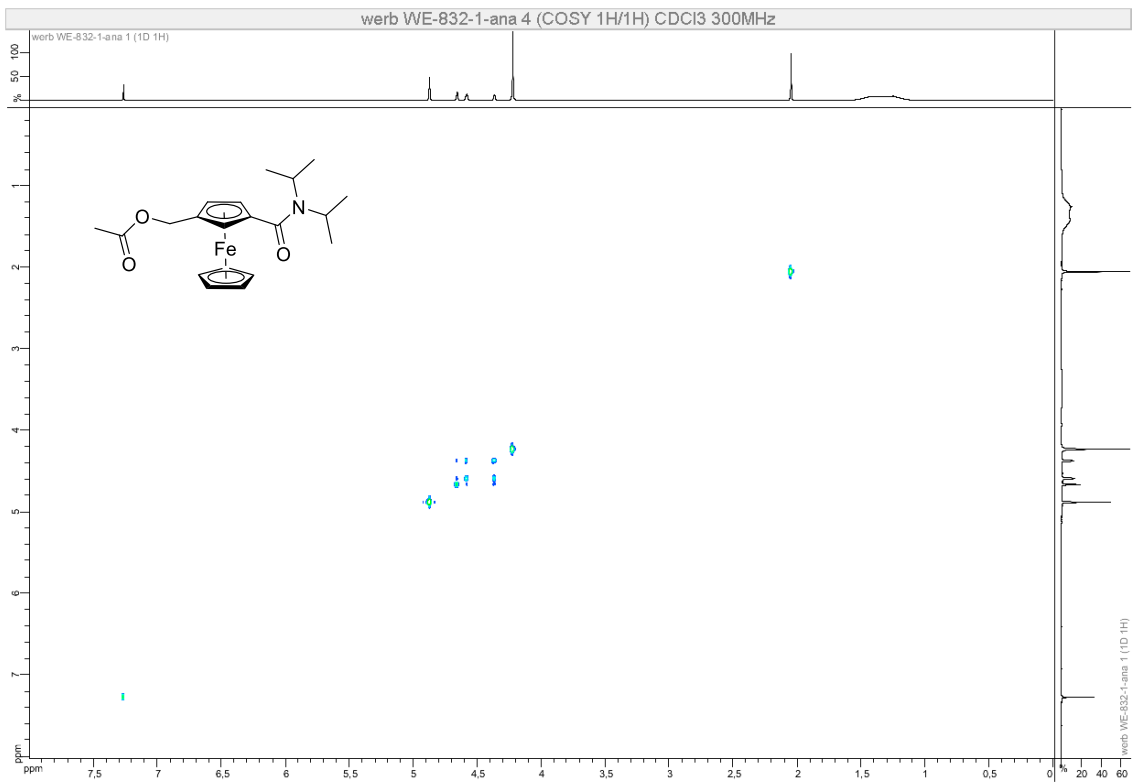
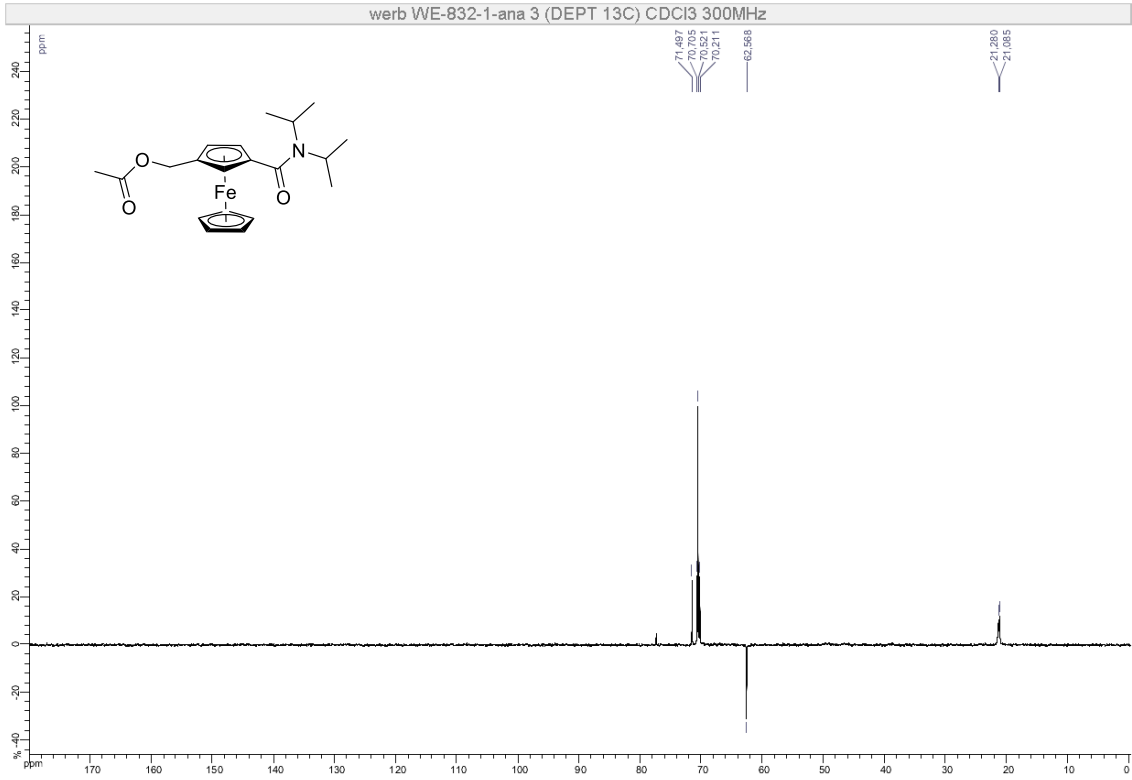


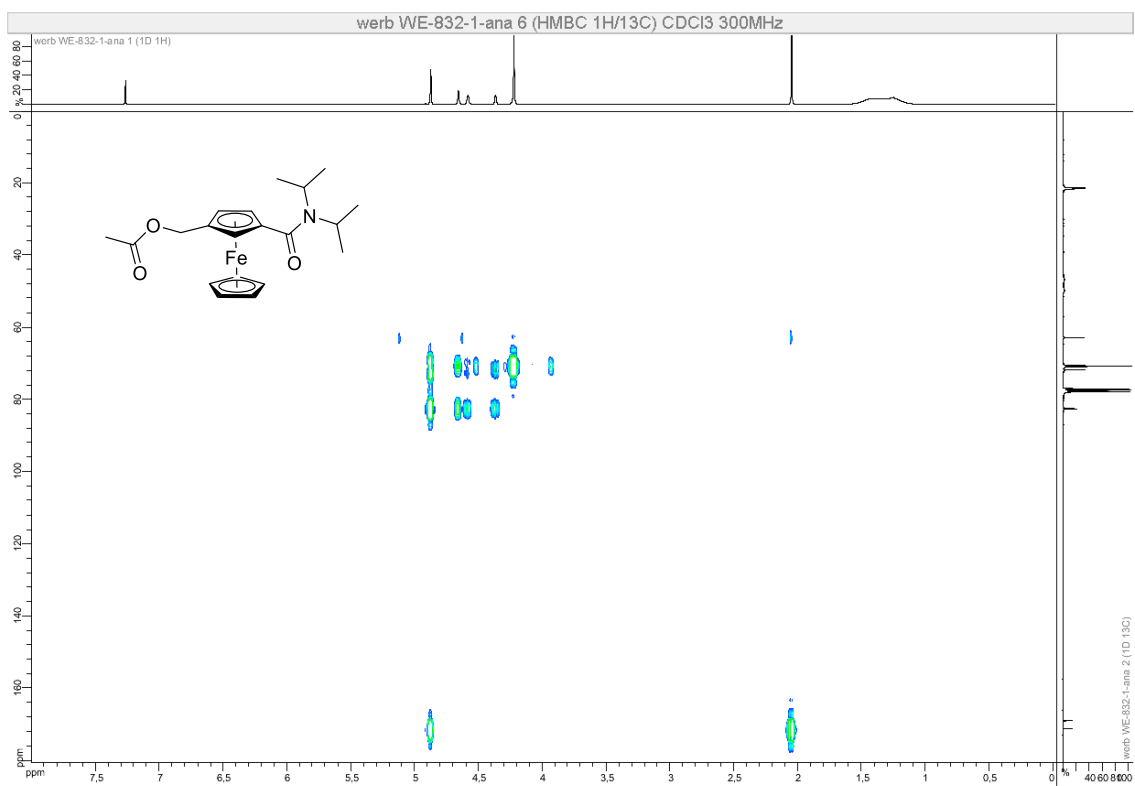
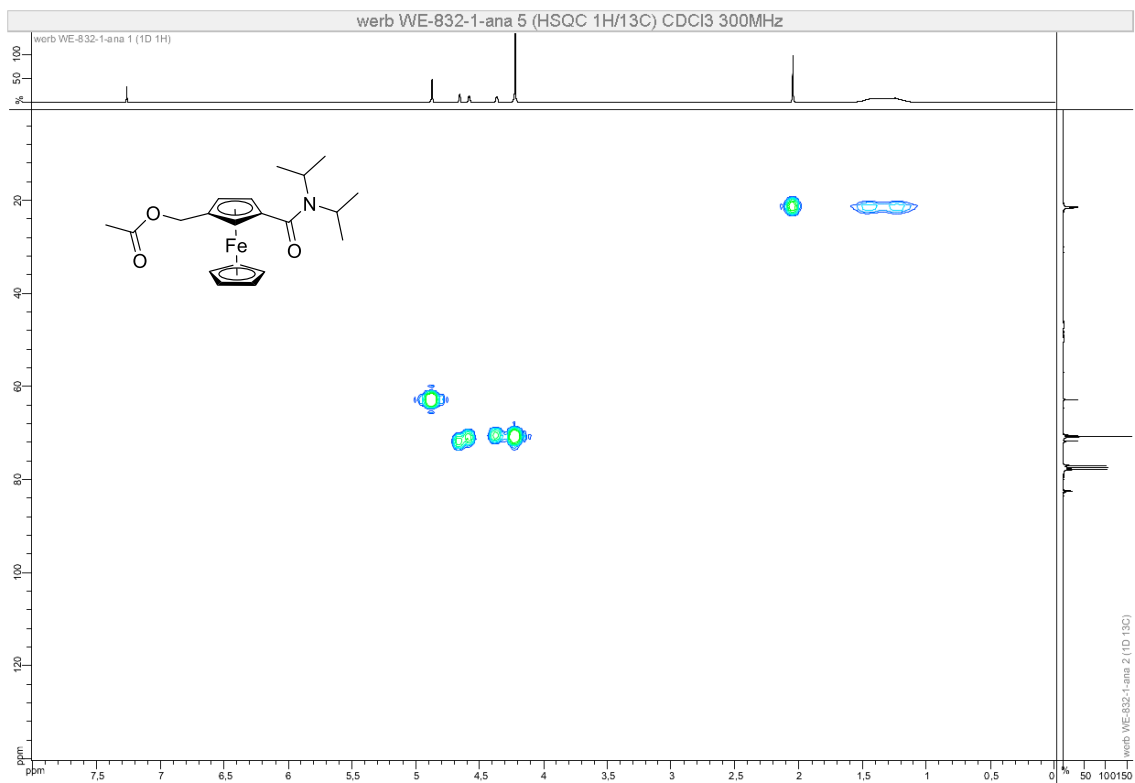


### 3-(Acetoxymethyl)-N,N-diisopropylferrocenecarboxamide (31)

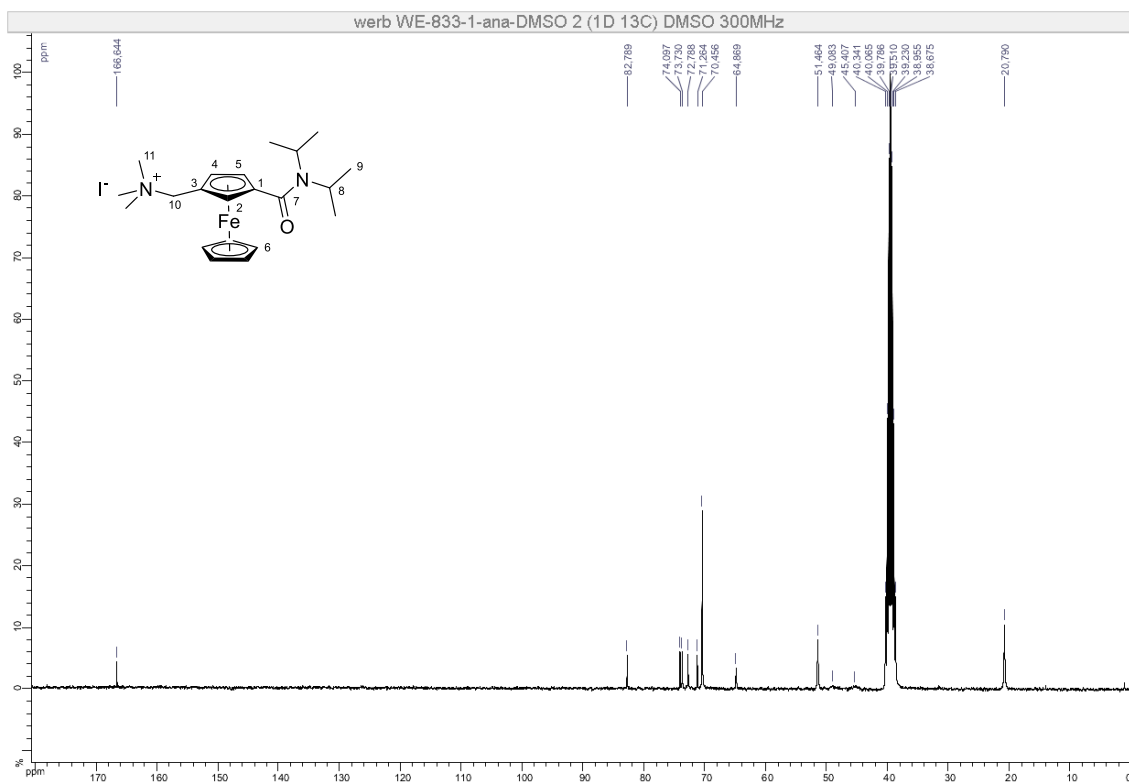
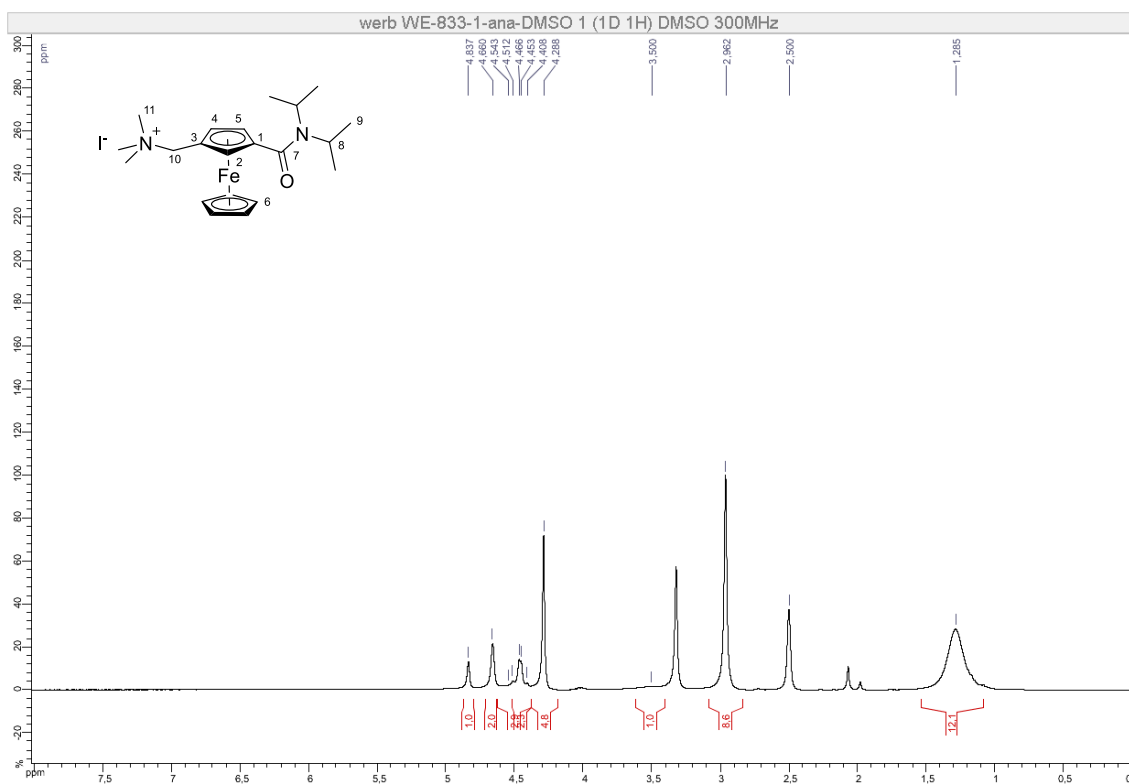


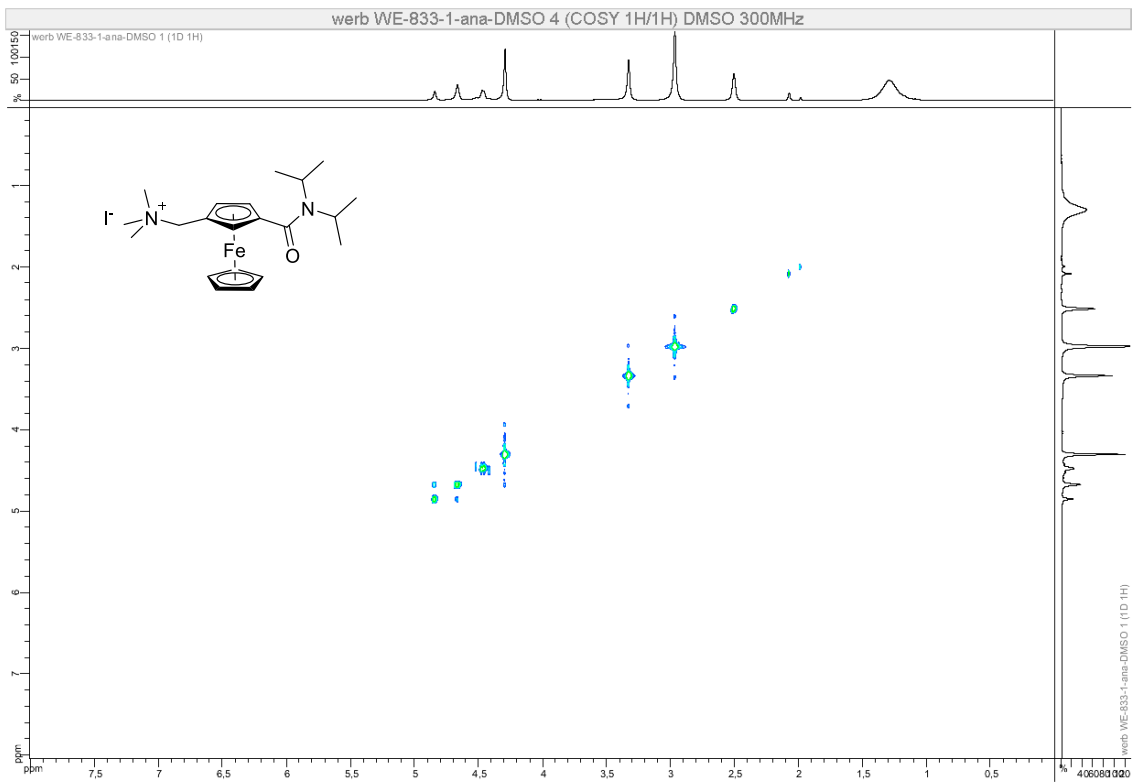
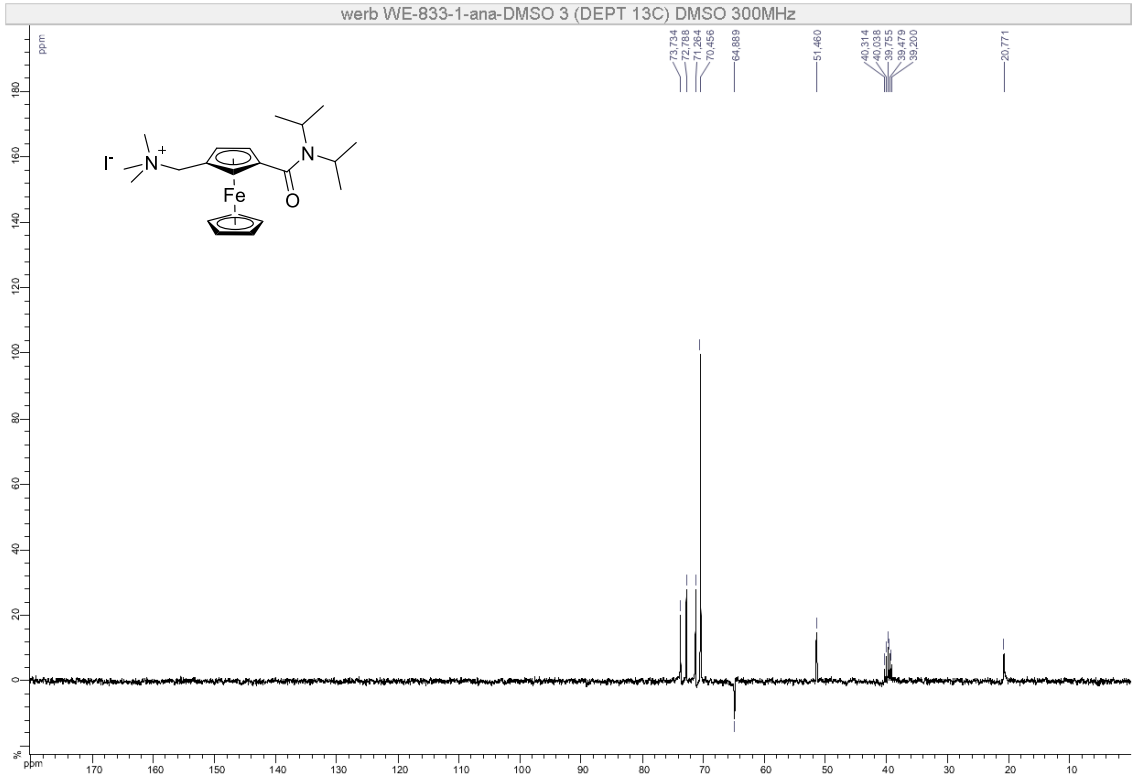


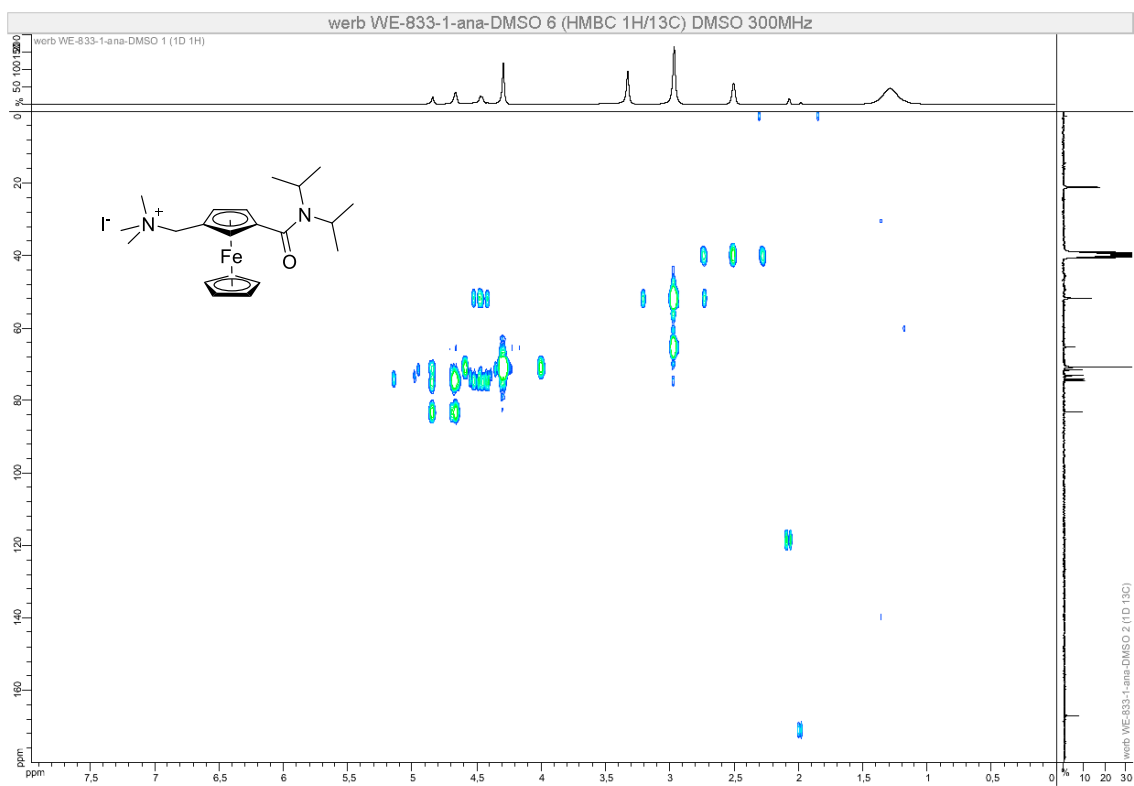
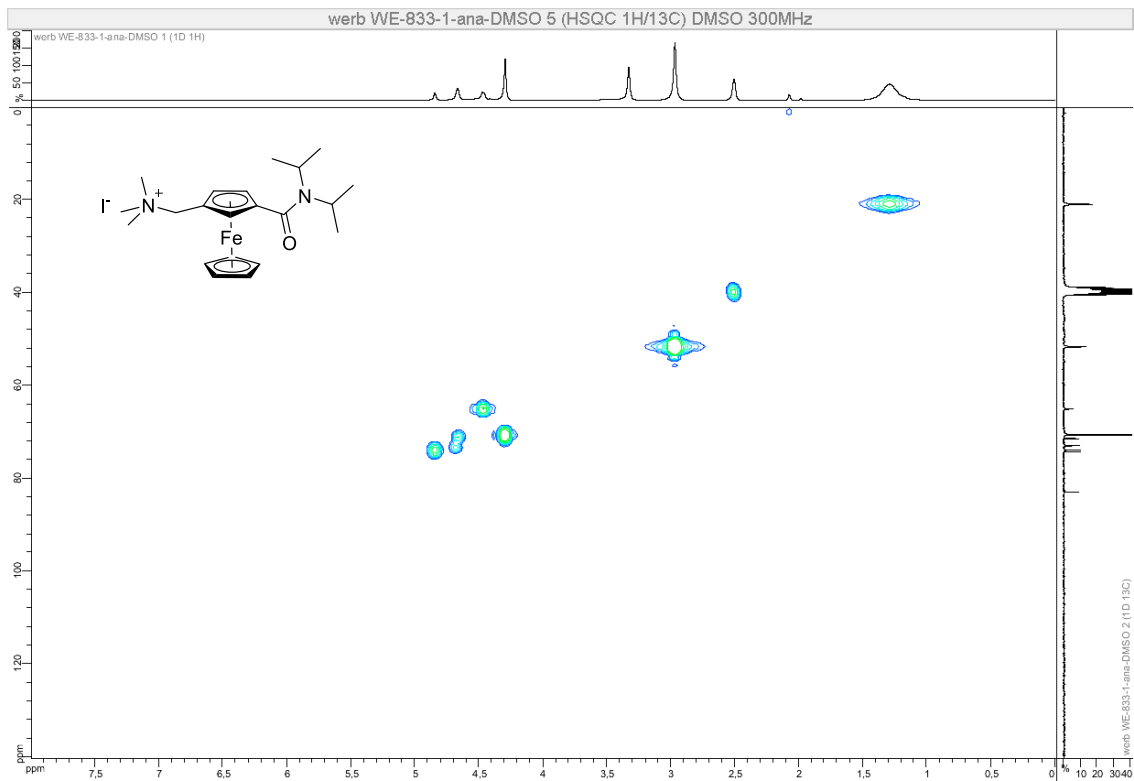


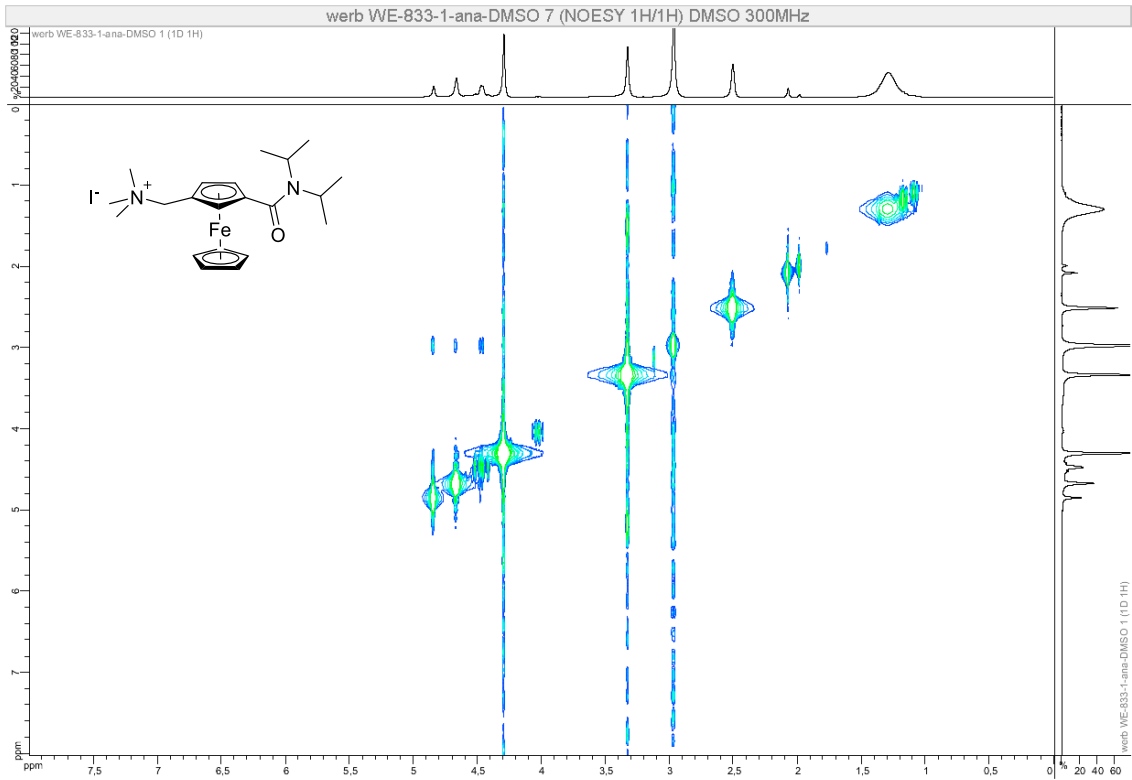


**3-(Diisopropylaminocarbonyl)ferrocenylmethyl)trimethyl-ammonium iodide (32)**

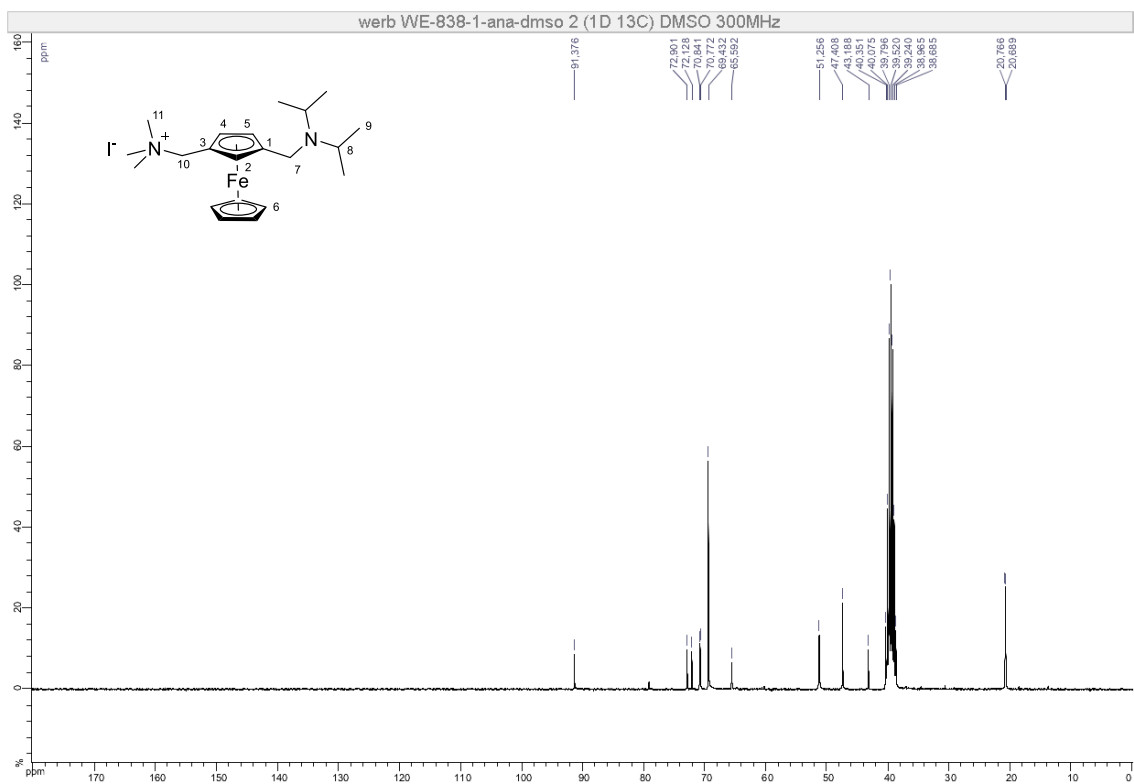
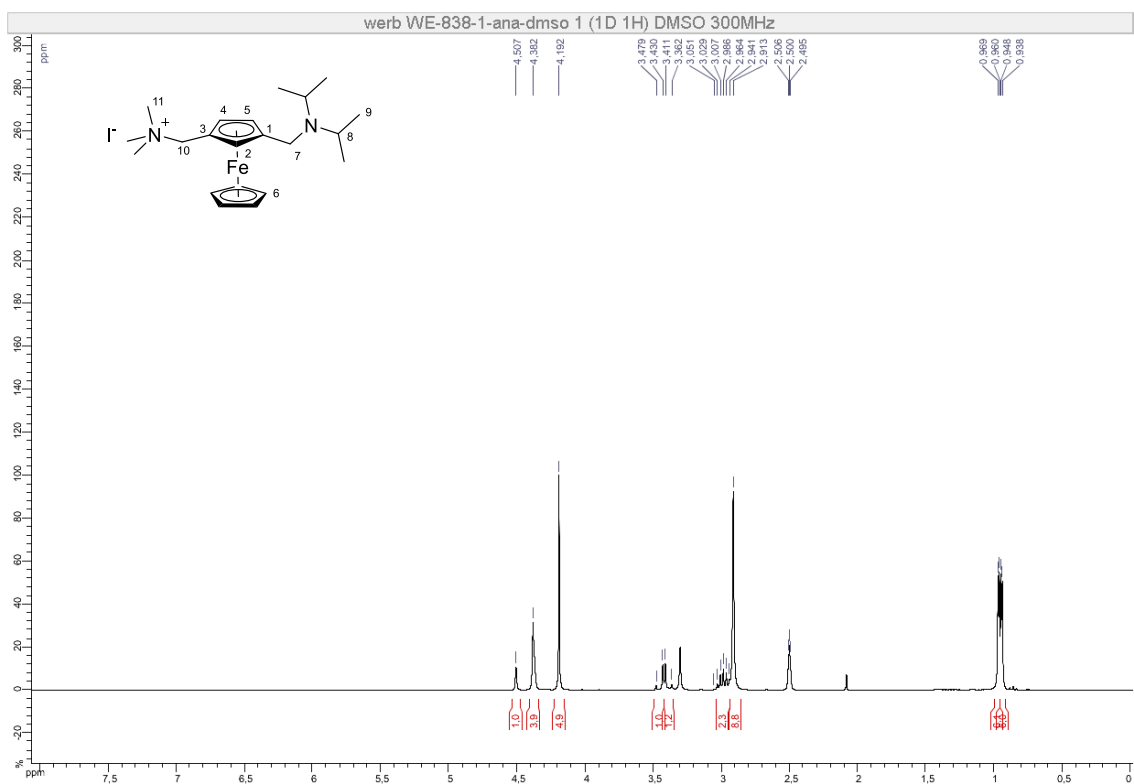


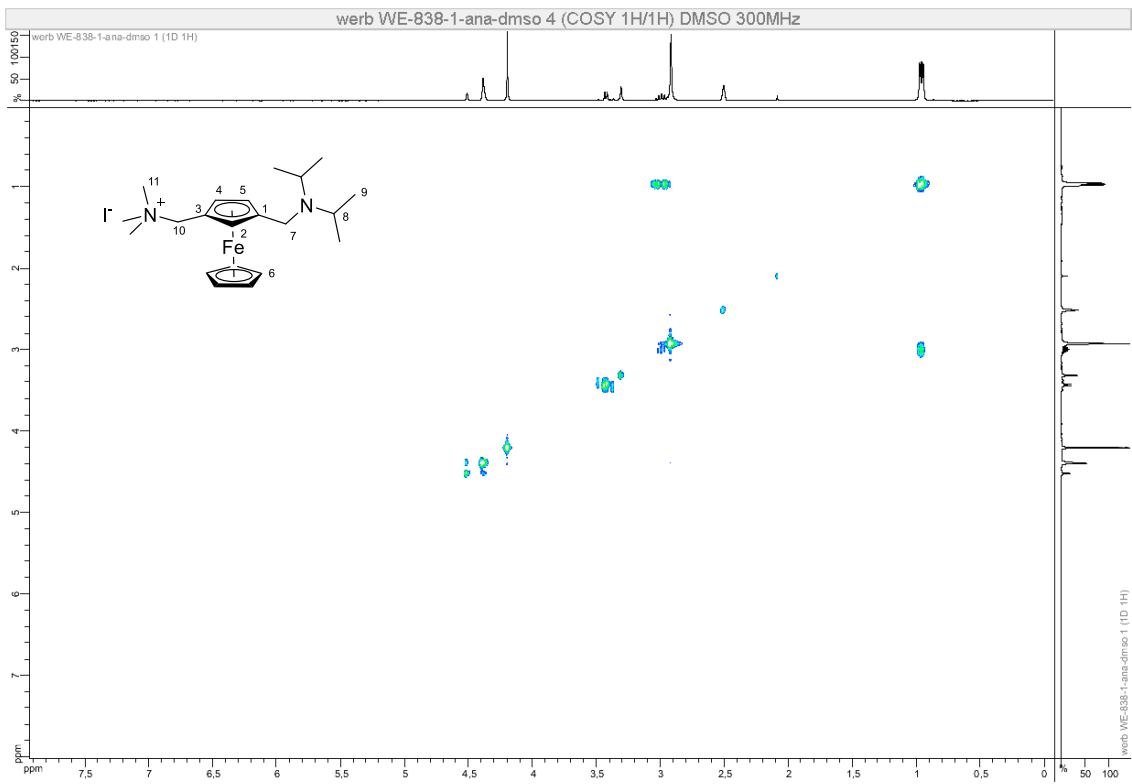
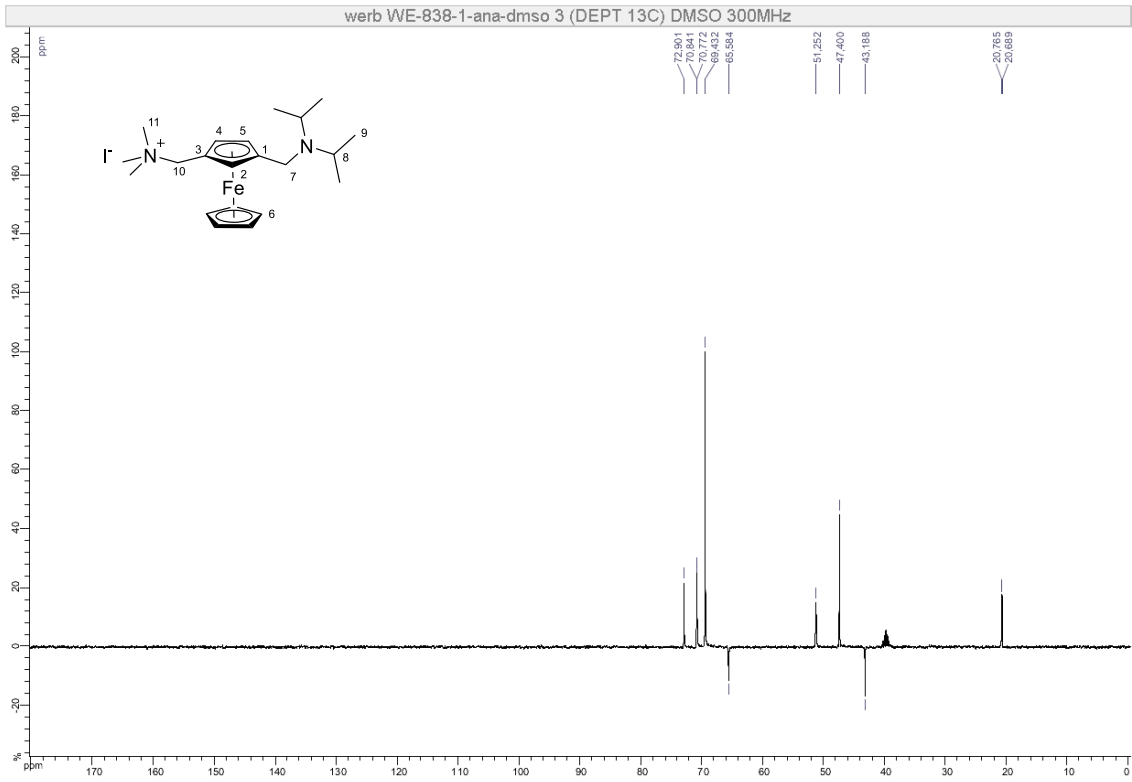




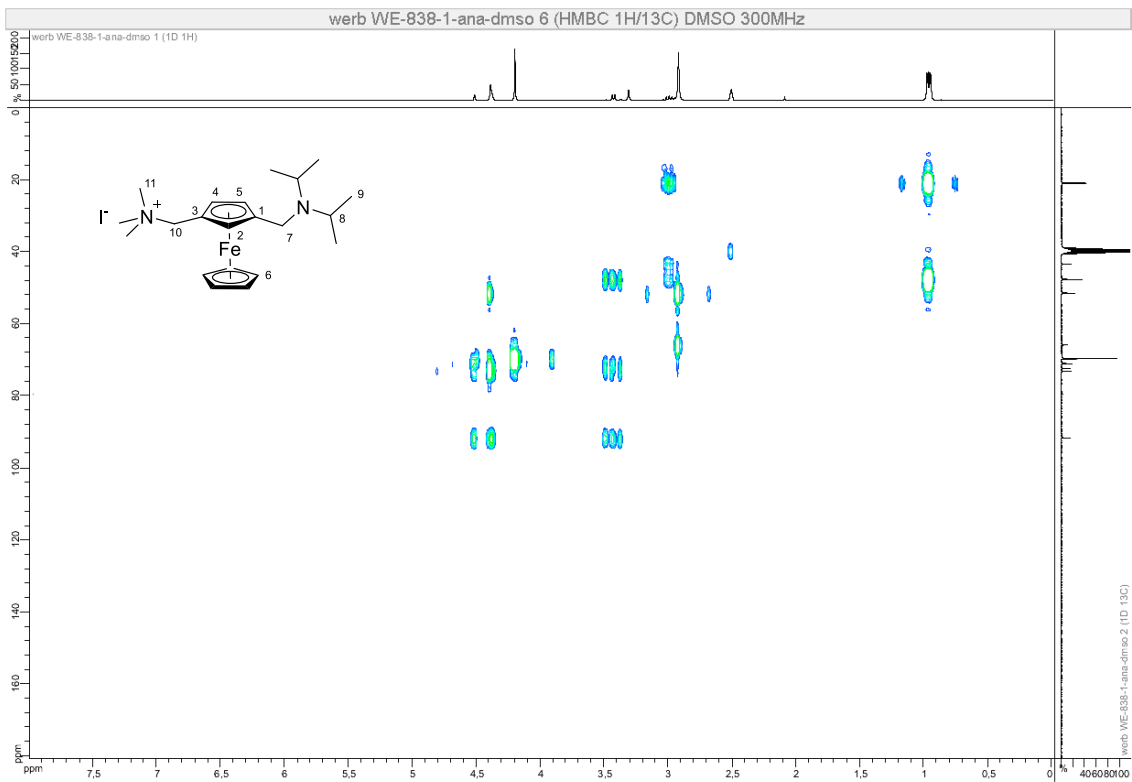
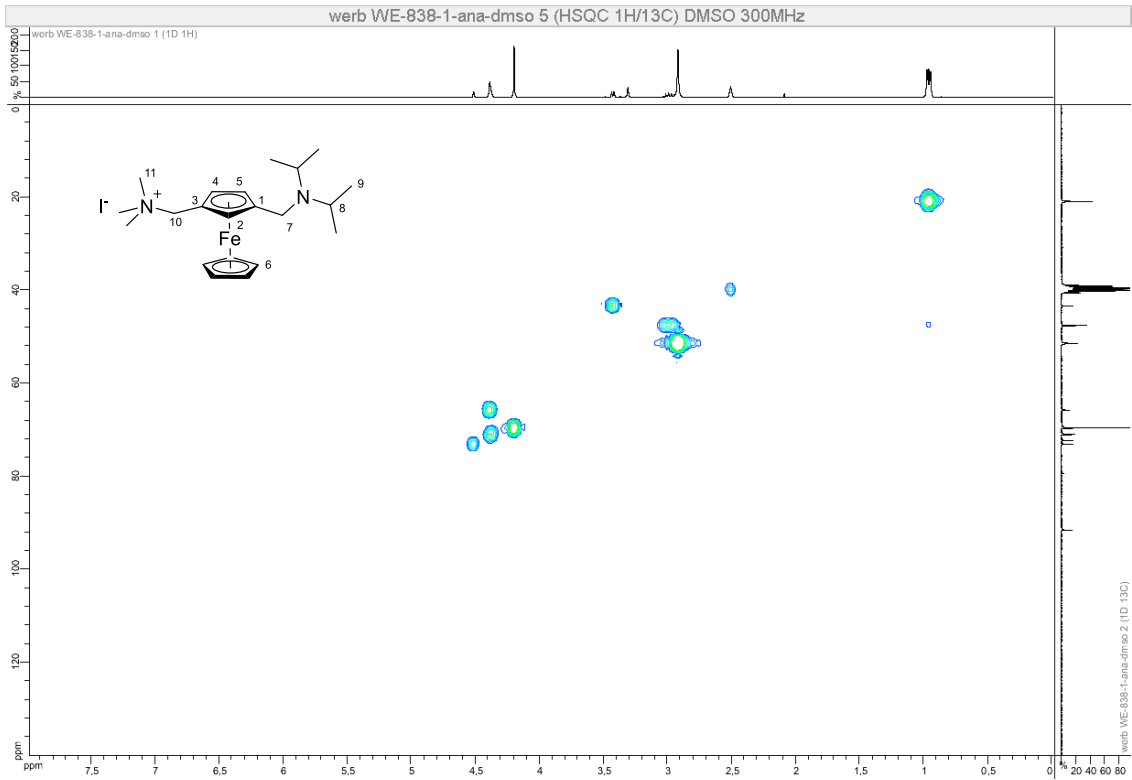


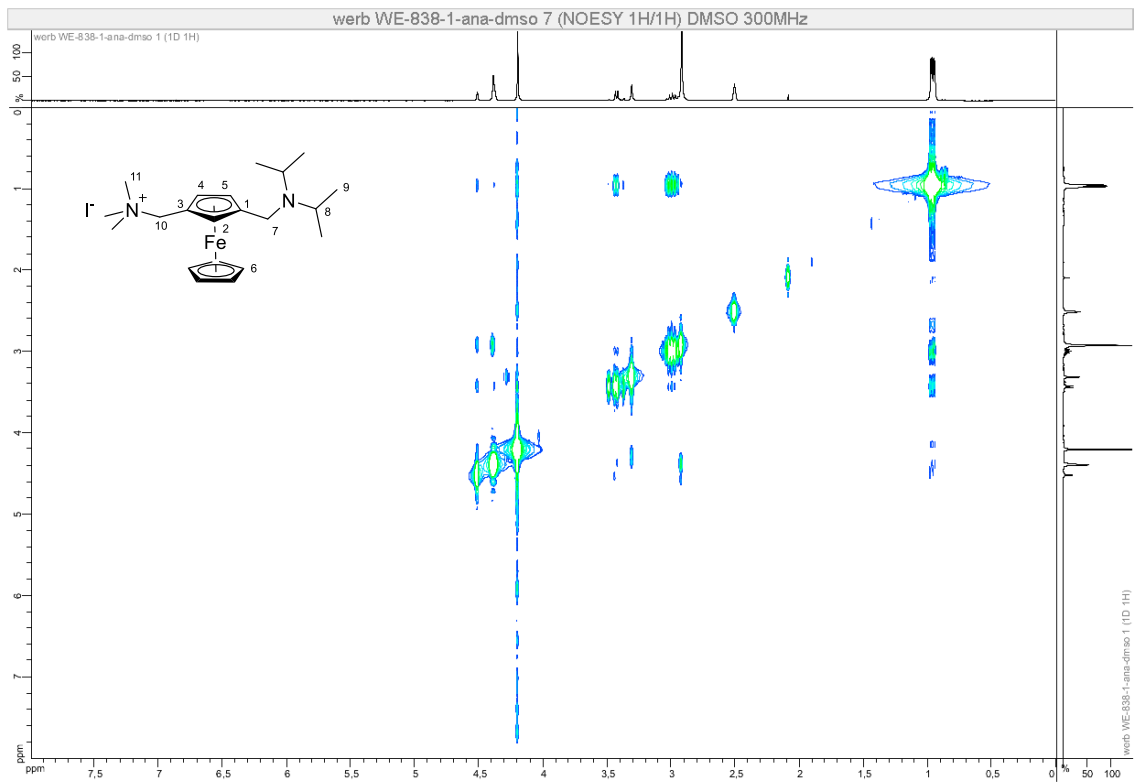
**3-(Diisopropylaminomethyl)ferrocenylmethyl)trimethyl-ammonium iodide (33)**



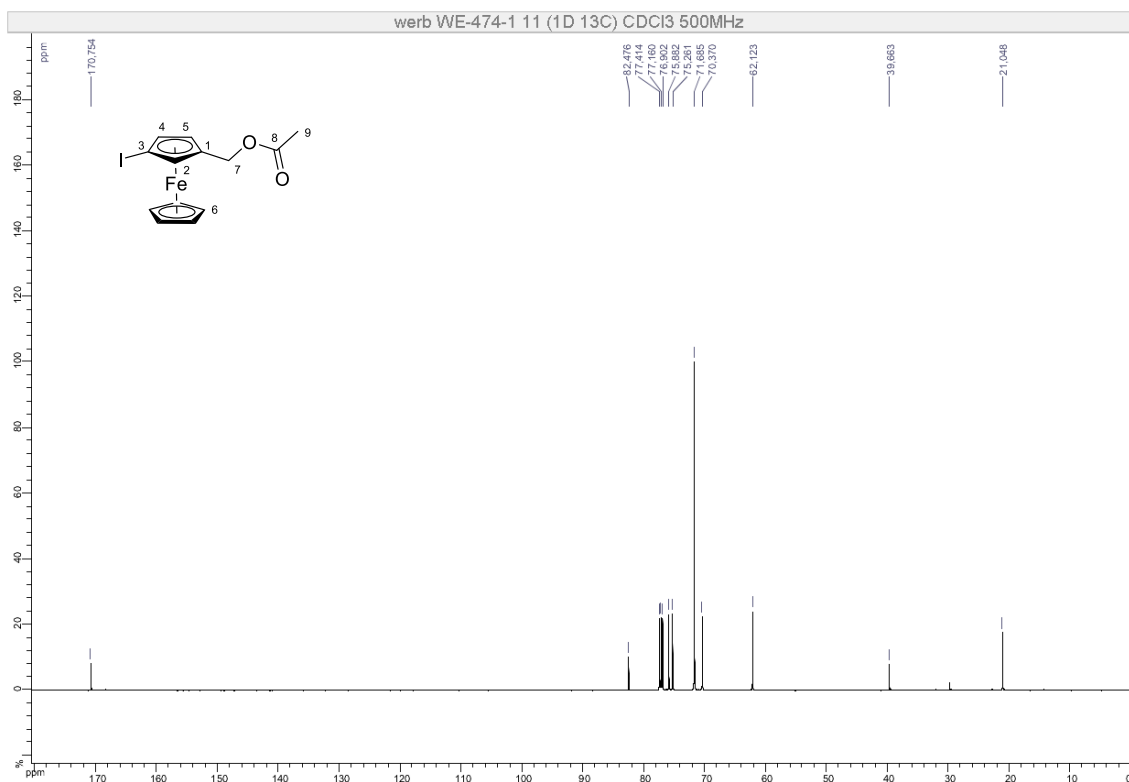
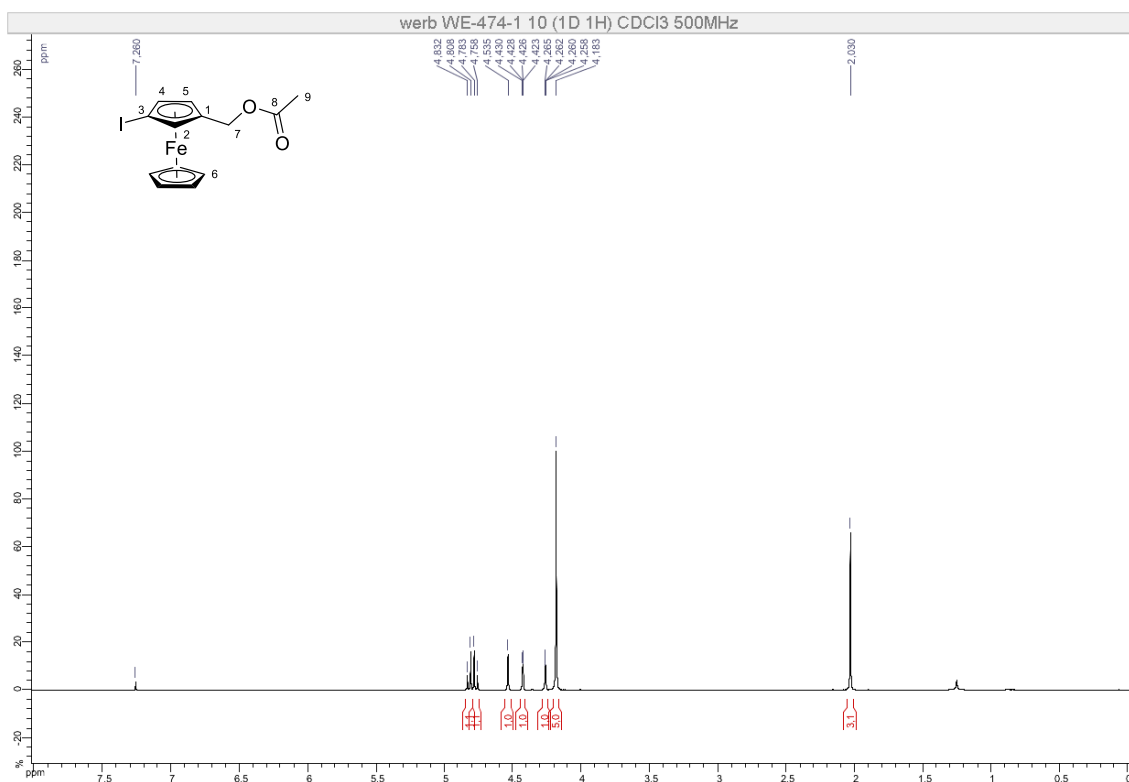


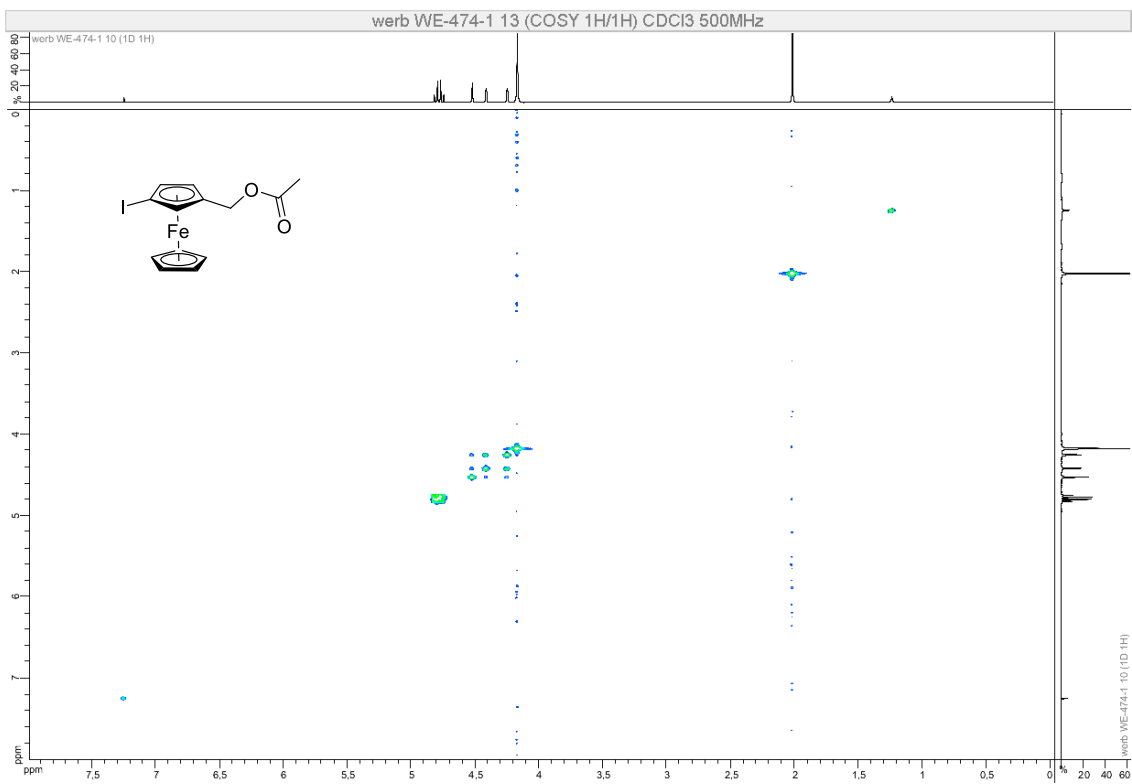
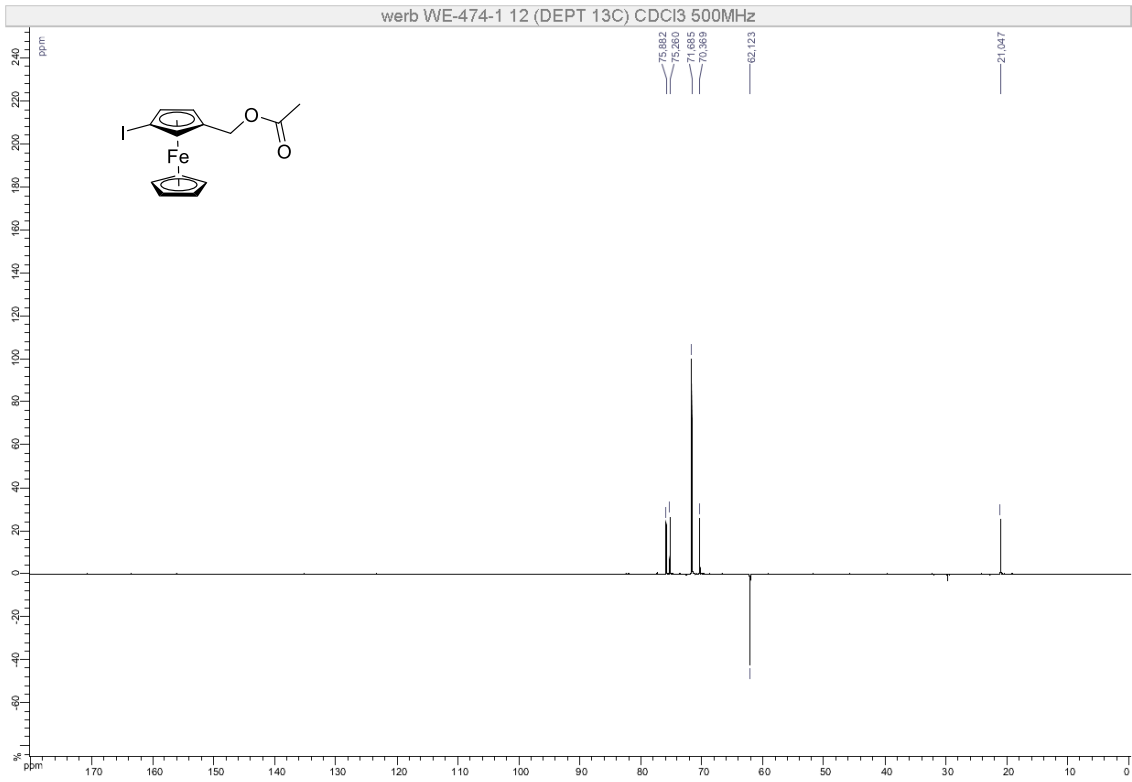


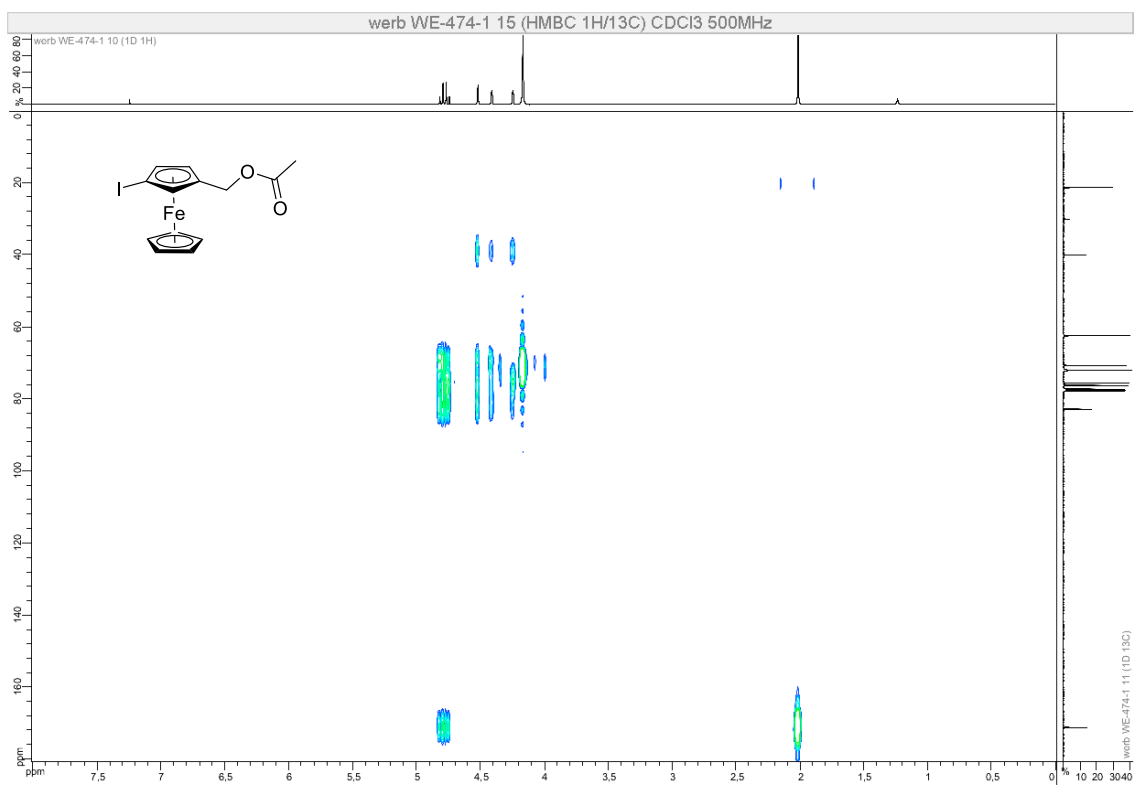
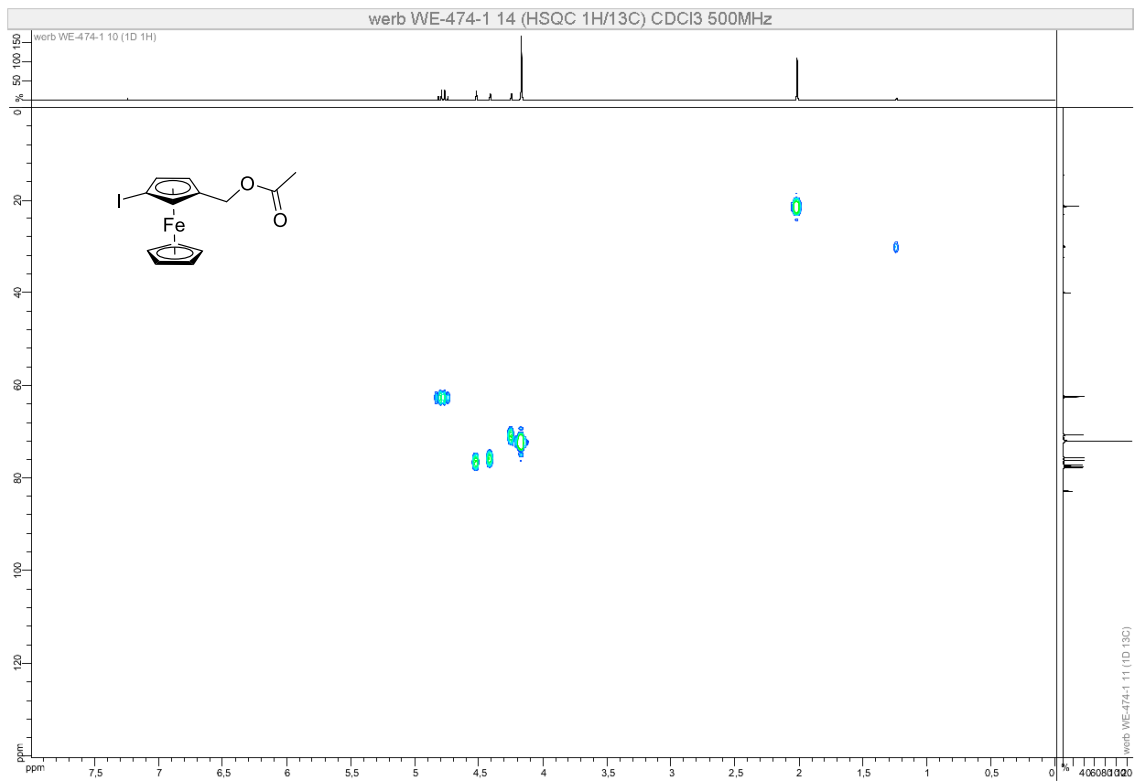




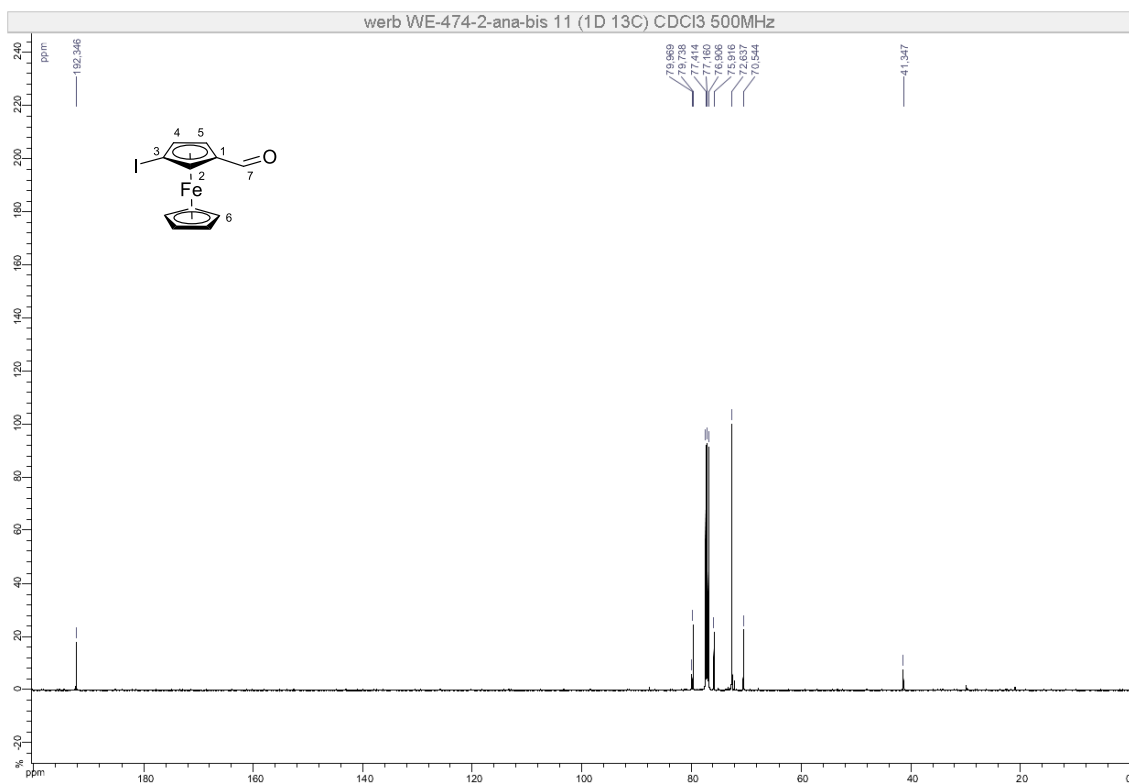
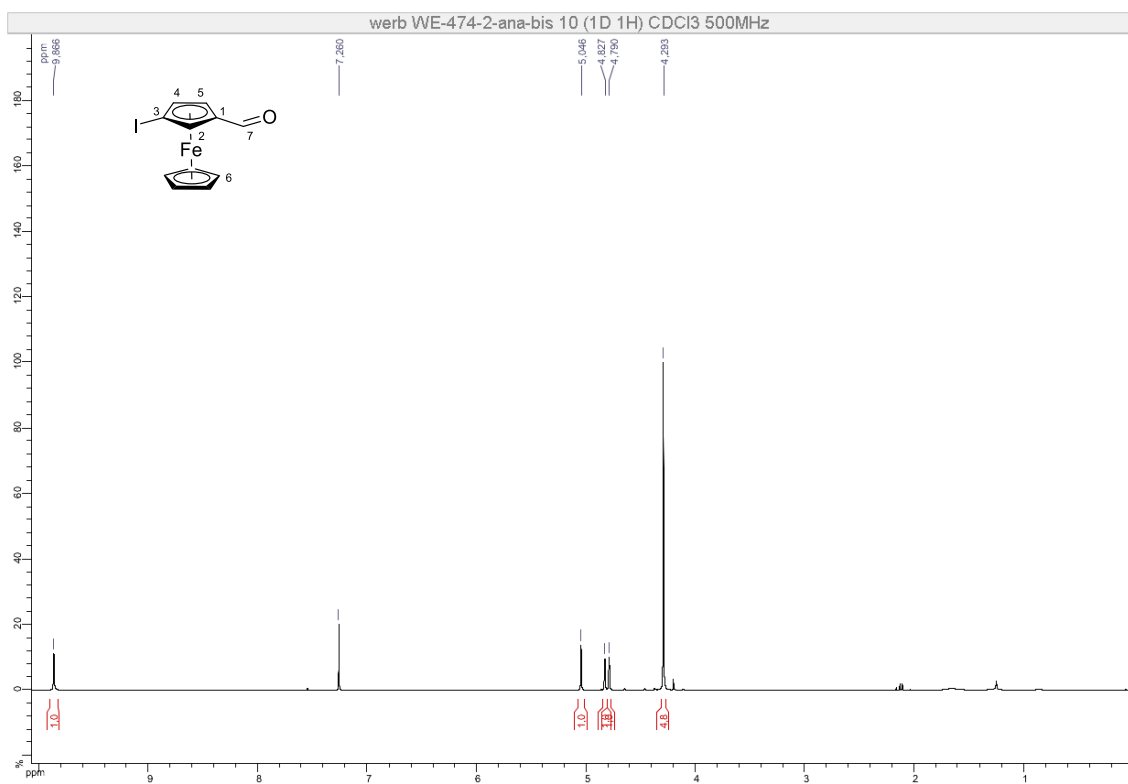
**1-(Acetoxymethyl)-3-iodoferrocene (34)**

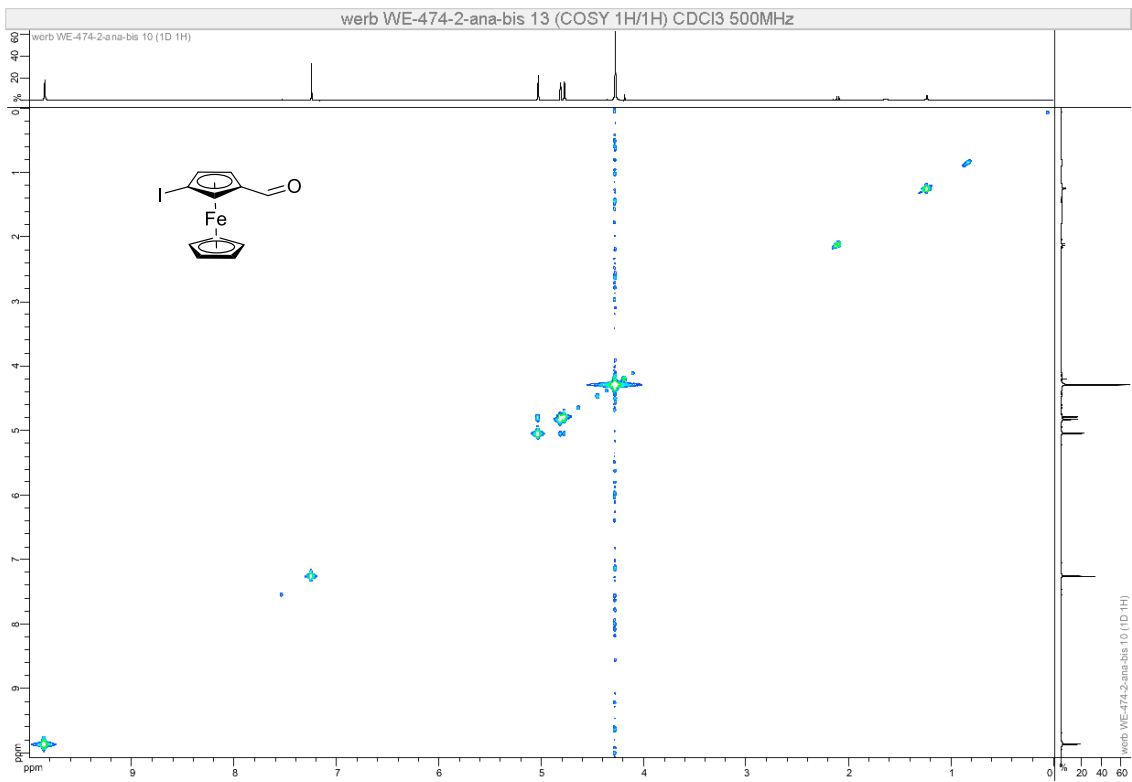
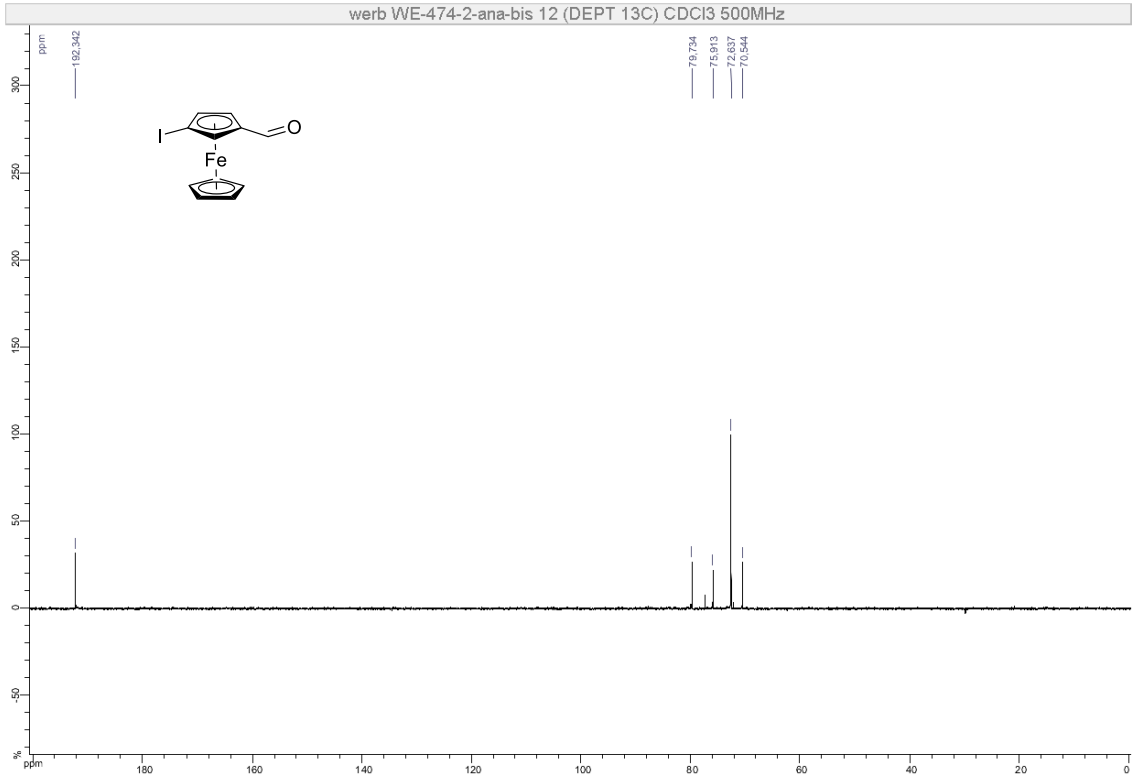


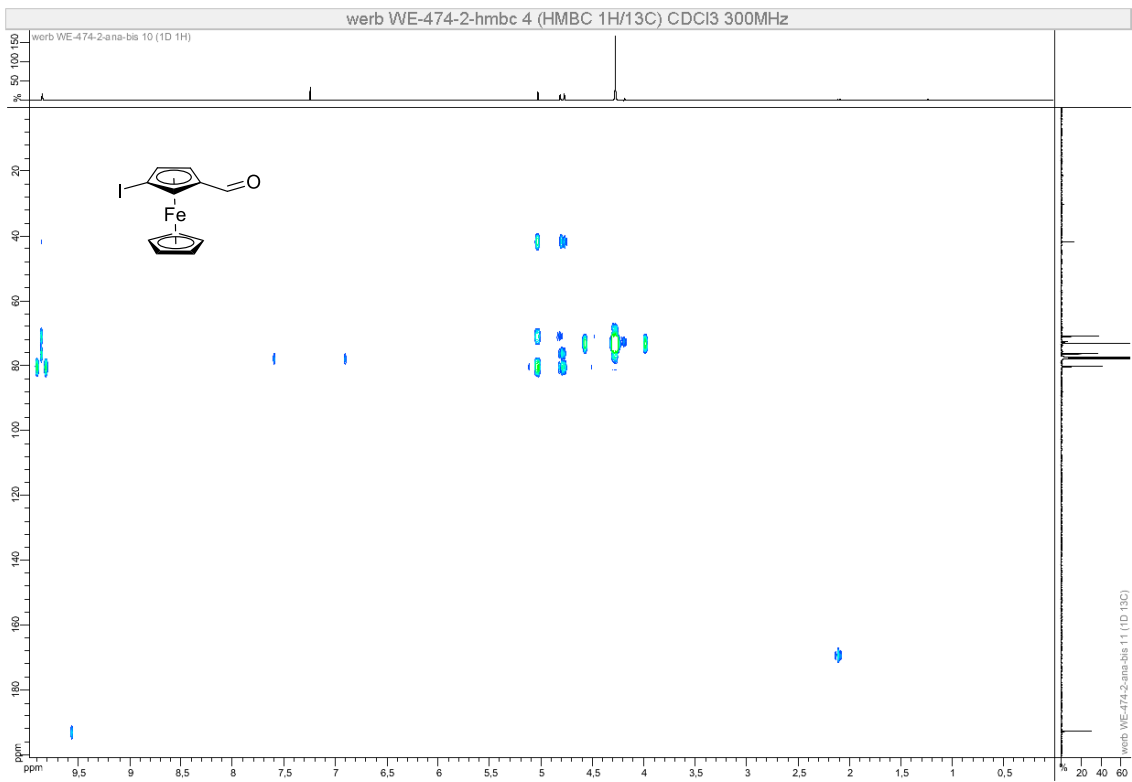
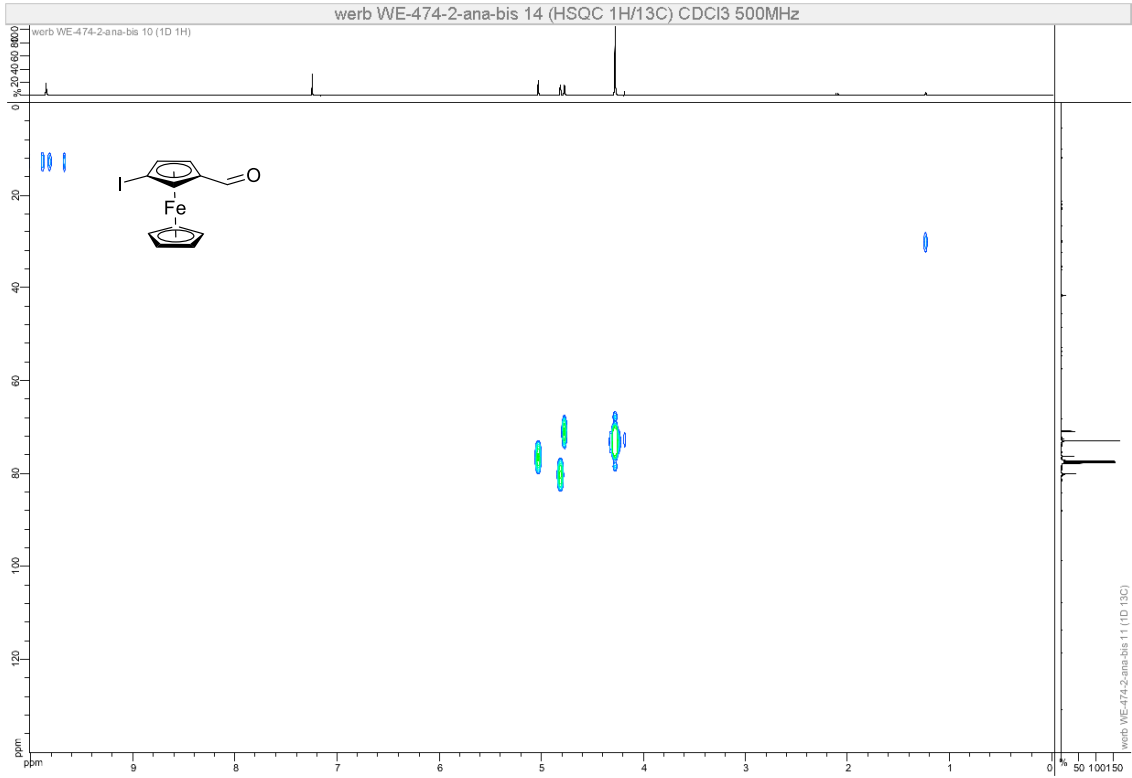




### 3-Iodoferrocenecarboxaldehyde (35)

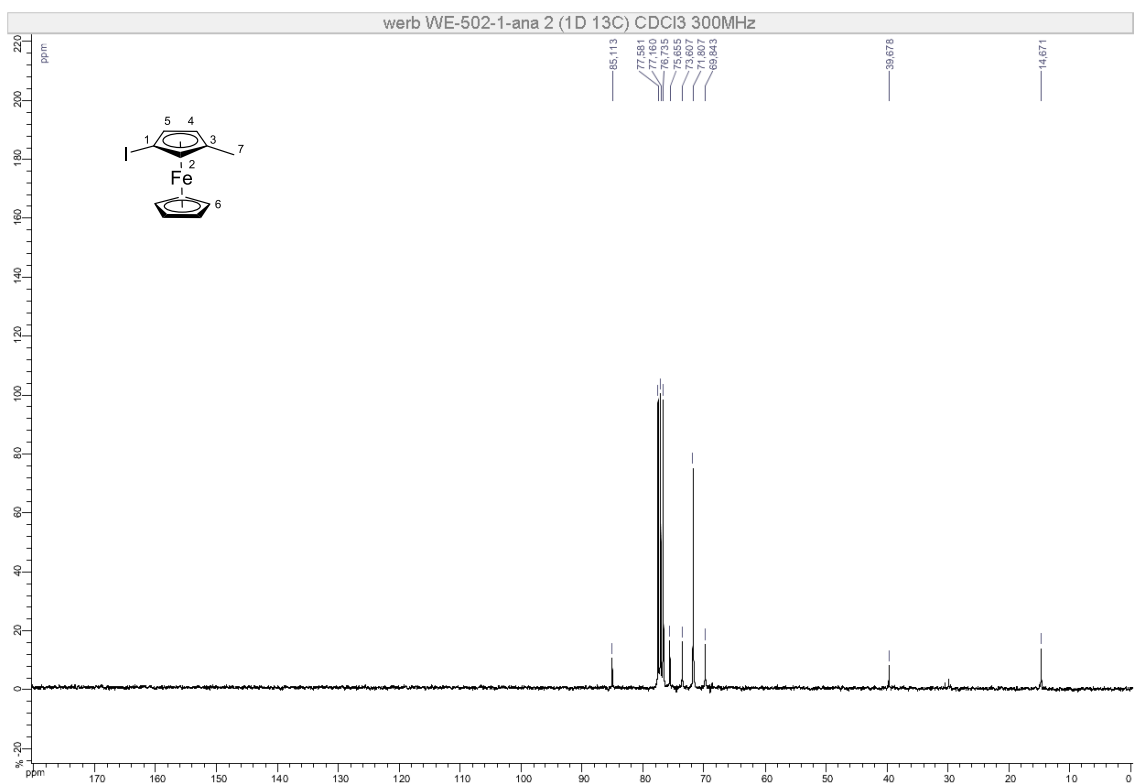
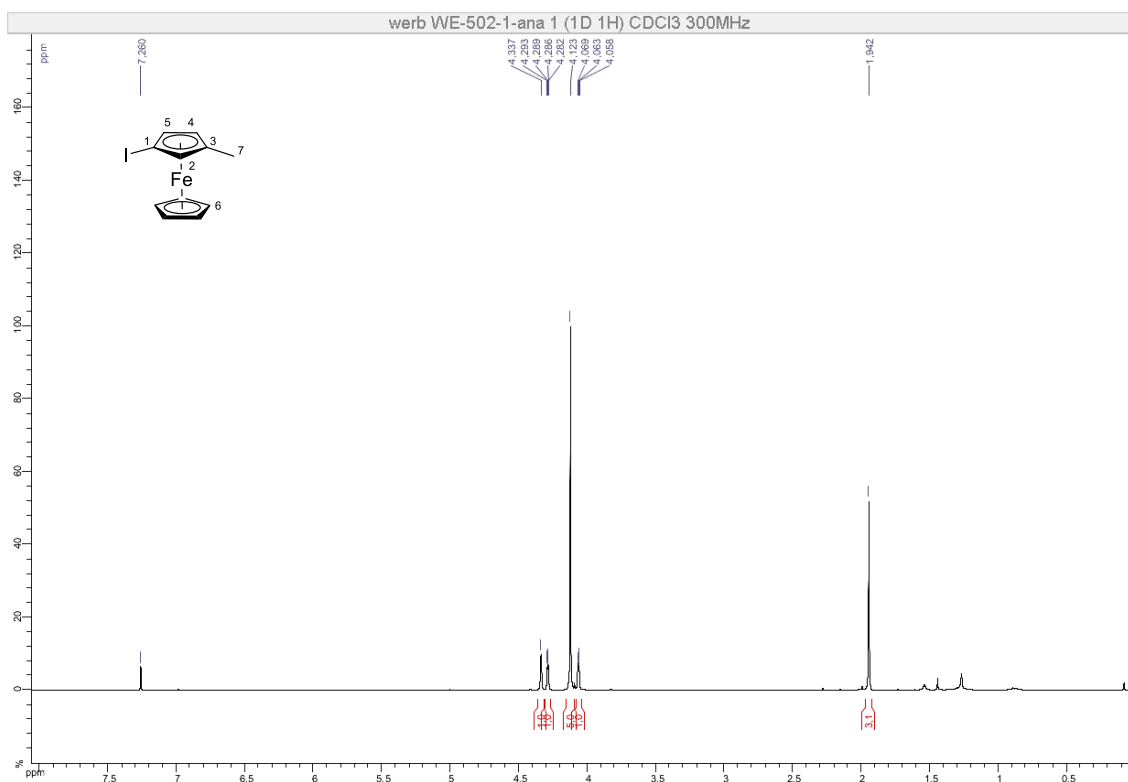


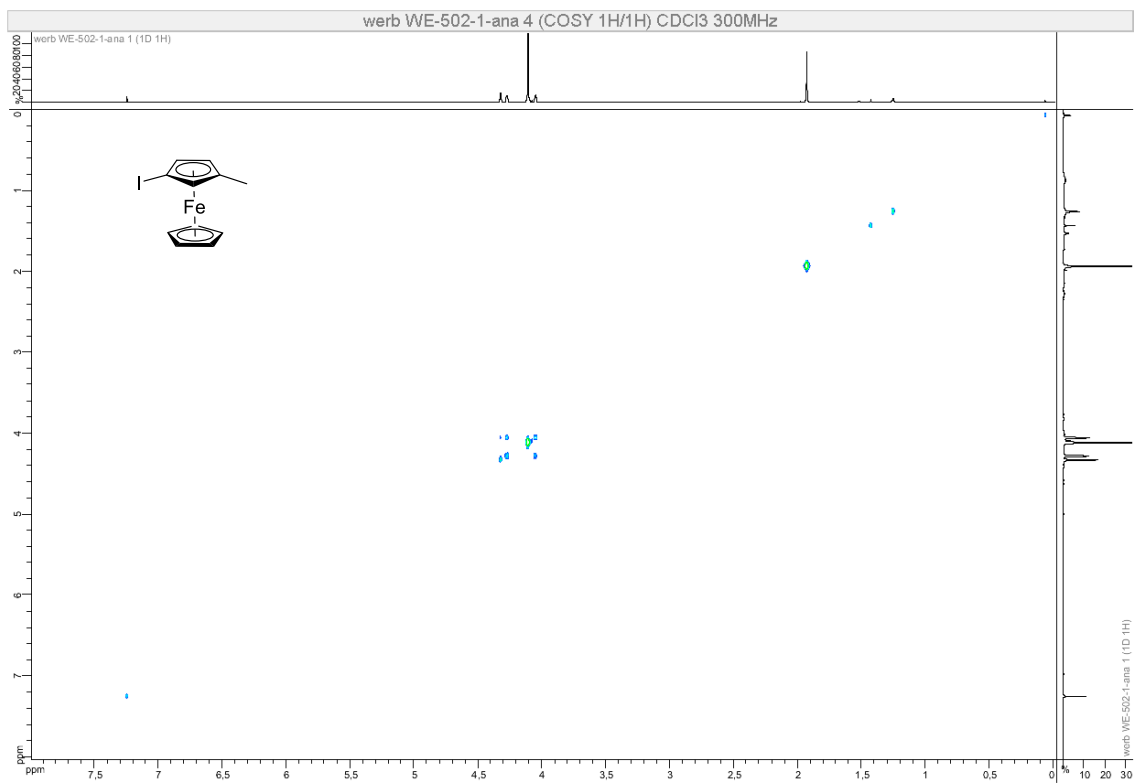
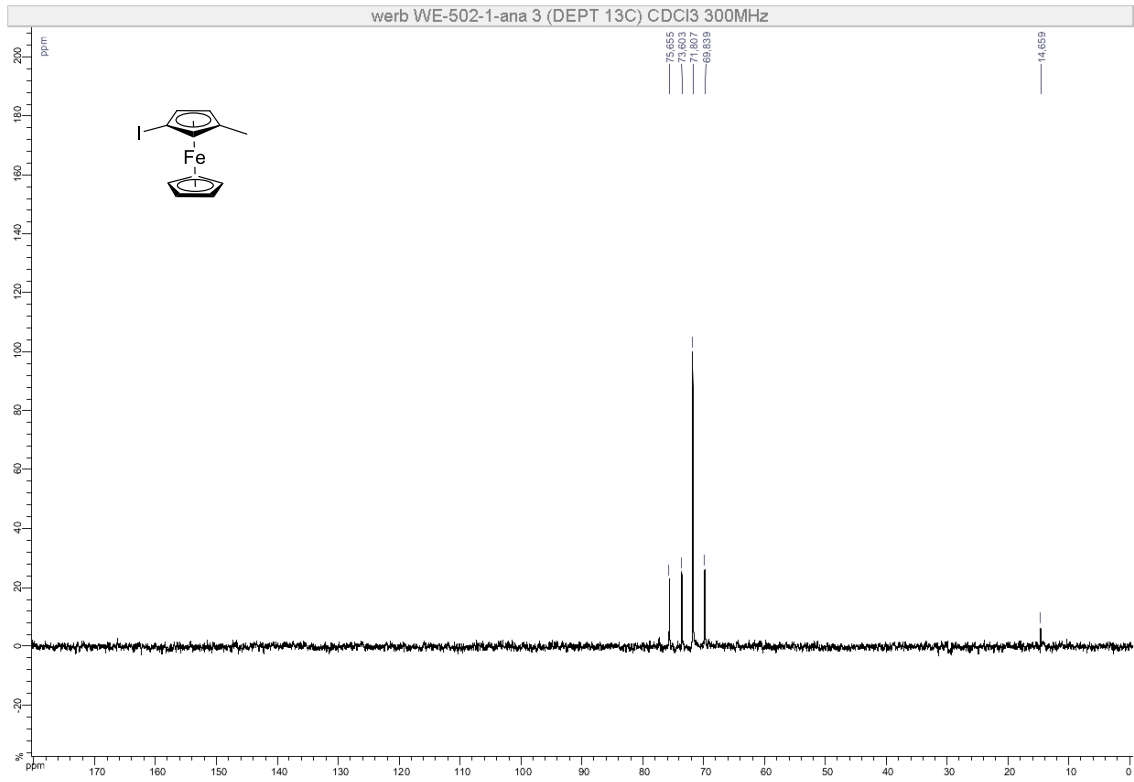


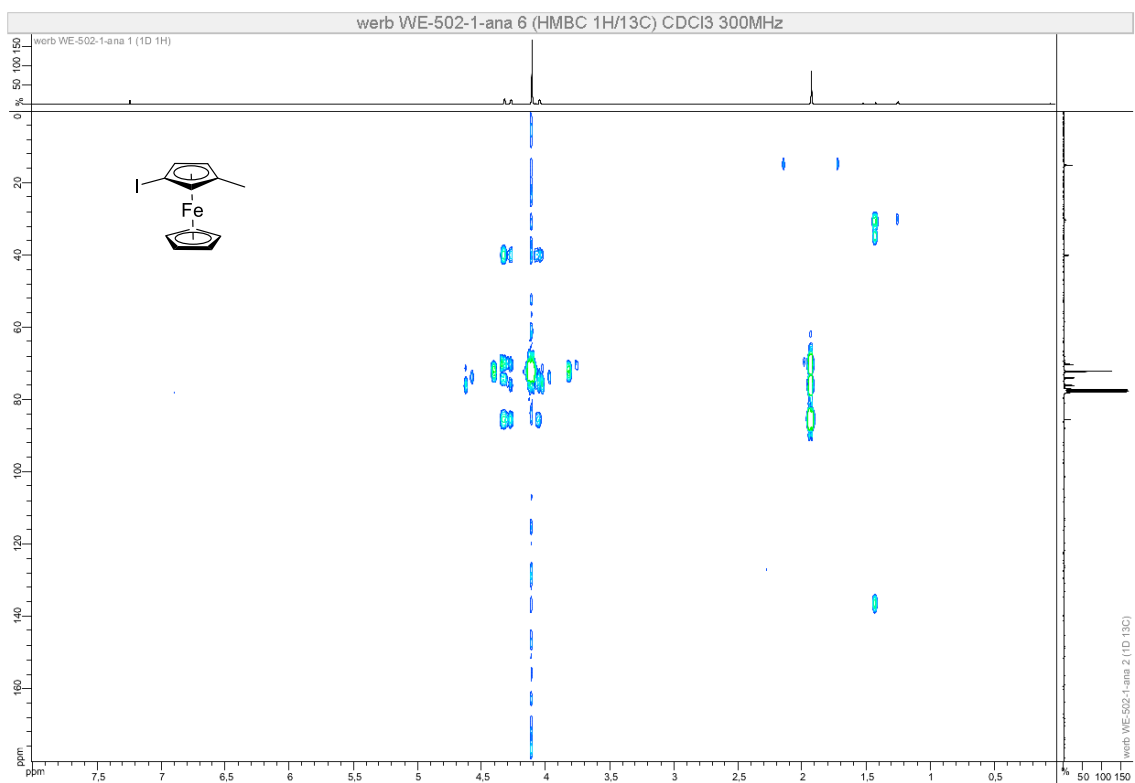
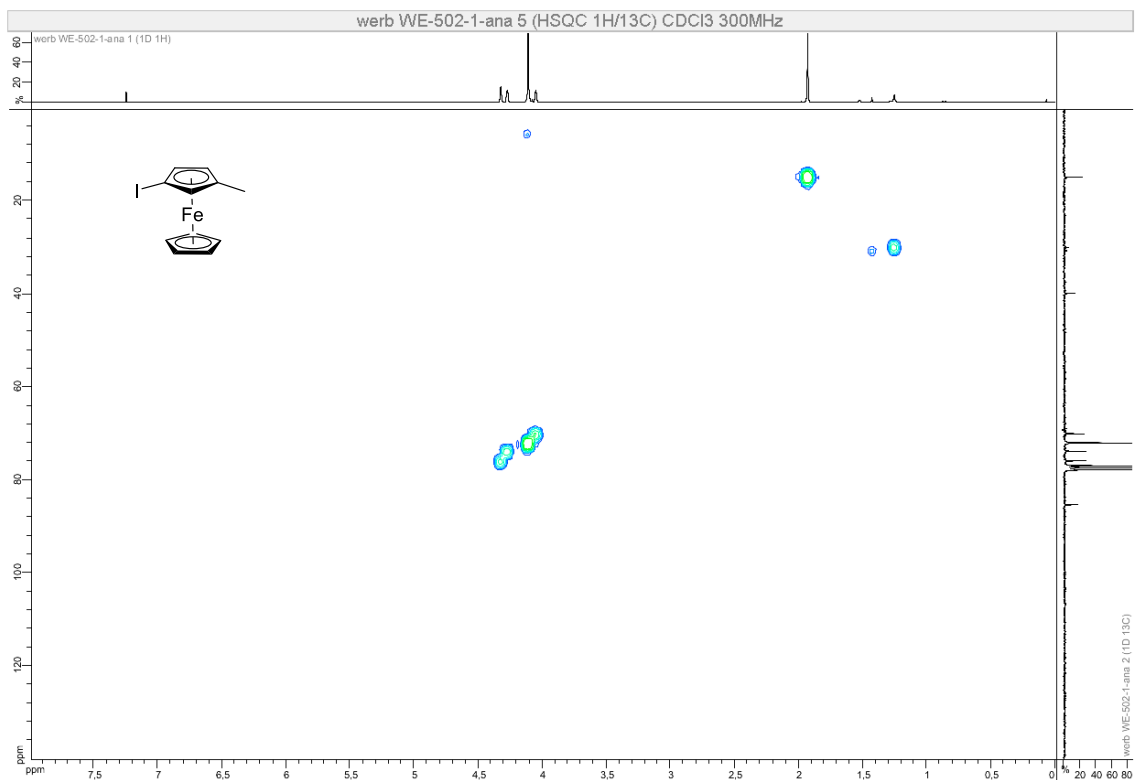




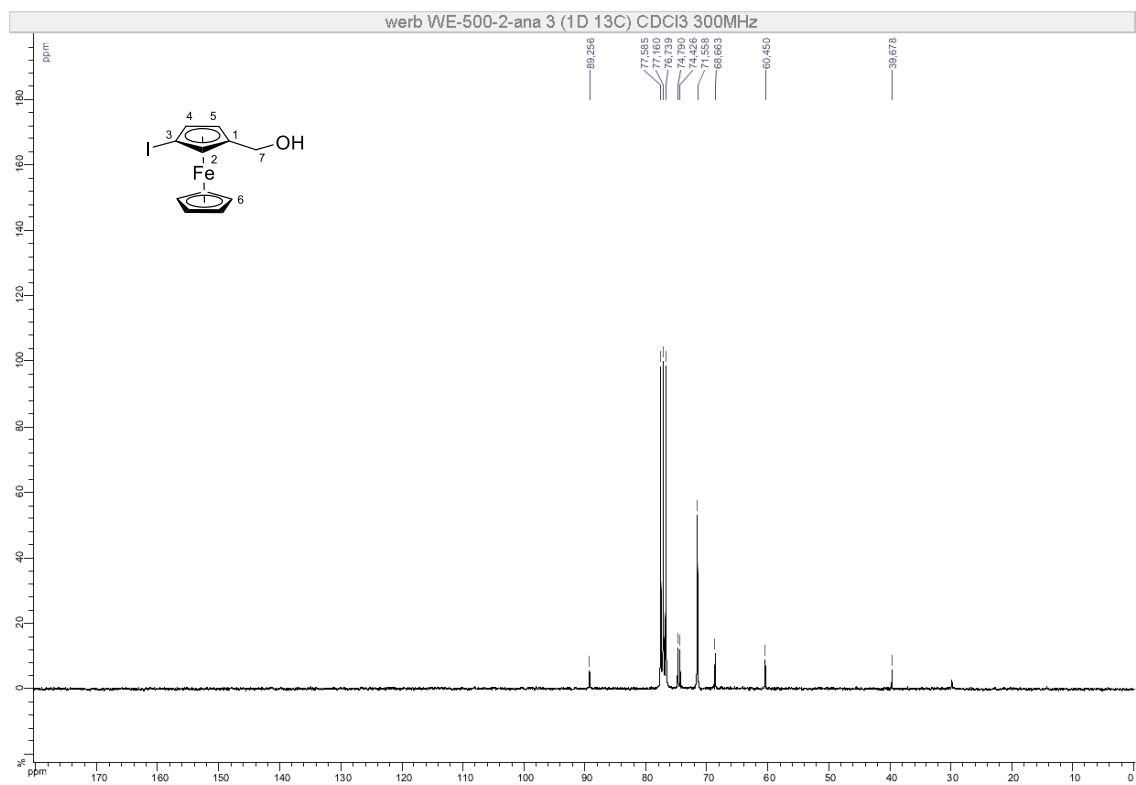
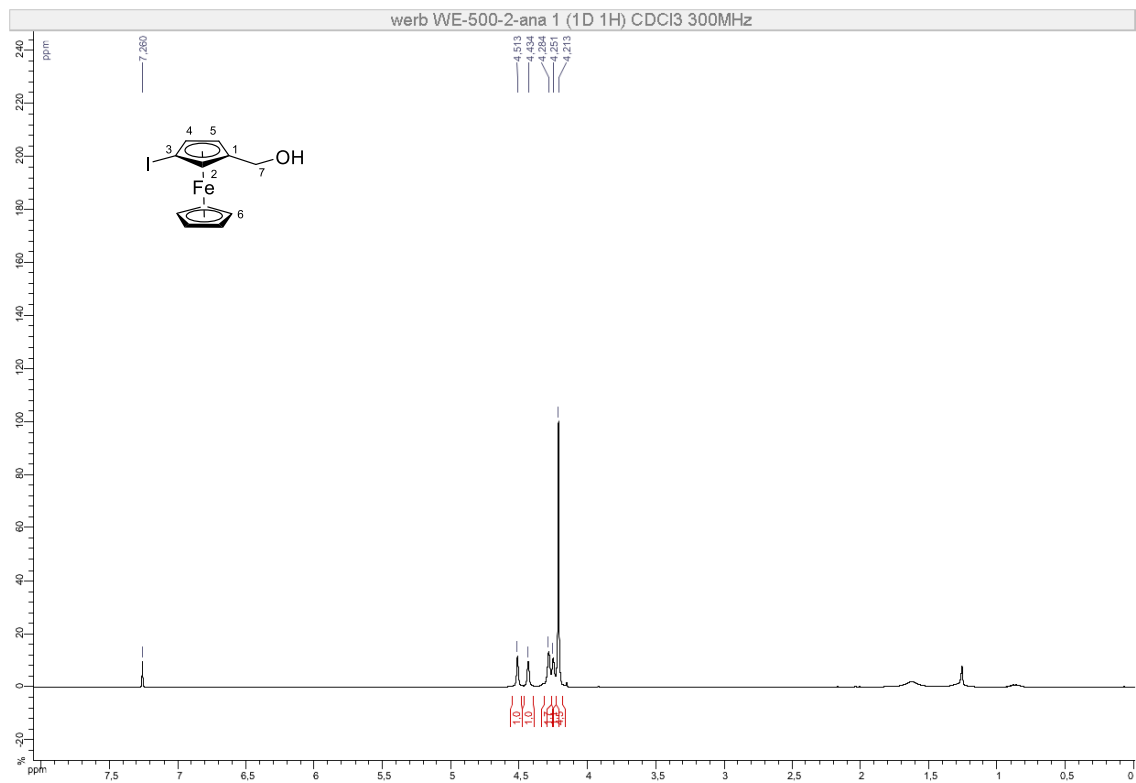
**1-Iodo-3-methylferrocene (36)**

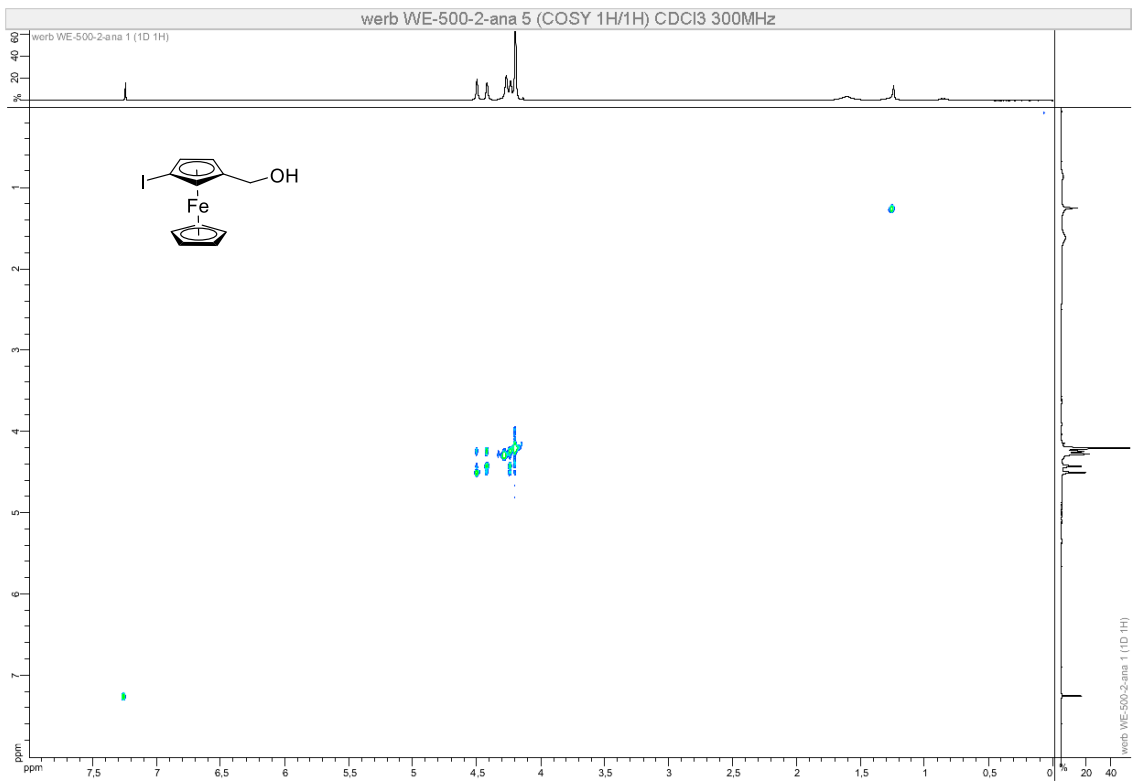
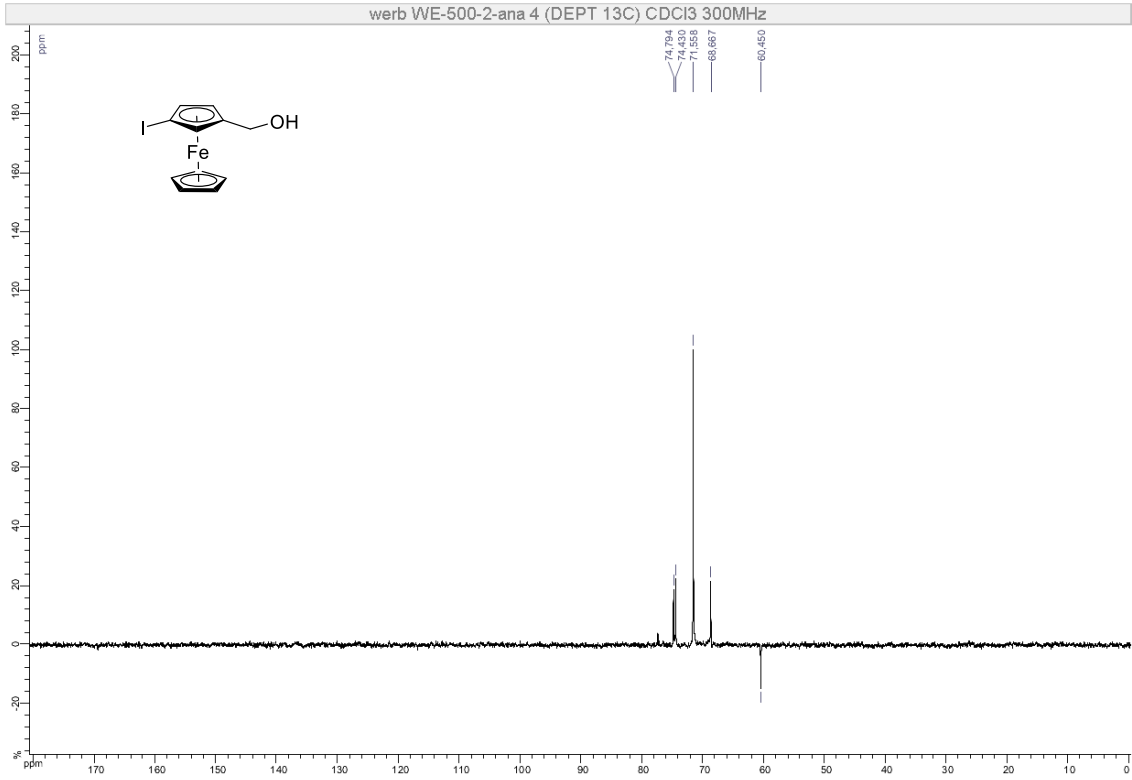


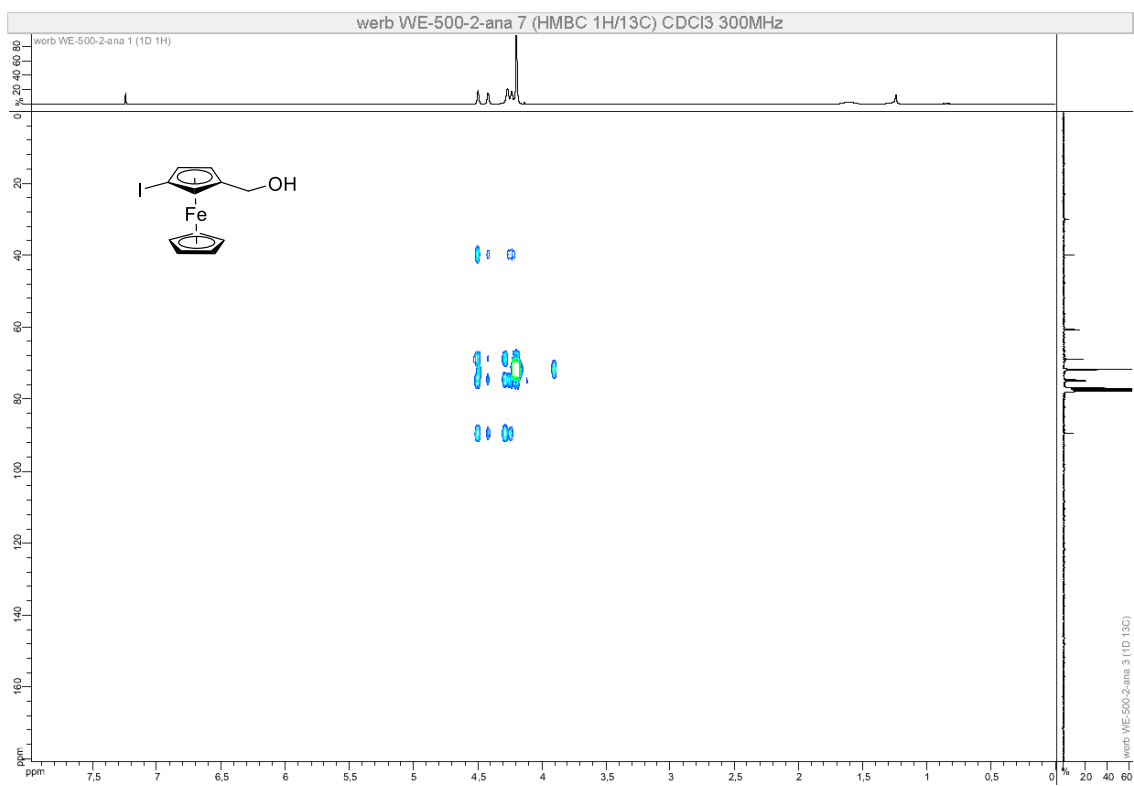
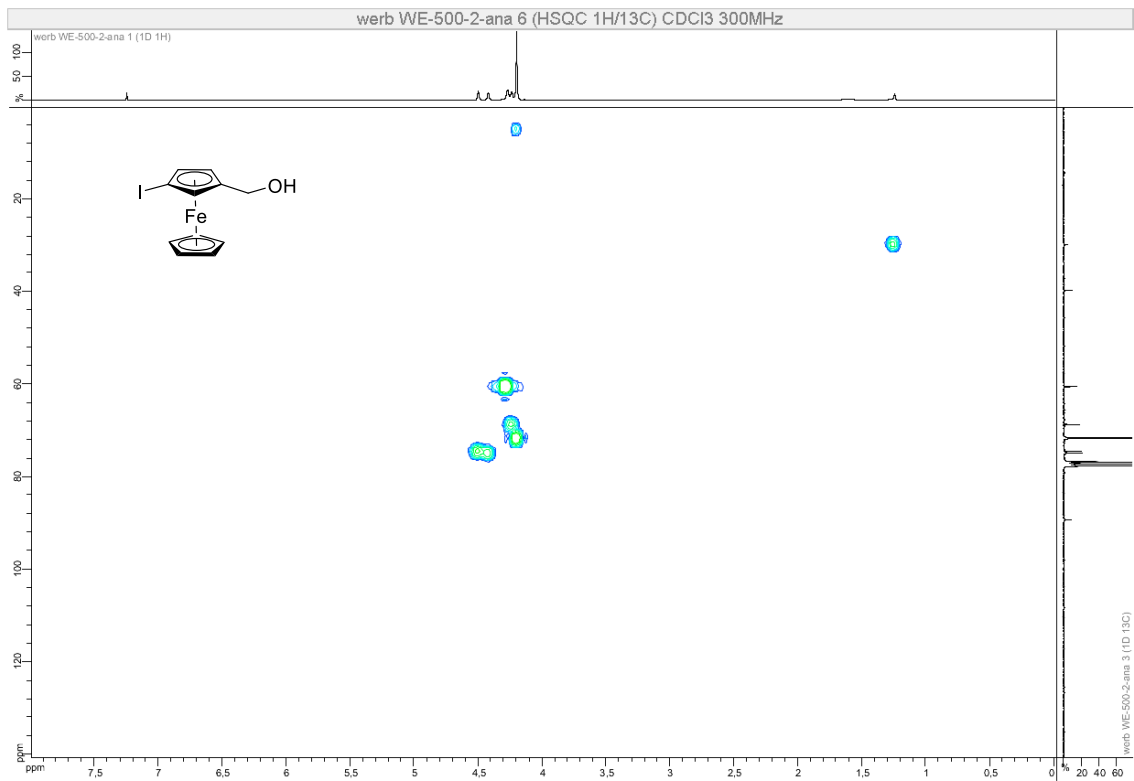




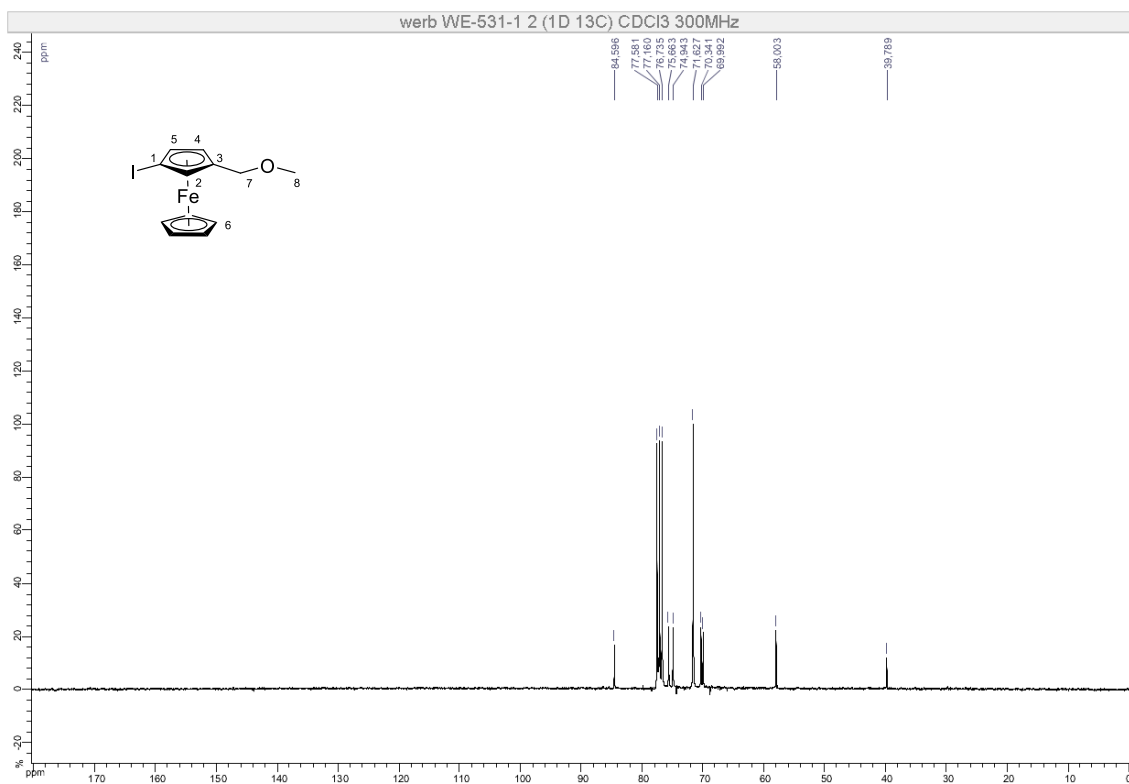
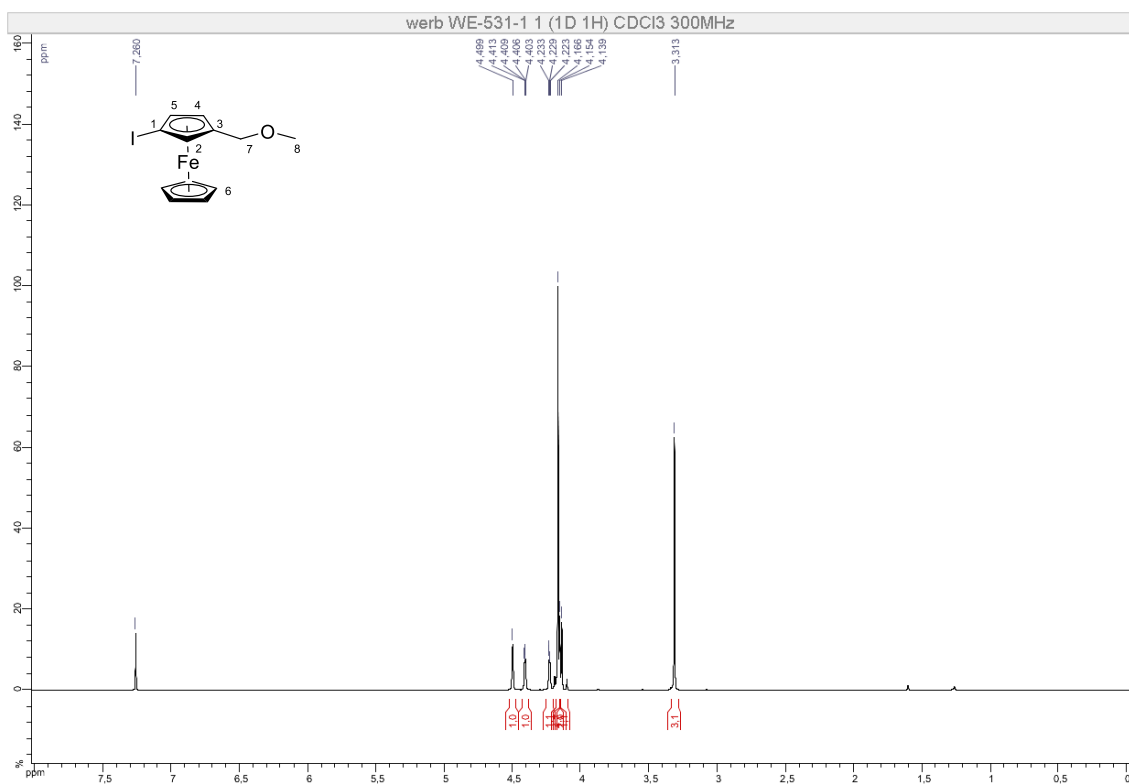
**1-(Hydromethyl)-3-iodoferrocene (37)**

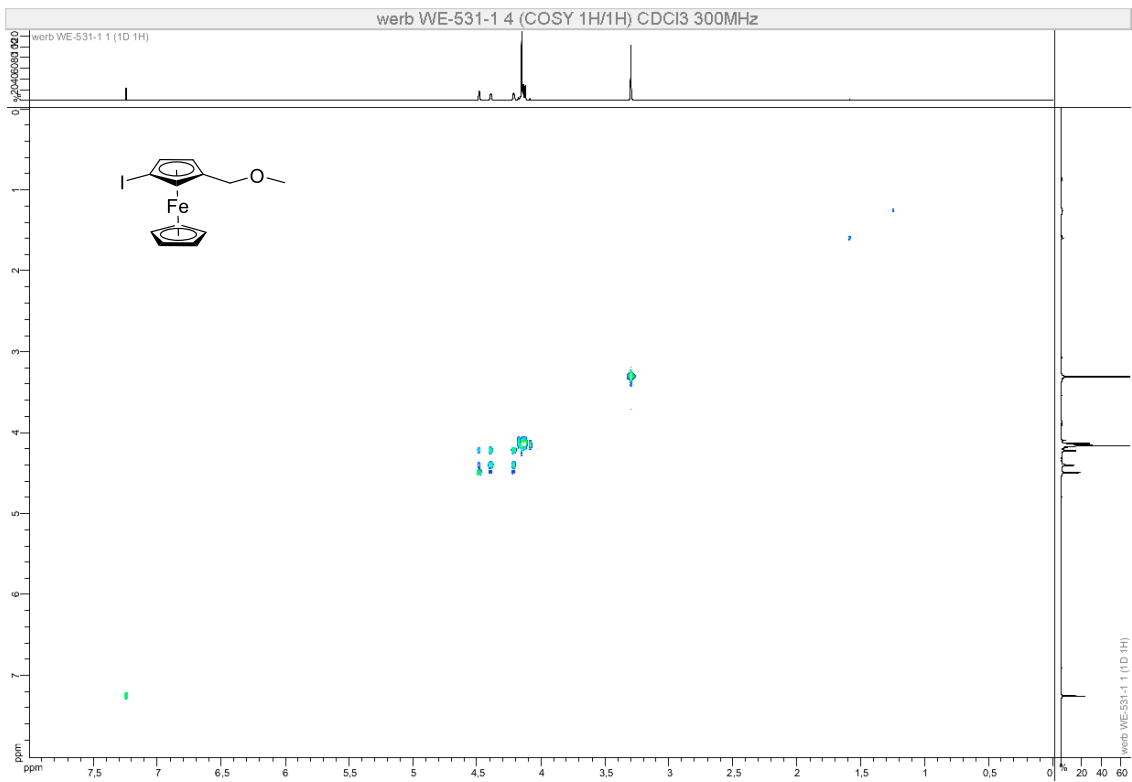
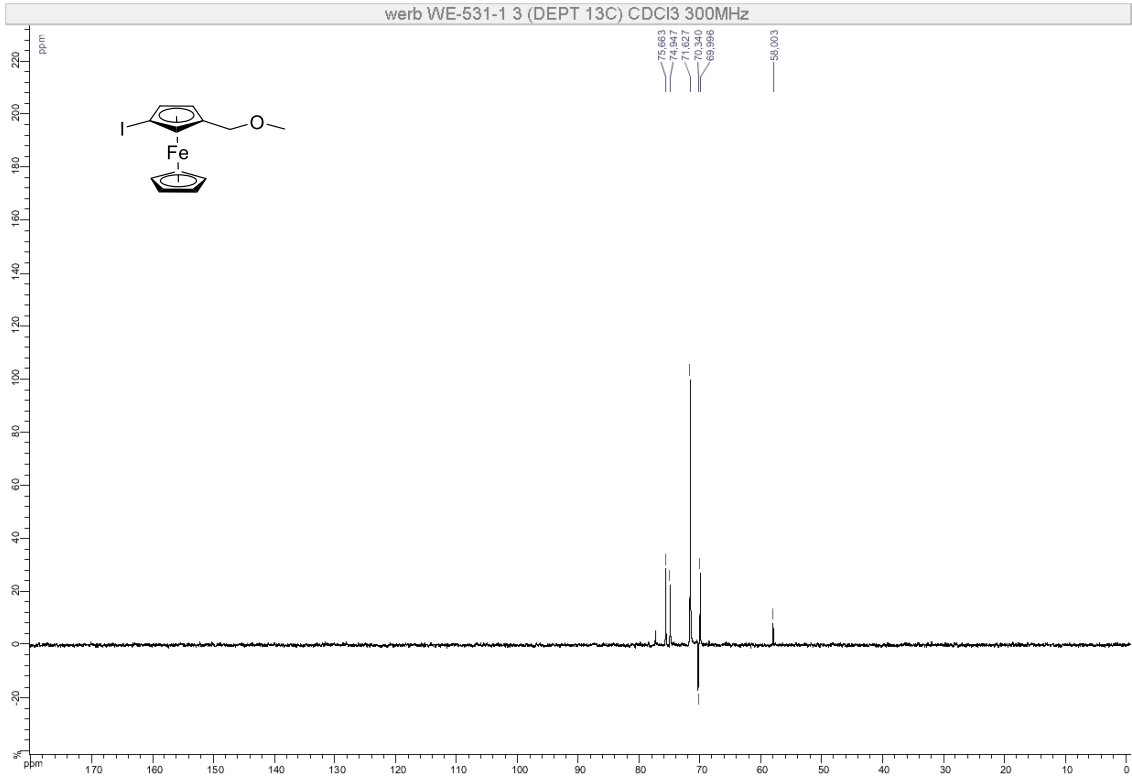




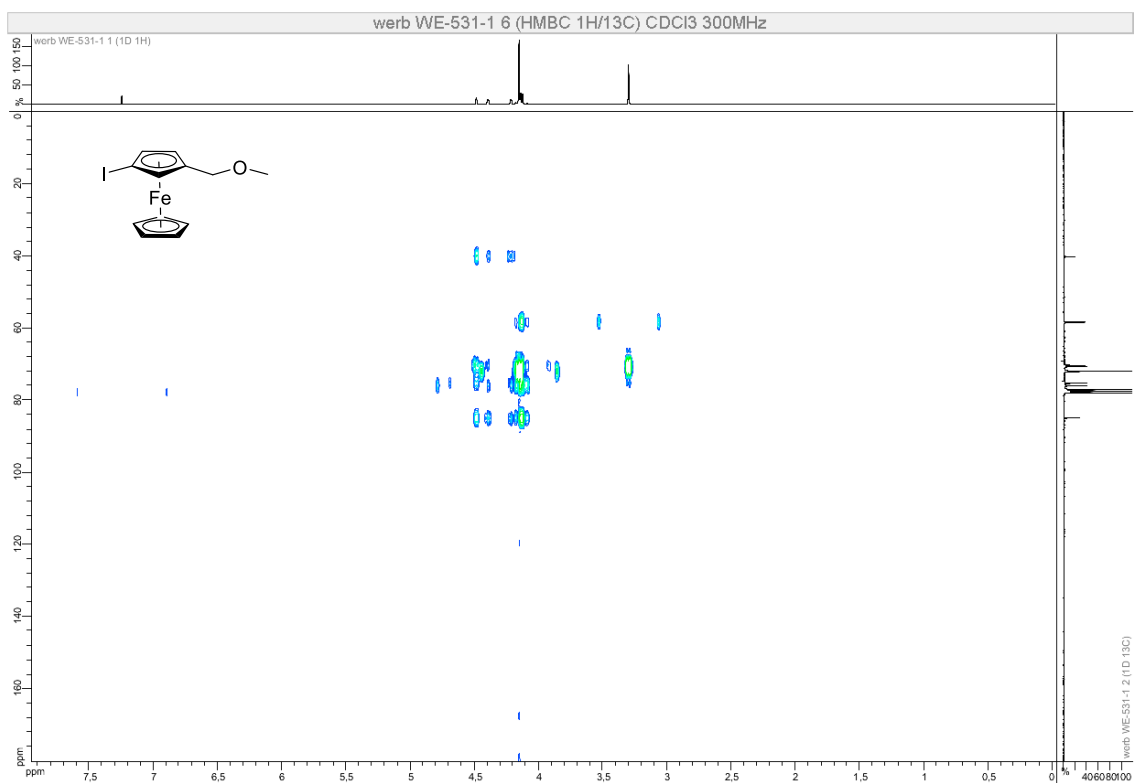
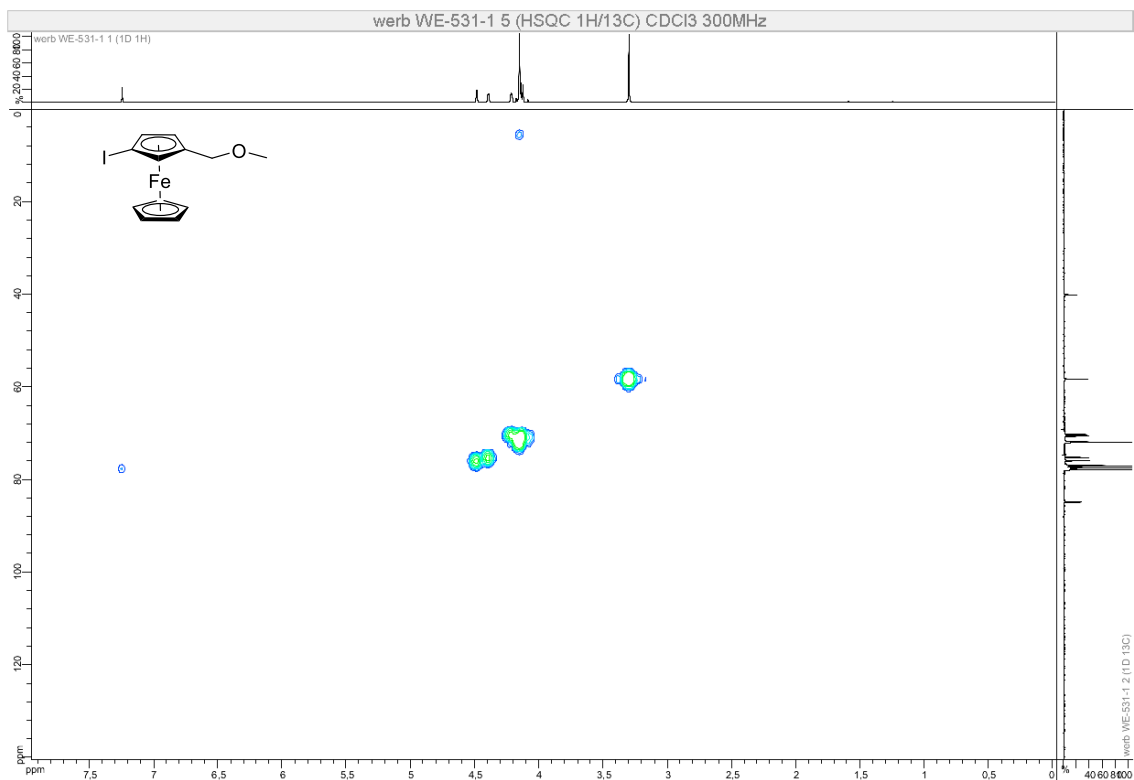


**1-Iodo-3-(methoxymethyl)ferrocene (38)**

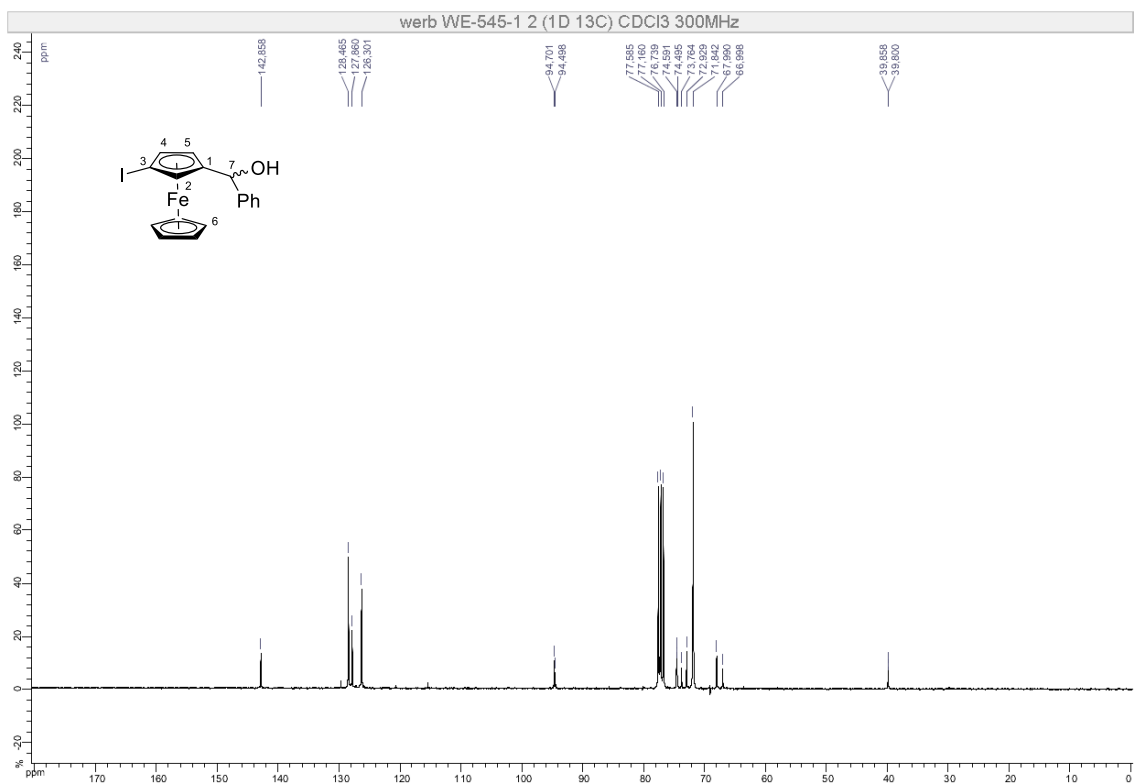
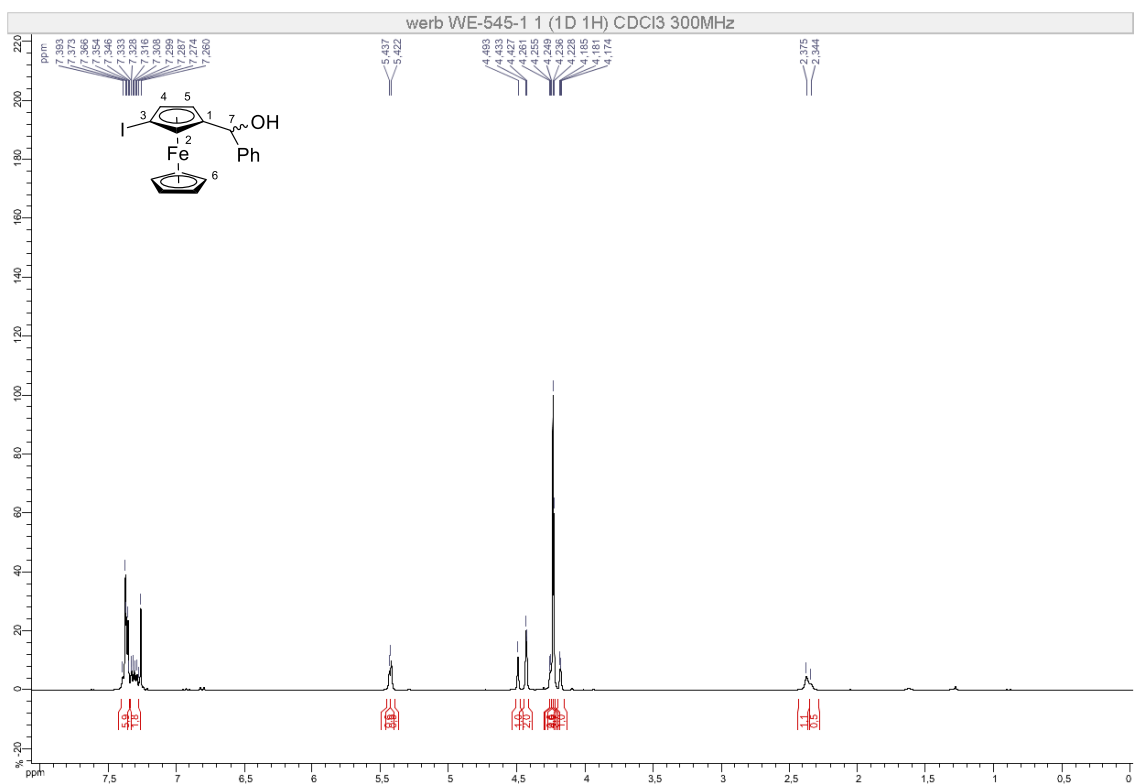


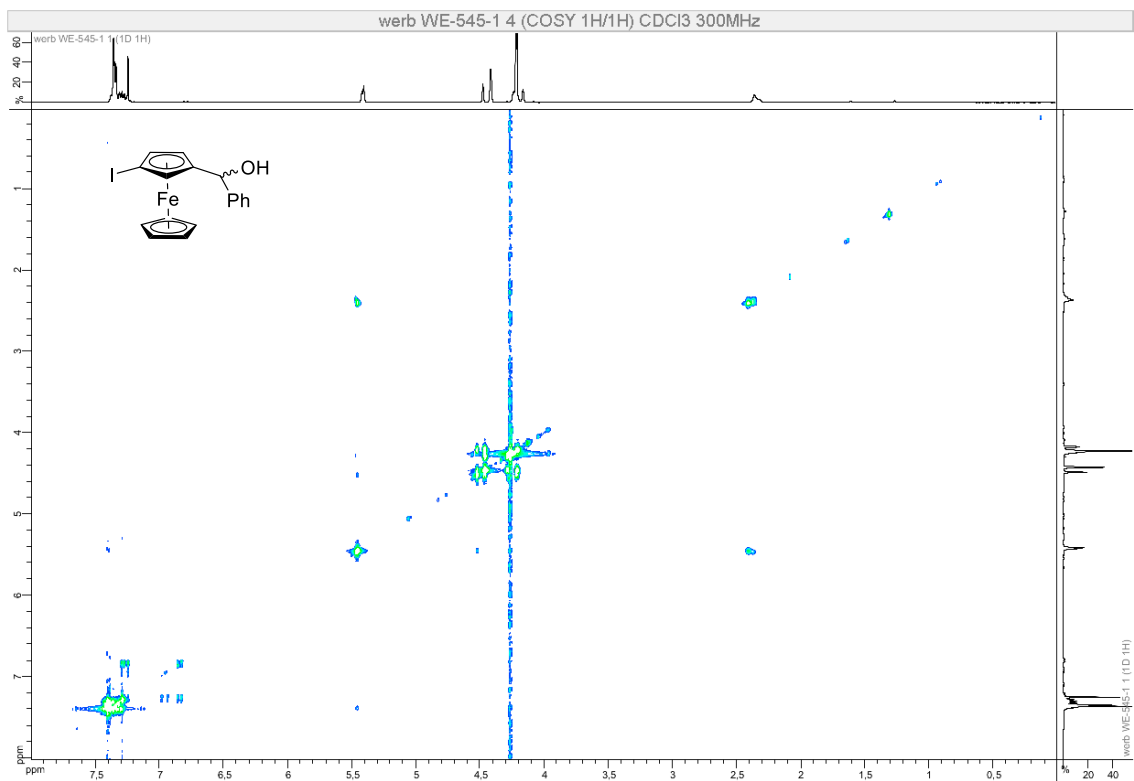
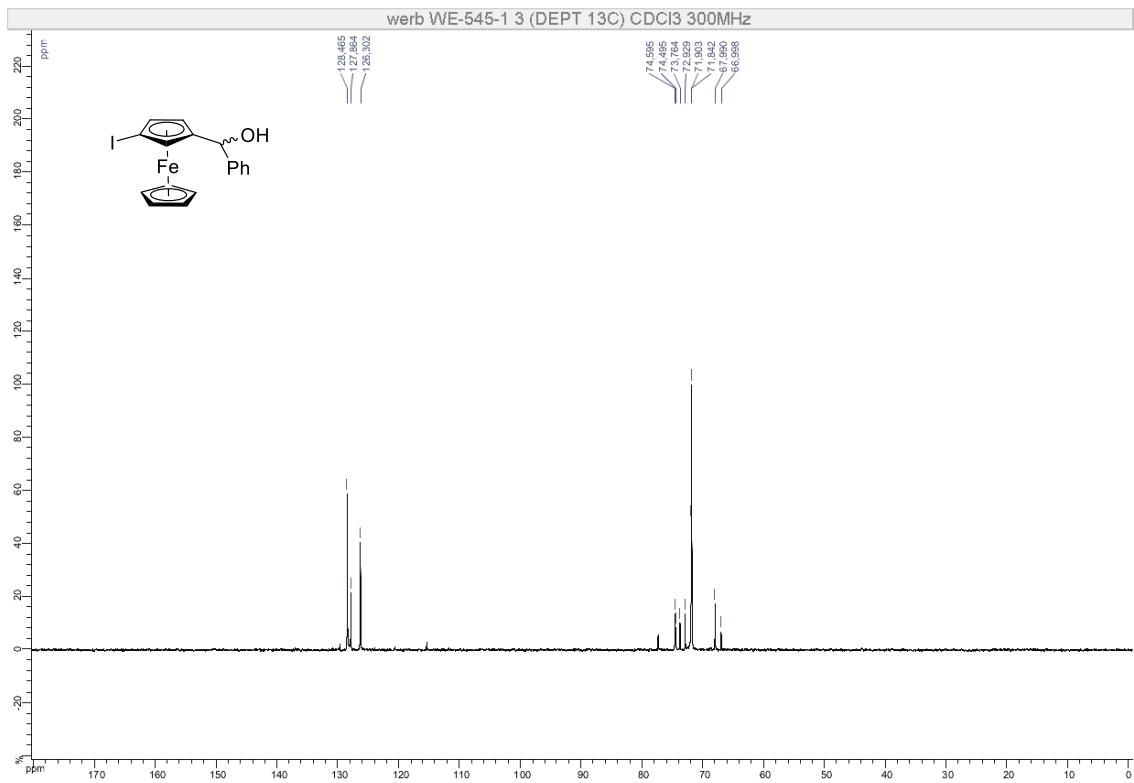


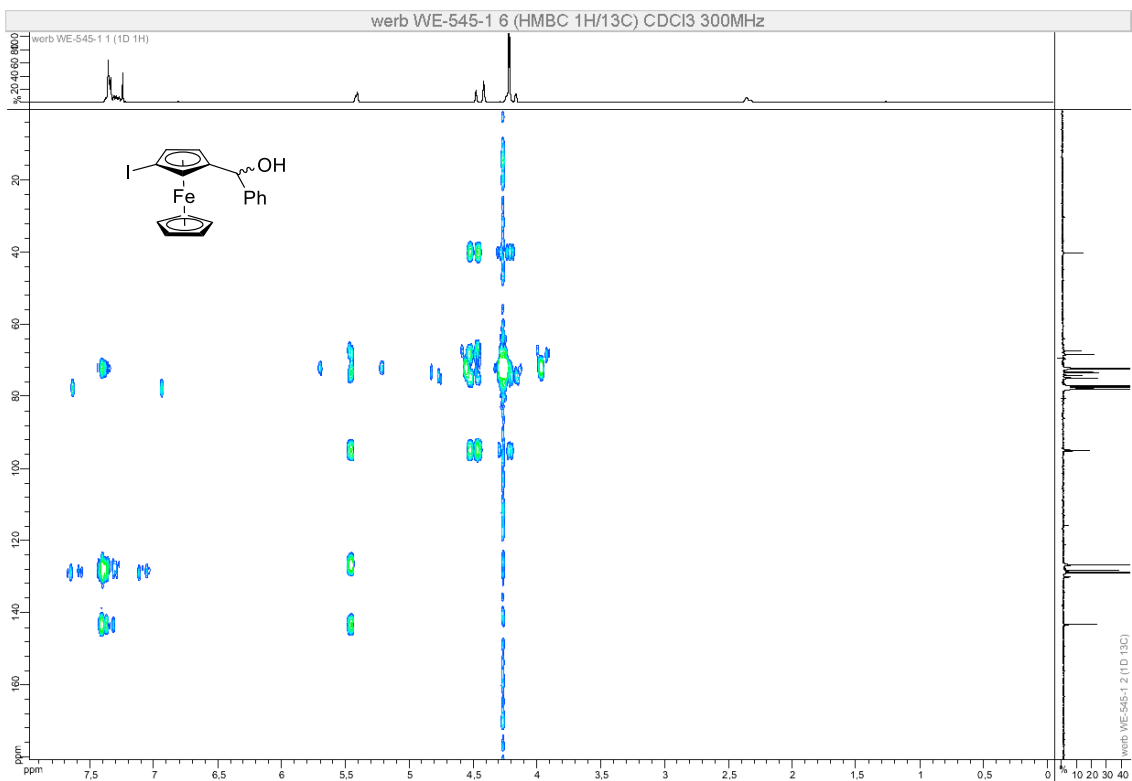
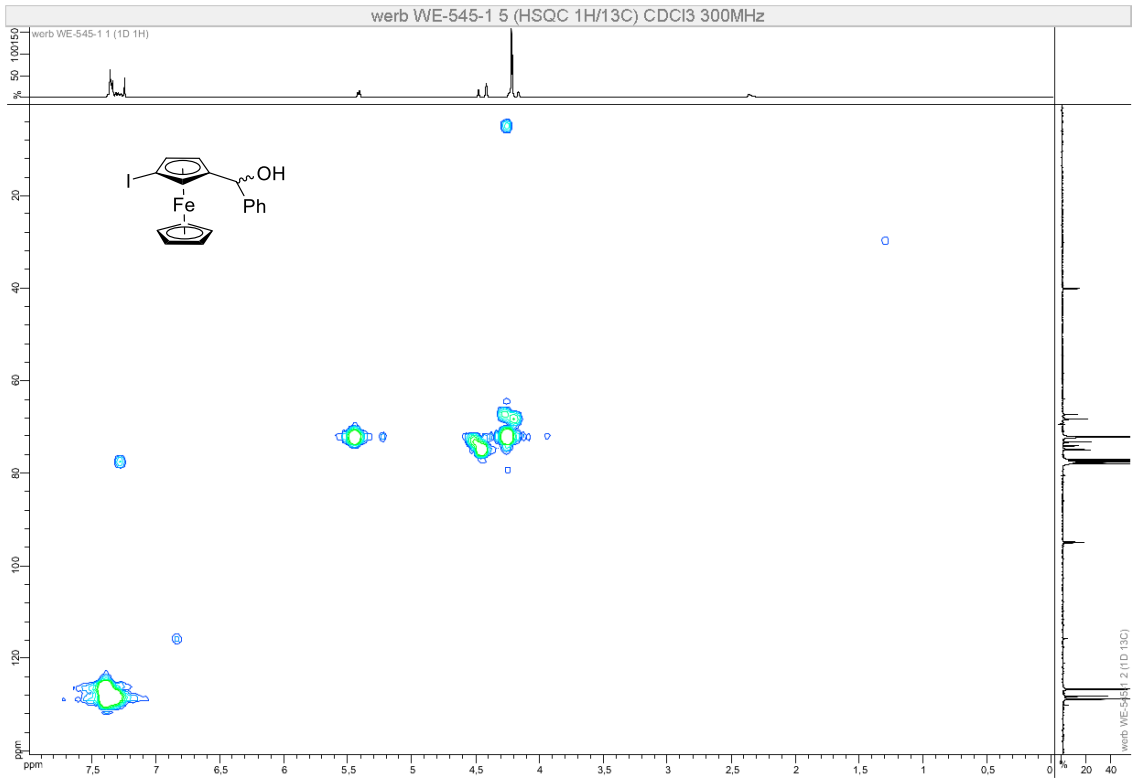




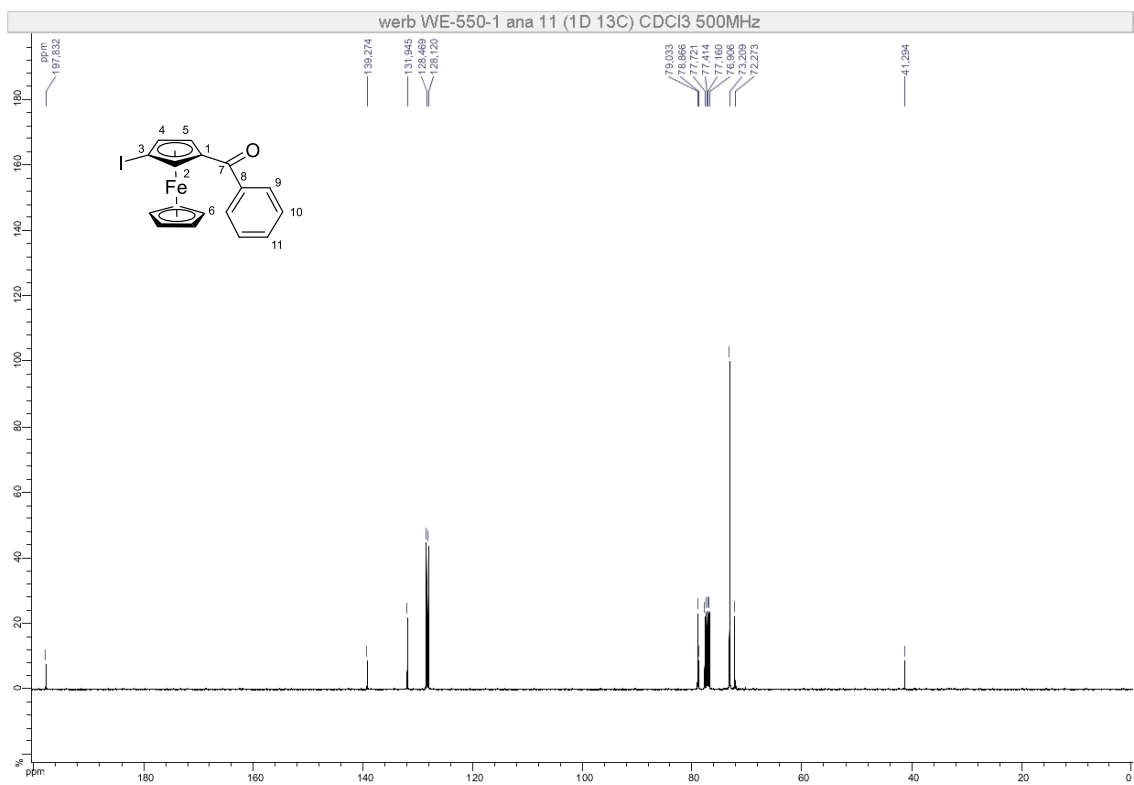
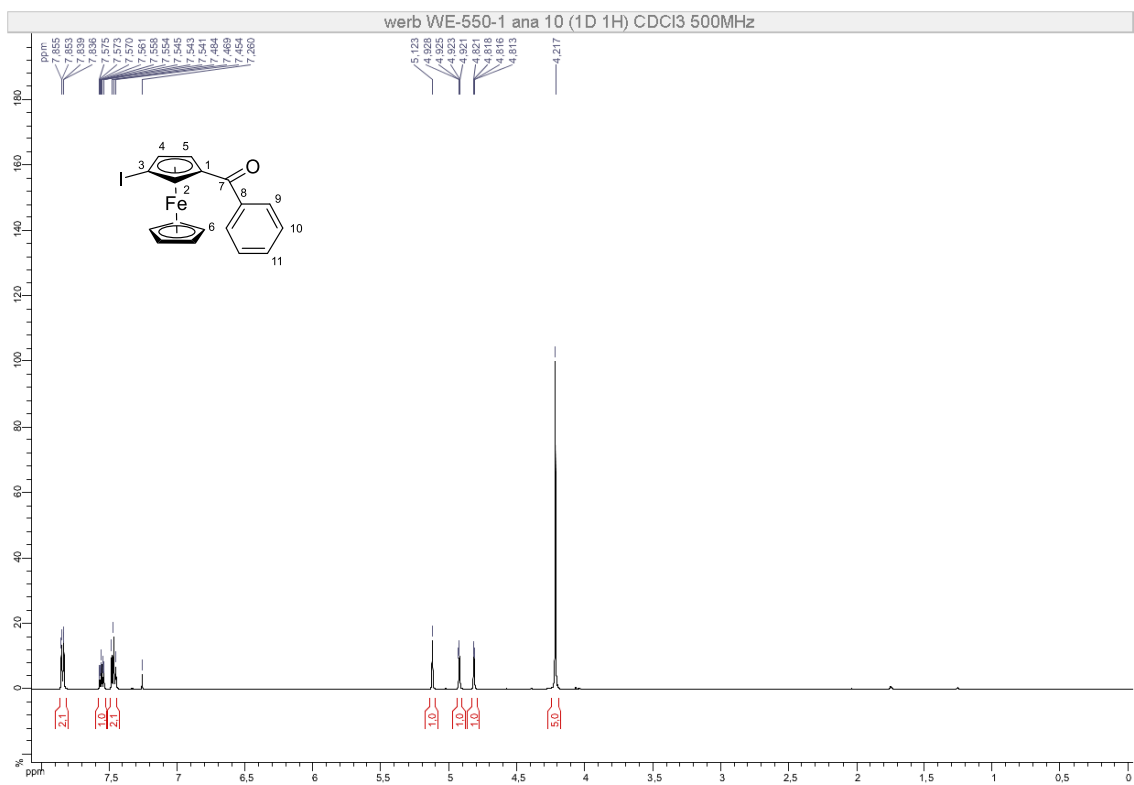
### 3-Iodo- $\alpha$ -Phenylferrocenemethanol (39)

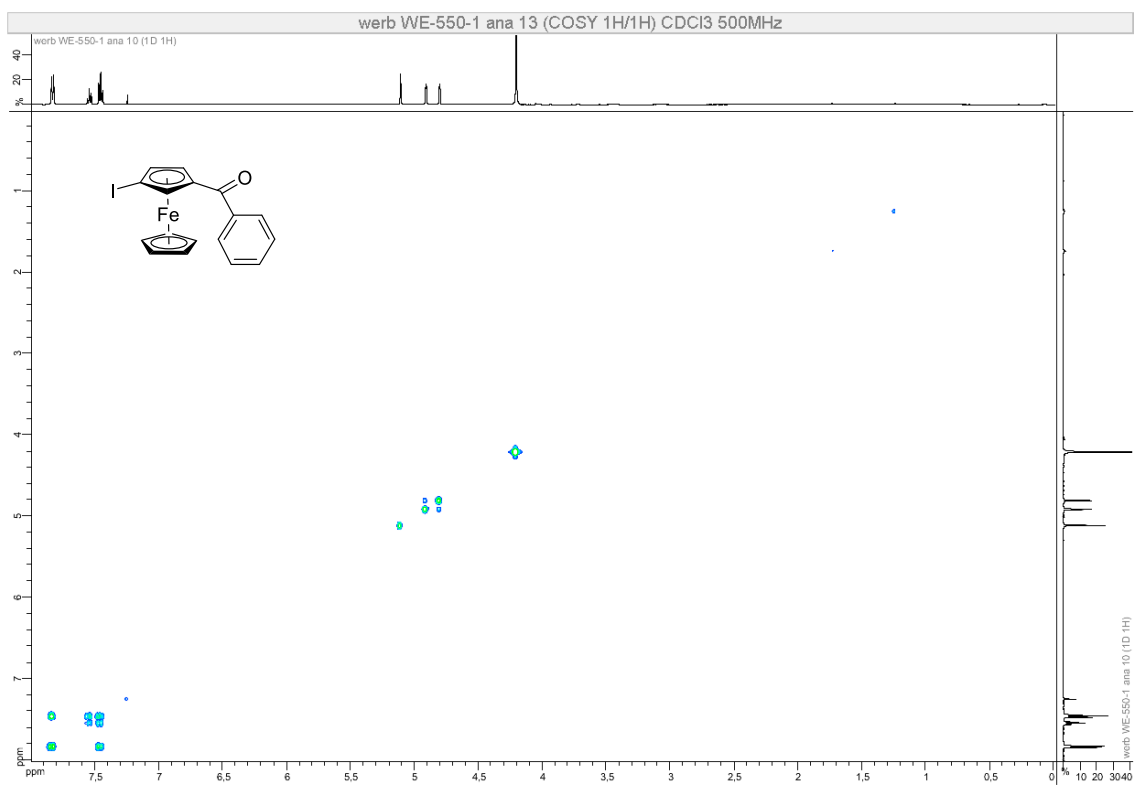
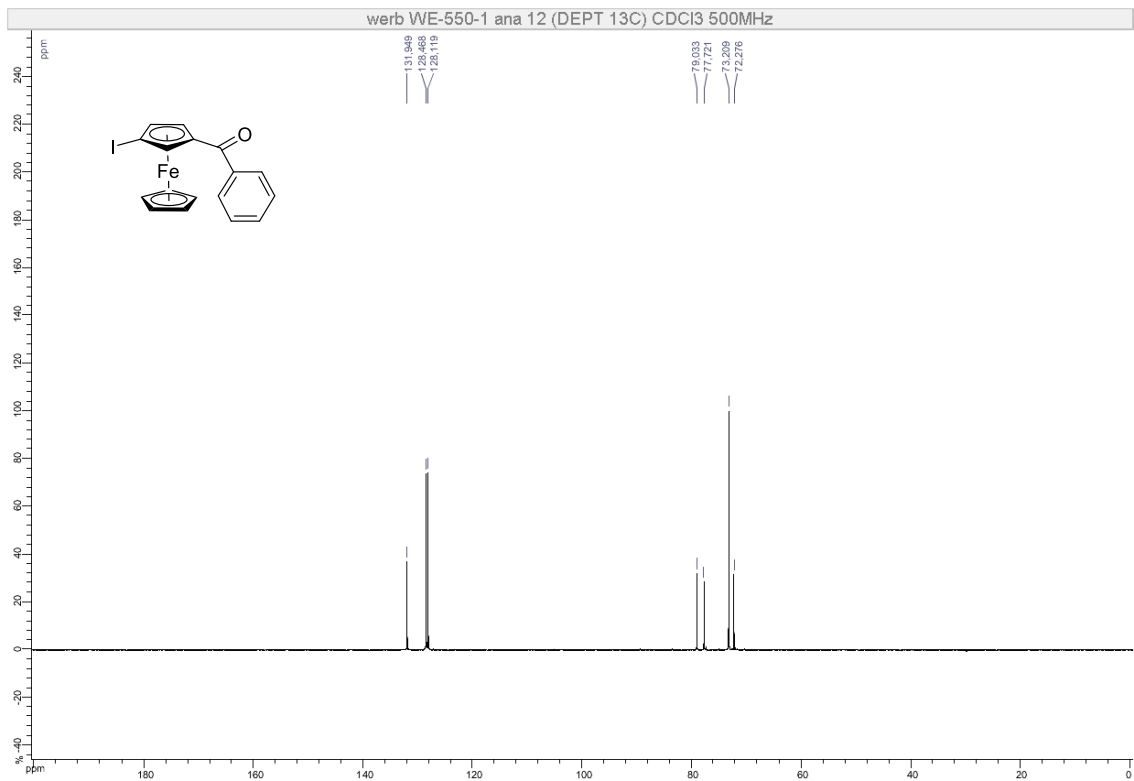


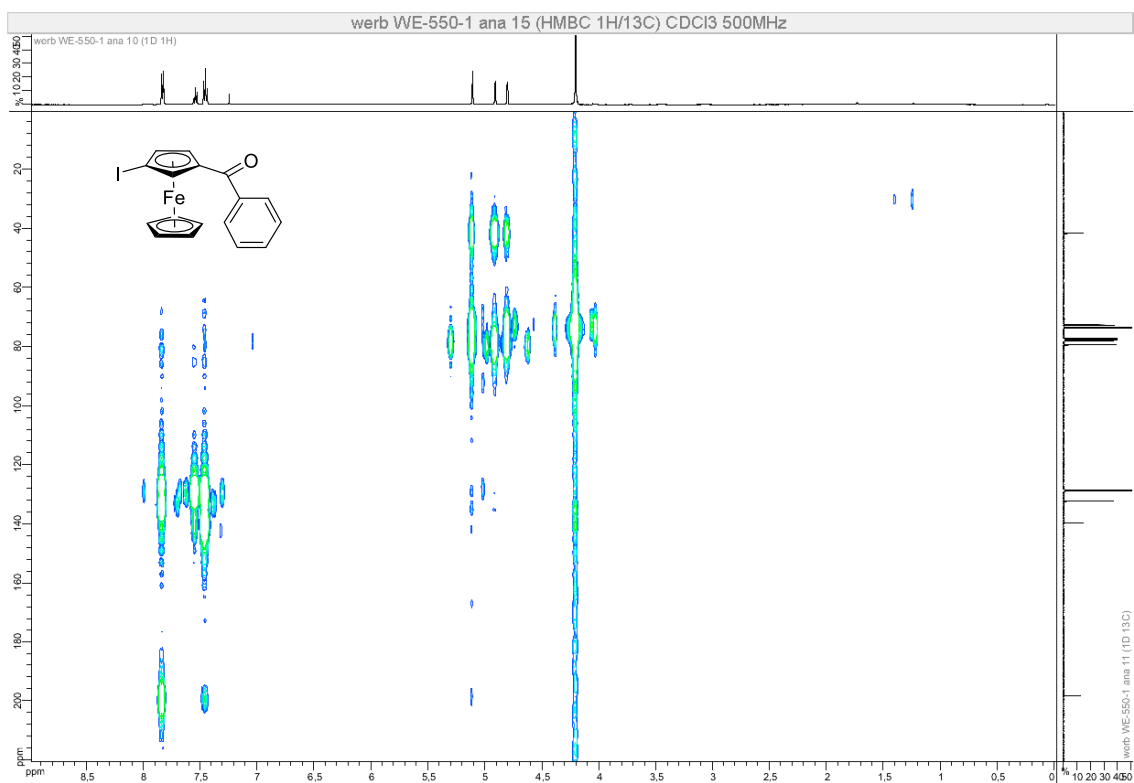


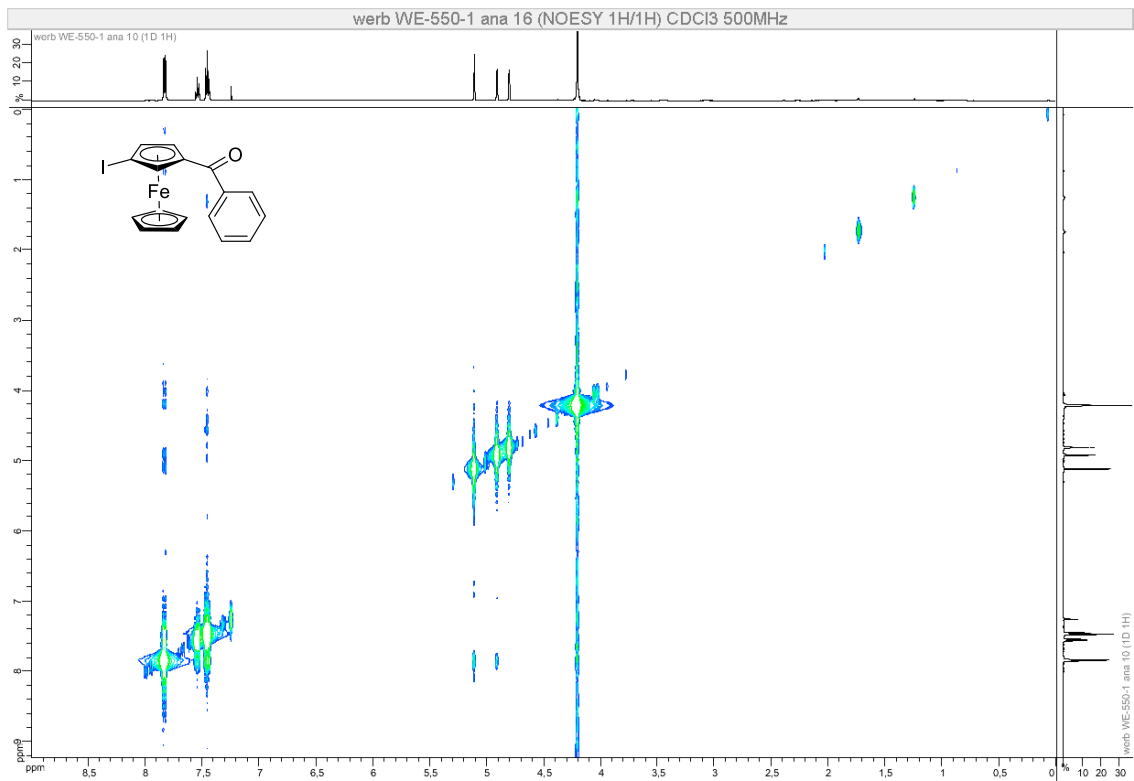


# 1-Benzoyl-3-iodoferrocene (40)



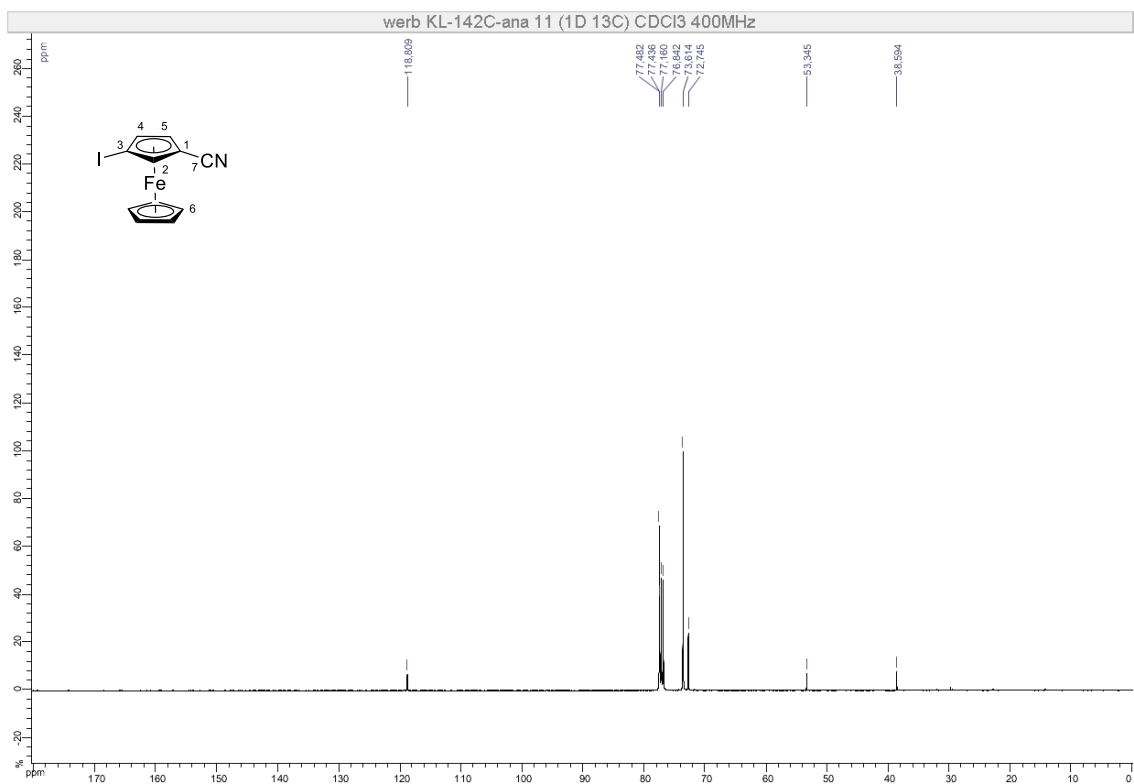
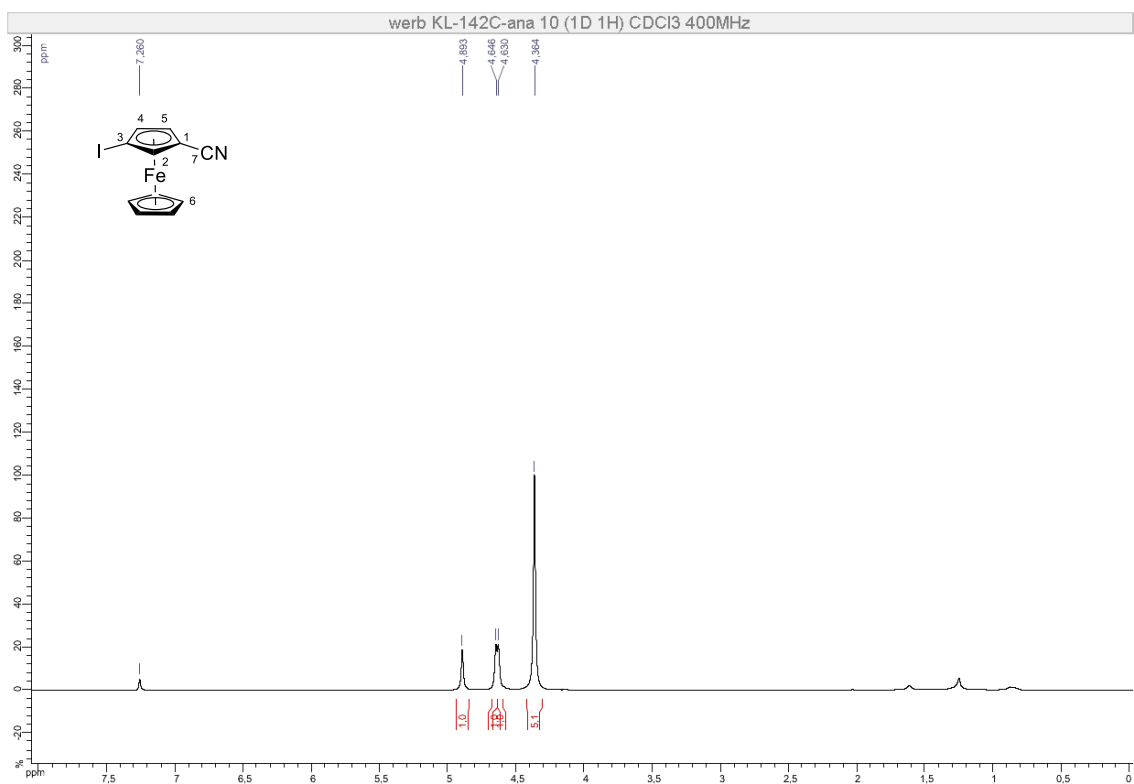


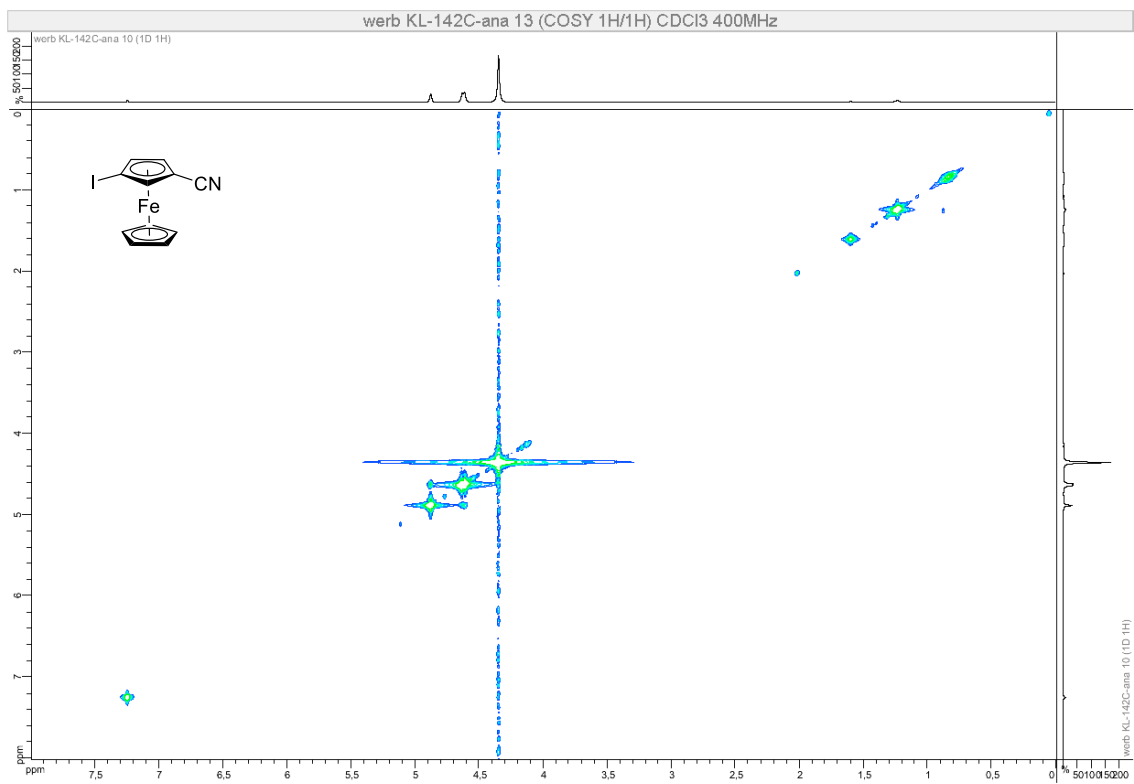
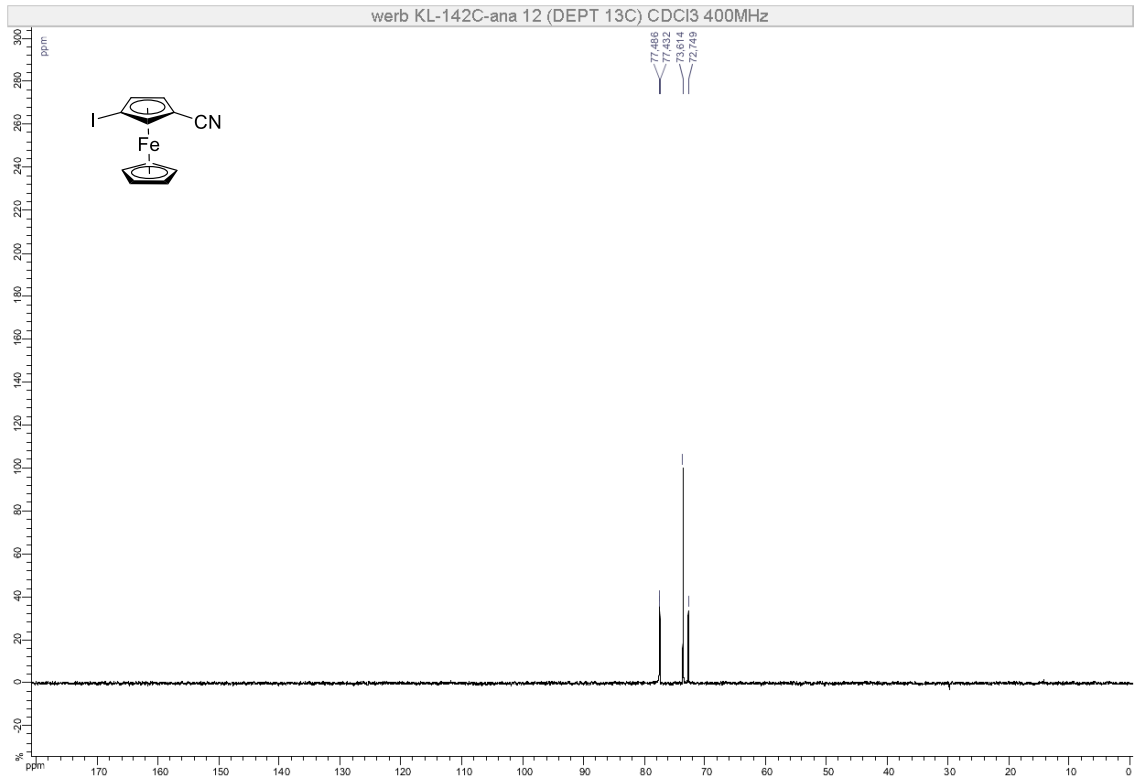


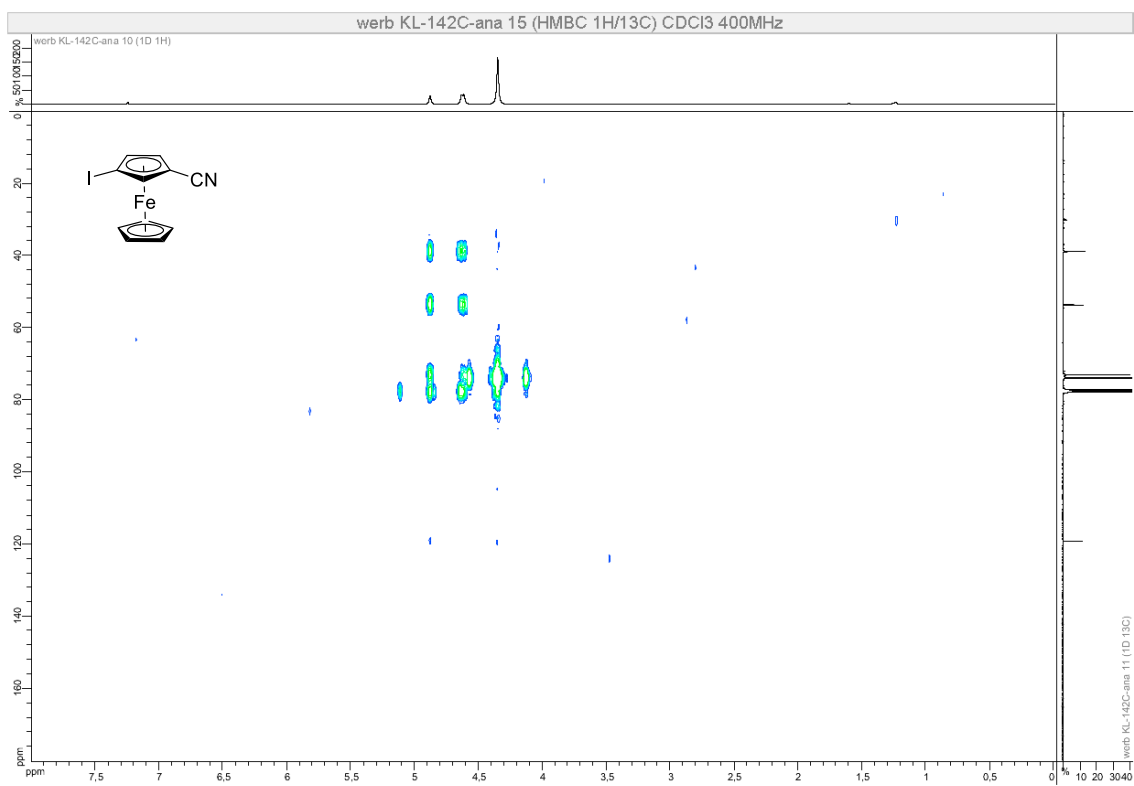
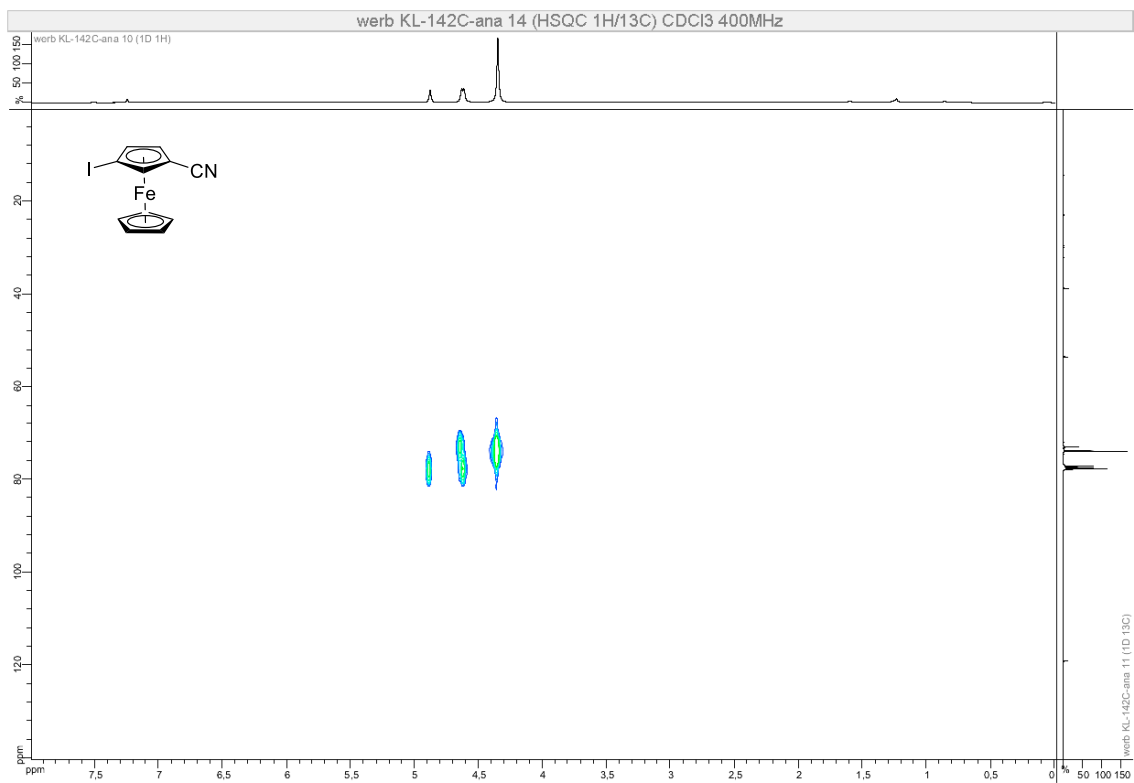




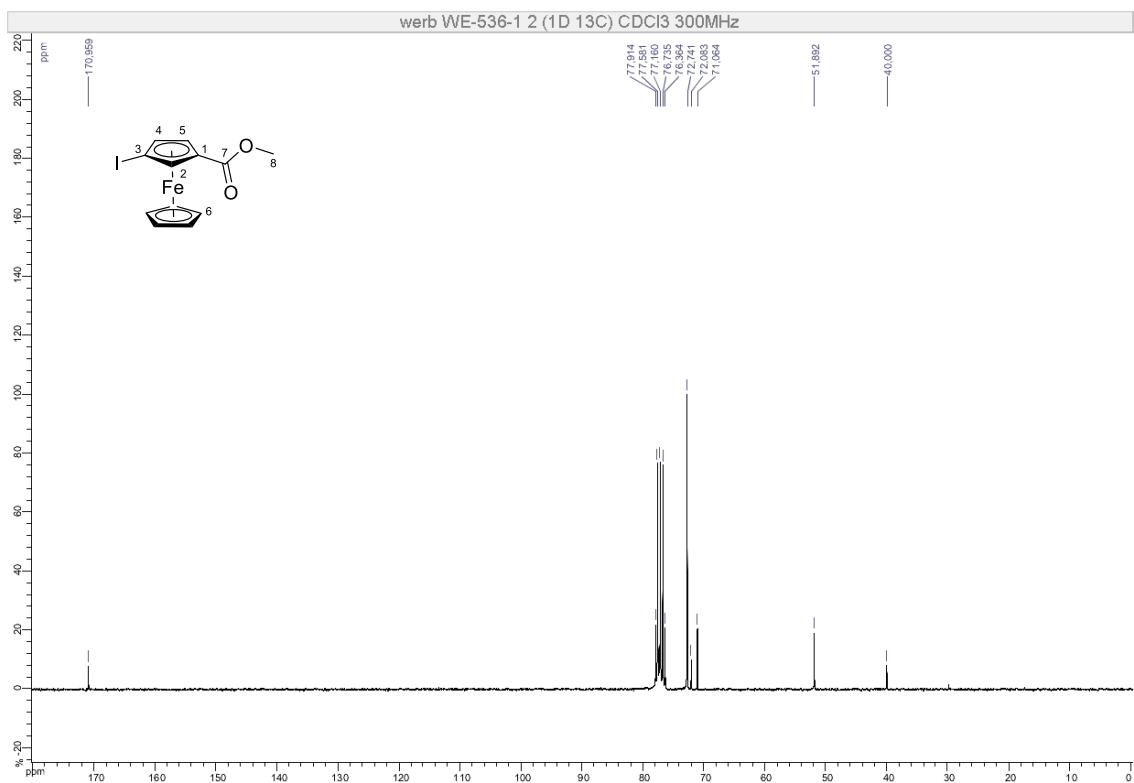
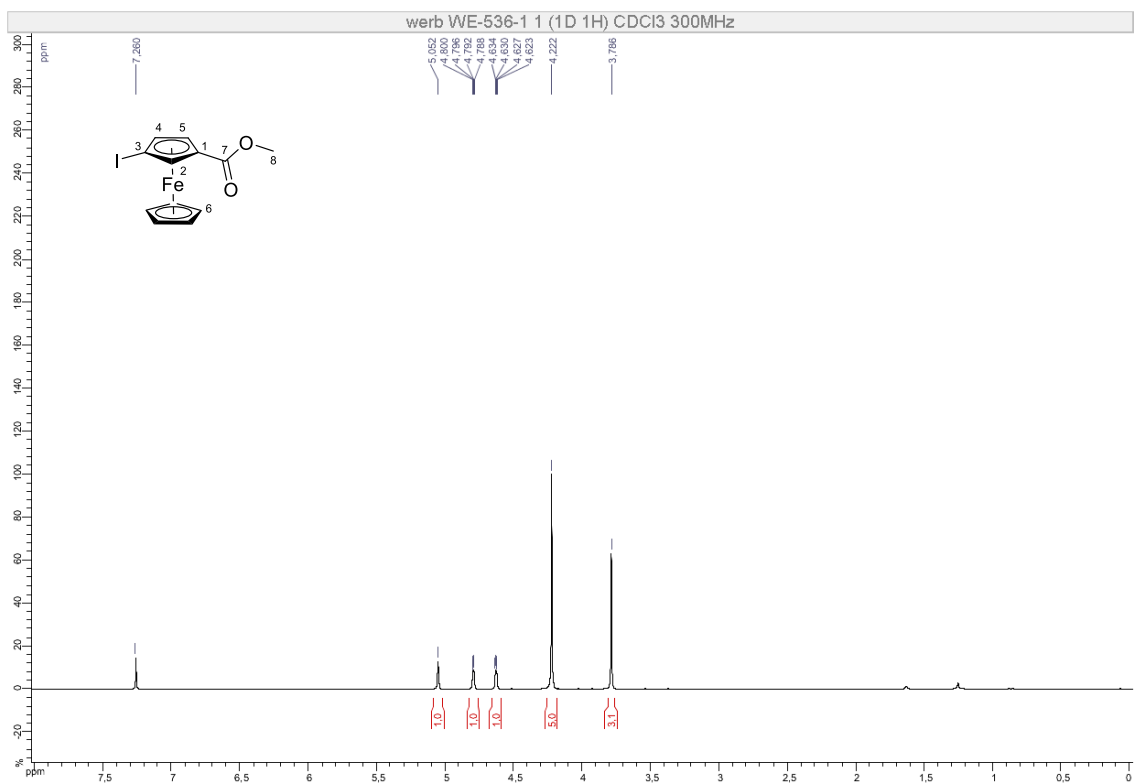
### 3-Iodoferrocenecarbonitrile (41)

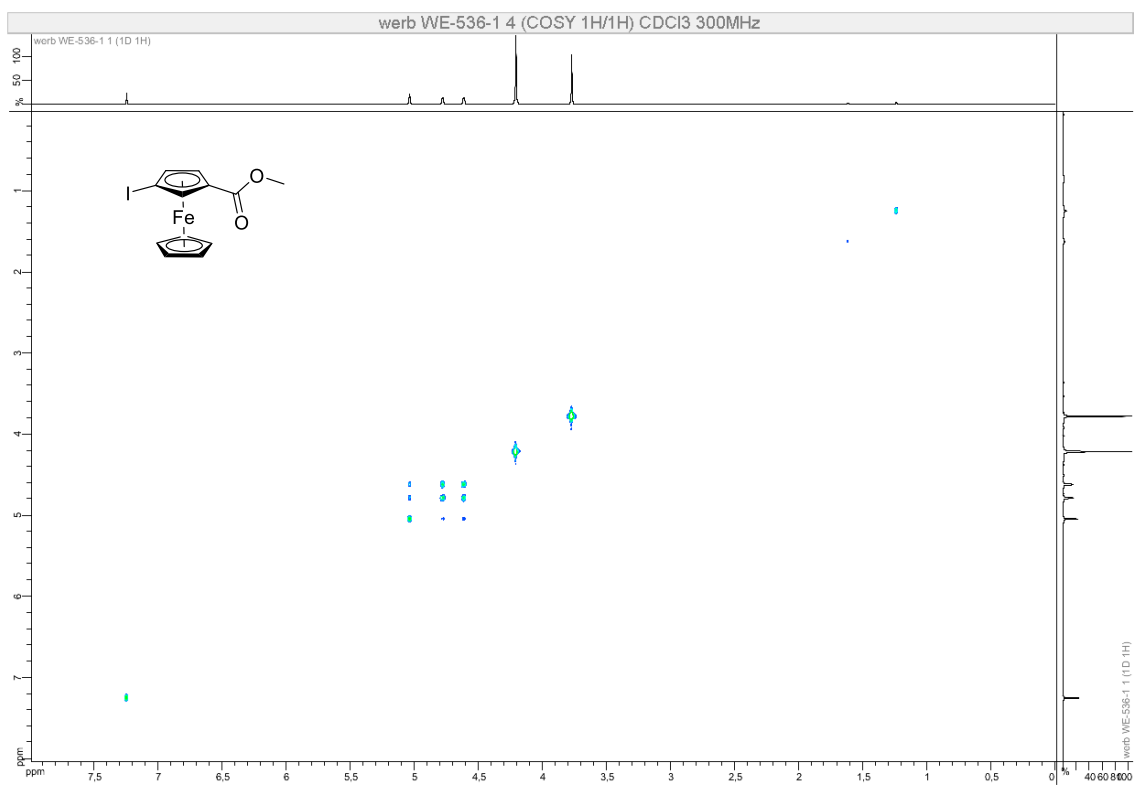
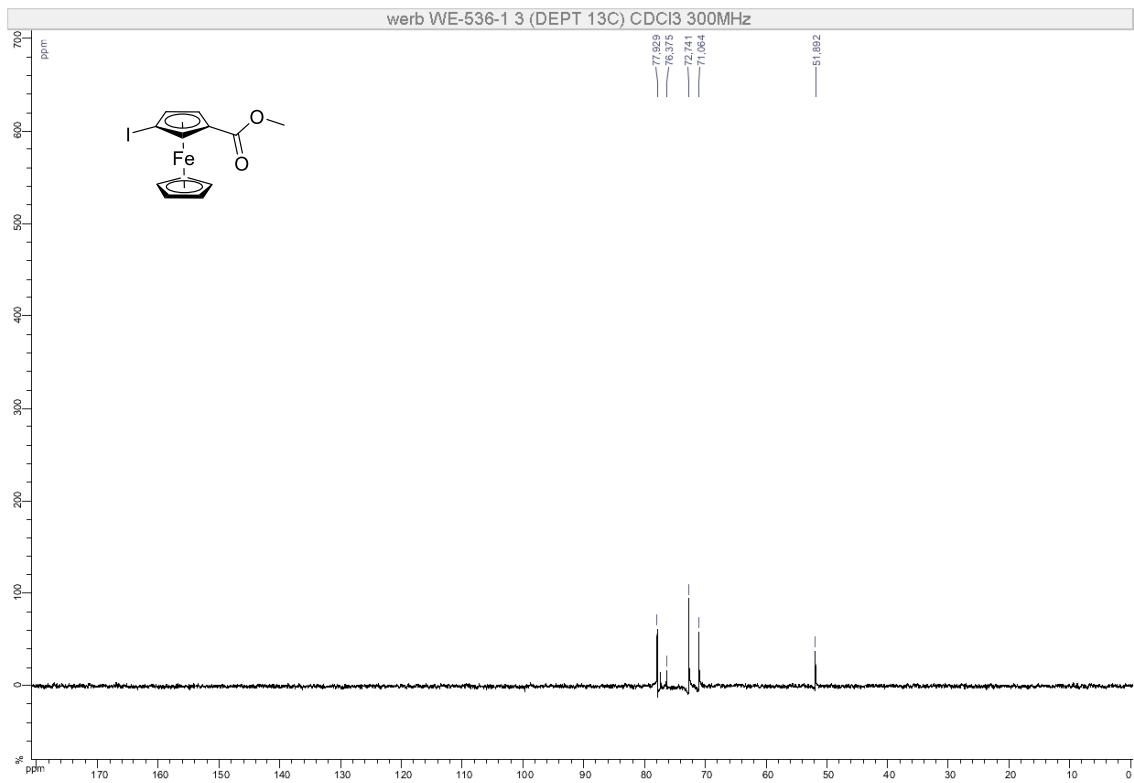


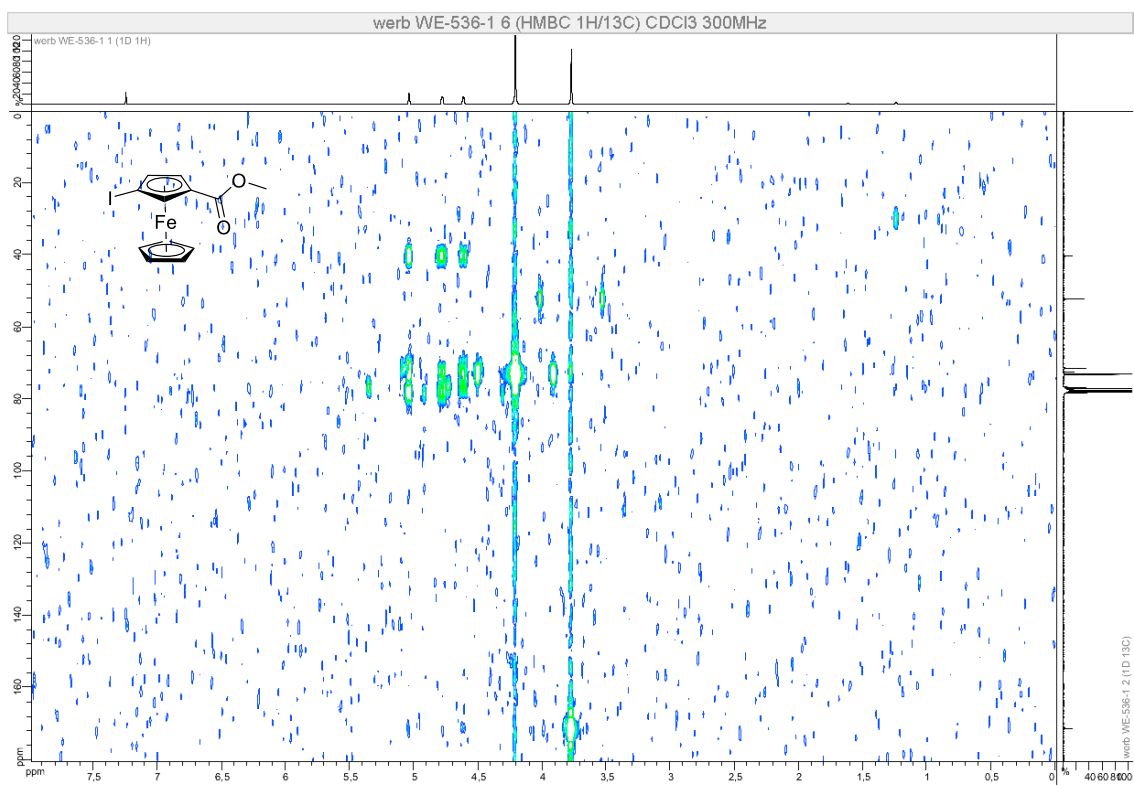
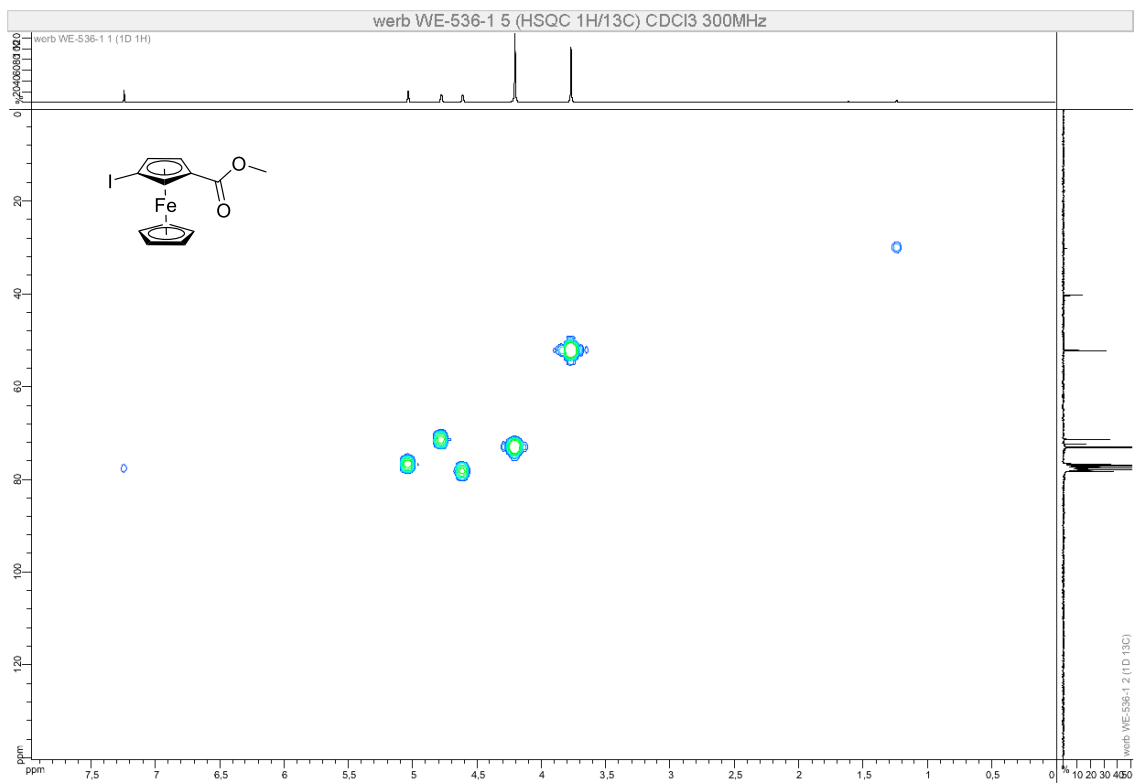




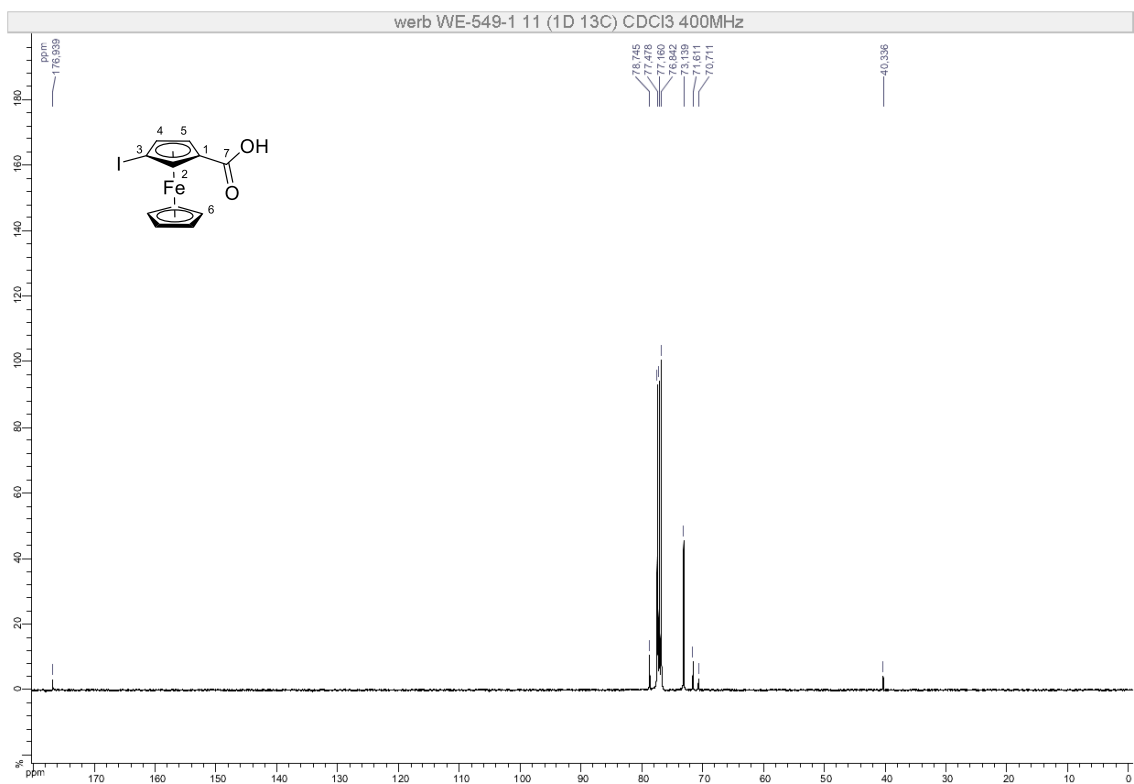
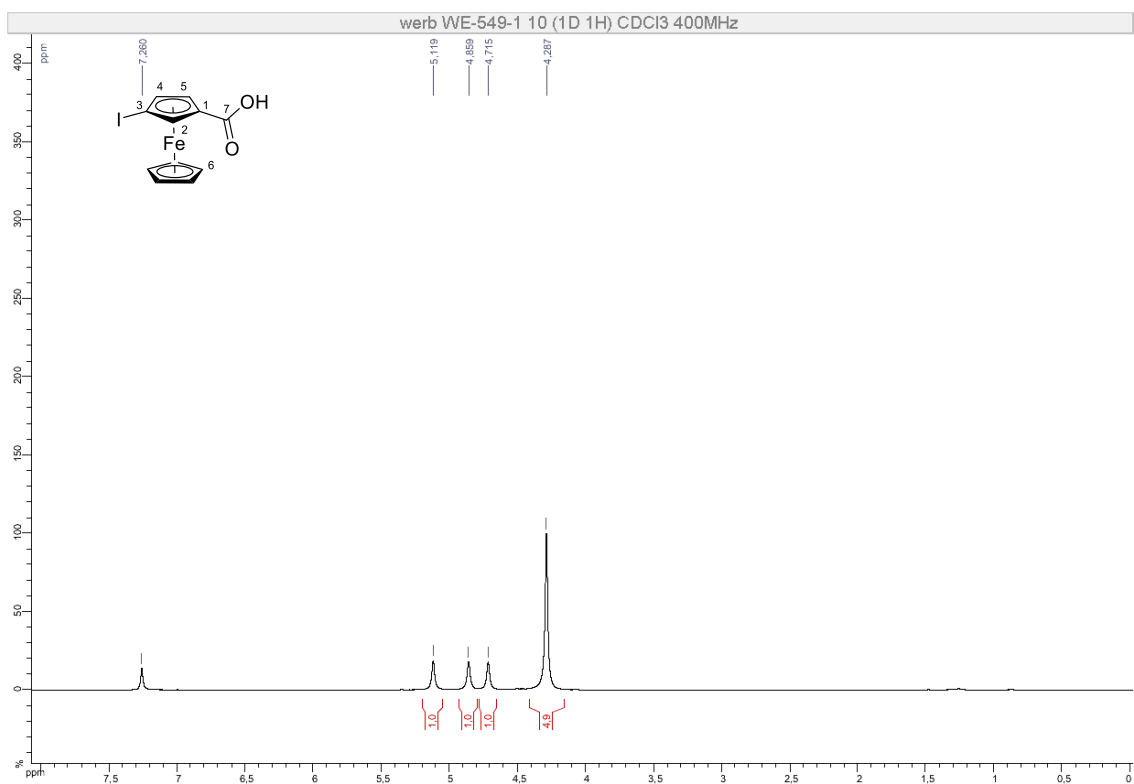
**Methyl 3-iodoferrocenecarboxylate (42)**

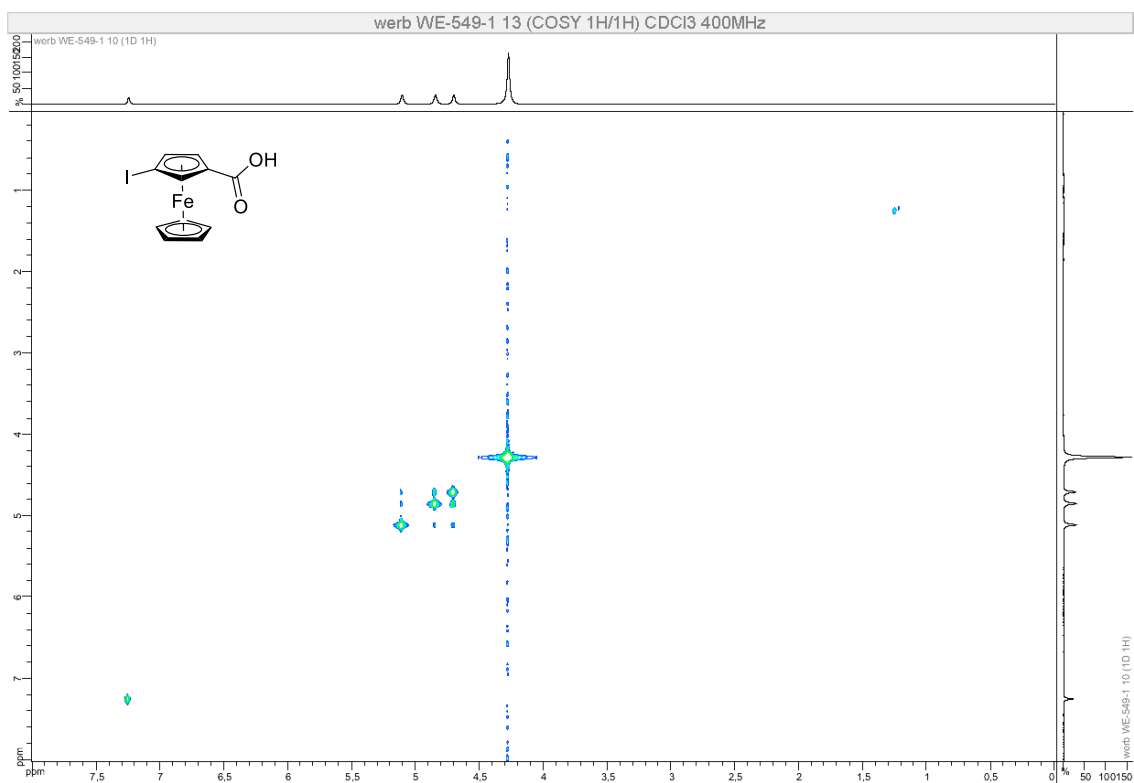
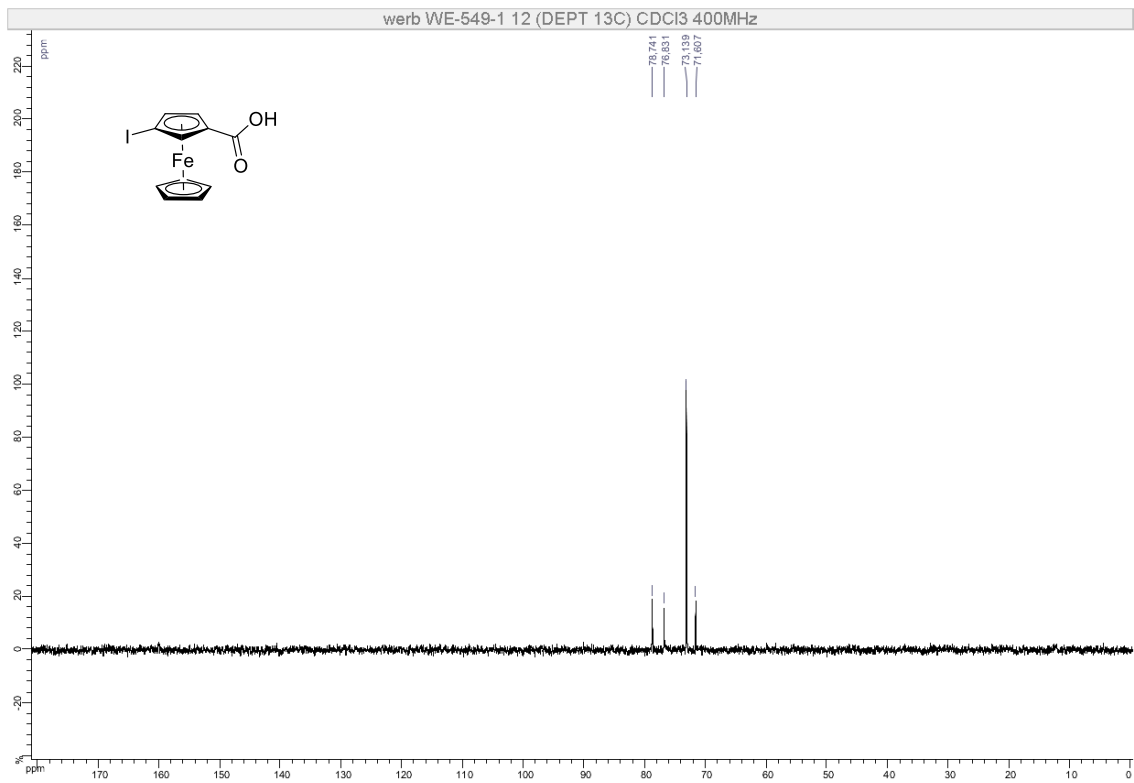




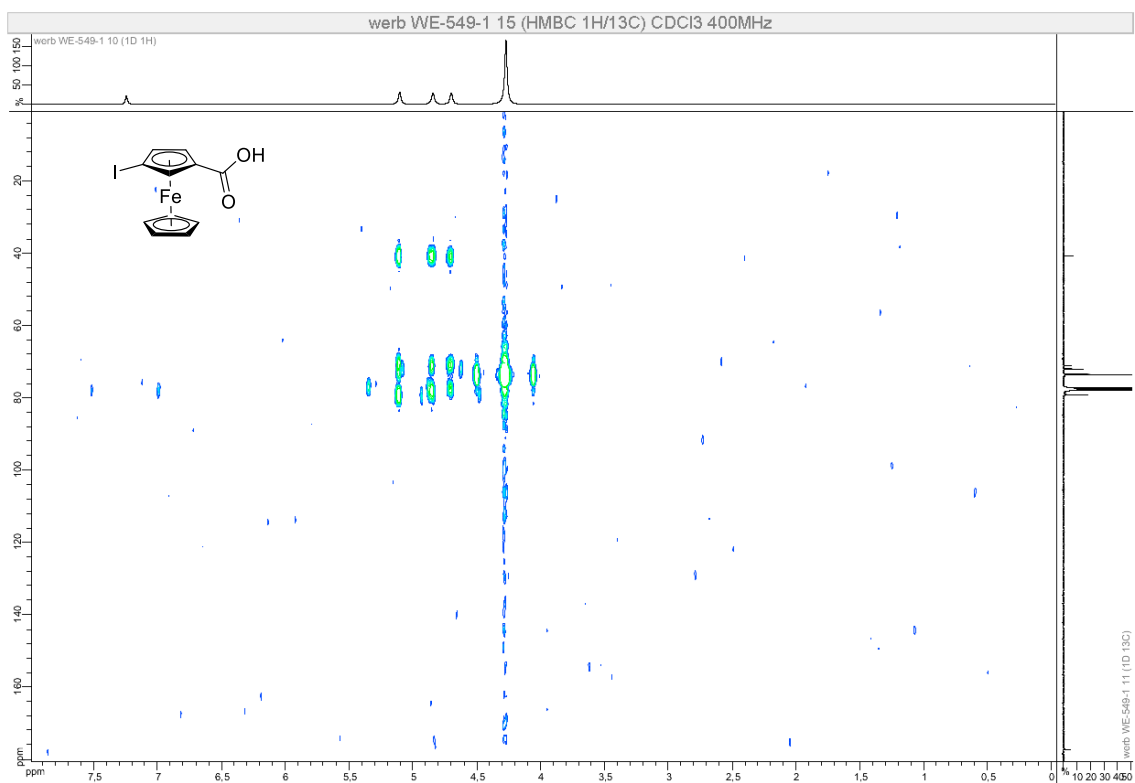
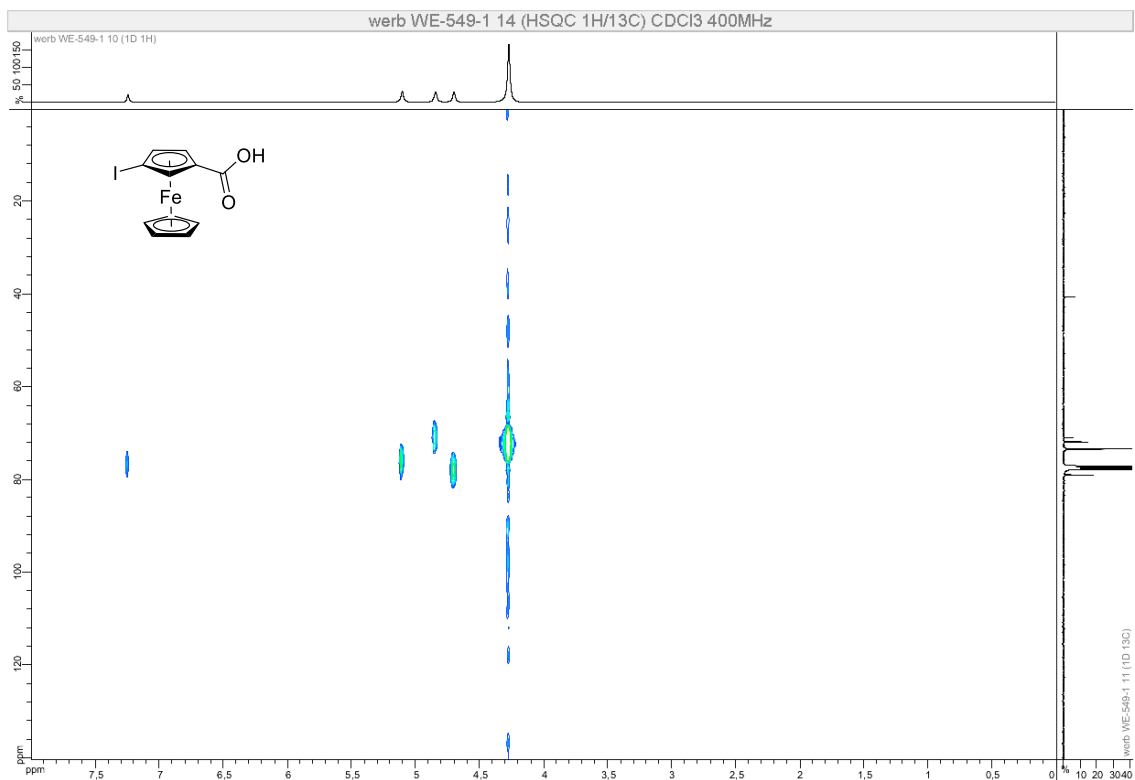


### 3-Iodoferrocenecarboxylic acid (43)

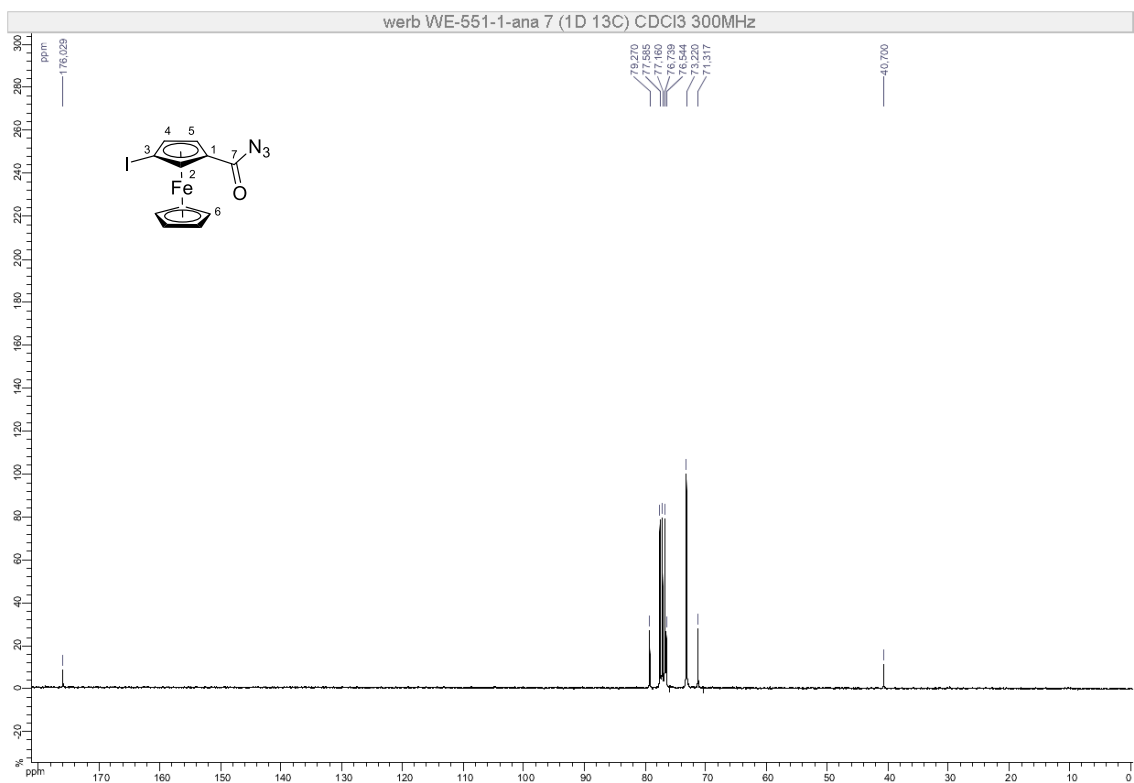
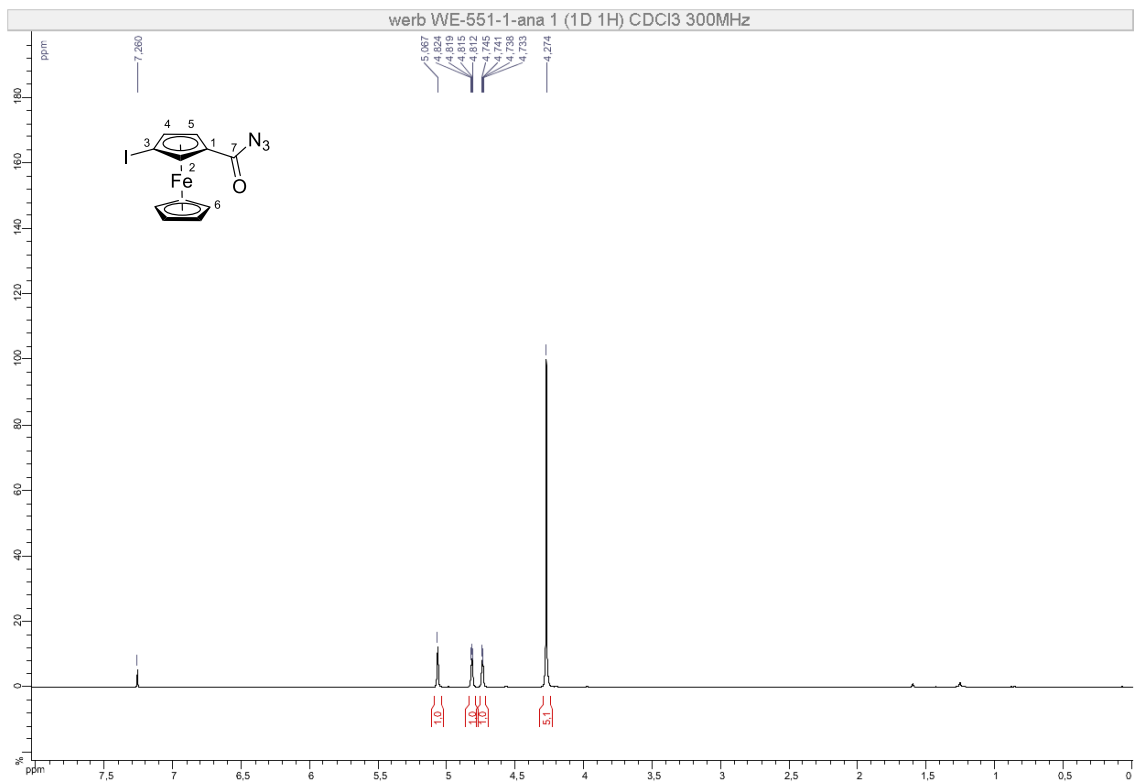


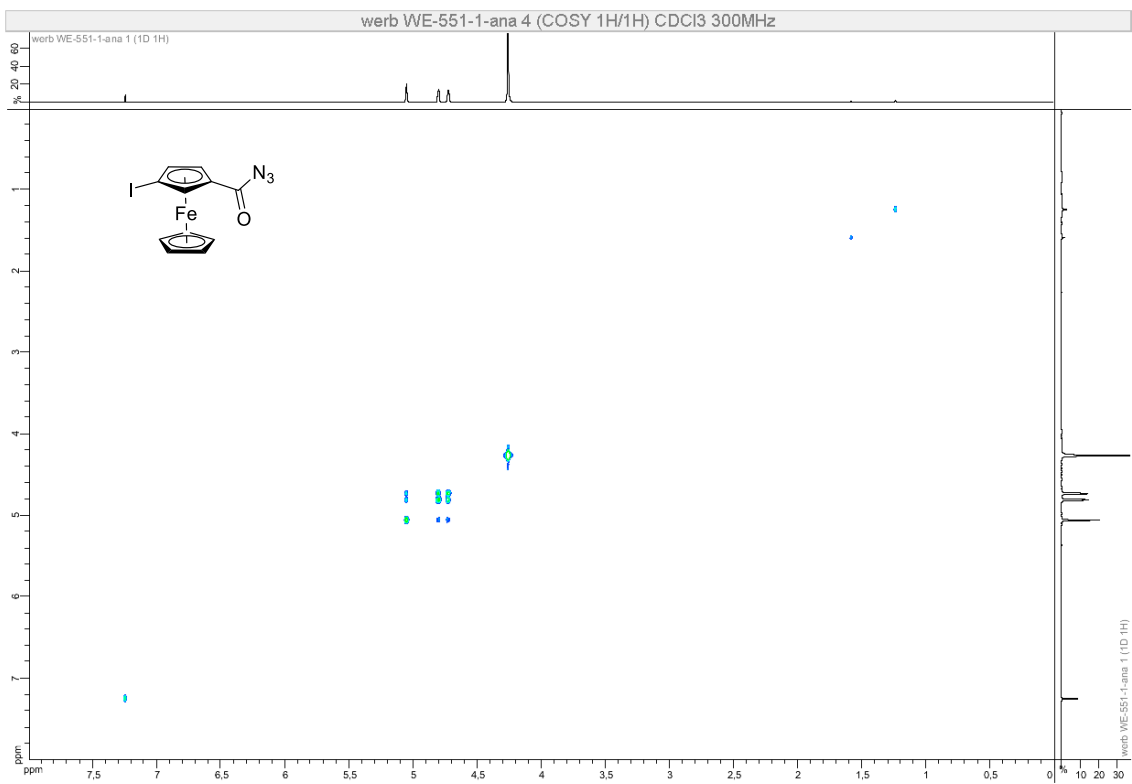
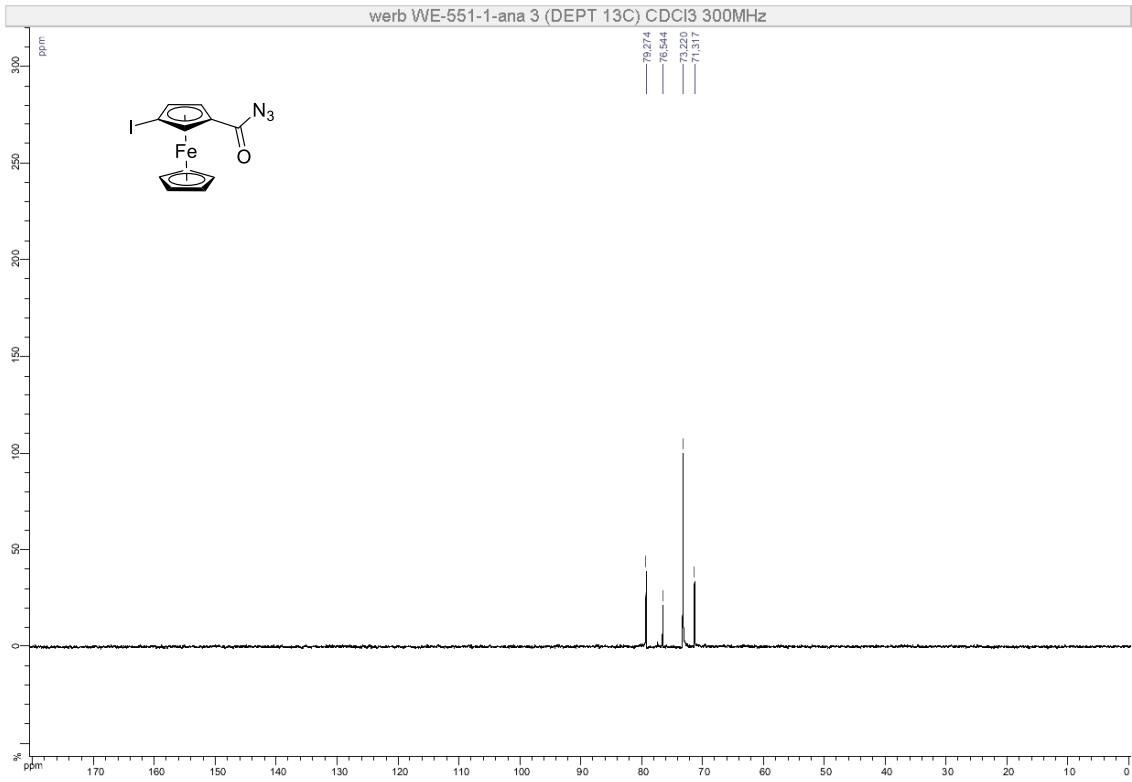


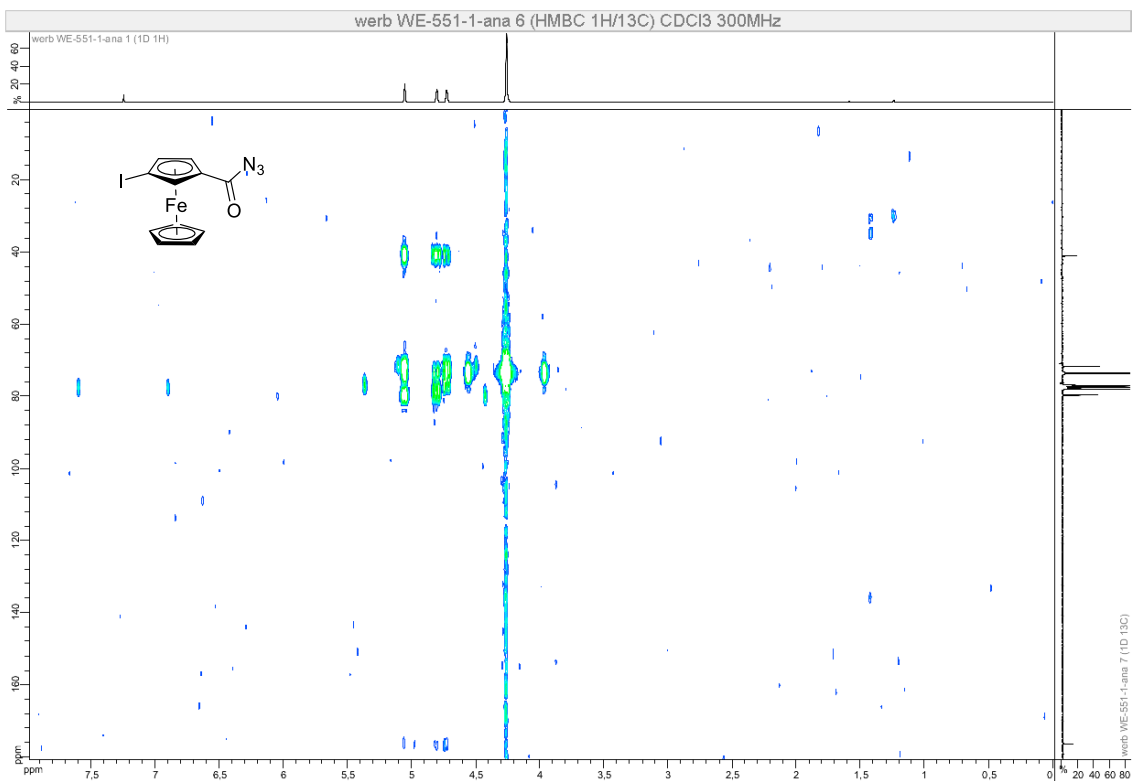
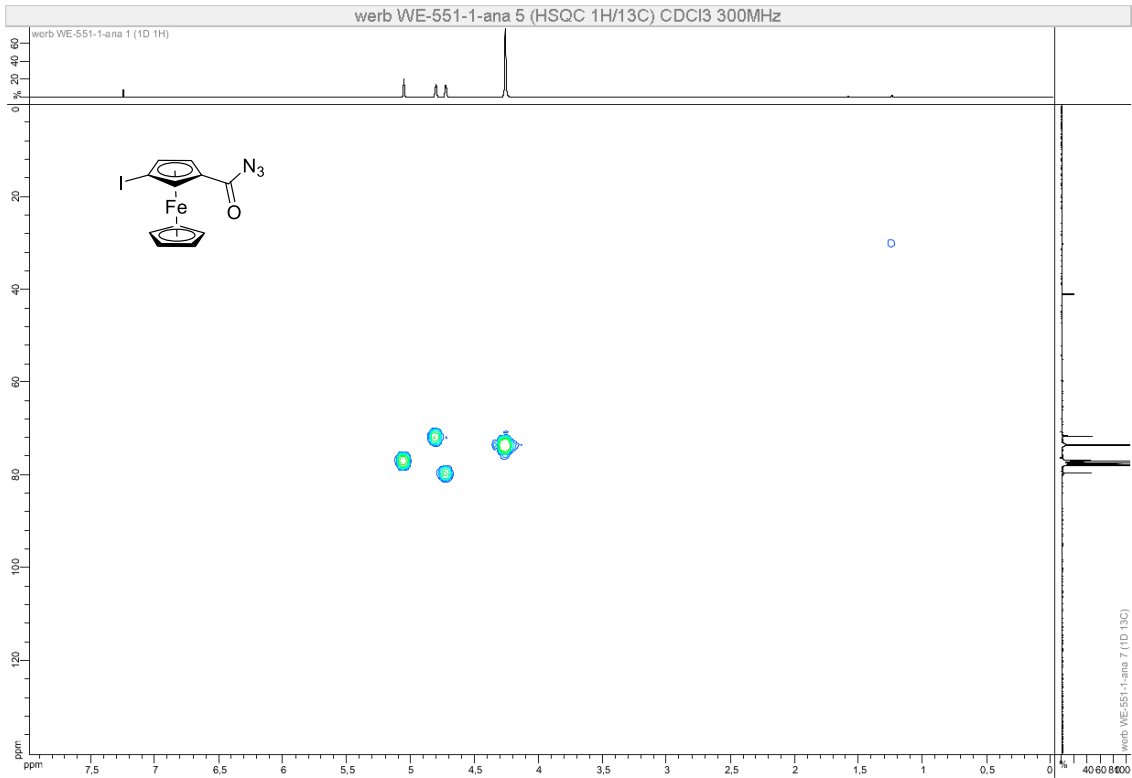




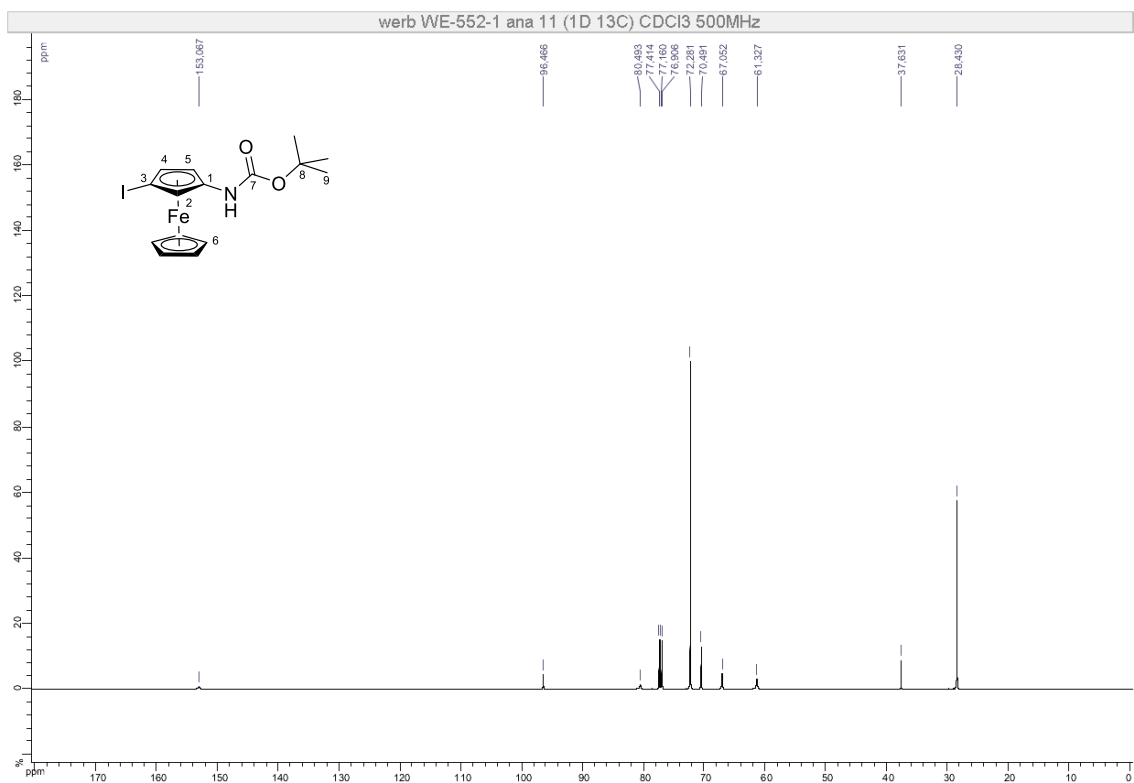
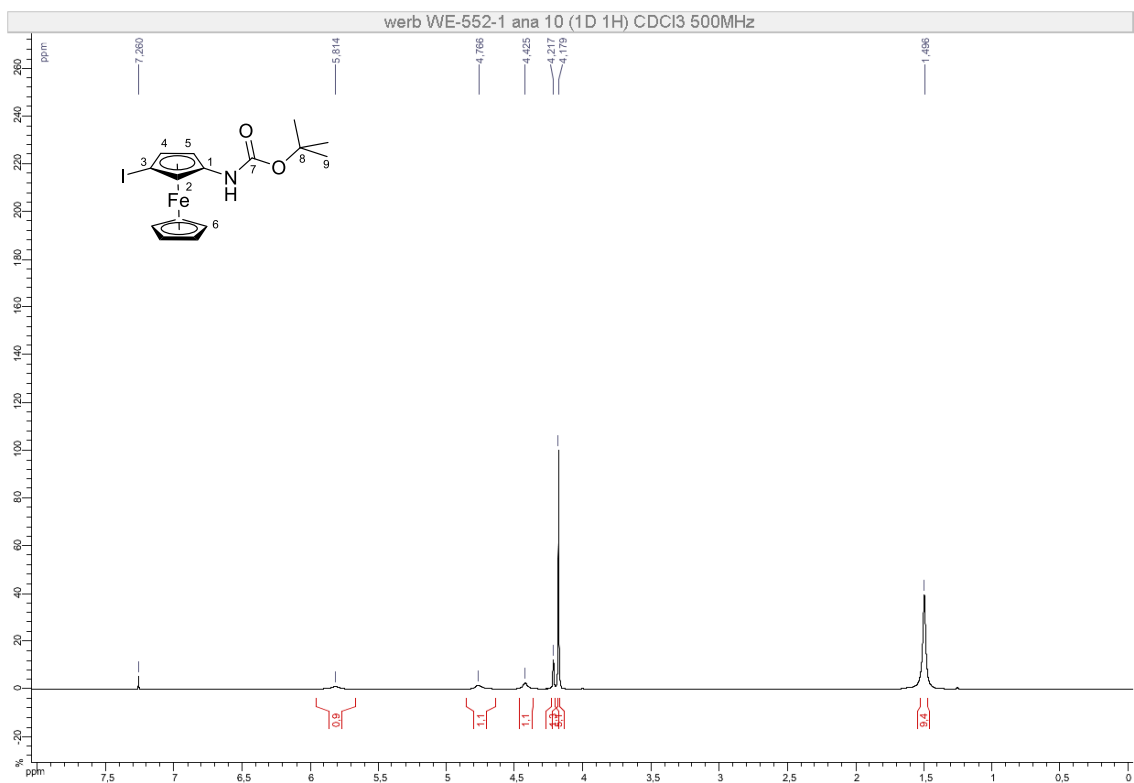
### 3-Iodoferrocenoyl azide (44)

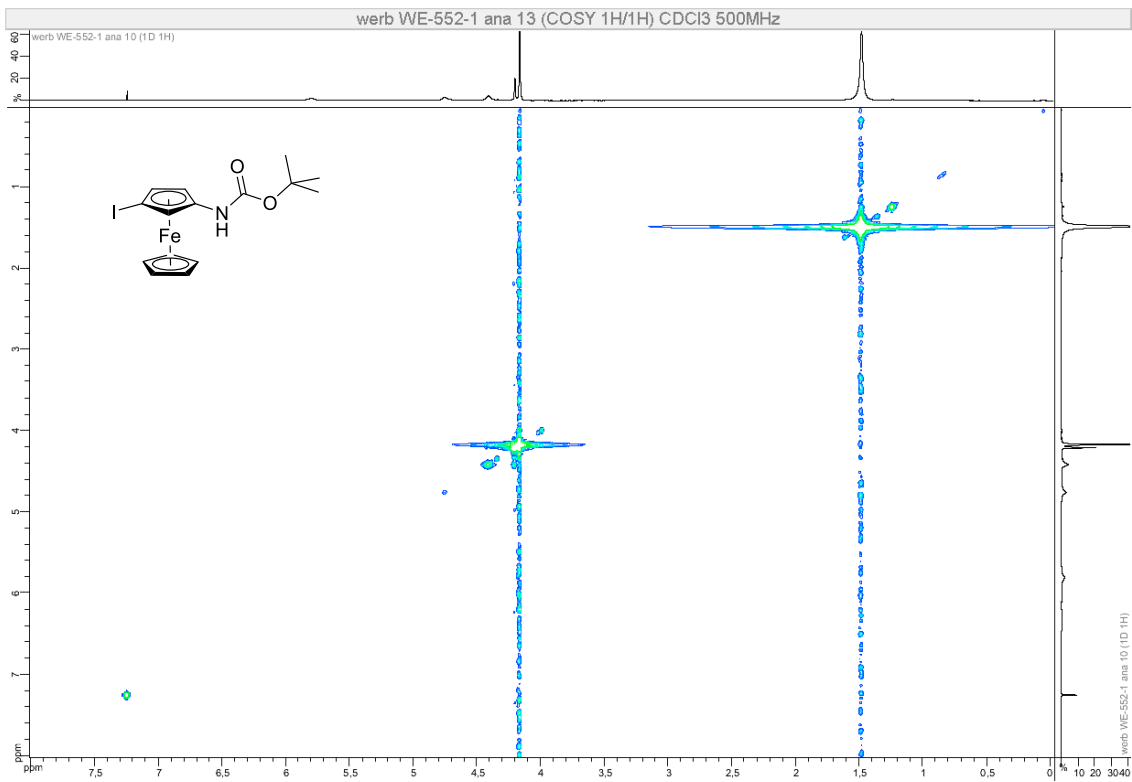
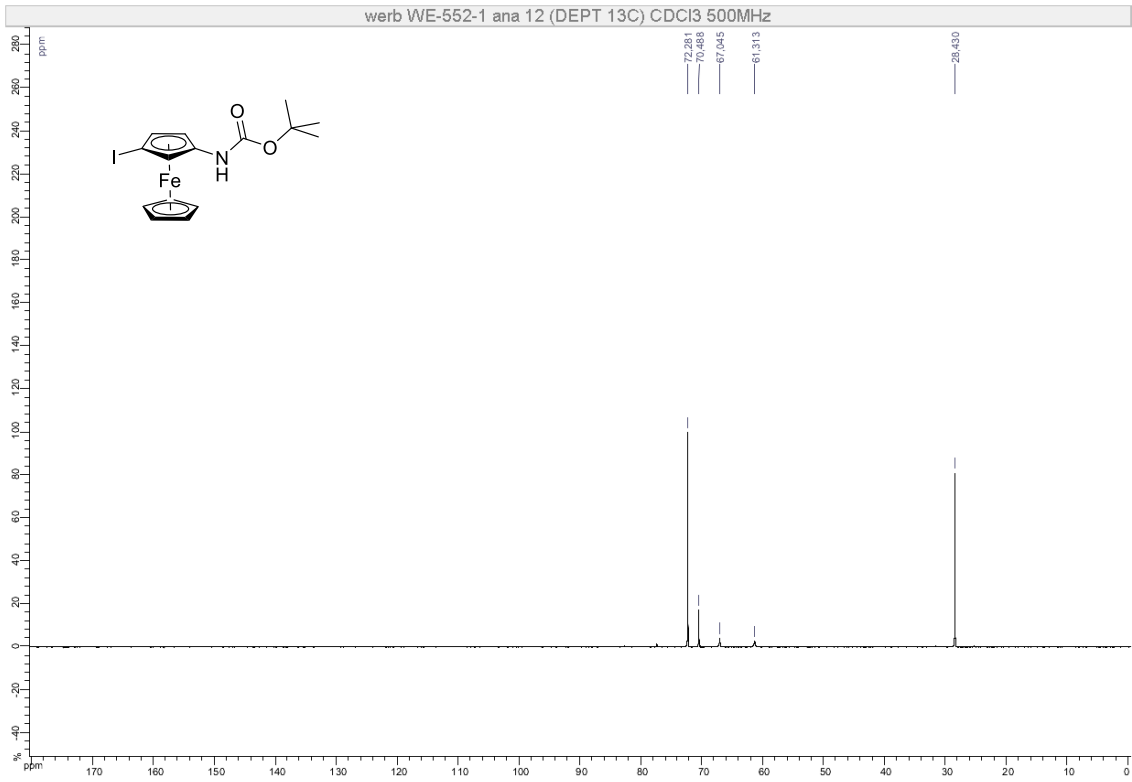


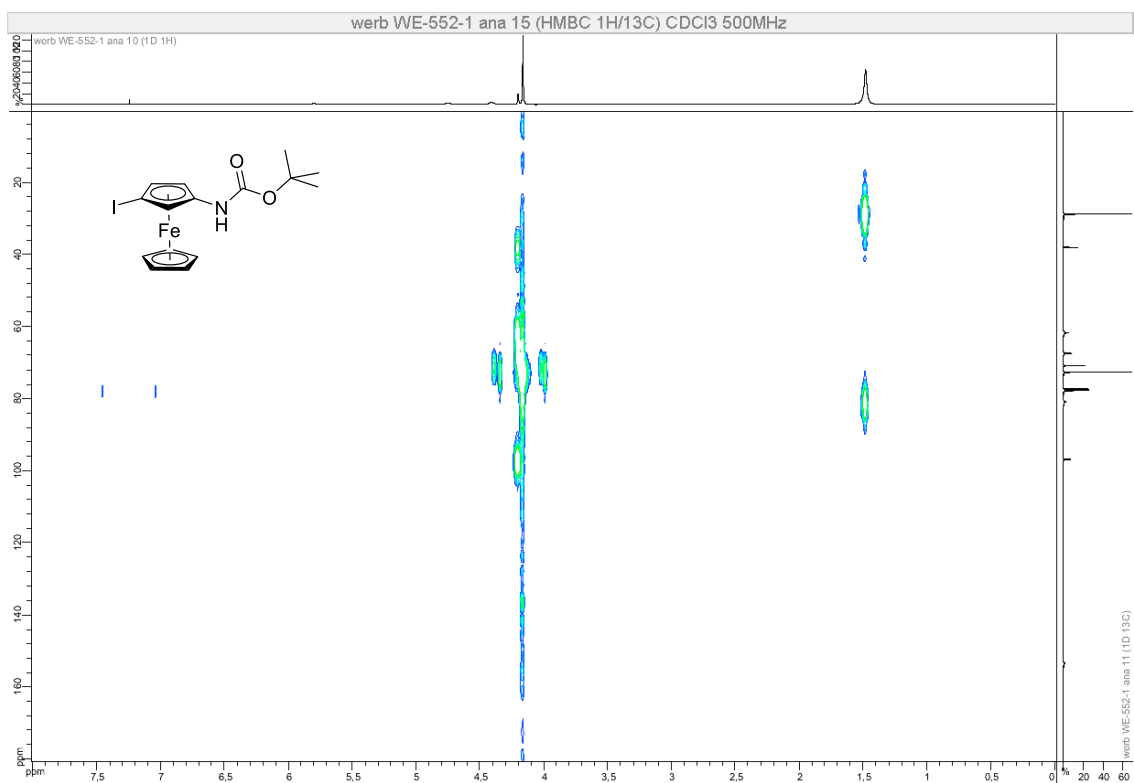
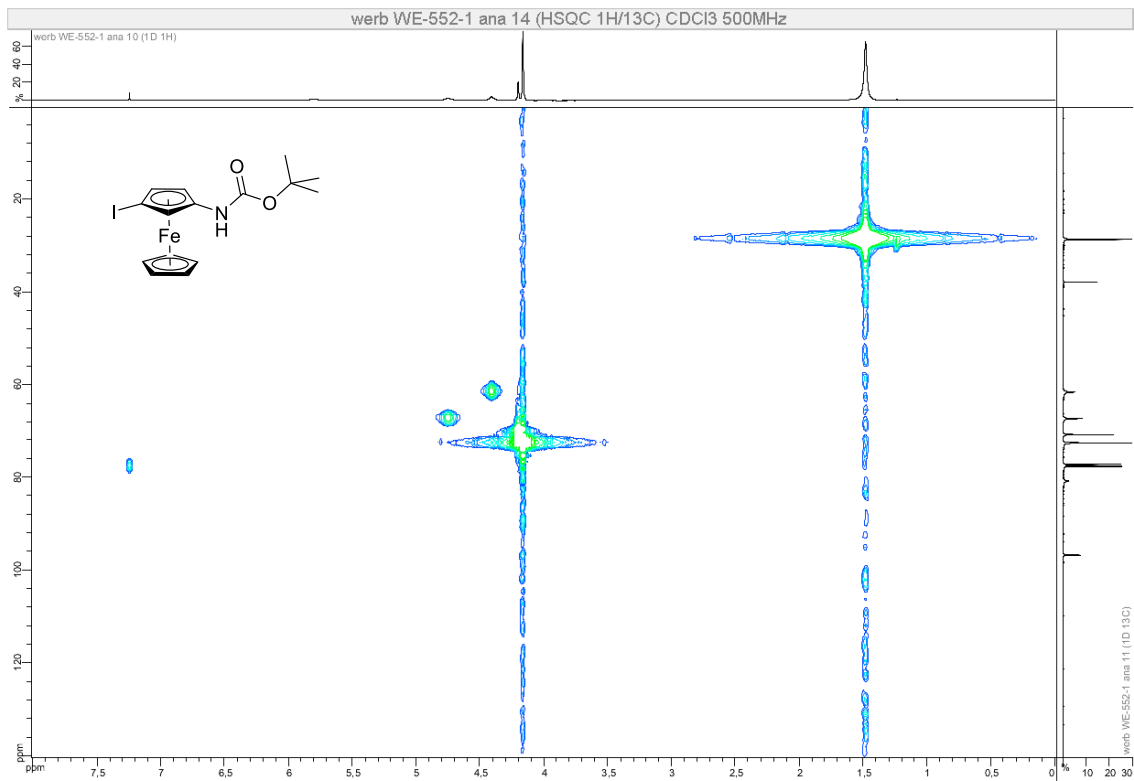




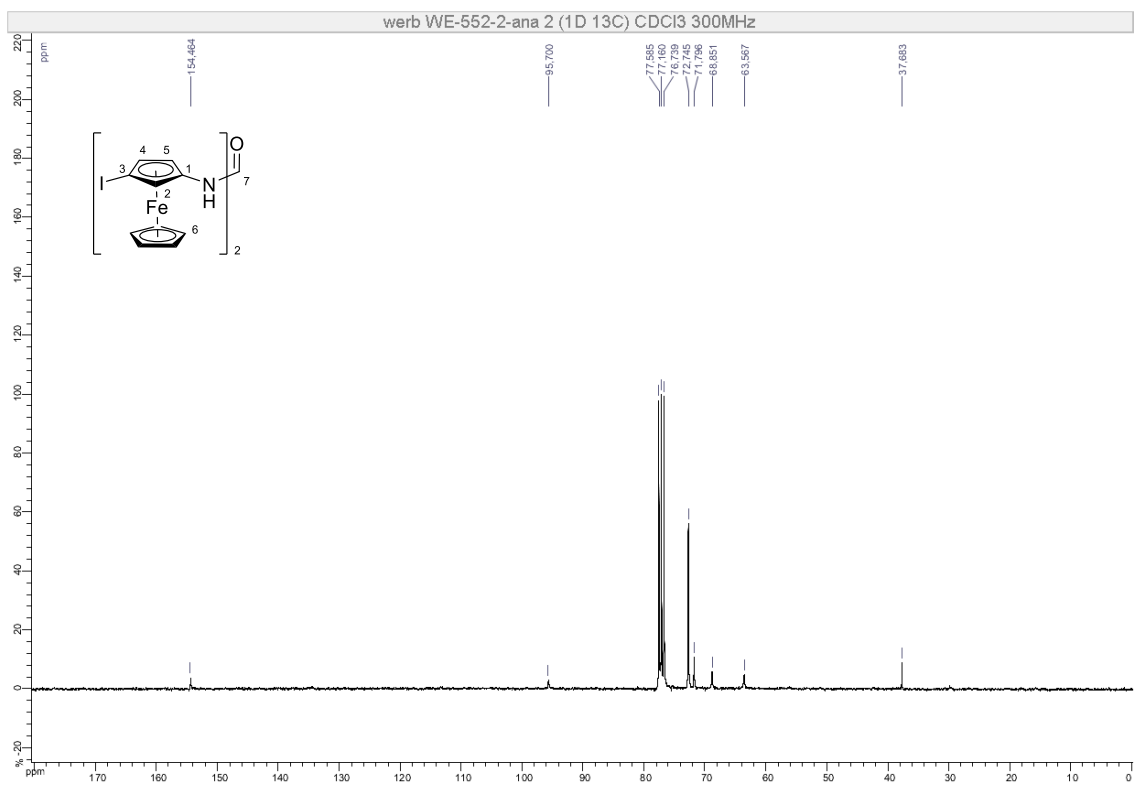
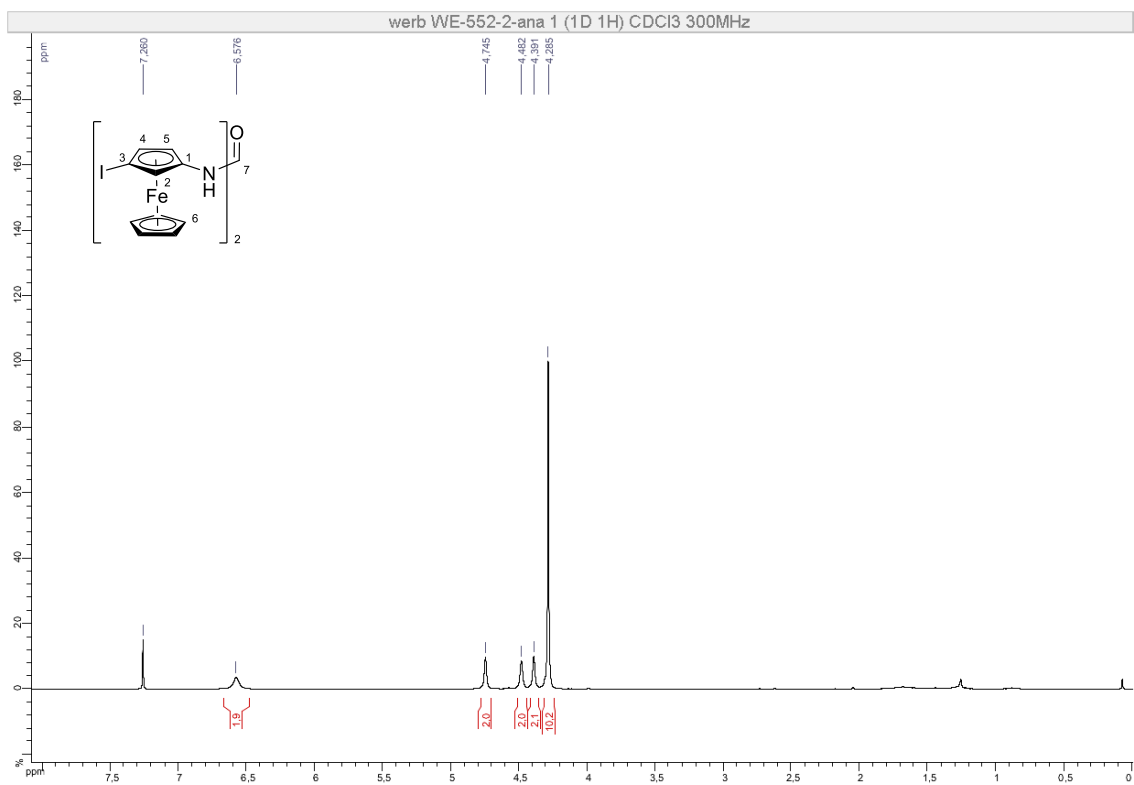
**1-(tert-Butoxycarbonyl)amino-3-iodoferrocene (45)**



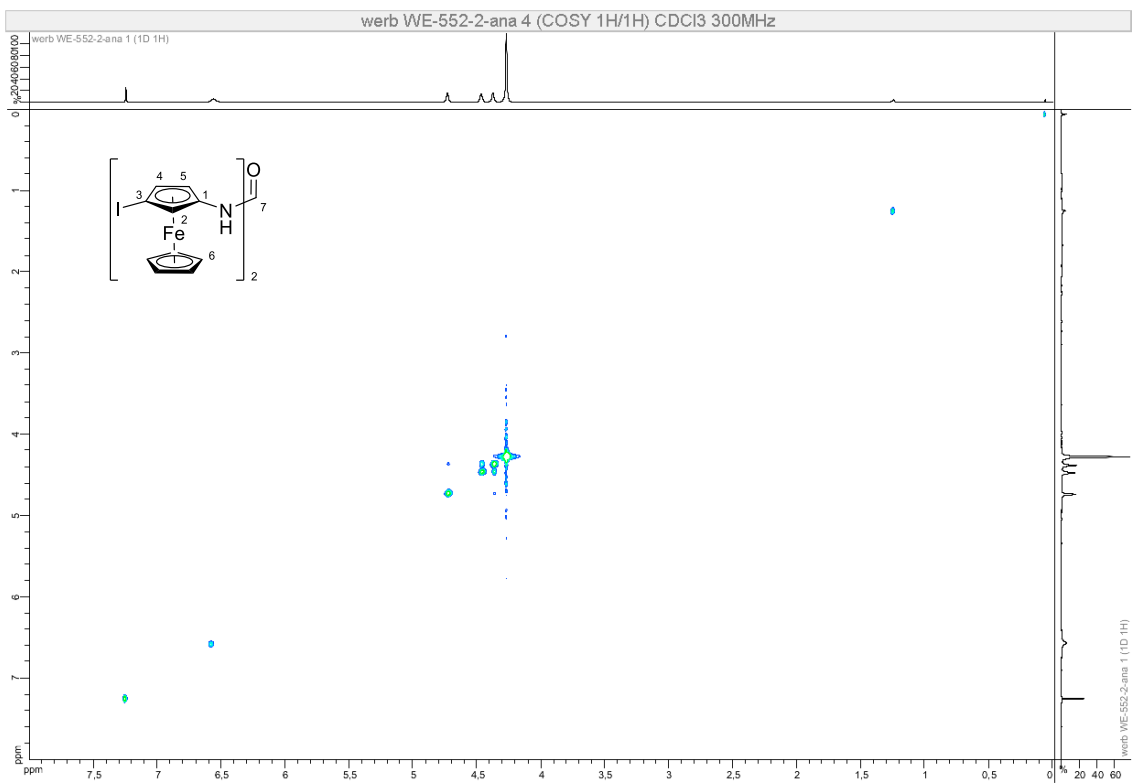
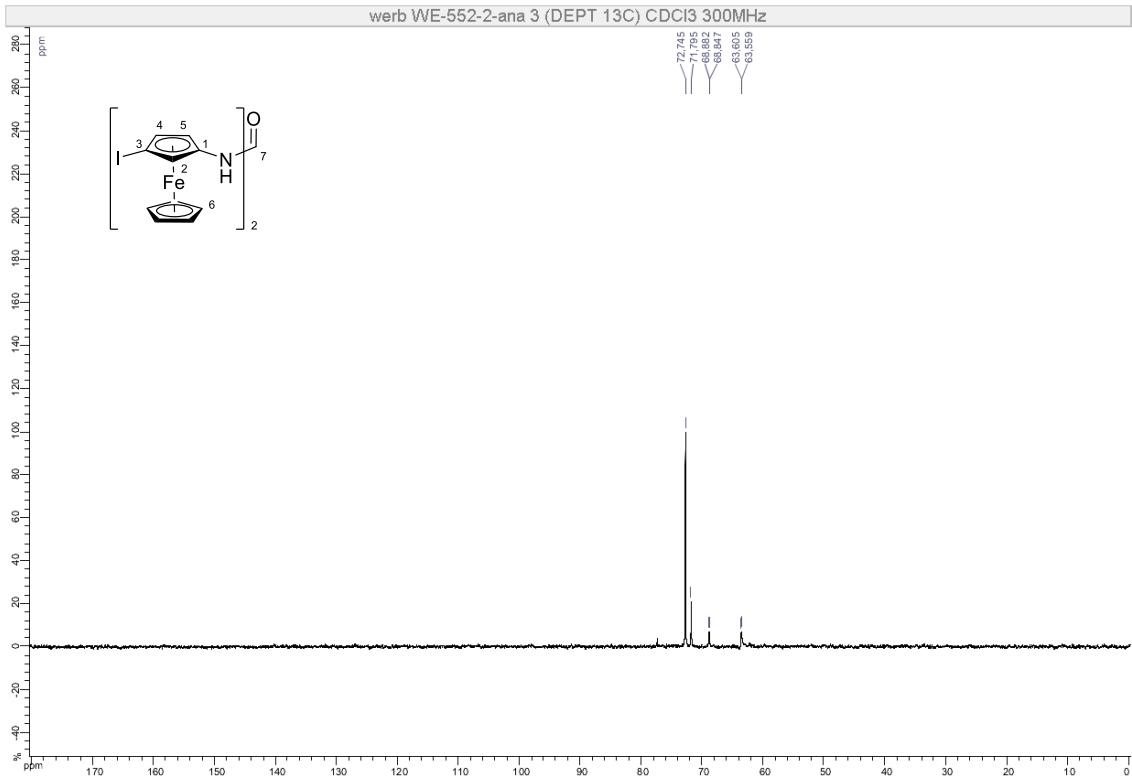


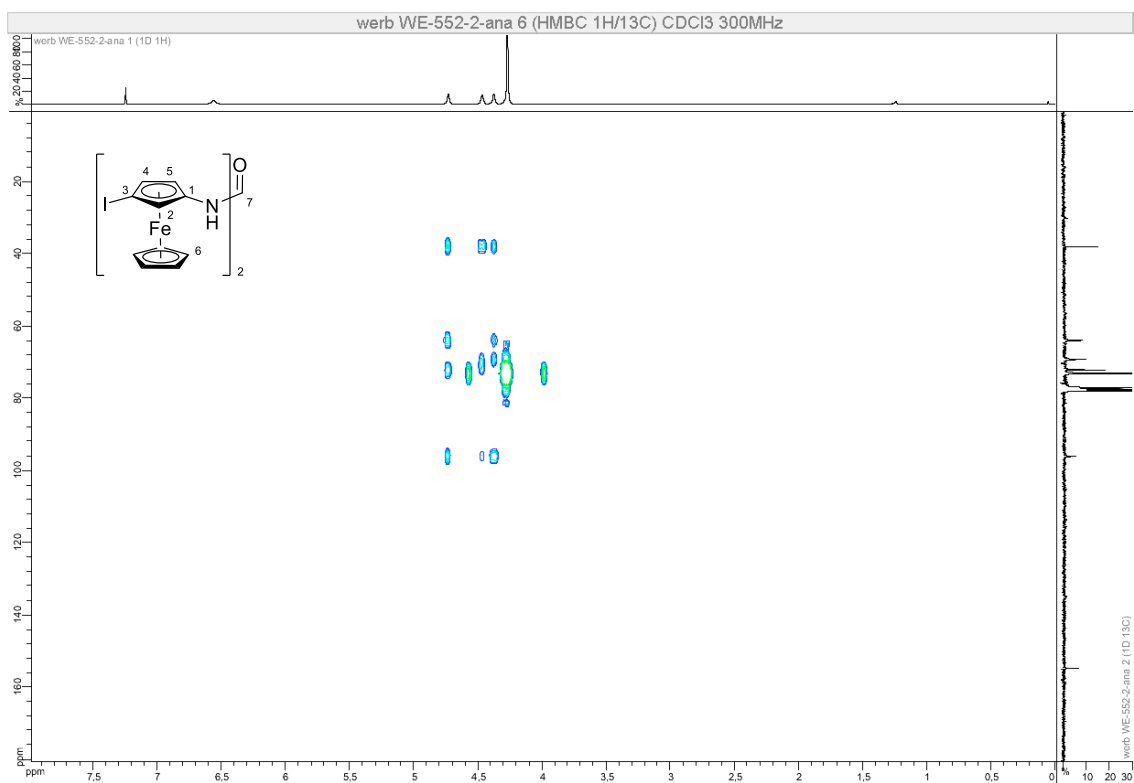
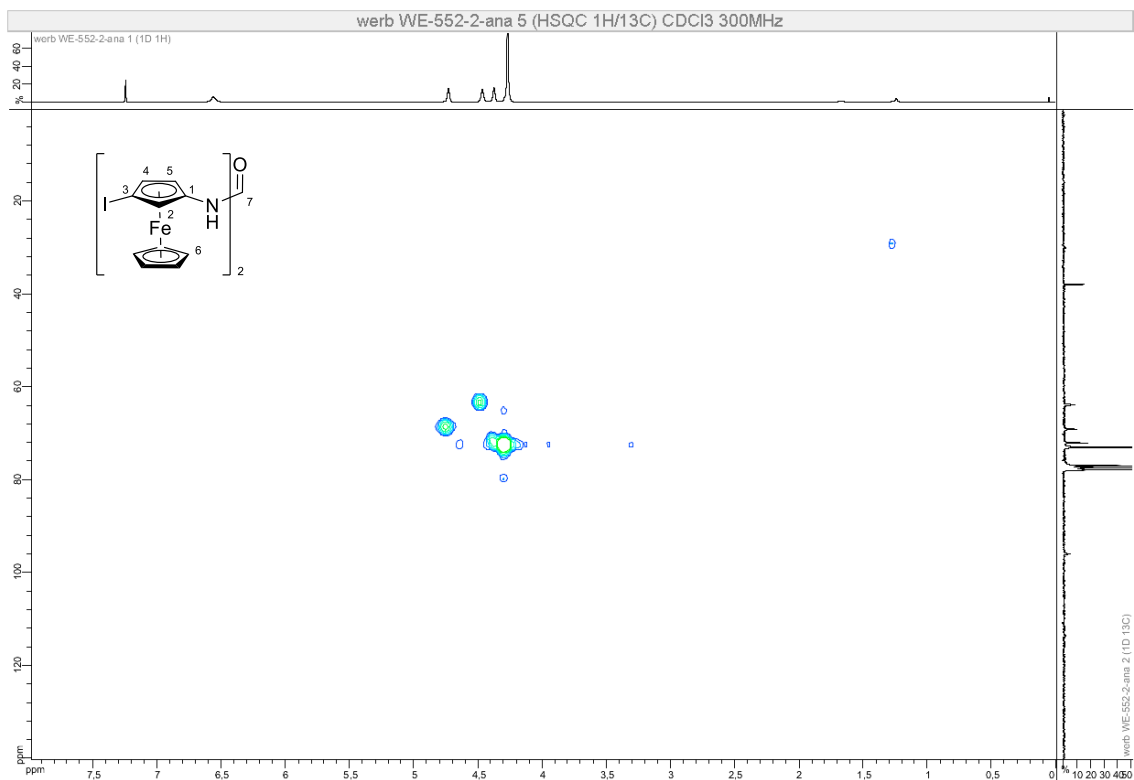


**N,N'-di(3-iodoferrocenyl)urea (46)**

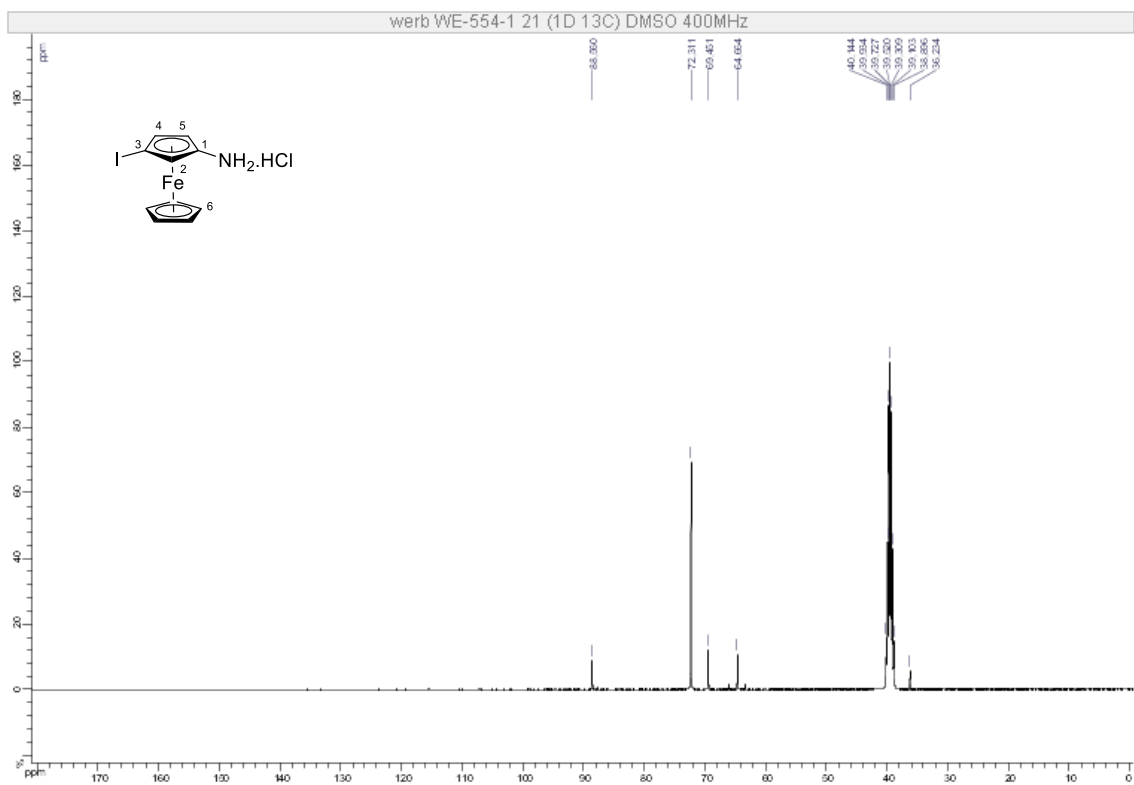
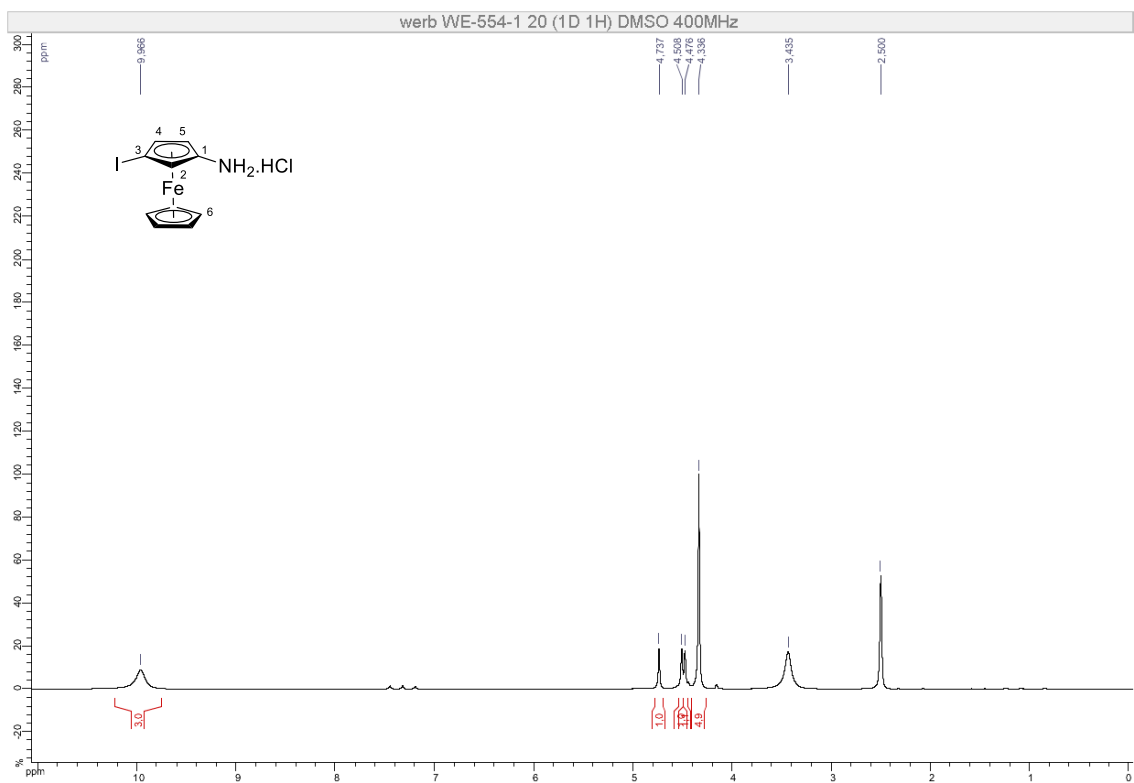


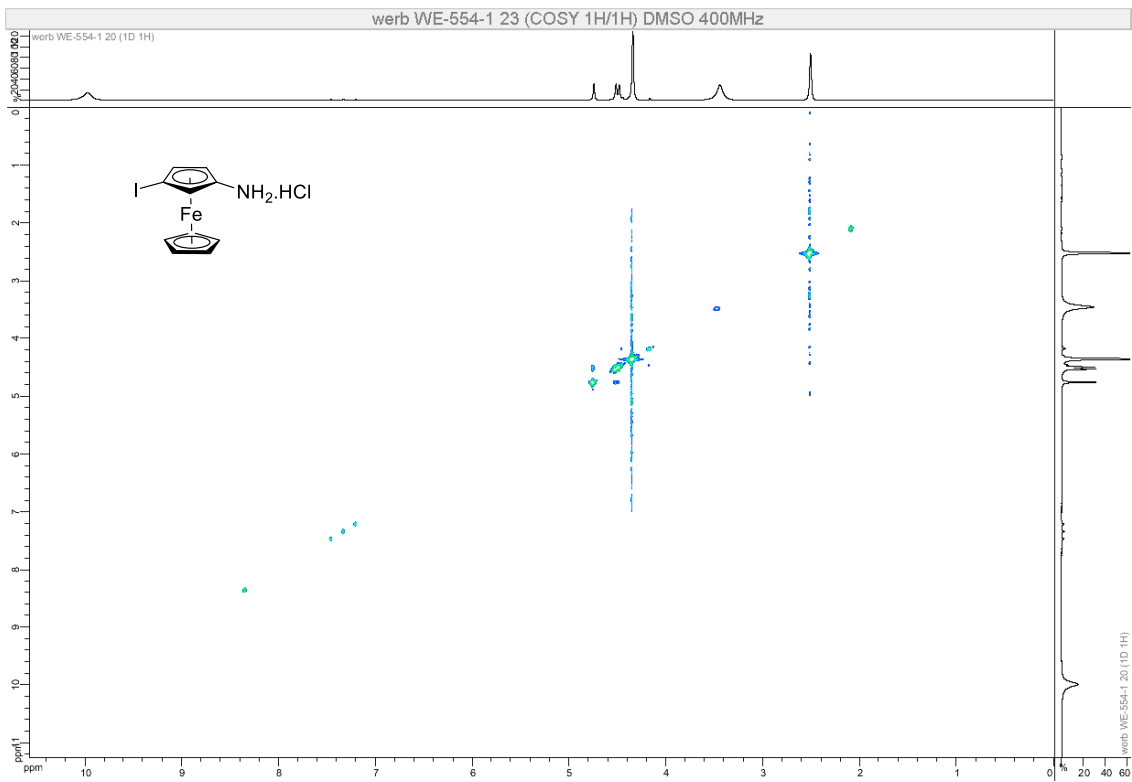
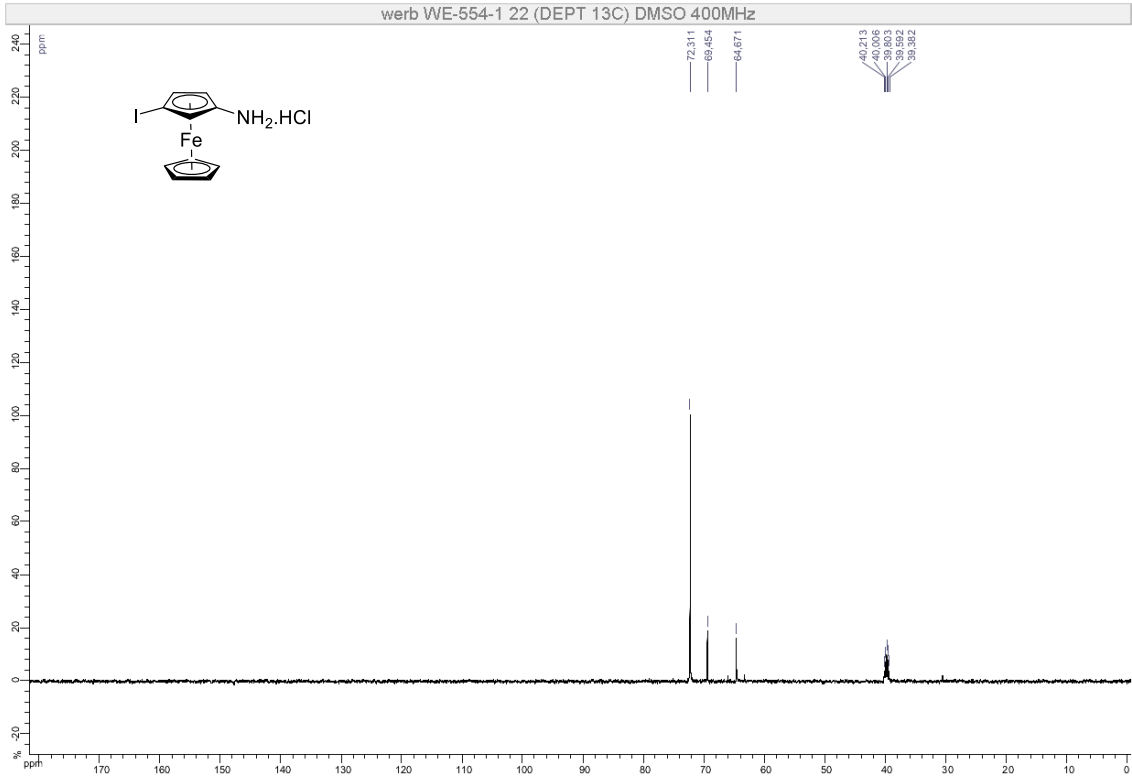


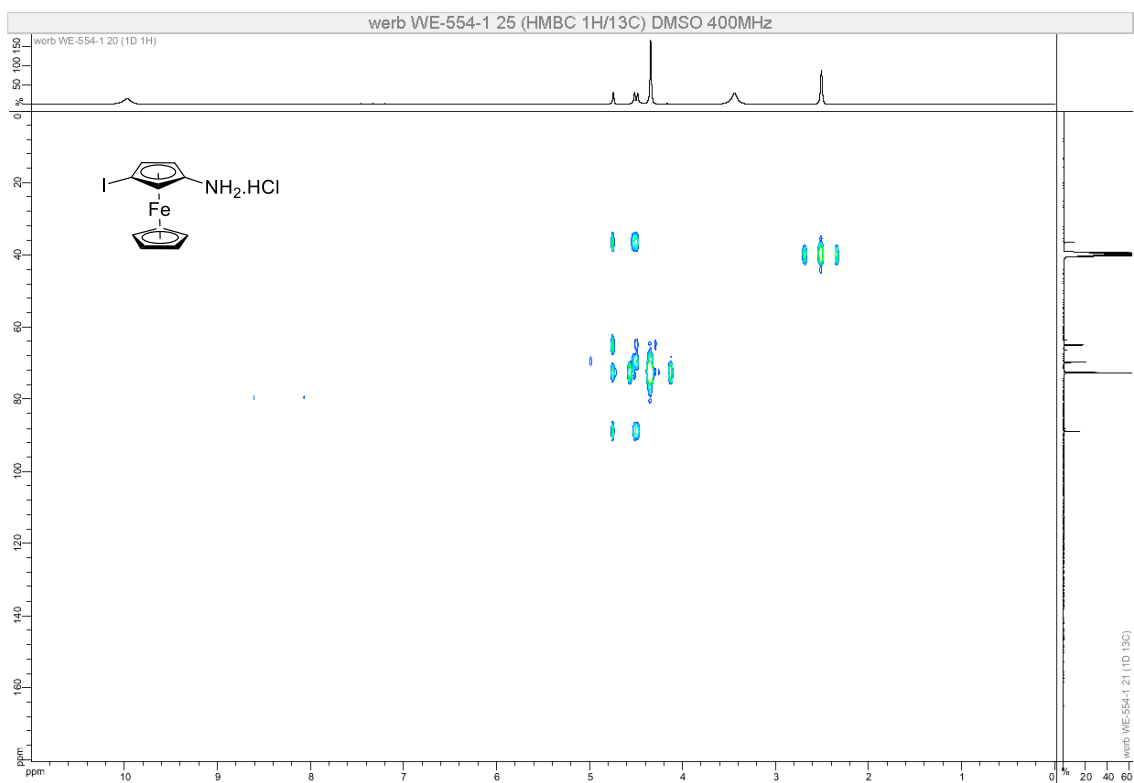
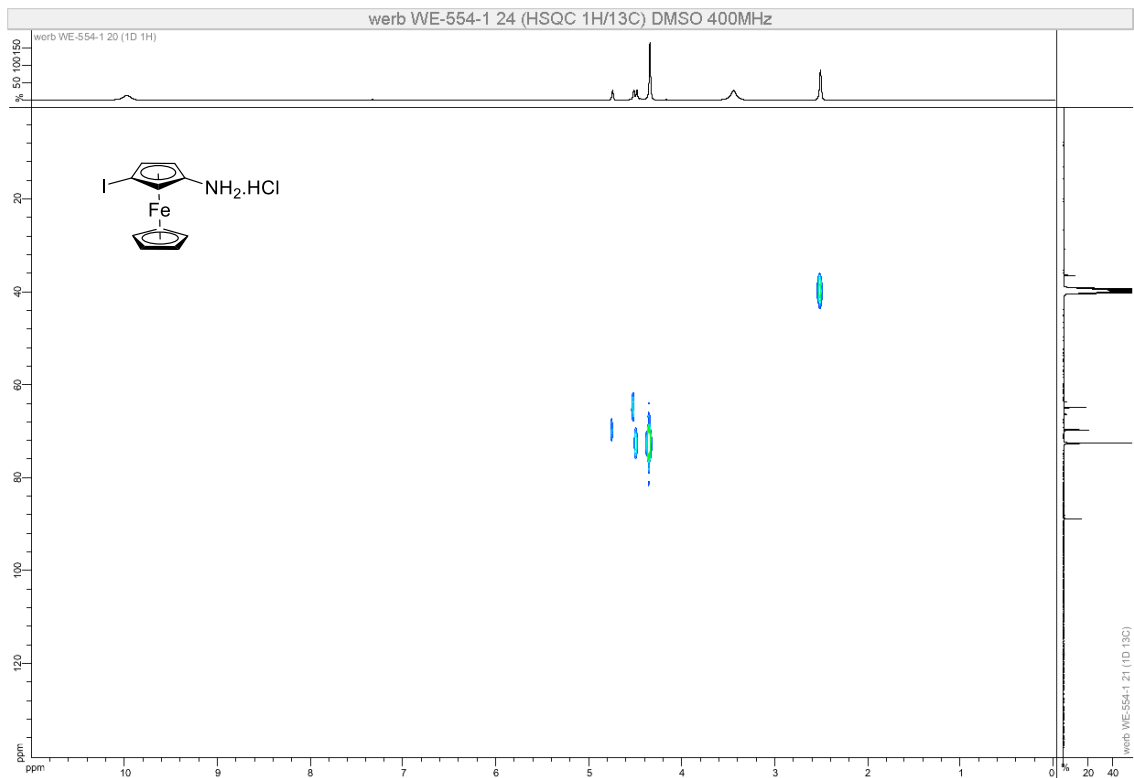




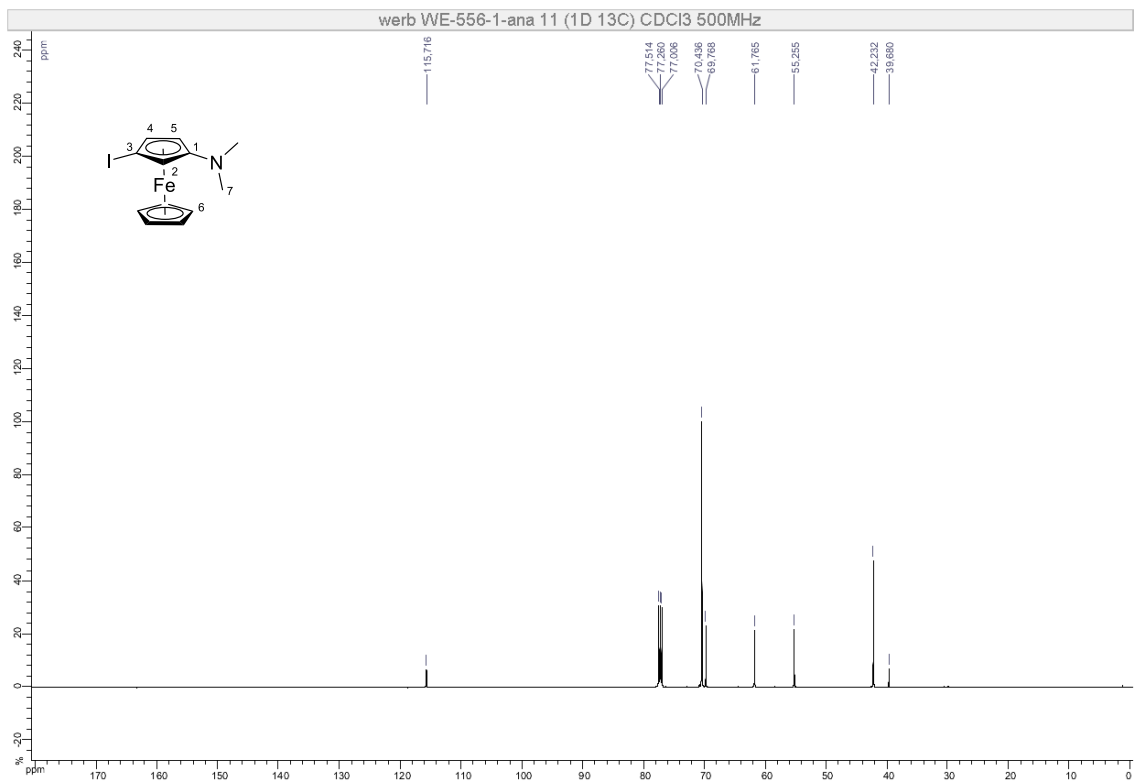
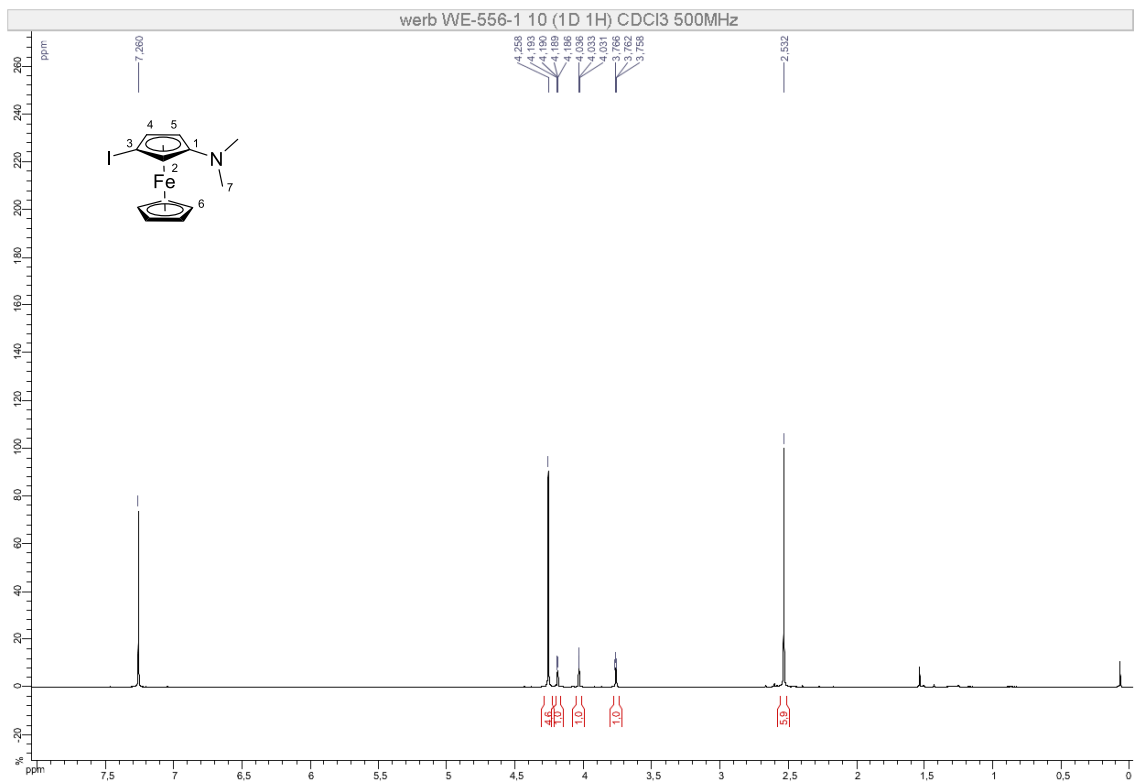
**3-Iodoferrocenamine hydrochloride (47)**

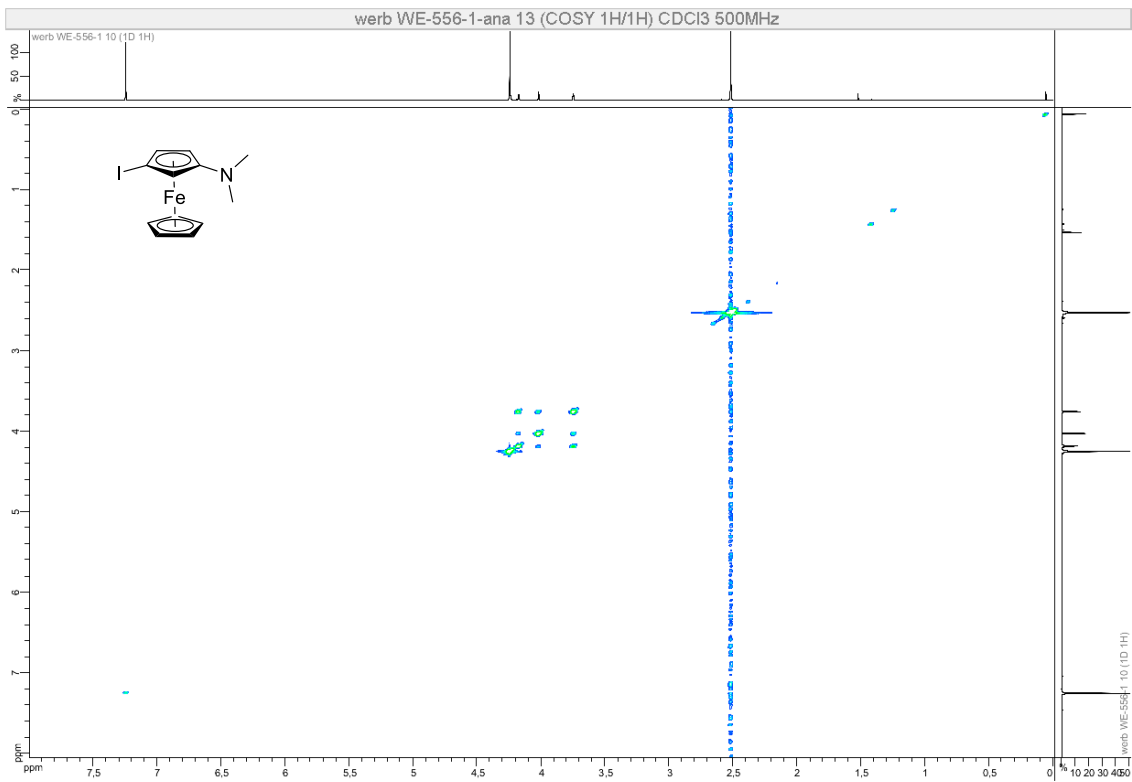
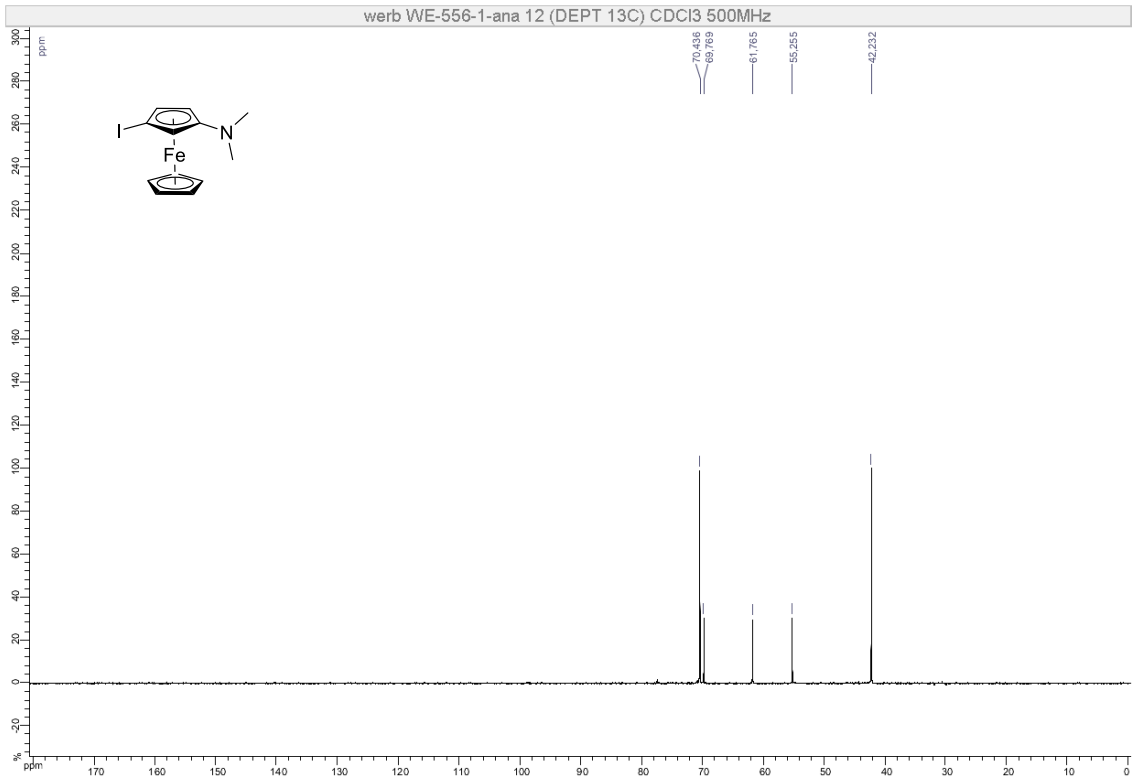


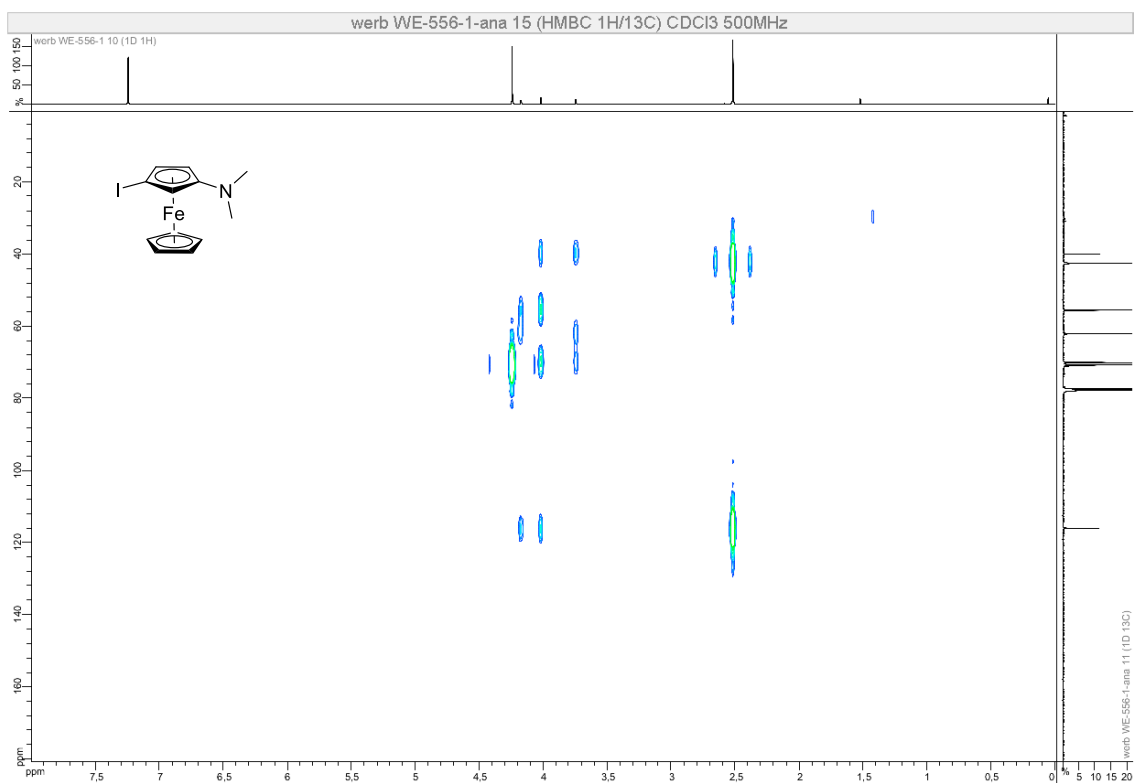
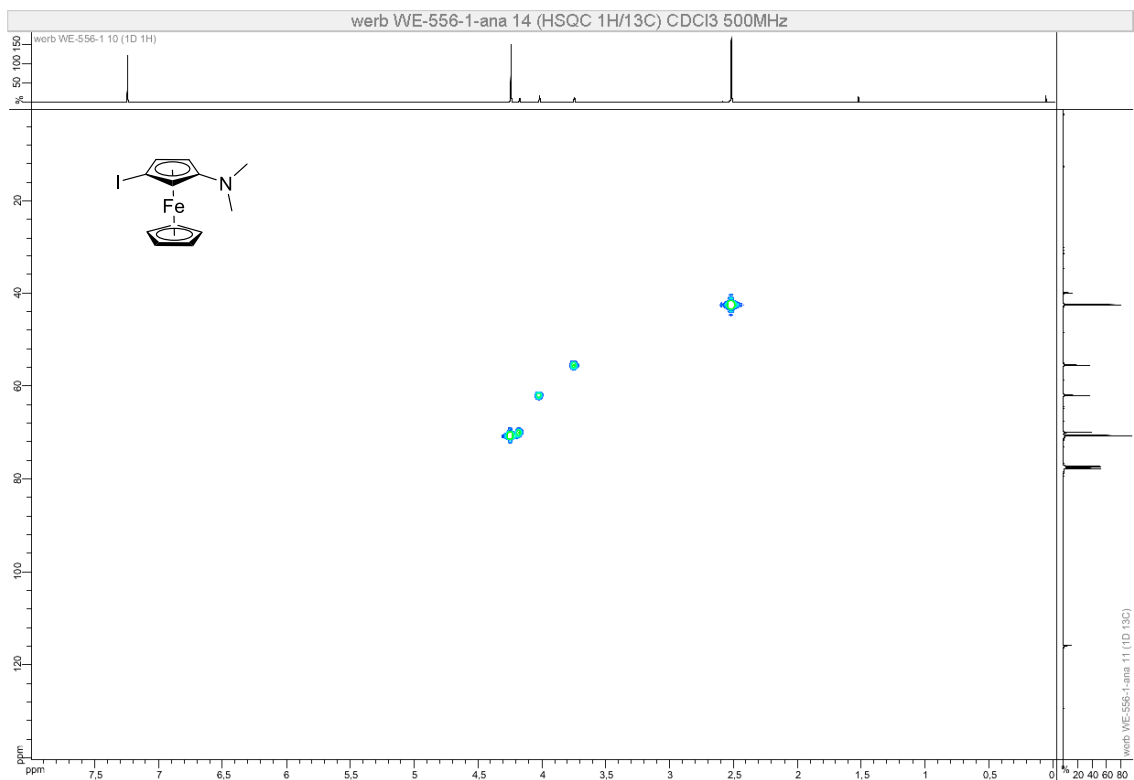




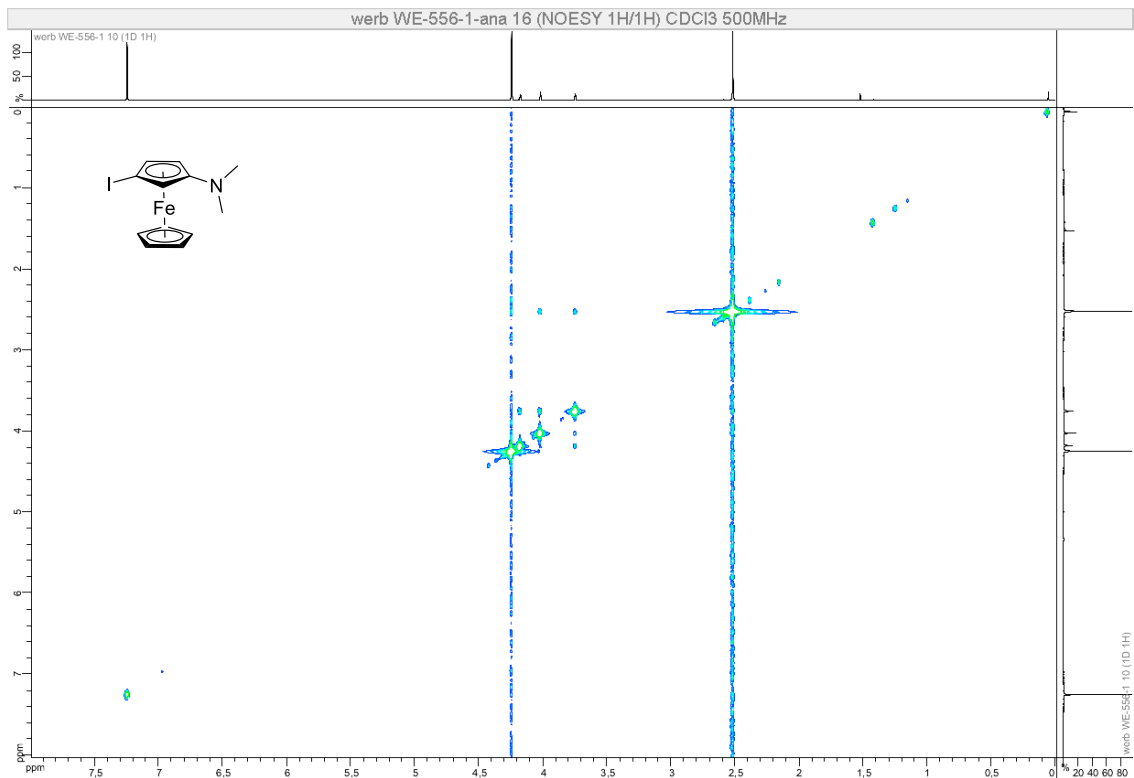
**1-(Dimethylamino)-3-iodoferrocene (48)**



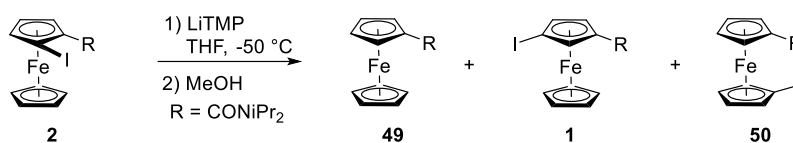




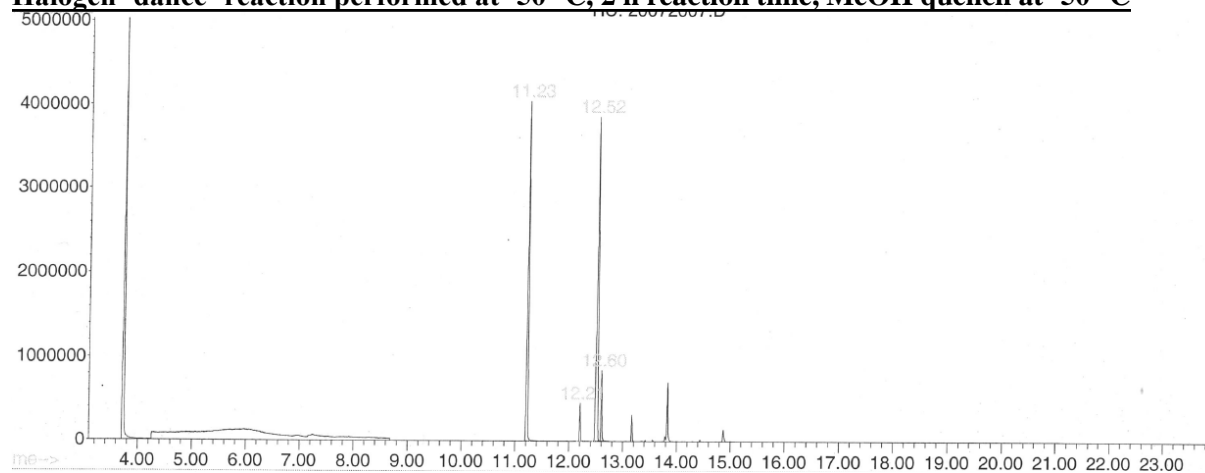




## GC-MS Chromatograms

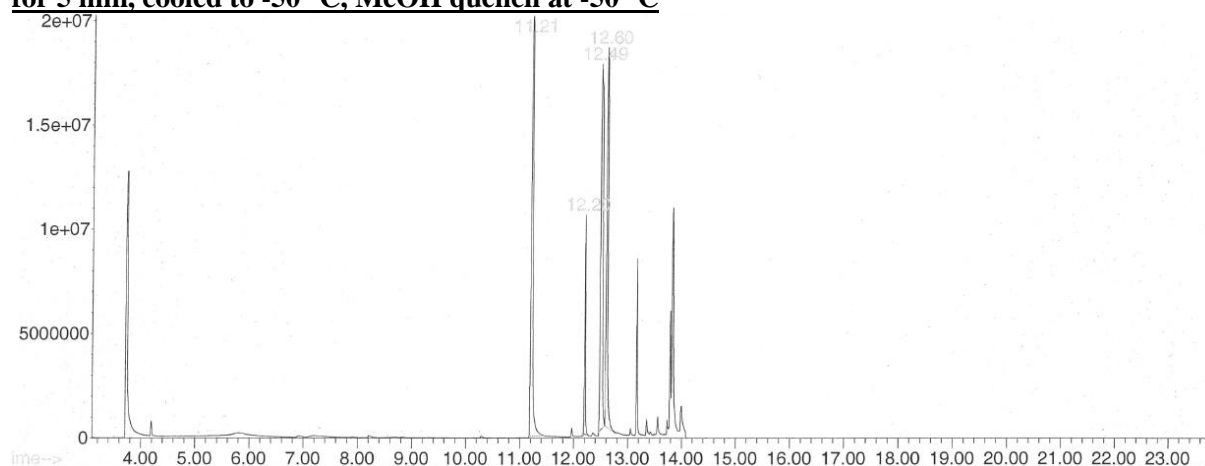


### Halogen 'dance' reaction performed at -50 °C, 2 h reaction time, MeOH quench at -50 °C



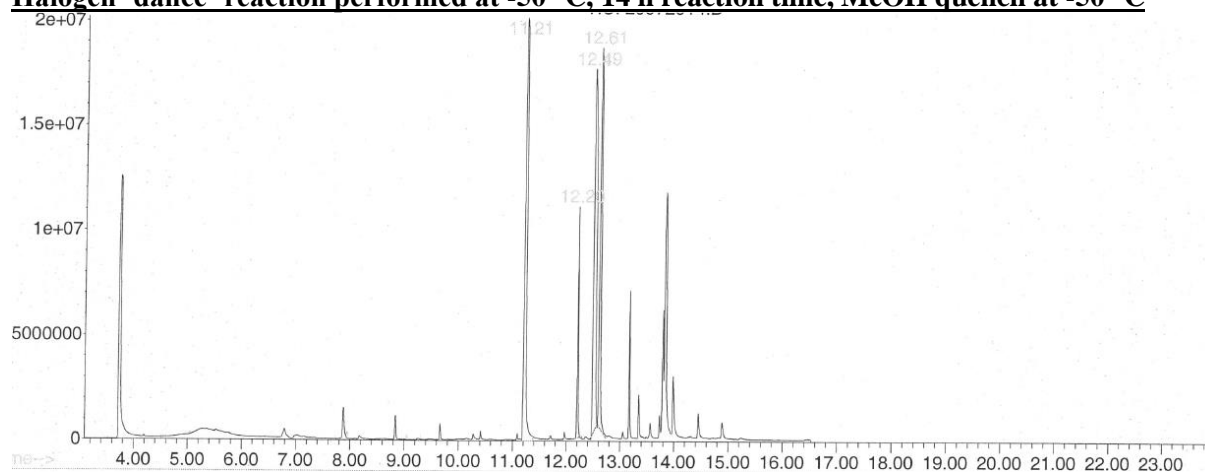
Peak	Products	Retention time (min)	% of total
1	49	11.23	42.8
2	2	12.21	3.6
3	1	12.52	47.3
4	50	12.60	6.3

### Halogen 'dance' reaction performed at -50 °C, 2 h reaction time, reaction mixture stirred at rt for 5 min, cooled to -50 °C, MeOH quench at -50 °C



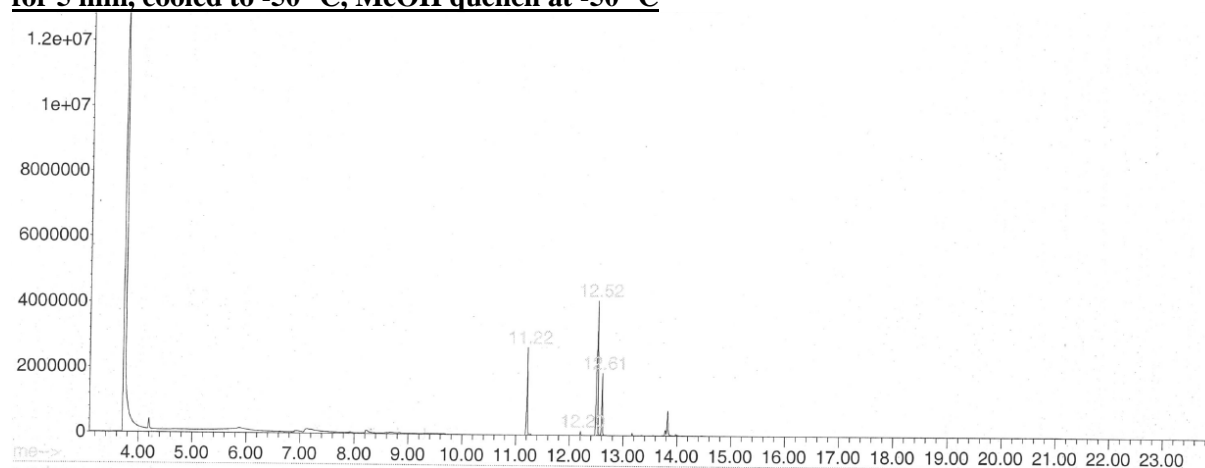
Peak	Products	Retention time (min)	% of total
1	49	11.21	33.6
2	2	12.20	8.5
3	1	12.49	32.8
4	50	12.60	25.1

**Halogen 'dance' reaction performed at -50 °C, 14 h reaction time, MeOH quench at -50 °C**



Peak	Products	Retention time (min)	% of total
1	49	11.21	34.0
2	2	12.20	7.4
3	1	12.49	35.0
4	50	12.61	23.6

**Halogen 'dance' reaction performed at -50 °C, 14 h reaction time, reaction mixture stirred at rt for 5 min, cooled to -50 °C, MeOH quench at -50 °C**



Peak	Products	Retention time (min)	% of total
1	49	11.22	27.4
2	2	12.20	1.2
3	1	12.52	53.3
4	50	12.61	18.1