

Supporting Information

On the *N*-arylation of acetamide using 2-, 3- and 1'-substituted iodoferrocenes

Lingaswamy Kadari,^{a,b} William Erb,^{a*} Yury S. Halauko,^{c*} Oleg A. Ivashkevich,^c Vadim E. Matulis,^d

Dmitry Lyakhov,^e Thierry Roisnel,^a Palakodety Radha Krishna^{b*} and Florence Mongin^a

^a *Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France*

^b *Organic Synthesis and Process Chemistry Division, CSIR-Indian Institute of Chemical Technology, Hyderabad, 500007, India*

^c *UNESCO Chair of Belarusian State University, 14 Leningradskaya Str., Minsk 220030, Belarus*

^d *Research Institute for Physico-Chemical Problems of Belarusian State University, 14 Leningradskaya Str., Minsk 220030, Belarus*

^e *Computer, Electrical and Mathematical Science and Engineering Division, 4700 King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia*

E-mails: william.erb@univ-rennes1.fr, hys@tut.by, prkgenius@iict.res.in

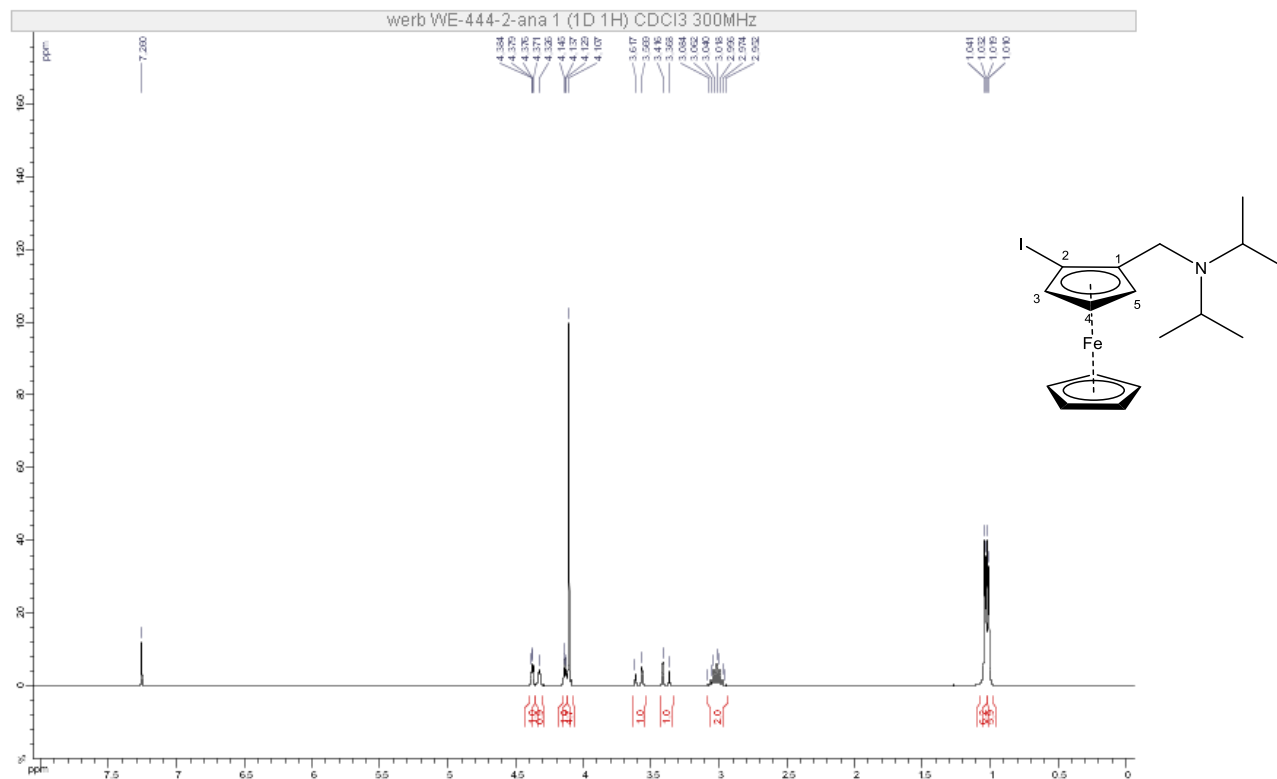
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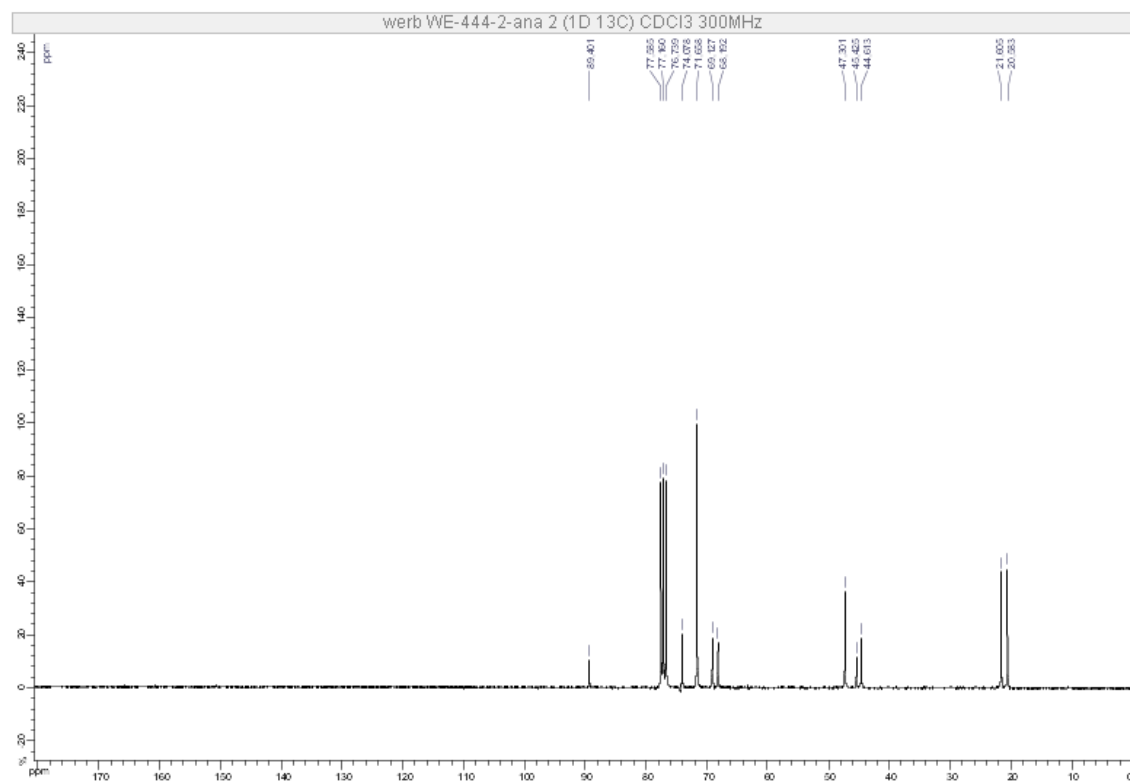
NMR spectra

1-(*N,N*-Diisopropylaminomethyl)-2-iodoferrocene (**1c**, racemic mixture)

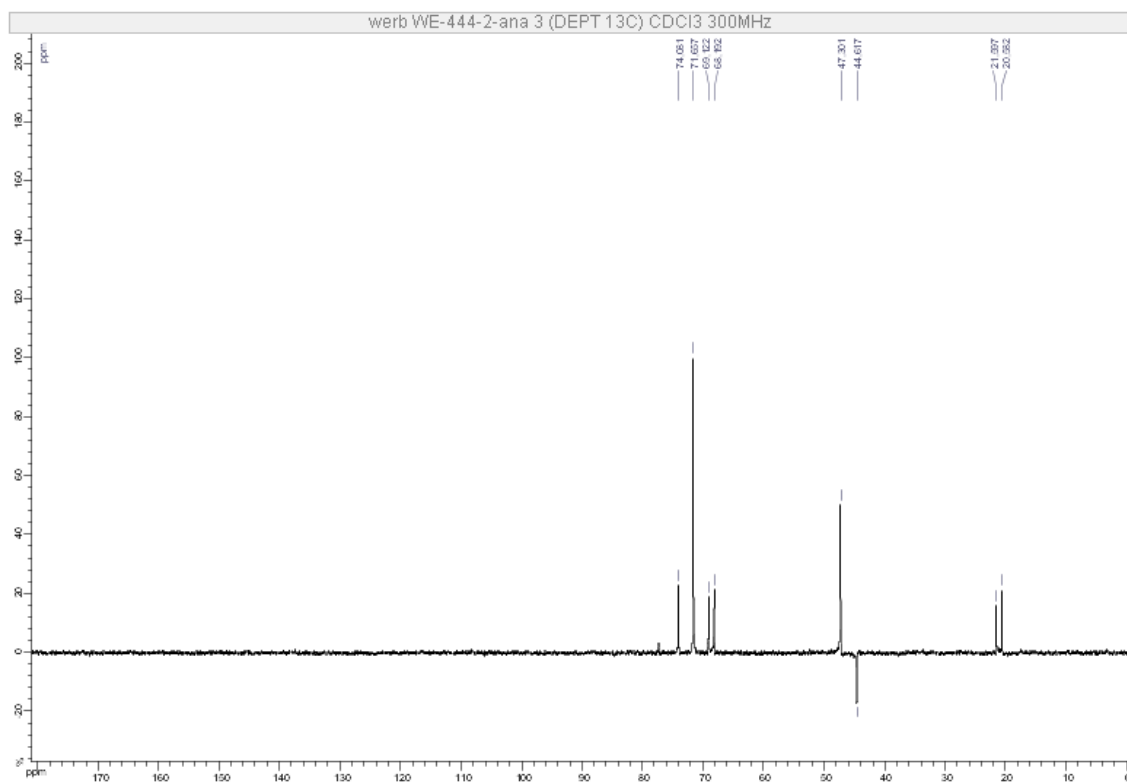
^1H NMR (300 MHz, CDCl_3)



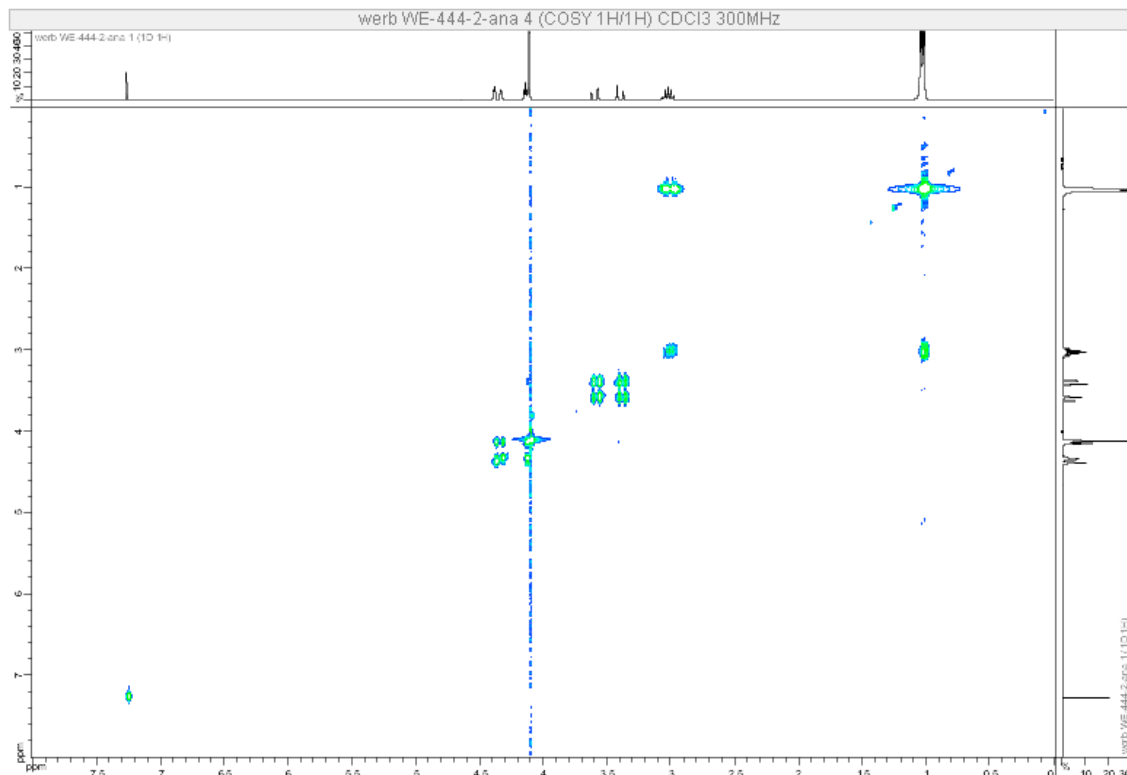
^{13}C NMR (75 MHz, CDCl_3)



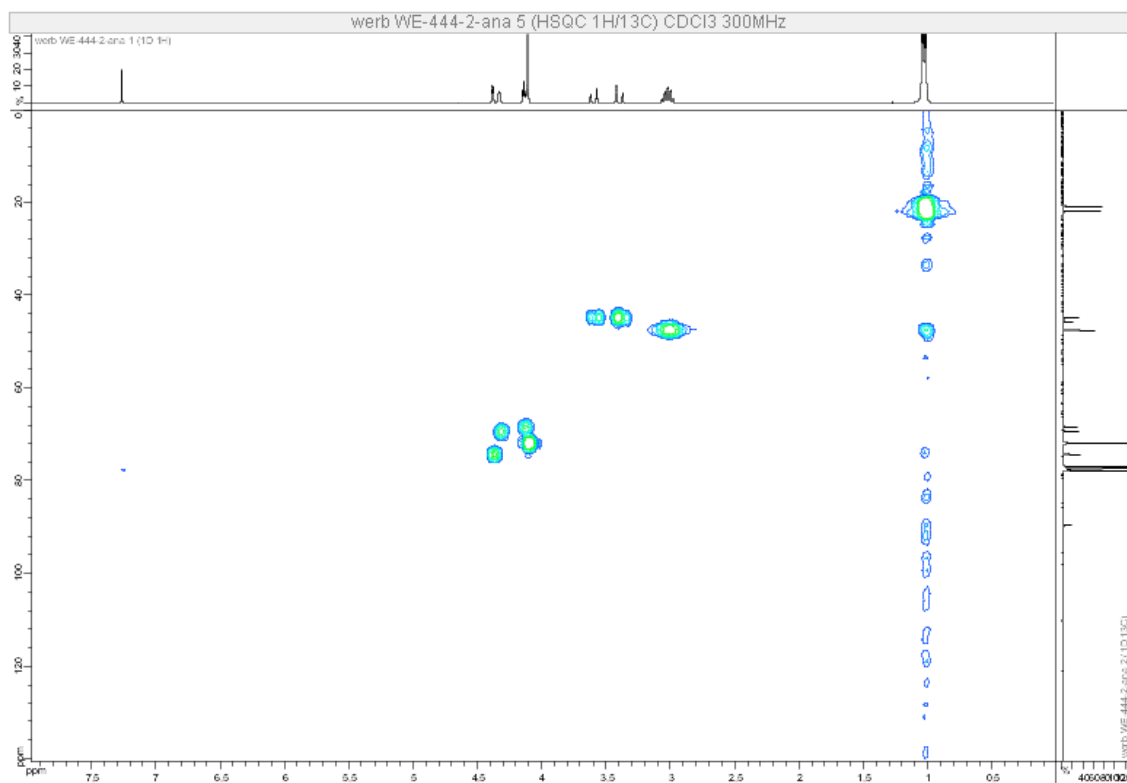
DEPT 135 (75 MHz, CDCl₃)



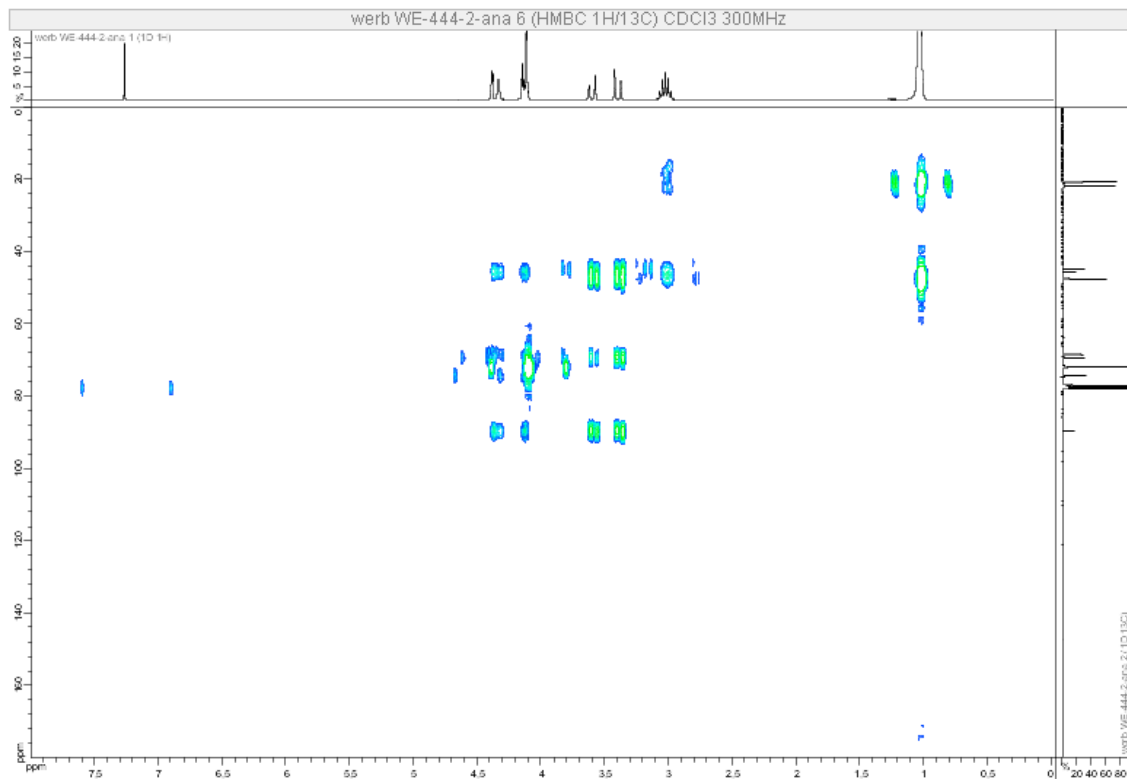
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

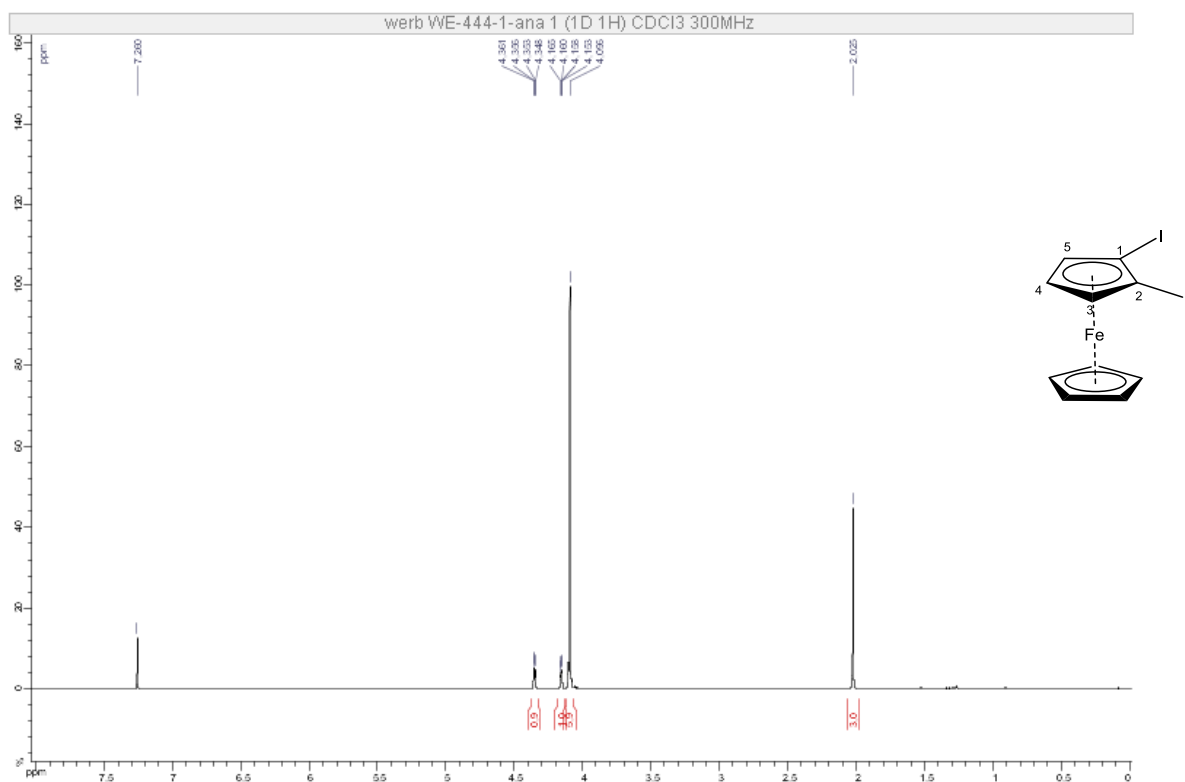


HMBC (300 MHz, CDCl₃)

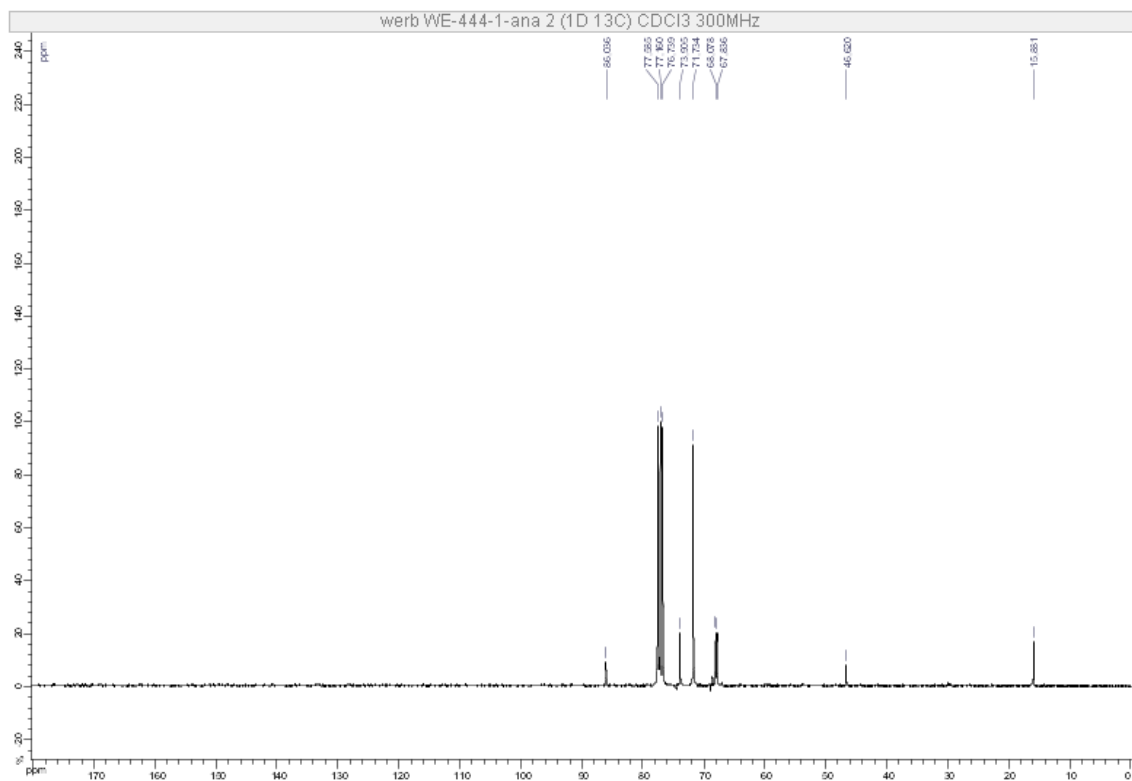


1-Iodo-2-methylferrocene (1b, racemic mixture)

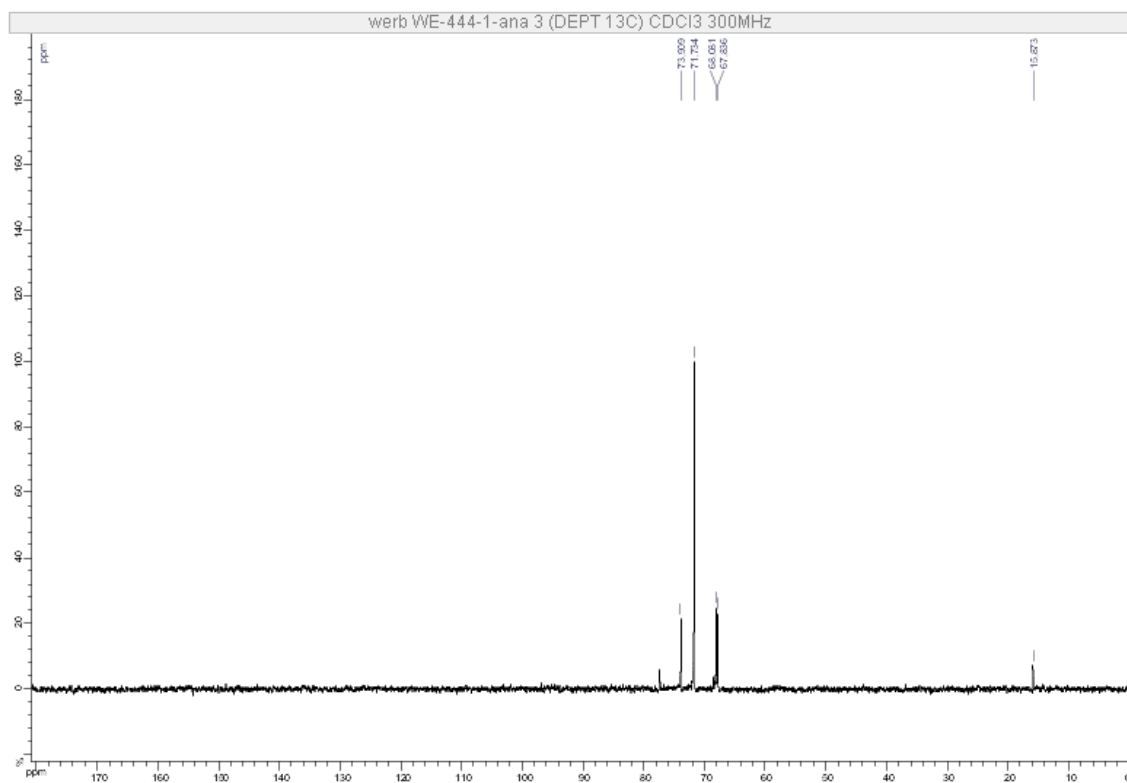
^1H NMR (300 MHz, CDCl_3)



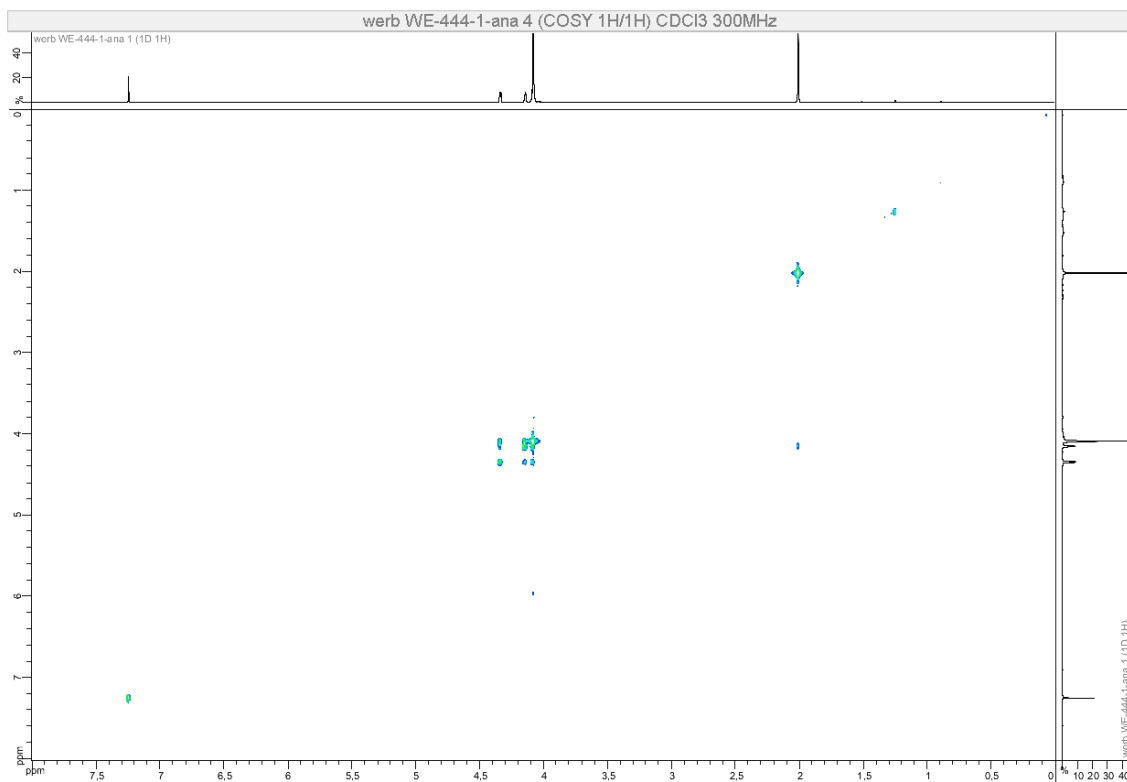
^{13}C NMR (75 MHz, CDCl_3)



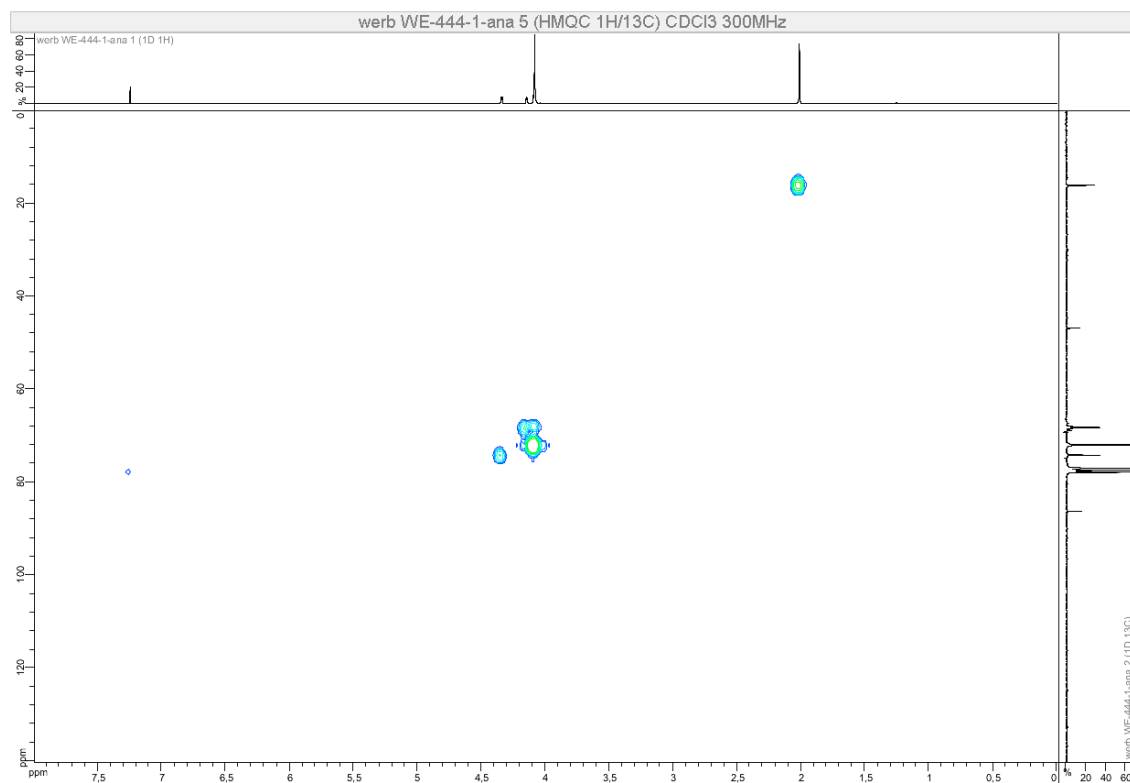
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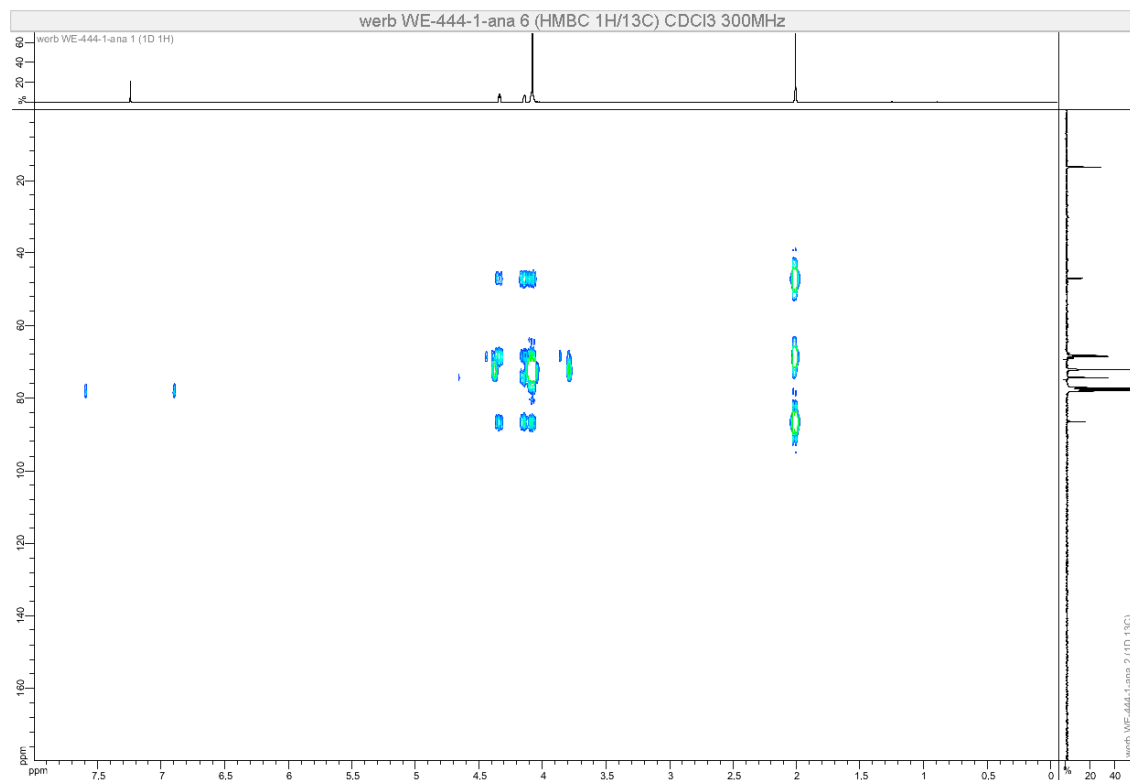
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HSQC (300 MHz, CDCl₃)

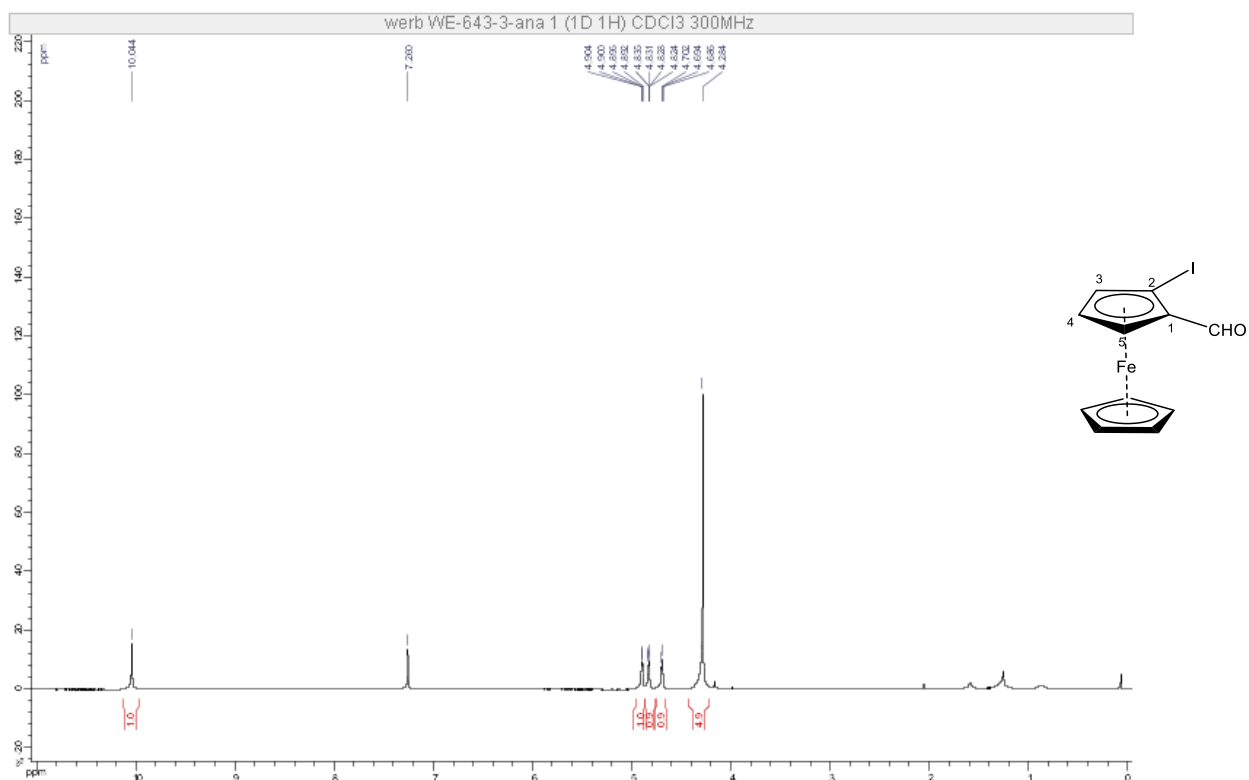


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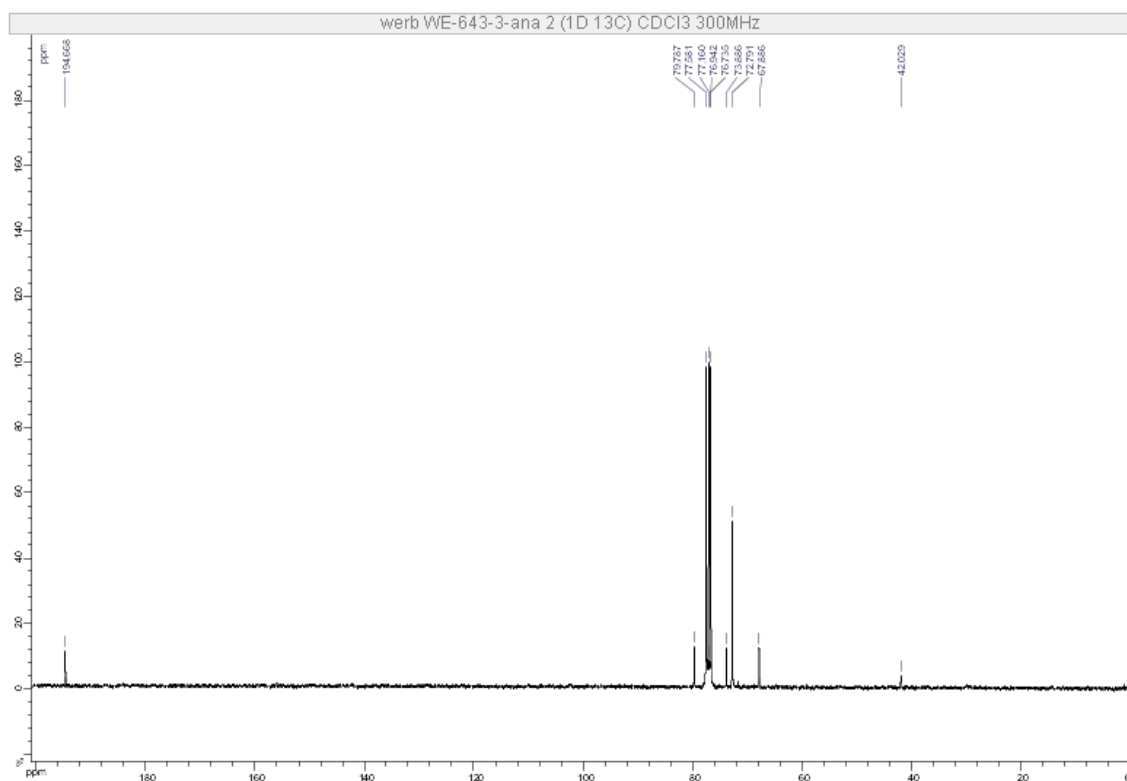


2-Iodoferrocenecarboxaldehyde (**1f**, racemic mixture)

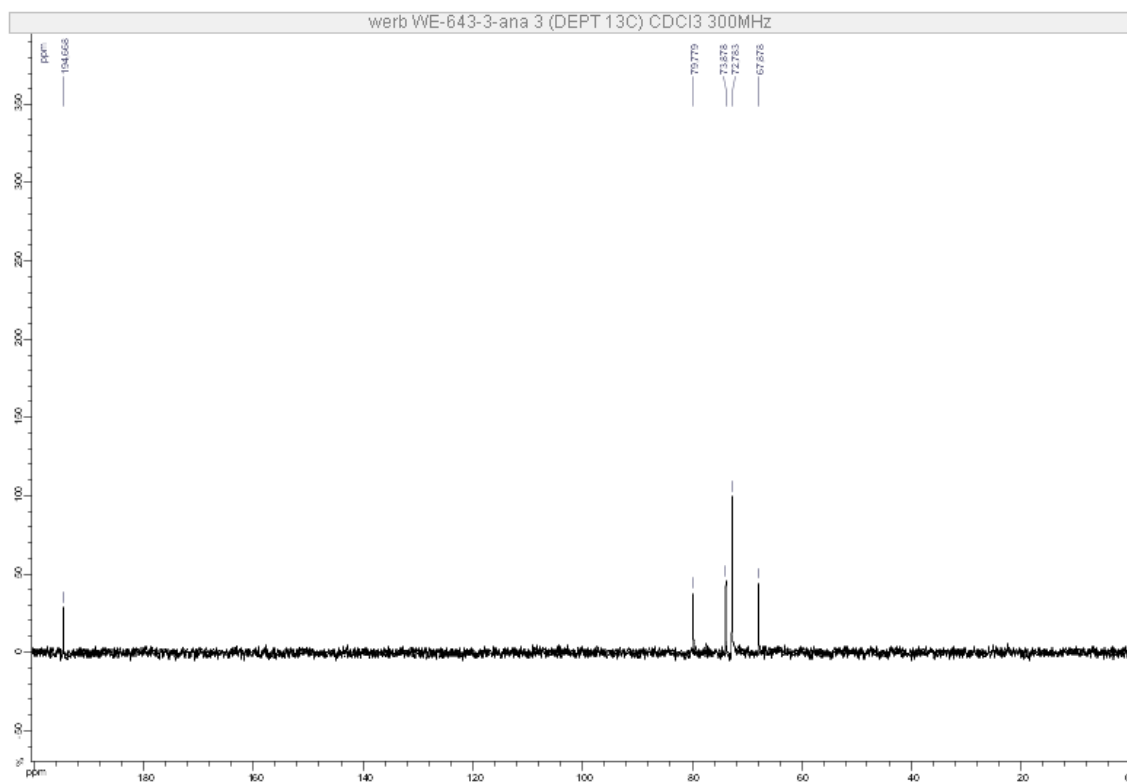
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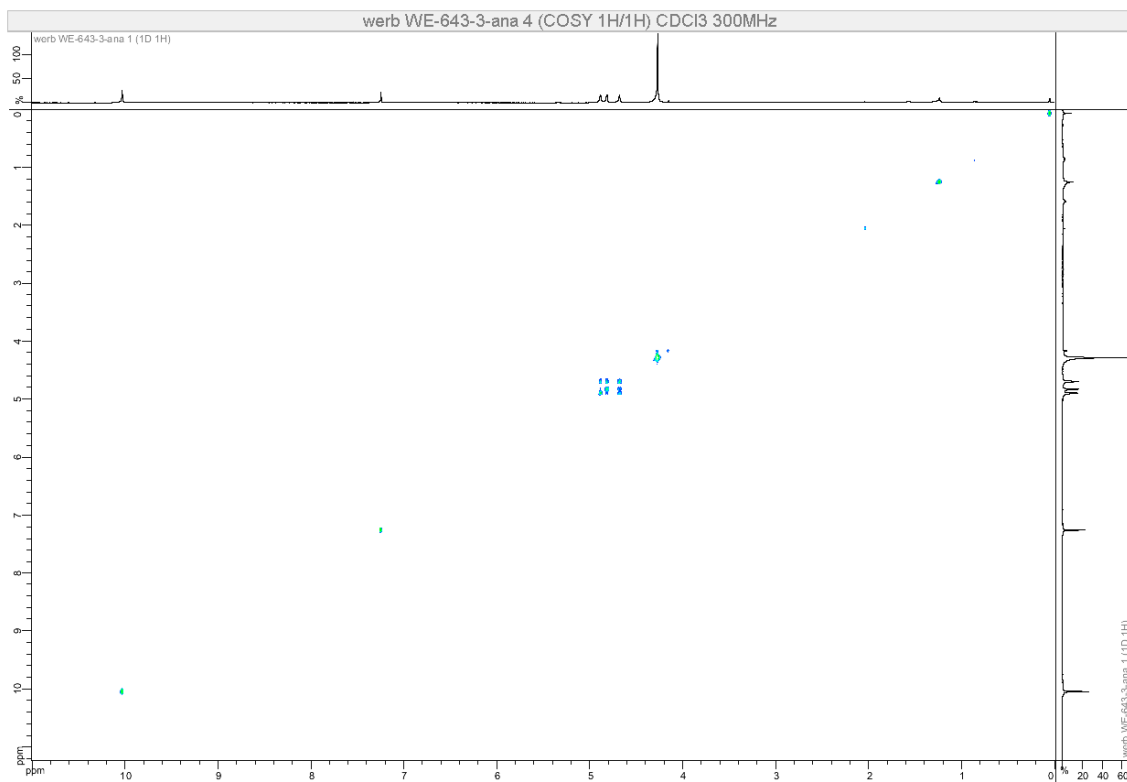
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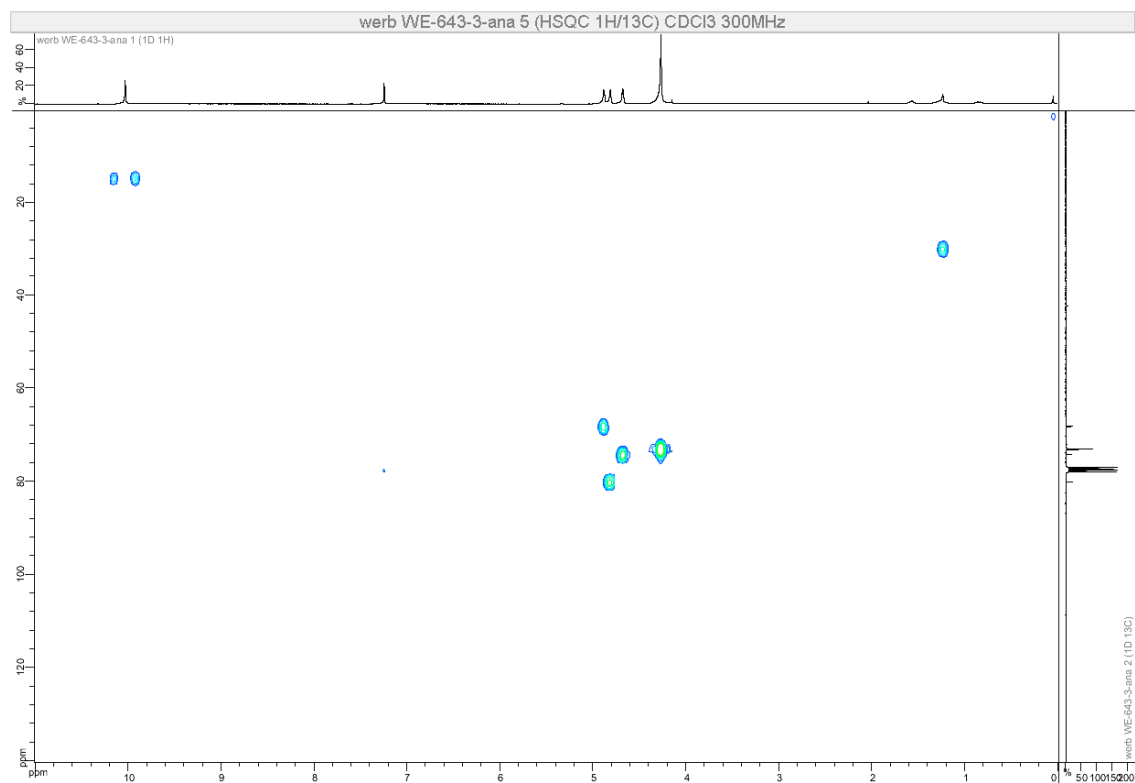
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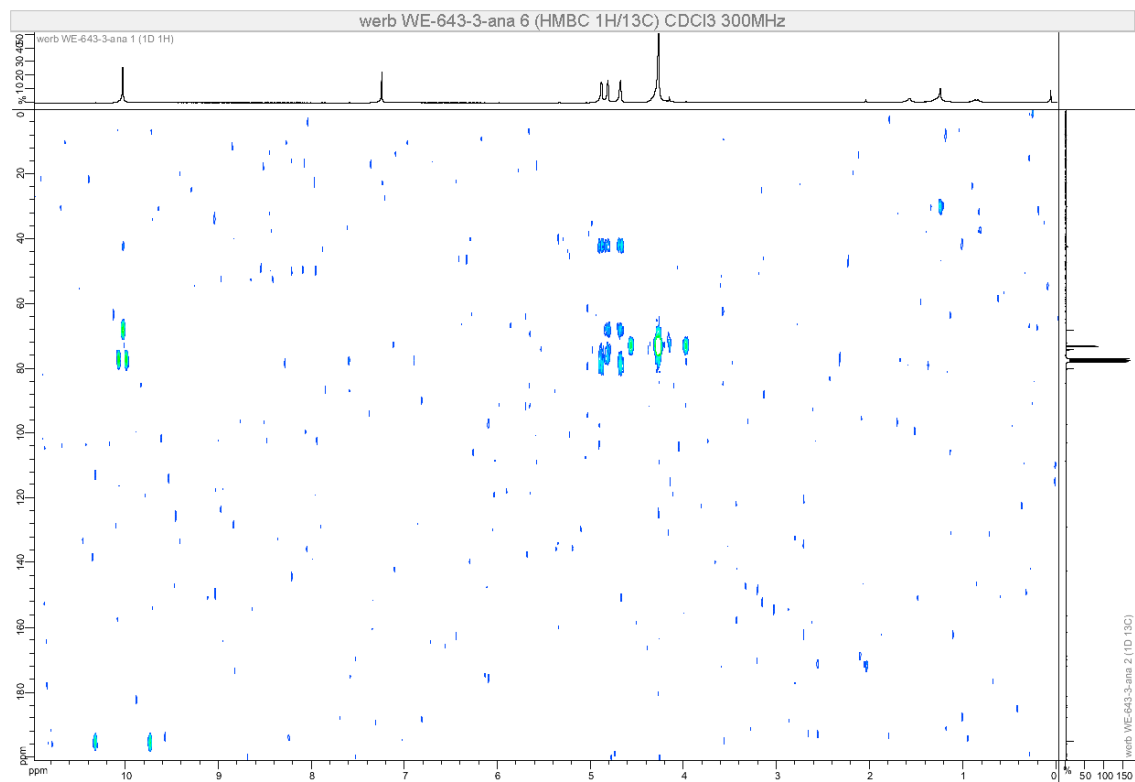
COSY (100 MHz, CDCl₃)



HSQC (100 MHz, CDCl₃)

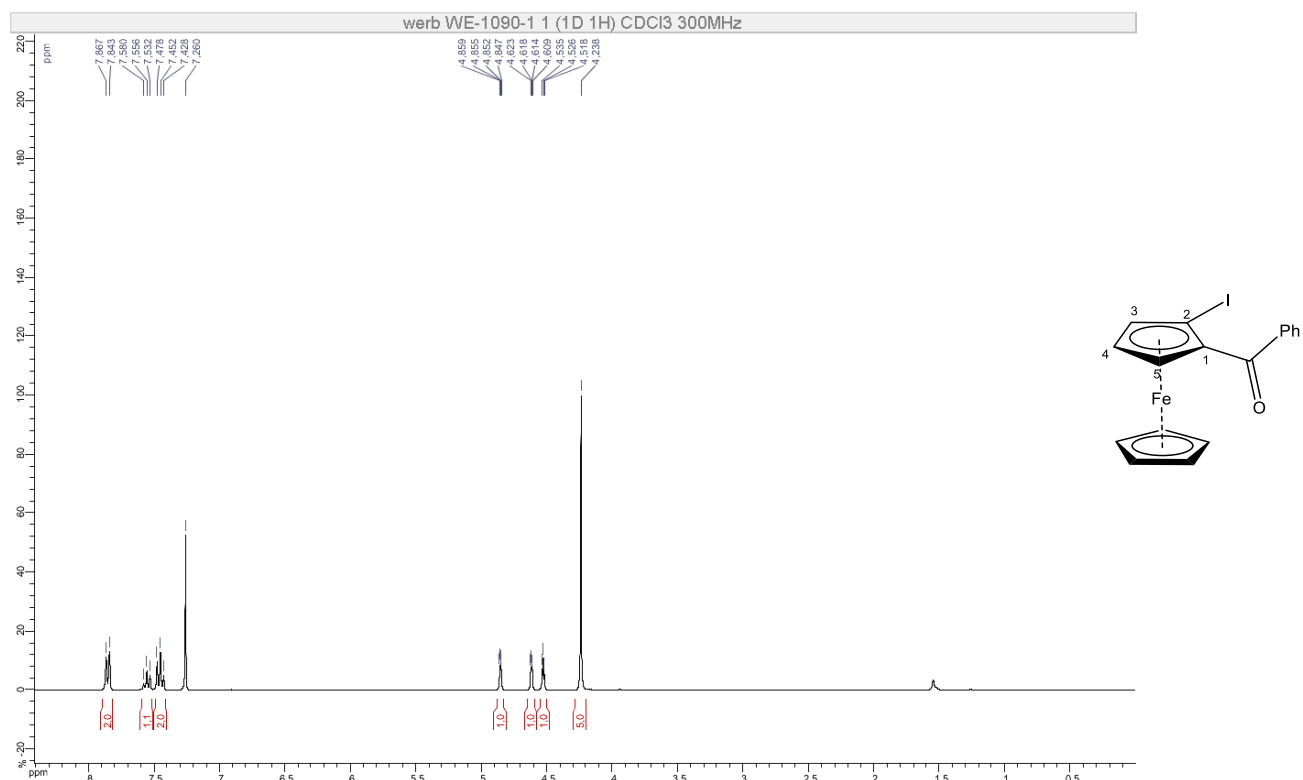


HMBC (100 MHz, CDCl₃)

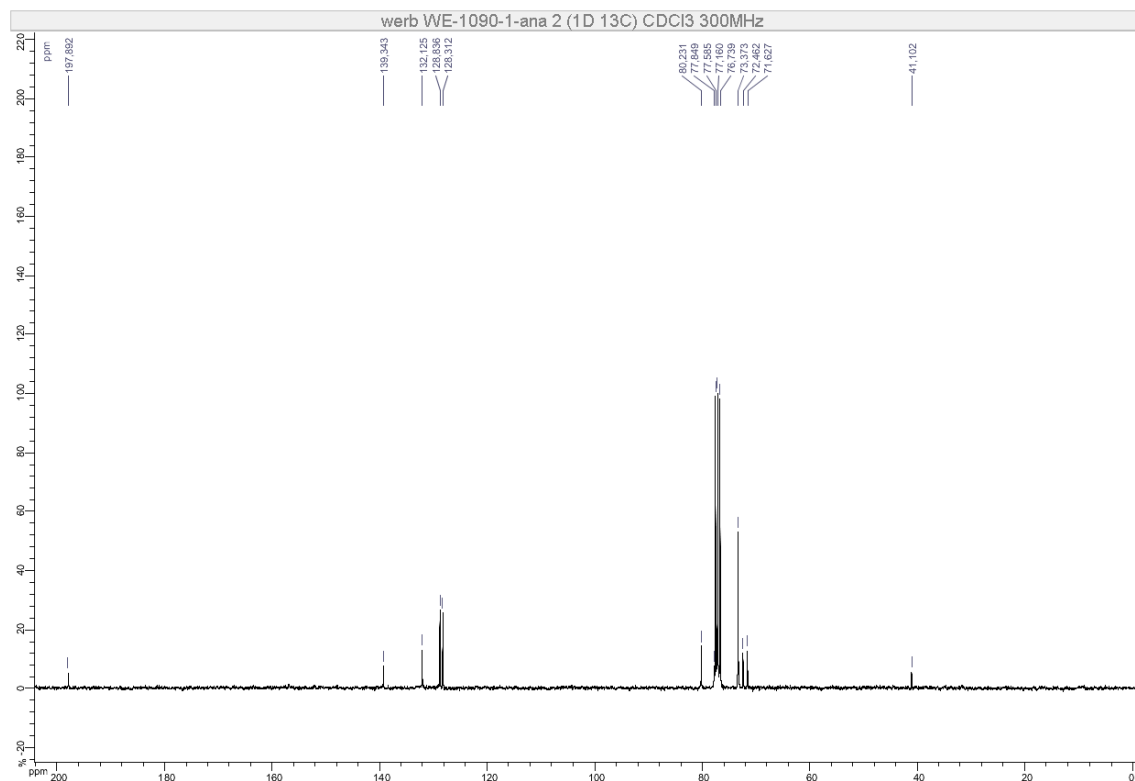


(2-Iodoferrocenyl)phenylketone (**1g**, racemic mixture)

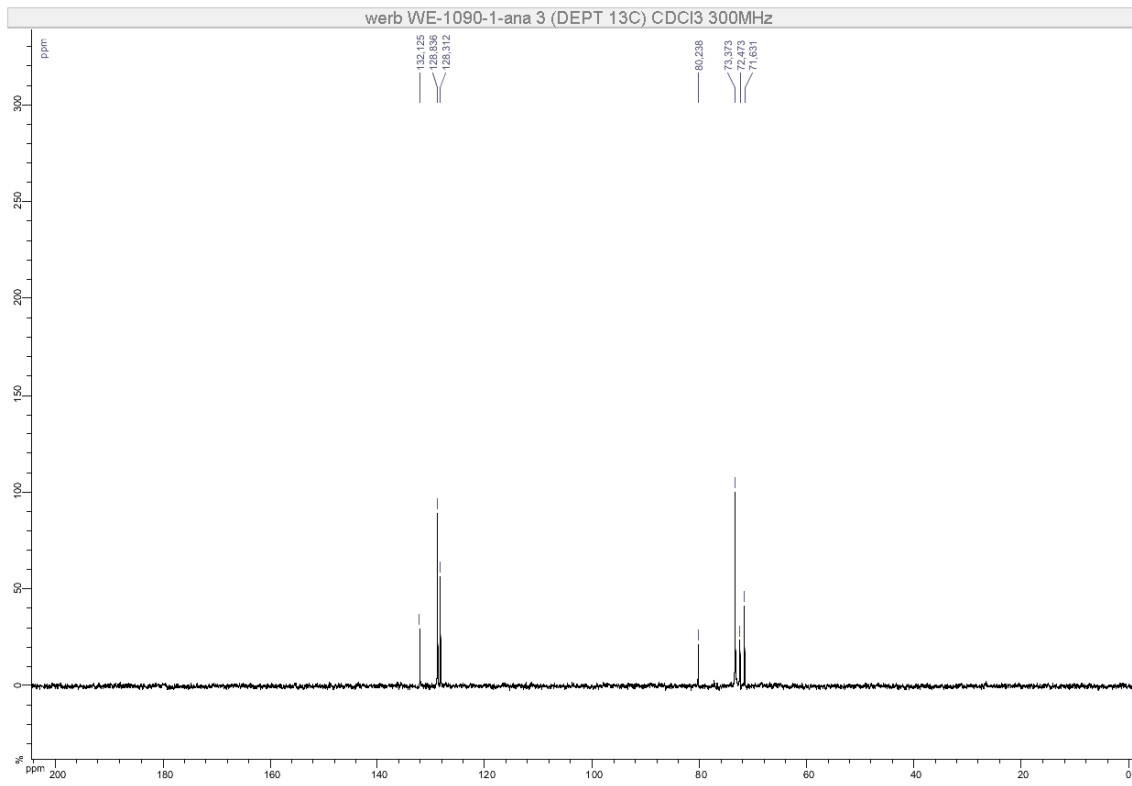
^1H NMR (300 MHz, CDCl_3)



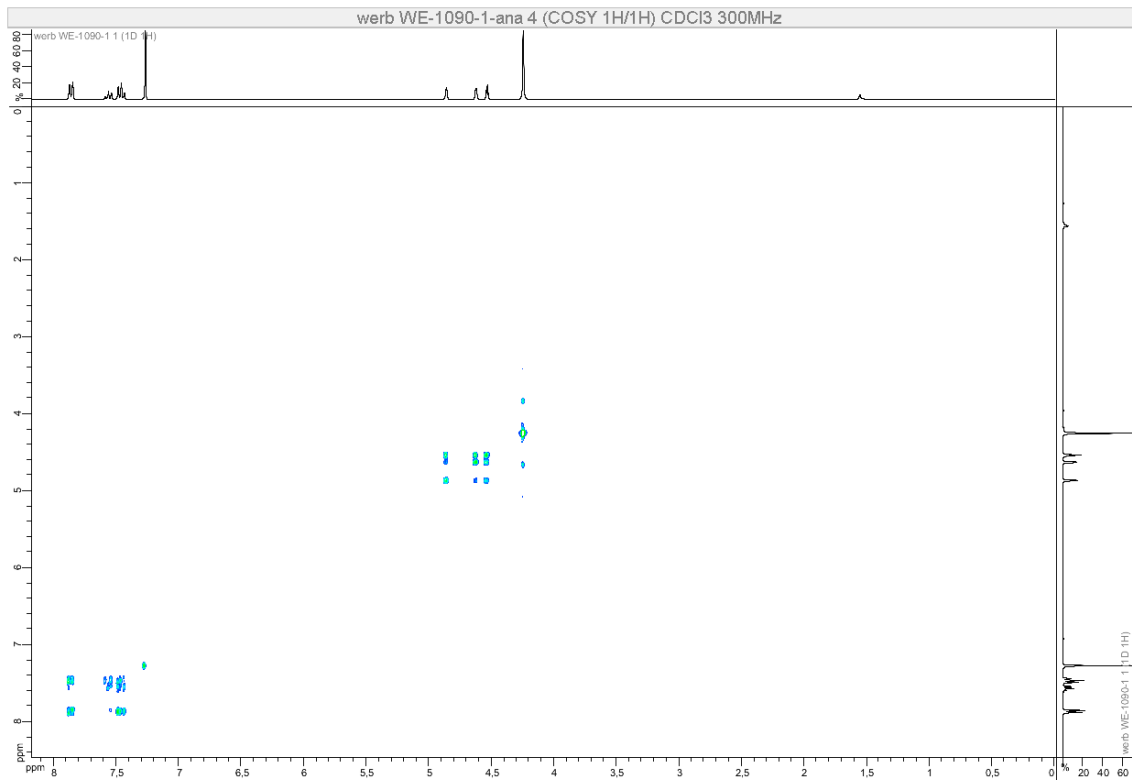
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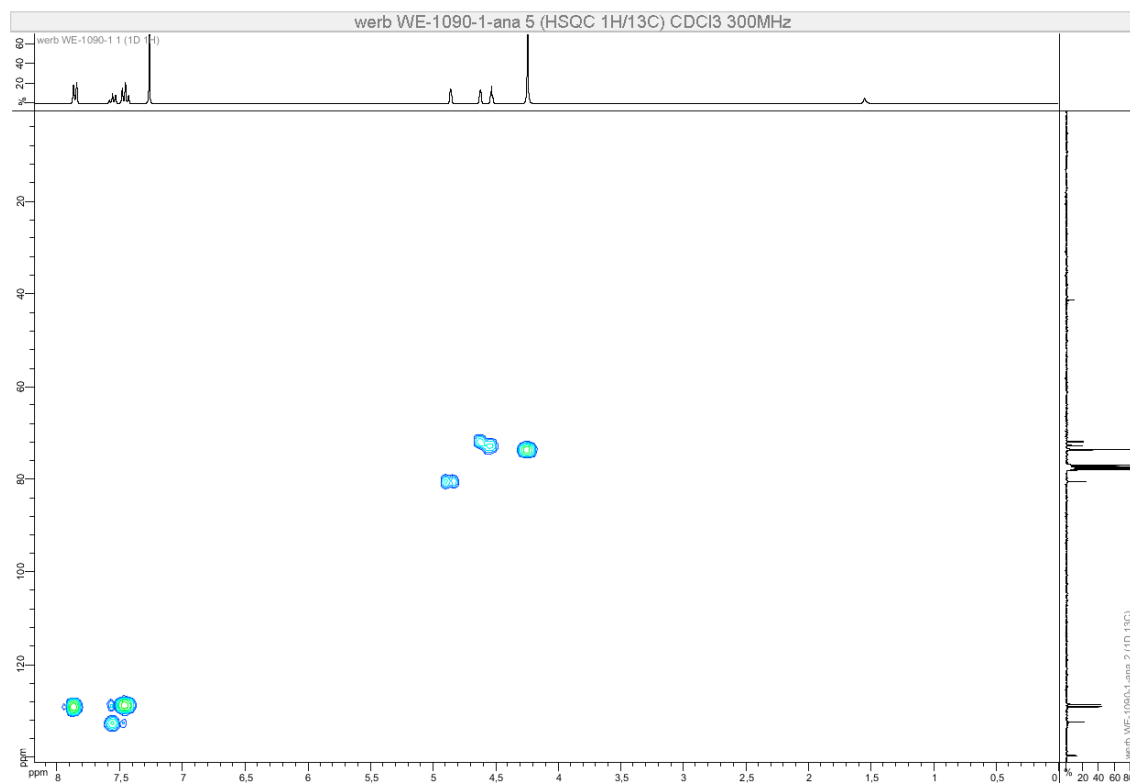
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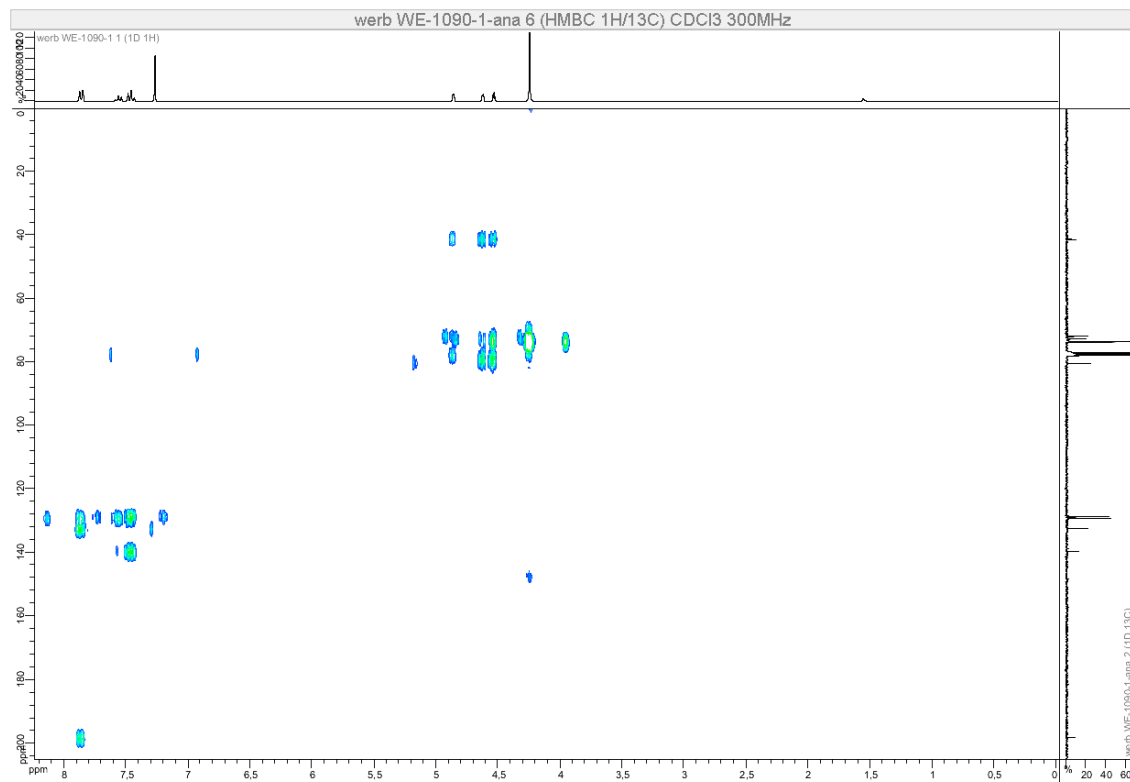
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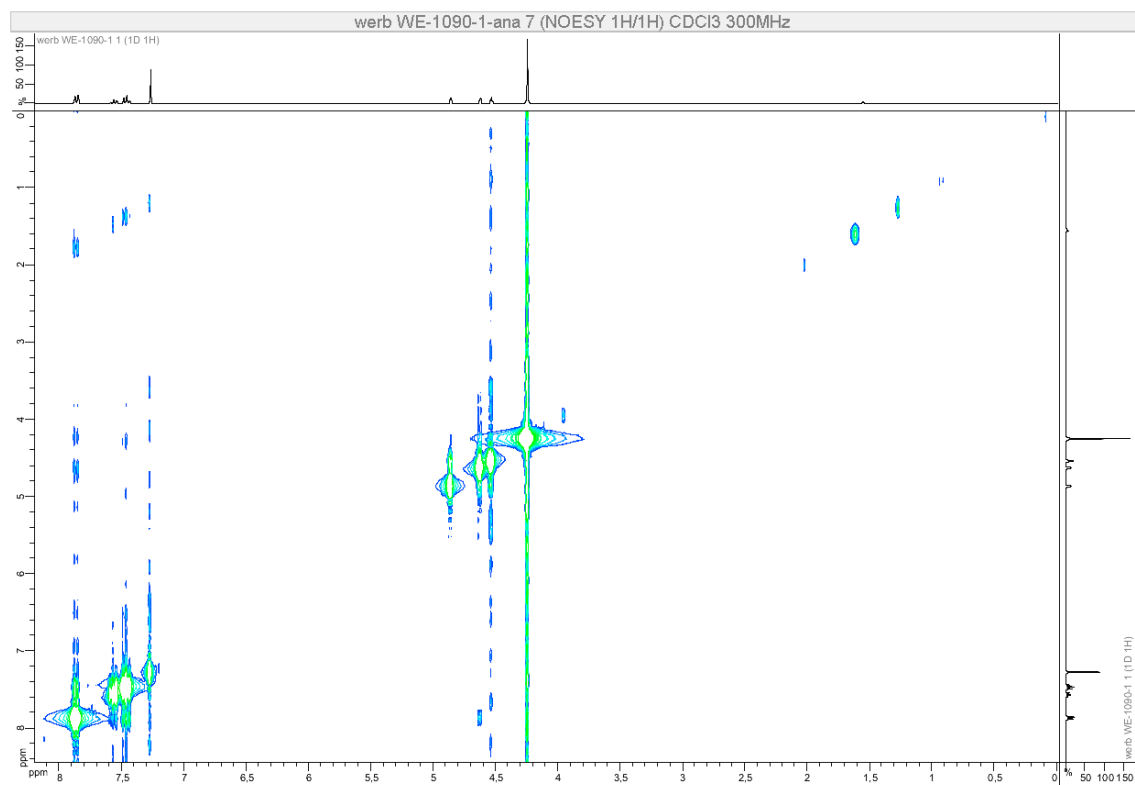
HSQC (300 MHz, CDCl₃)



HMBC (300 MHz, CDCl₃)

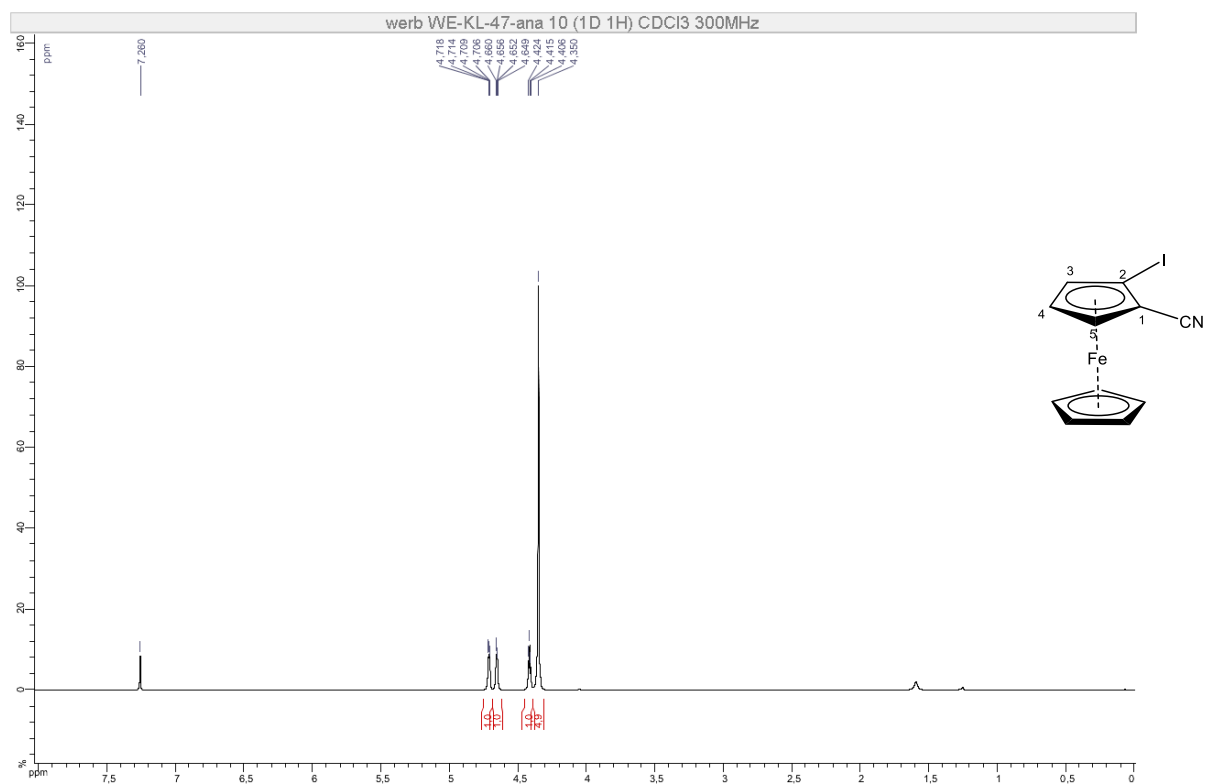


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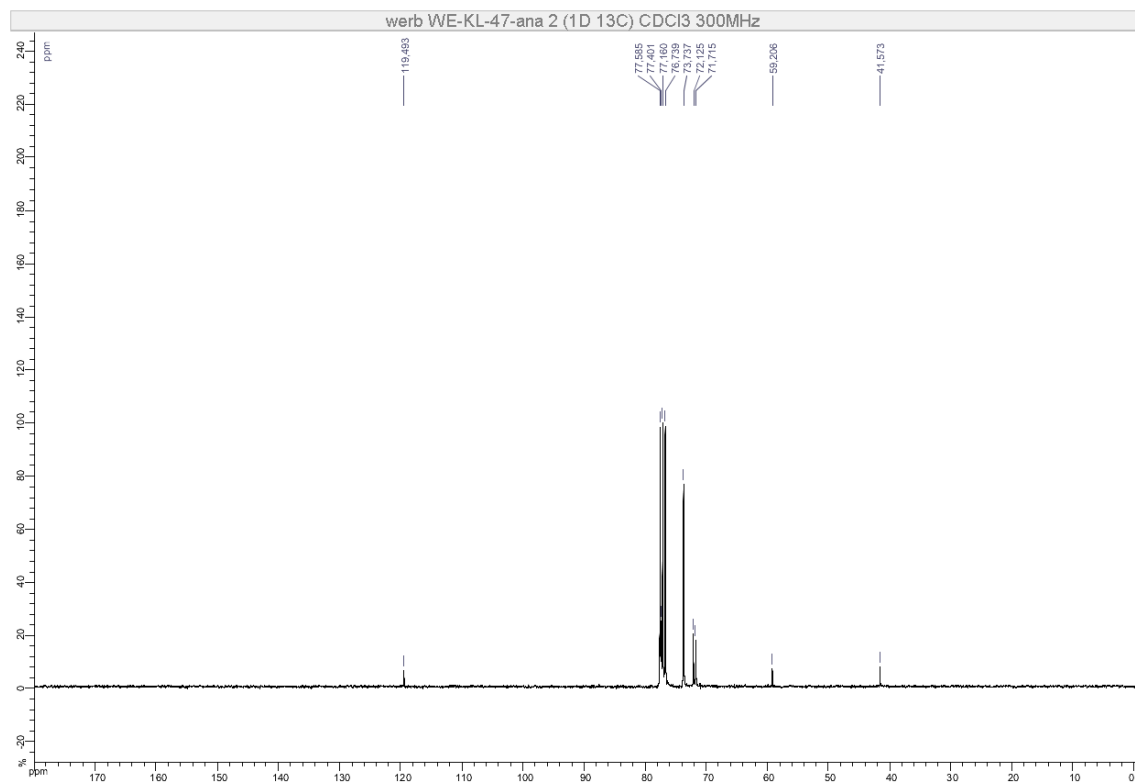


2-Iodoferrocenecarbonitrile (**1h**, racemic mixture)

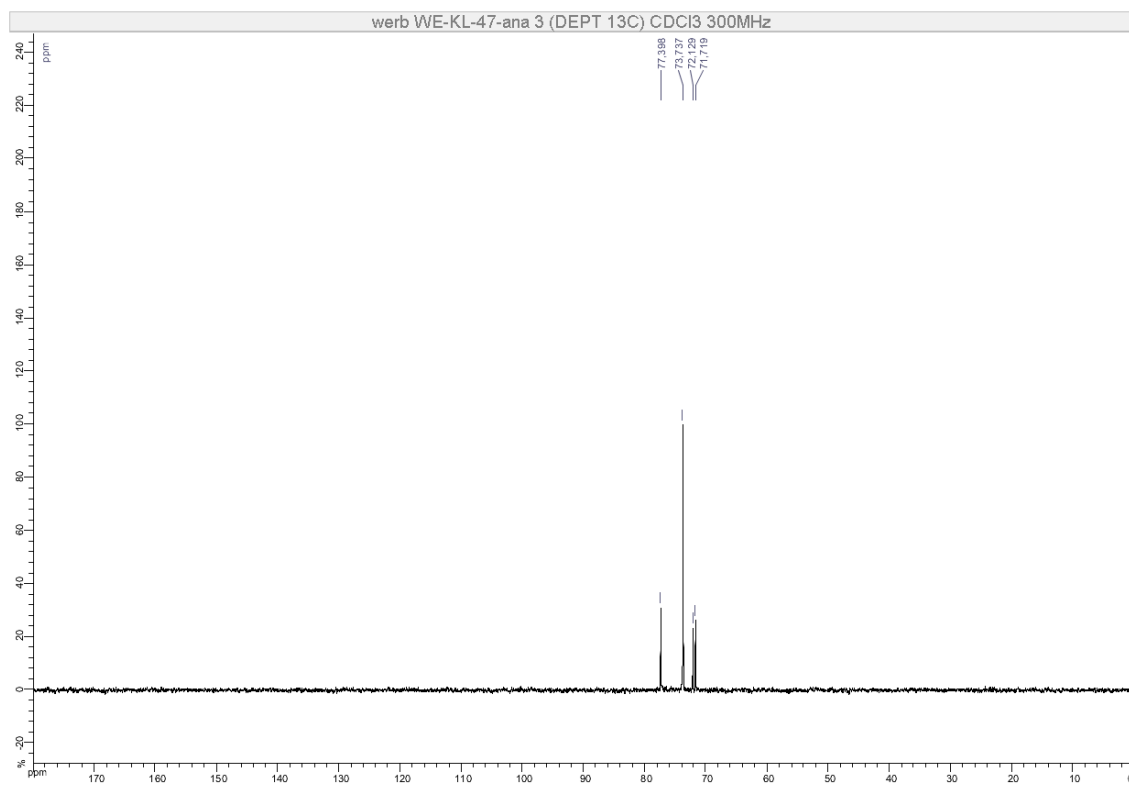
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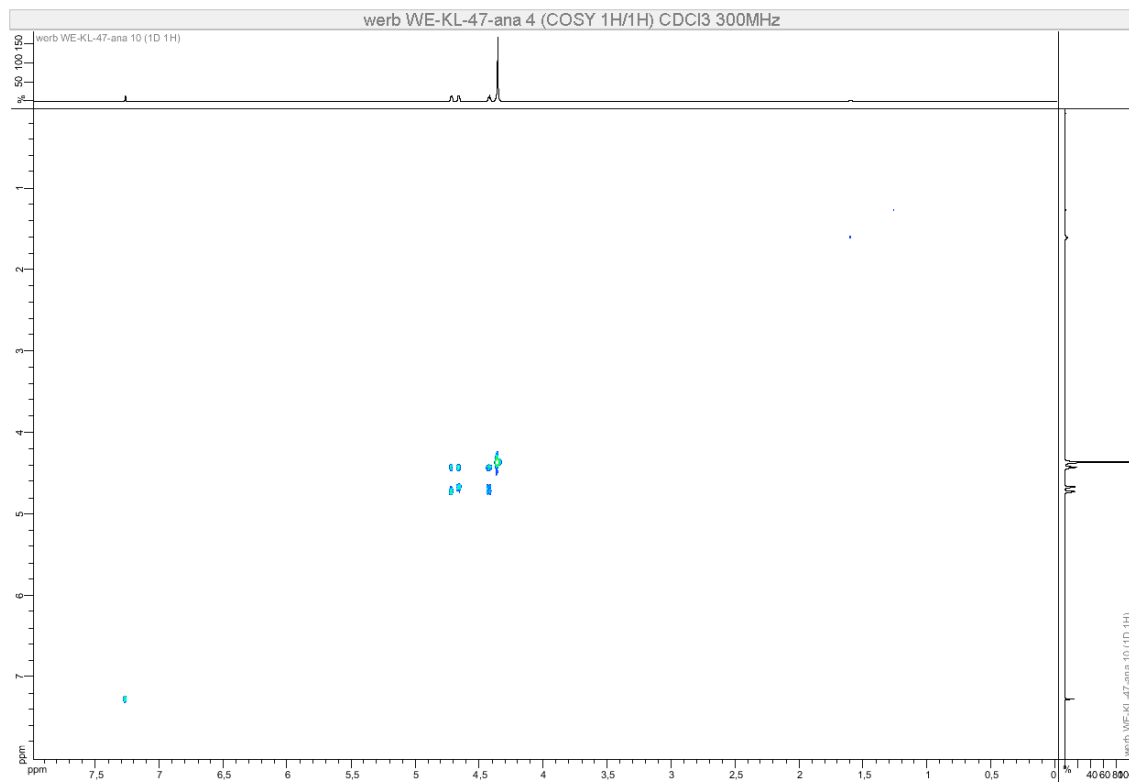
^{13}C NMR (75 MHz, CDCl_3)



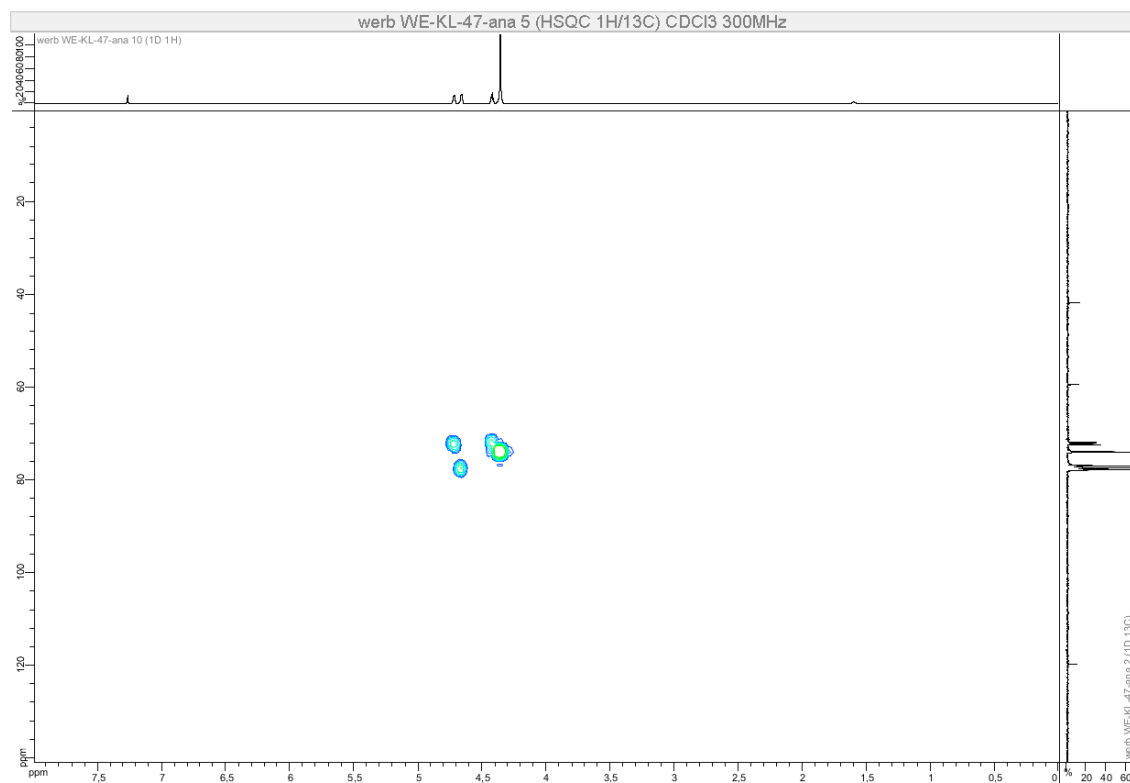
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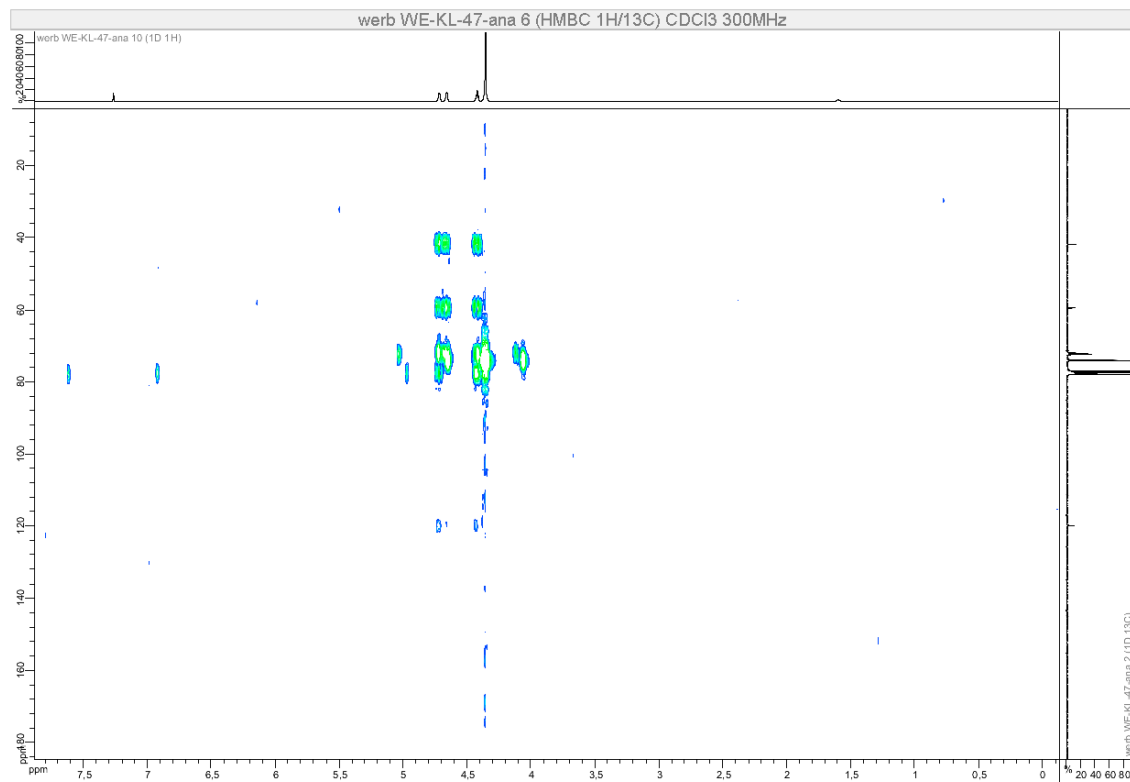
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HSQC (300 MHz, CDCl₃)

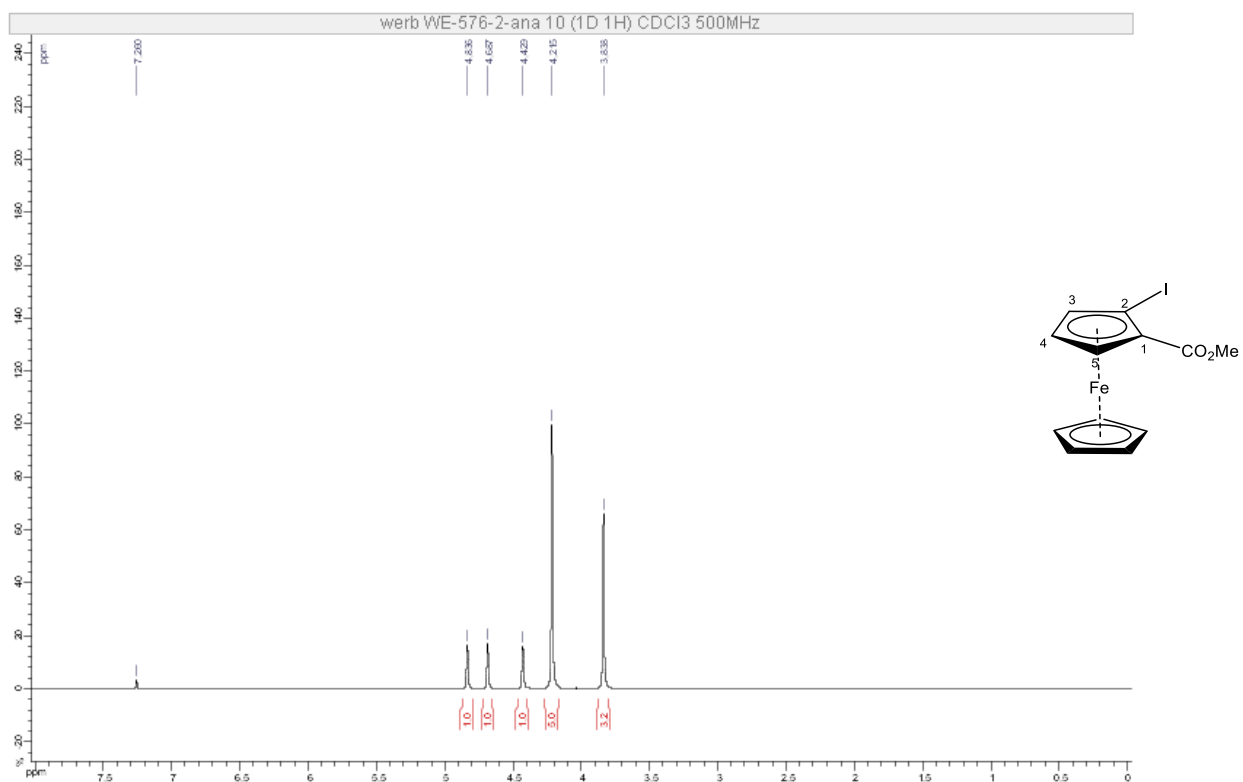


HMBC (300 MHz, CDCl₃)

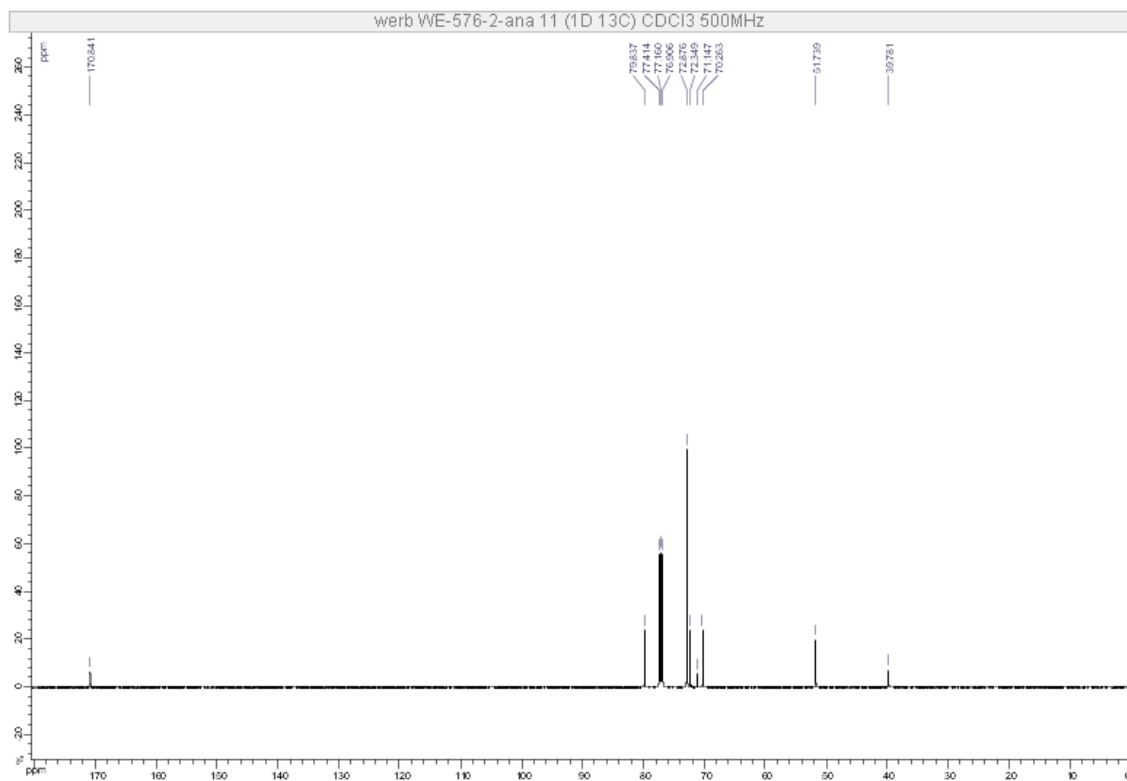


Methyl 2-iodoferrocenecarboxylate (**1i**, racemic mixture)

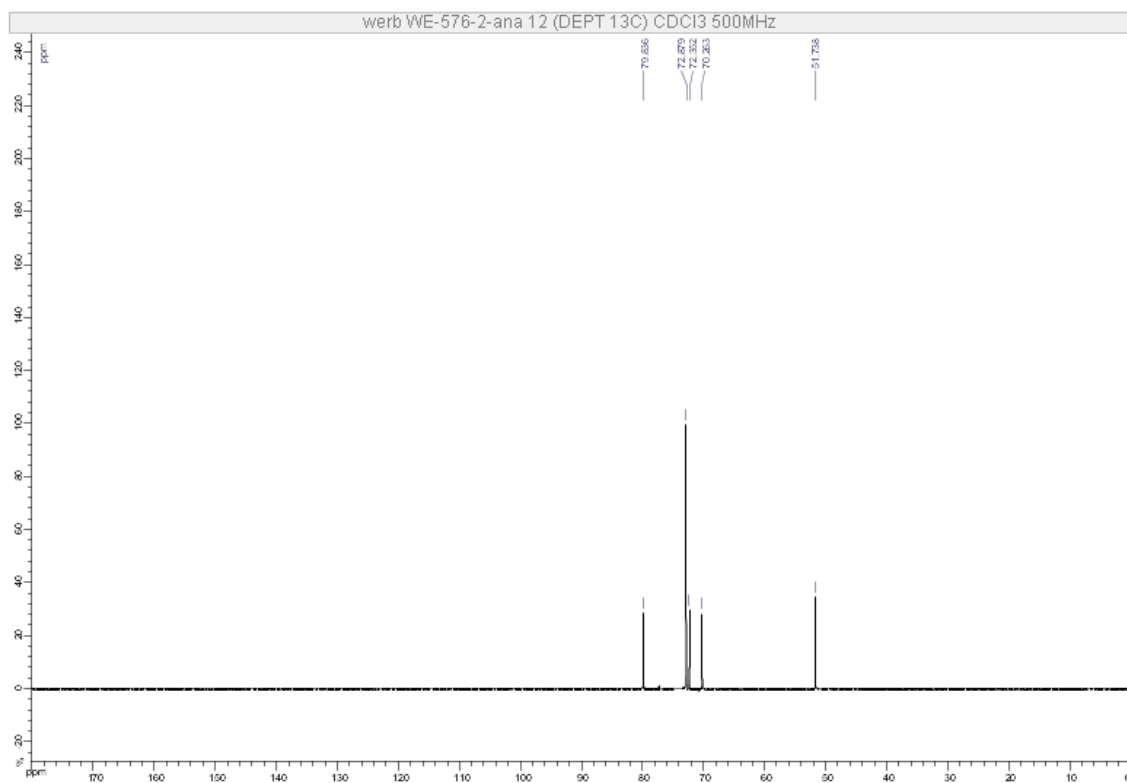
^1H NMR (500 MHz, CDCl_3)



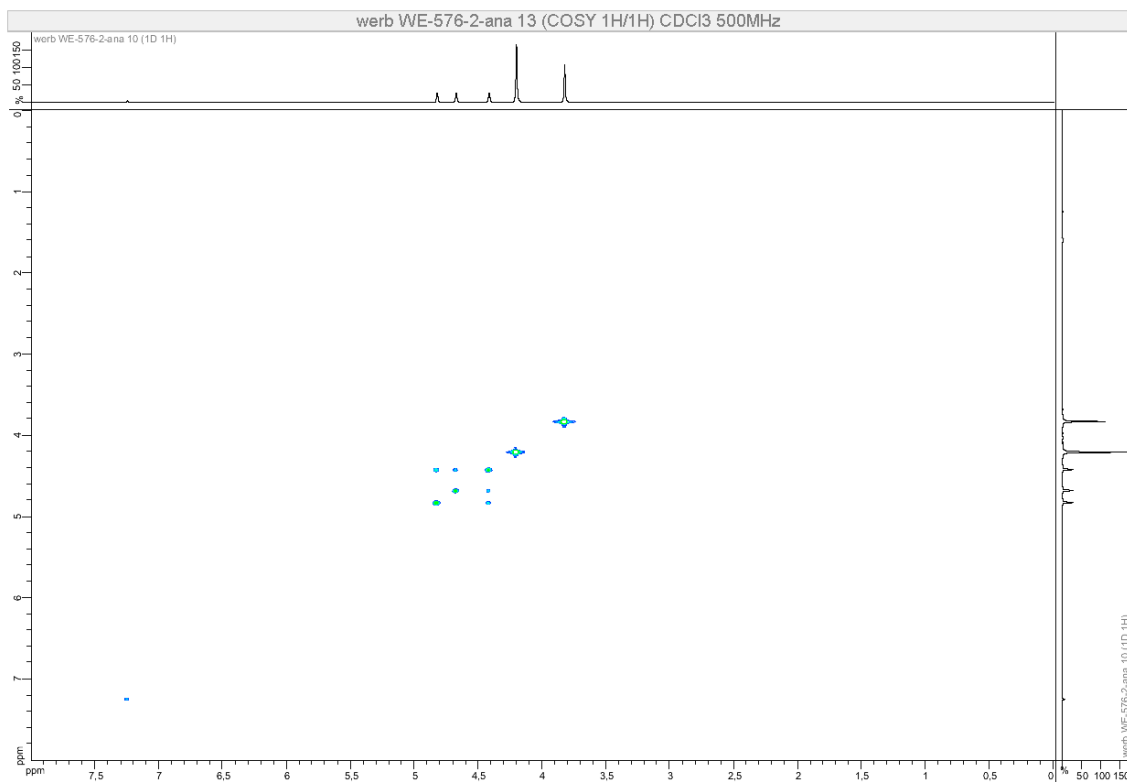
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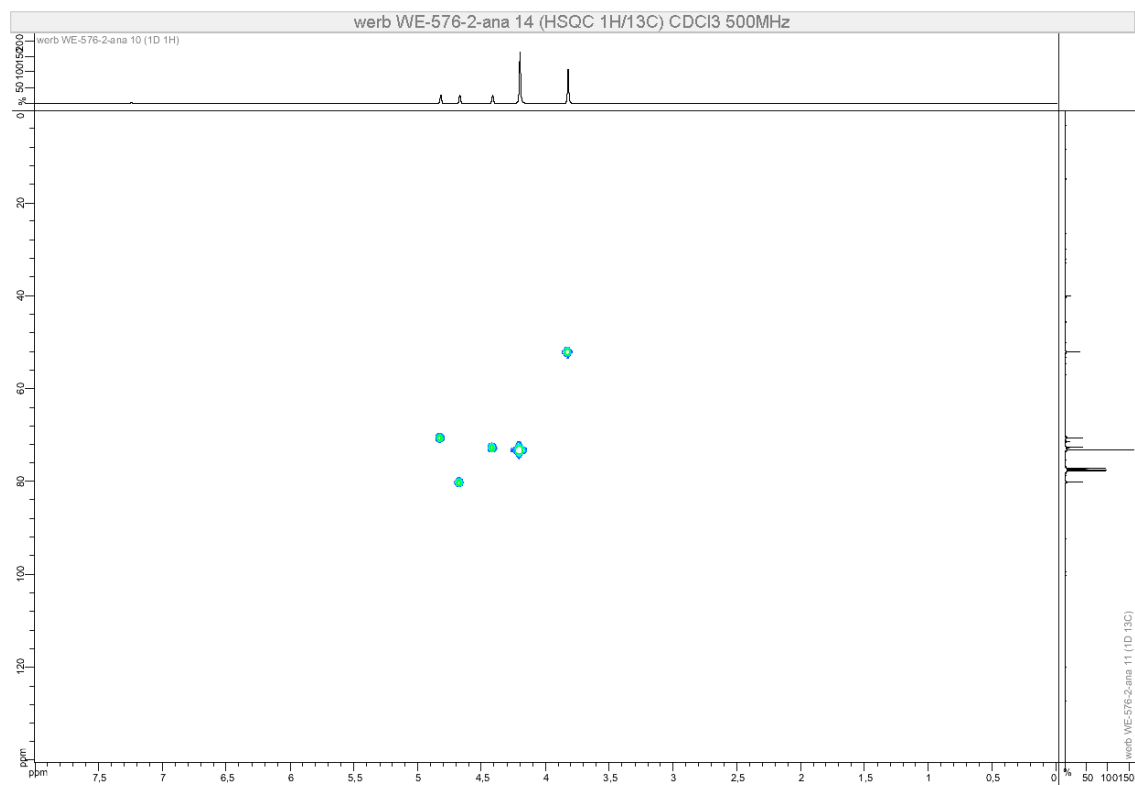
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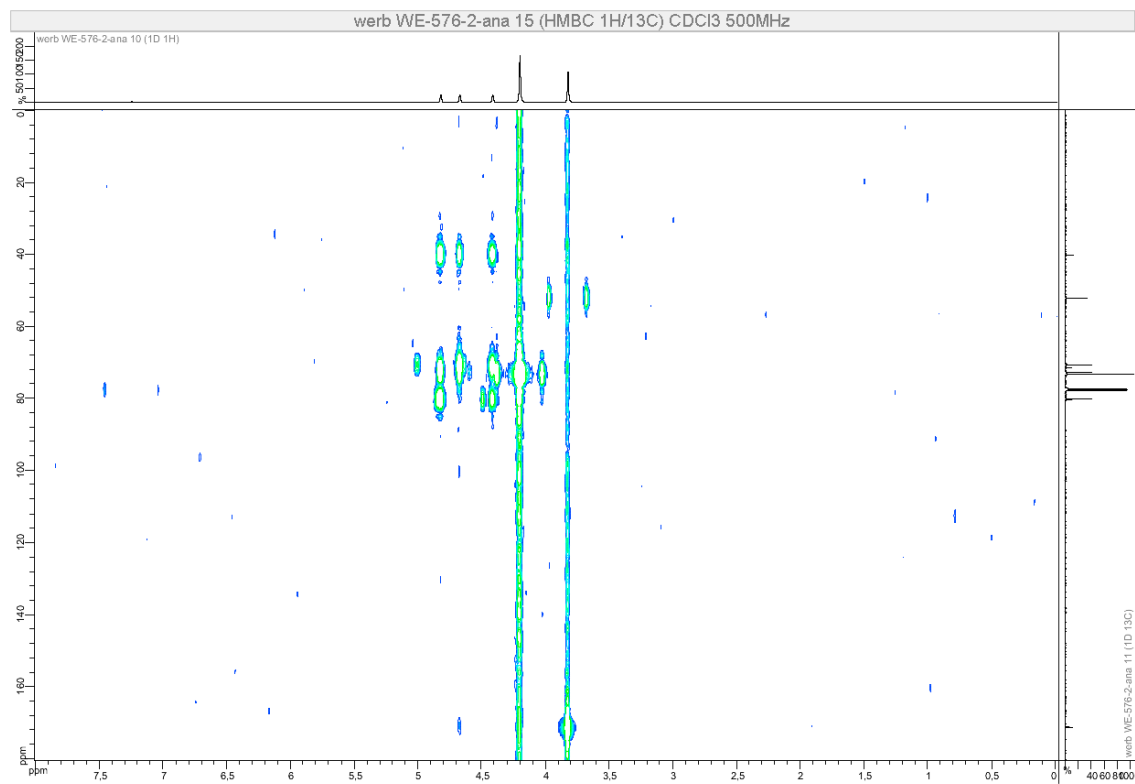
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

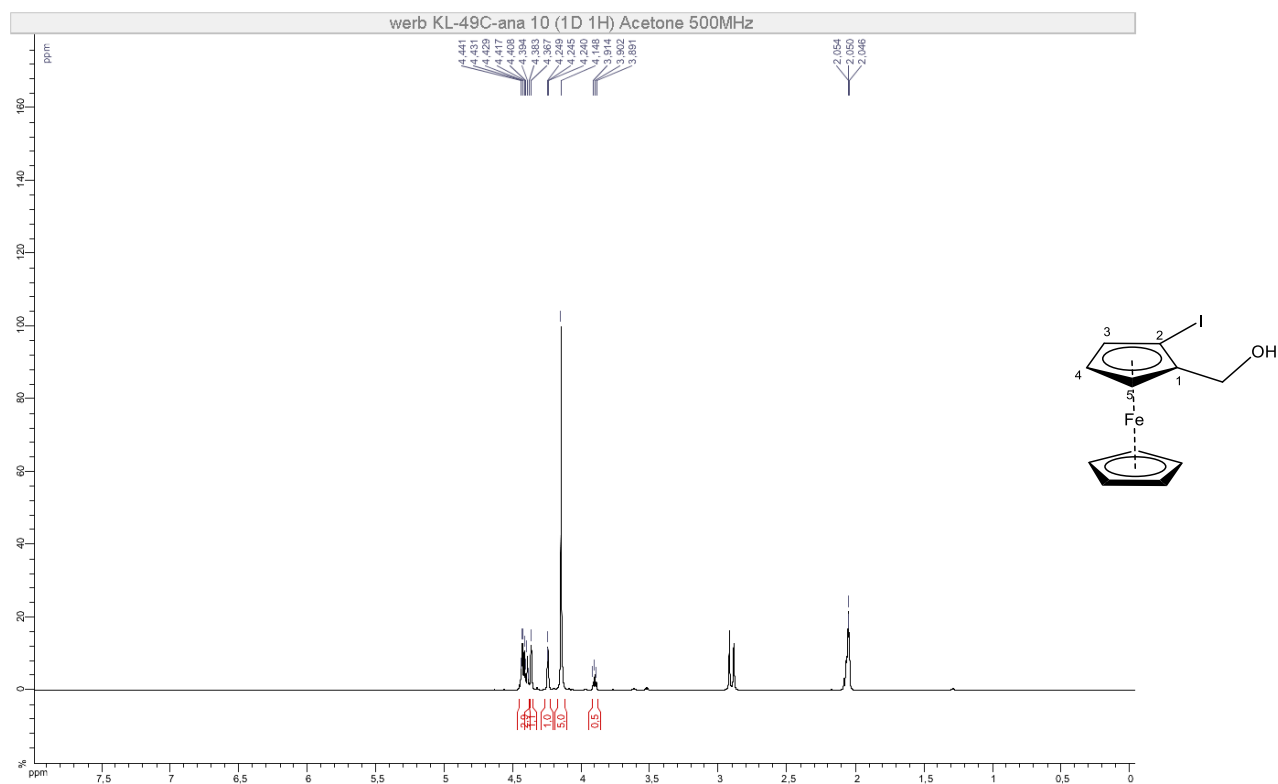


HMBC (500 MHz, CDCl₃)

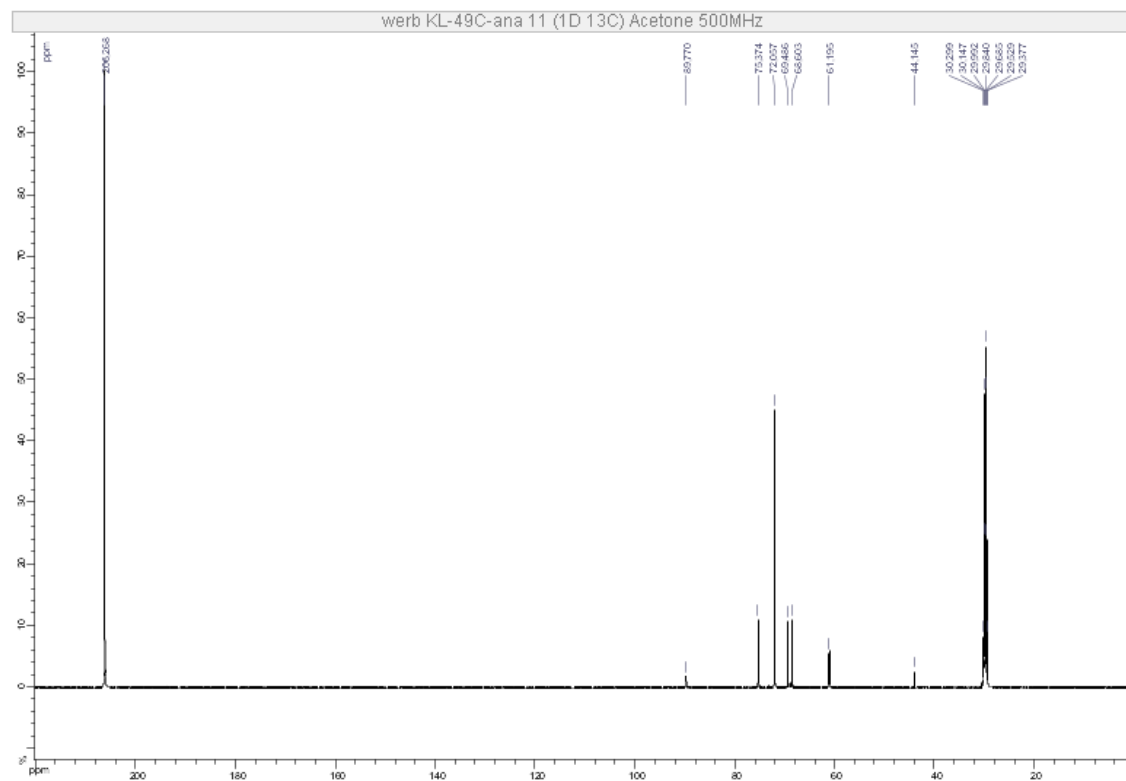


2-Iodoferrocenemethanol (1e, racemic mixture)

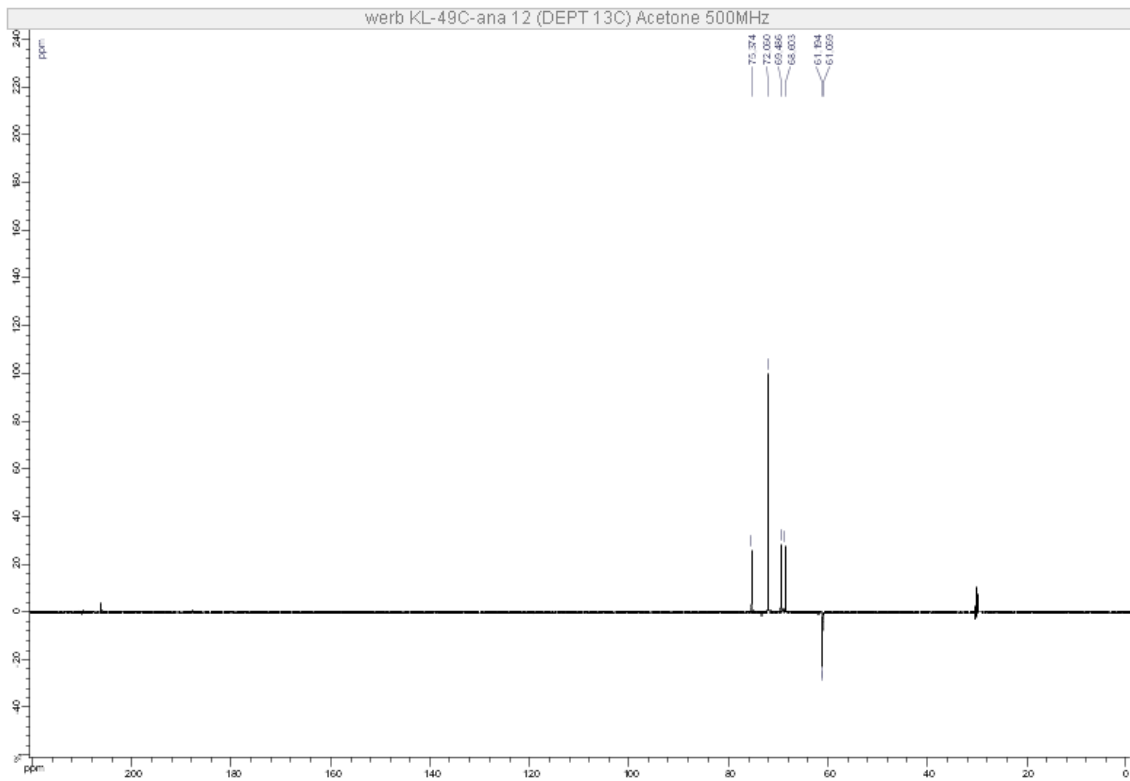
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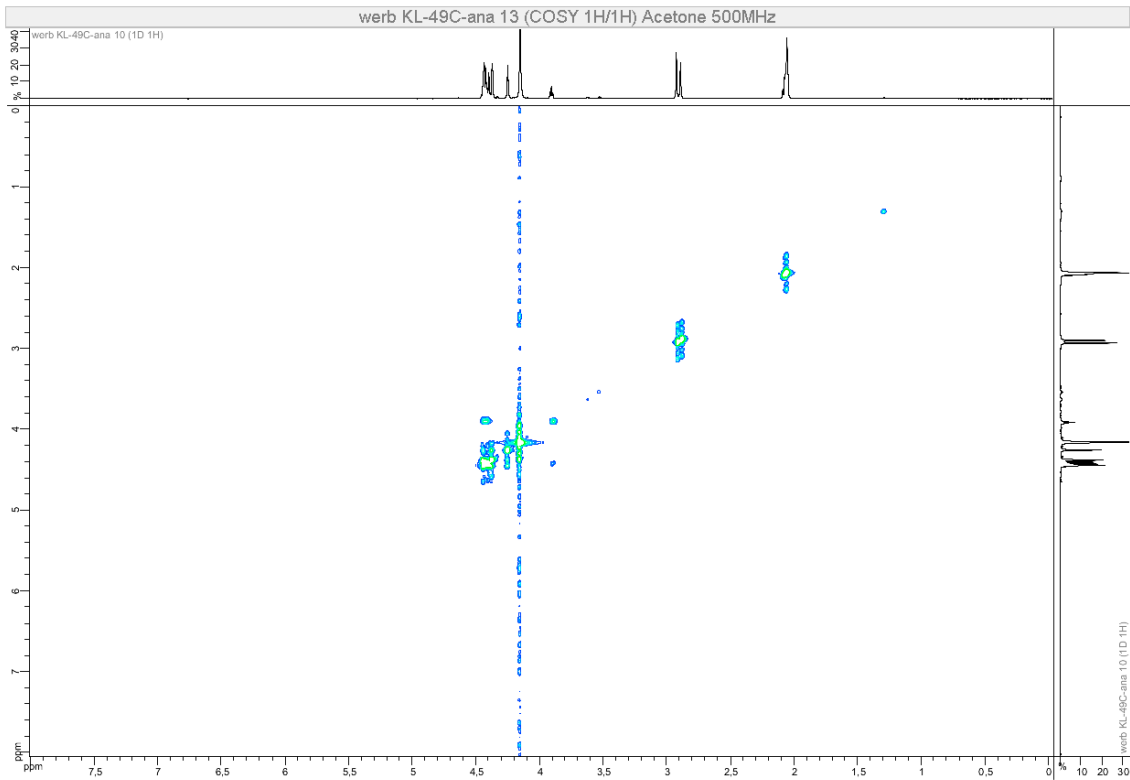
^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{CO}$)



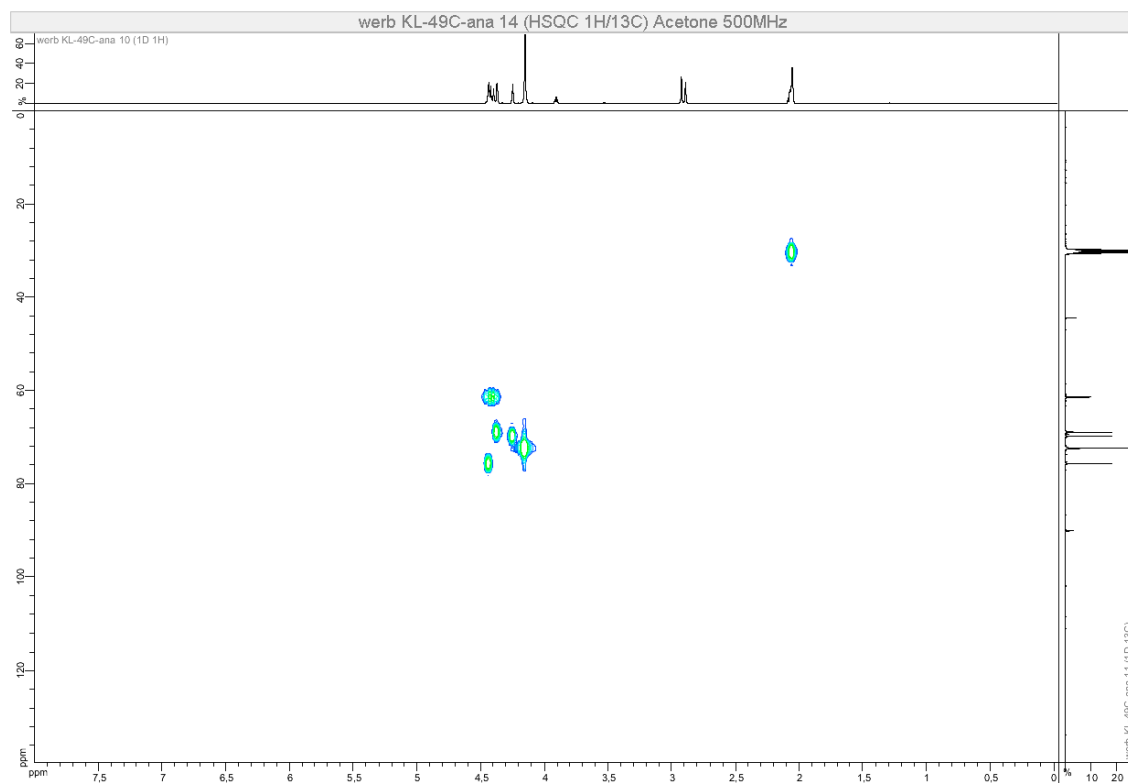
DEPT 135 (126 MHz, (CD₃)₂CO)



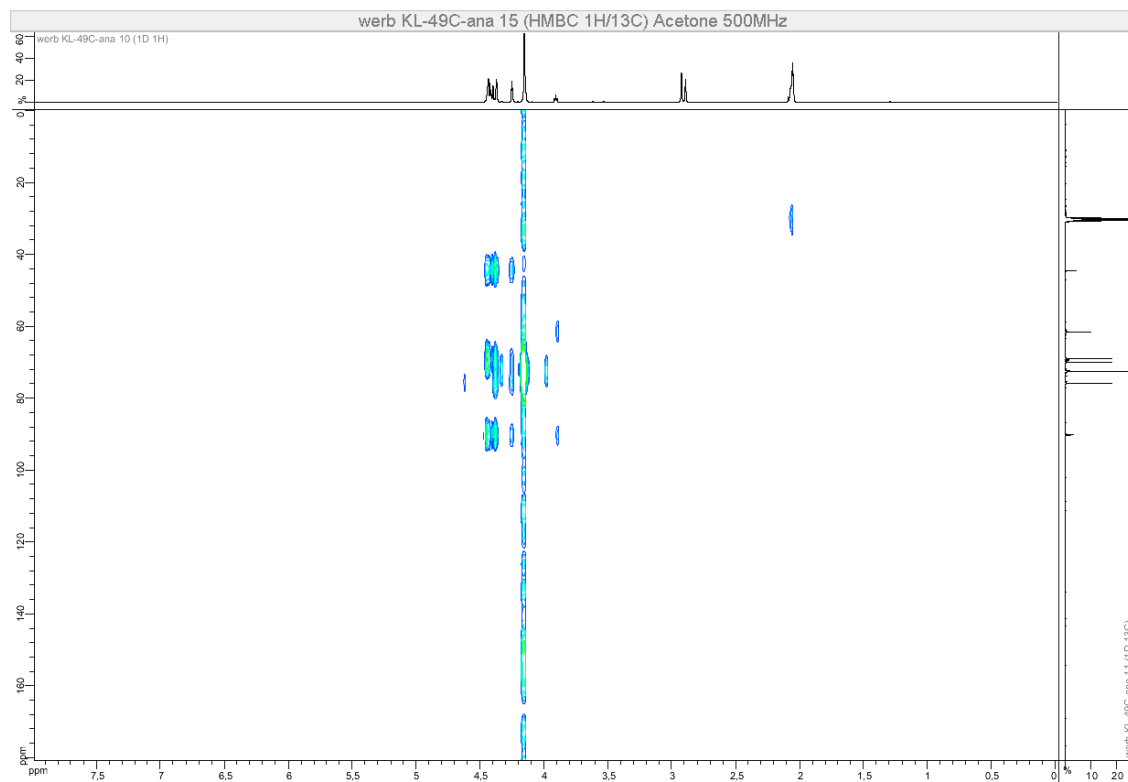
COSY (500 MHz, (CD₃)₂CO)



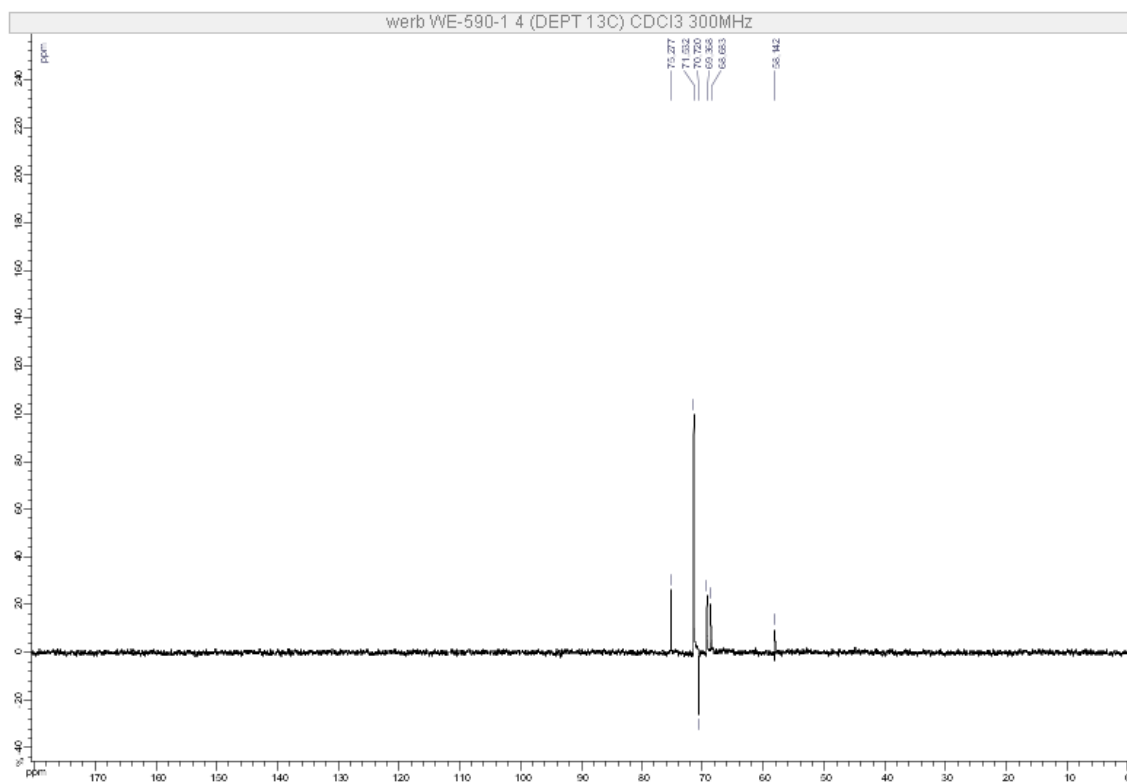
HSQC (500 MHz, (CD₃)₂CO)



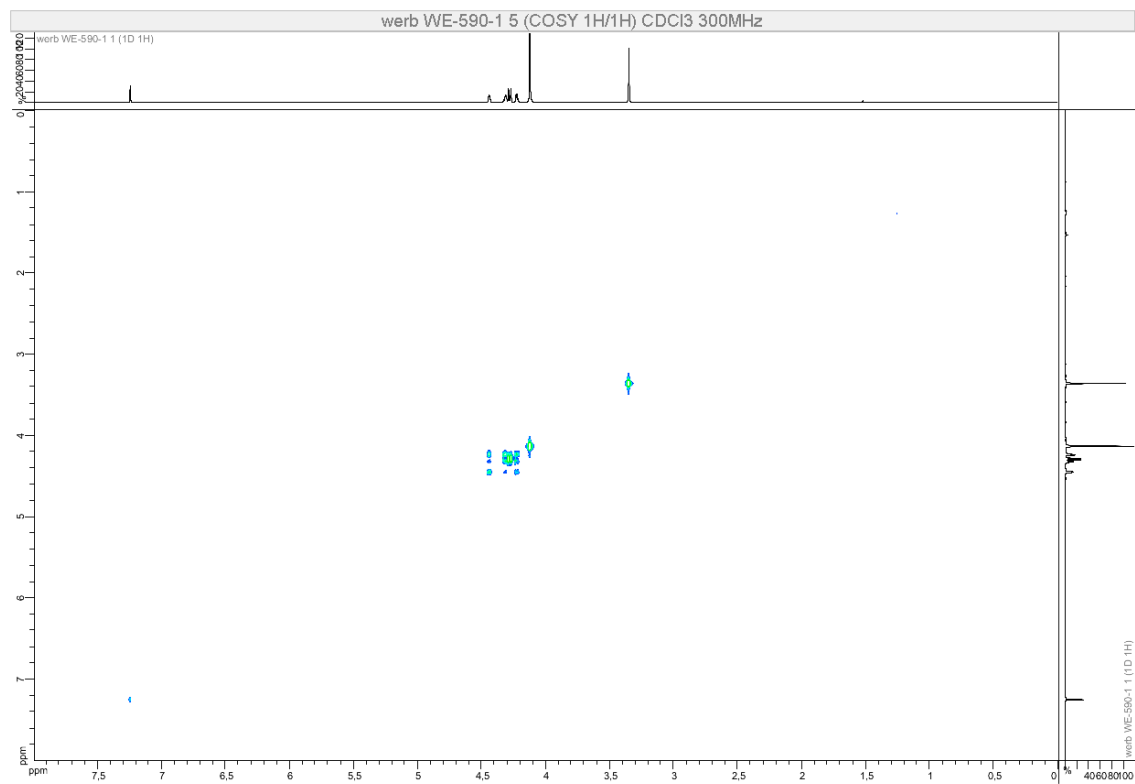
HMBC (500 MHz, (CD₃)₂CO)



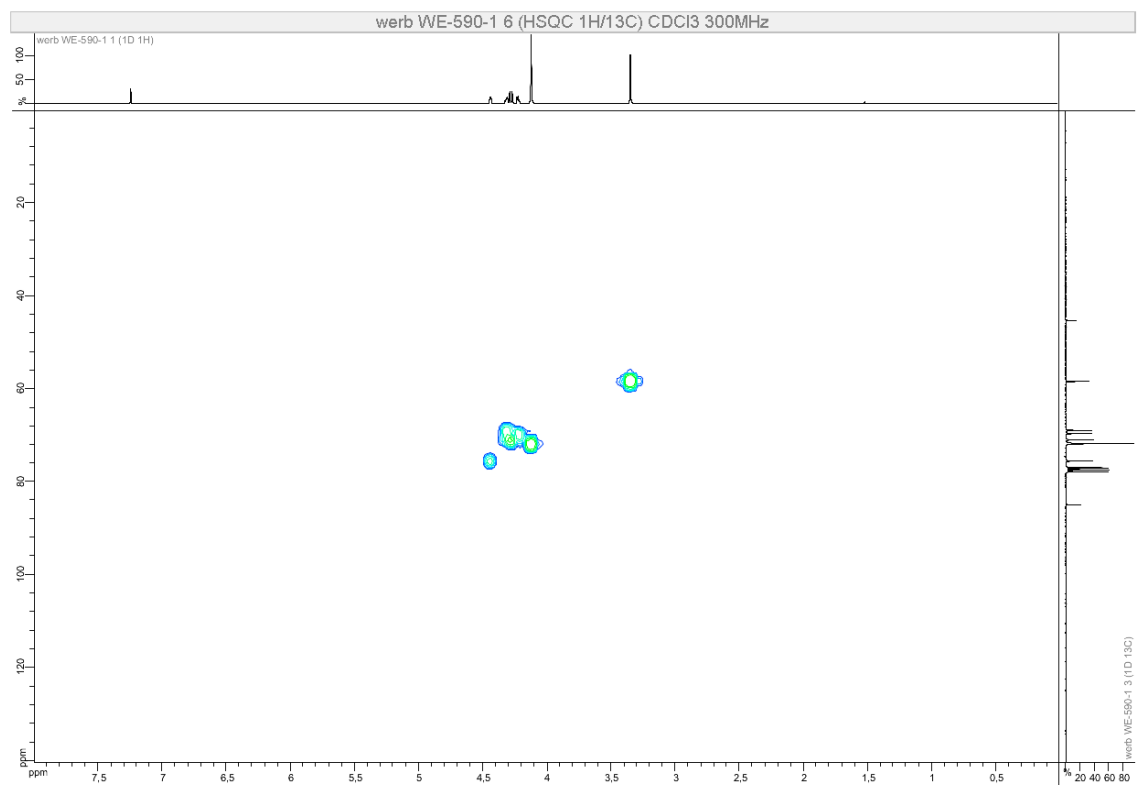
DEPT 135 (75 MHz, CDCl₃)



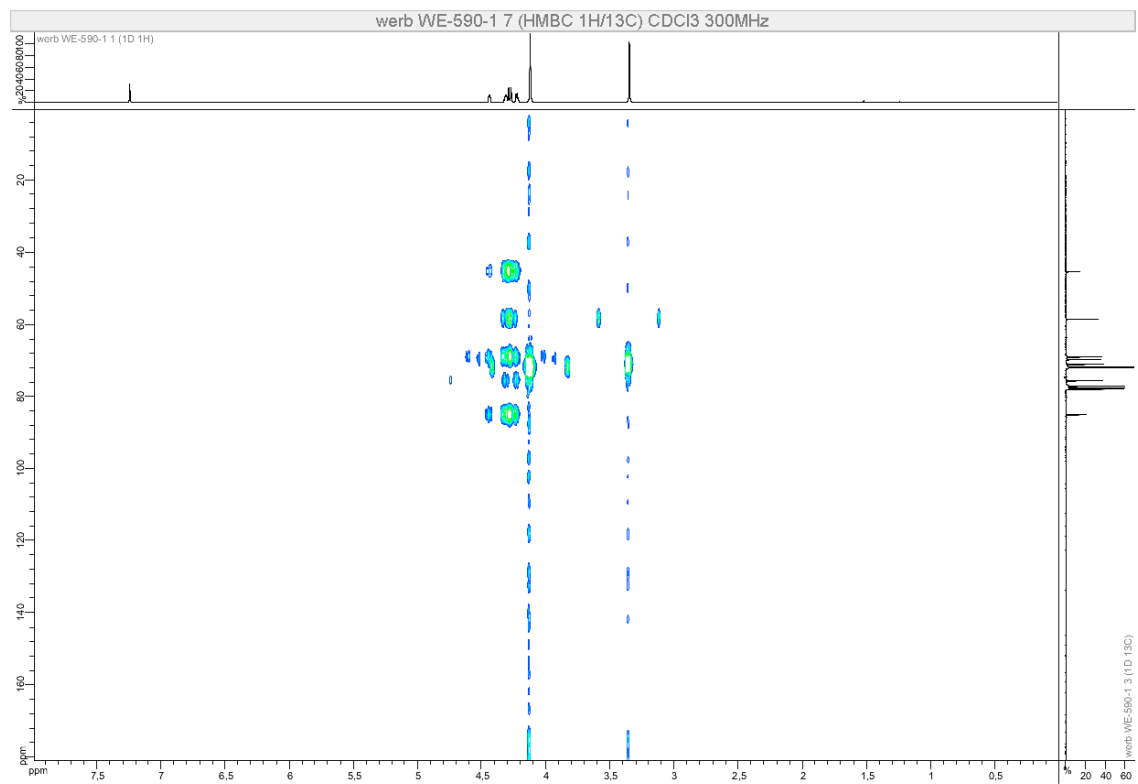
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

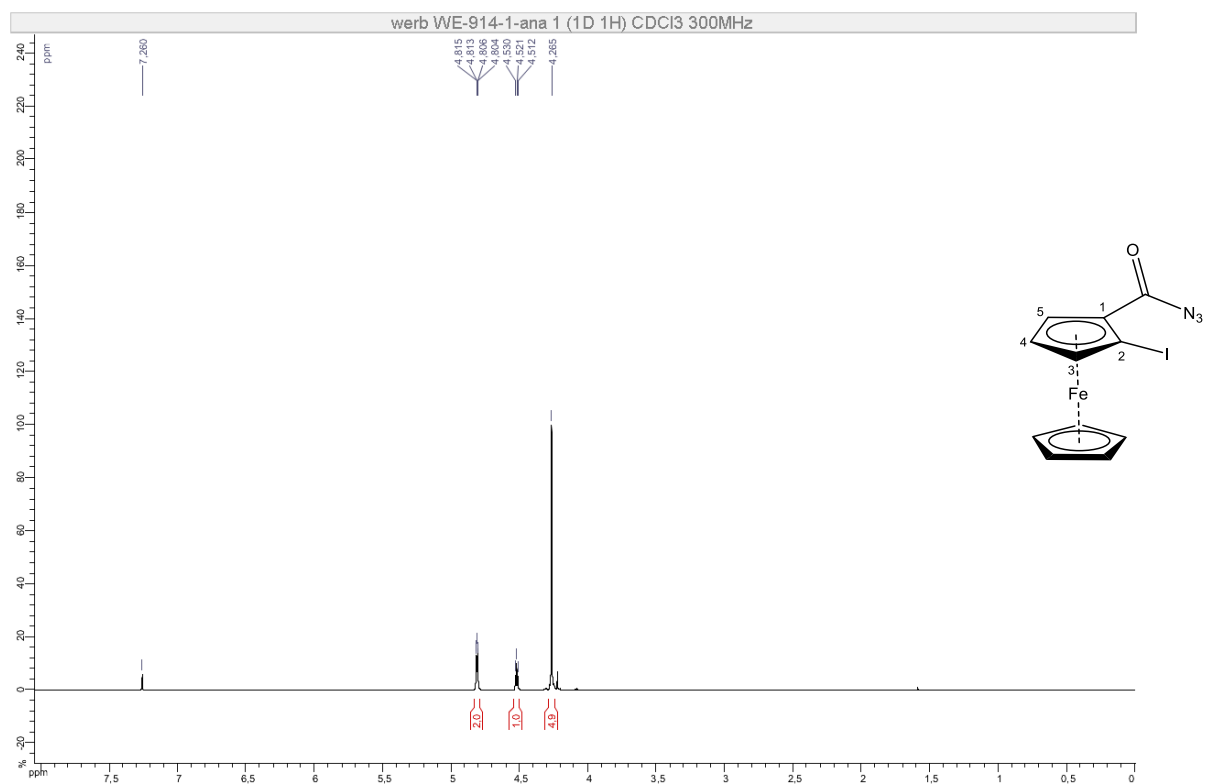


HMBC (300 MHz, CDCl₃)

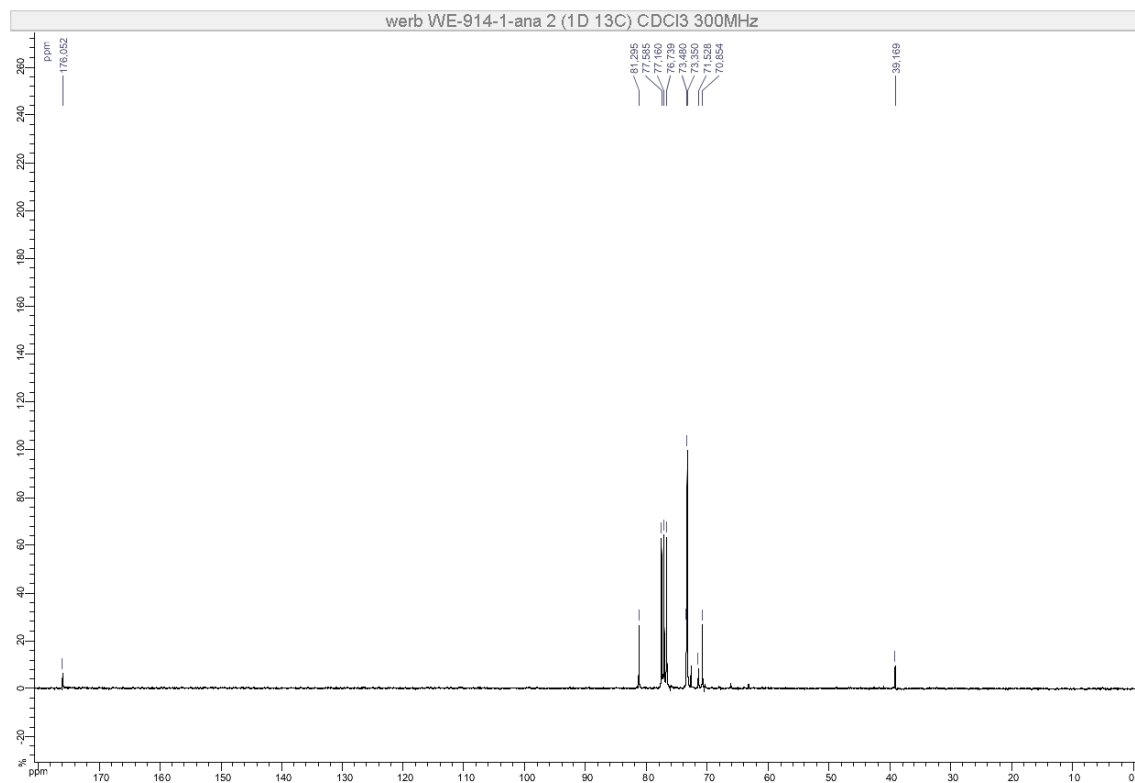


1-Azidocarbonyl-2-iodoferrocene (racemic mixture)

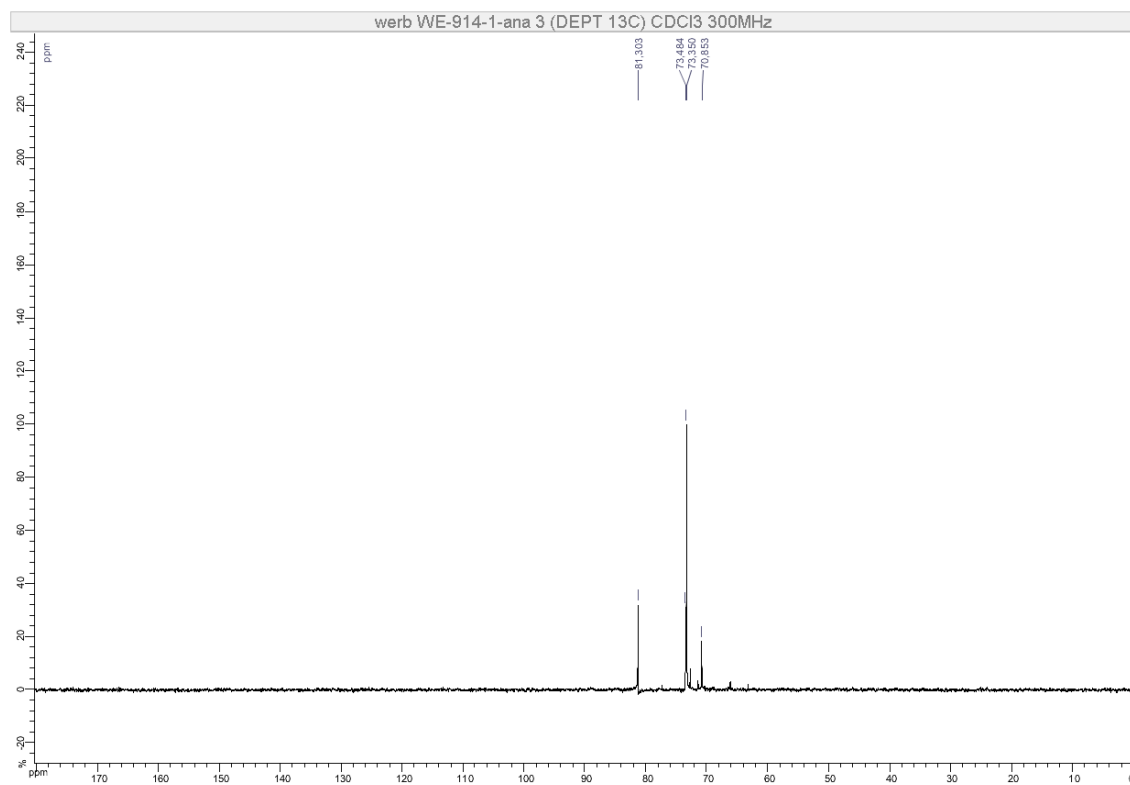
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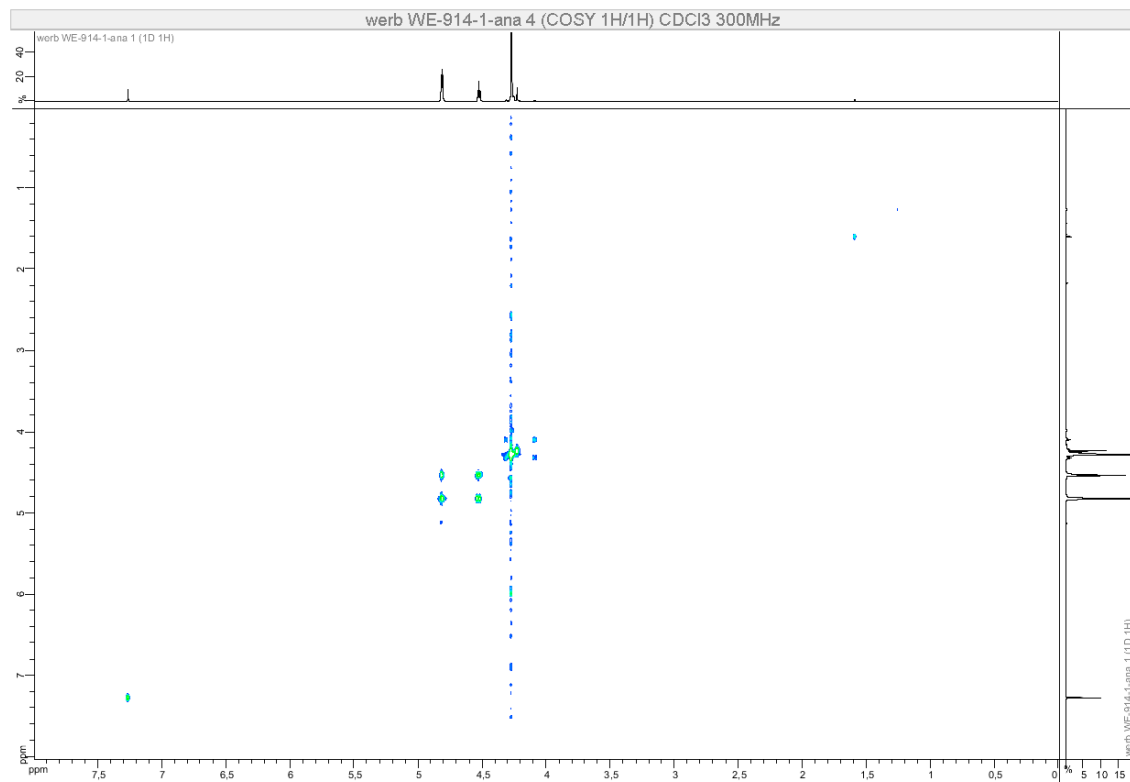
^{13}C NMR (126 MHz, CDCl_3)



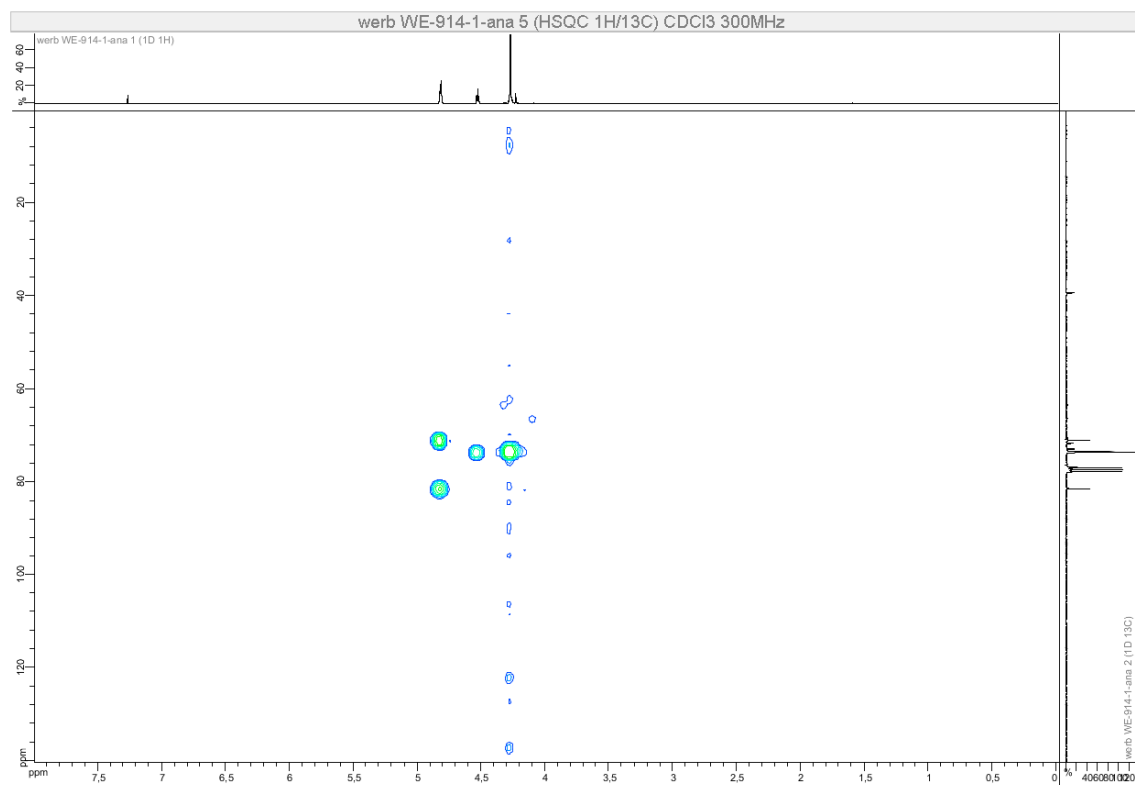
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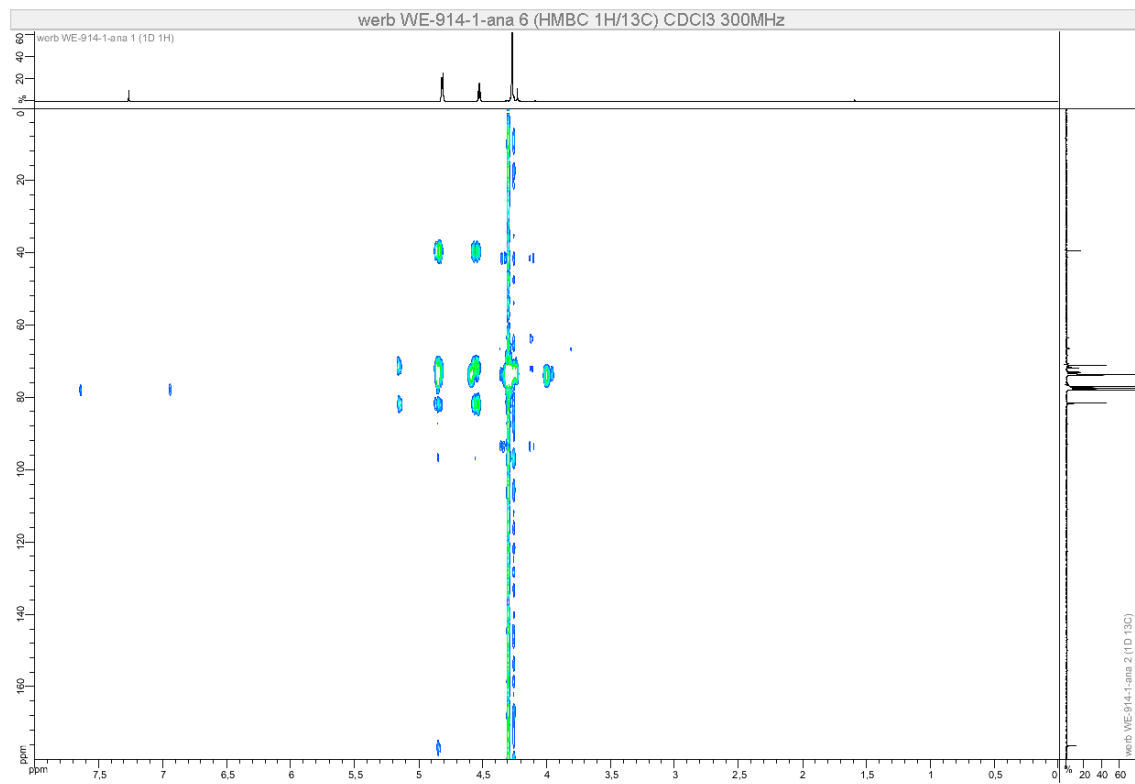
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

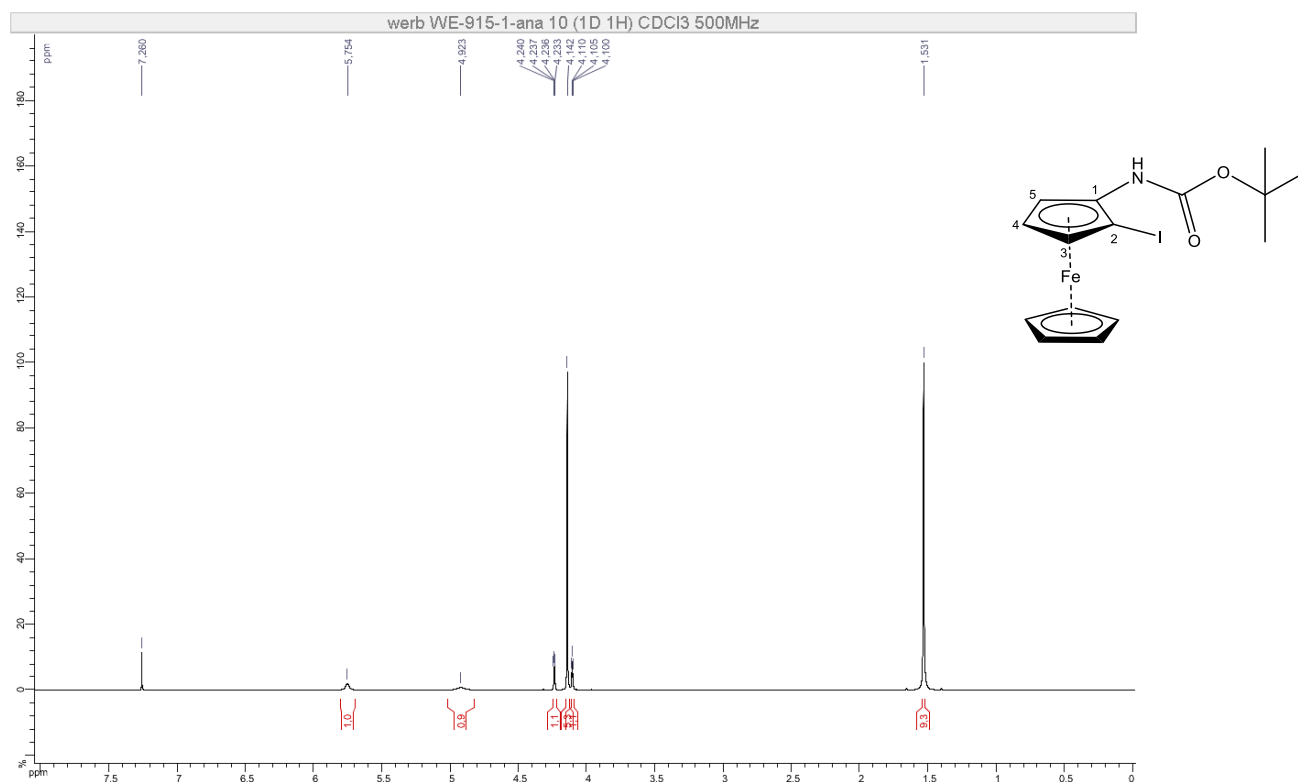


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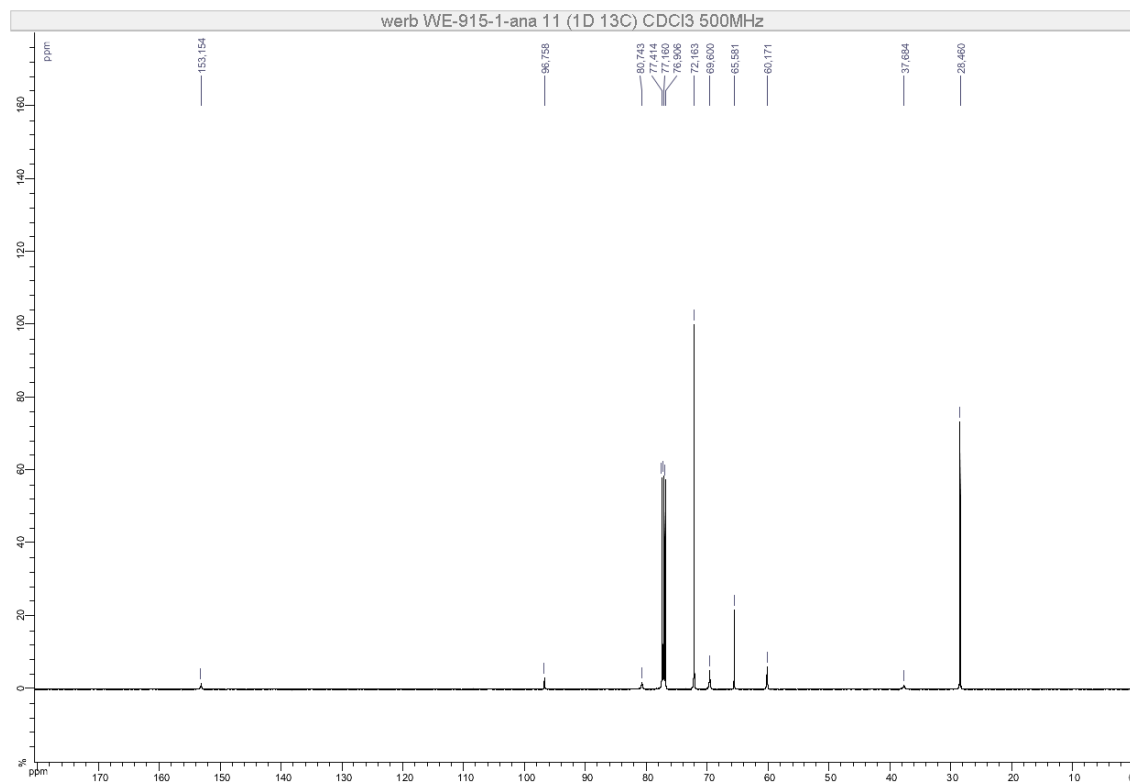


1-(*tert*-Butoxycarbonylamino)-2-iodoferrocene (**11**, racemic mixture)

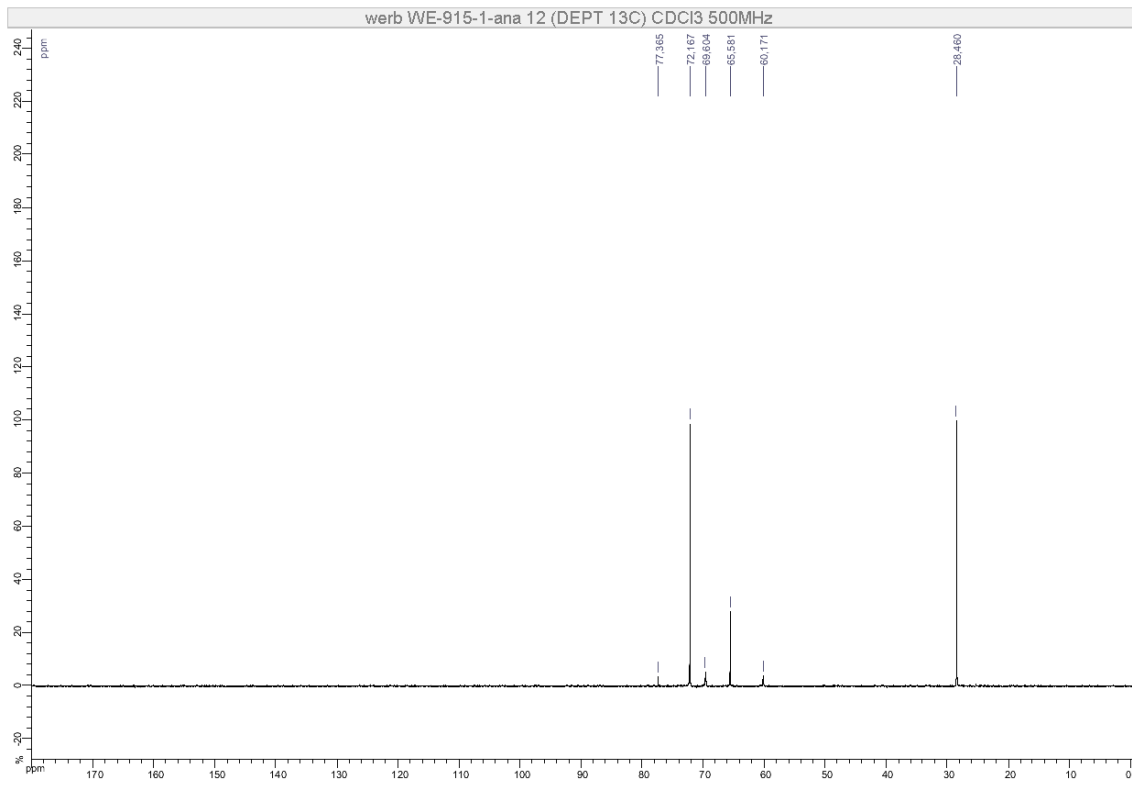
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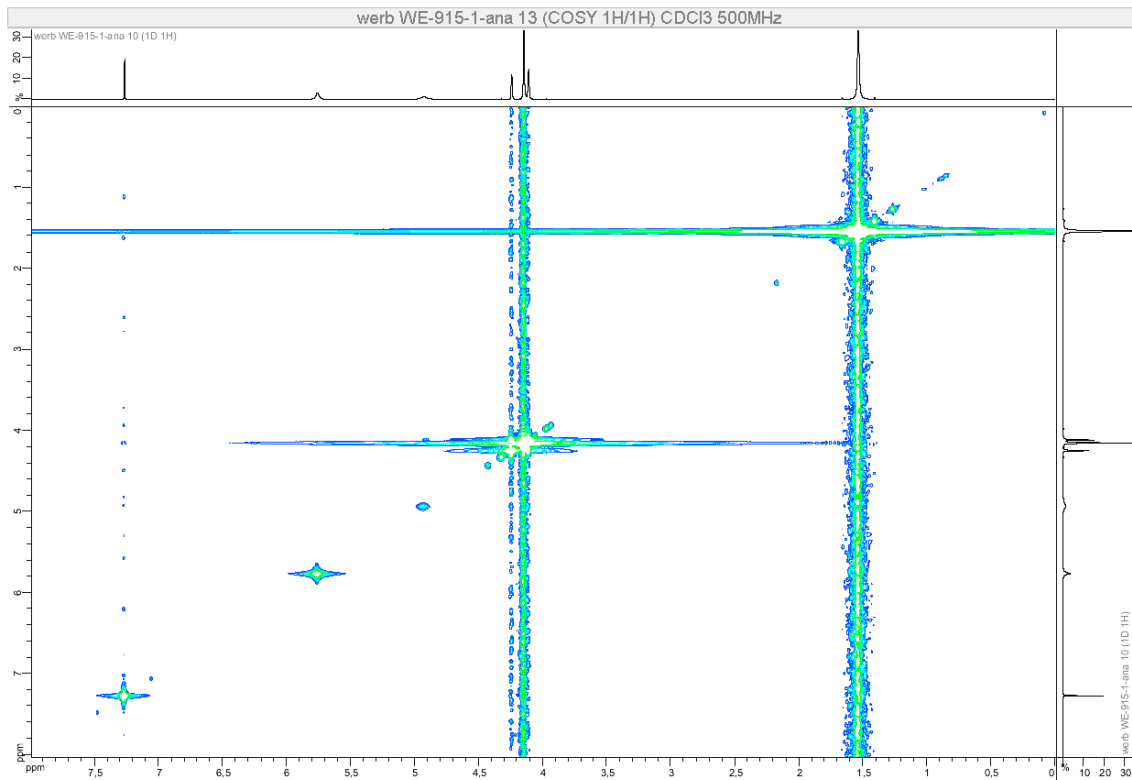
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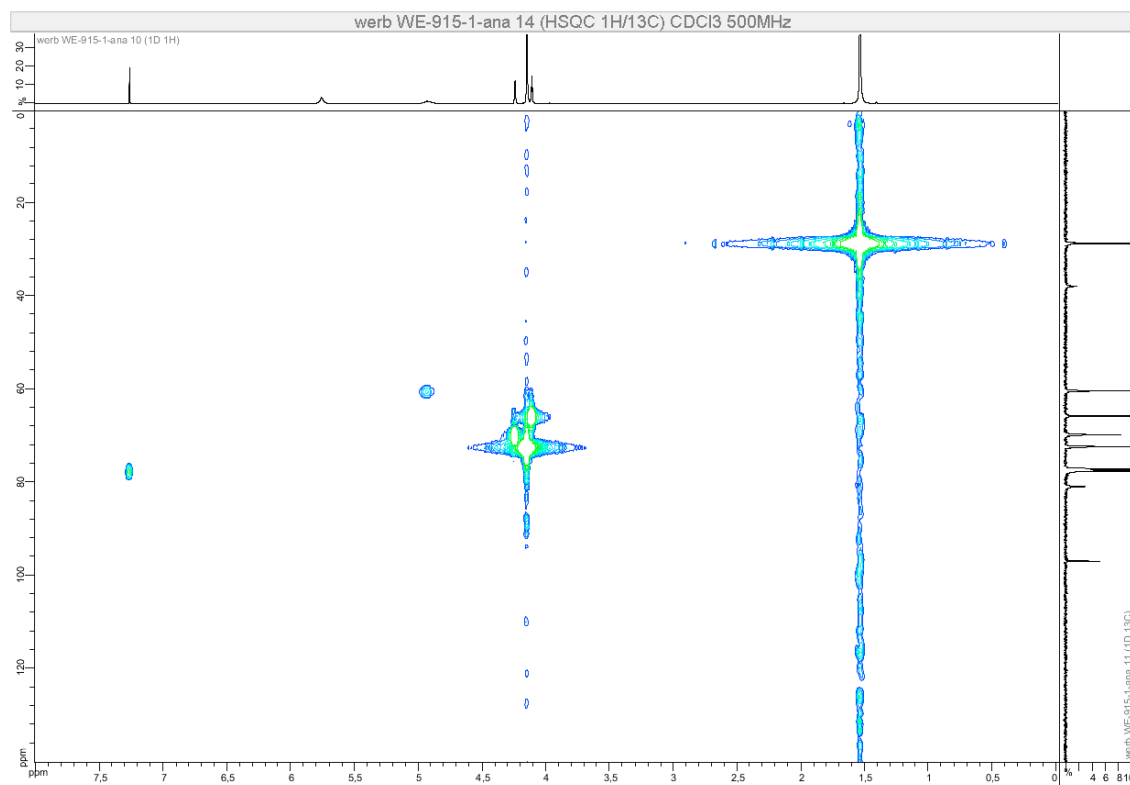
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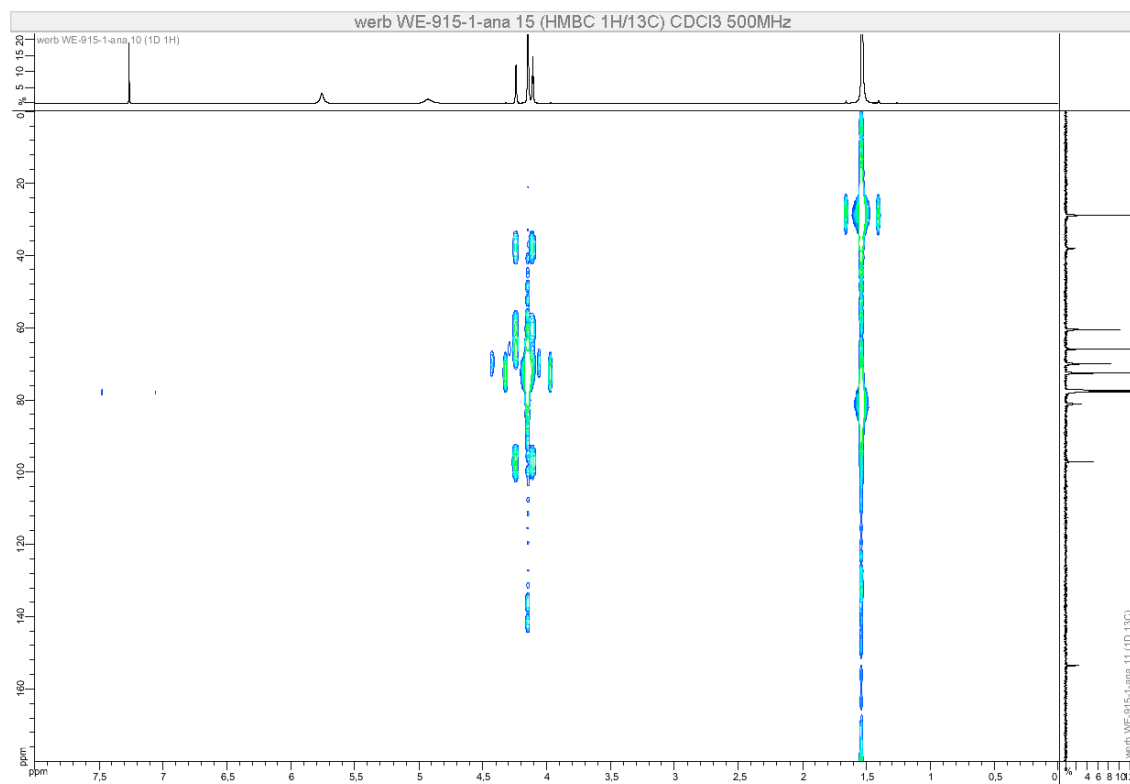
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HSQC (500 MHz, CDCl₃)

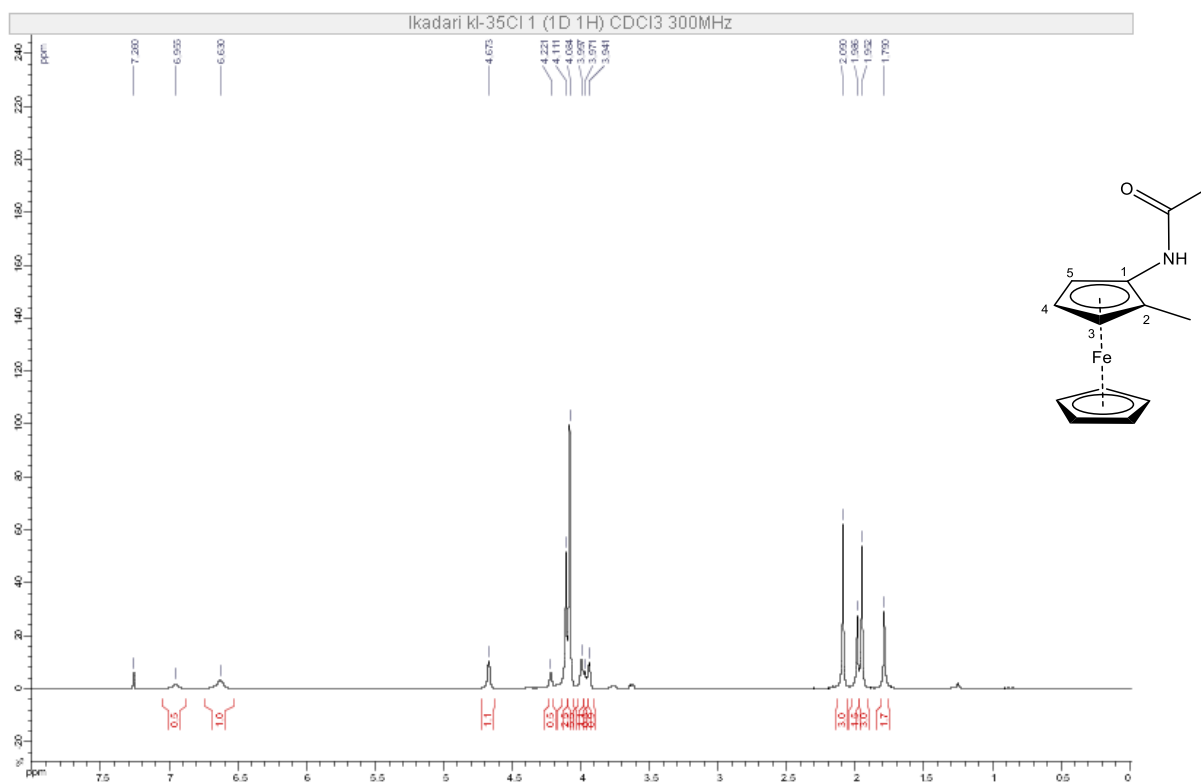


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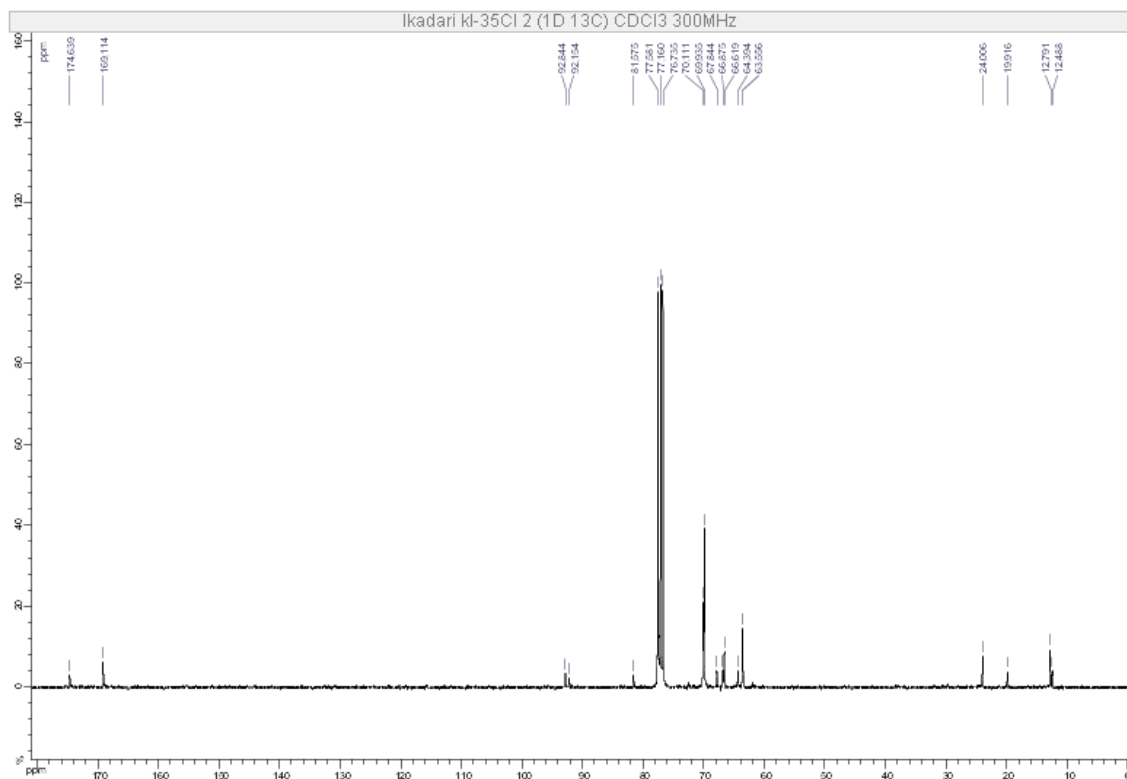


N-(2-Methylferrocenyl)acetamide (**2b**, stereoisomeric mixture due to rotamers)

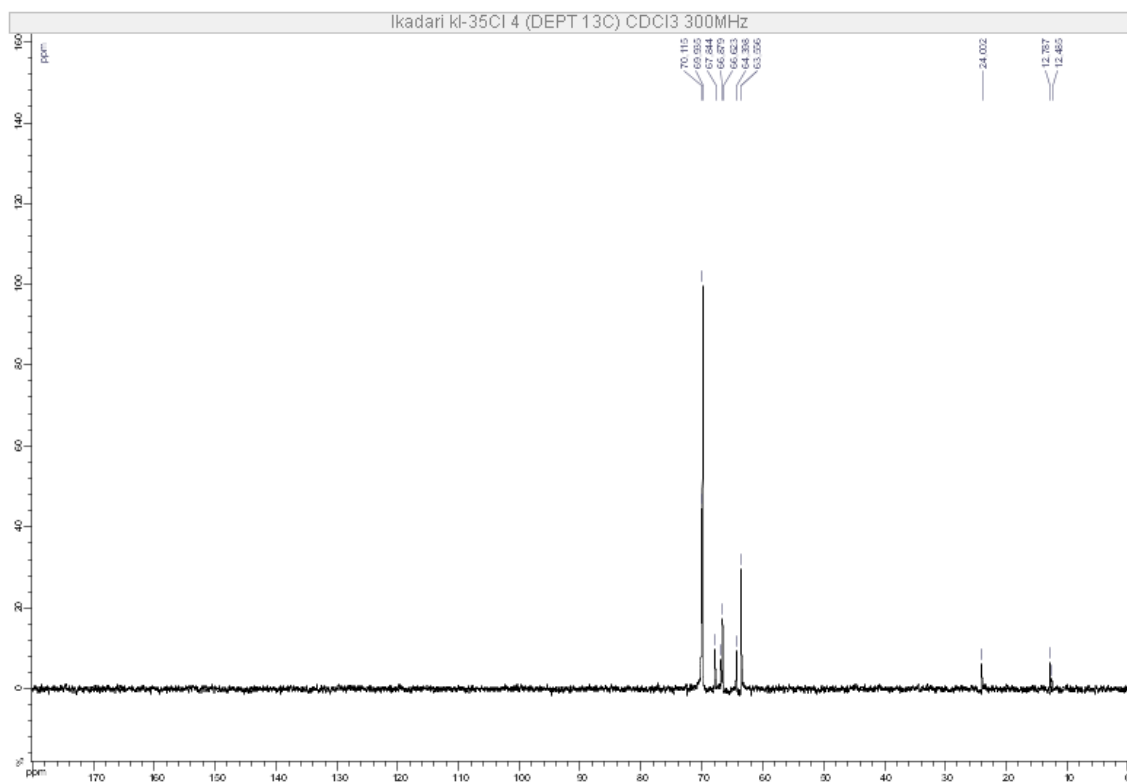
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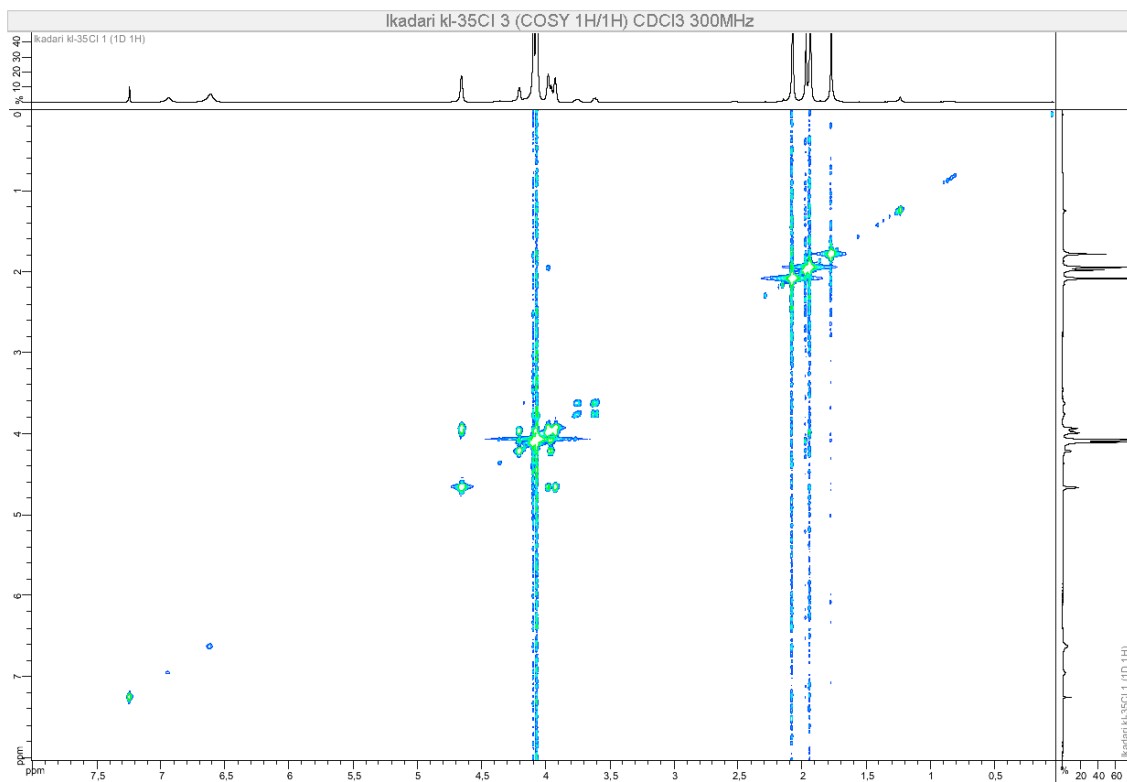
^{13}C NMR (75 MHz, CDCl_3)



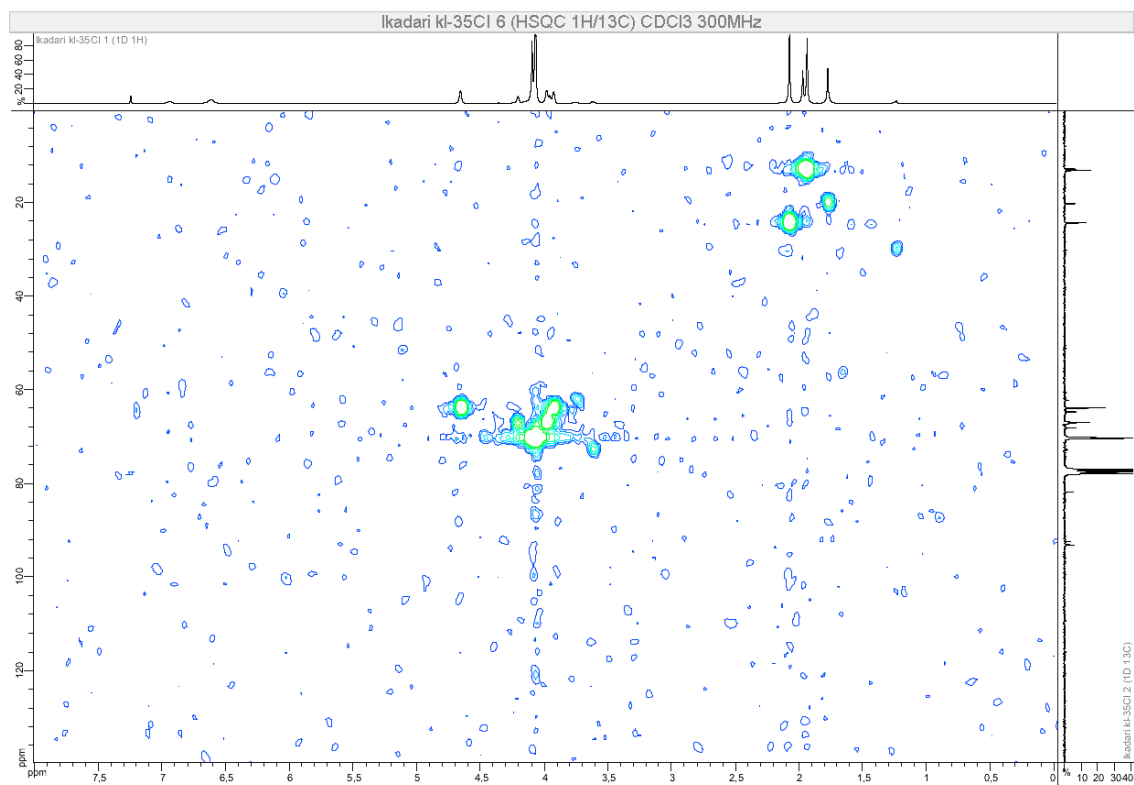
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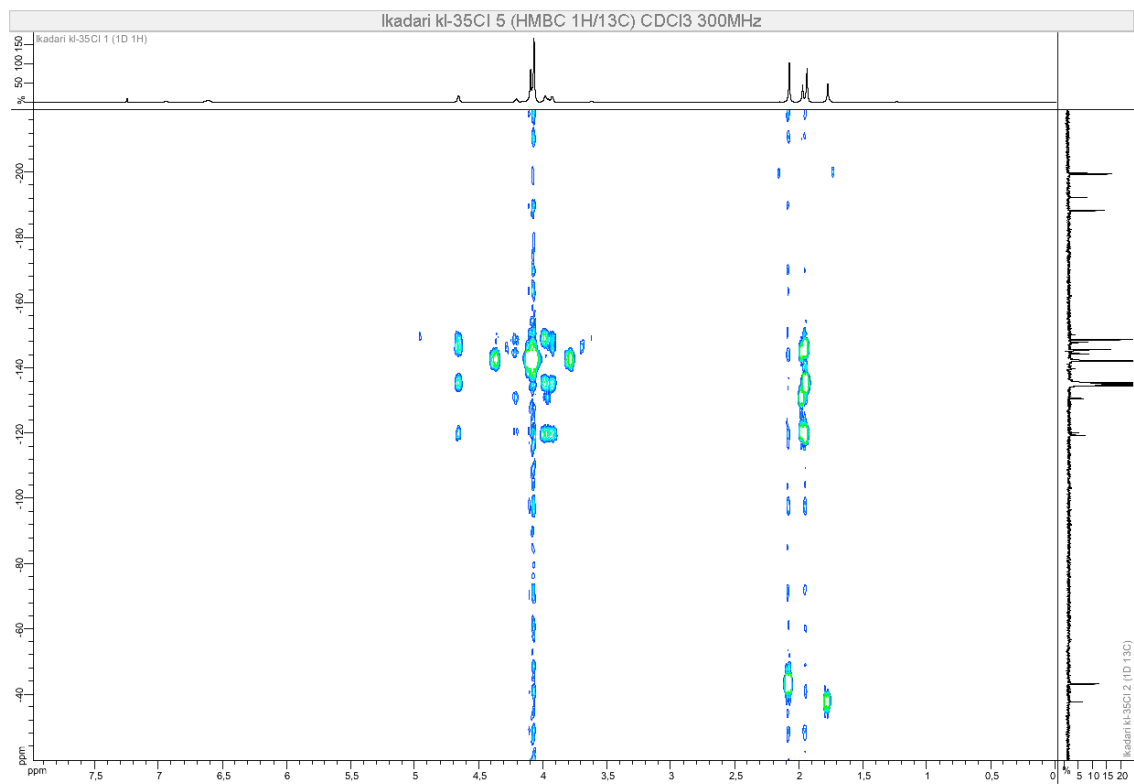
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HSQC (300 MHz, CDCl₃)

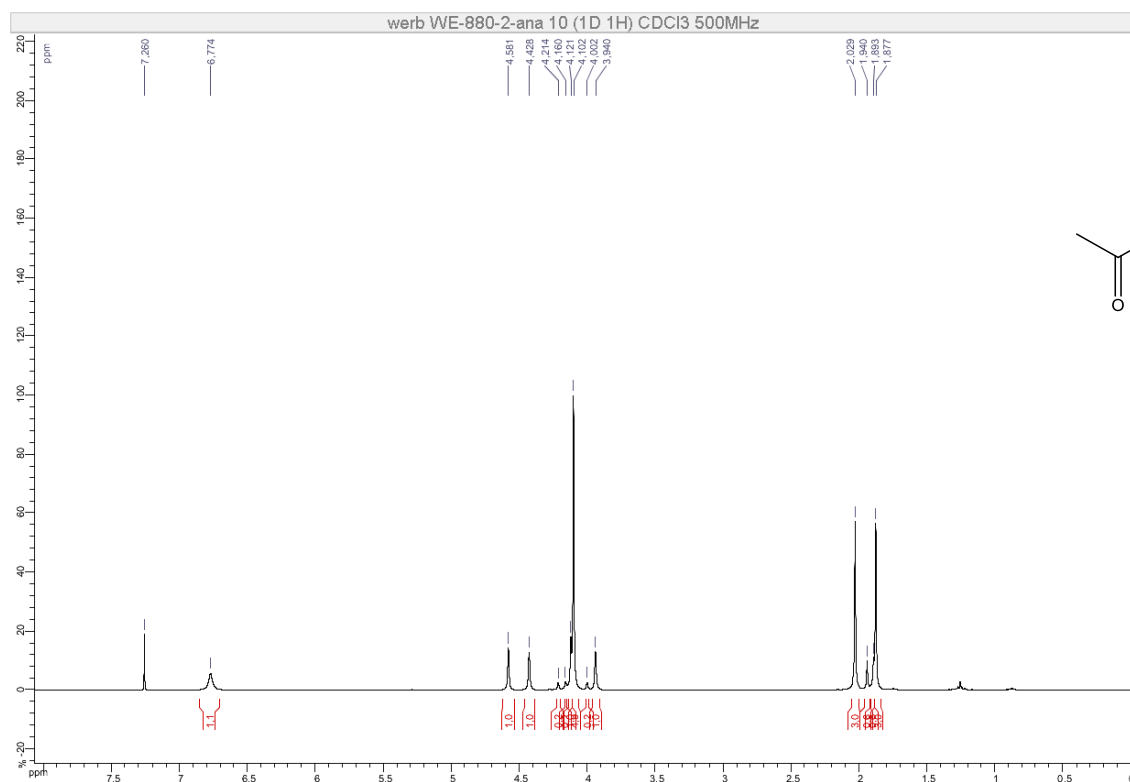


HMBC (300 MHz, CDCl₃)

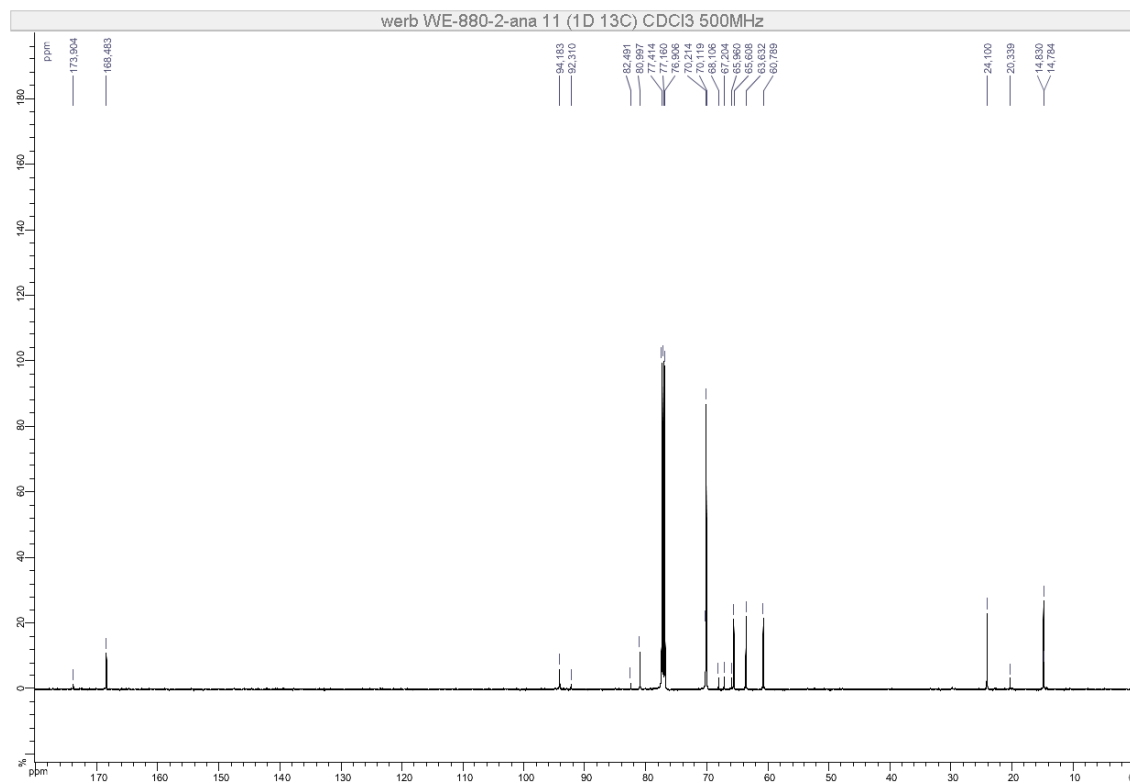


N-(3-Methylferrocenyl)acetamide (**4b**, stereoisomeric mixture due to rotamers)

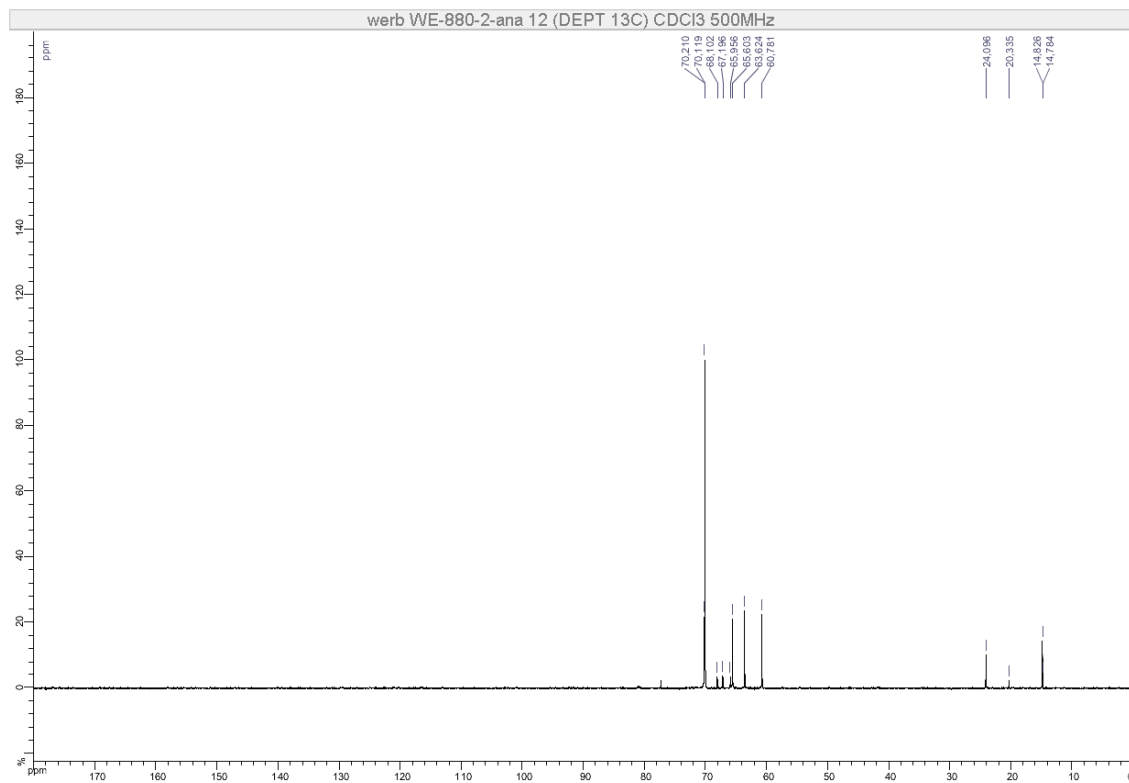
^1H NMR (500 MHz, CDCl_3)



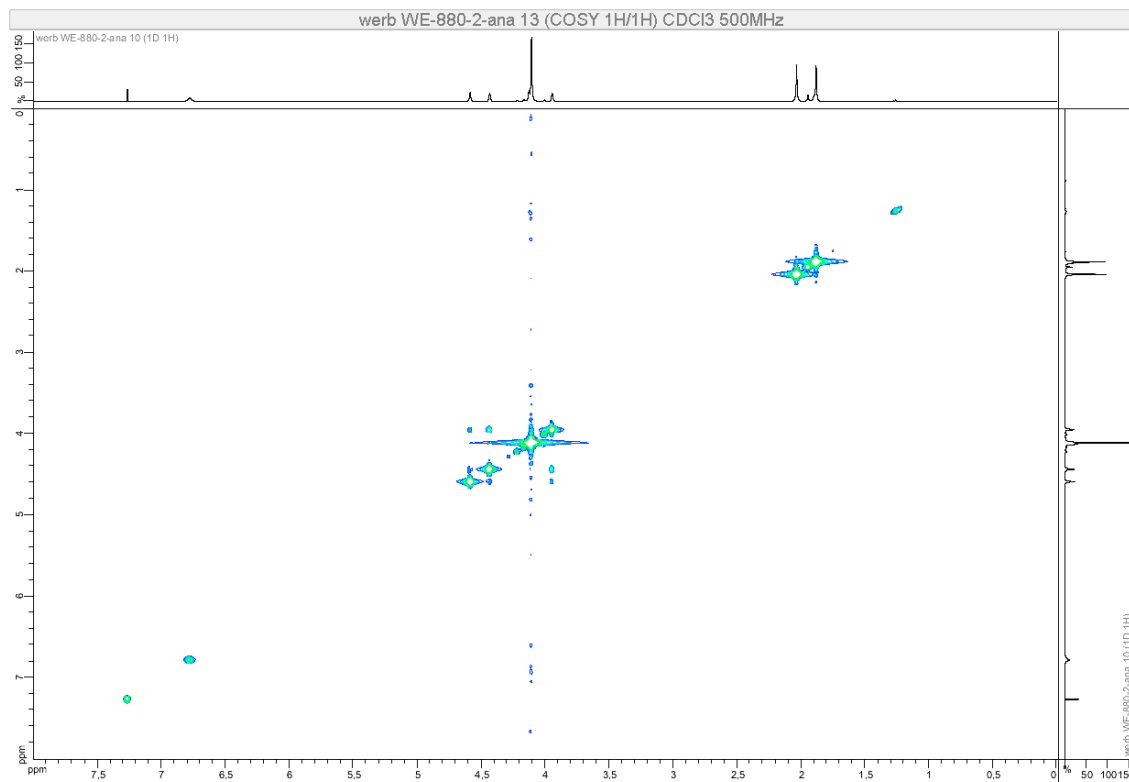
^{13}C NMR (126 MHz, CDCl_3)



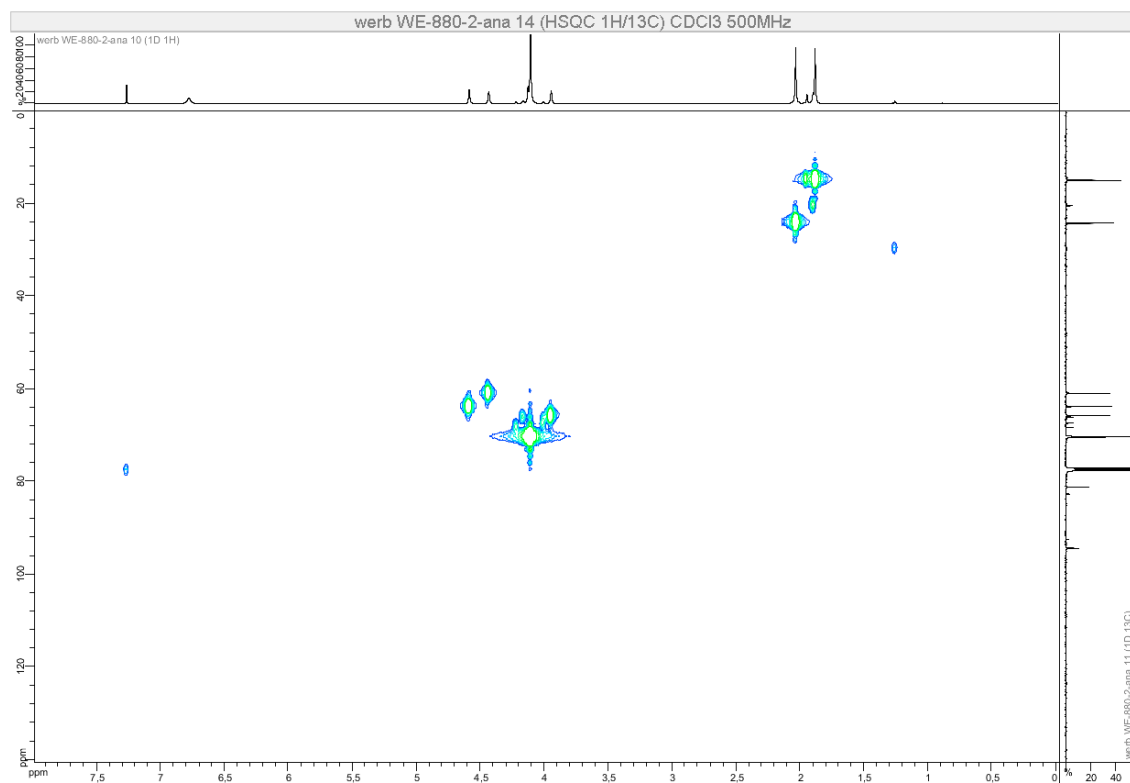
DEPT 135 (126 MHz, CDCl₃)



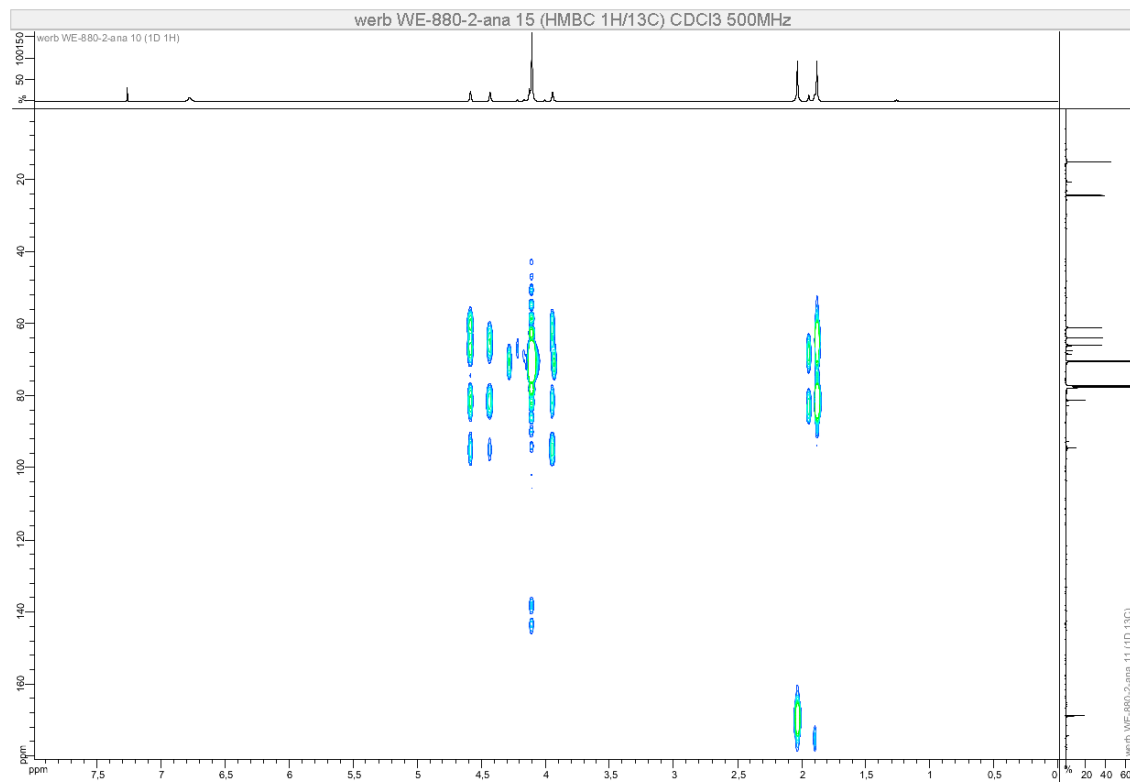
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

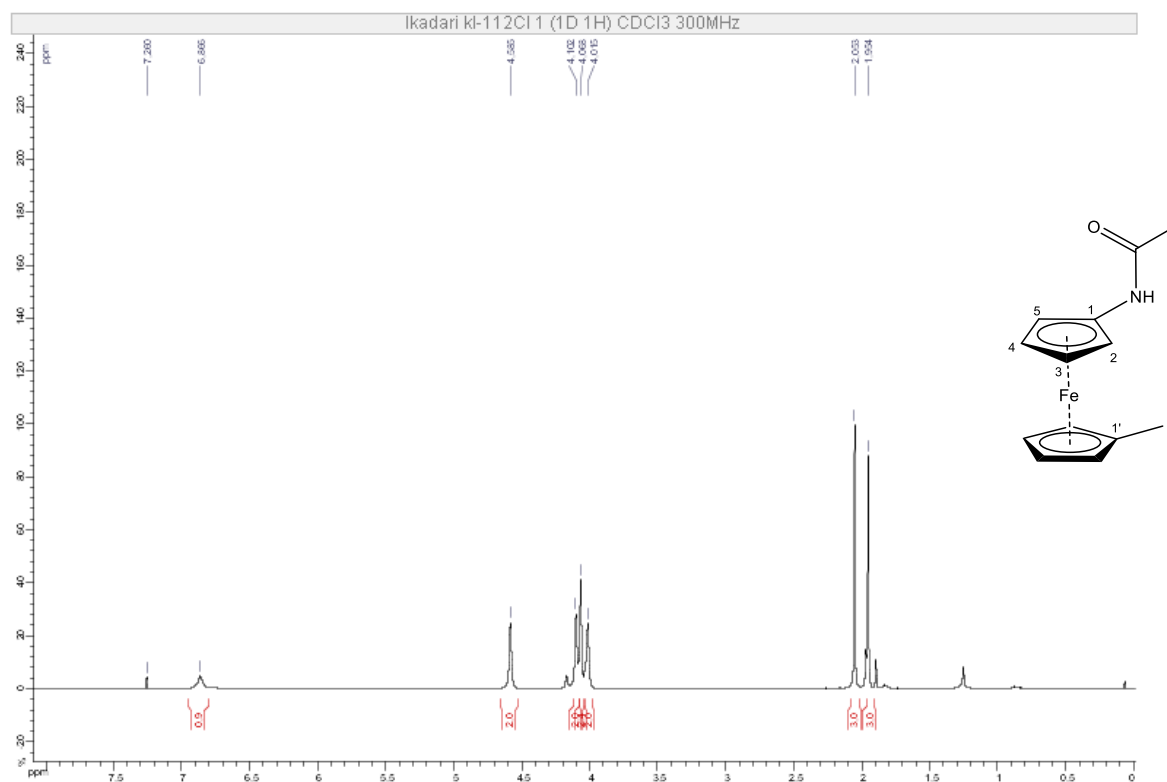


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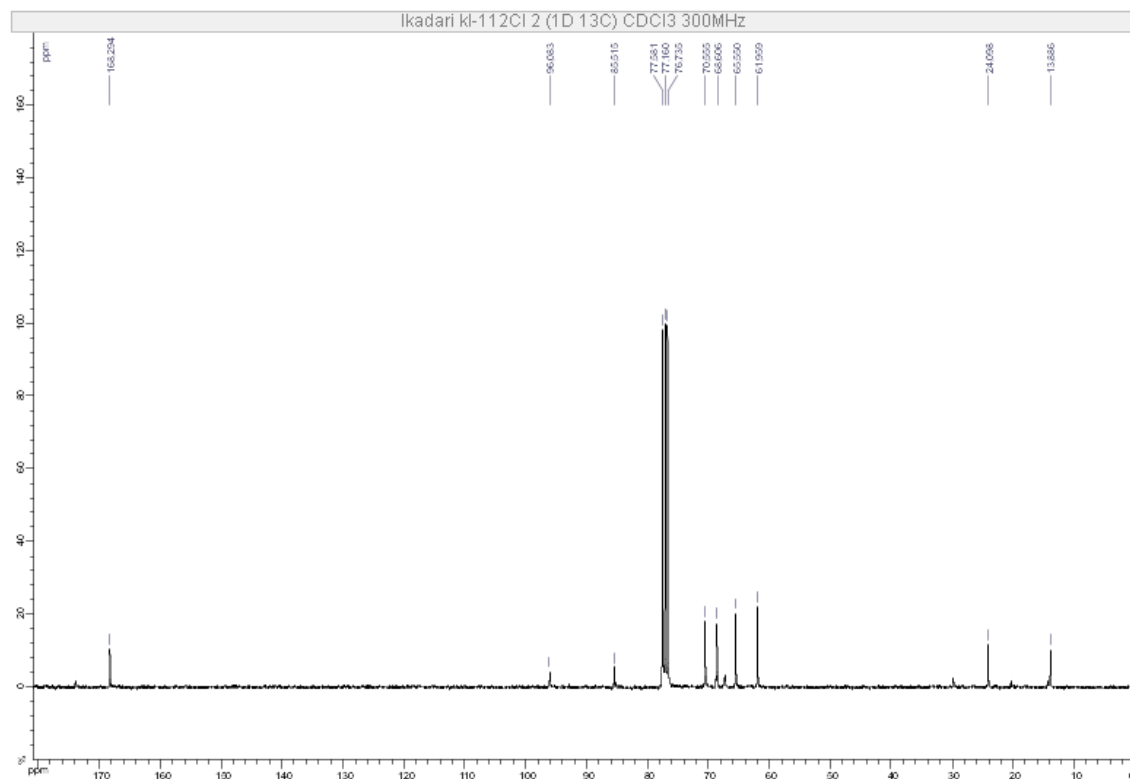


N-(1'-Methylferrocenyl)acetamide (6b)

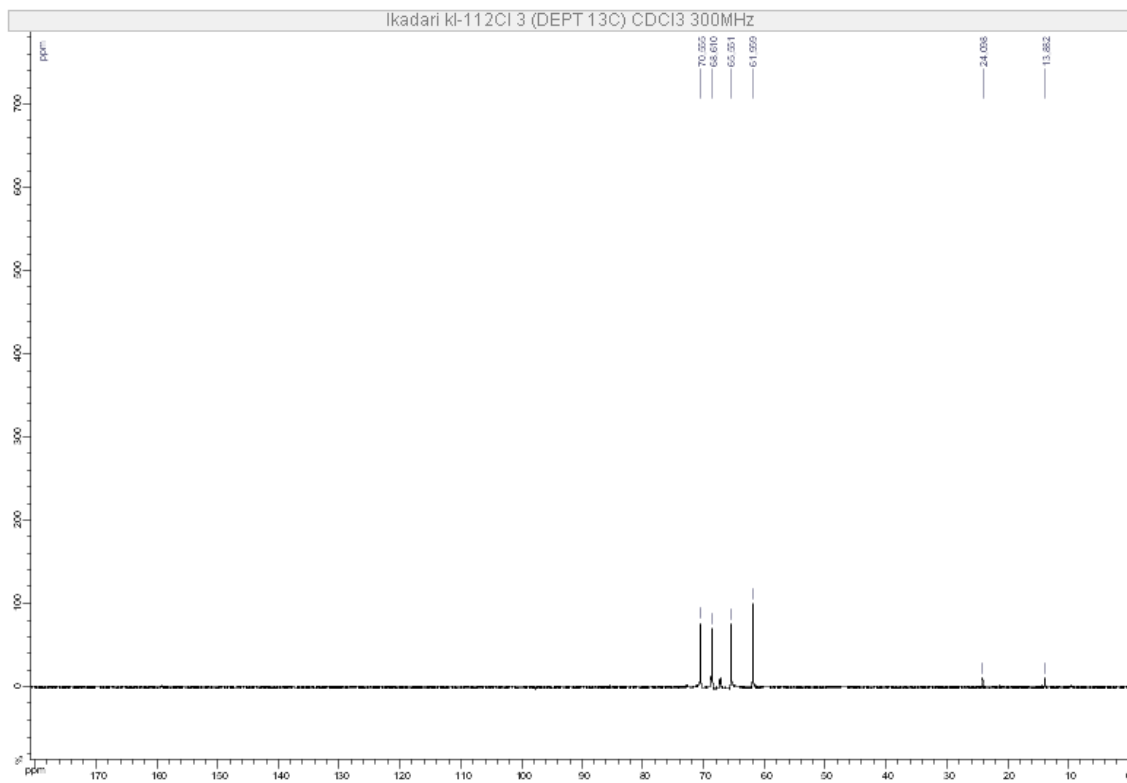
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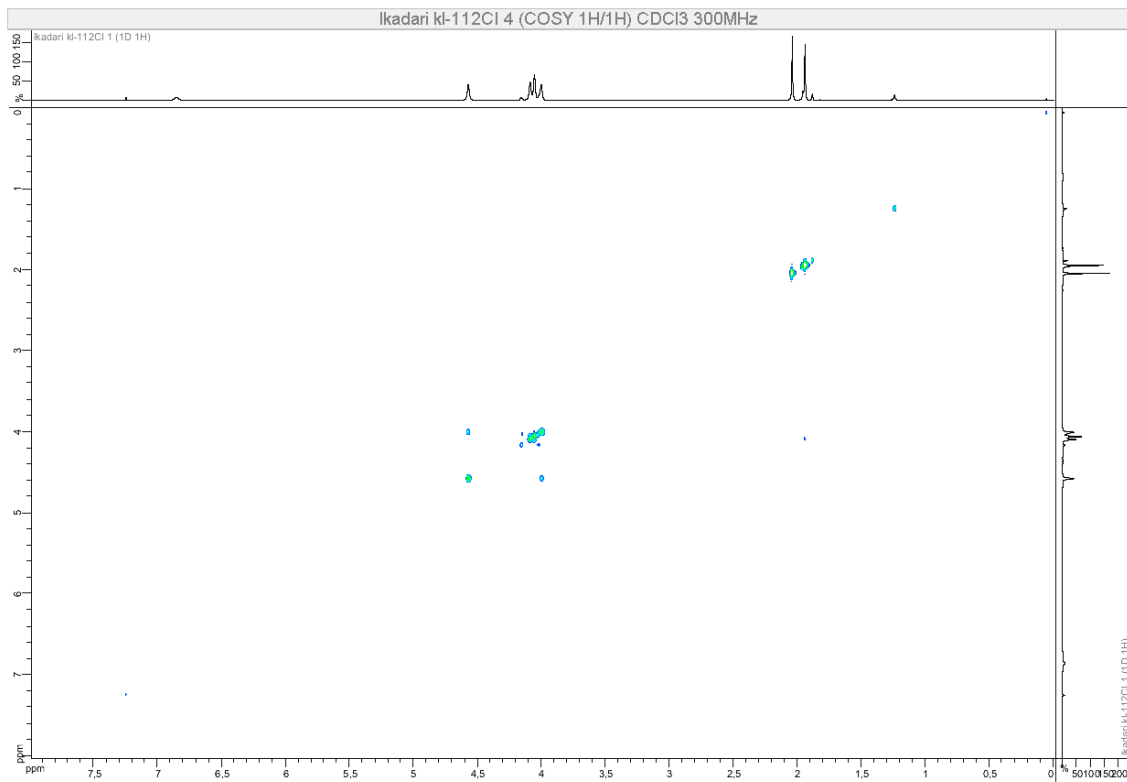
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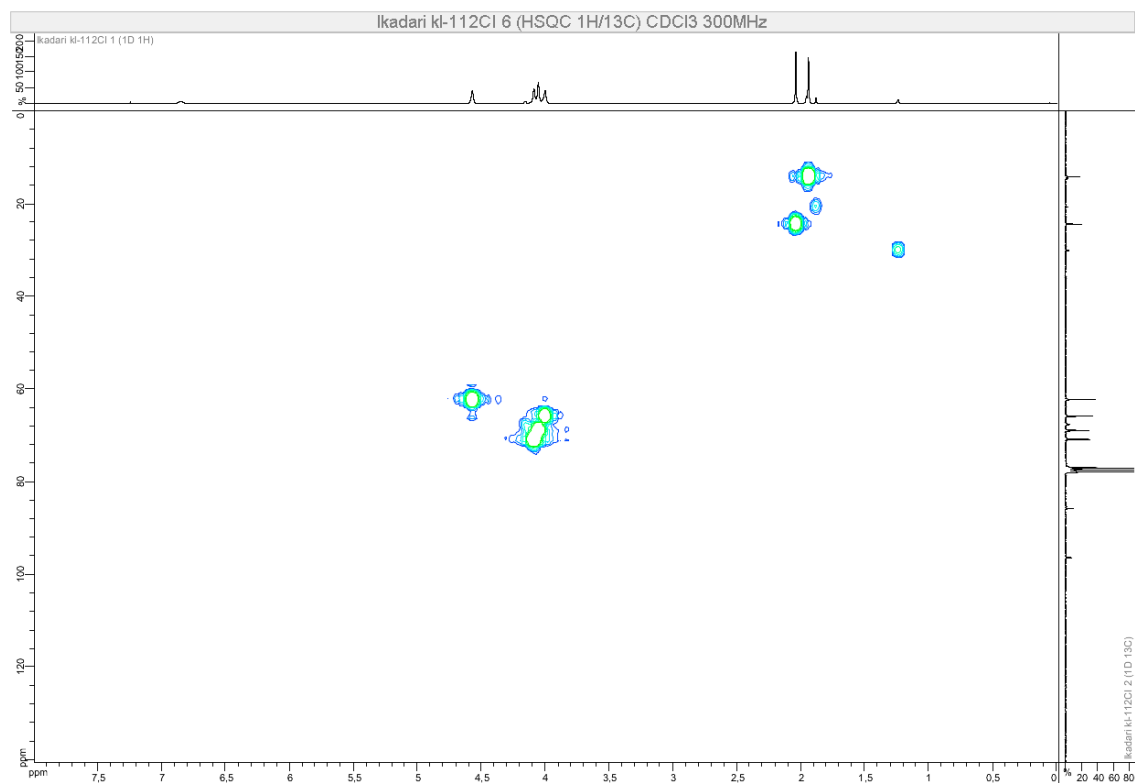
DEPT 135 (75 MHz, CDCl₃)



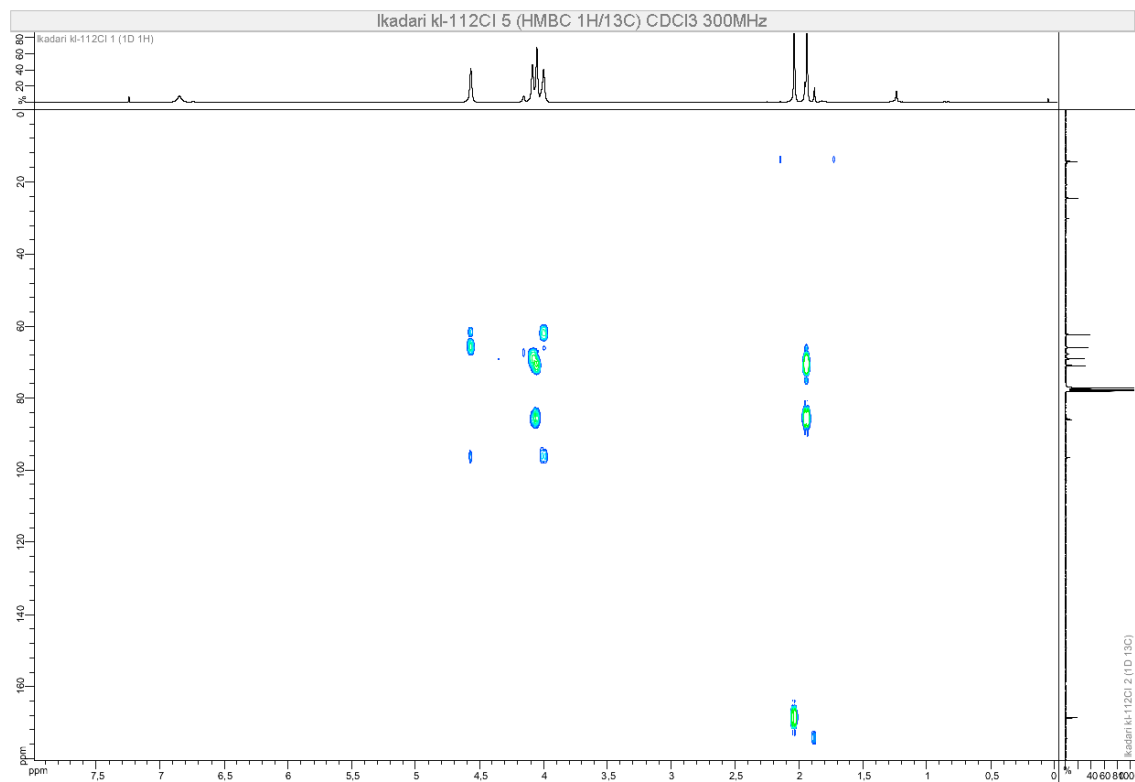
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

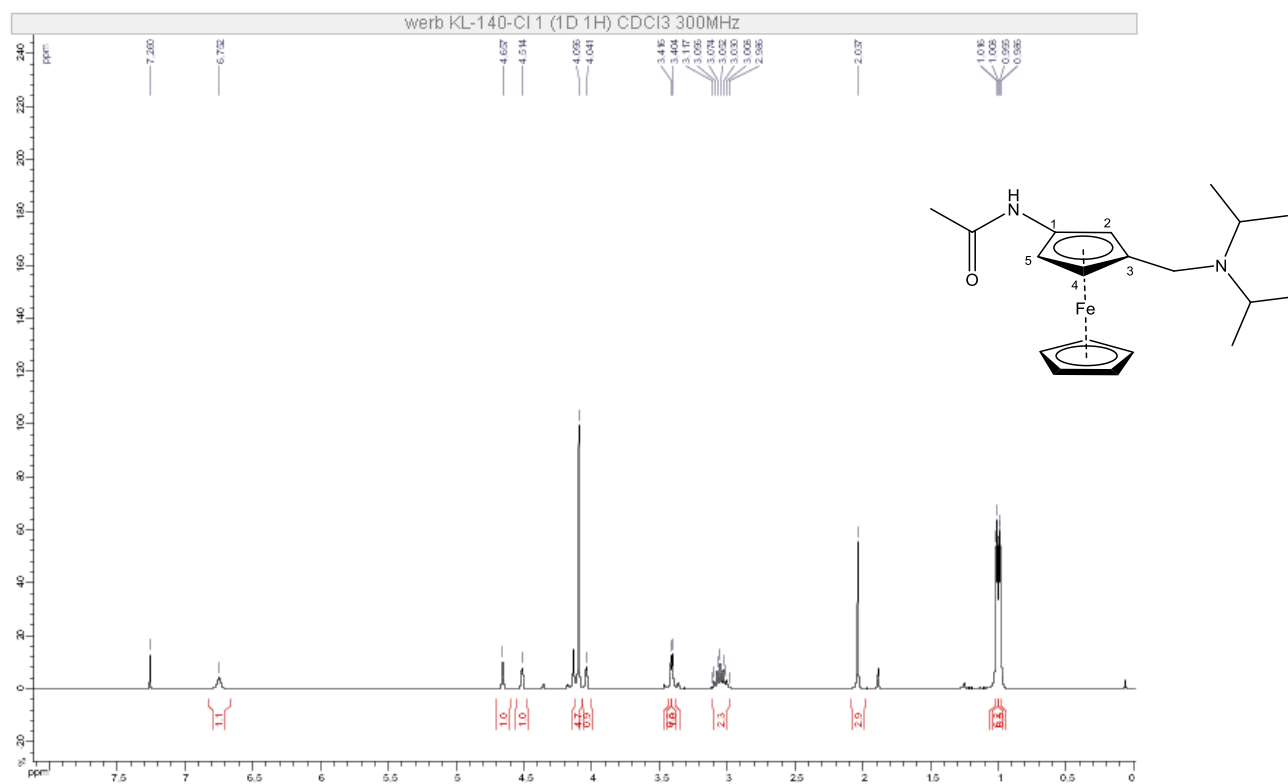


HMBC (300 MHz, CDCl₃)

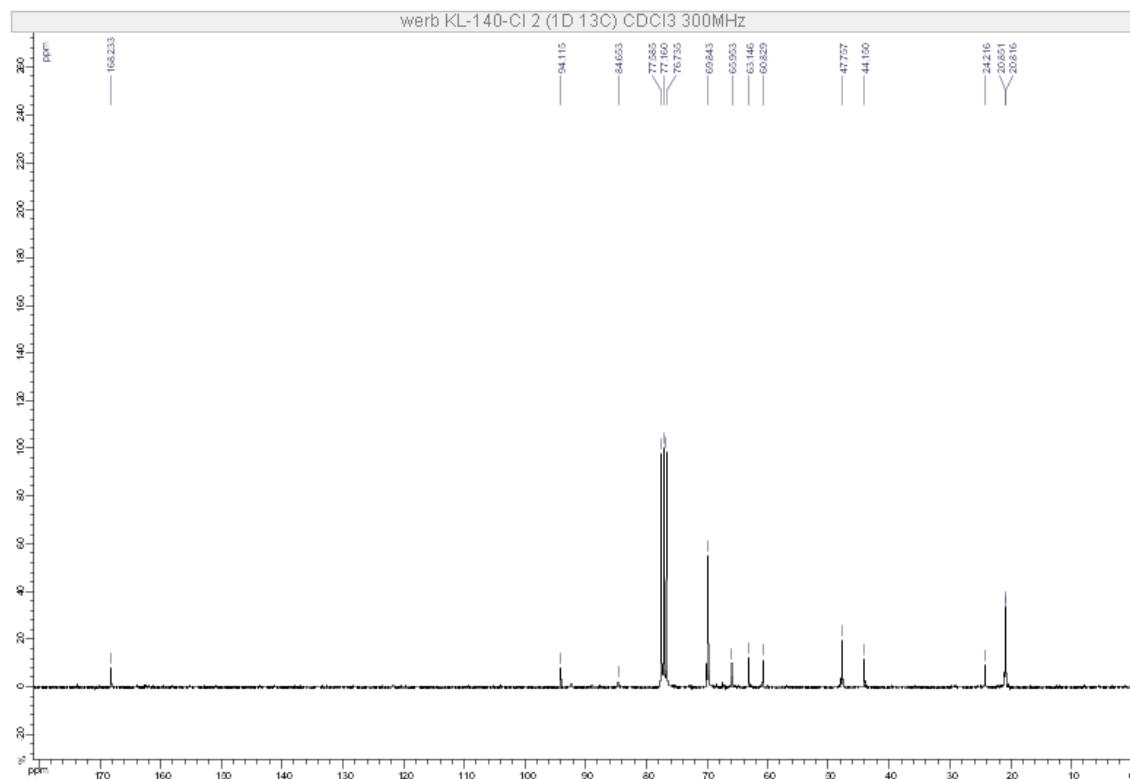


N-(3-(Diisopropylaminomethyl)ferrocenyl)acetamide (**4c**, racemic mixture)

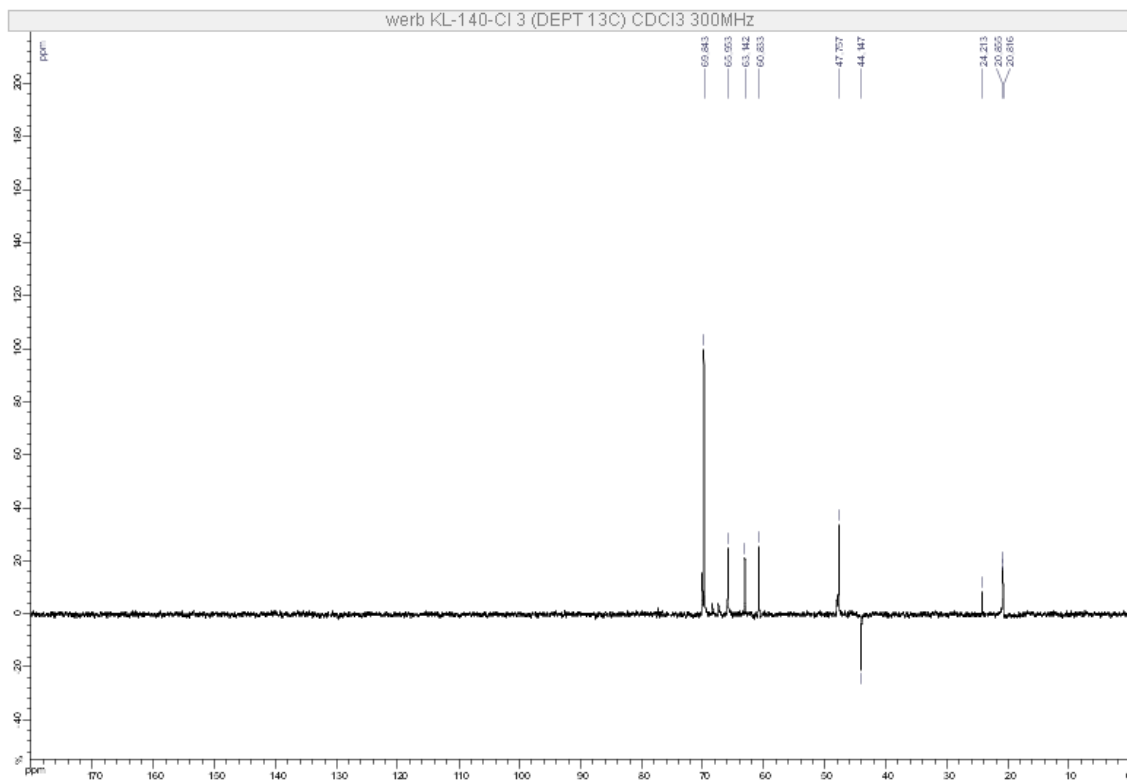
^1H NMR (300 MHz, CDCl_3)



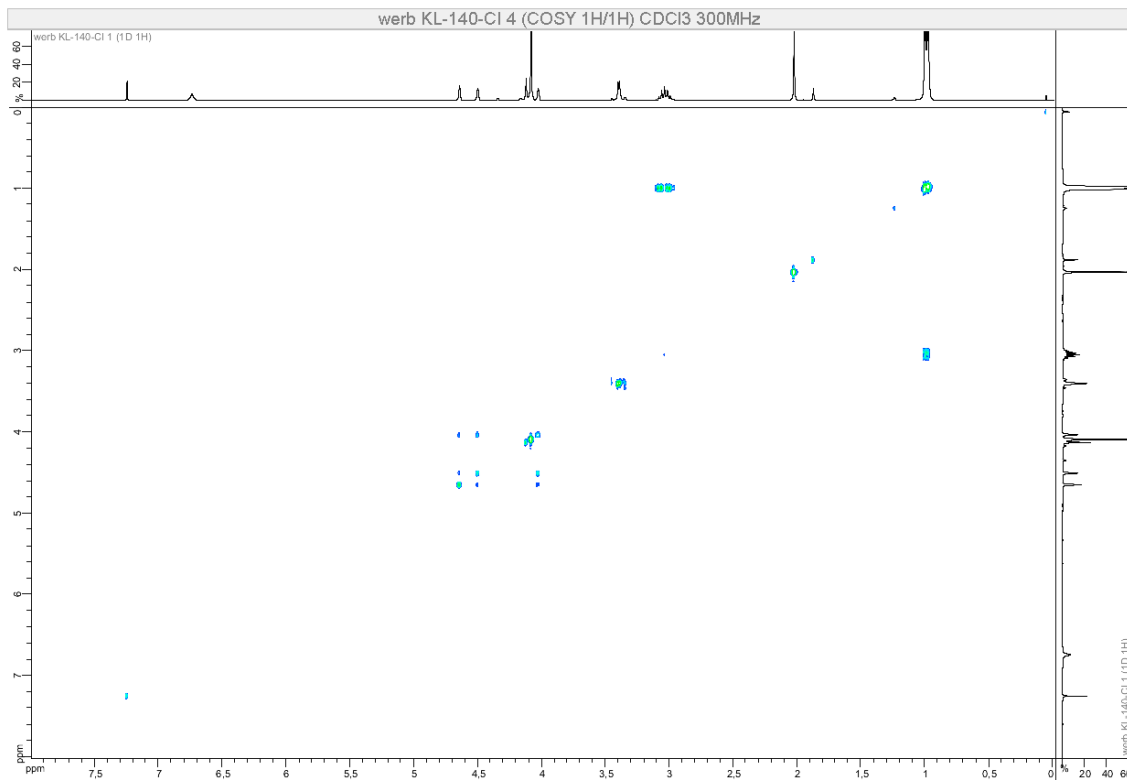
^{13}C NMR (75 MHz, CDCl_3)



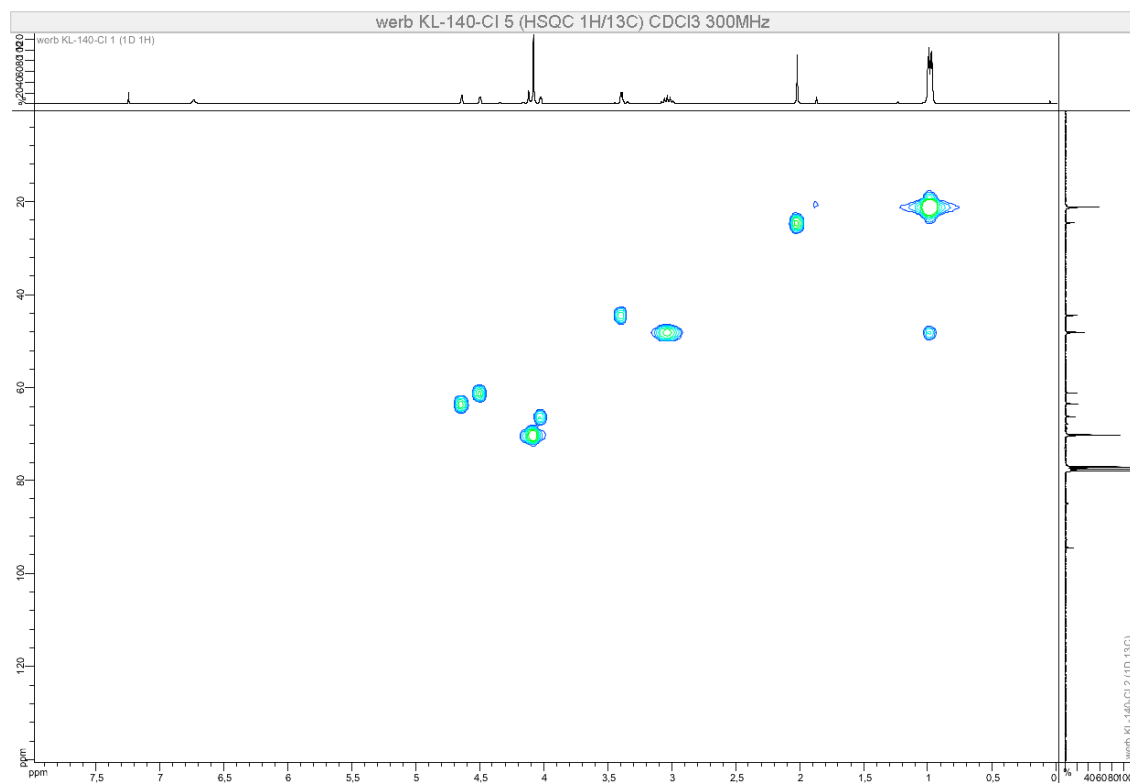
DEPT 135 (75 MHz, CDCl₃)



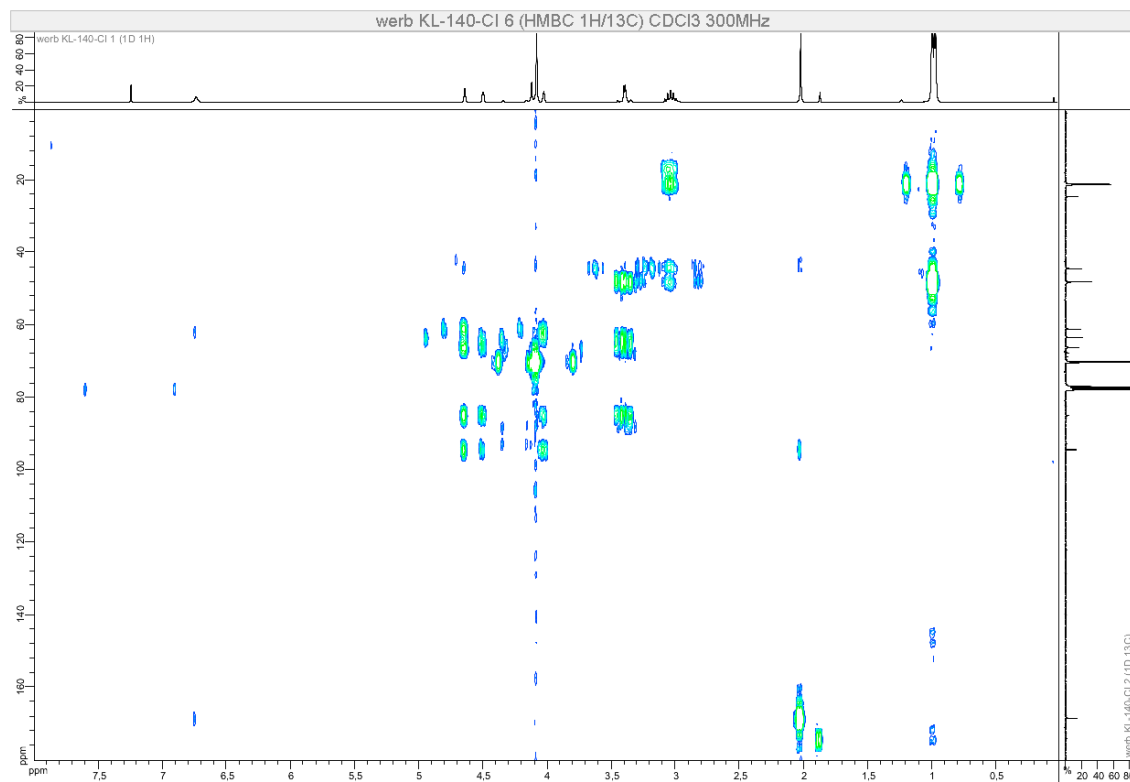
COSY (300 MHz, CDCl₃)



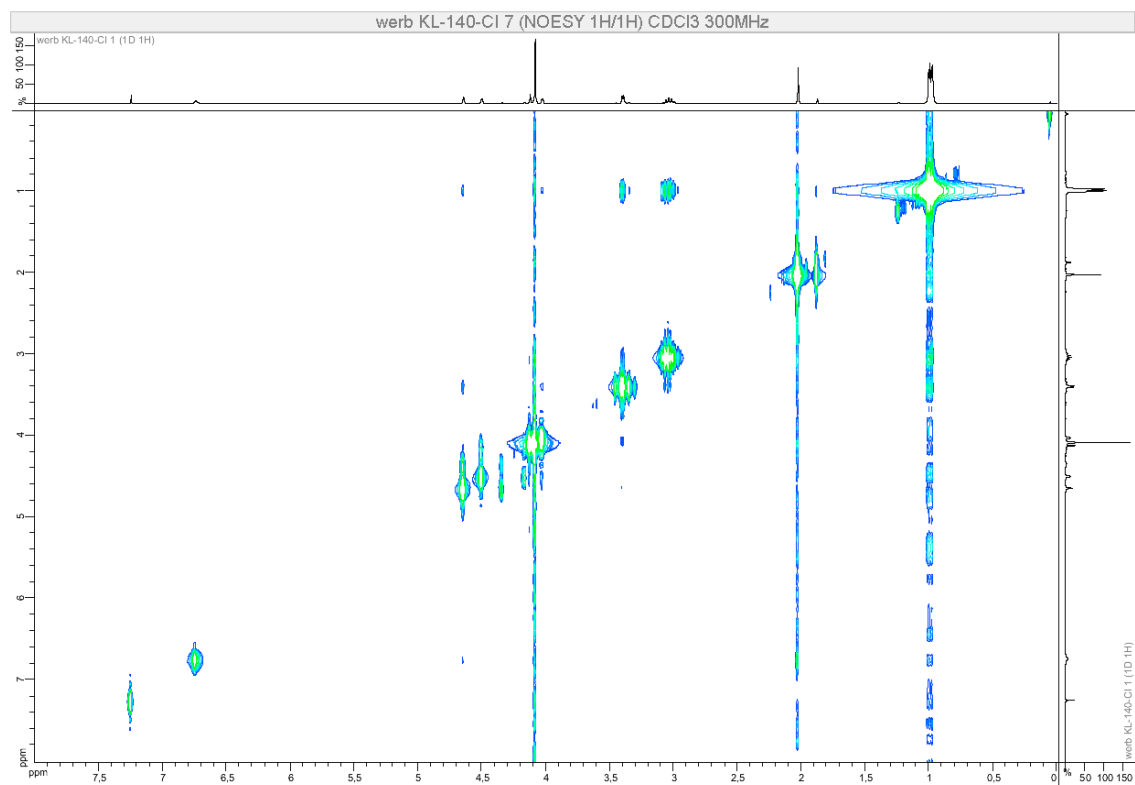
HSQC (300 MHz, CDCl₃)



HMBC (300 MHz, CDCl₃)

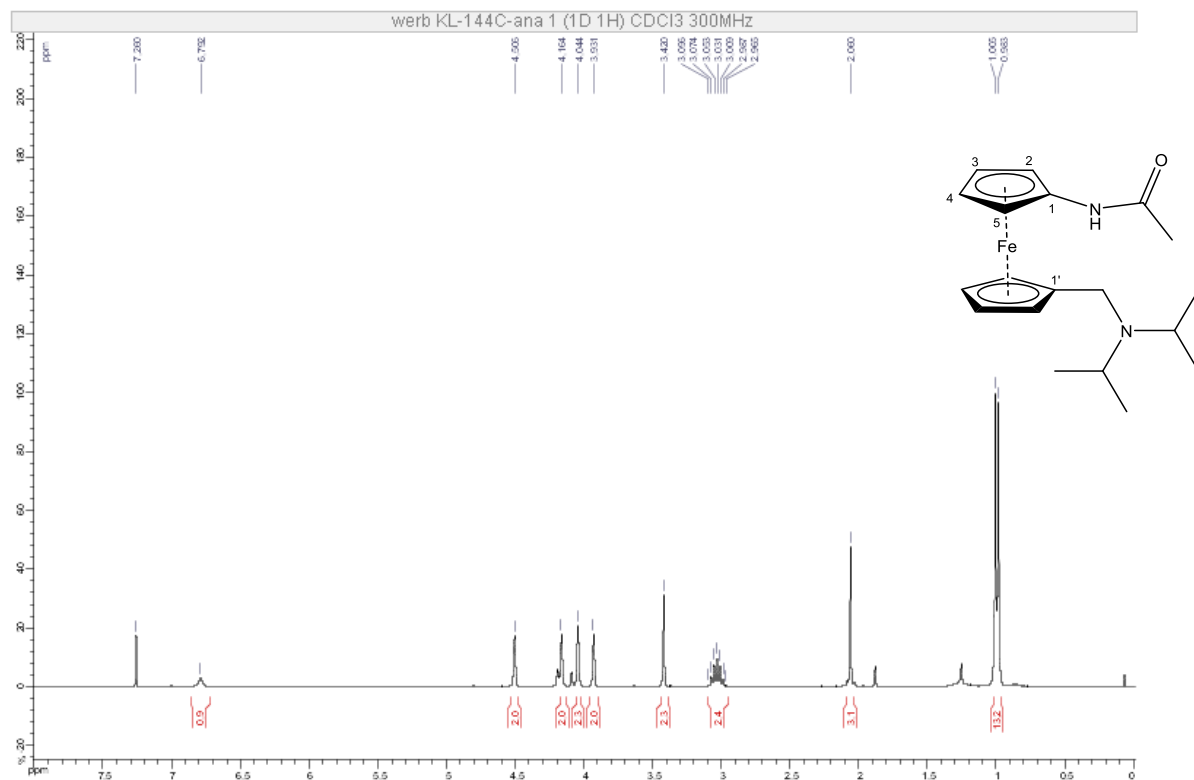


NOESY (300 MHz, CDCl₃)

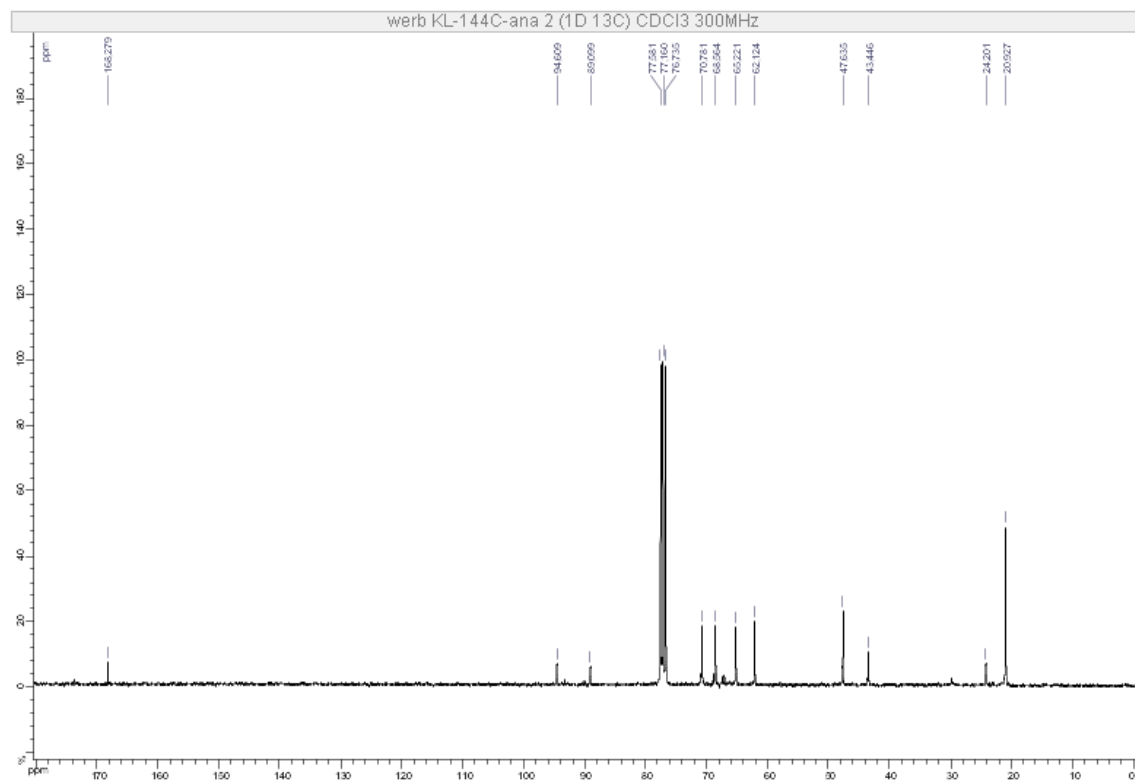


N-(1'-(Diisopropylaminomethyl)ferrocenyl)acetamide (6c)

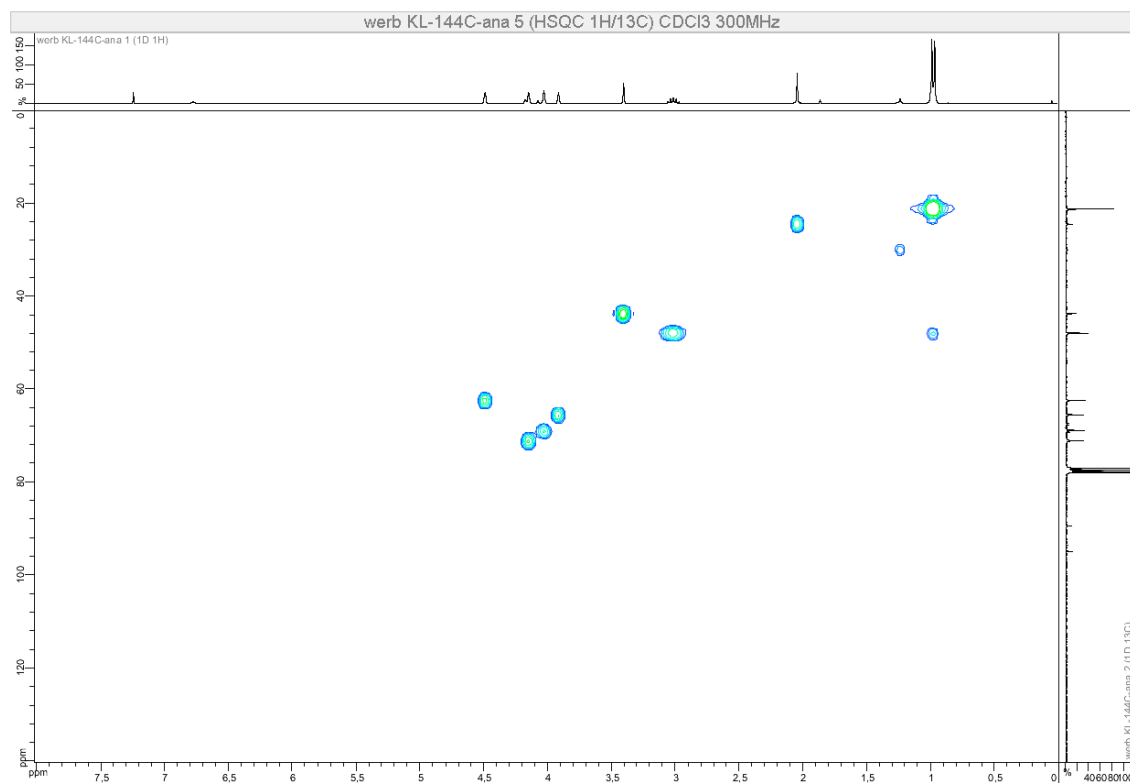
^1H NMR (300 MHz, CDCl_3)



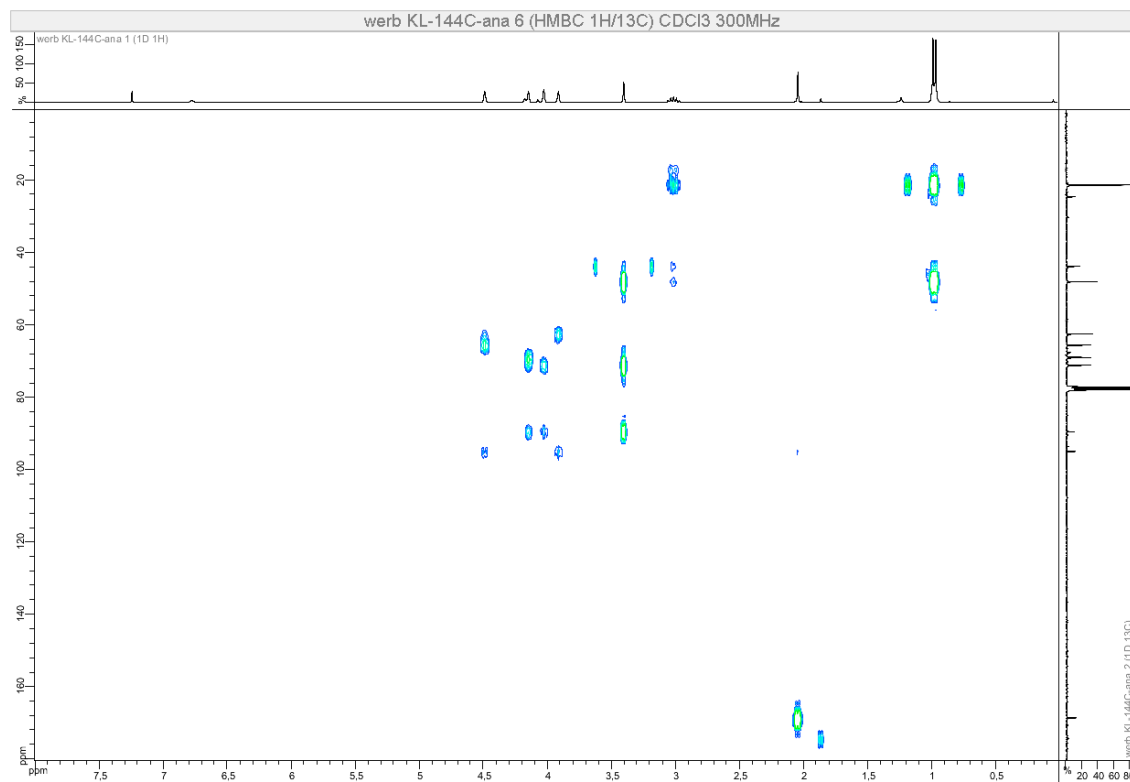
^{13}C NMR (75 MHz, CDCl_3)



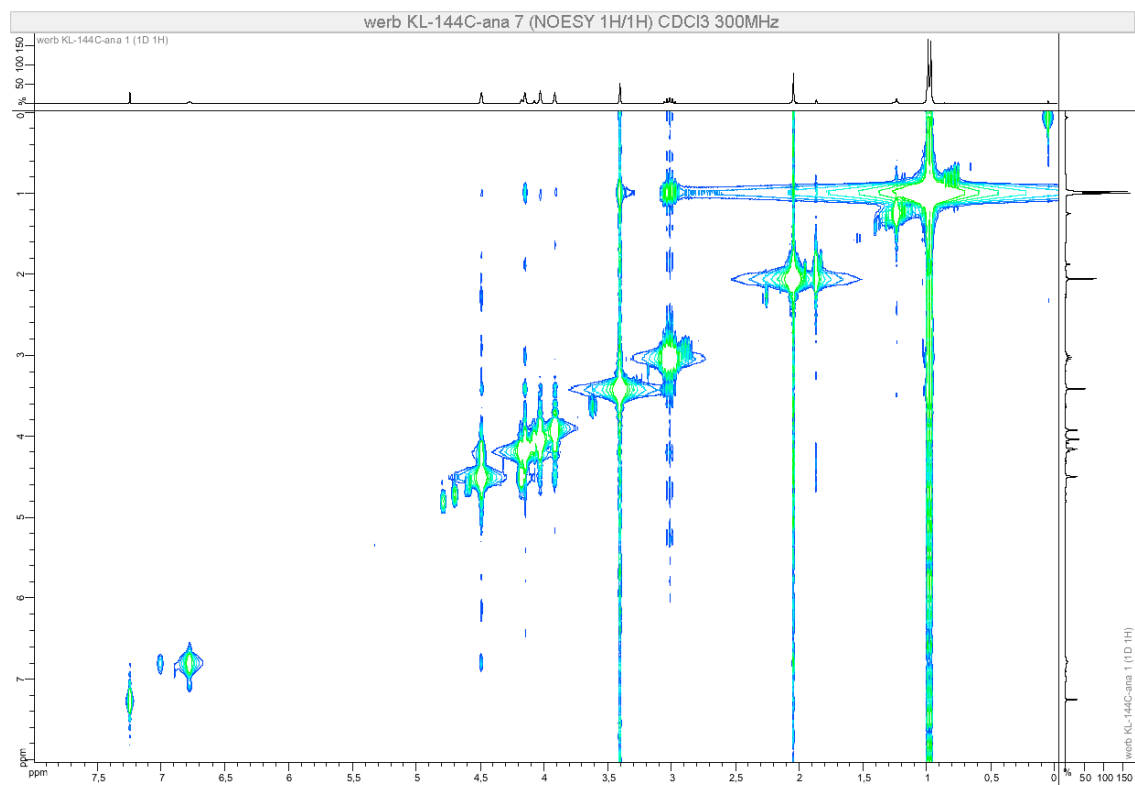
HSQC (300 MHz, CDCl₃)



HMBC (300 MHz, CDCl₃)

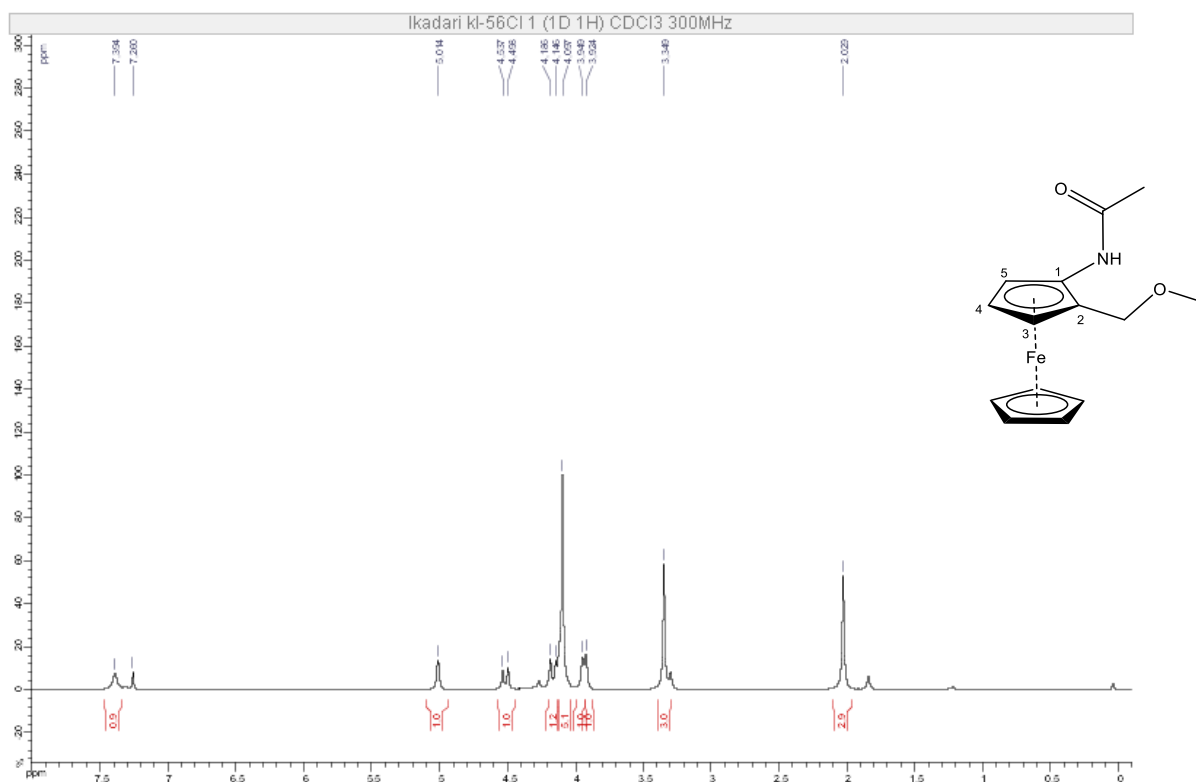


NOESY (300 MHz, CDCl₃)

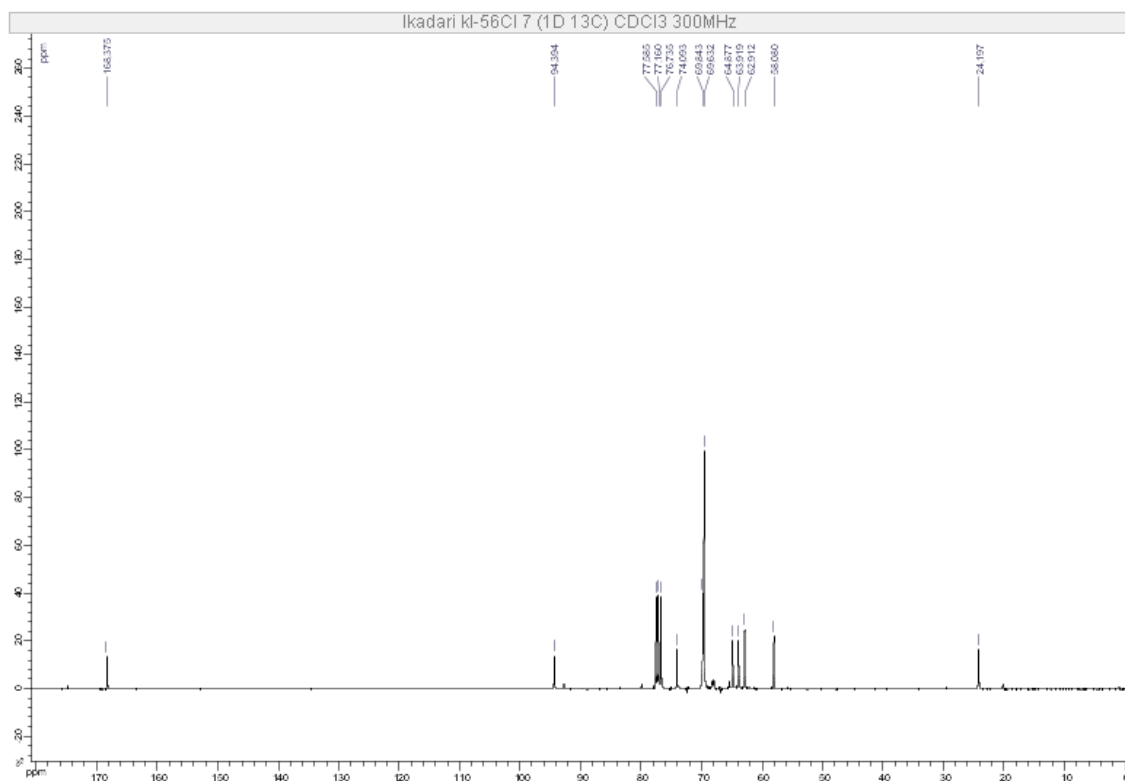


N-(2-(Methoxymethyl)ferrocenyl)acetamide (**2d**, racemic mixture)

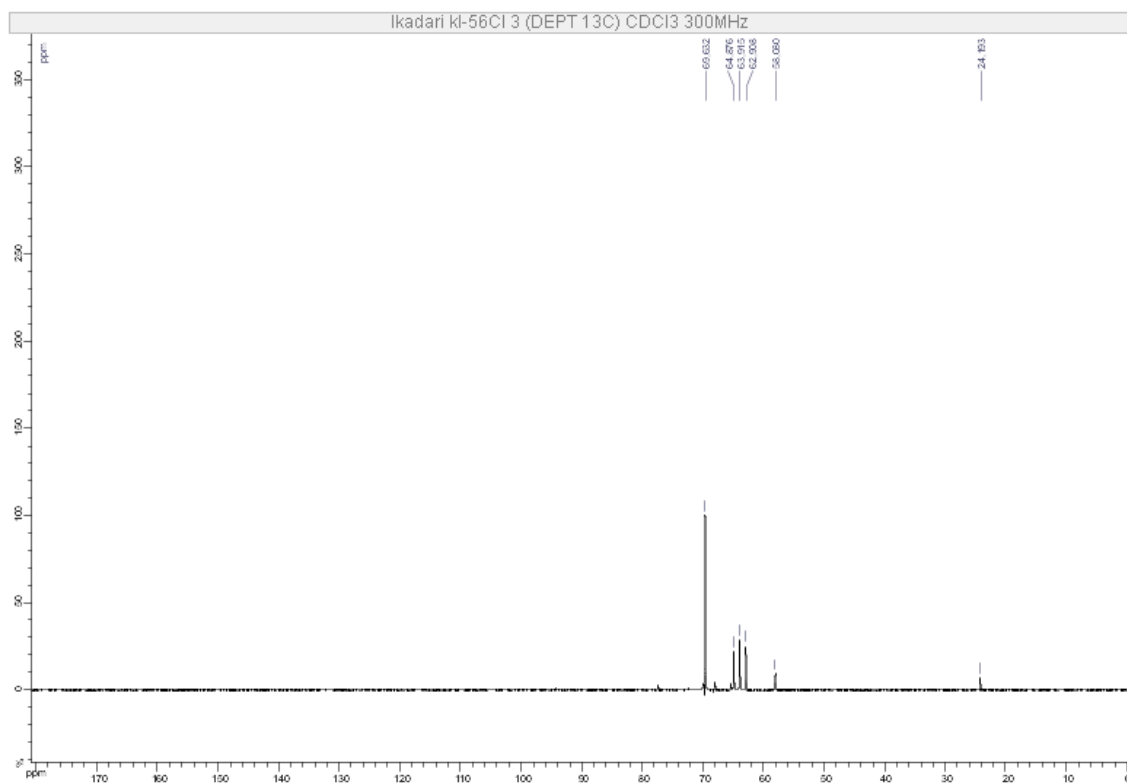
^1H NMR (300 MHz, CDCl_3)



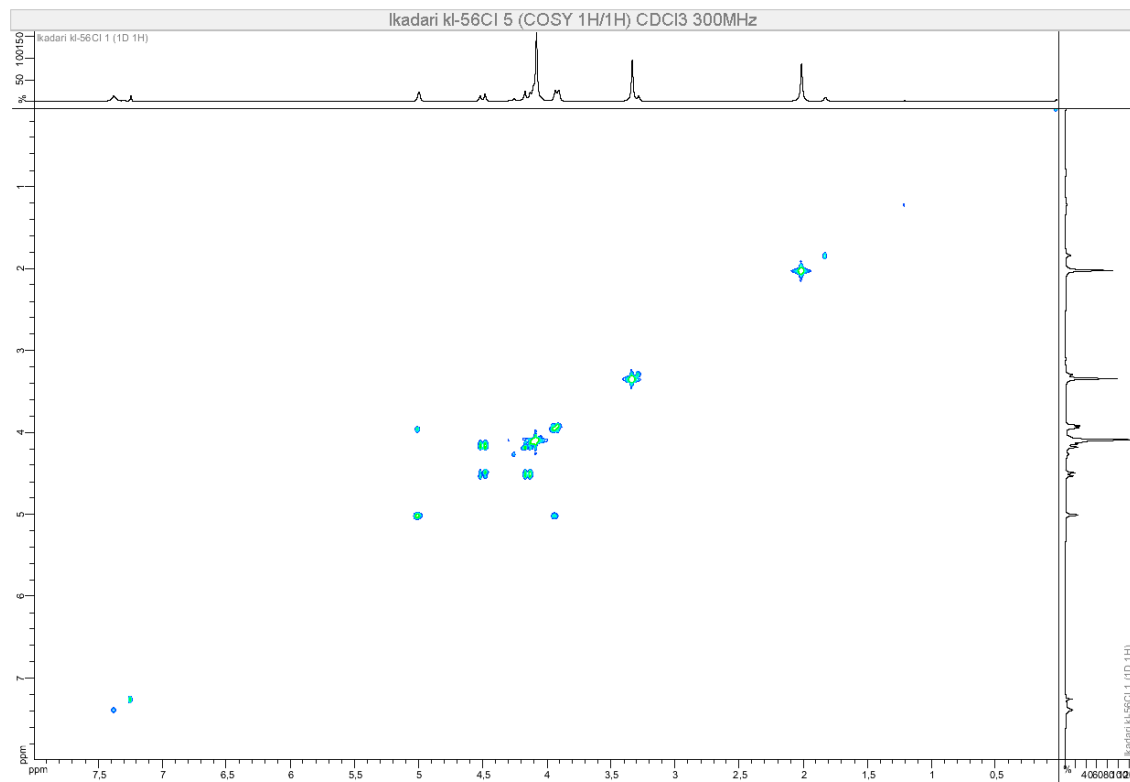
^{13}C NMR (75 MHz, CDCl_3)



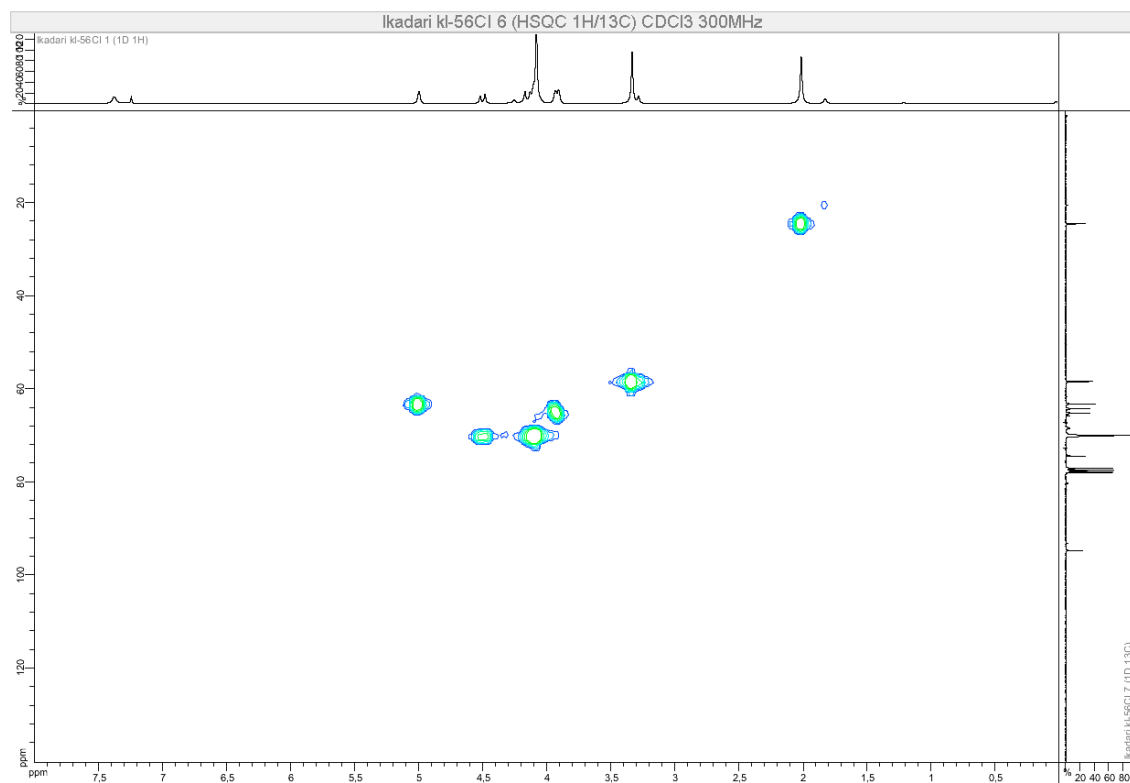
DEPT 135 (75 MHz, CDCl₃)



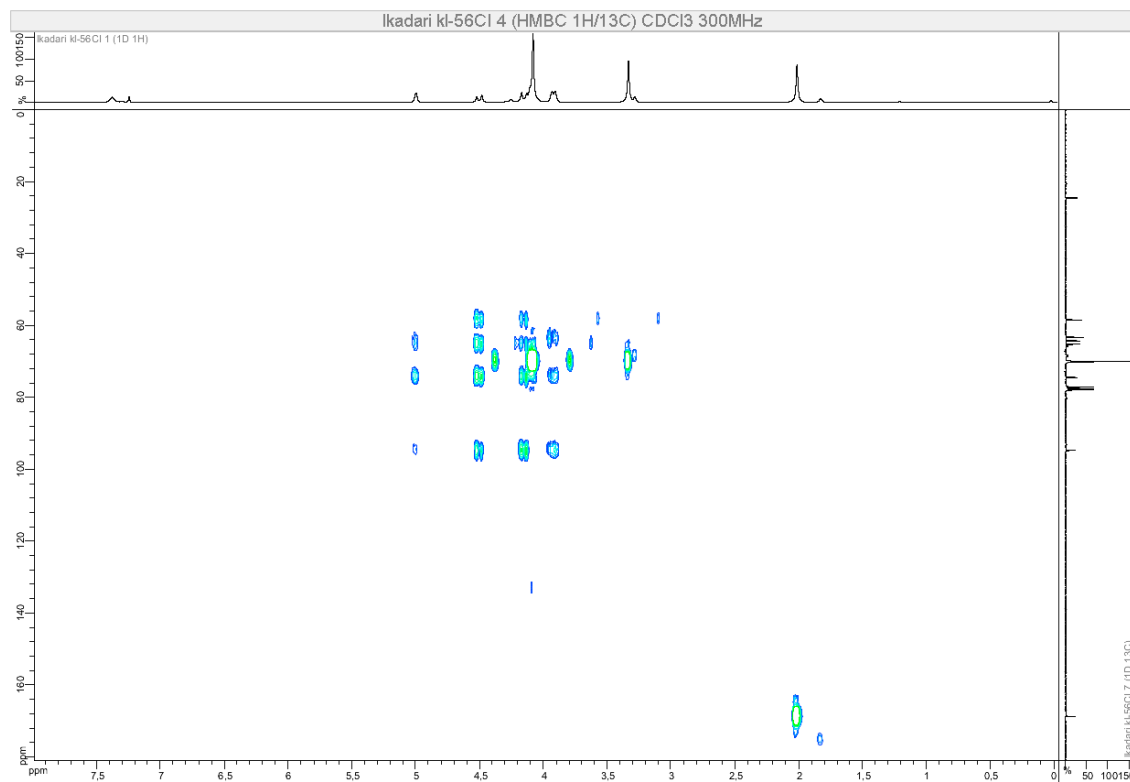
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

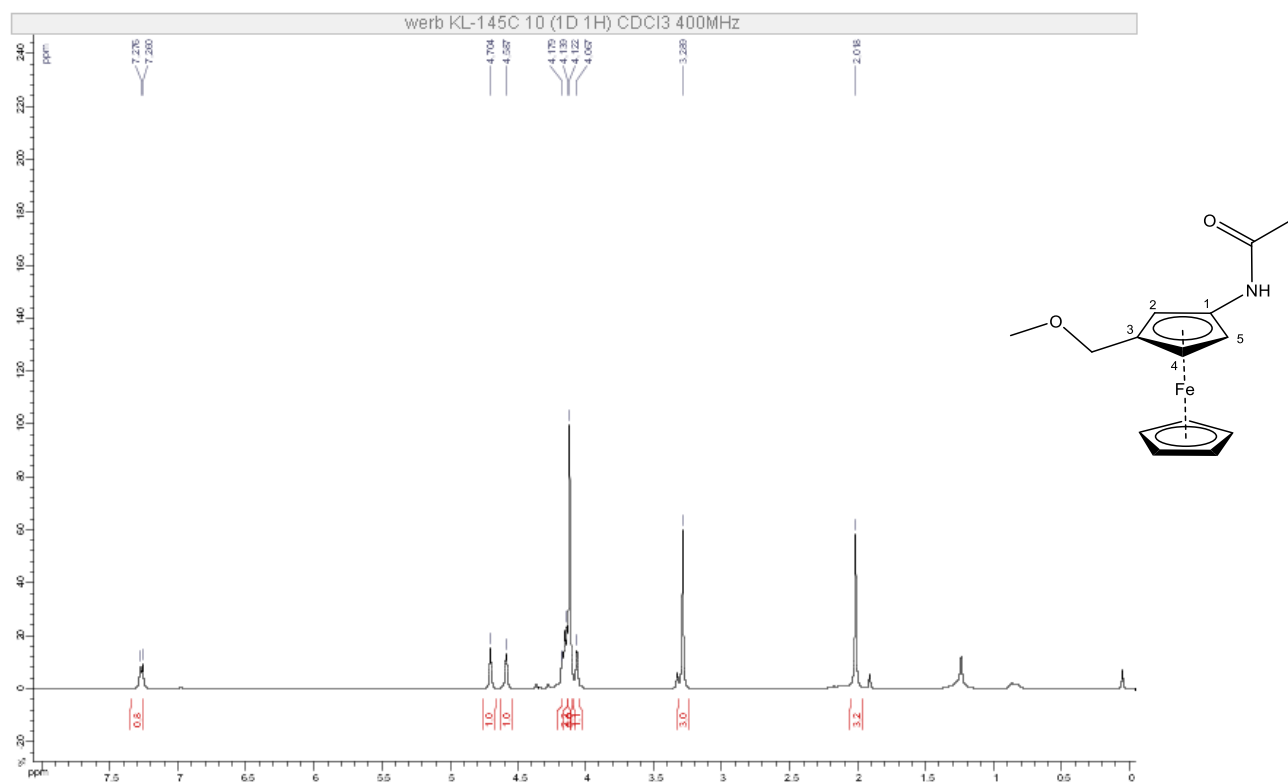


HMBC (300 MHz, CDCl₃)

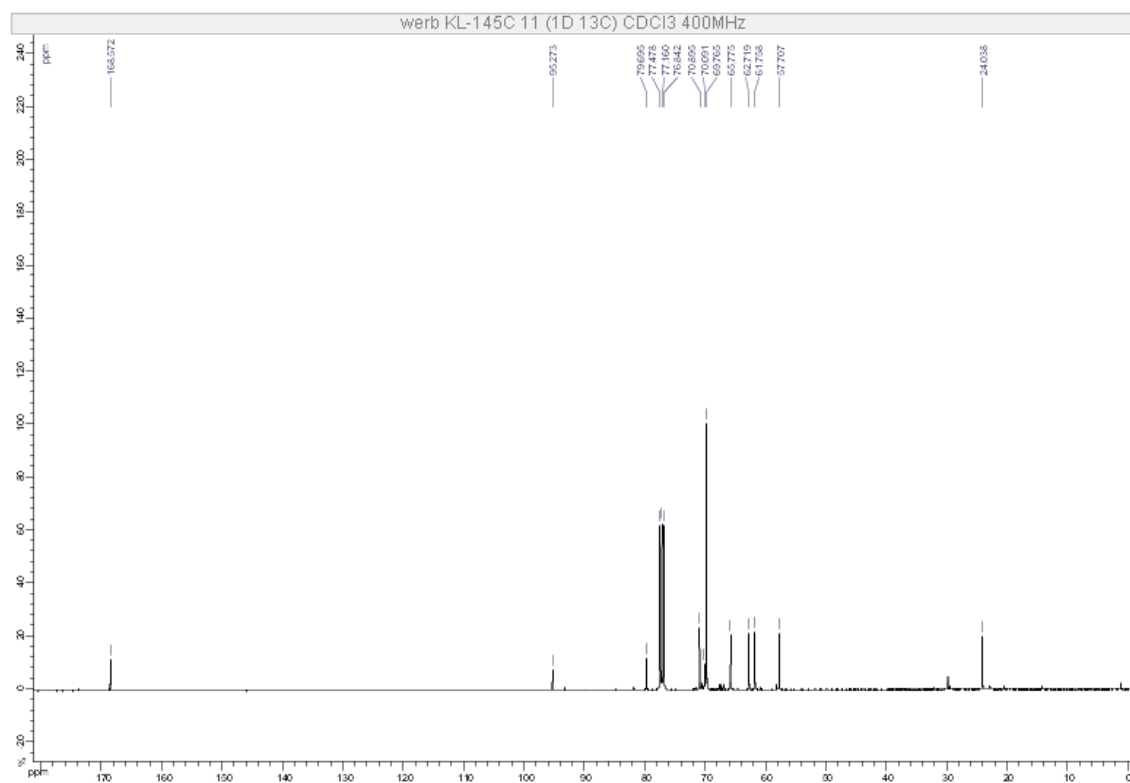


N-(3-(Methoxymethyl)ferrocenyl)acetamide (**4d**, racemic mixture)

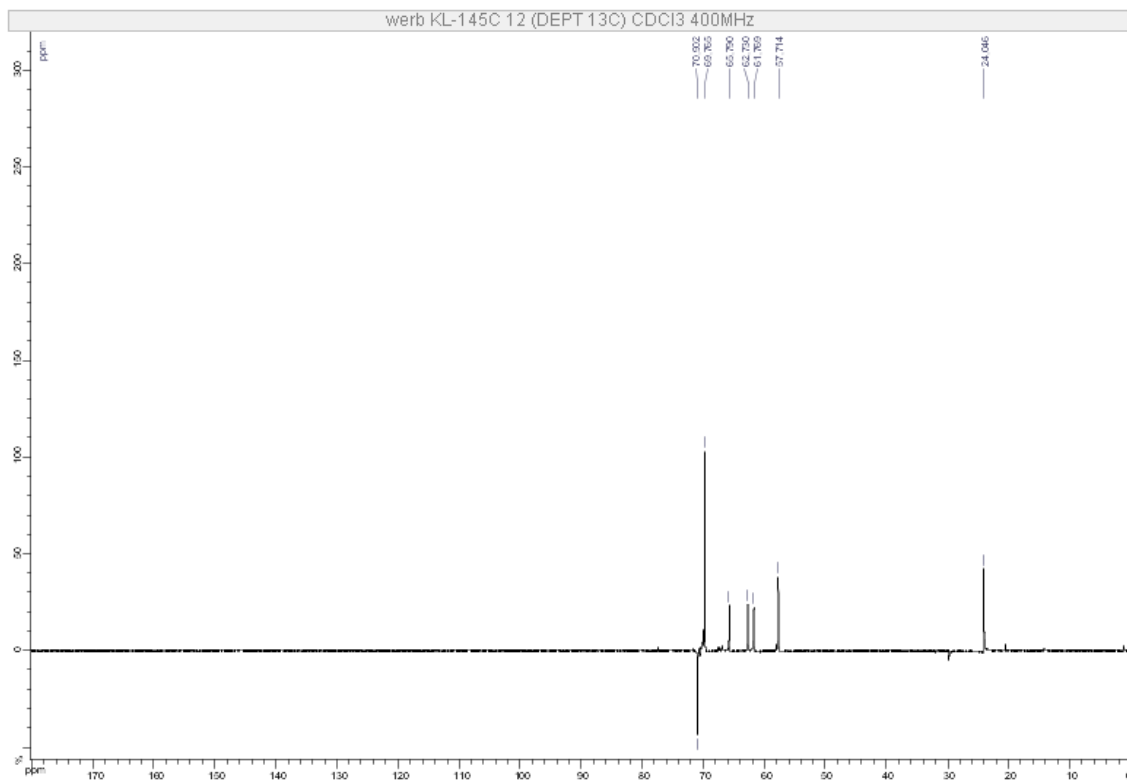
^1H NMR (400 MHz, CDCl_3)



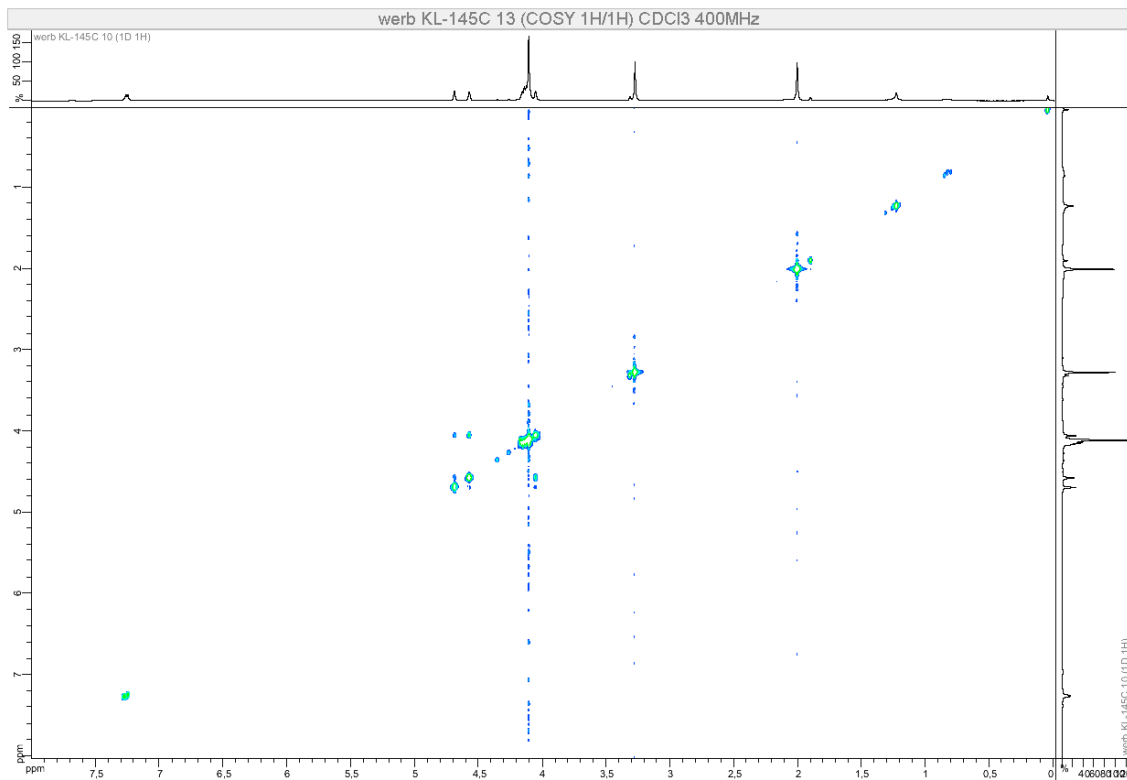
^{13}C NMR (100 MHz, CDCl_3)



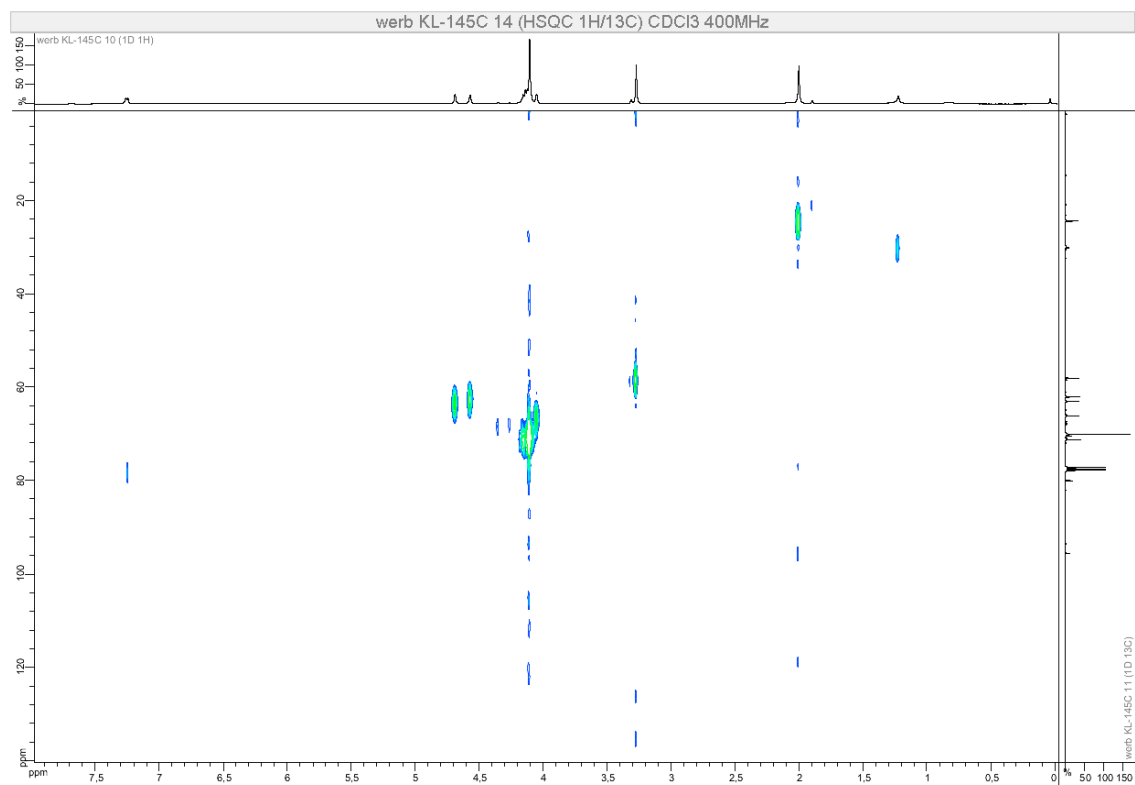
DEPT 135 (100 MHz, CDCl₃)



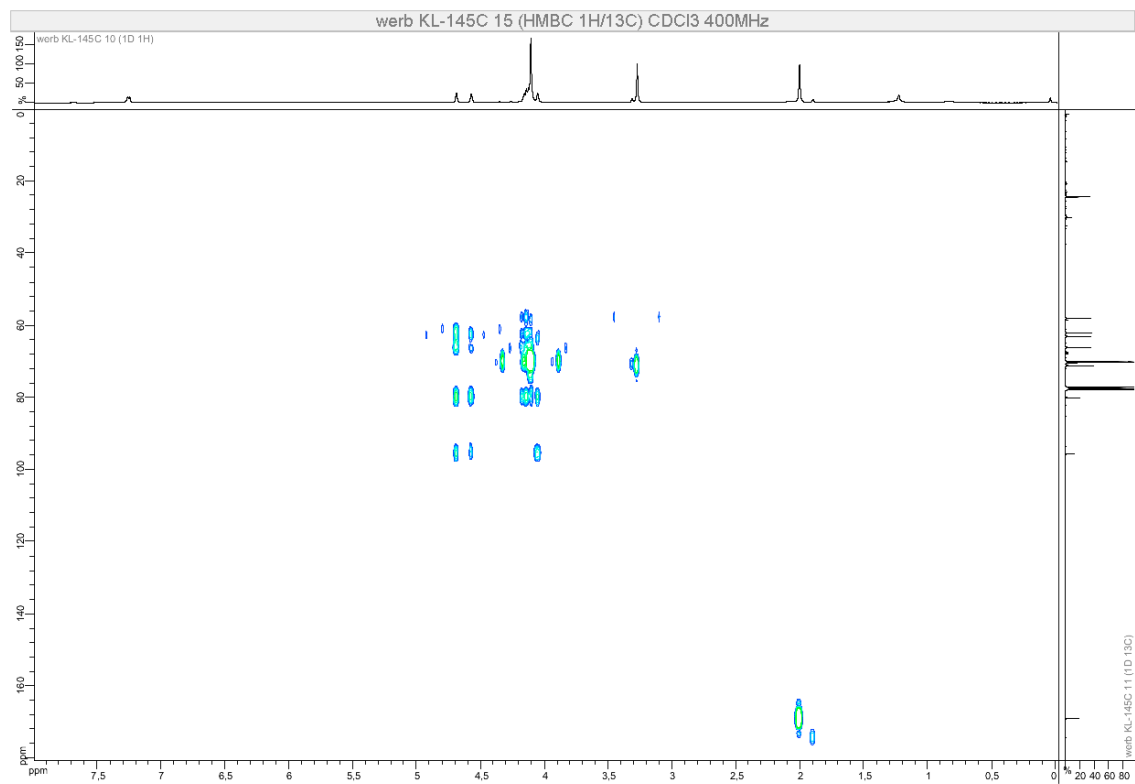
COSY (400 MHz, CDCl₃)



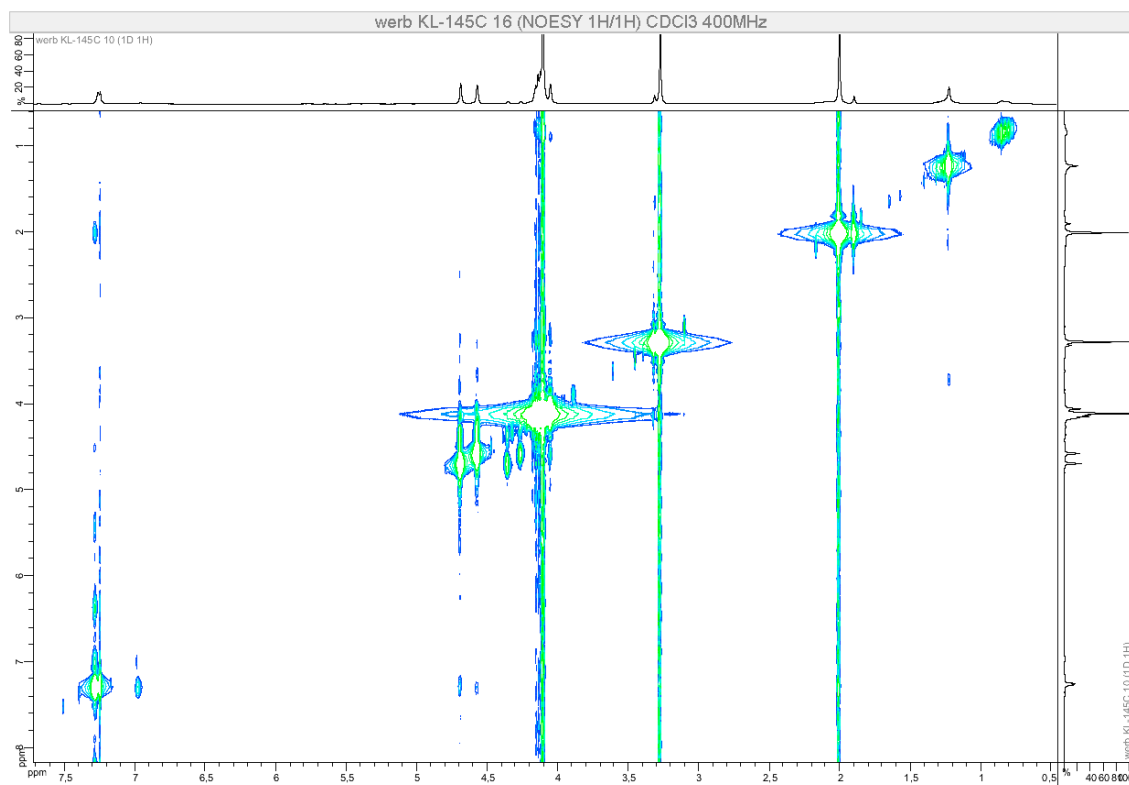
HSQC (400 MHz, CDCl₃)



HMBC (400 MHz, CDCl₃)

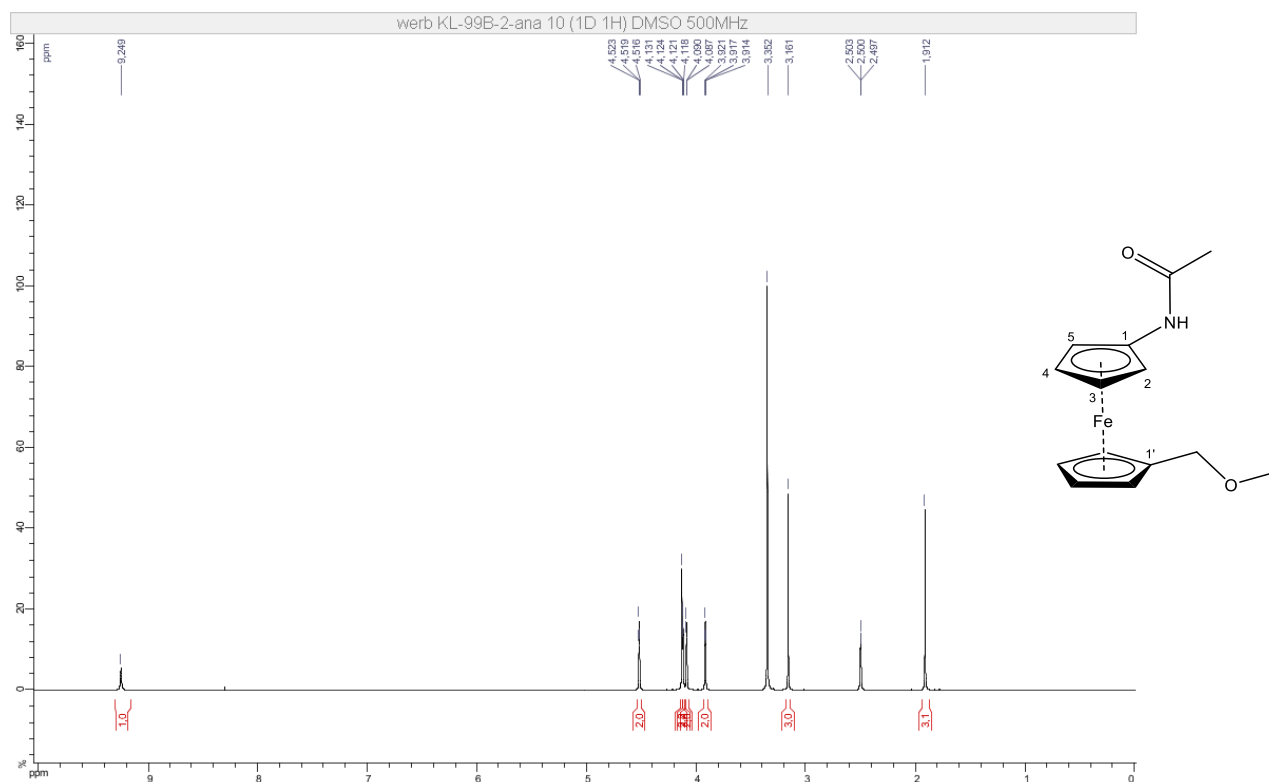


NOESY (400 MHz, CDCl₃)

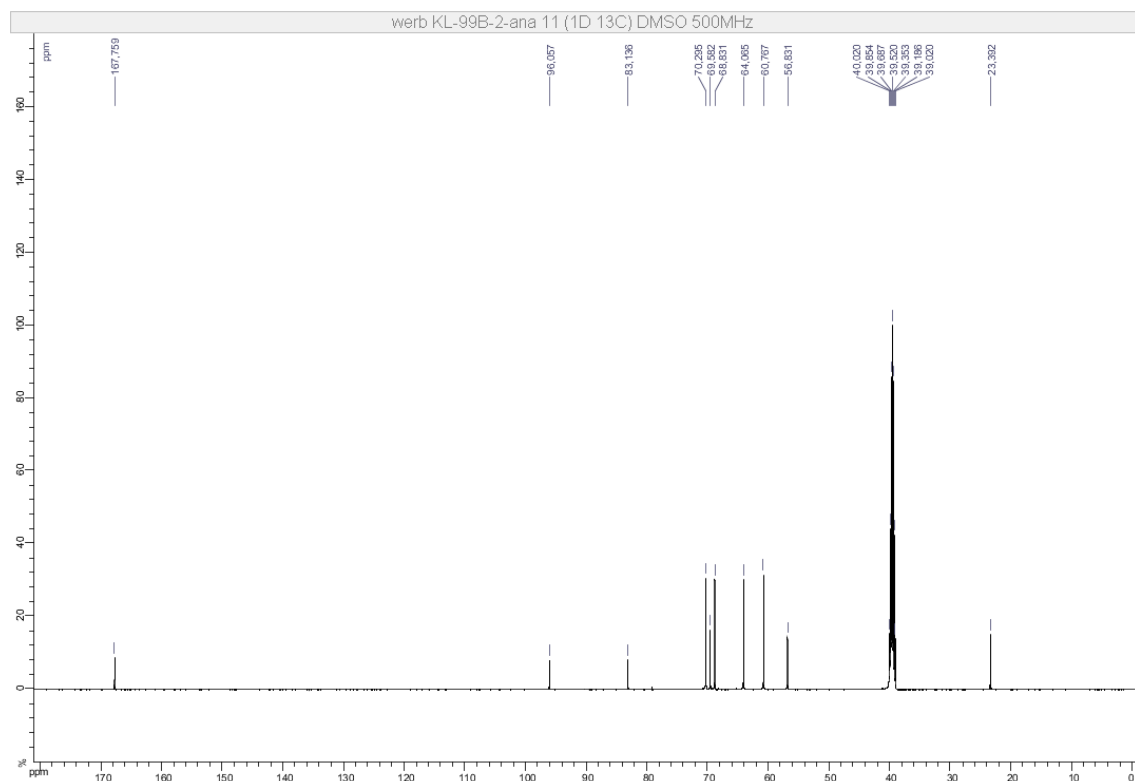


N-(1'-Methoxymethylferrocenyl)acetamide (6d)

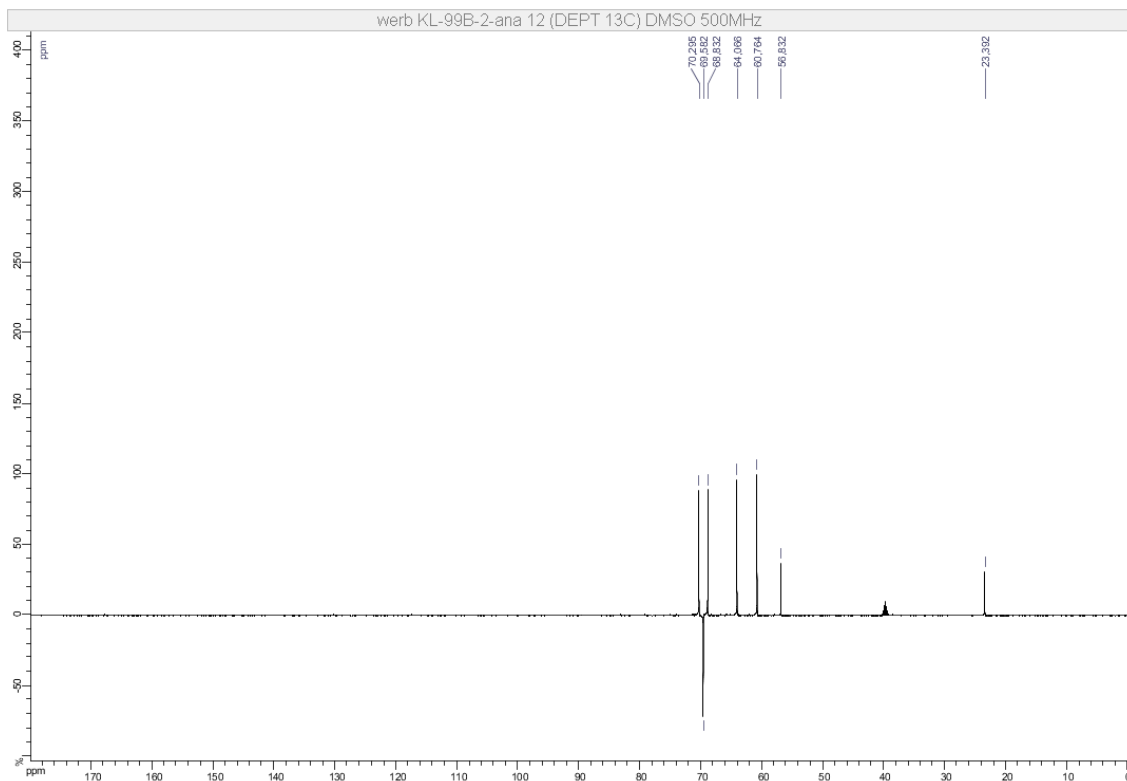
¹H NMR (500 MHz, (CD₃)₂SO)



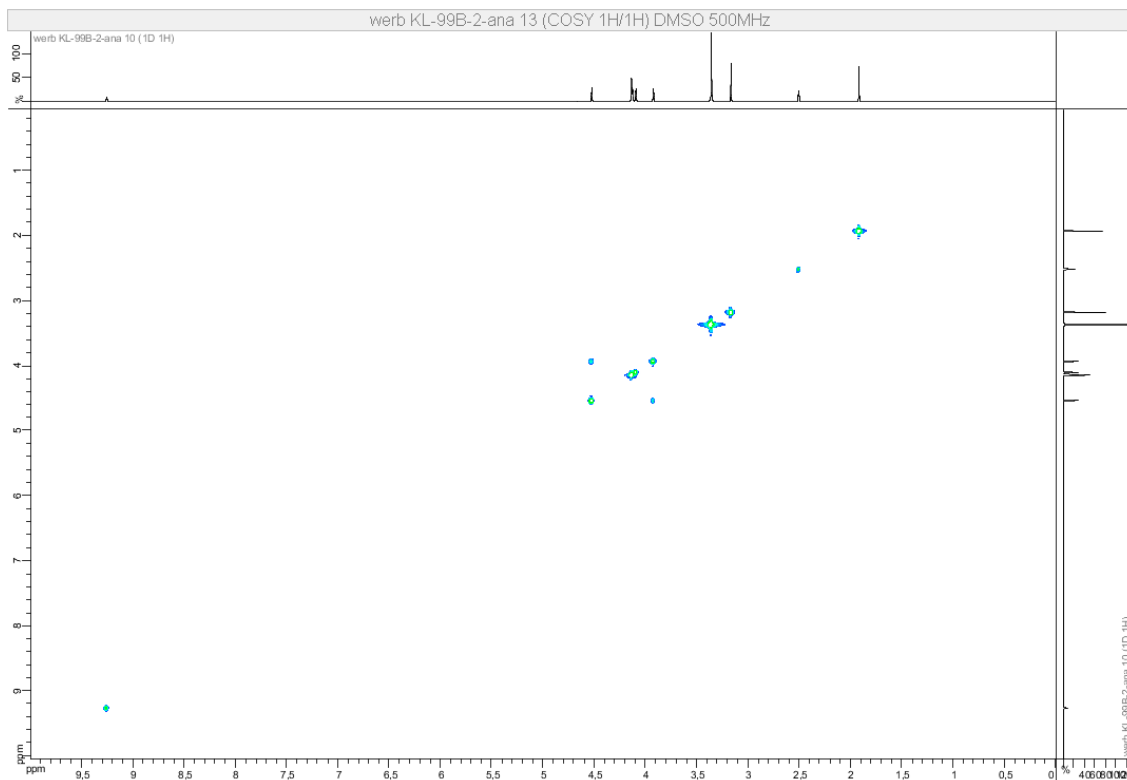
¹³C NMR (126 MHz, (CD₃)₂SO)



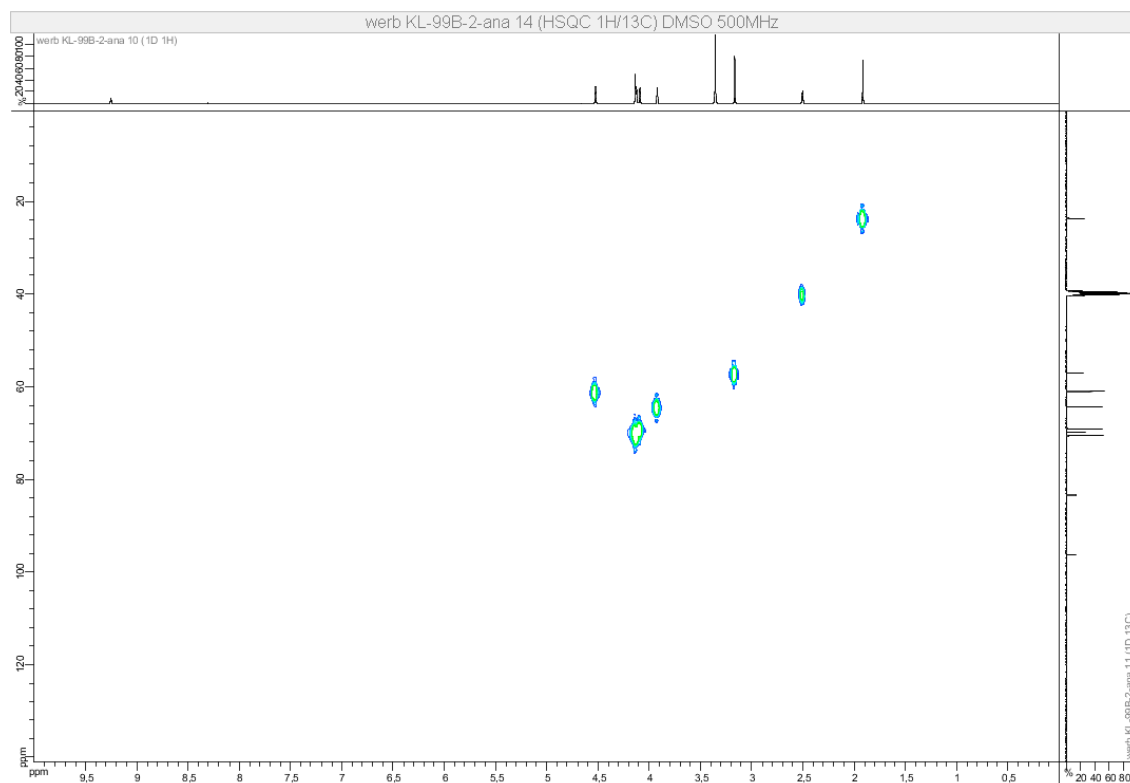
DEPT 135 (126 MHz, (CD₃)₂SO)



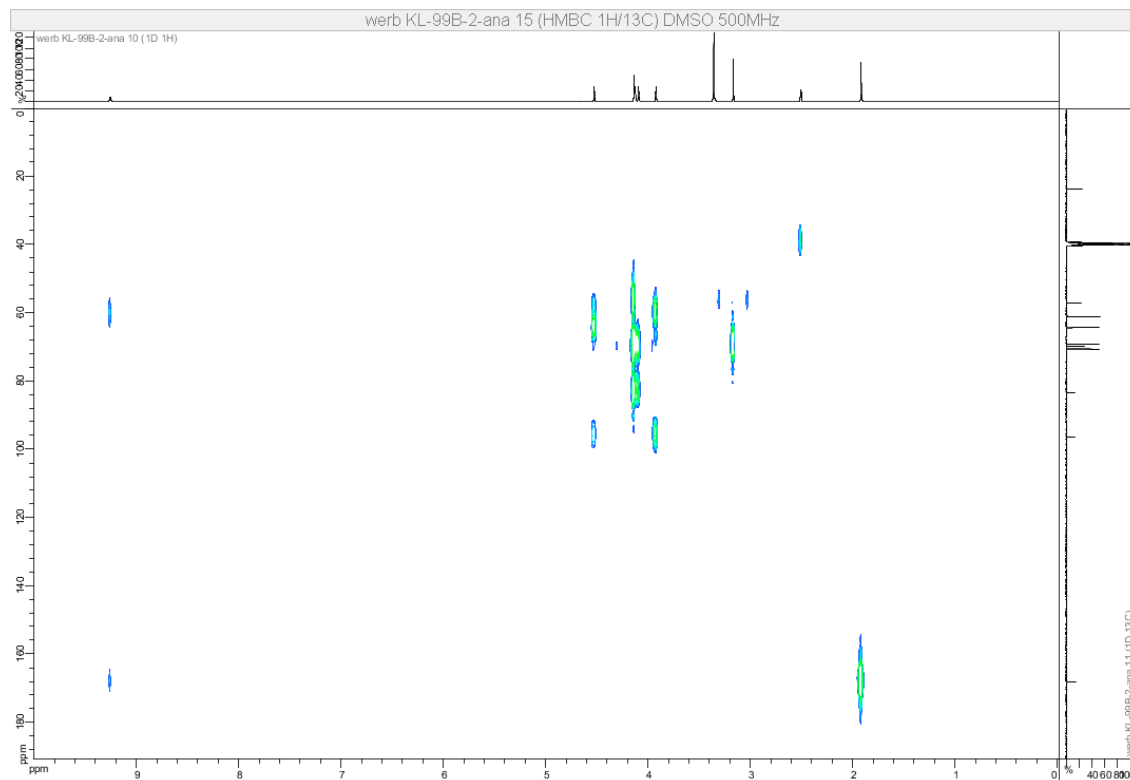
COSY (500 MHz, (CD₃)₂SO)



HSQC (500 MHz, (CD₃)₂SO)

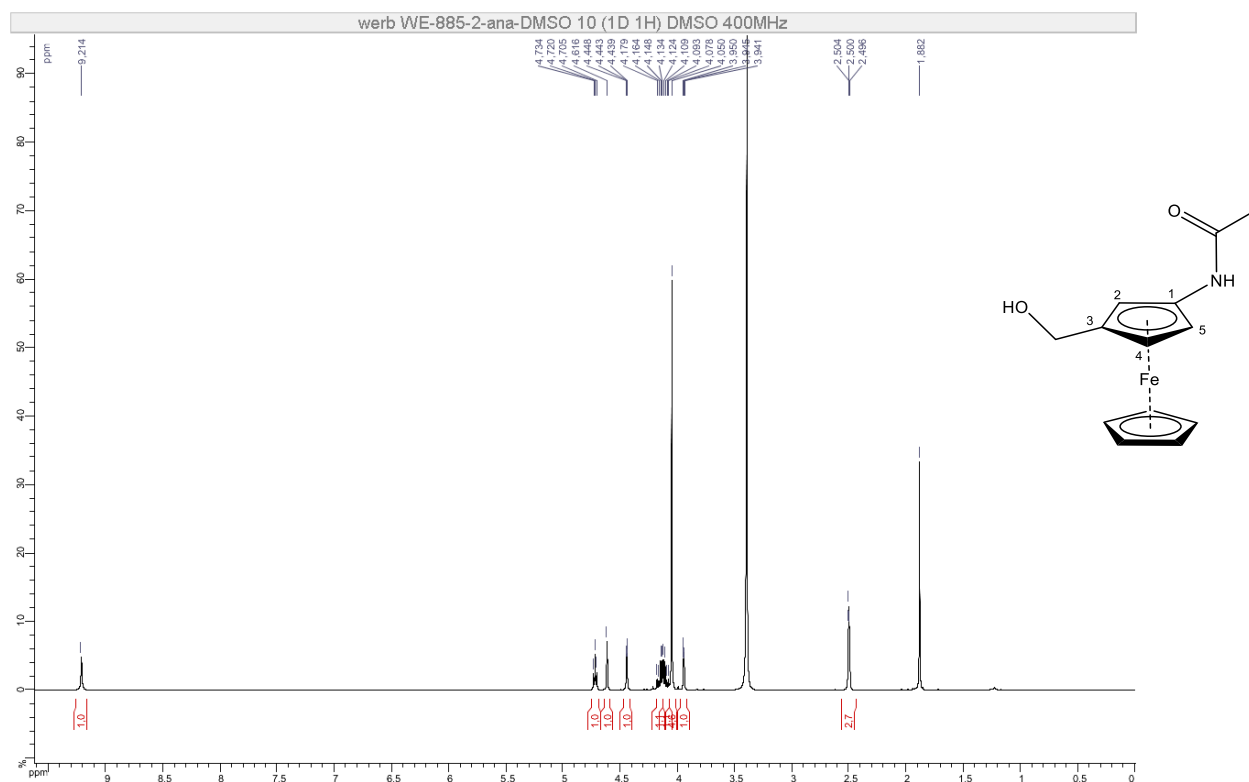


HMBC (500 MHz, (CD₃)₂SO)

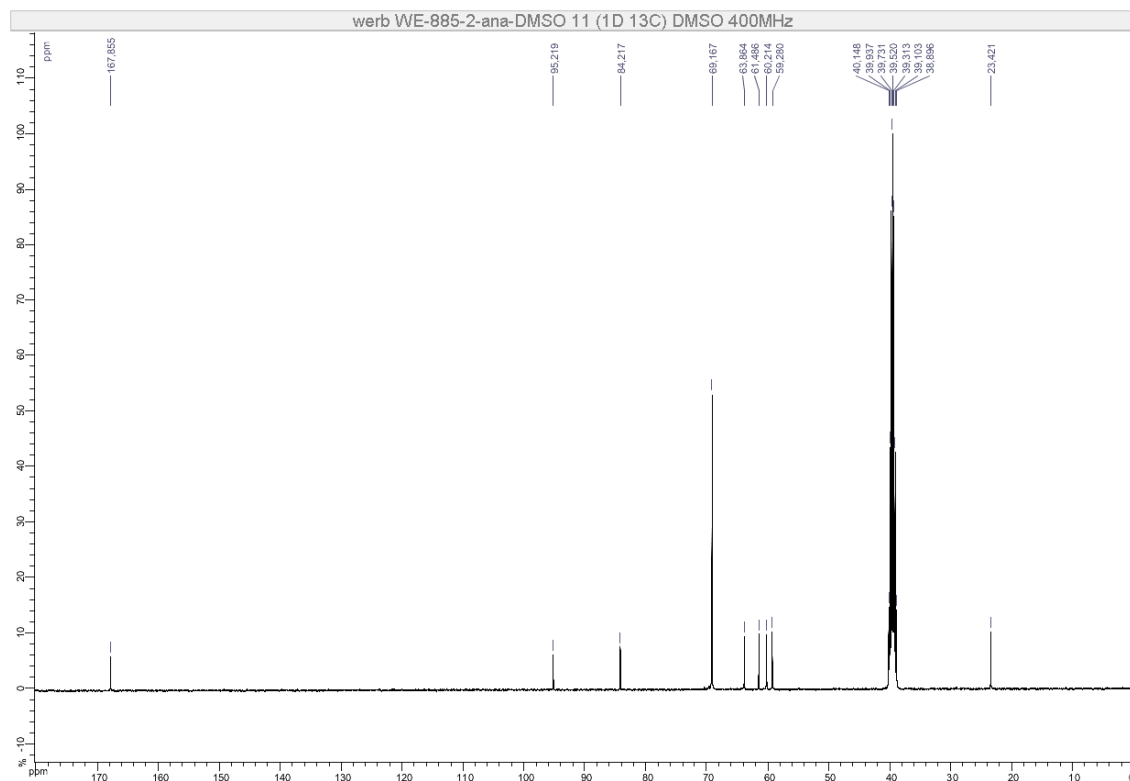


N-(3-(Hydroxymethyl)ferrocenyl)acetamide (**4e**, racemic mixture)

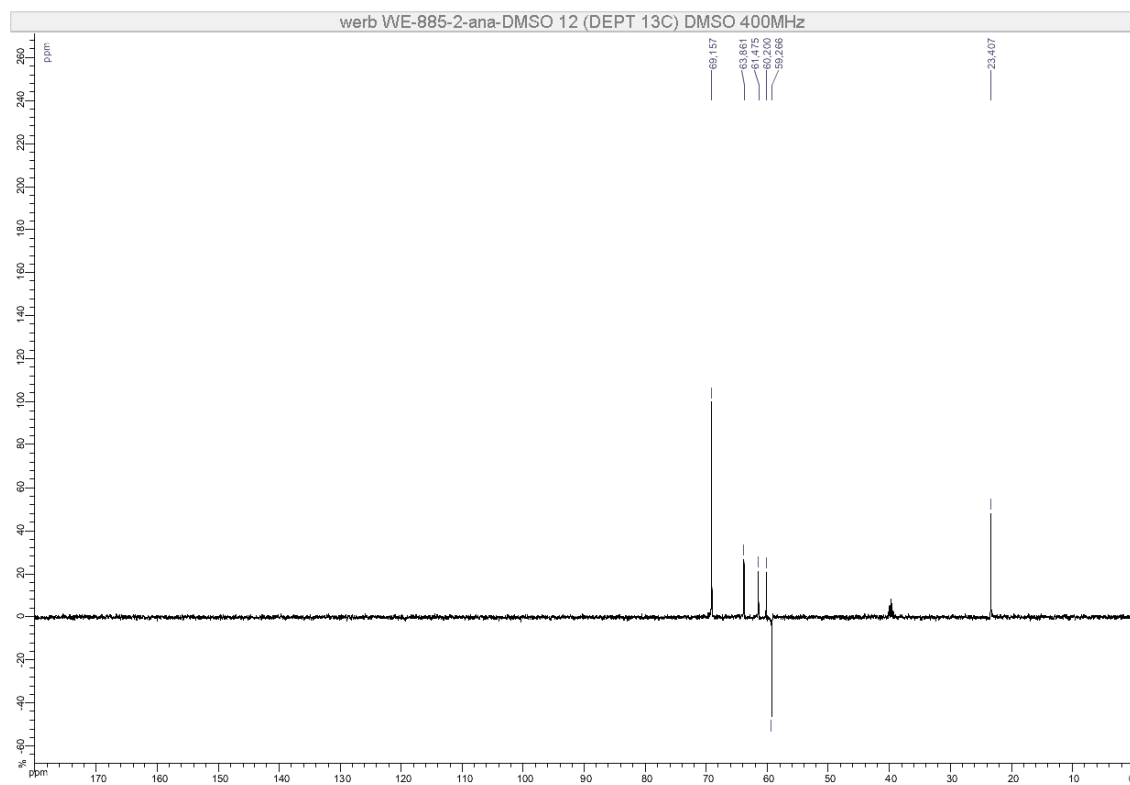
^1H NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$)



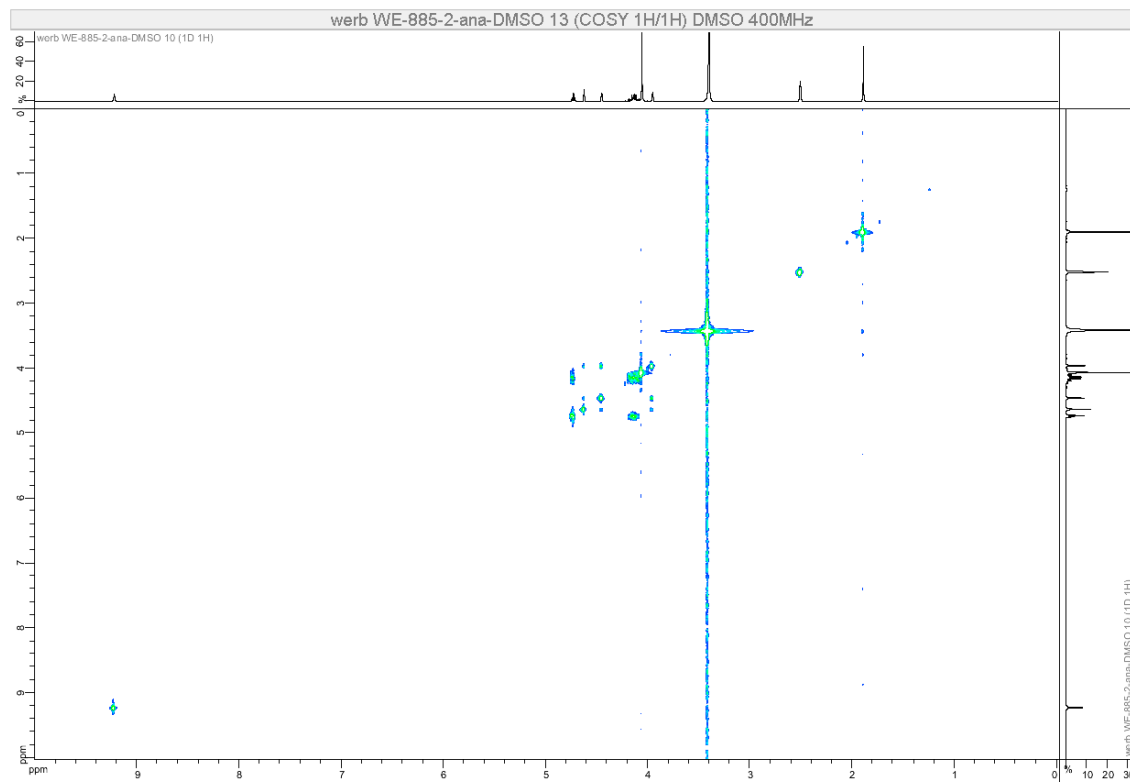
^{13}C NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$)



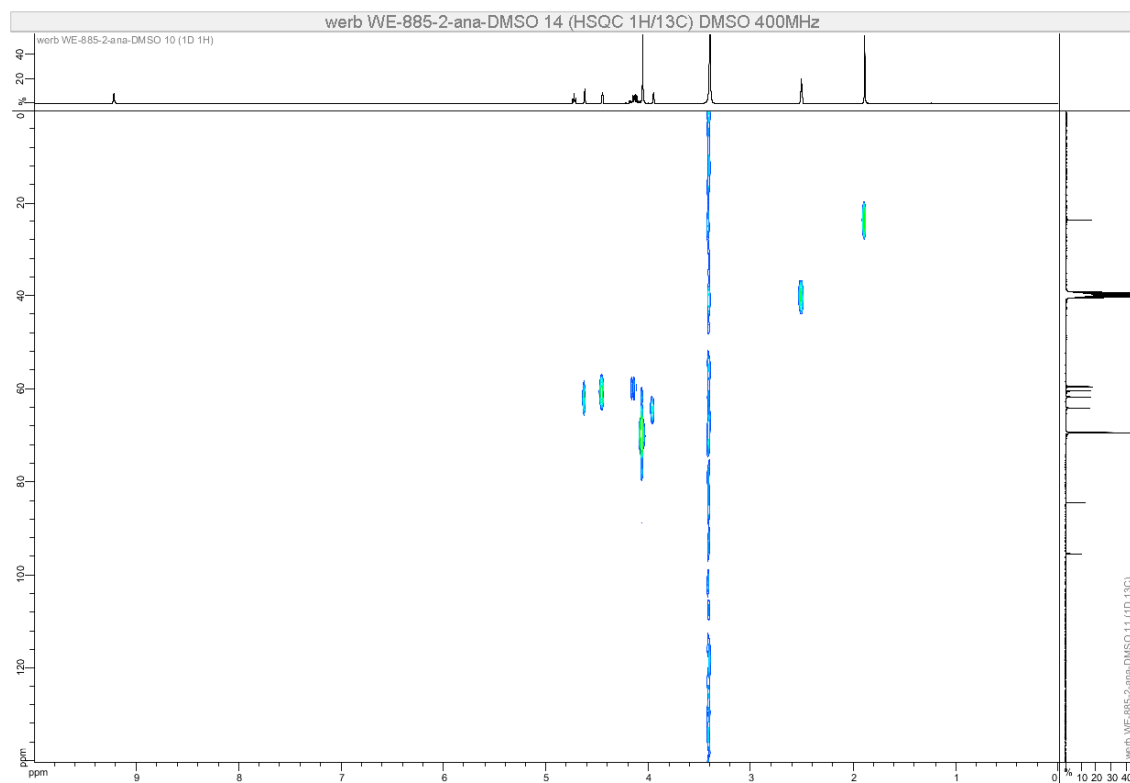
DEPT 135 (100 MHz, (CD₃)₂SO)



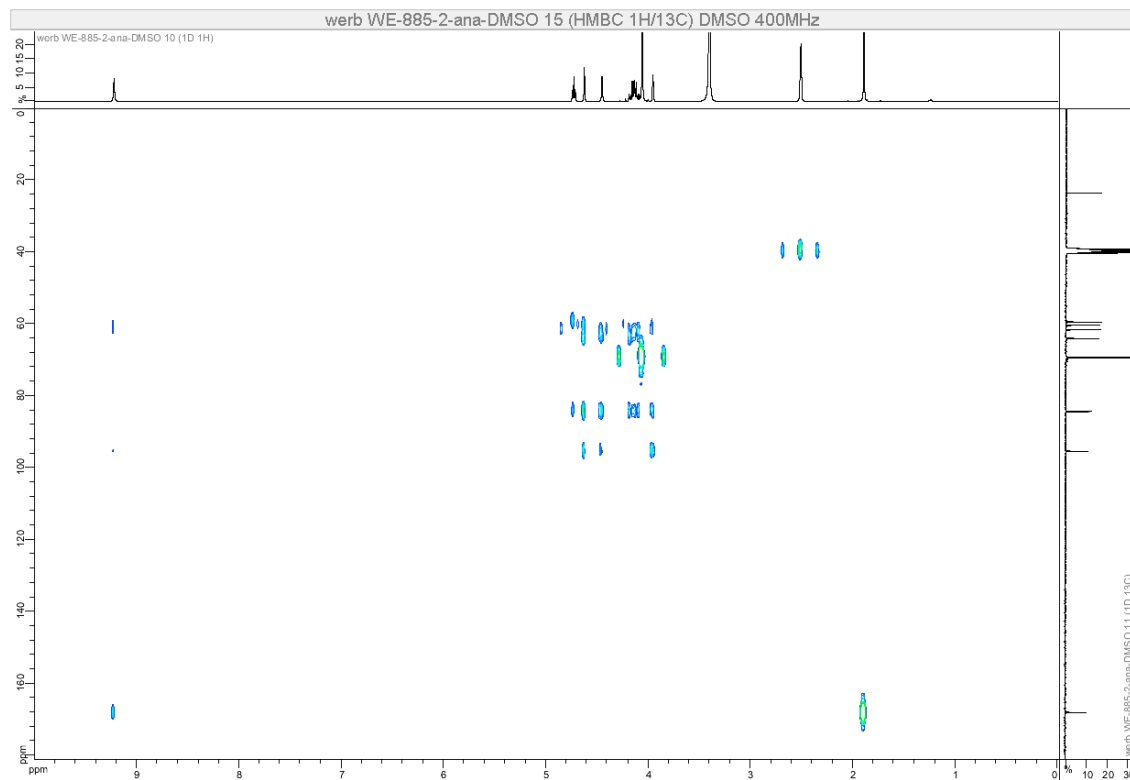
COSY (400 MHz, (CD₃)₂SO)



HSQC (400 MHz, (CD₃)₂SO)

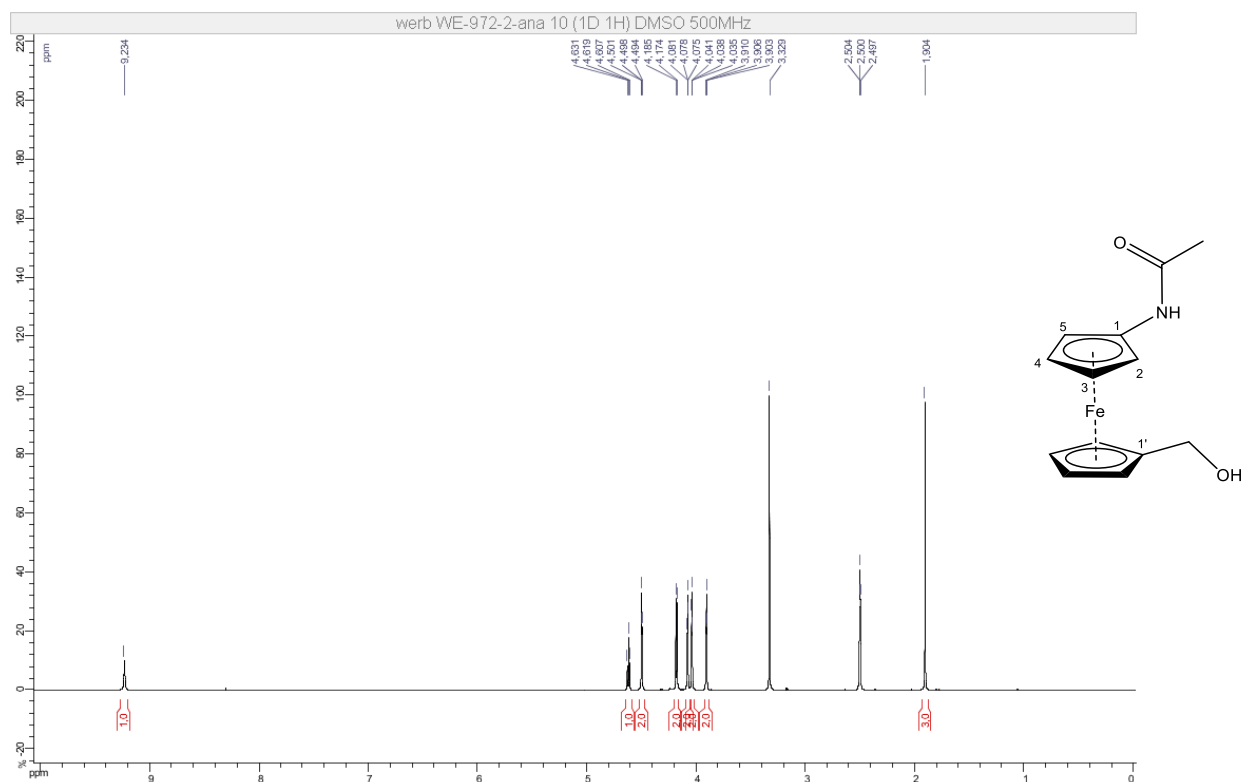


HMBC (400 MHz, (CD₃)₂SO)

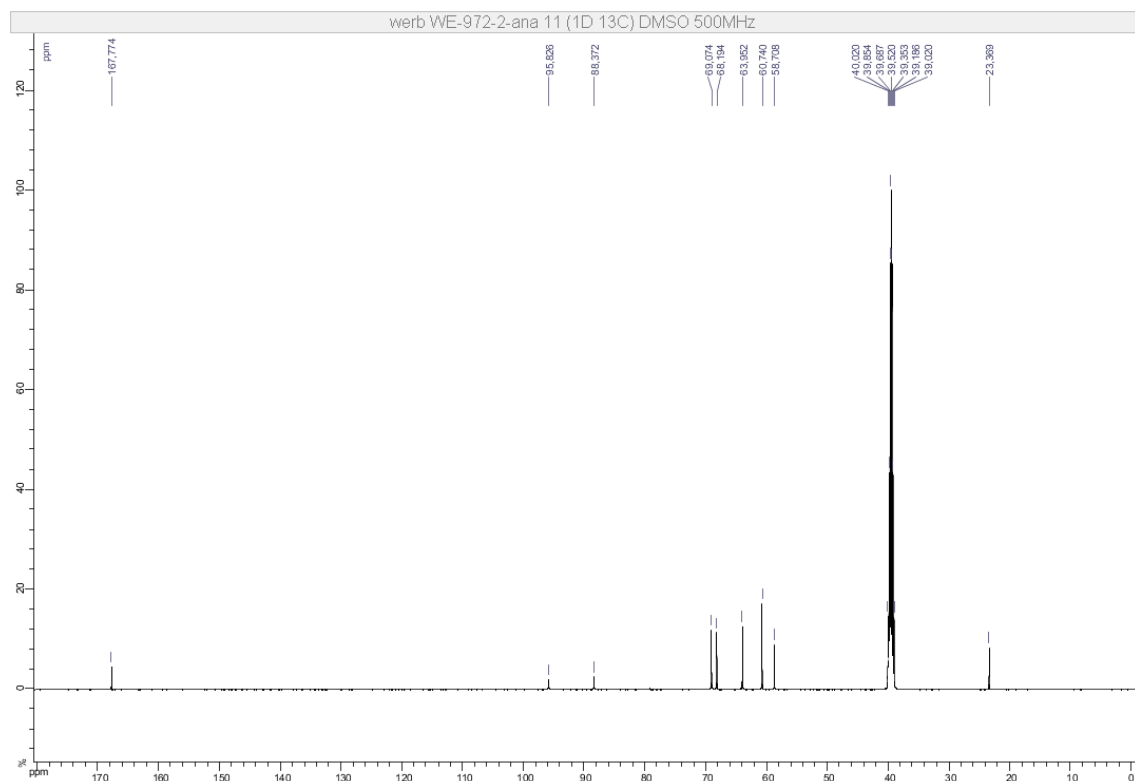


N-(1'-Hydroxymethylferrocenyl)acetamide (**6e**)

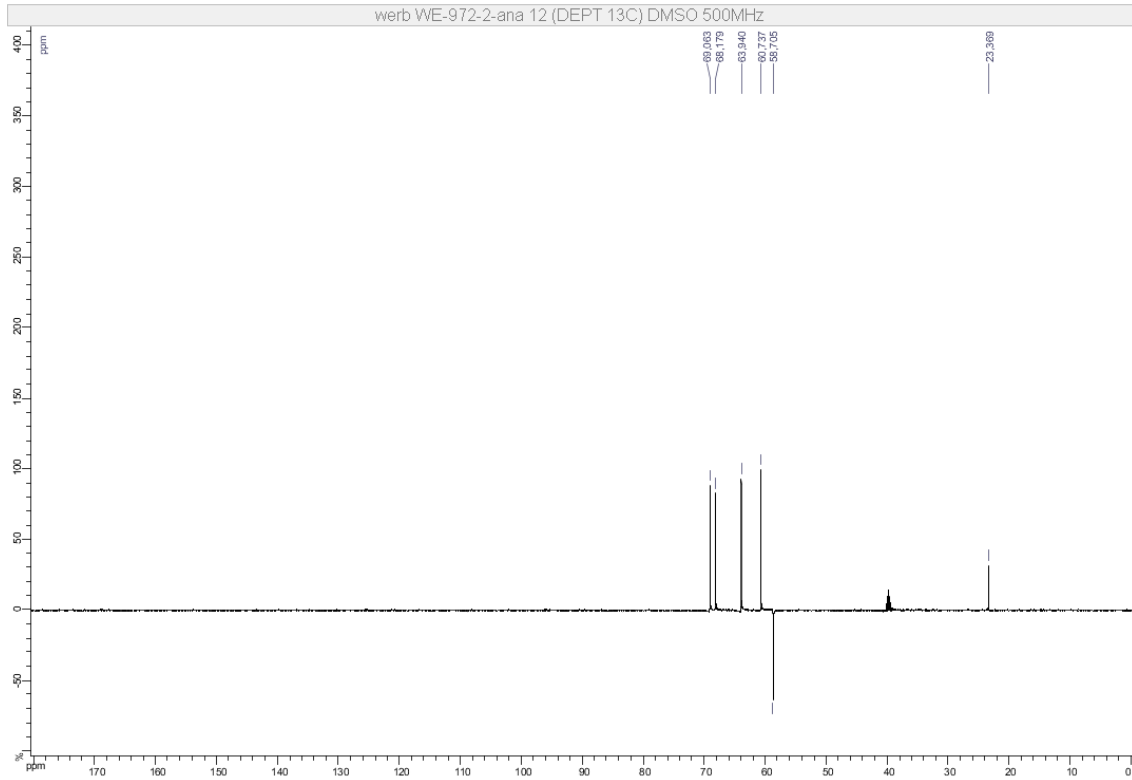
^1H NMR (500 MHz, $(\text{CD}_3)_2\text{SO}$)



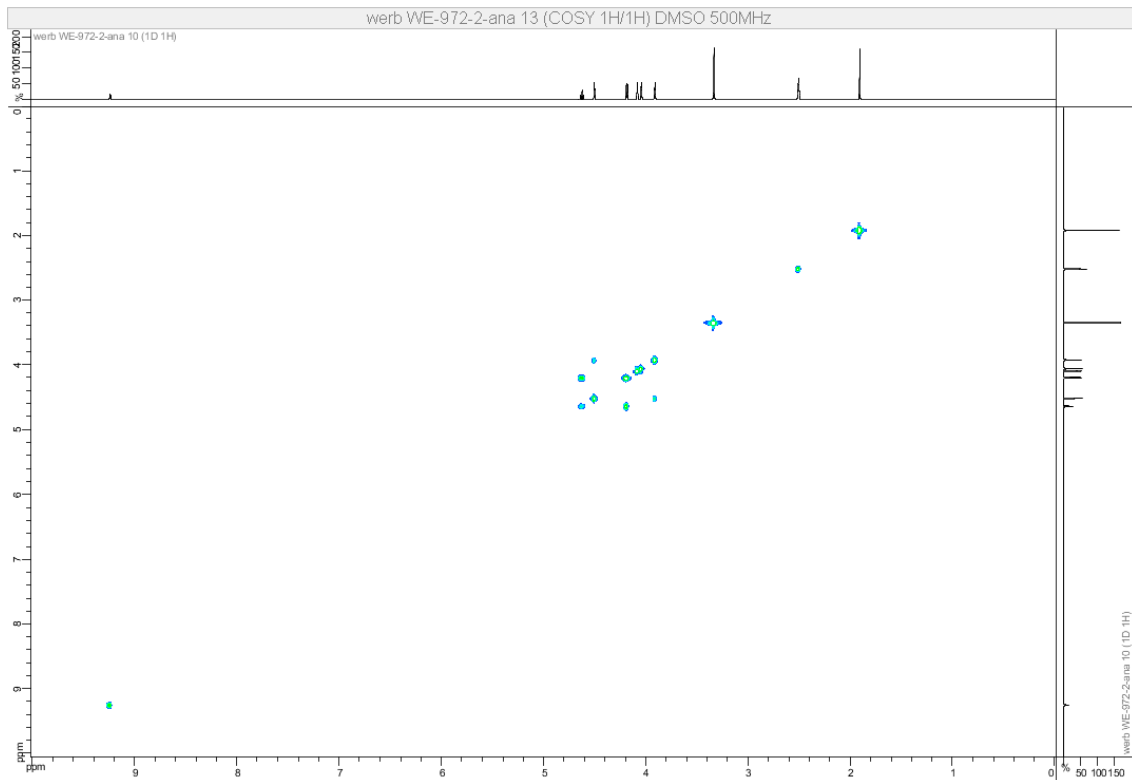
^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{SO}$)



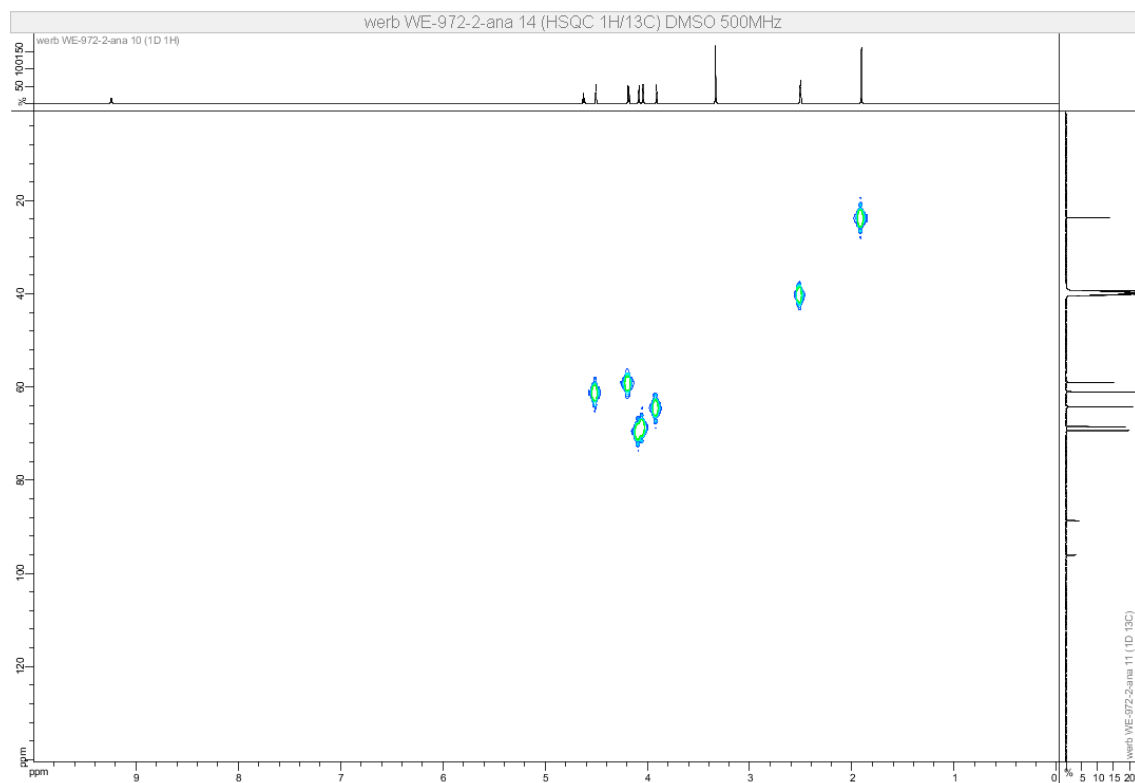
DEPT 135 (126 MHz, (CD₃)₂SO)



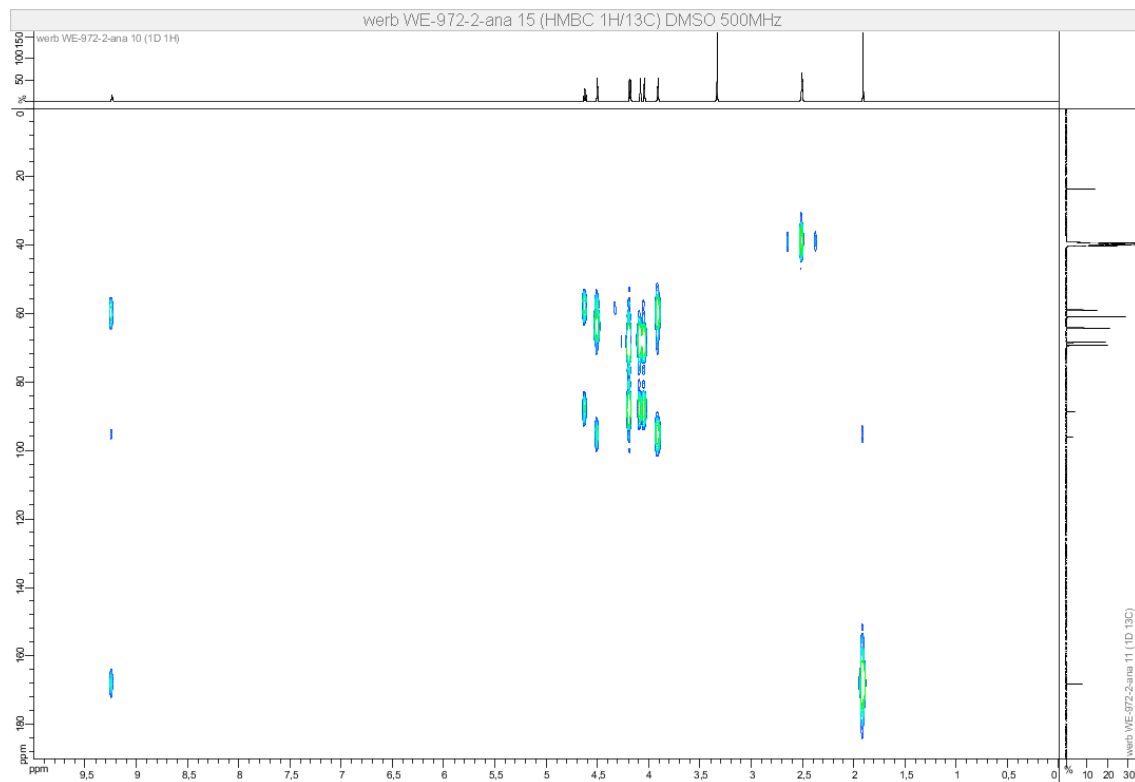
COSY (500 MHz, (CD₃)₂SO)



HSQC (500 MHz, (CD₃)₂SO)

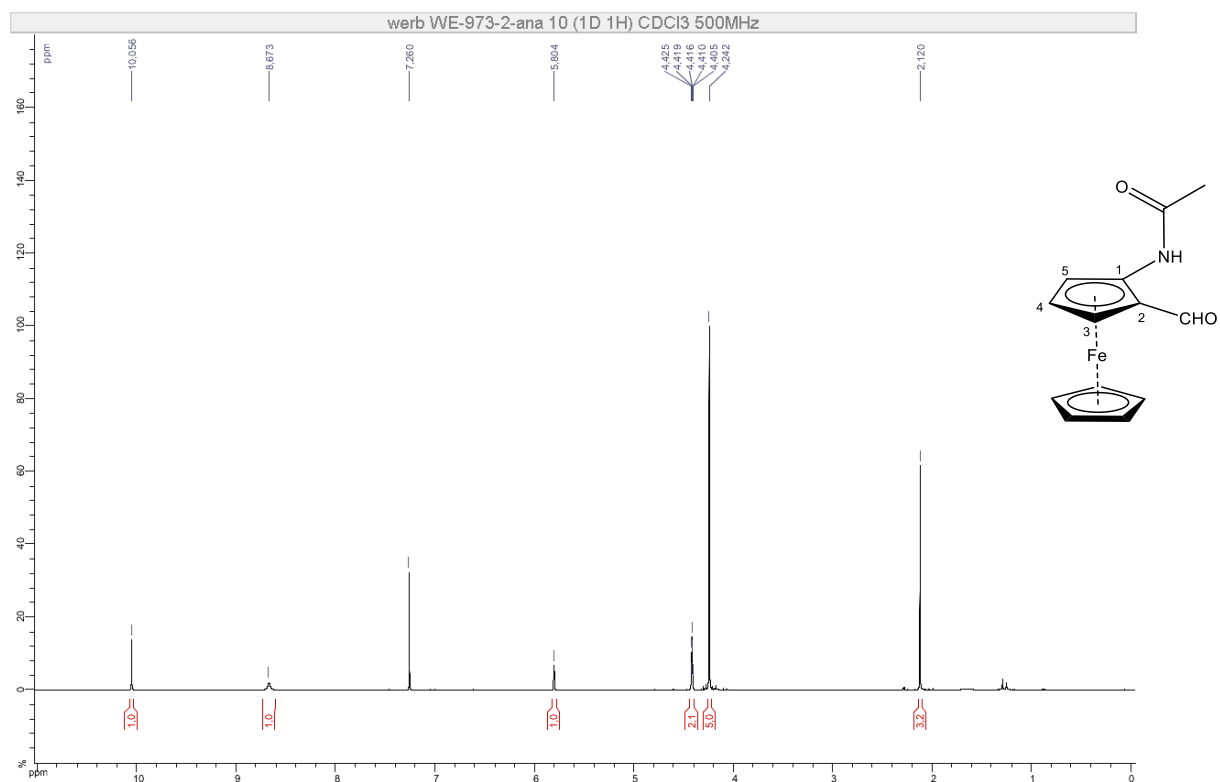


HMBC (500 MHz, (CD₃)₂SO)

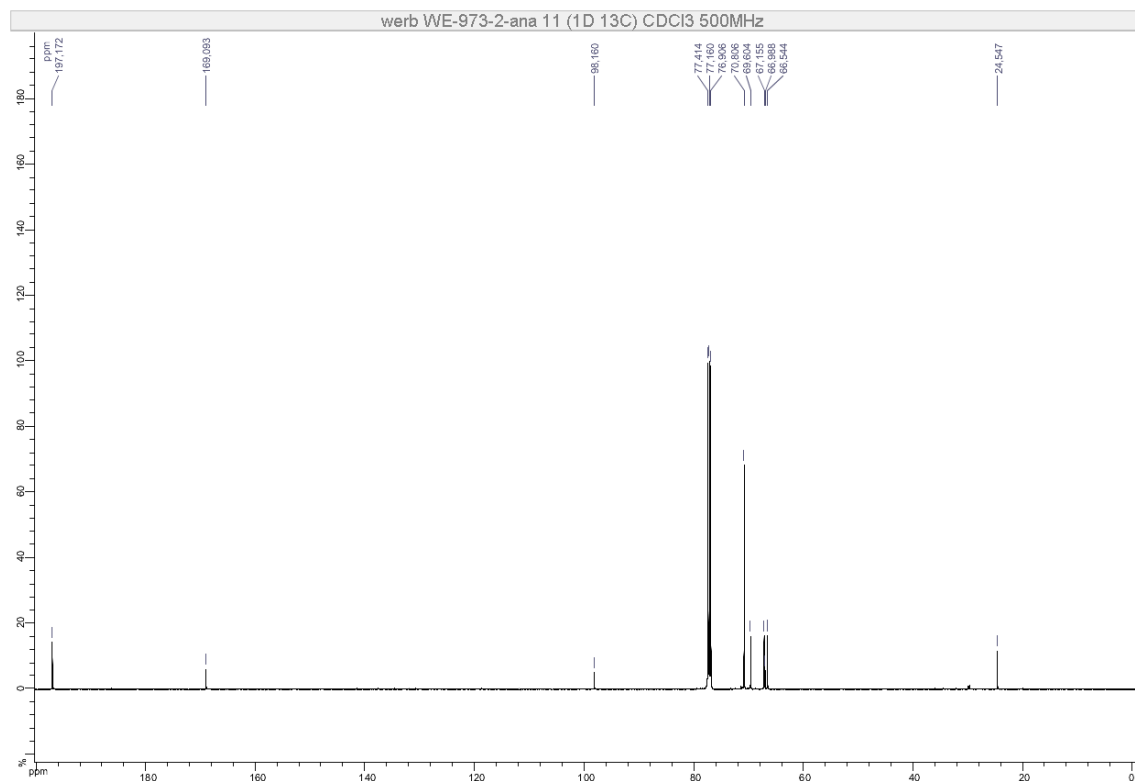


N-(2-Formylferrocenyl)acetamide (**2f**, racemic mixture)

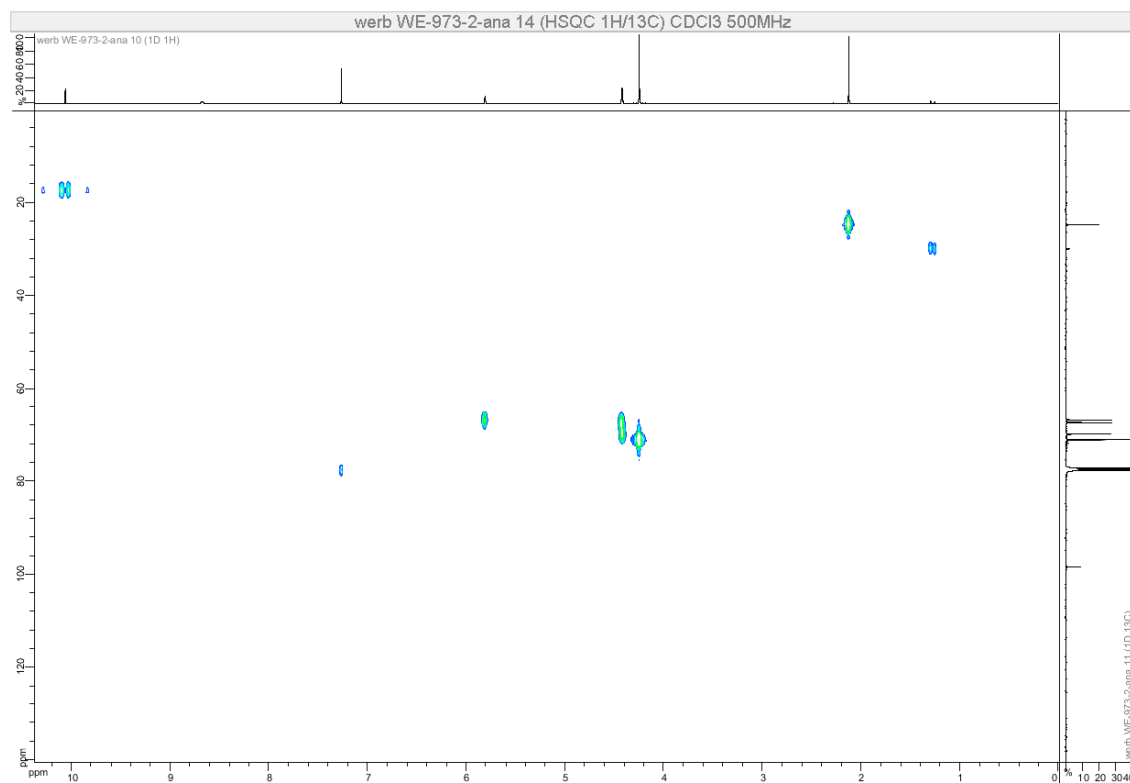
^1H NMR (500 MHz, CDCl_3)



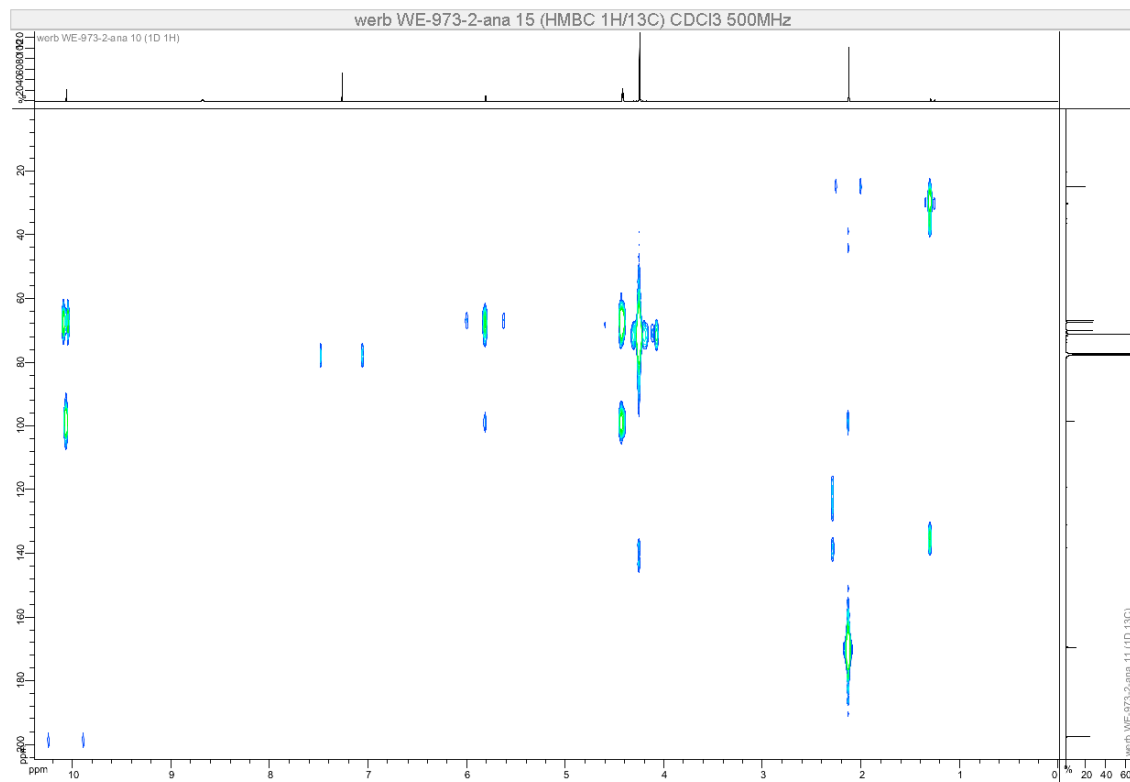
^{13}C NMR (126 MHz, CDCl_3)



HSQC (500 MHz, CDCl₃)

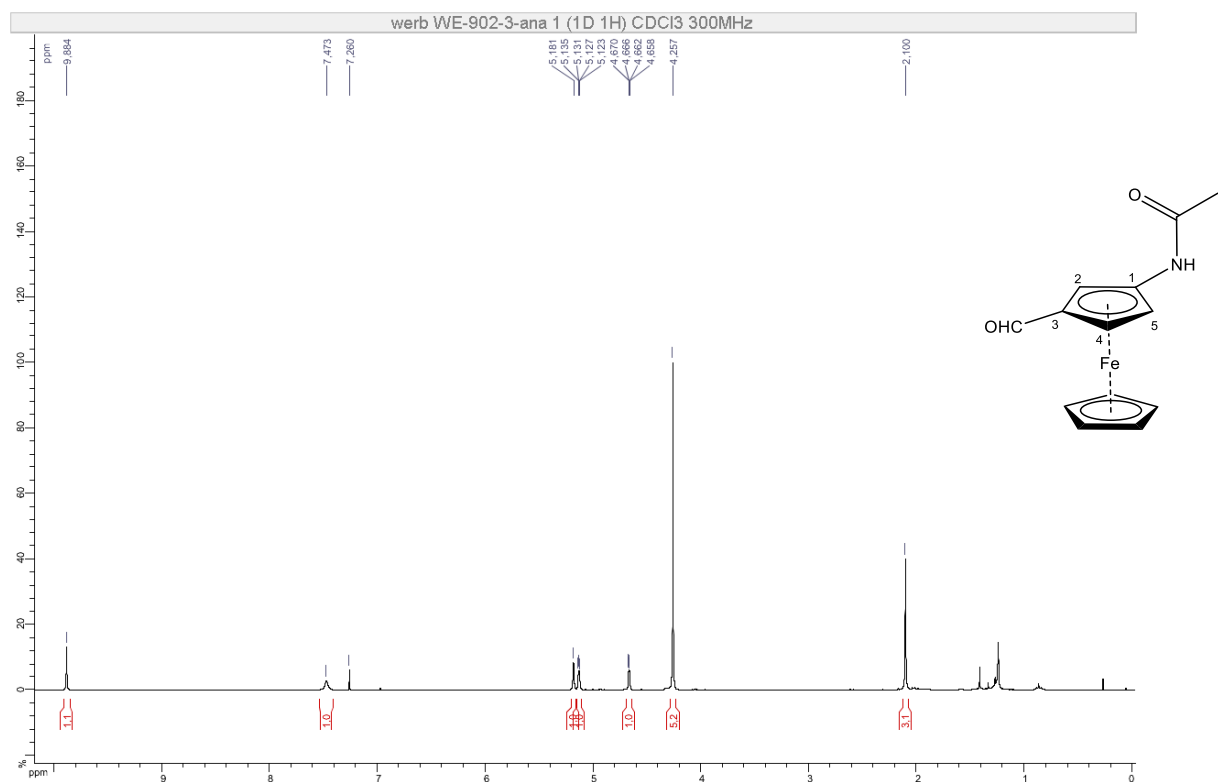


HMBC (500 MHz, CDCl₃)

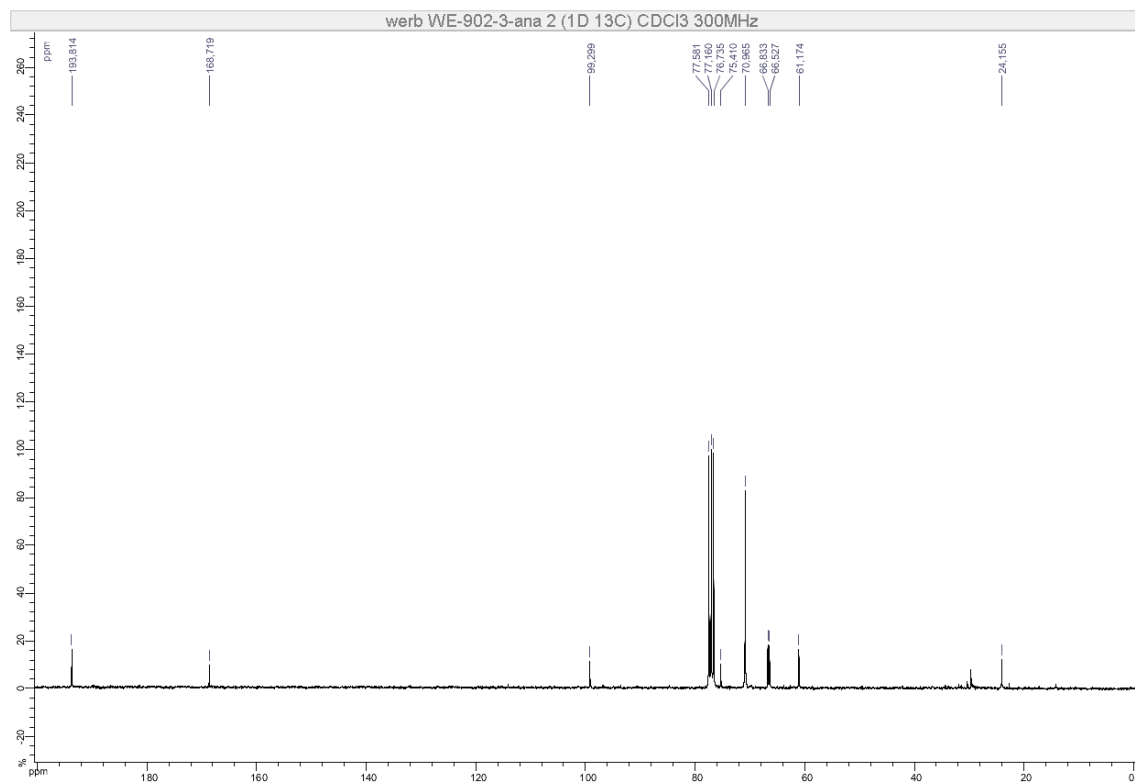


N-(3-Formylferrocenyl)acetamide (**4f**, racemic mixture)

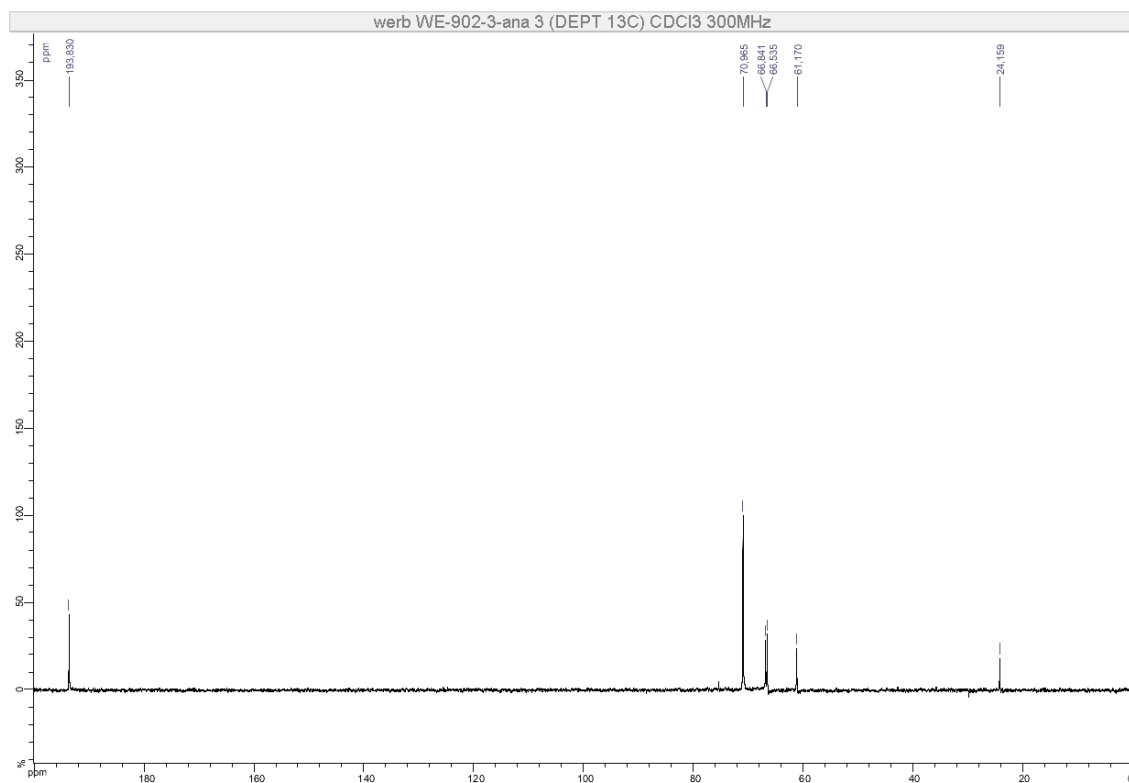
^1H NMR (300 MHz, CDCl_3)



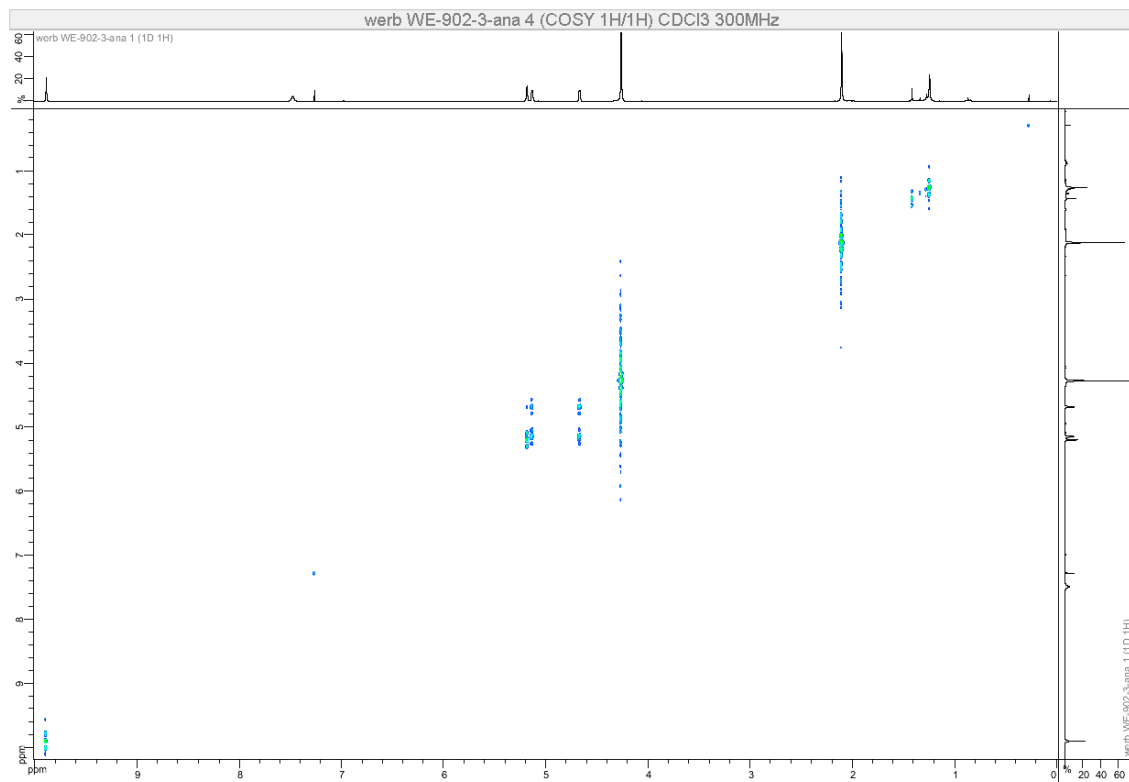
^{13}C NMR (75 MHz, CDCl_3)



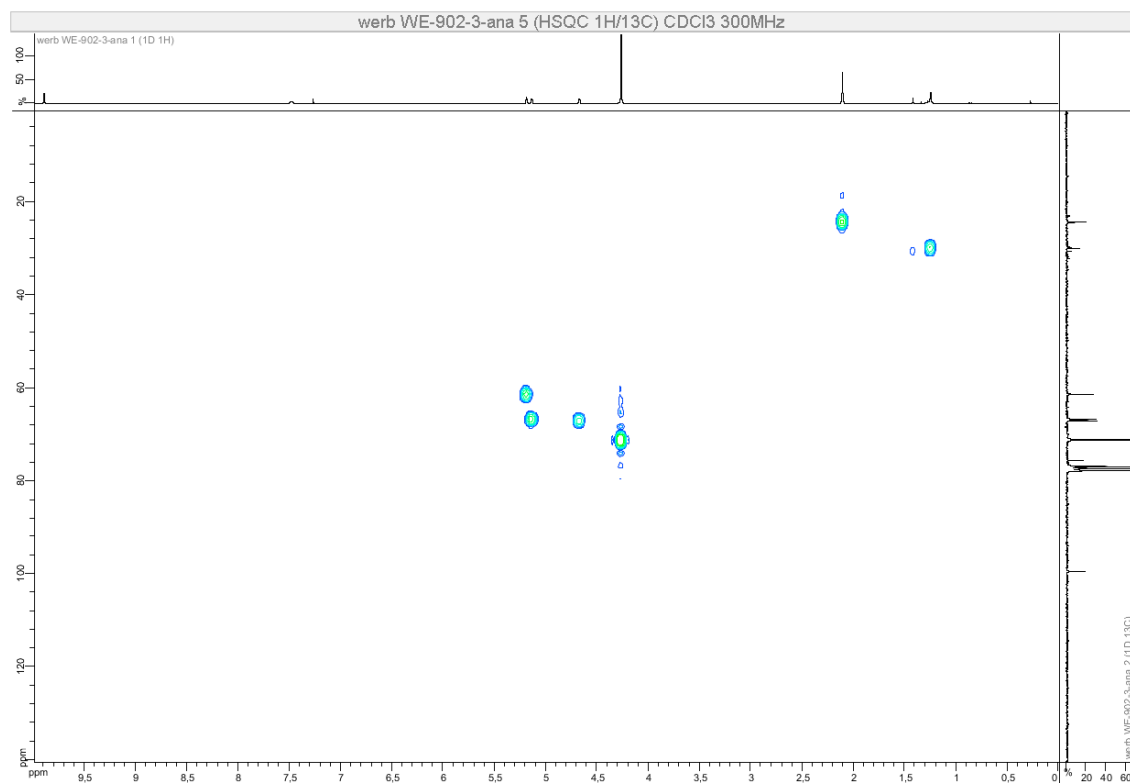
DEPT 135 (75 MHz, CDCl₃)



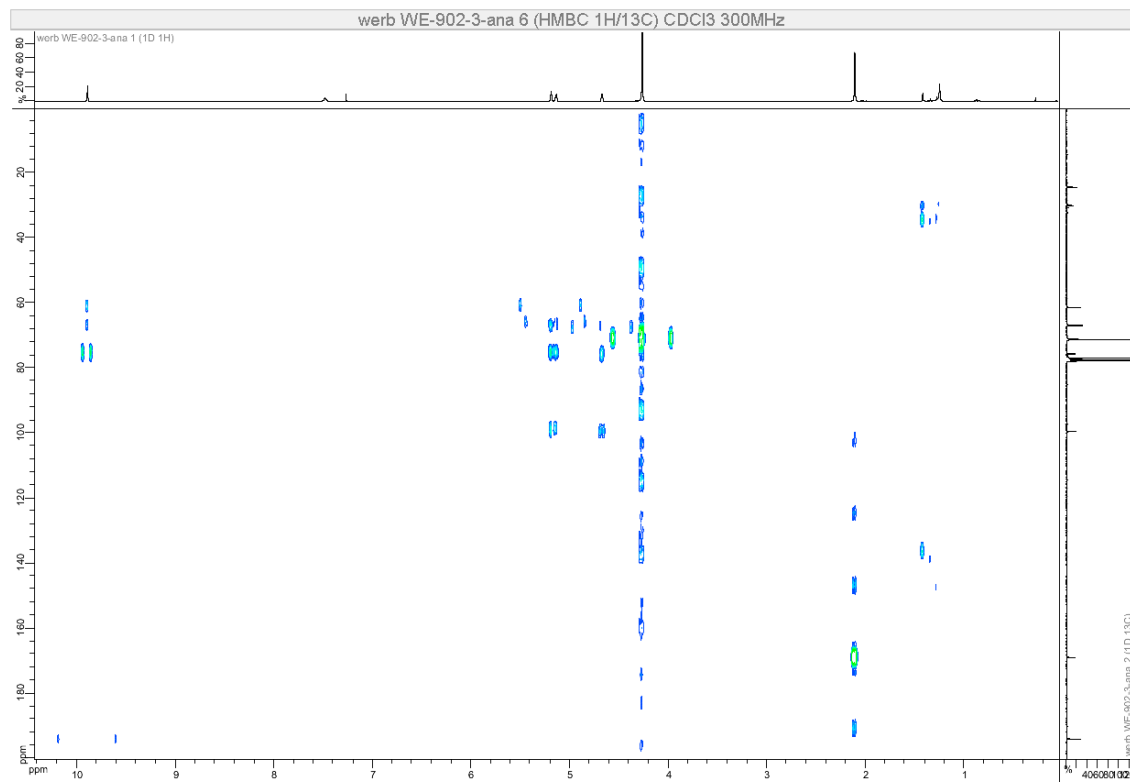
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

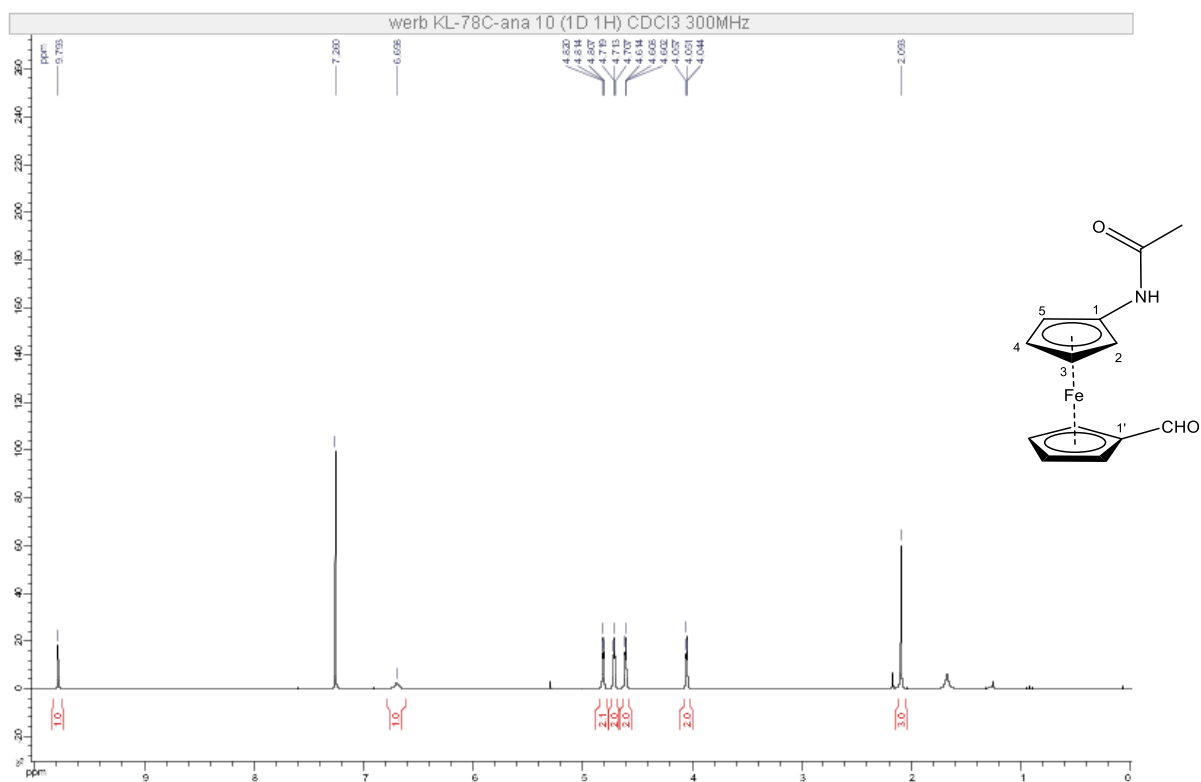


HMBC (300 MHz, CDCl₃)

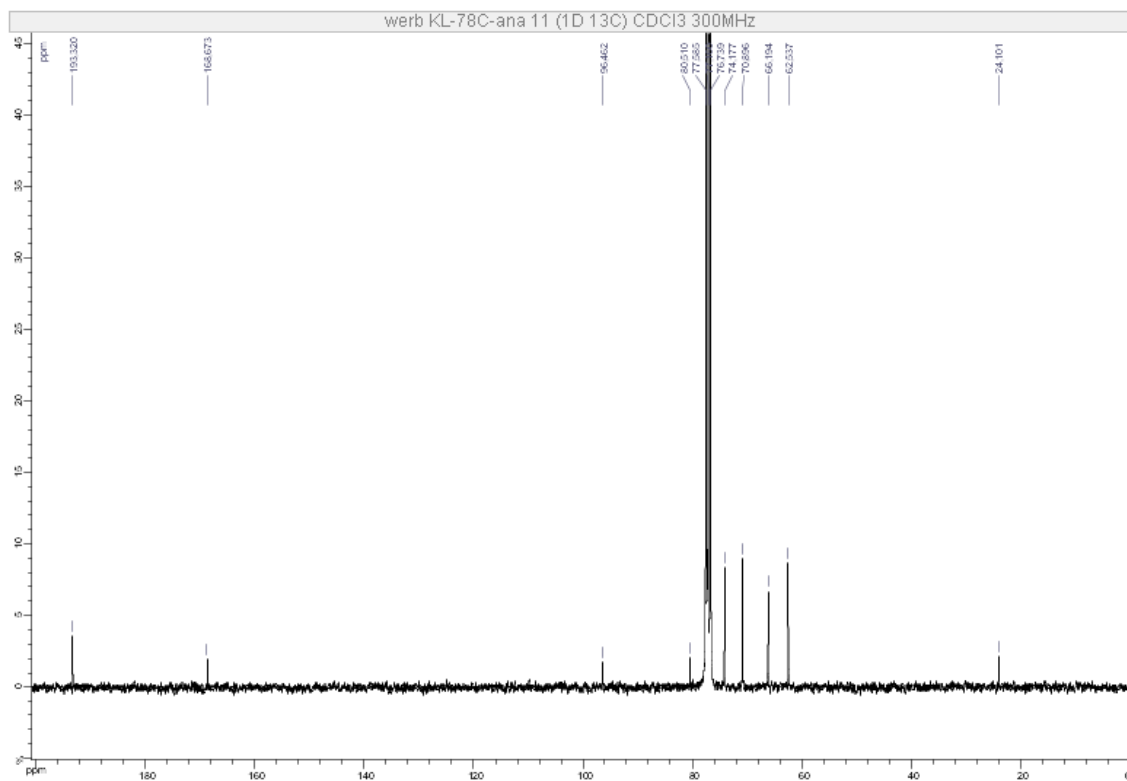


N-(1'-Formylferrocenyl)acetamide (**6f**)

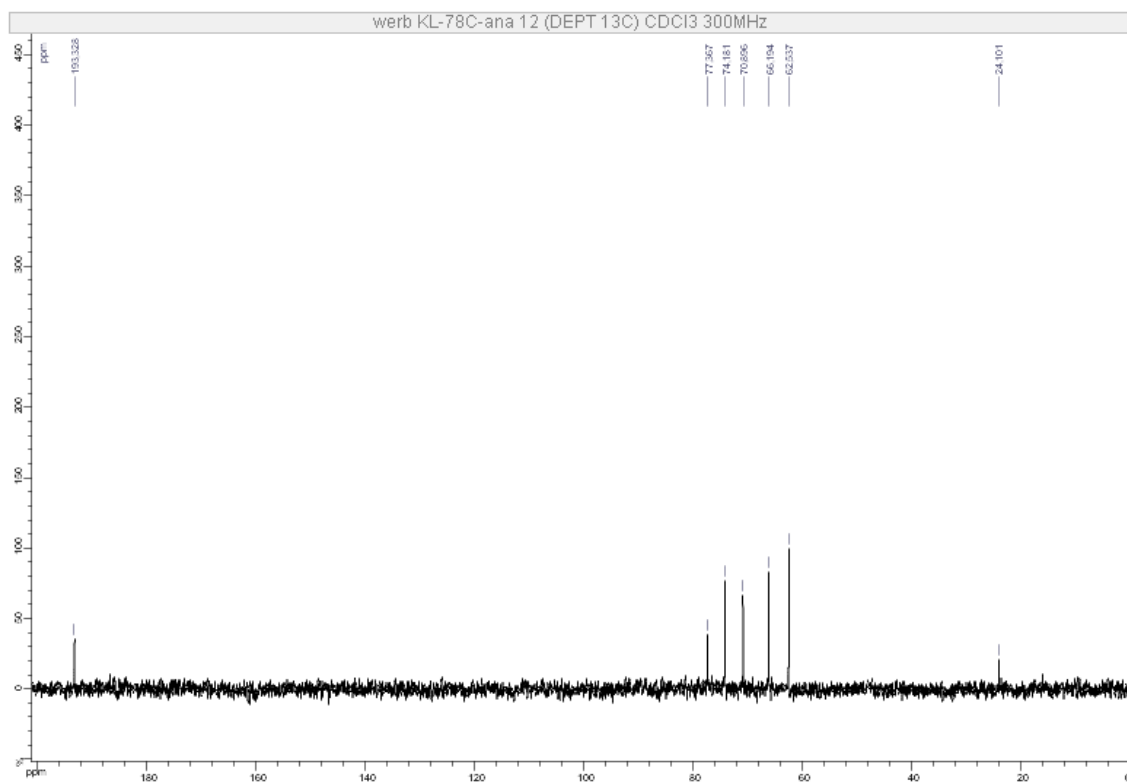
^1H NMR (300 MHz, CDCl_3)



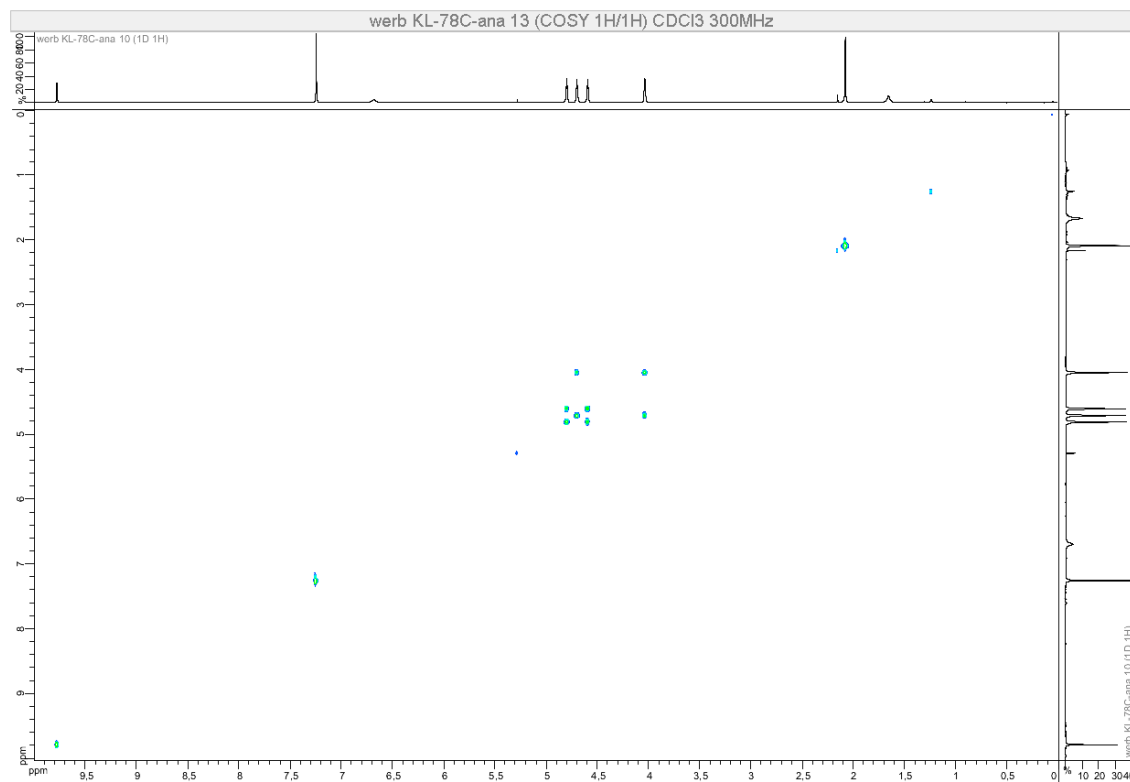
^{13}C NMR (75 MHz, CDCl_3)



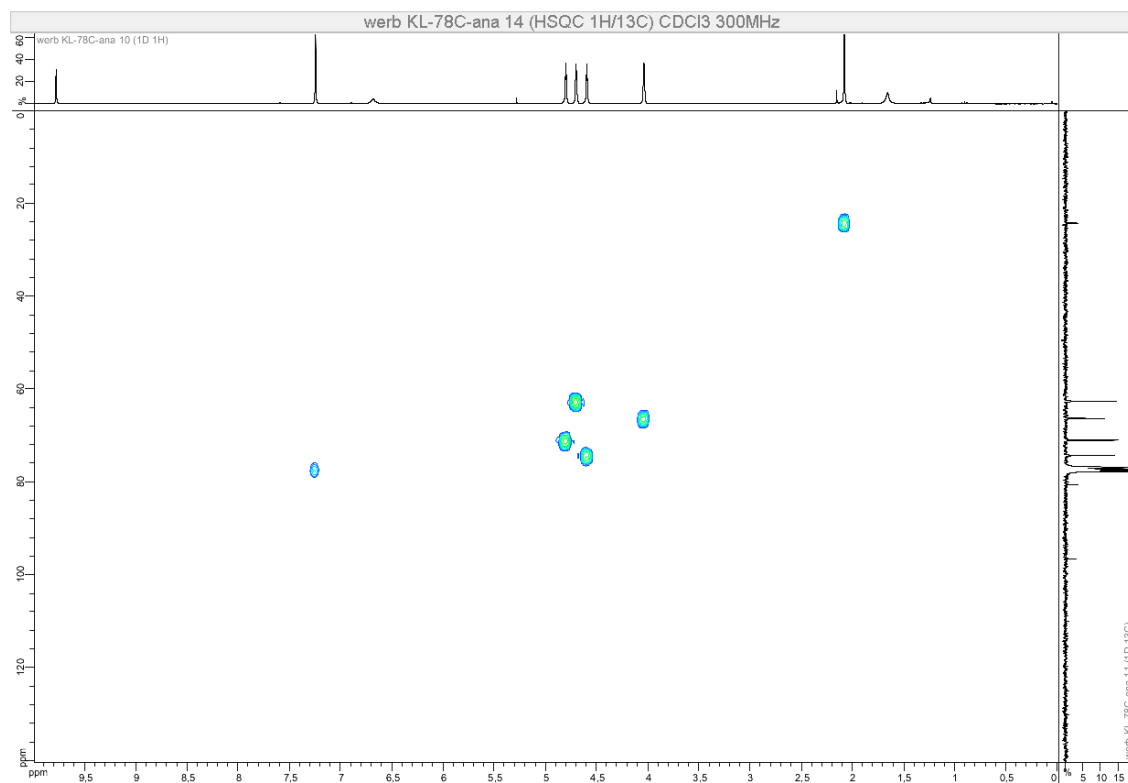
DEPT 135 (75 MHz, CDCl₃)



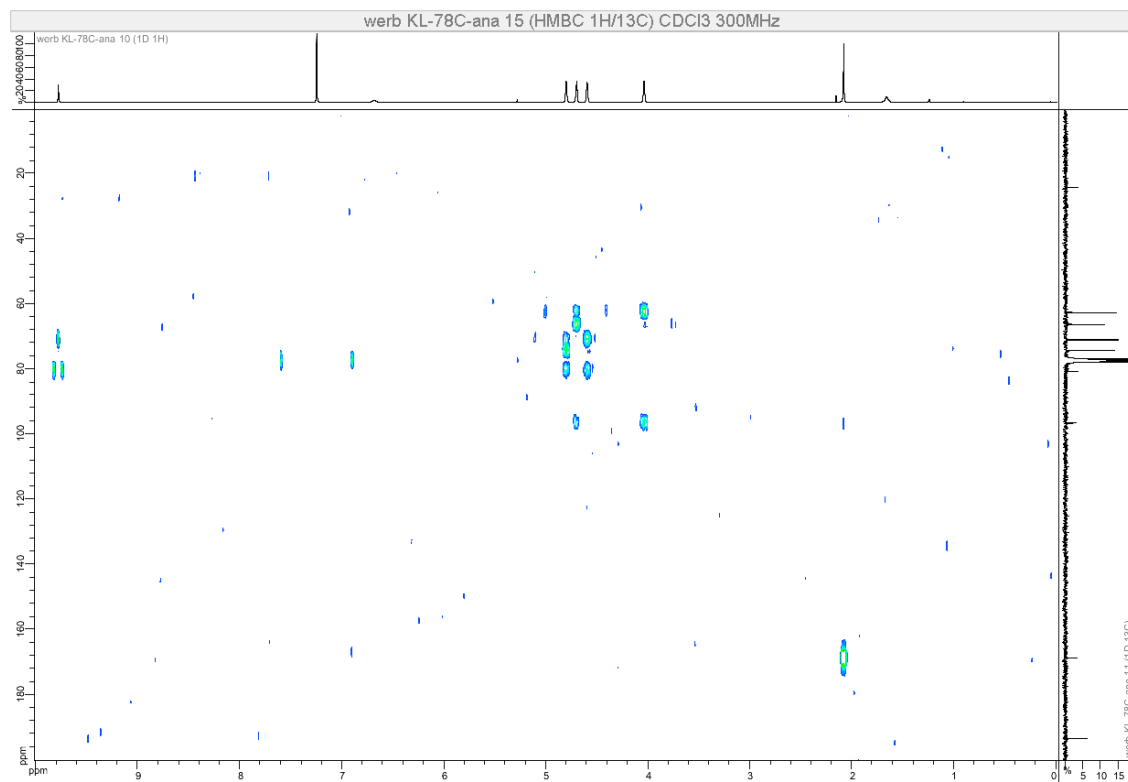
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

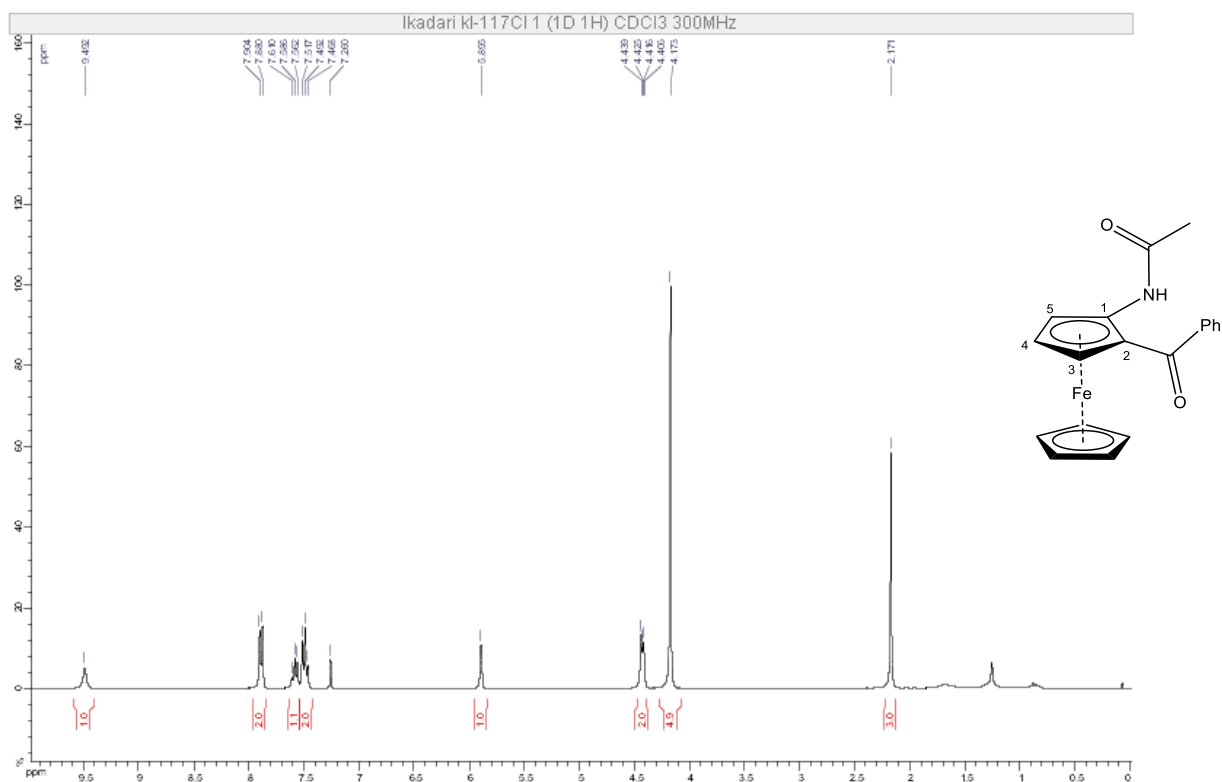


HMBC (300 MHz, CDCl₃)

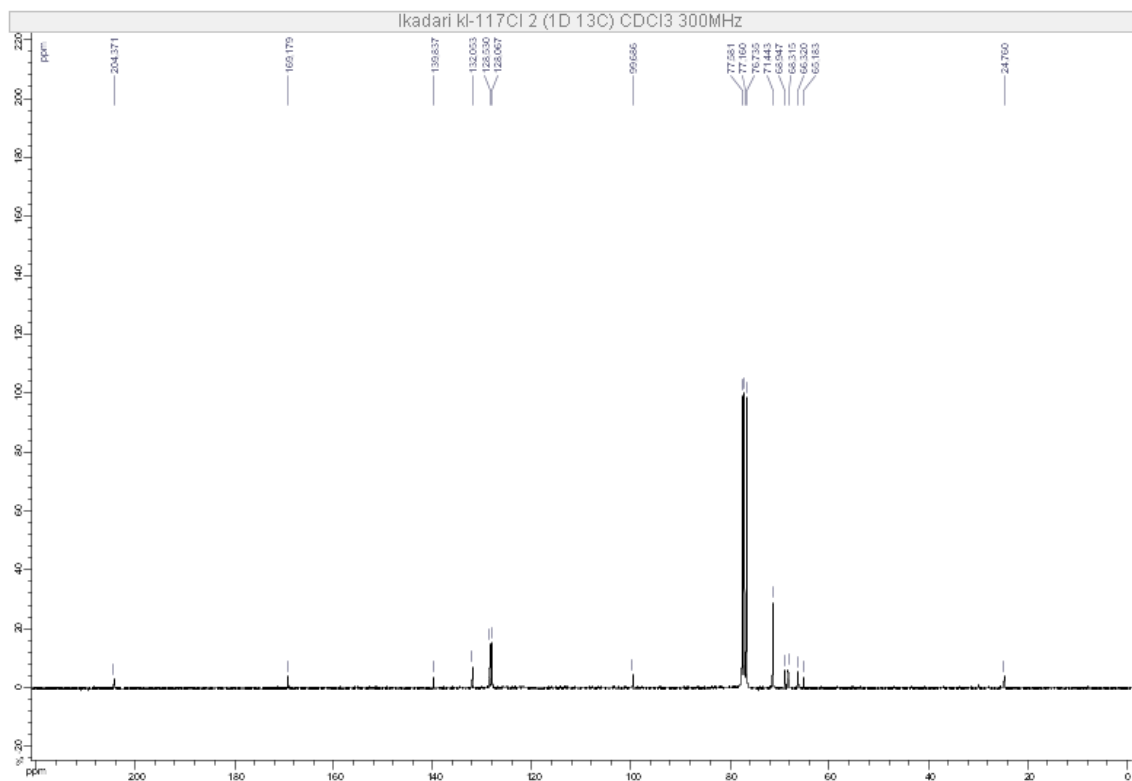


***N*-(2-Benzoylferrocenyl)acetamide (2g, racemic mixture)**

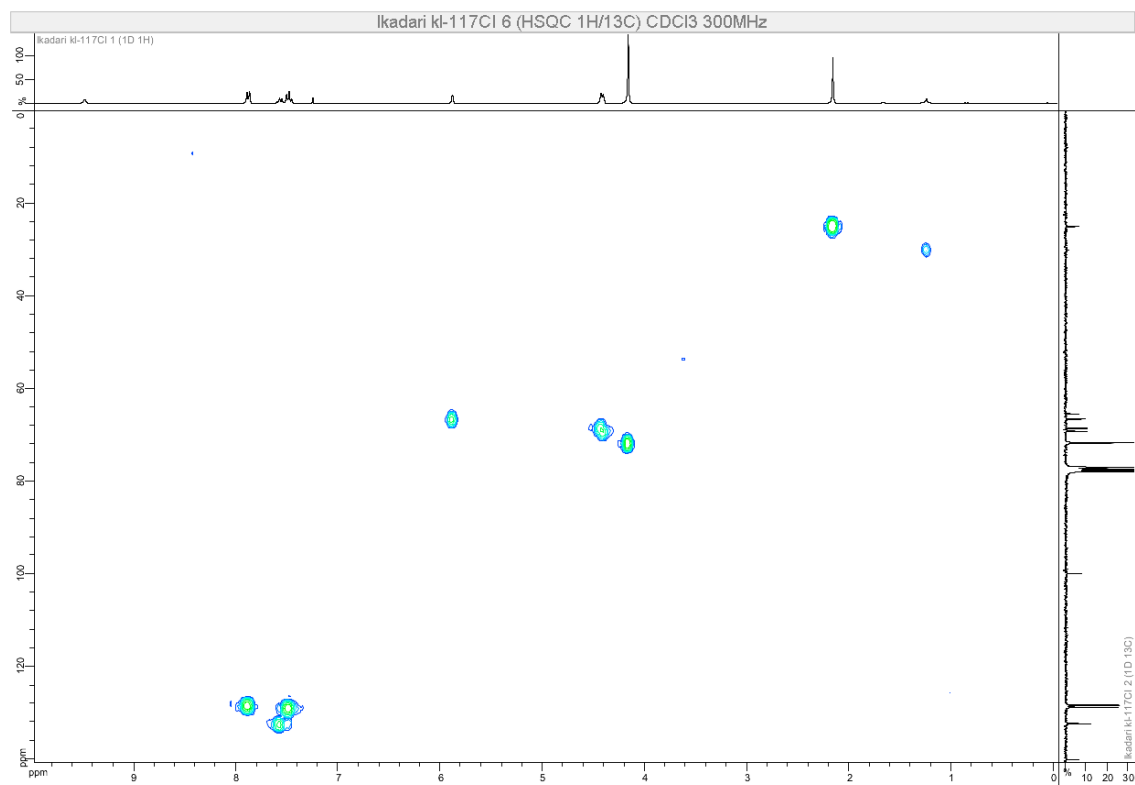
¹H NMR (300 MHz, CDCl₃)



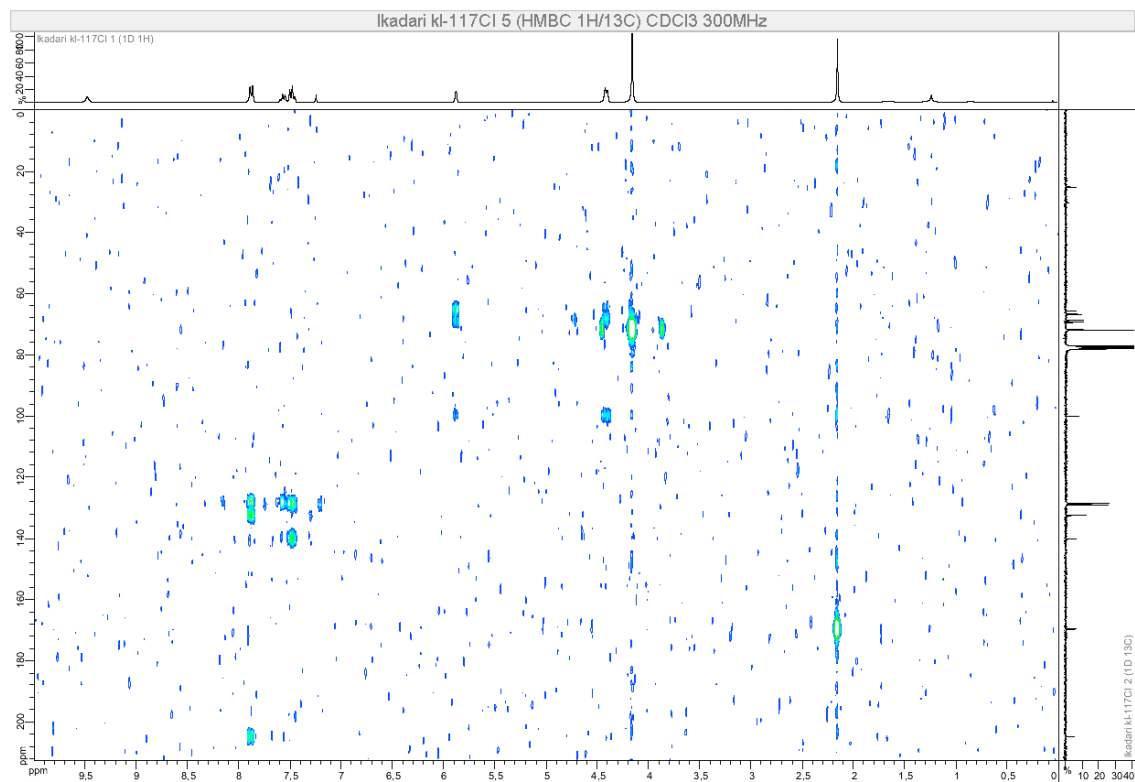
¹³C NMR (75 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

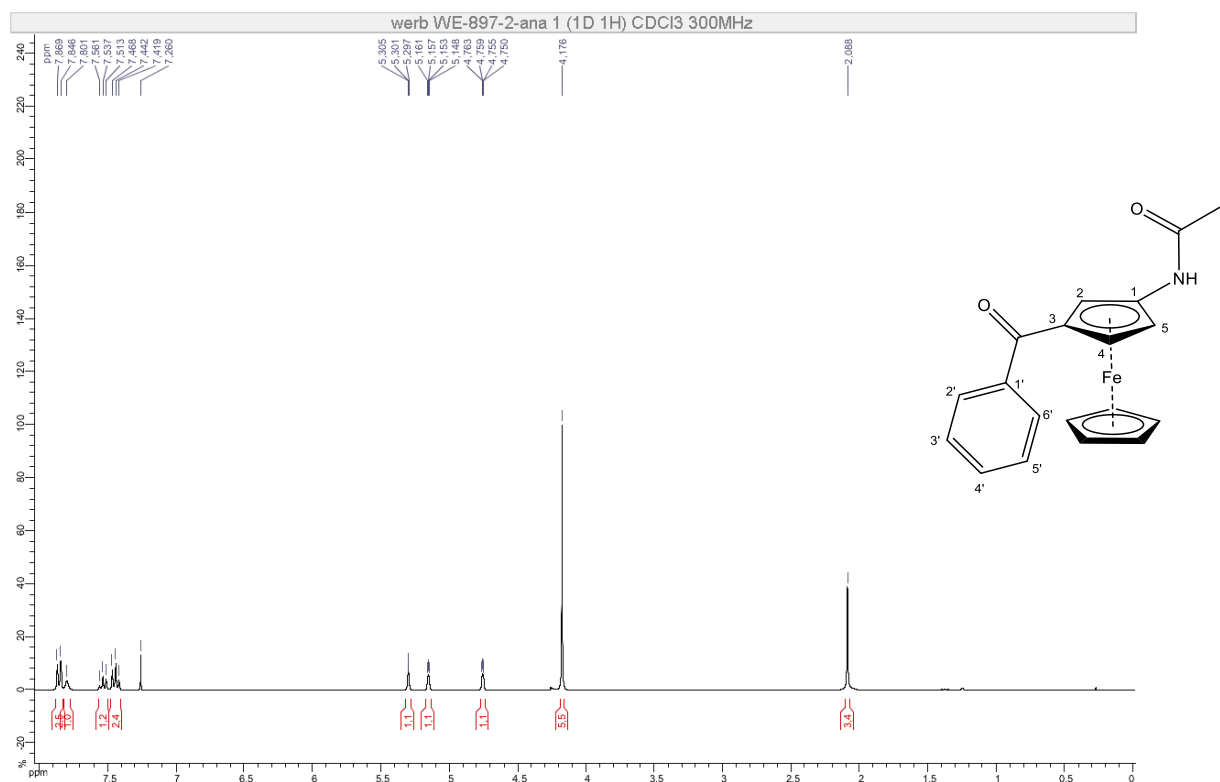


HMBC (300 MHz, CDCl₃)

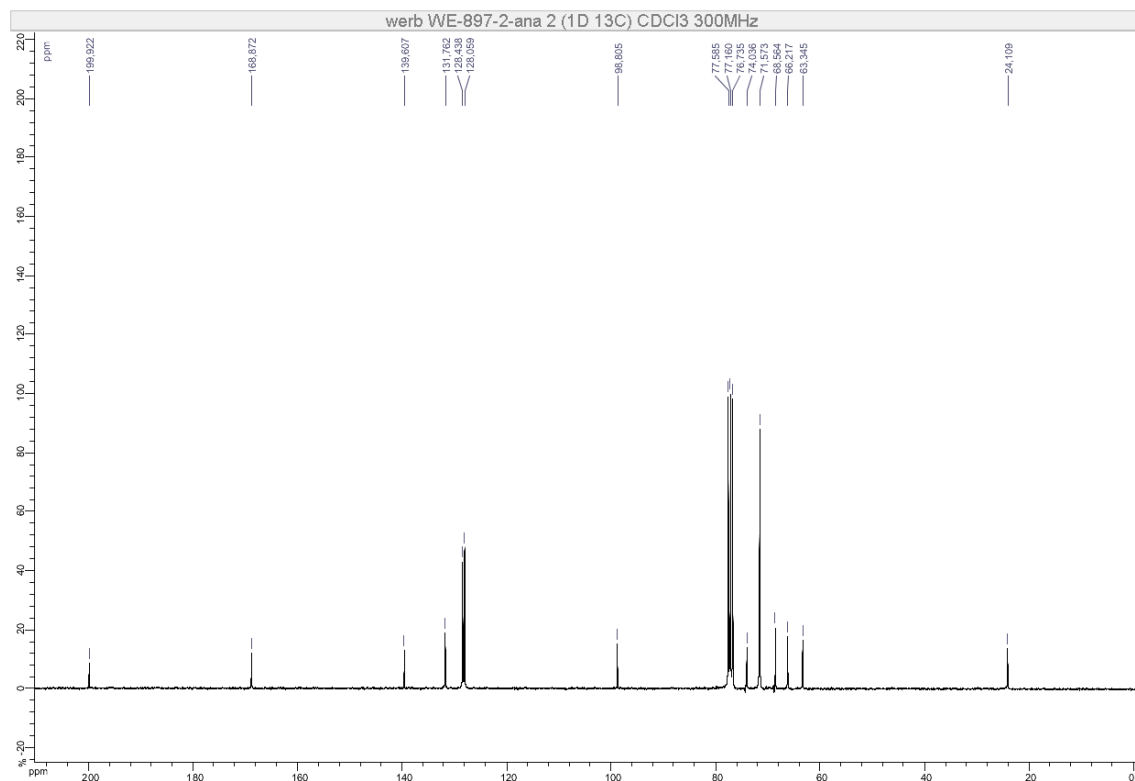


N-(3-Benzoylferrocenyl)acetamide (**4g**, racemic mixture)

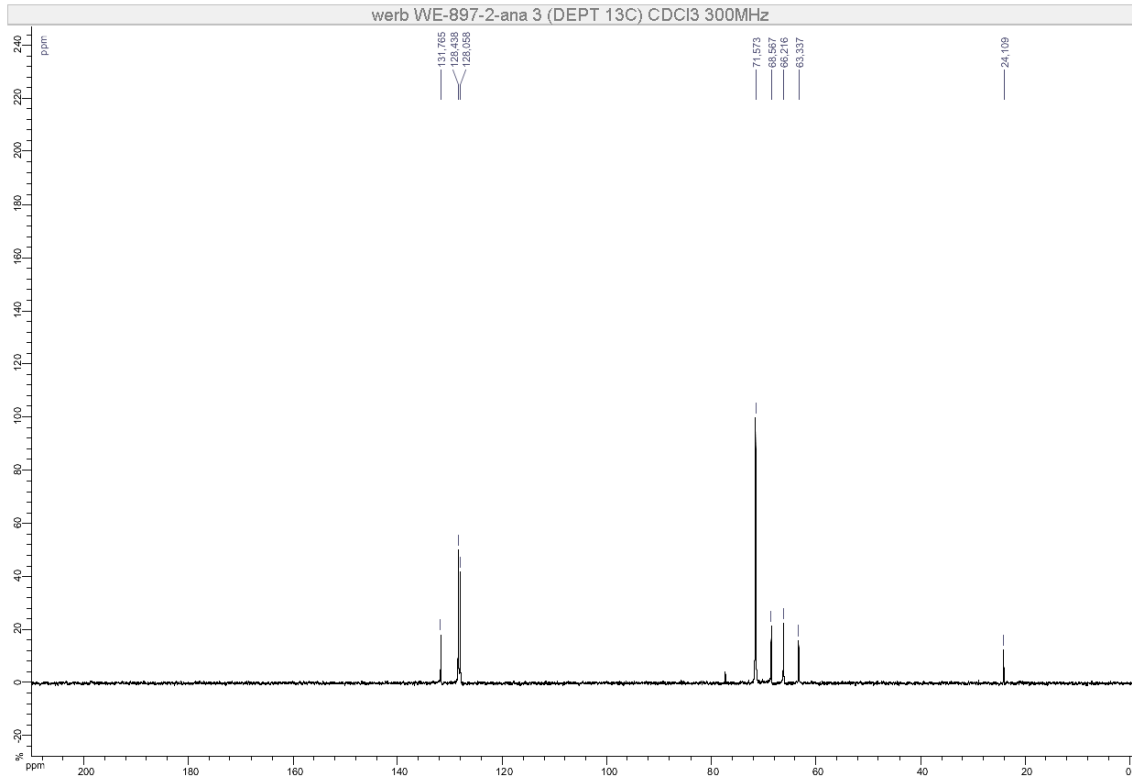
^1H NMR (300 MHz, CDCl_3)



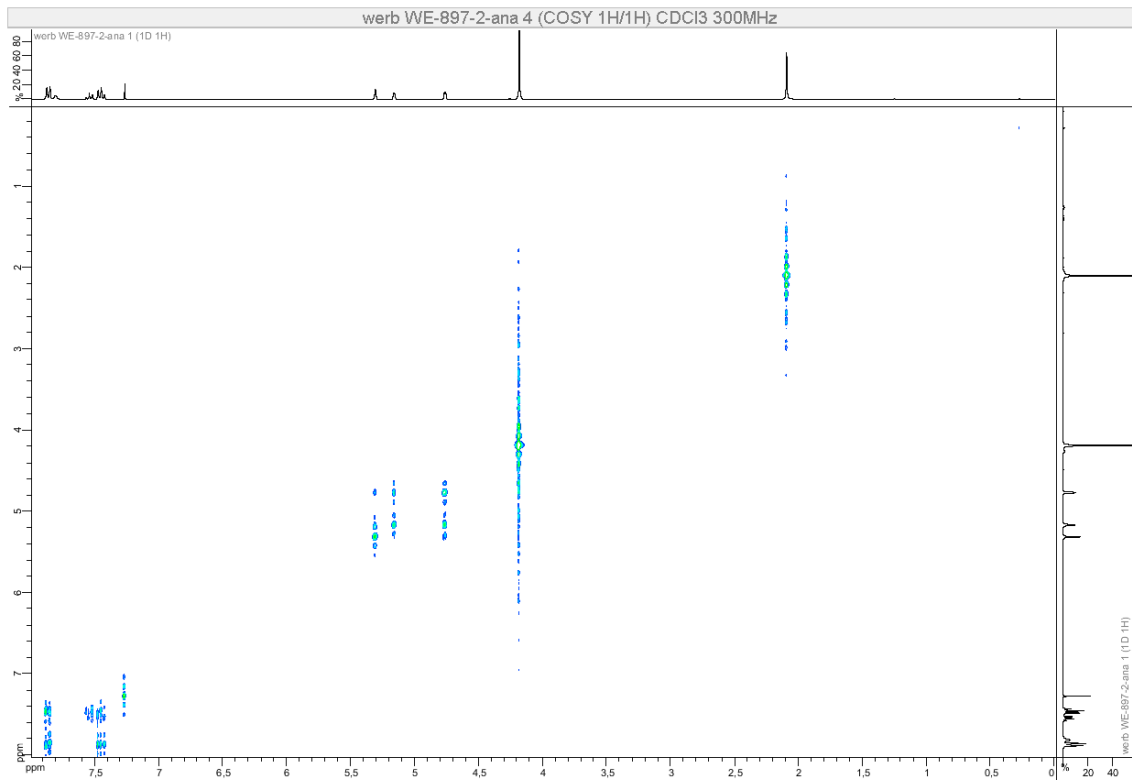
^{13}C NMR (75 MHz, CDCl_3)



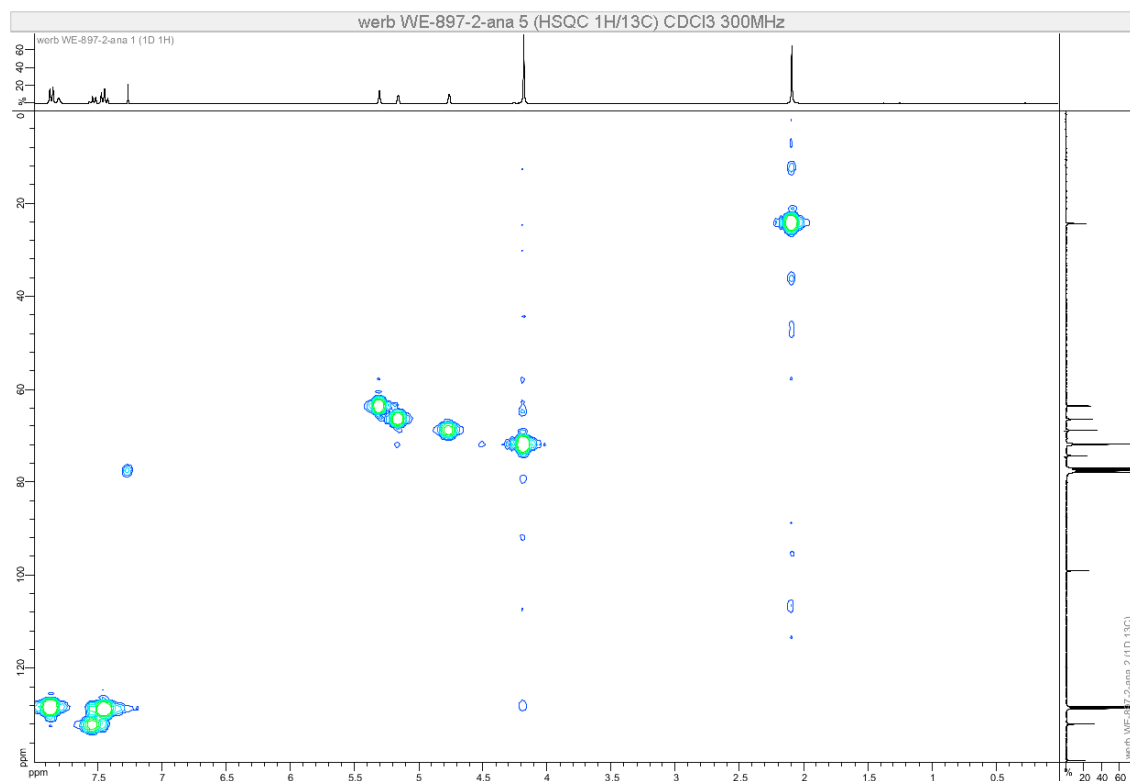
DEPT 135 (75 MHz, CDCl₃)



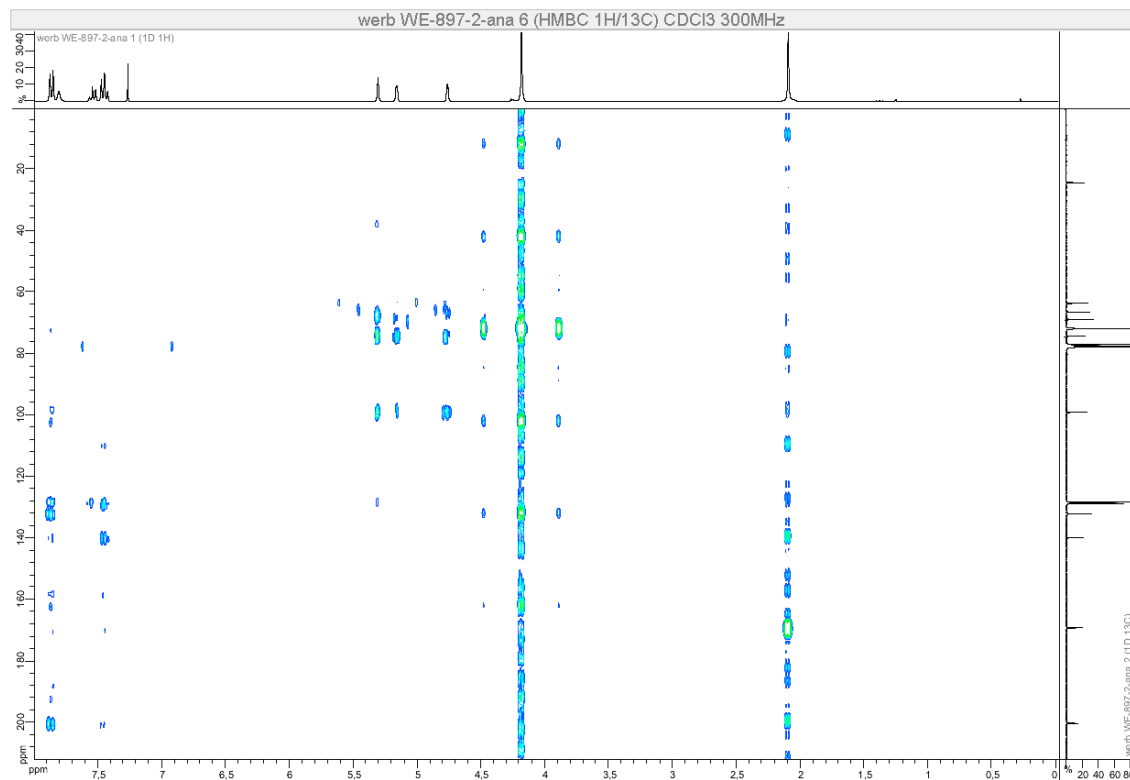
COSY (300 MHz, CDCl₃)



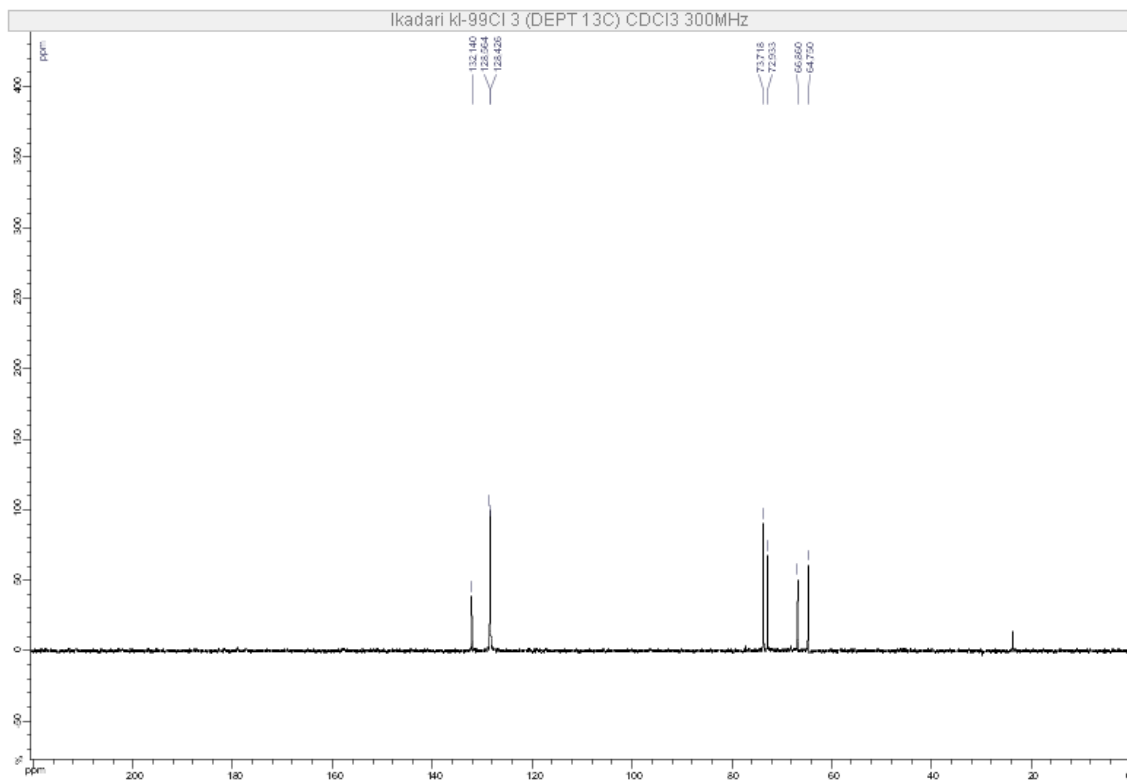
HSQC (300 MHz, CDCl₃)



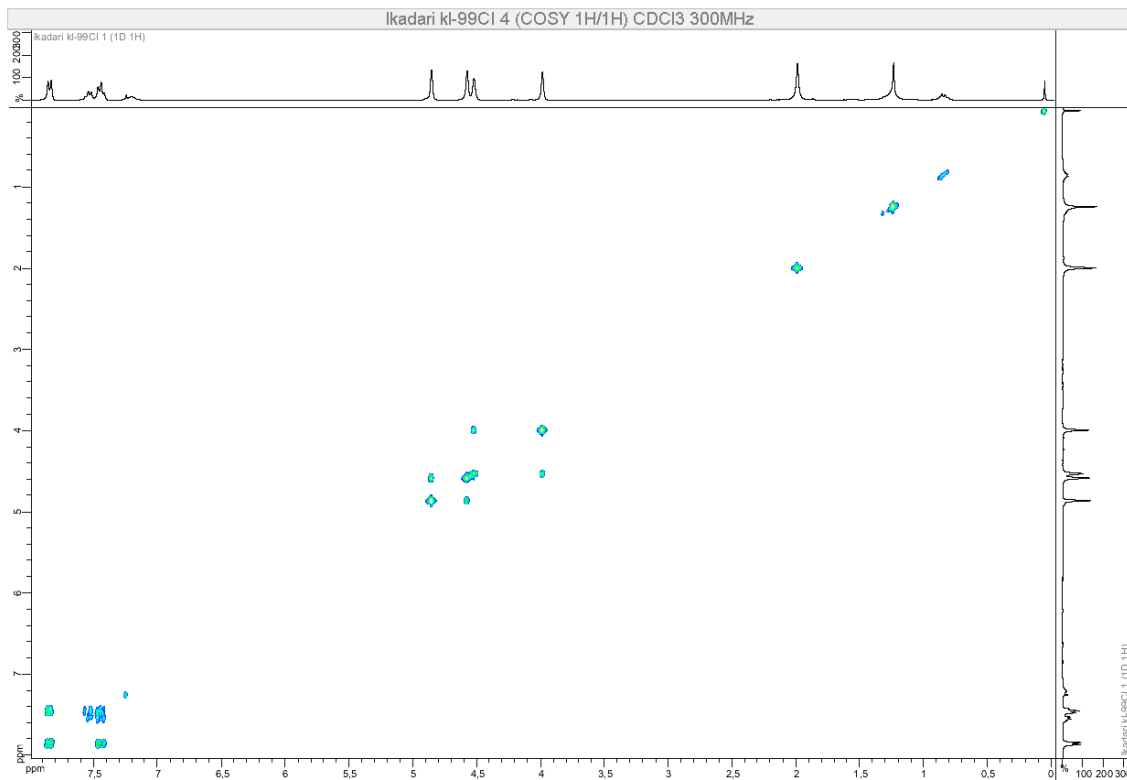
HMBC (300 MHz, CDCl₃)



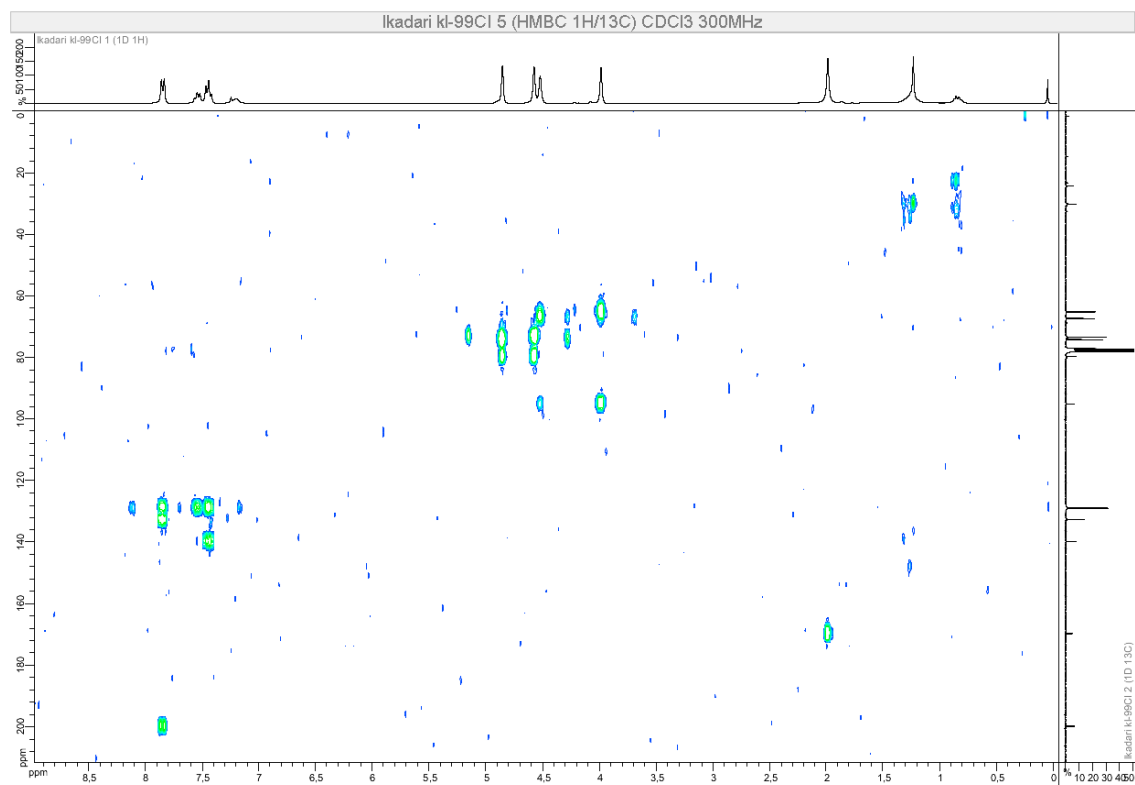
DEPT 135 (75 MHz, CDCl₃)



COSY (300 MHz, CDCl₃)

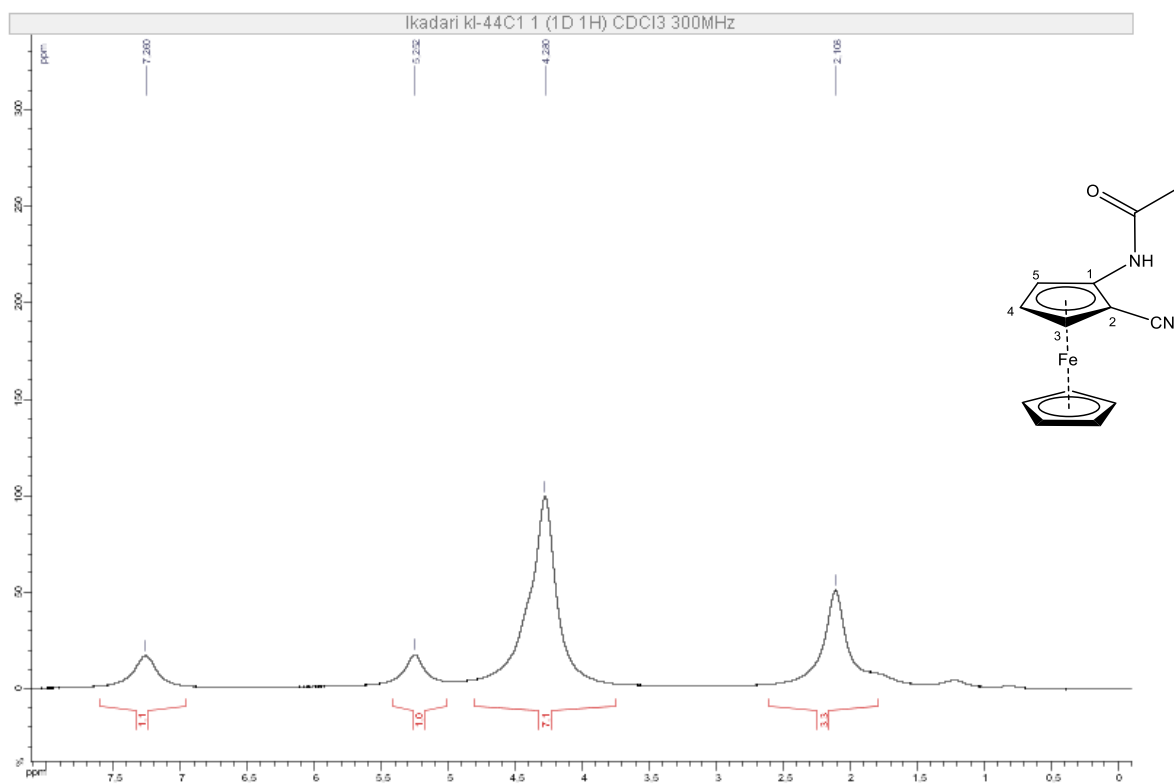


HMBC (300 MHz, CDCl₃)

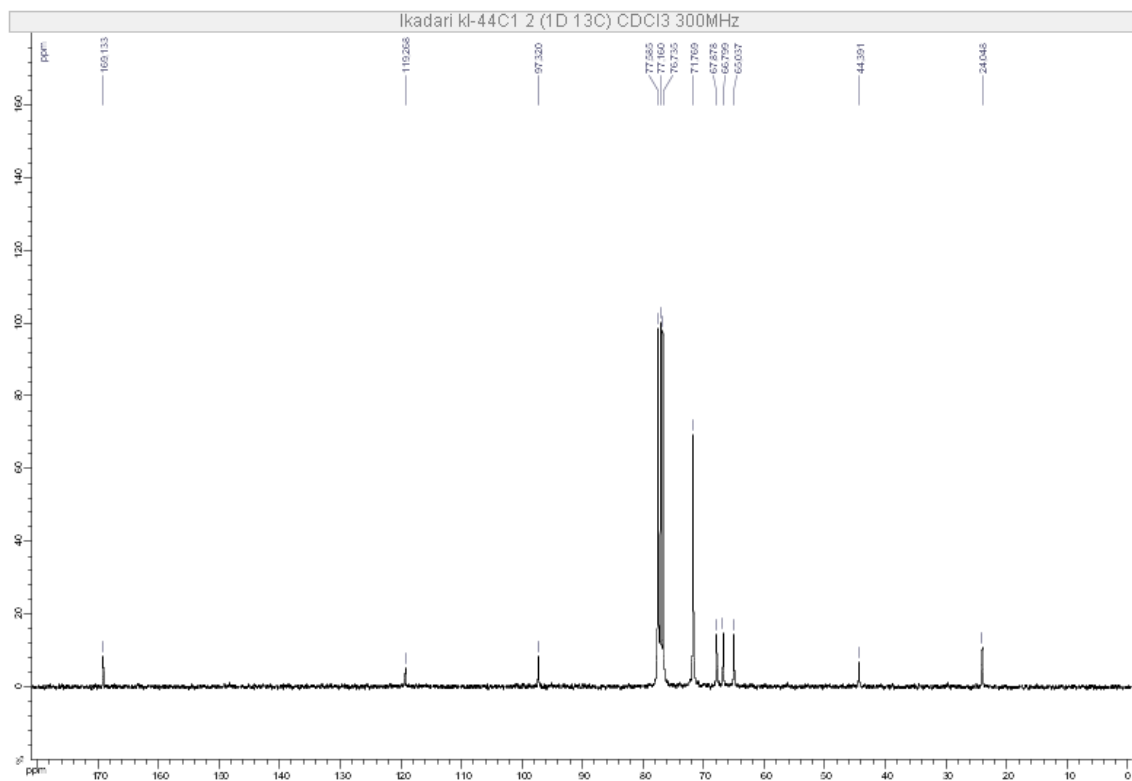


N-(2-Cyanoferrocenyl)acetamide (**2h**, racemic mixture)

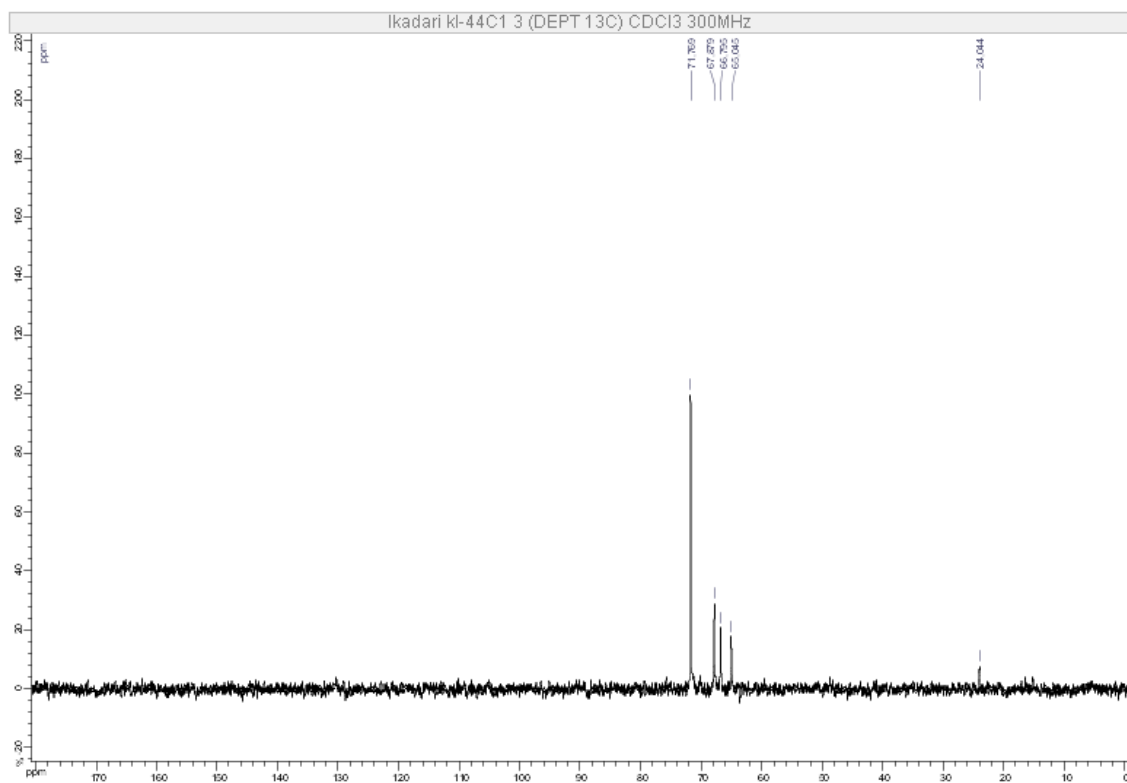
^1H NMR (300 MHz, CDCl_3)



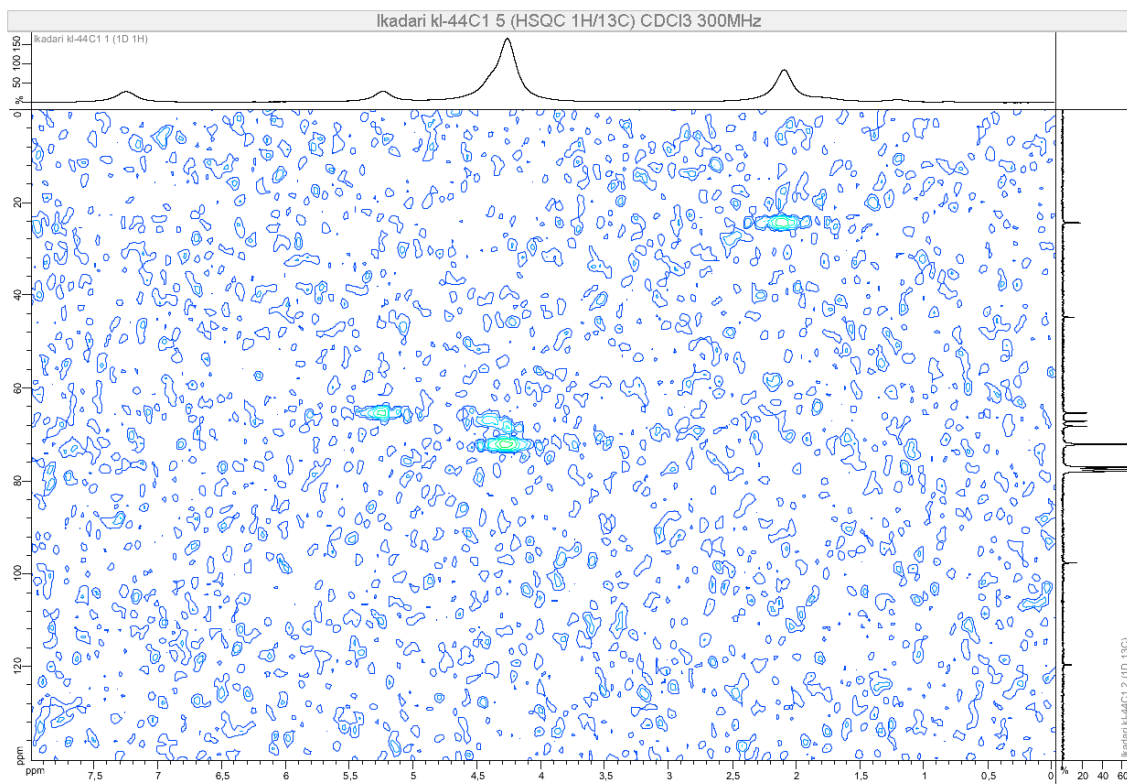
^{13}C NMR (75 MHz, CDCl_3)



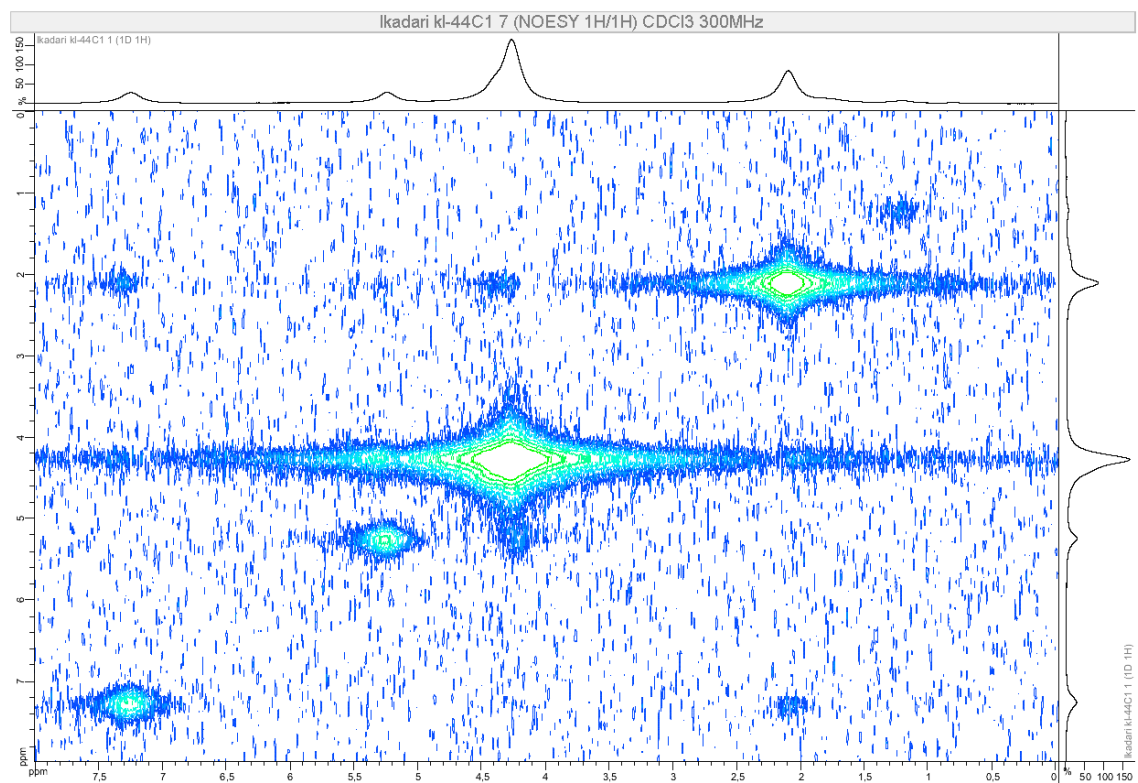
DEPT 135 (75 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

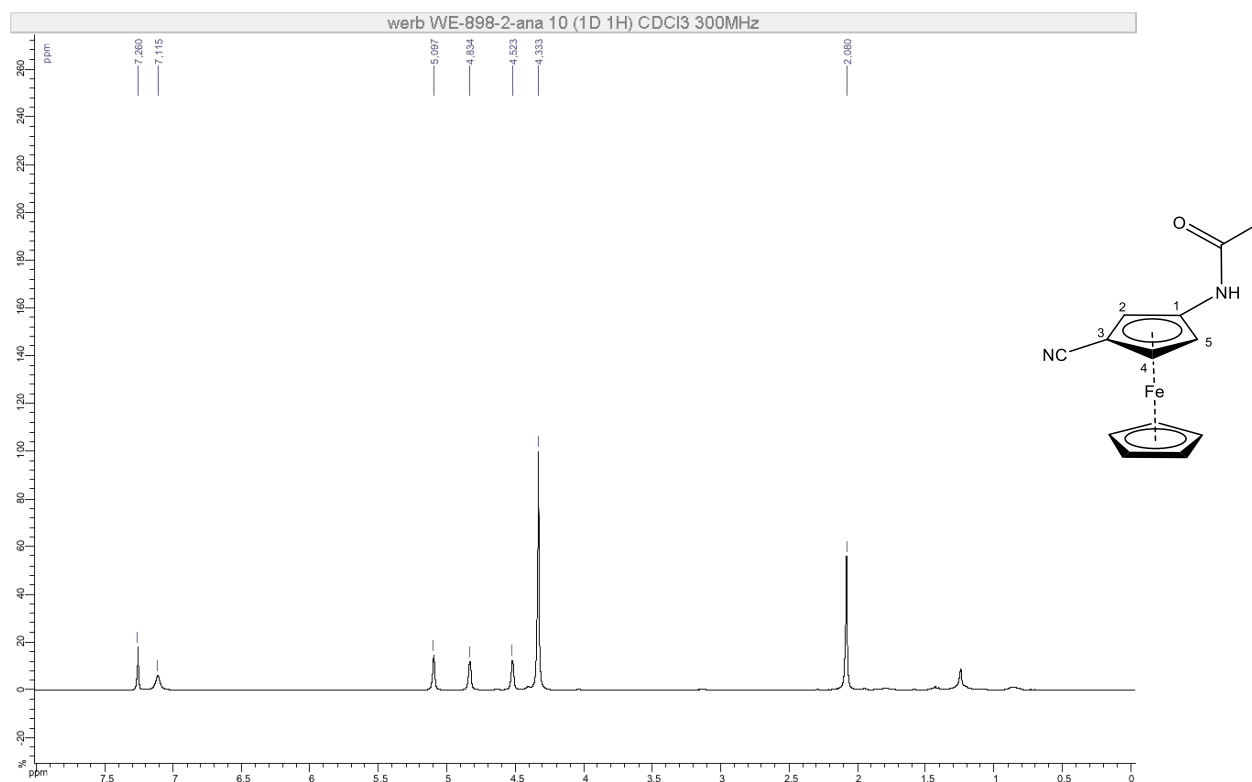


NOESY (300 MHz, CDCl₃)

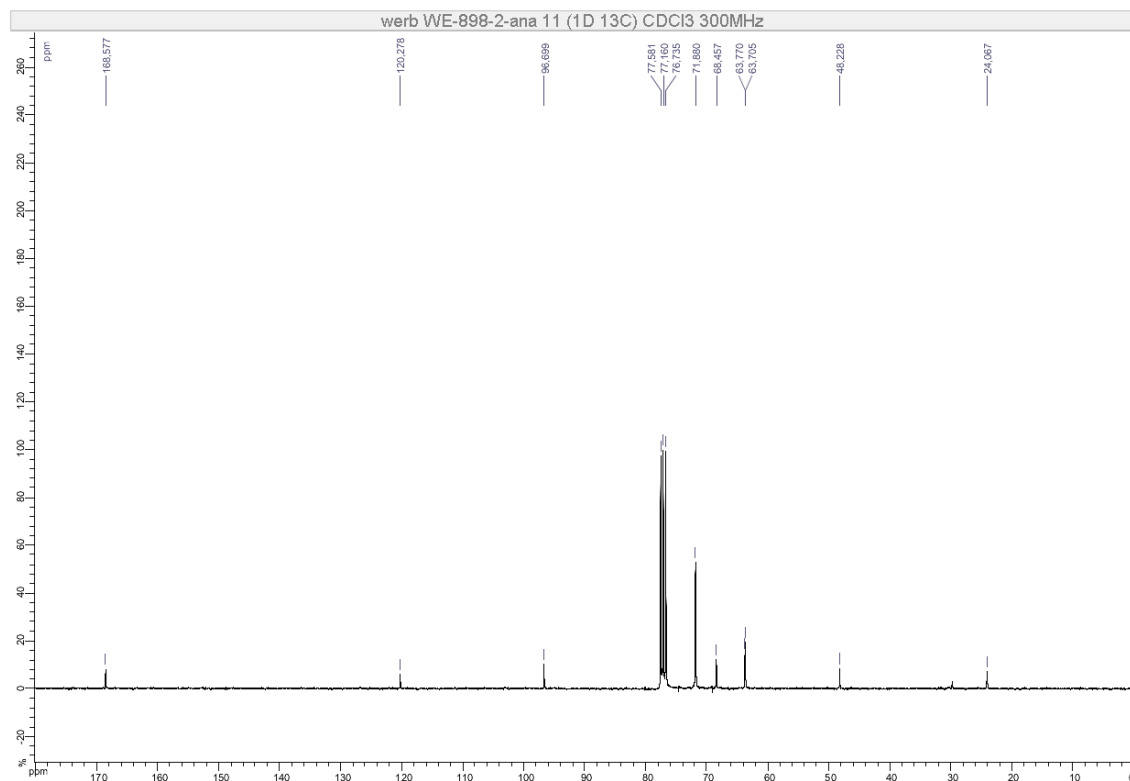


N-(3-Cyanoferrocenyl)acetamide (**4h**, racemic mixture)

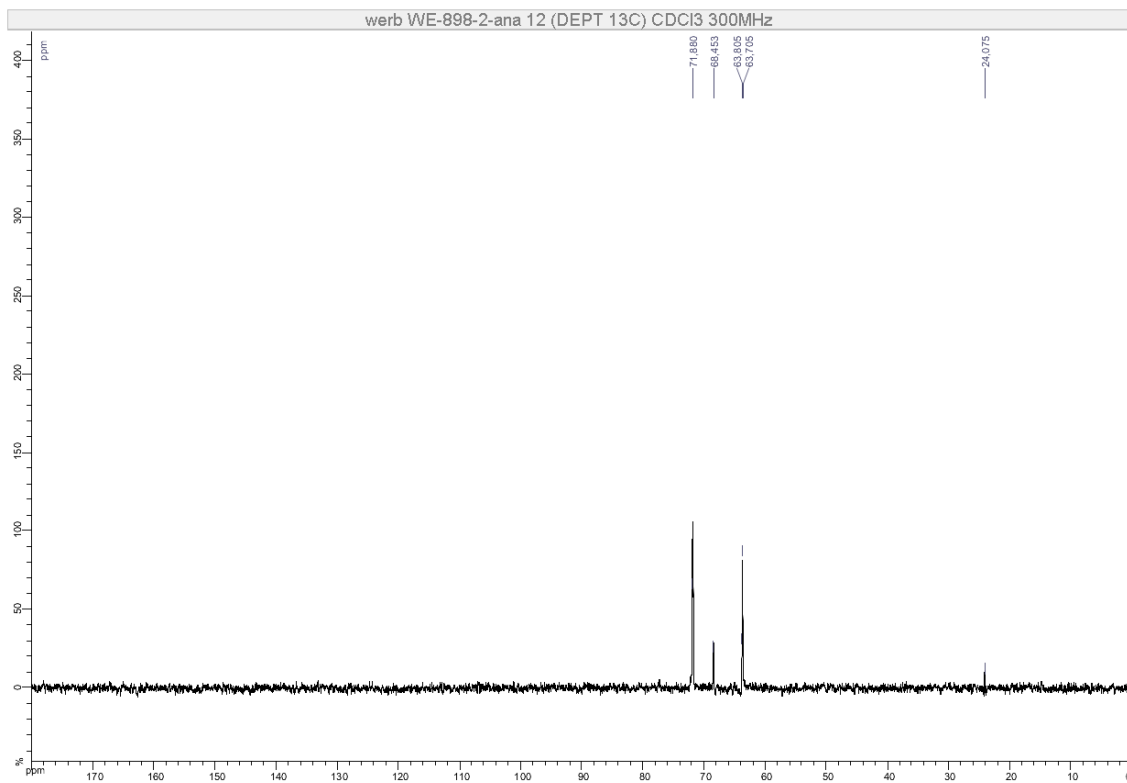
^1H NMR (300 MHz, CDCl_3)



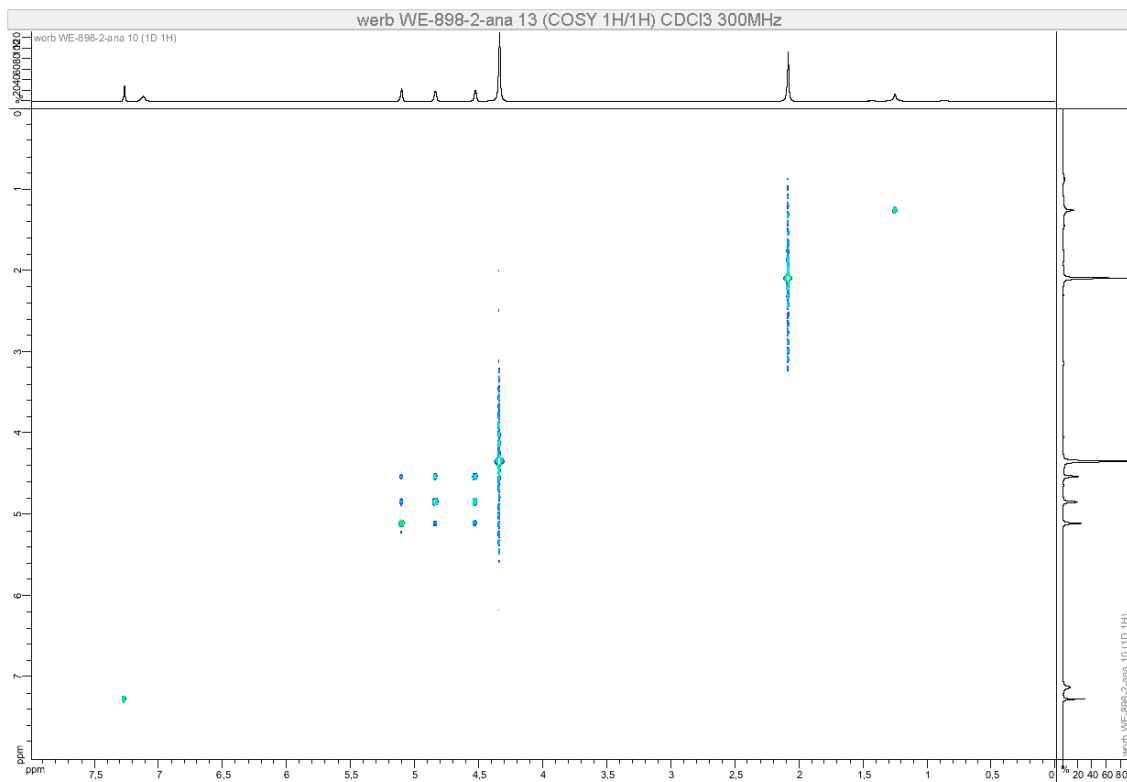
^{13}C NMR (75 MHz, CDCl_3)



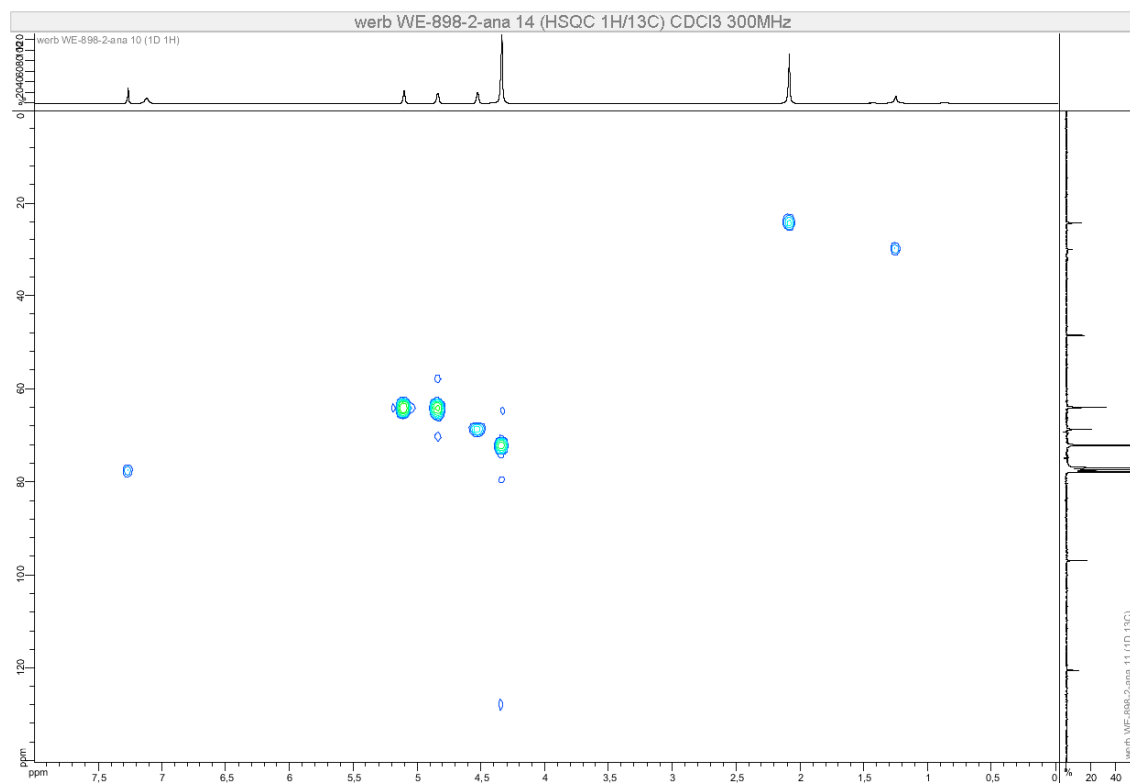
DEPT 135 (75 MHz, CDCl₃)



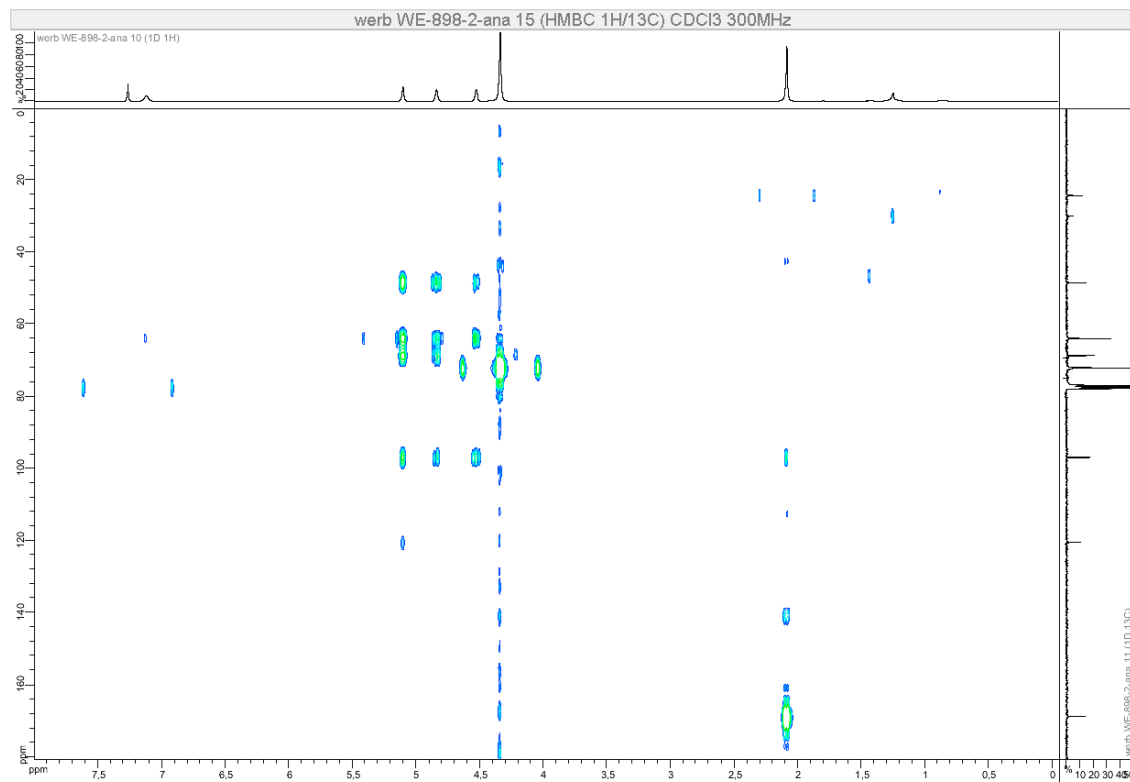
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

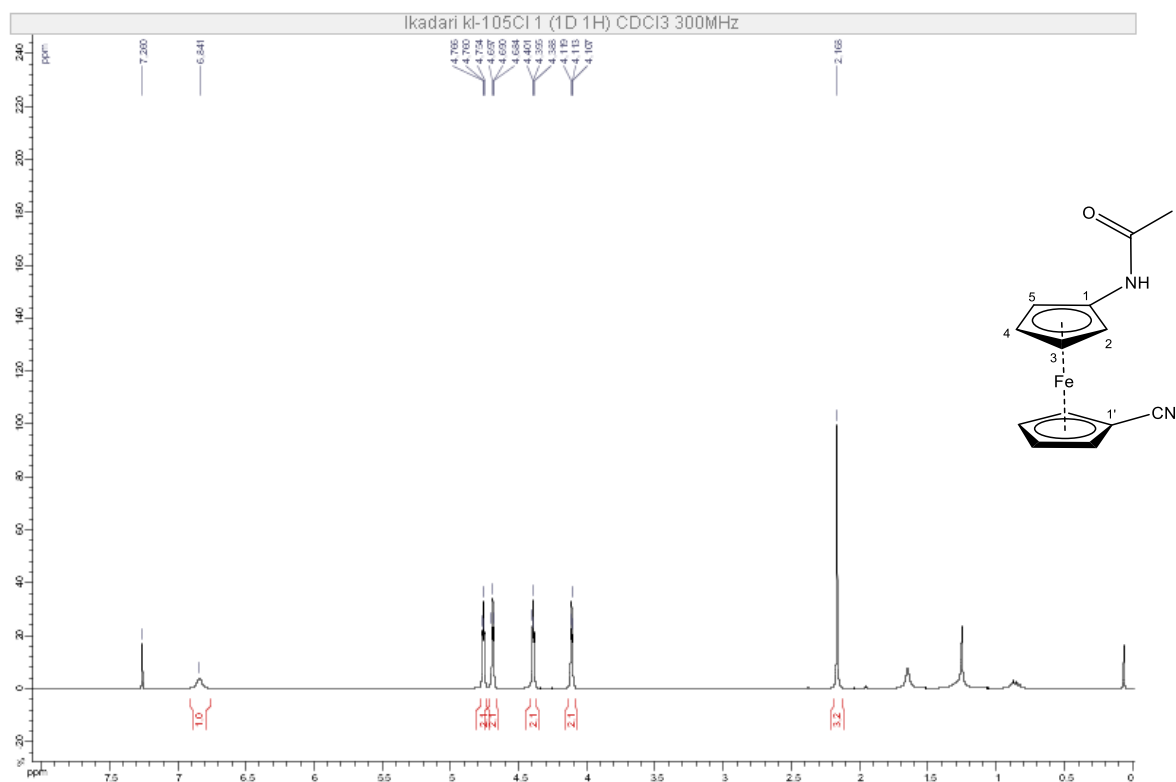


HMBC (300 MHz, CDCl₃)

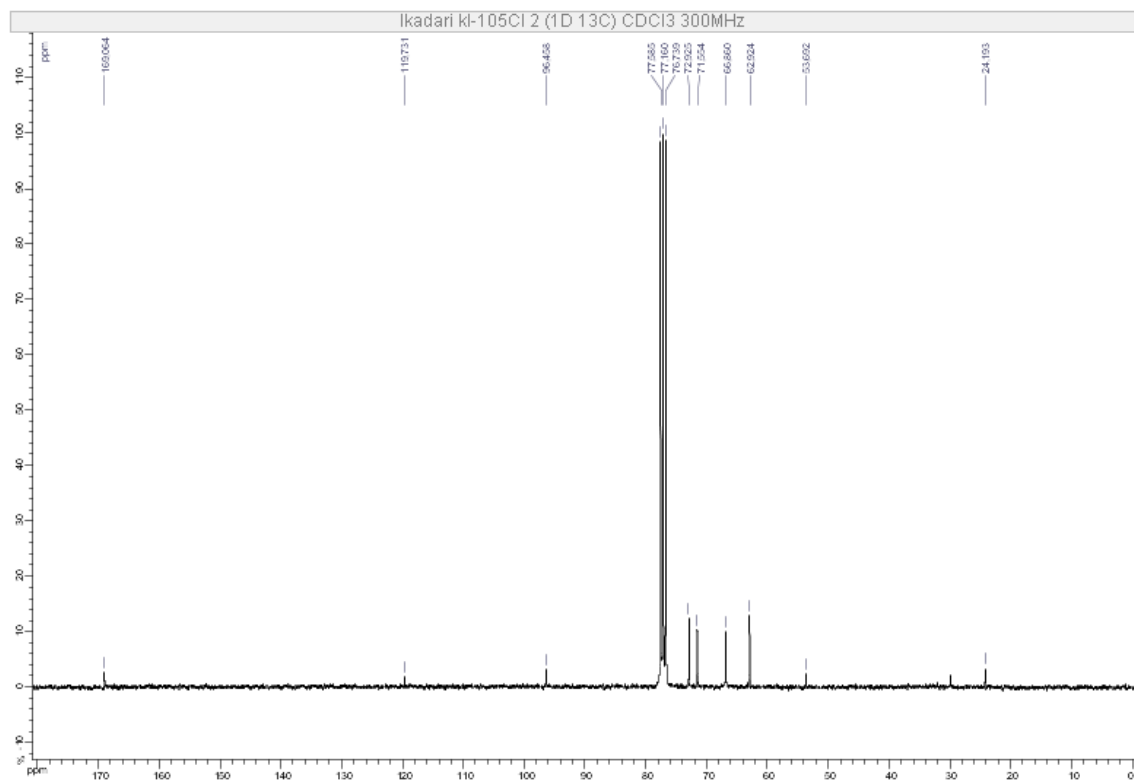


N-(1'-Cyanoferrocenyl)acetamide (6h)

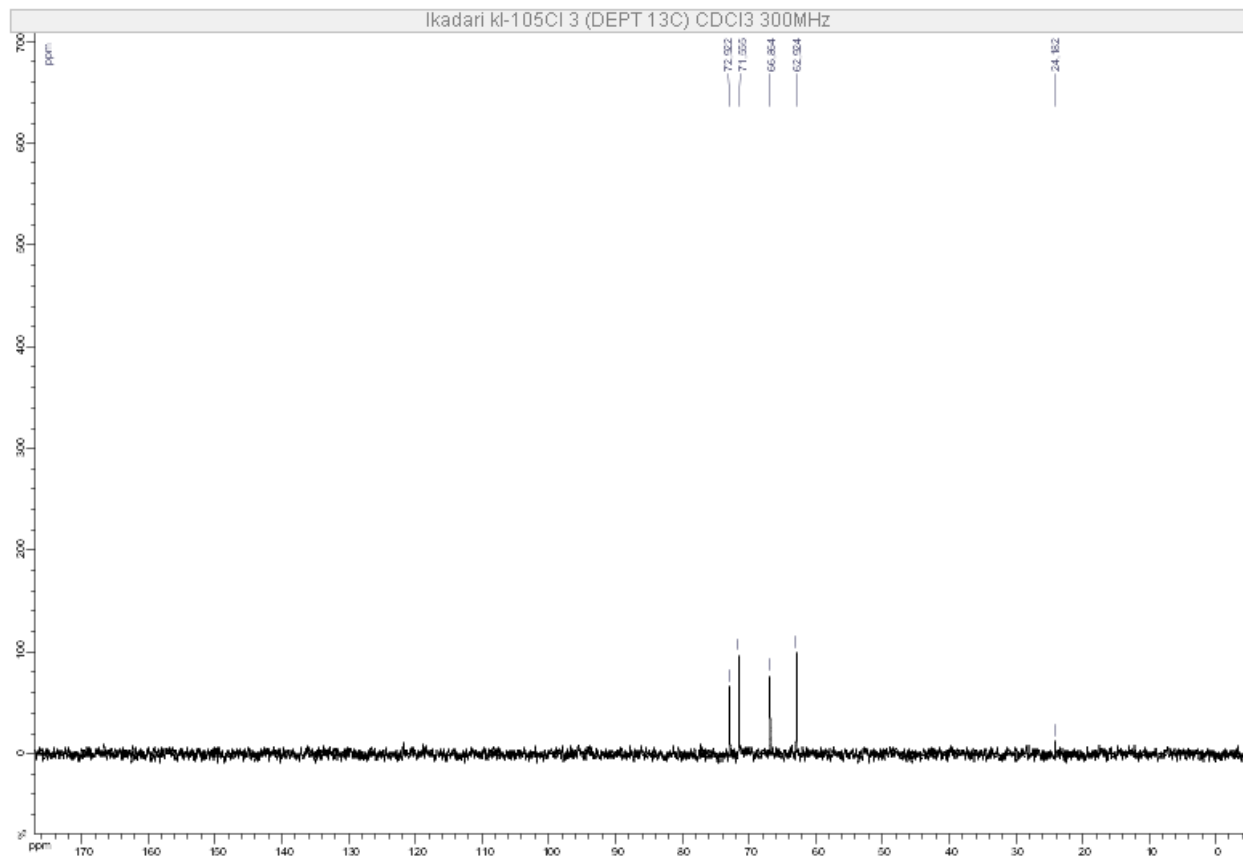
¹H NMR (300 MHz, CDCl₃)



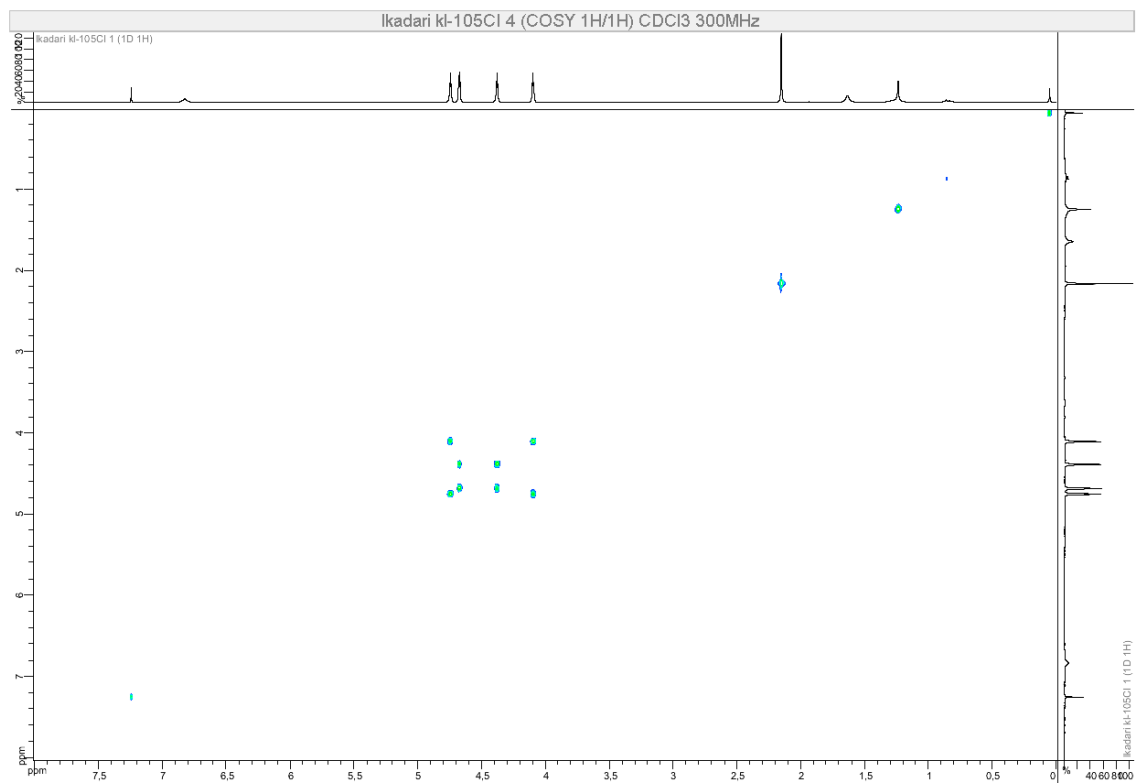
¹³C NMR (75 MHz, CDCl₃)



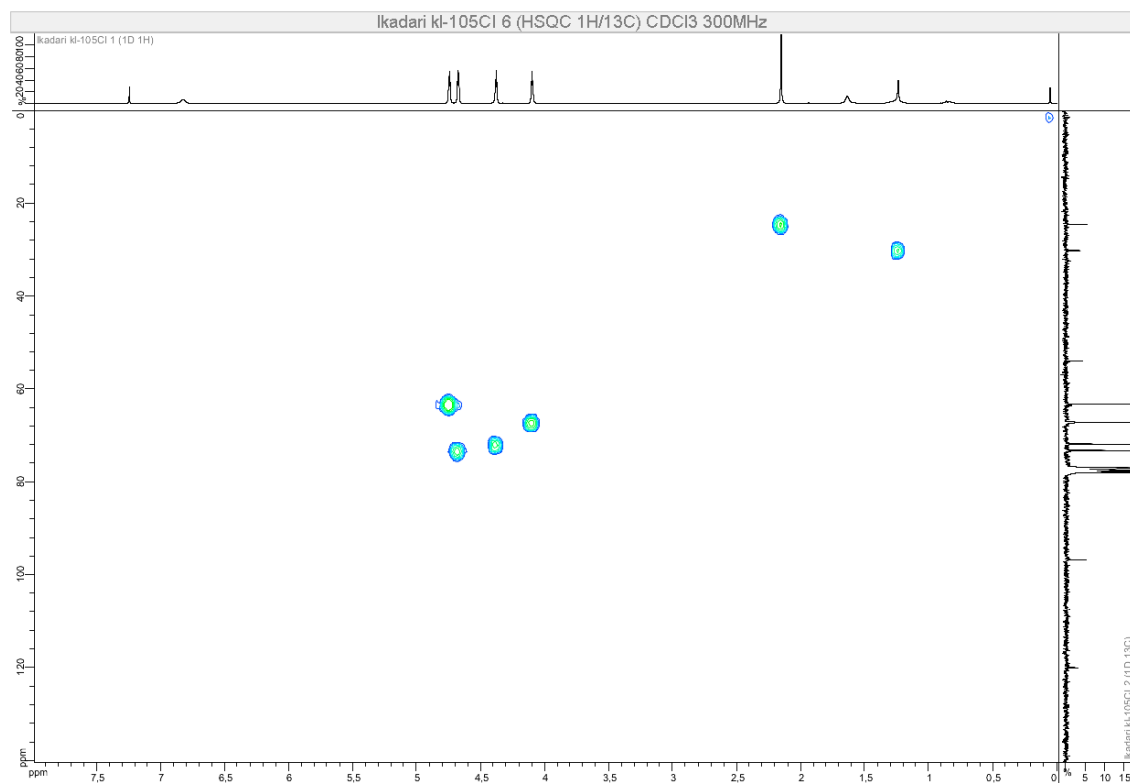
DEPT 135 (75 MHz, CDCl₃)



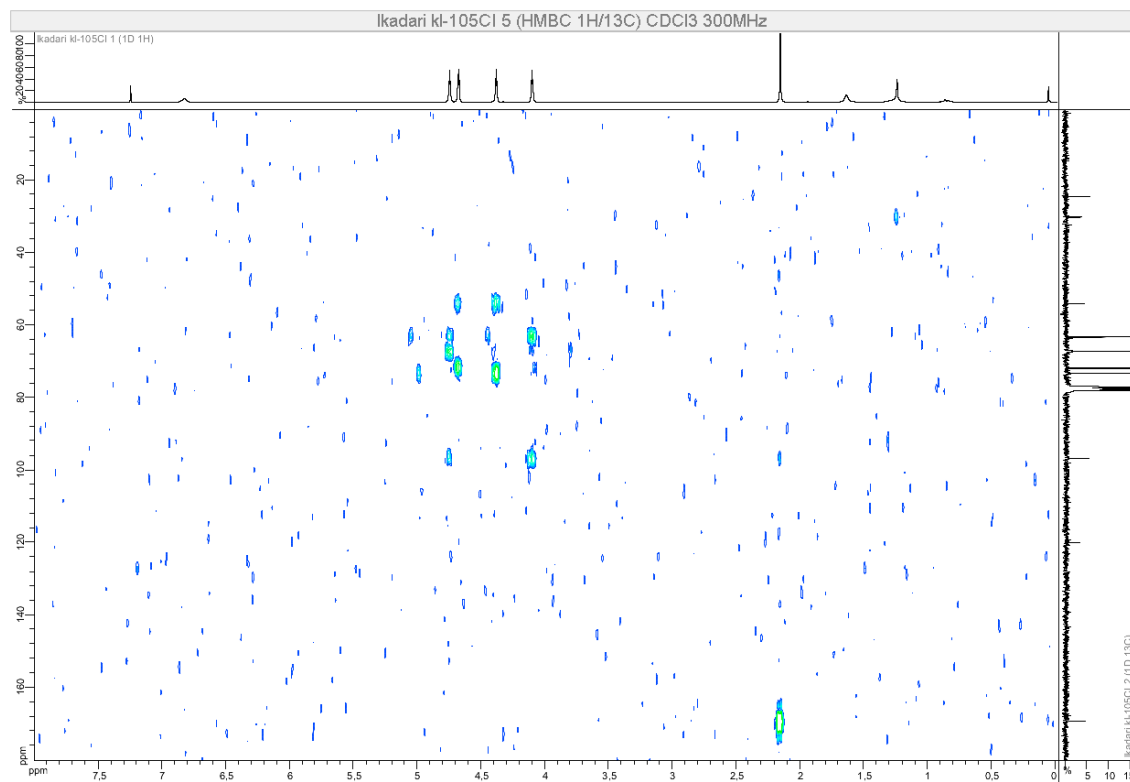
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

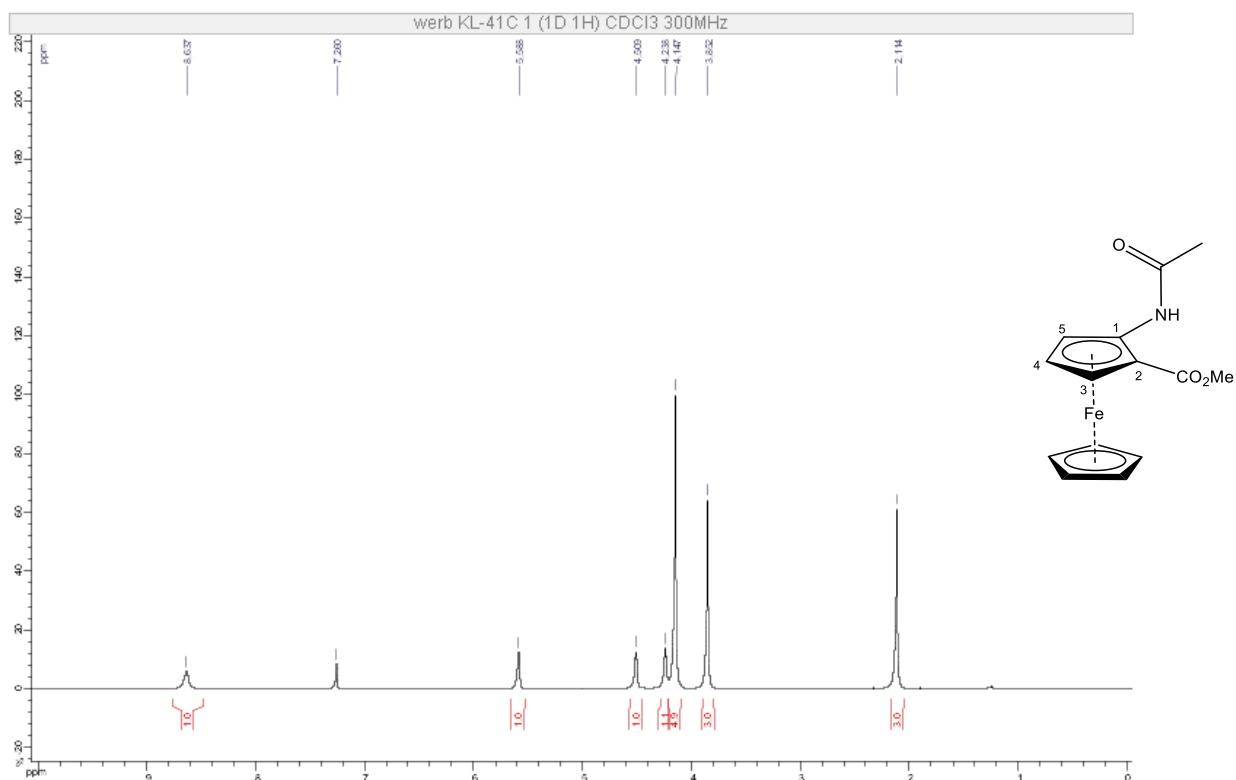


HMBC (300 MHz, CDCl₃)

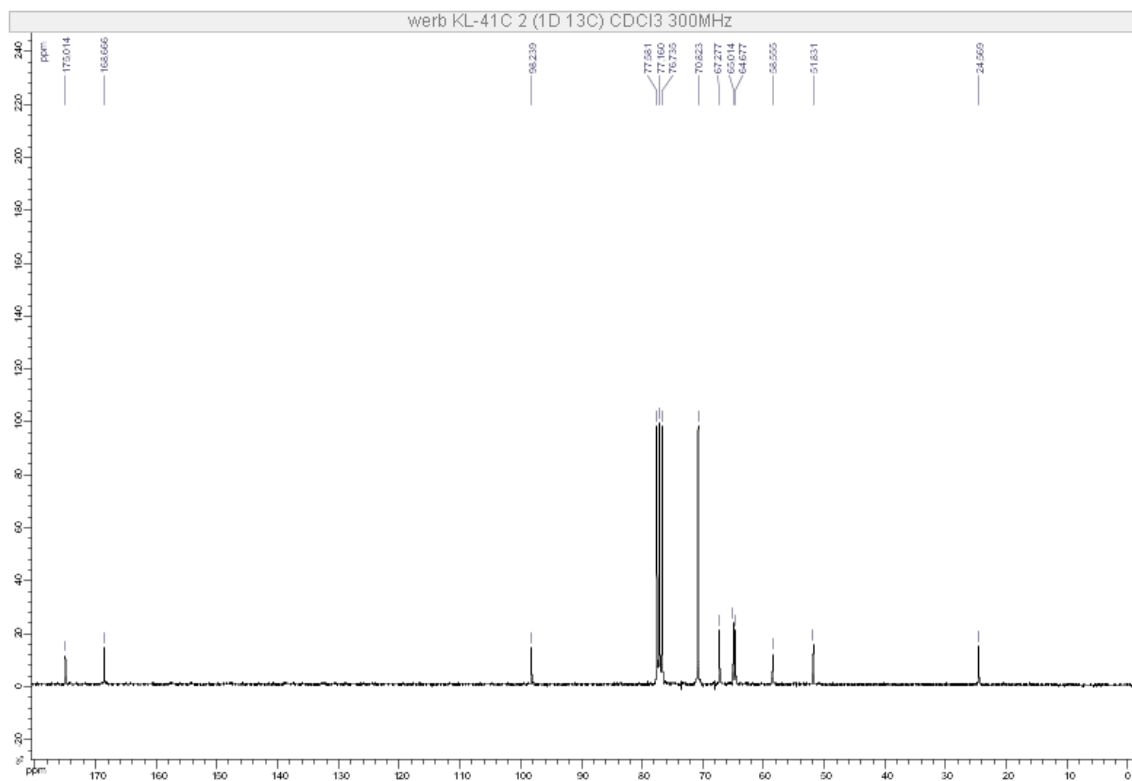


N-(2-(Methoxycarbonyl)ferrocenyl)acetamide (**2i**, racemic mixture)

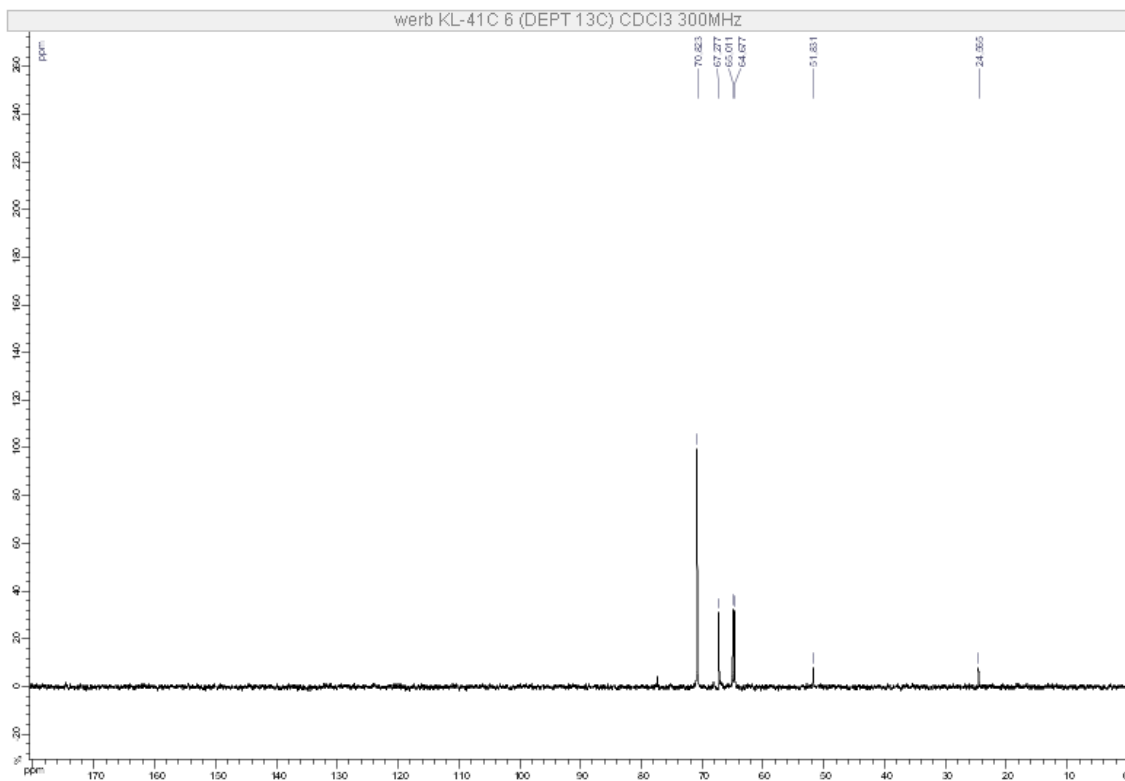
^1H NMR (300 MHz, CDCl_3)



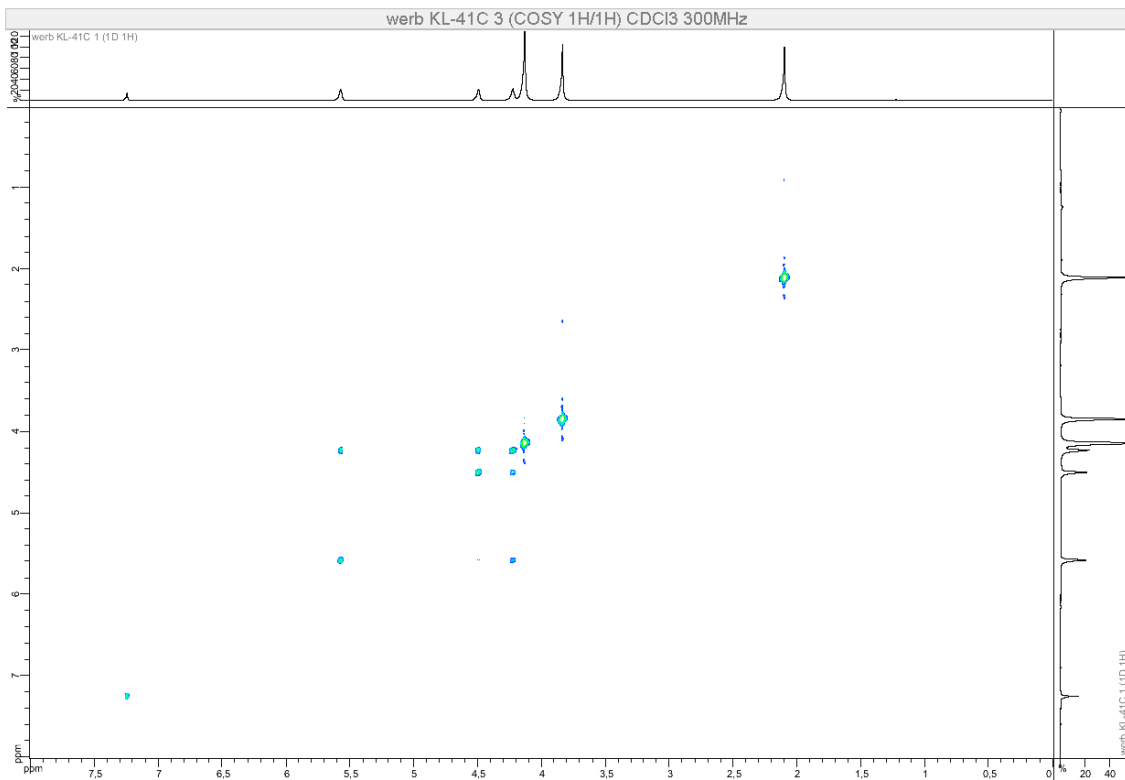
^{13}C NMR (75 MHz, CDCl_3)



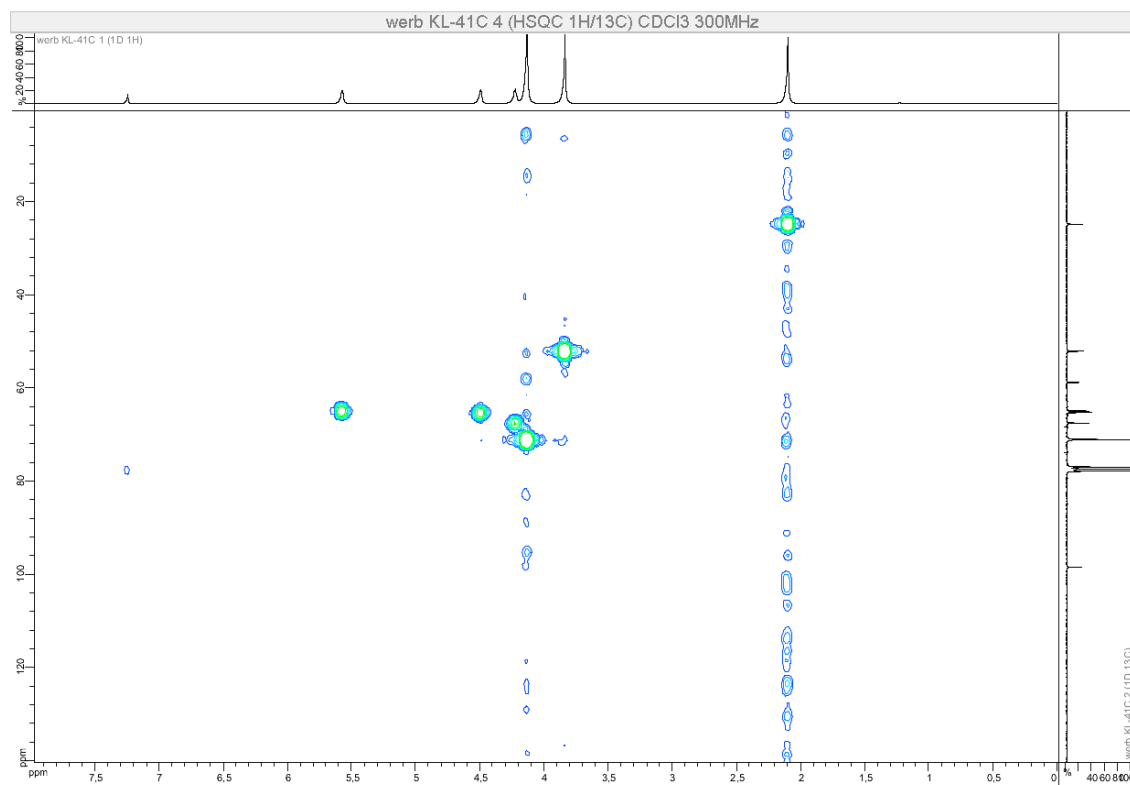
DEPT 135 (75 MHz, CDCl₃)



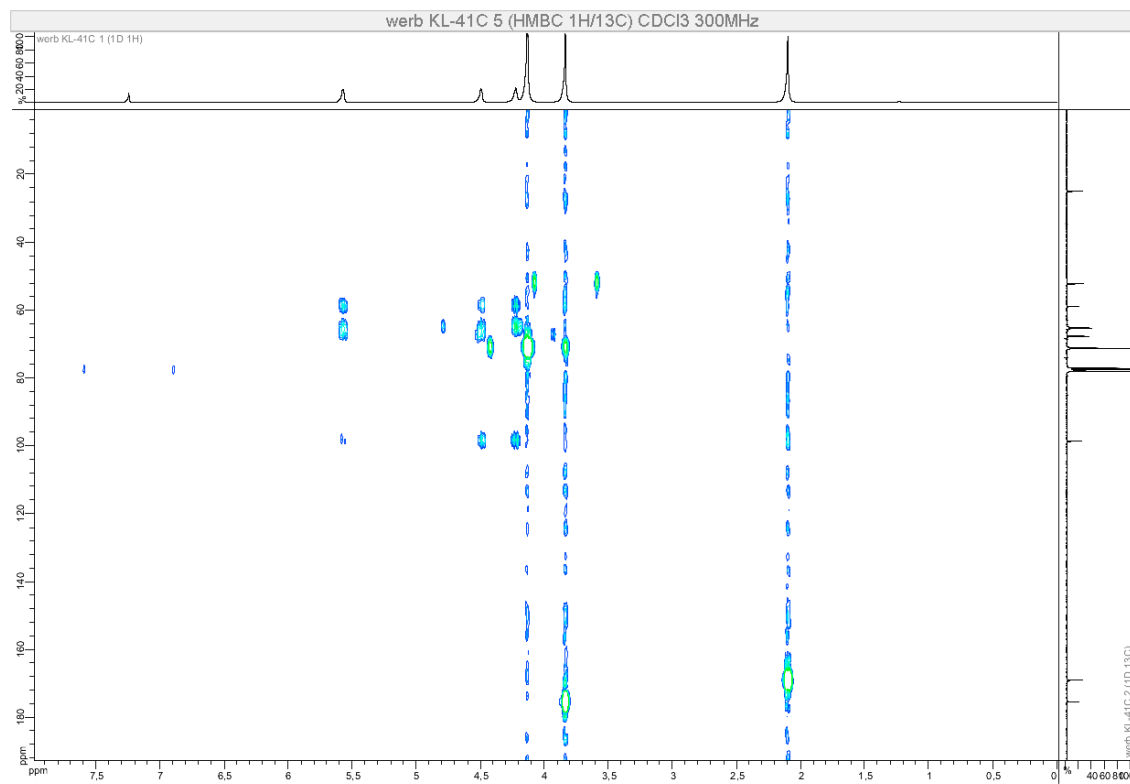
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

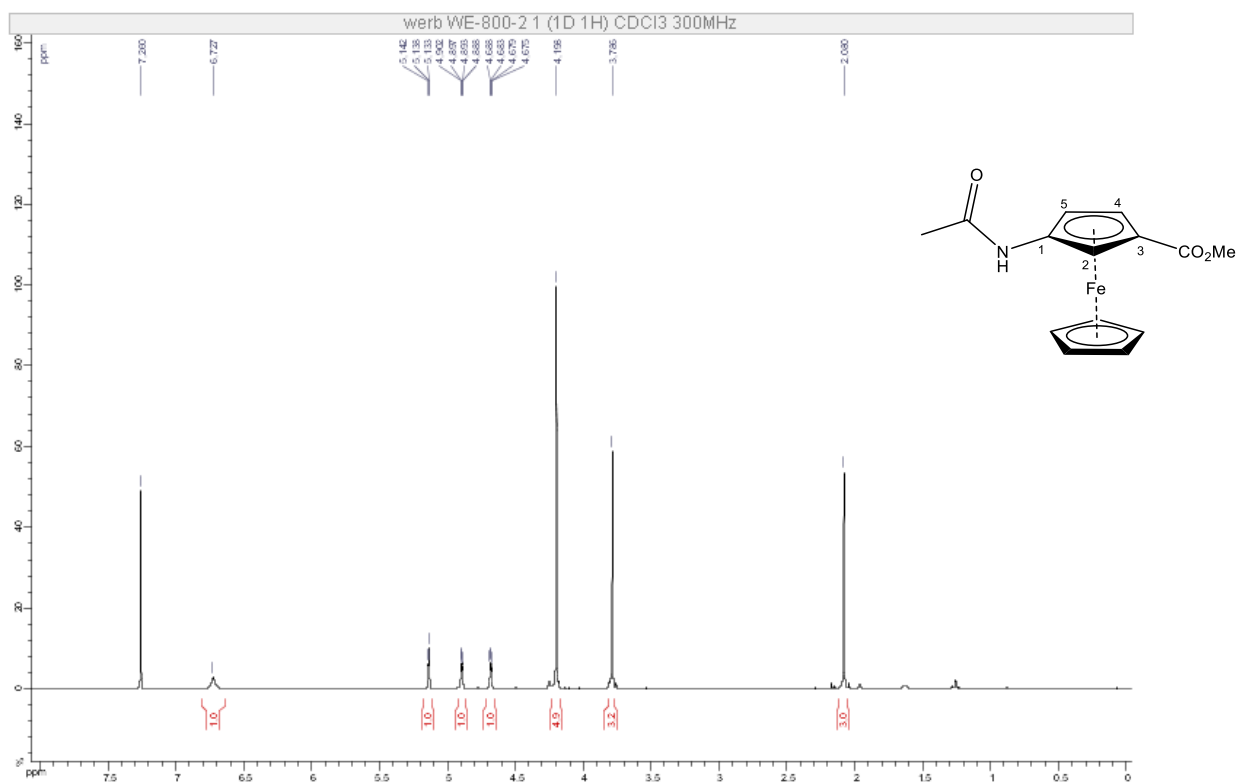


HMBC (300 MHz, CDCl₃)

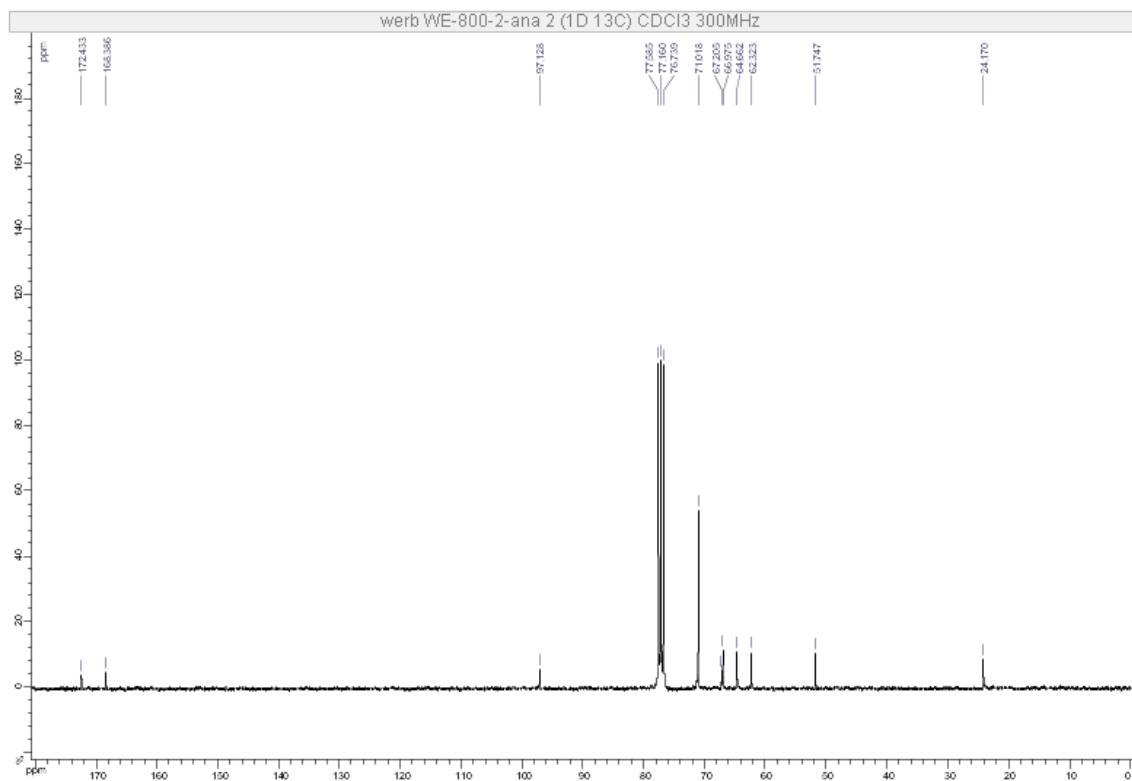


N-(3-(Methoxycarbonyl)ferrocenyl)acetamide (**4i**, racemic mixture)

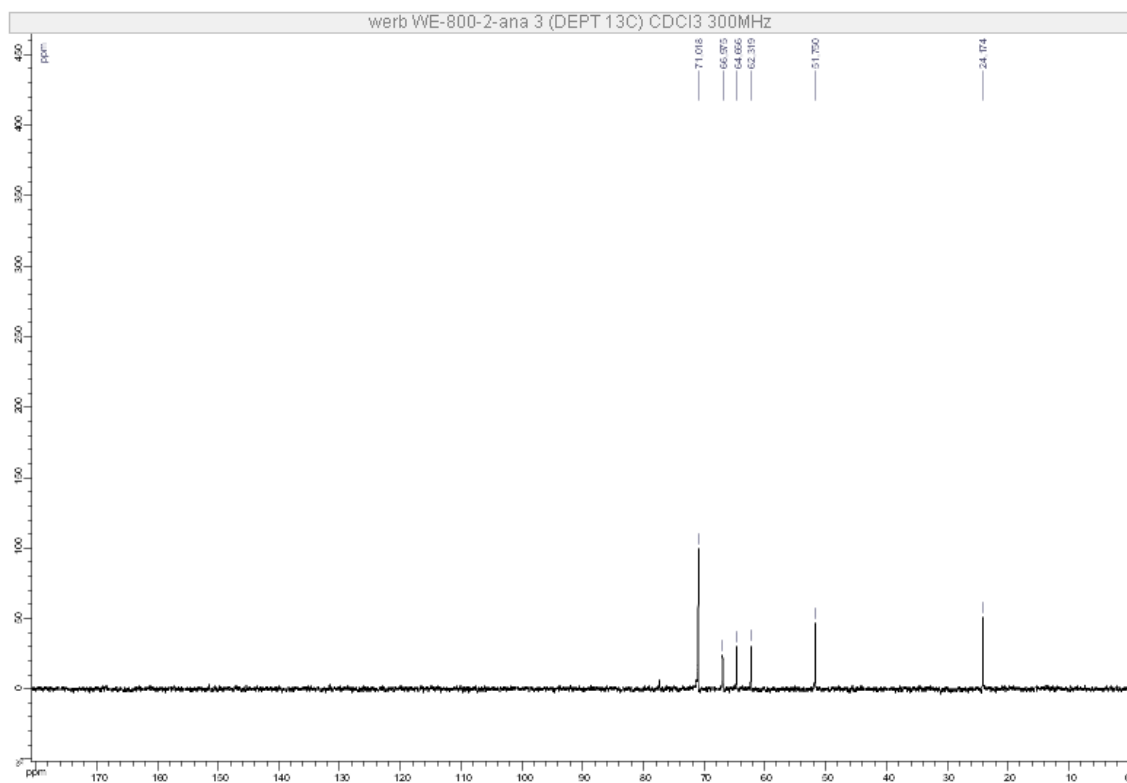
^1H NMR (300 MHz, CDCl_3)



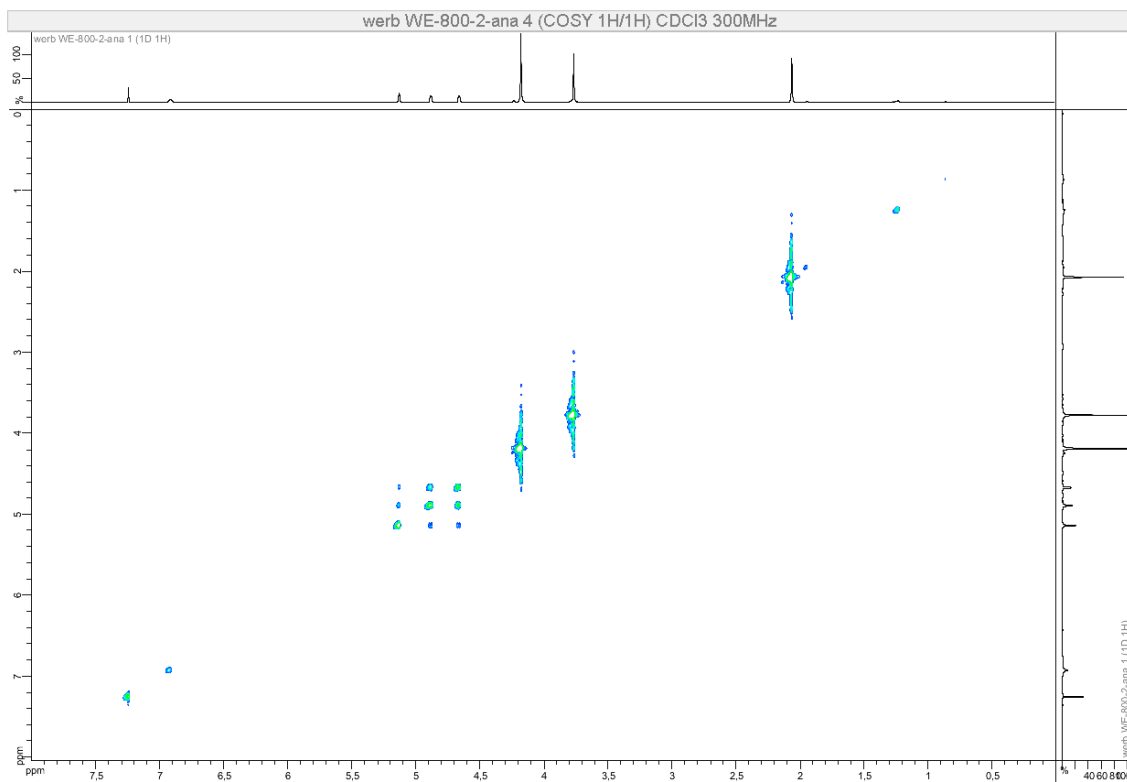
^{13}C NMR (75 MHz, CDCl_3)



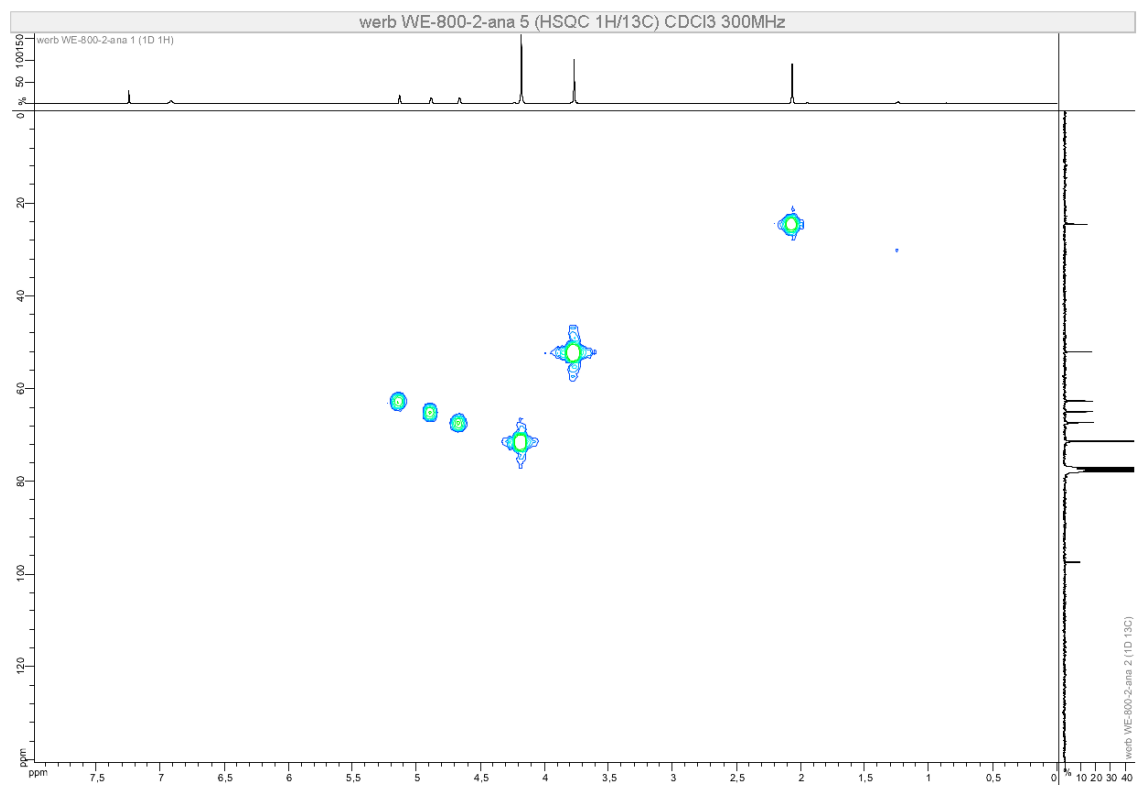
DEPT 135 (75 MHz, CDCl₃)



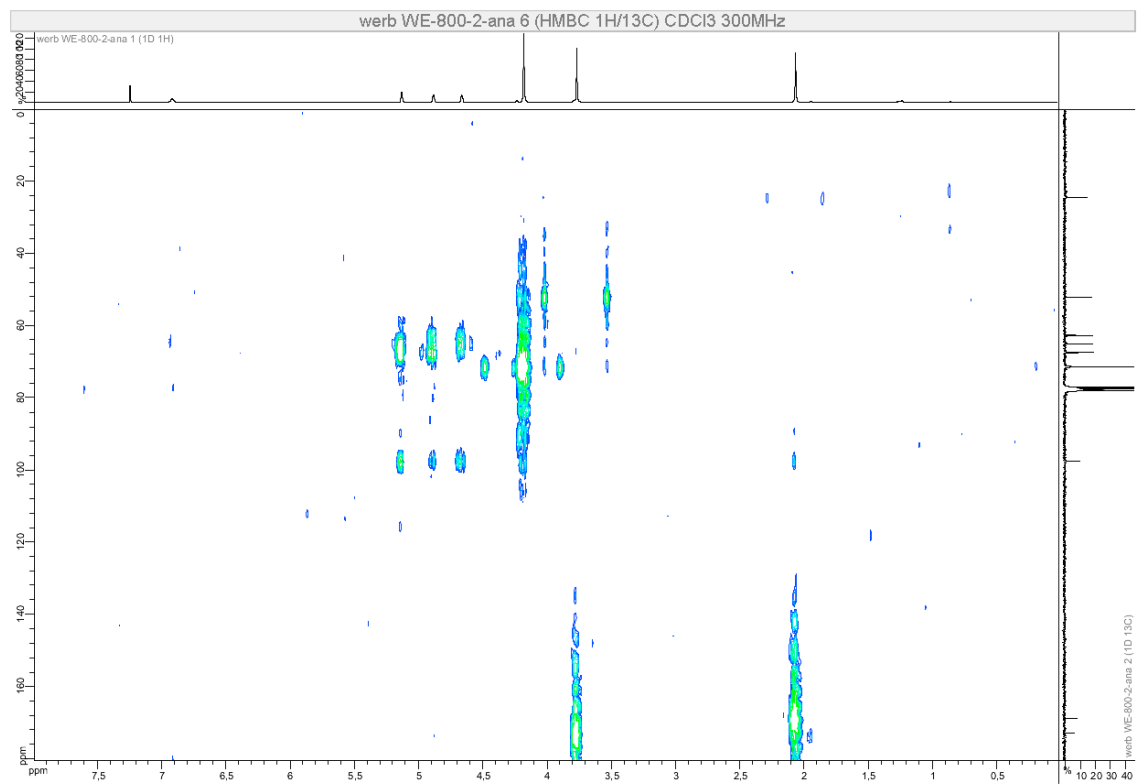
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

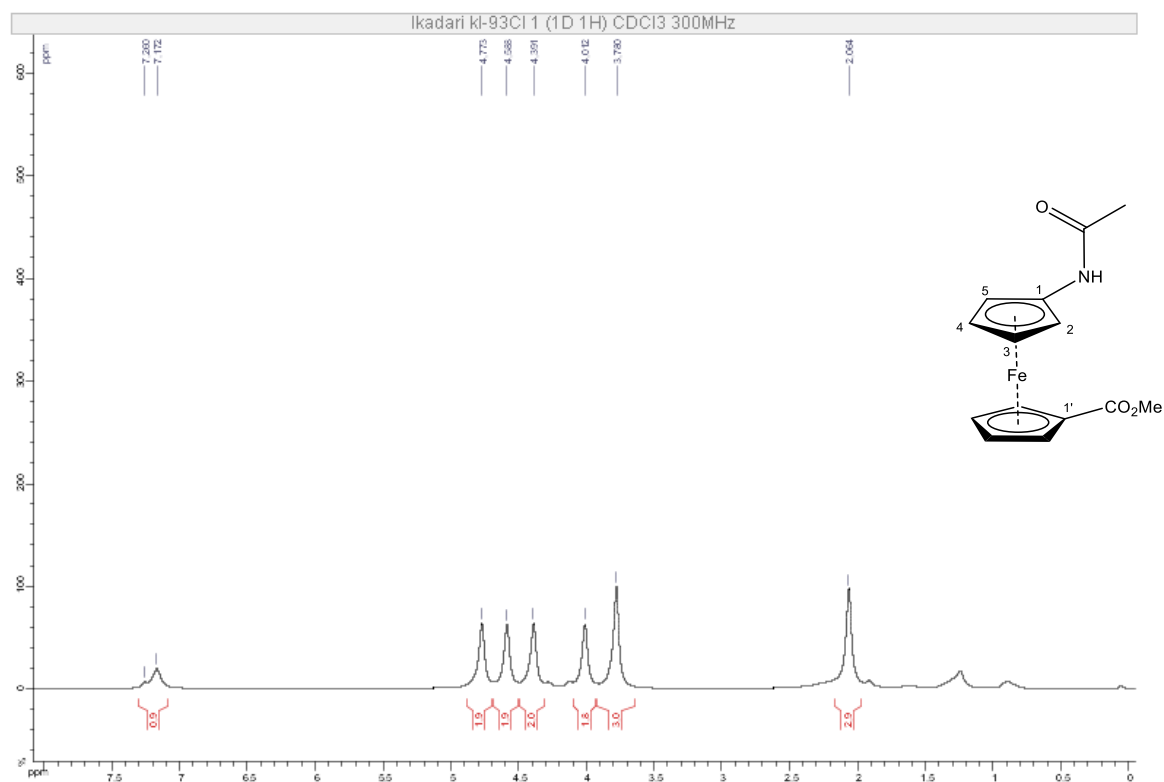


HMBC (300 MHz, CDCl₃)

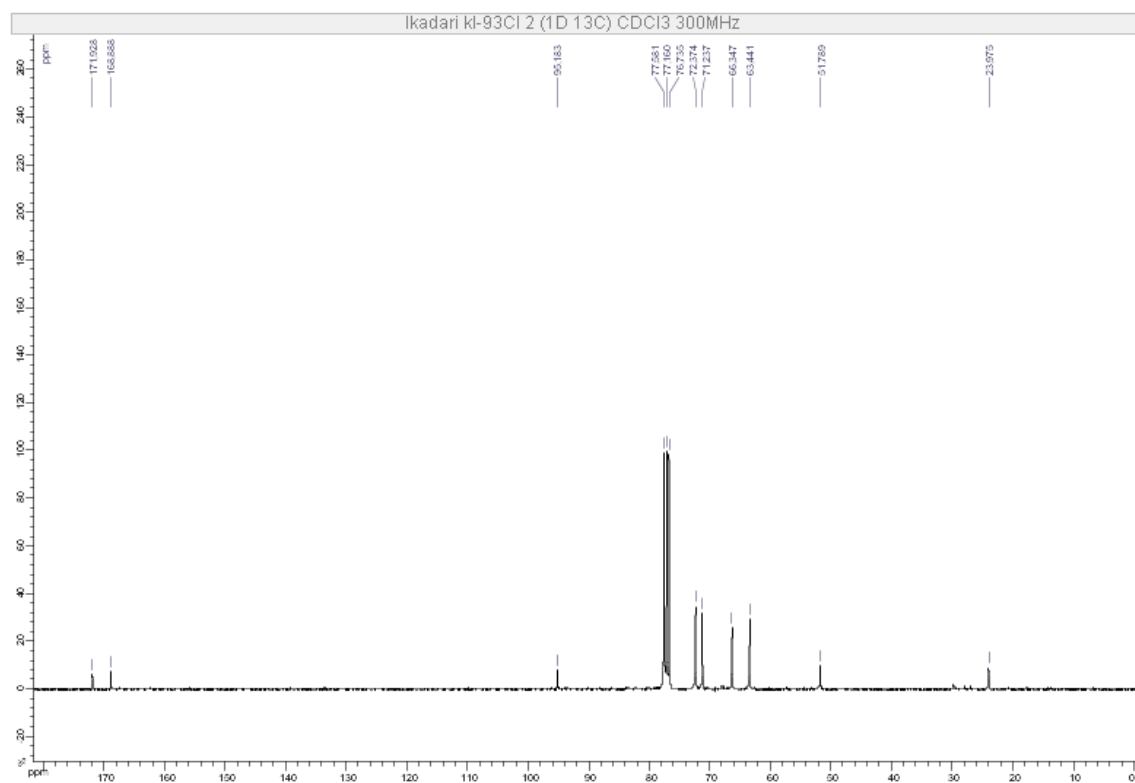


N-(1'-(Methoxycarbonyl)ferrocenyl)acetamide (**6i**)

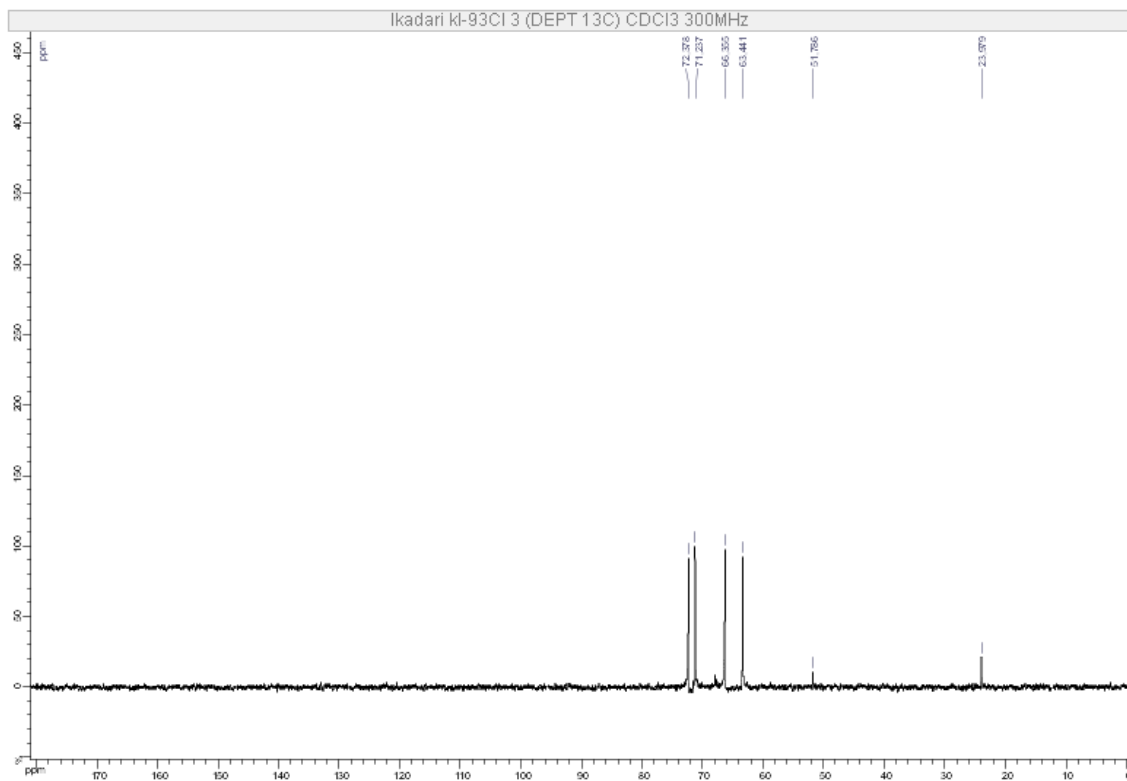
^1H NMR (300 MHz, CDCl_3)



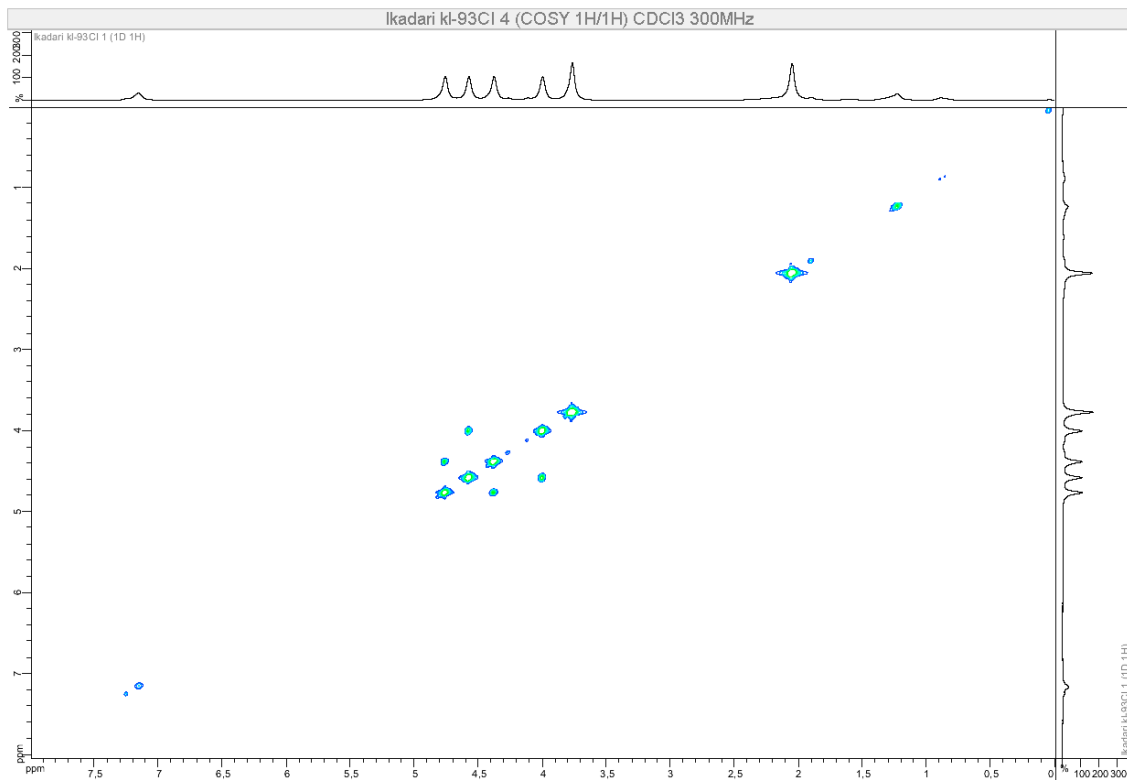
^{13}C NMR (75 MHz, CDCl_3)



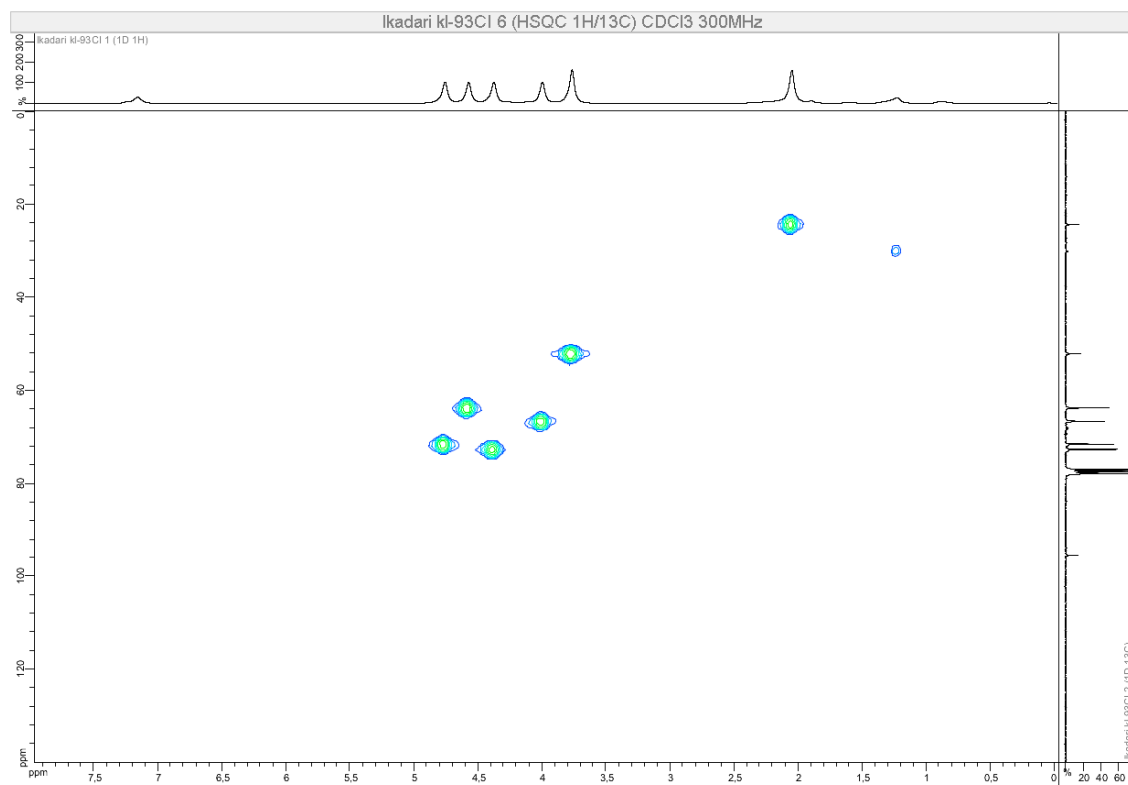
DEPT 135 (75 MHz, CDCl₃)



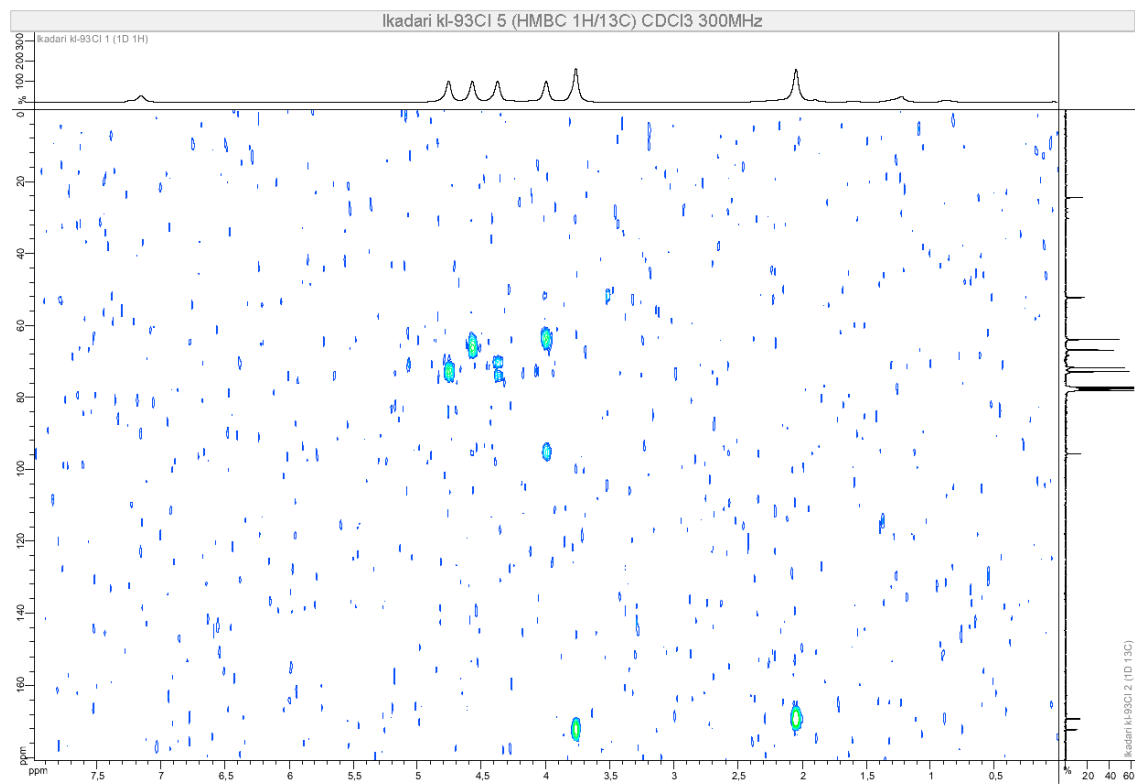
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

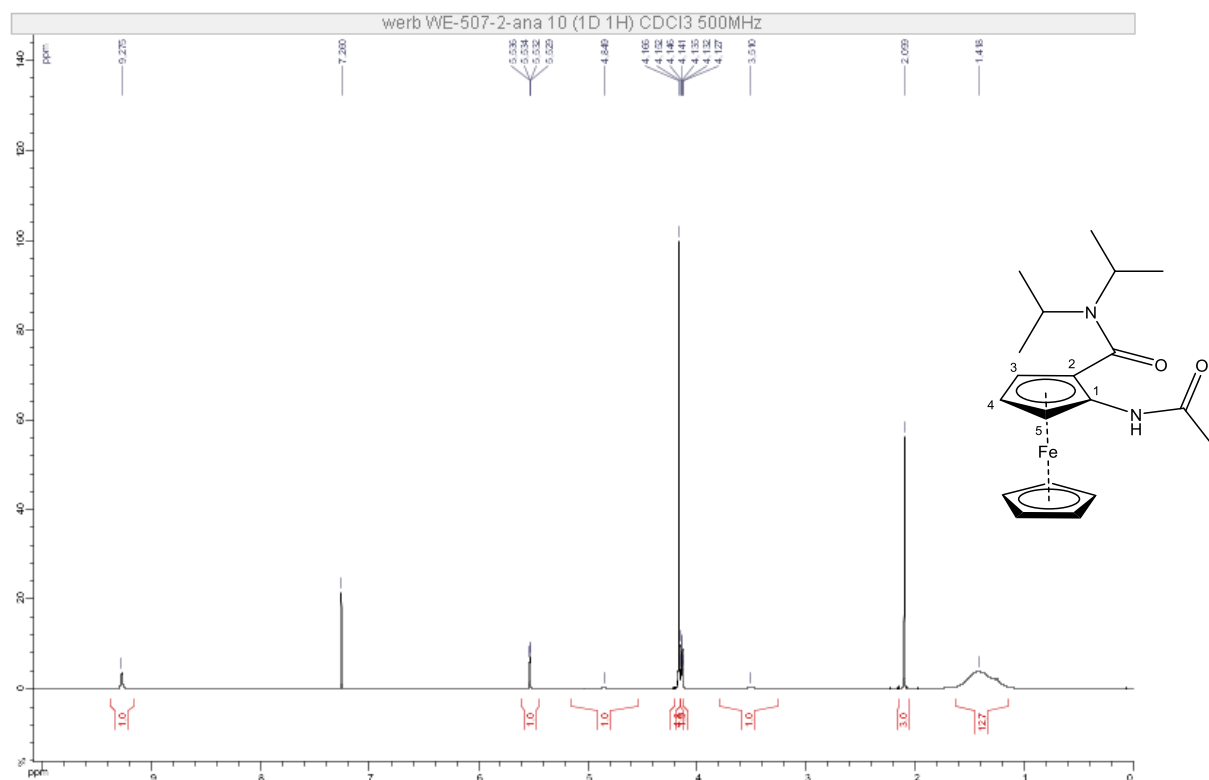


HMBC (300 MHz, CDCl₃)

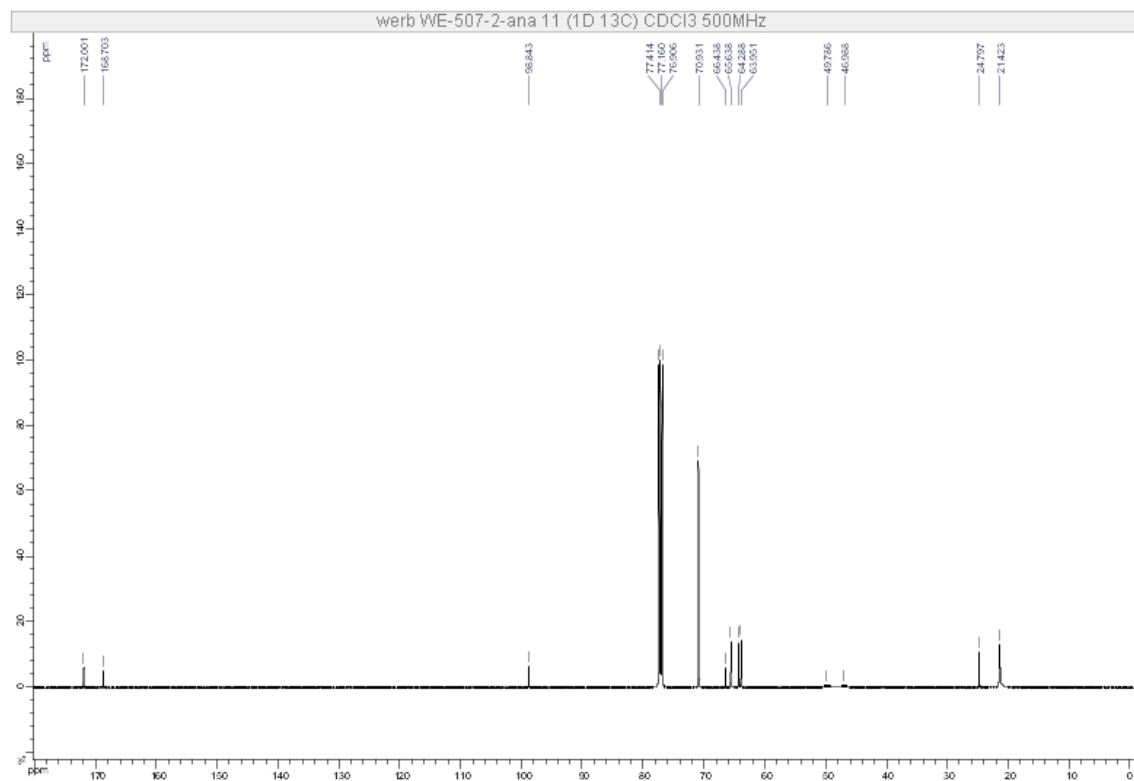


N-(2-(Diisopropylaminocarbonyl)ferrocenyl)acetamide (**2j**, racemic mixture)

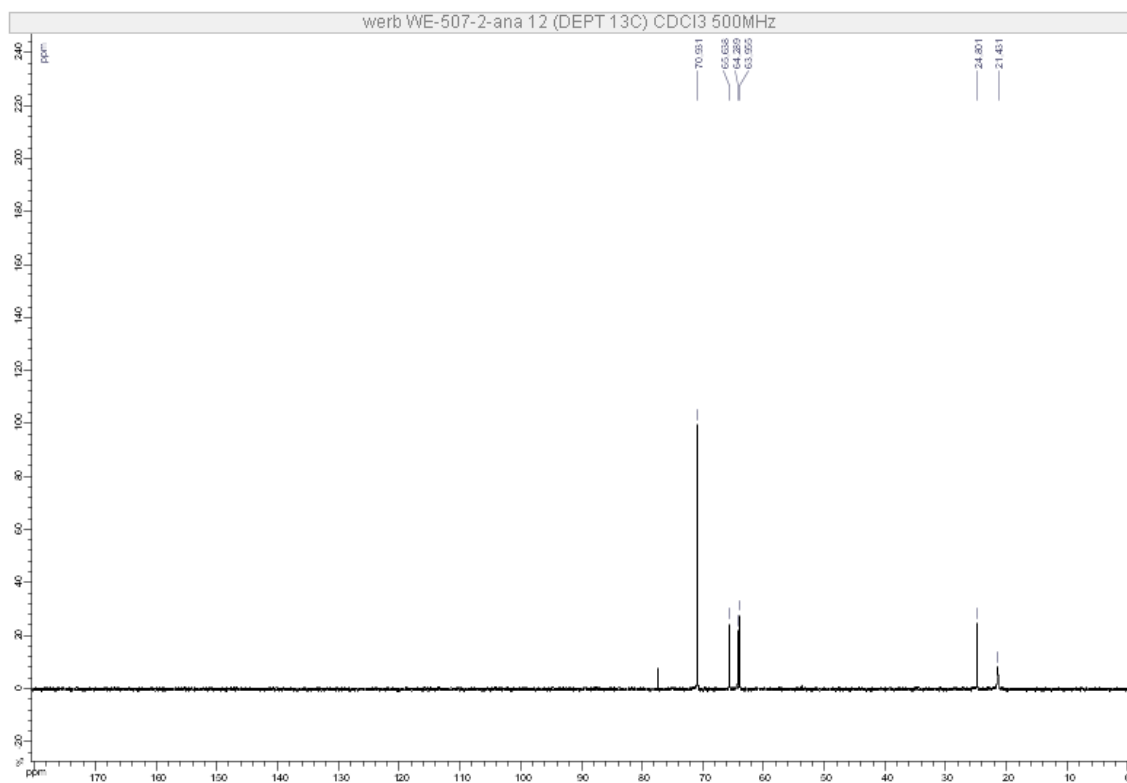
^1H NMR (500 MHz, CDCl_3)



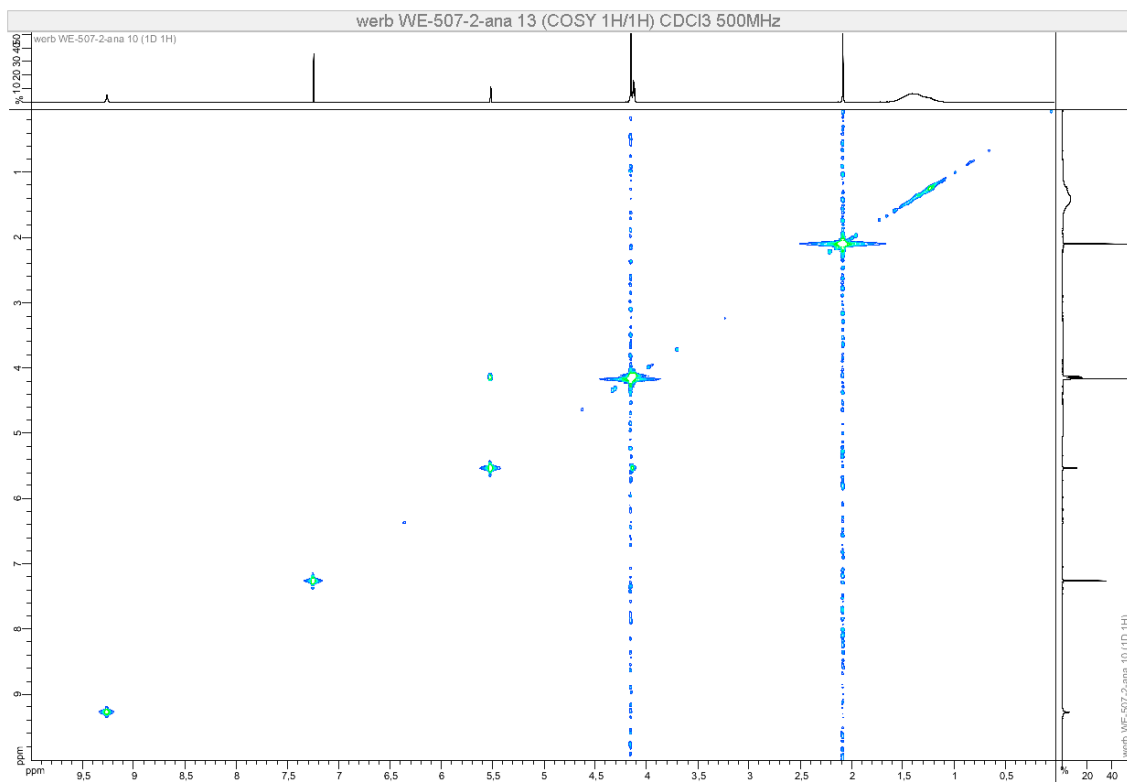
^{13}C NMR (126 MHz, CDCl_3)



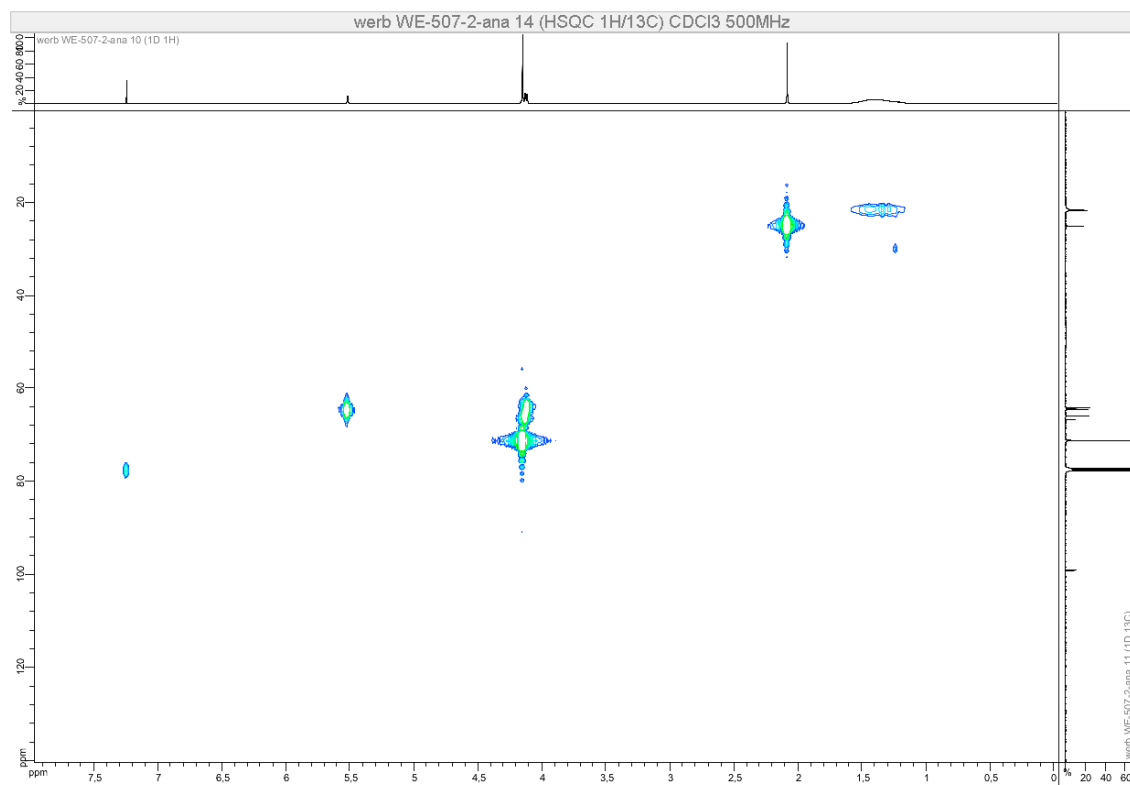
DEPT 135 (126 MHz, CDCl₃)



COSY (500 MHz, CDCl₃)



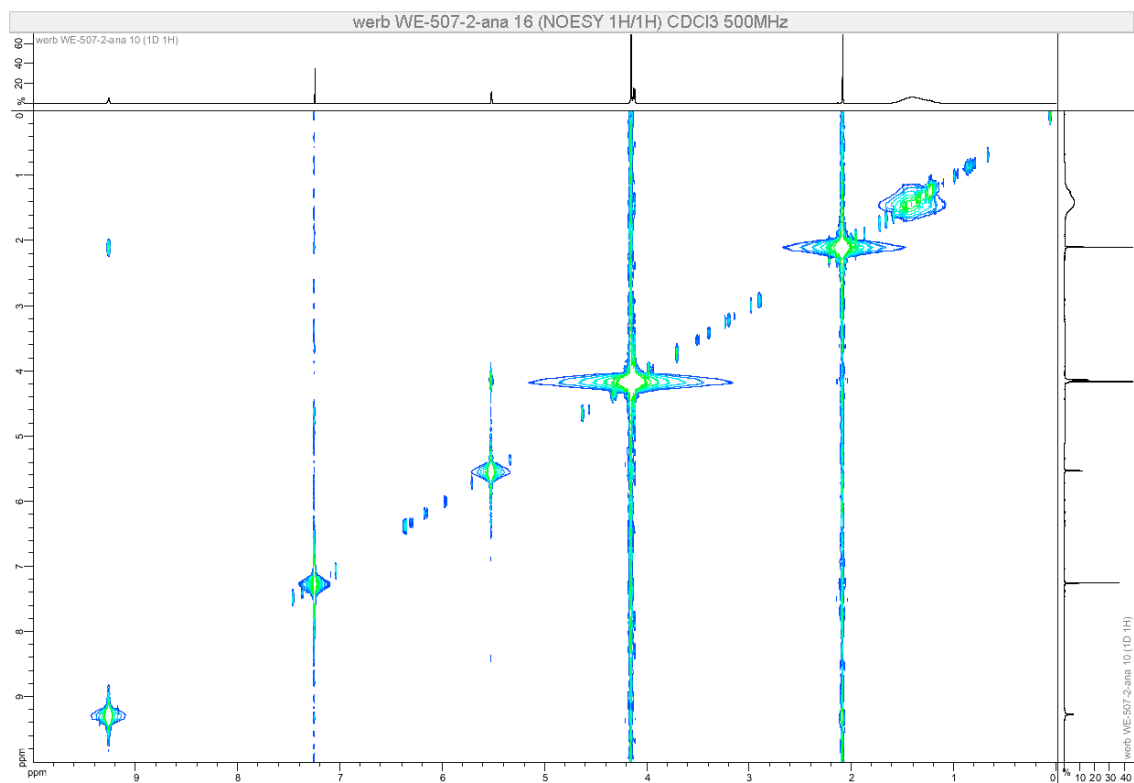
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

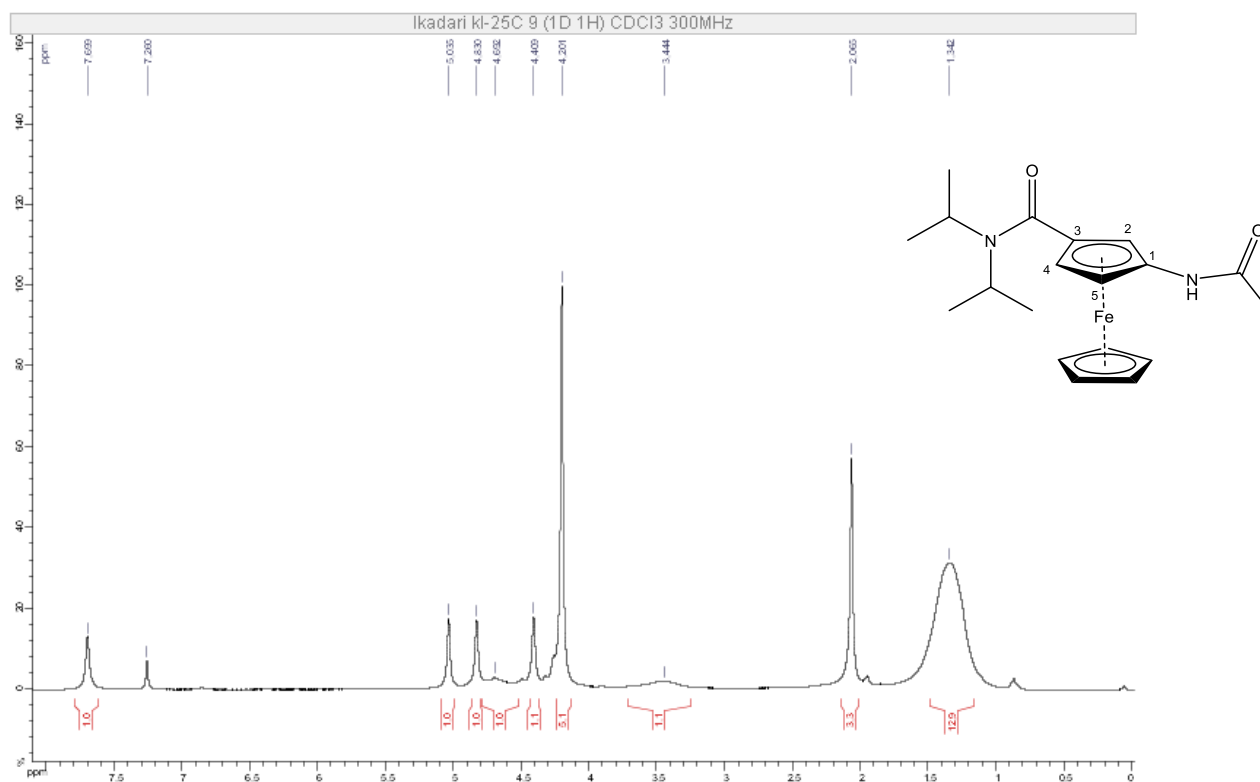


NOESY (500 MHz, CDCl₃)

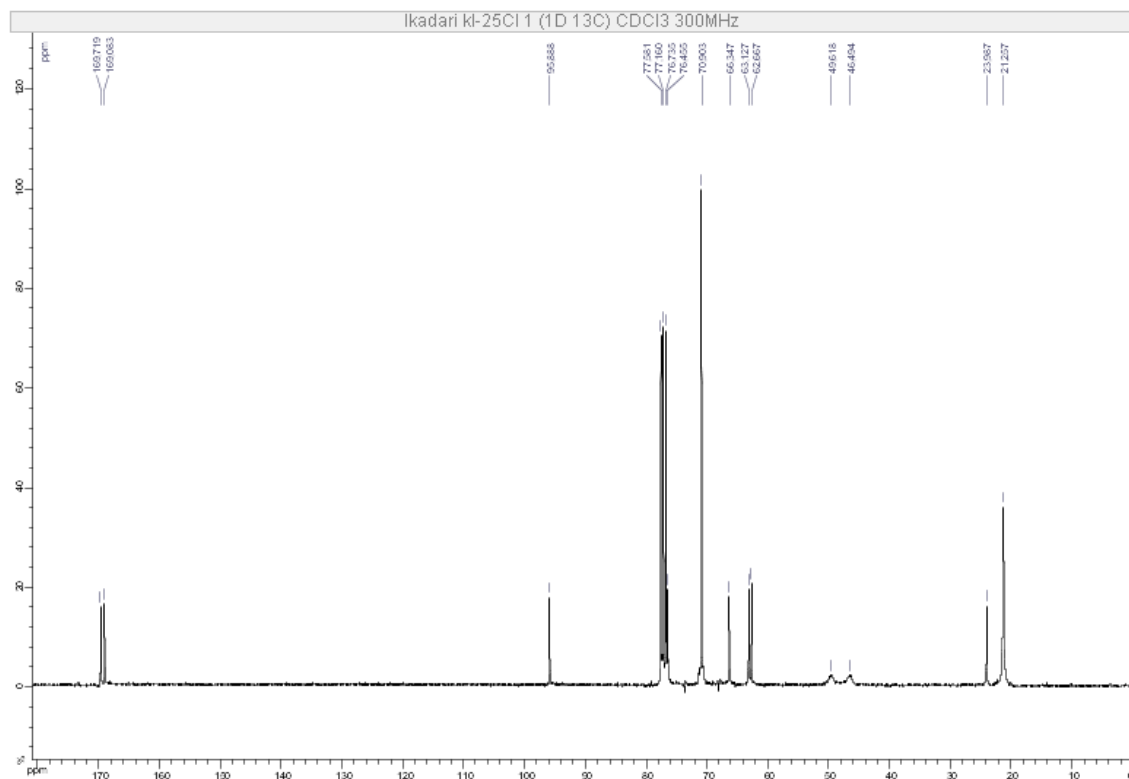


N-(3-(Diisopropylaminocarbonyl)ferrocenyl)acetamide (**4j**, racemic mixture)

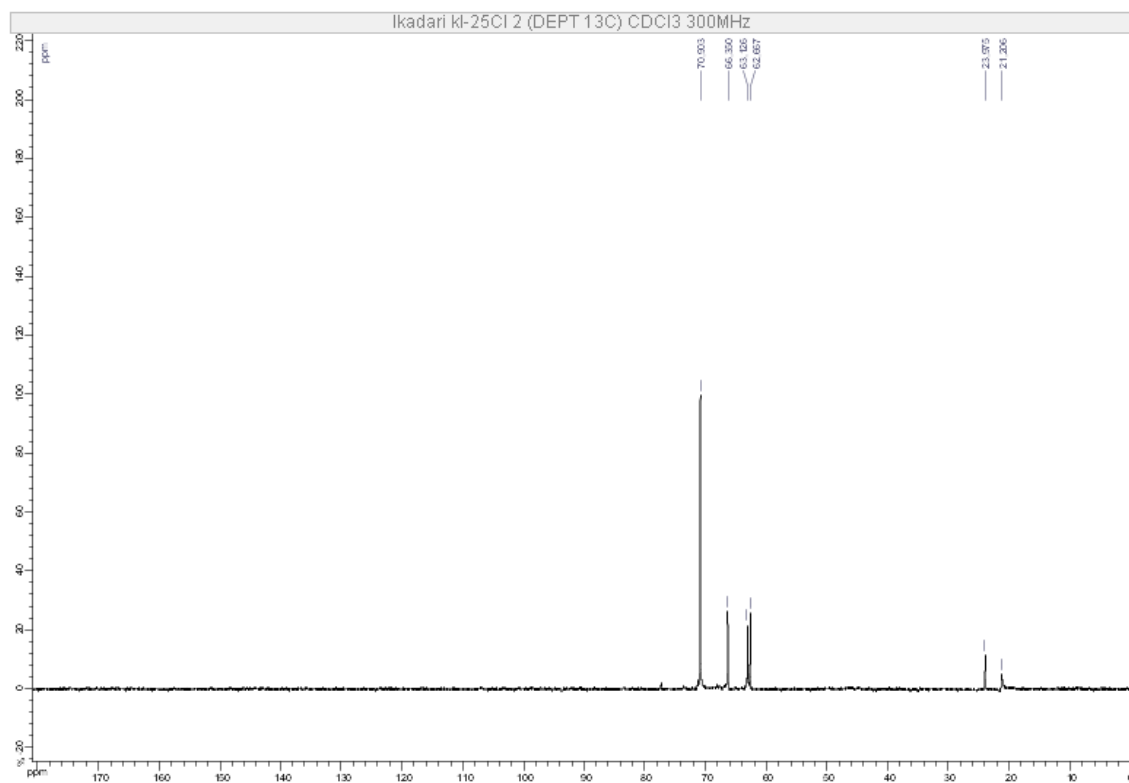
^1H NMR (300 MHz, CDCl_3)



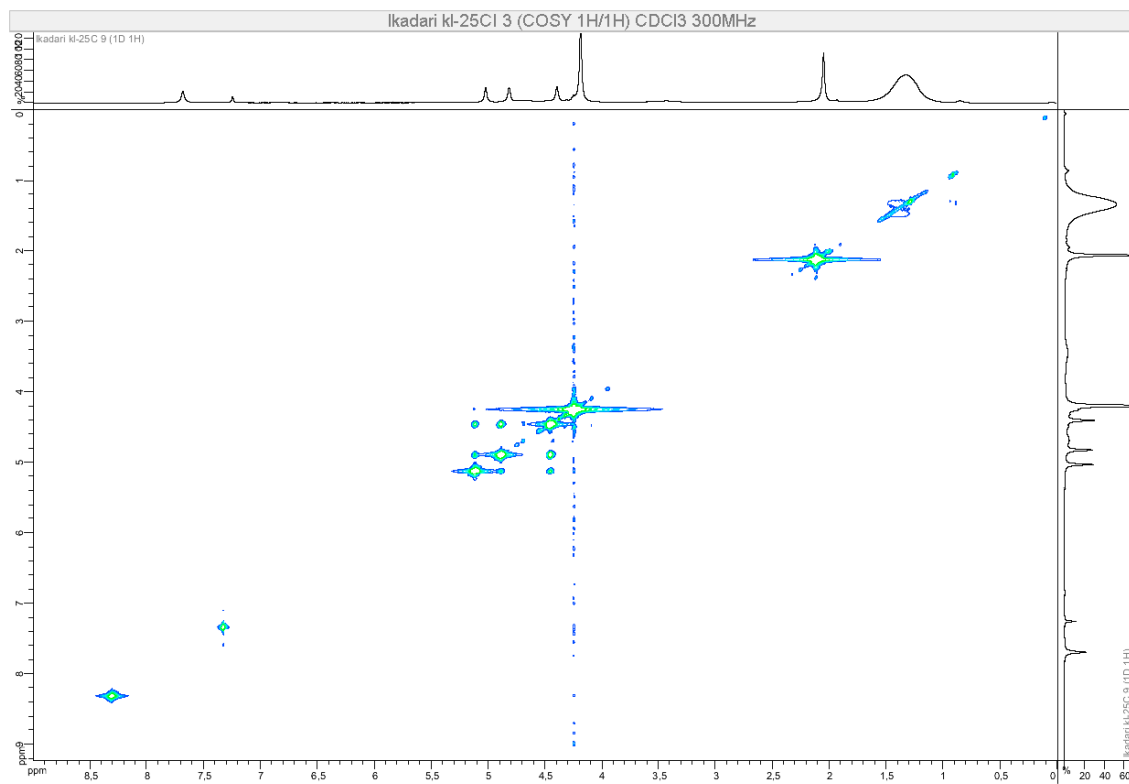
^{13}C NMR (75 MHz, CDCl_3)



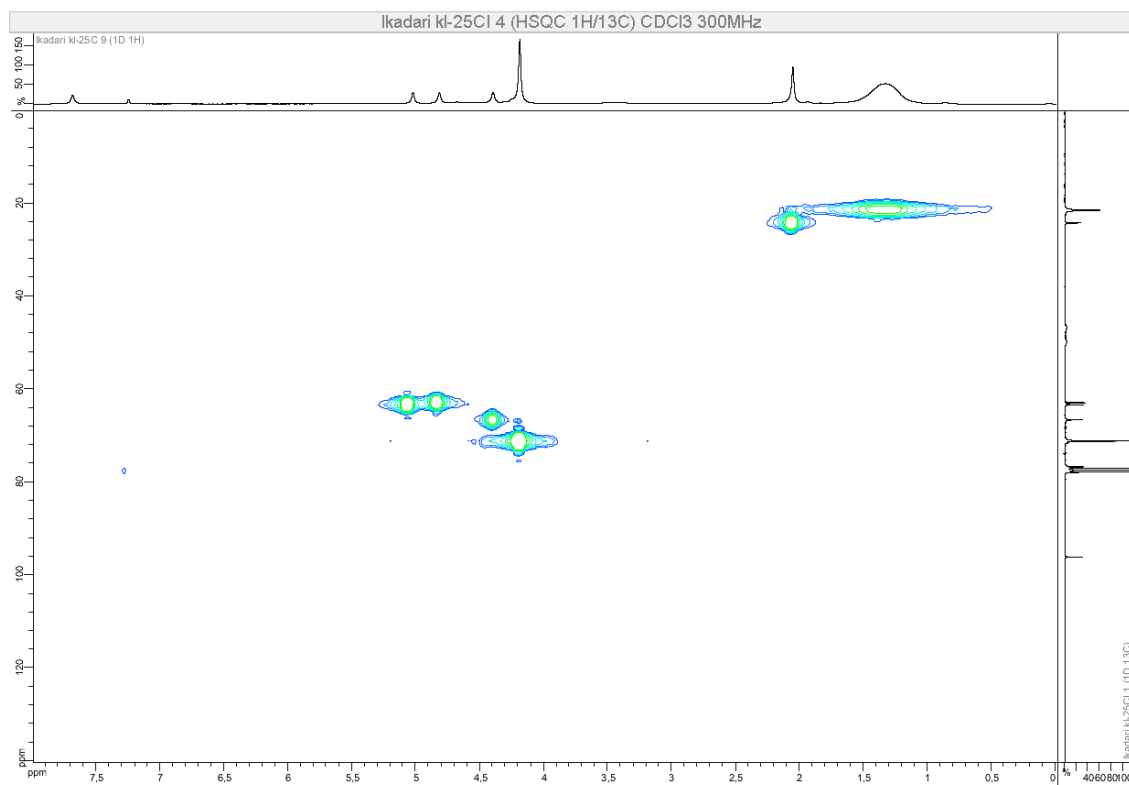
DEPT 135 (75 MHz, CDCl₃)



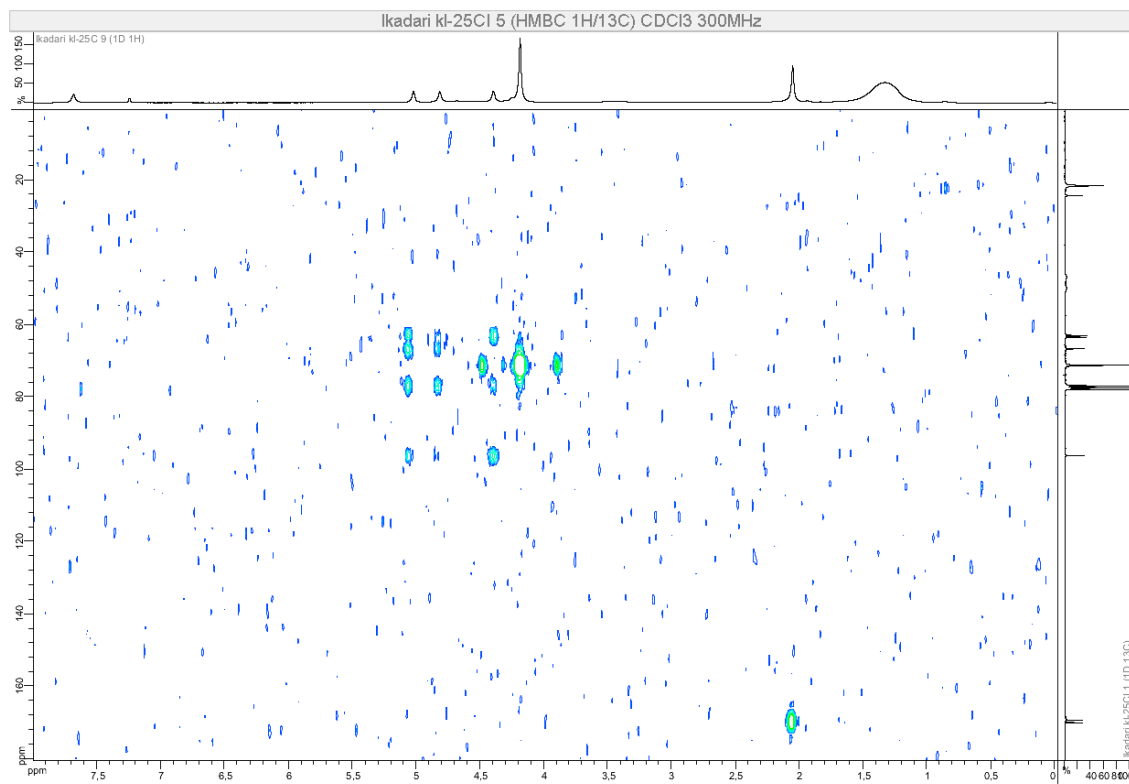
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

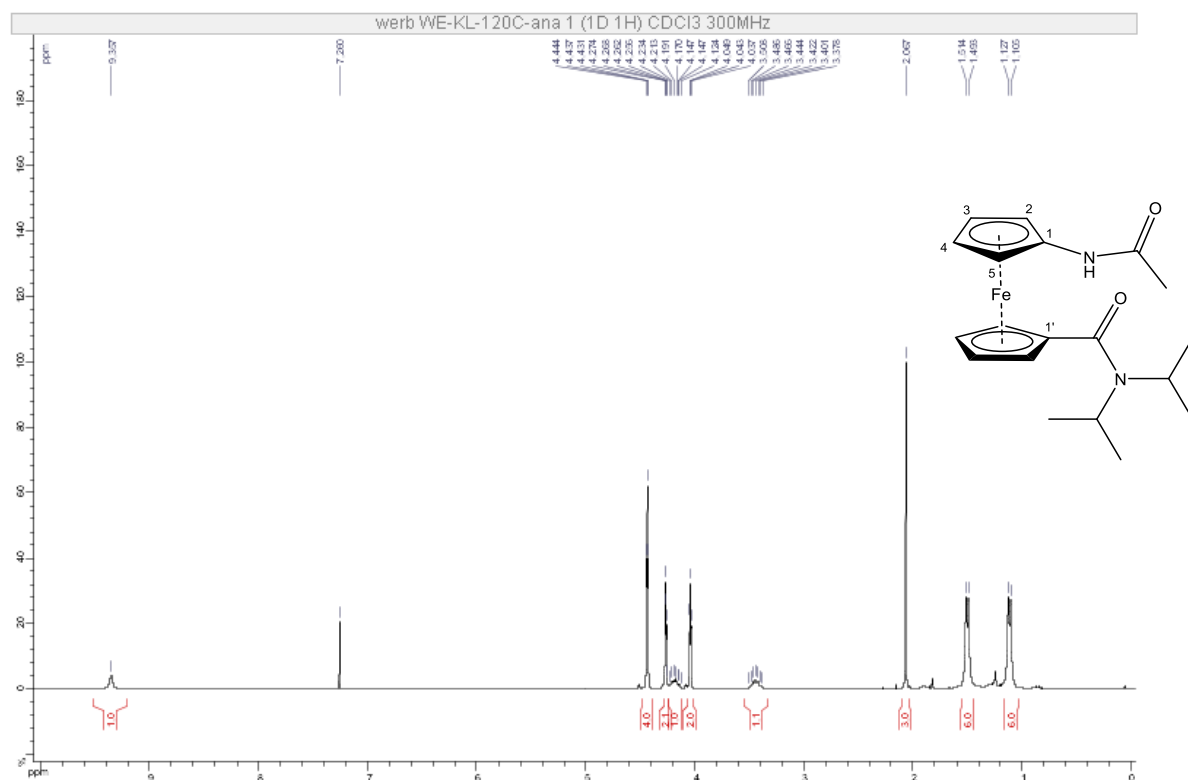


HMBC (300 MHz, CDCl₃)

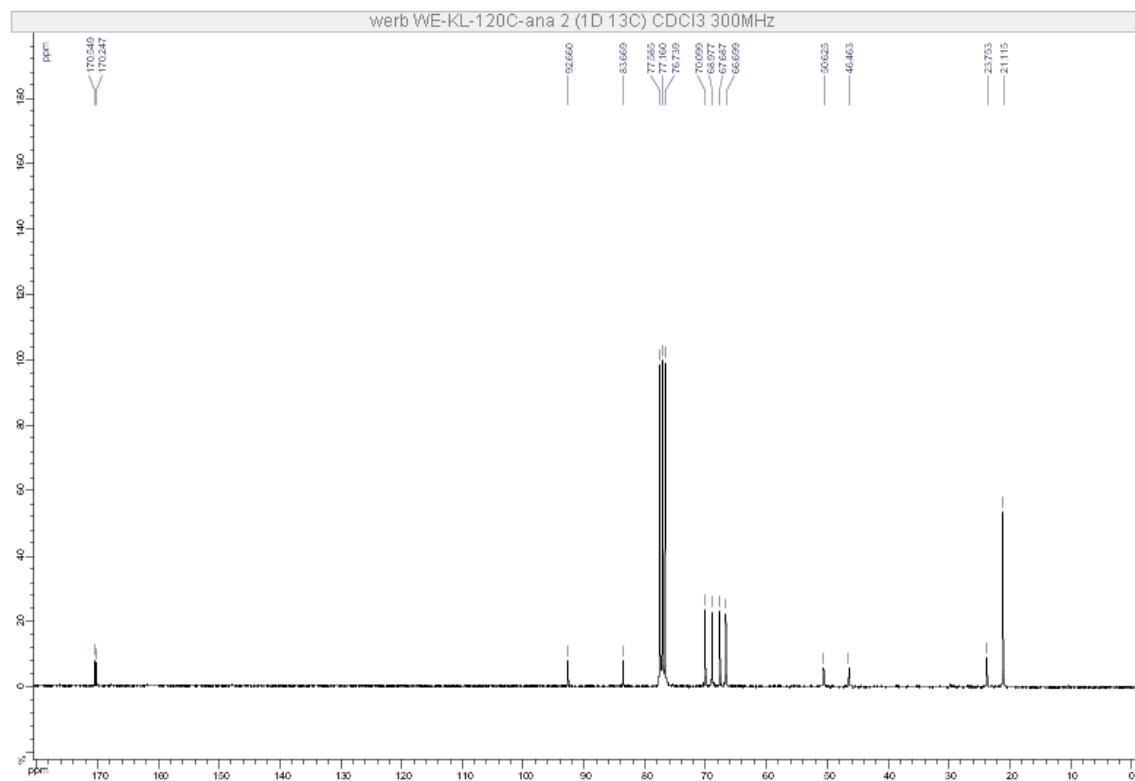


***N*-(1'-(Diisopropylaminocarbonyl)ferrocenyl)acetamide (6j, racemic mixture)**

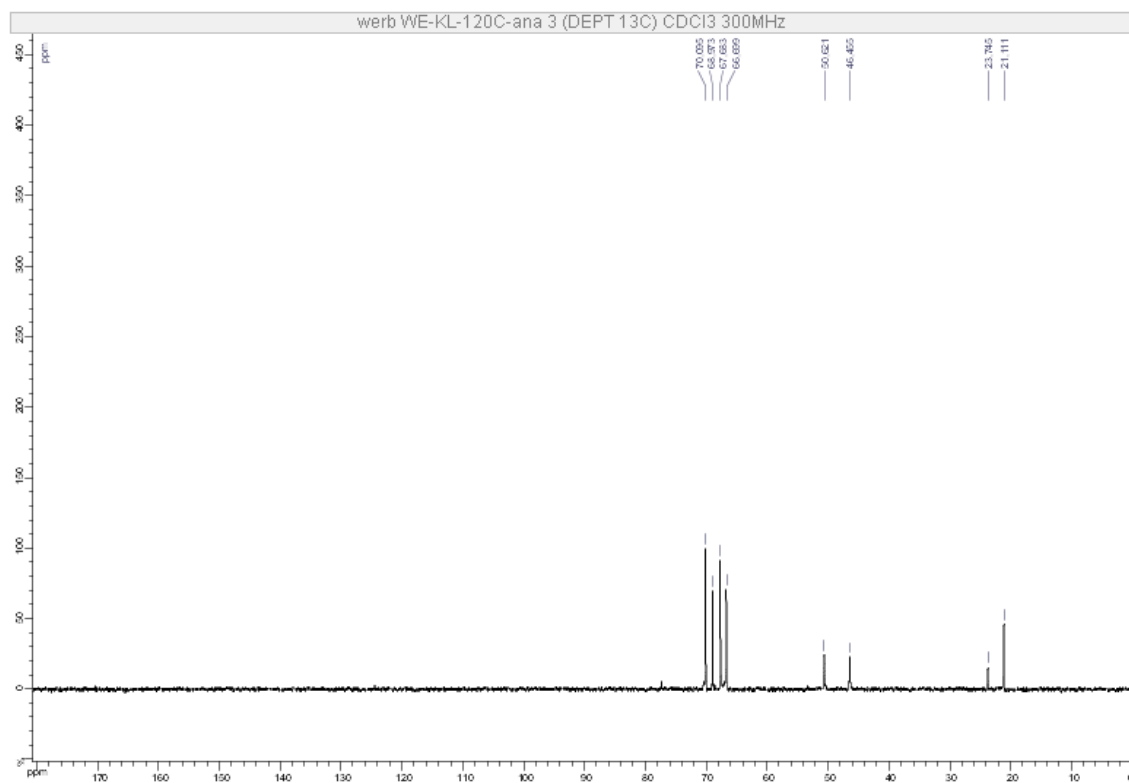
¹H NMR (300 MHz, CDCl₃)



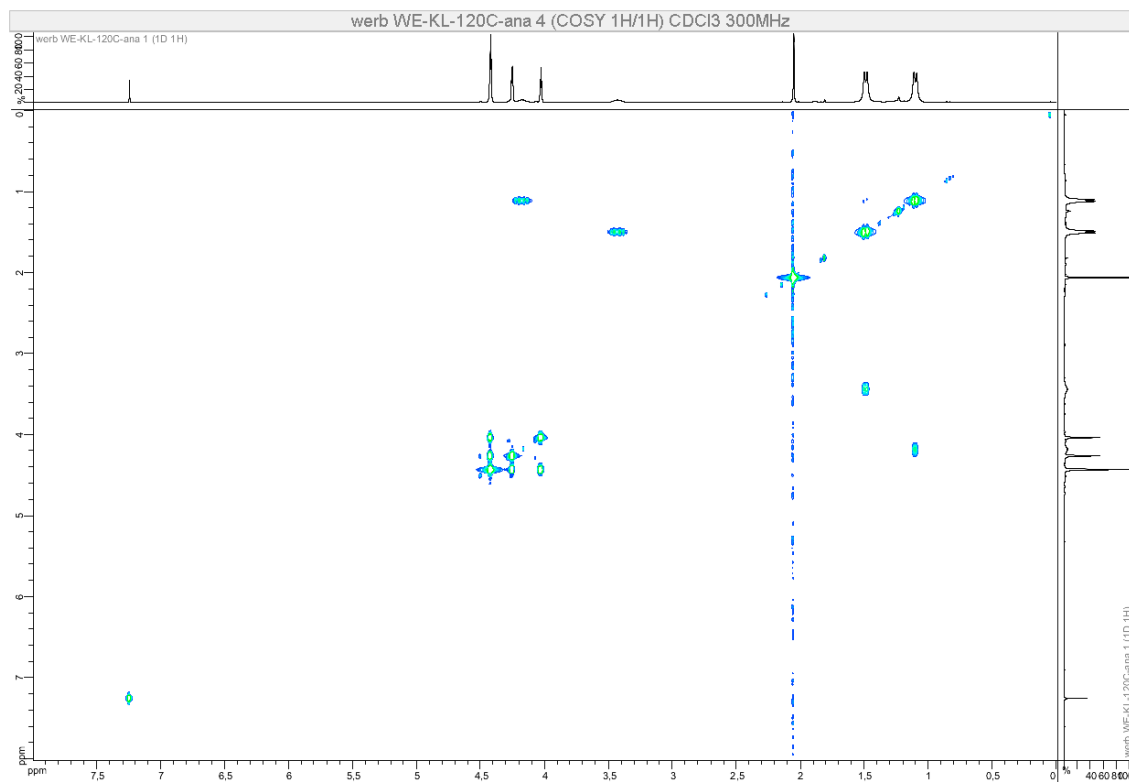
¹³C NMR (75 MHz, CDCl₃)



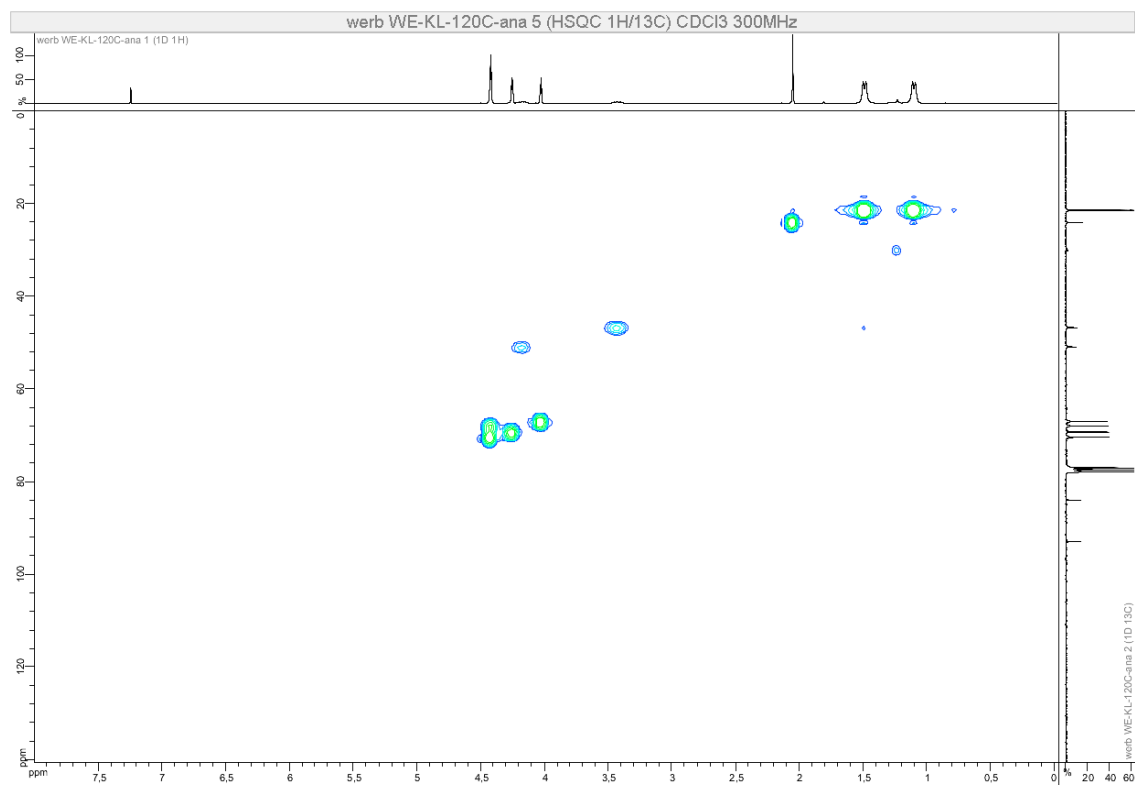
DEPT 135 (75 MHz, CDCl₃)



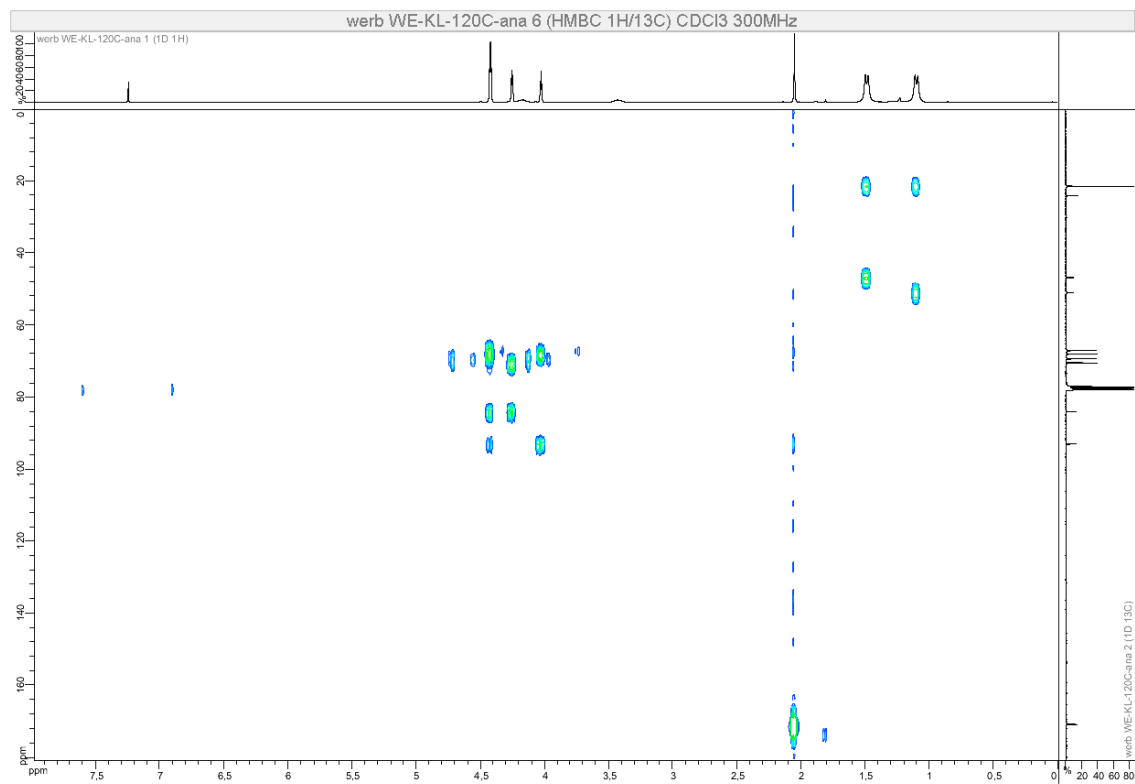
COSY (300 MHz, CDCl₃)



HSQC (300 MHz, CDCl₃)

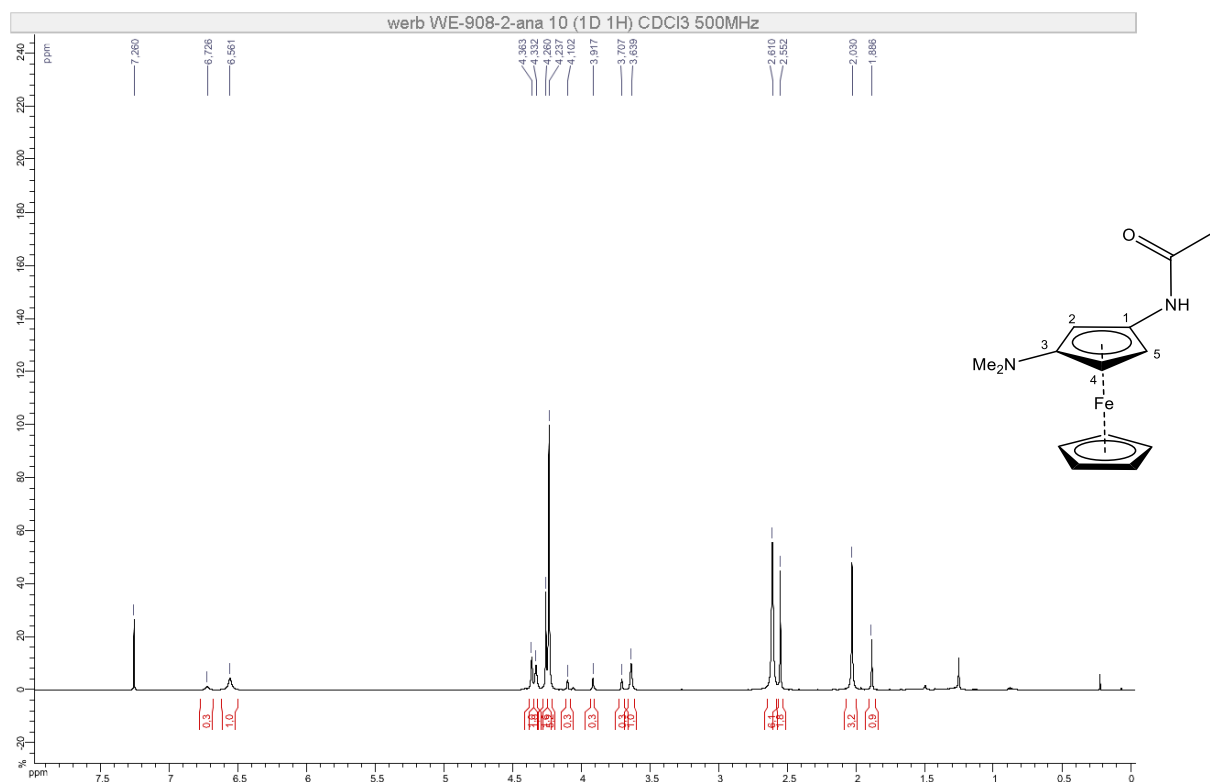


HMBC (300 MHz, CDCl₃)

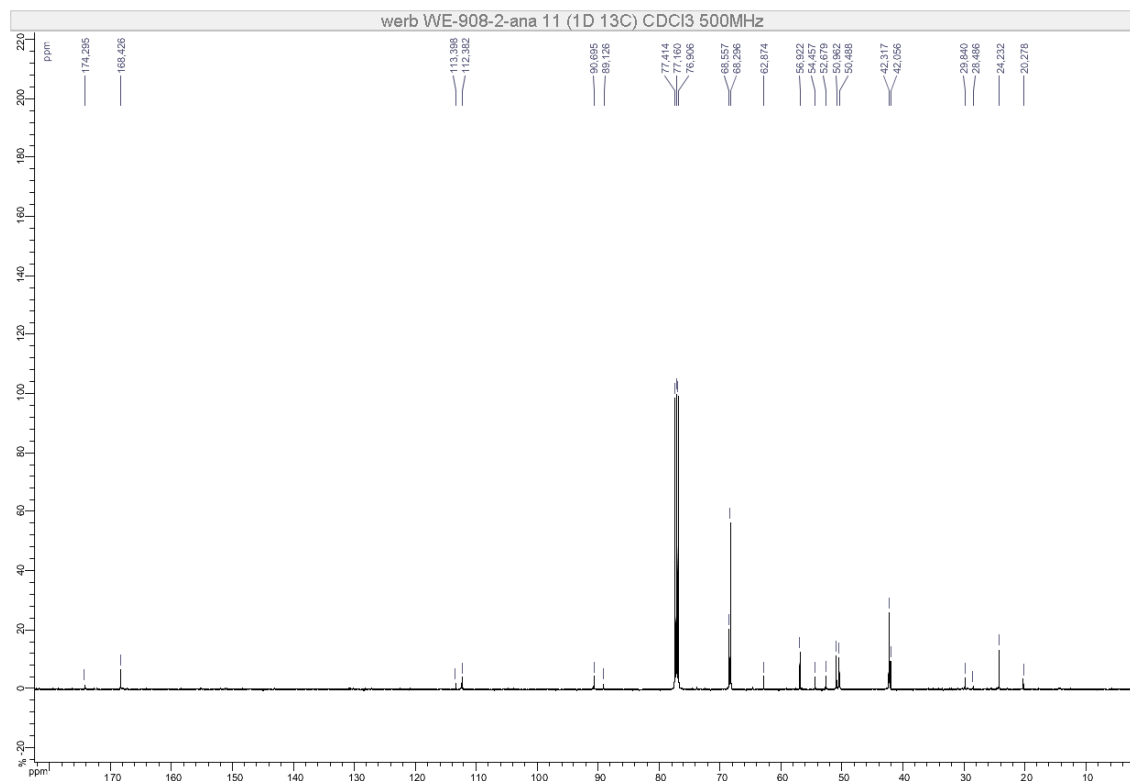


***N*-(3-(Dimethylamino)ferrocenyl)acetamide (4k, stereoisomeric mixture due to rotamers)**

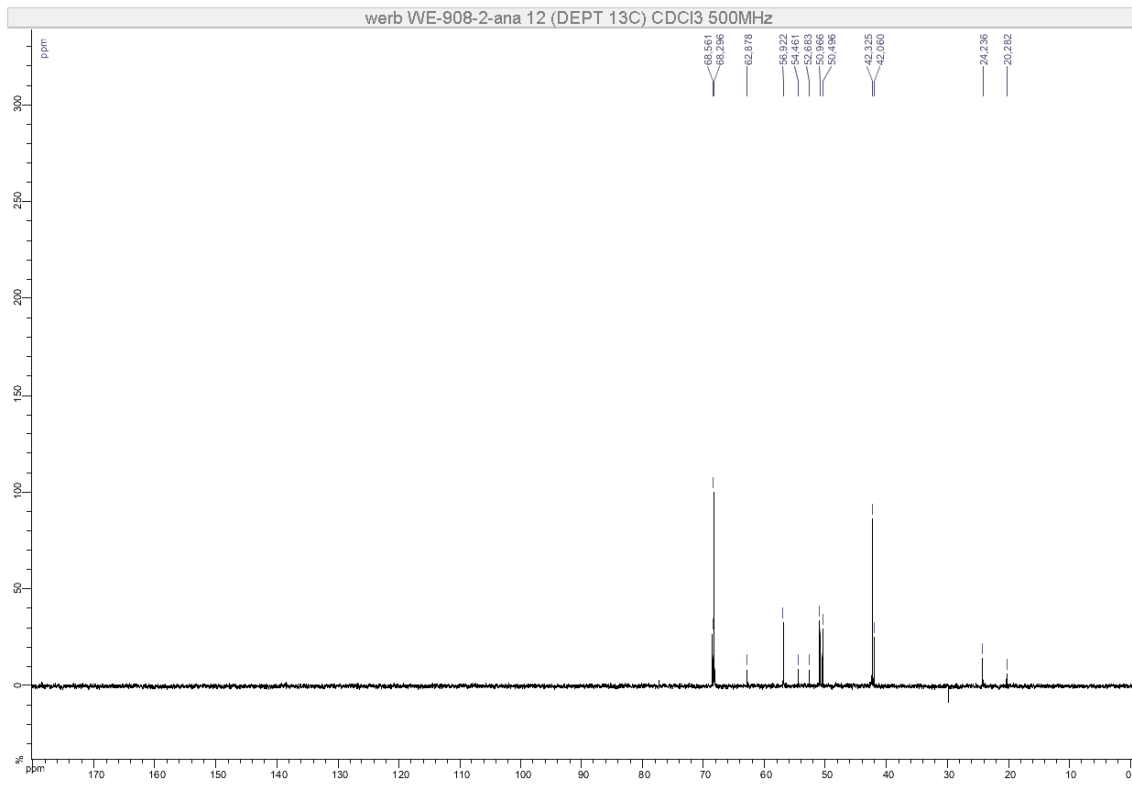
¹H NMR (500 MHz, CDCl₃)



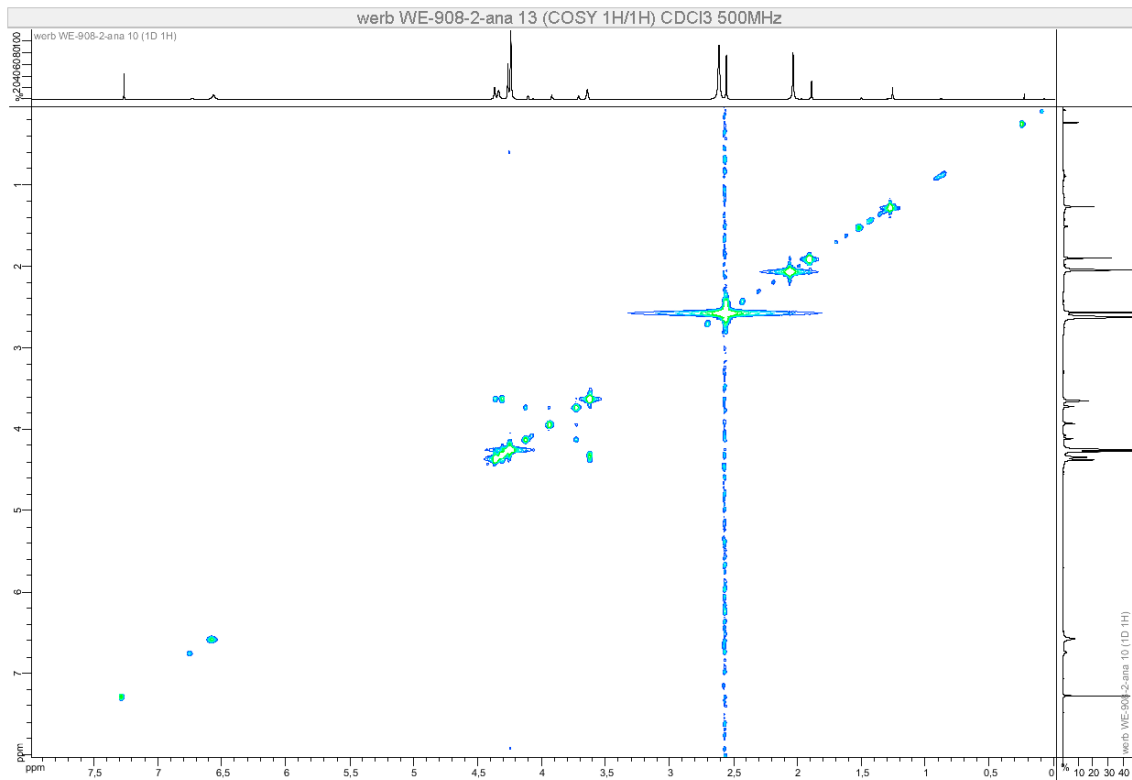
¹³C NMR (126 MHz, CDCl₃)



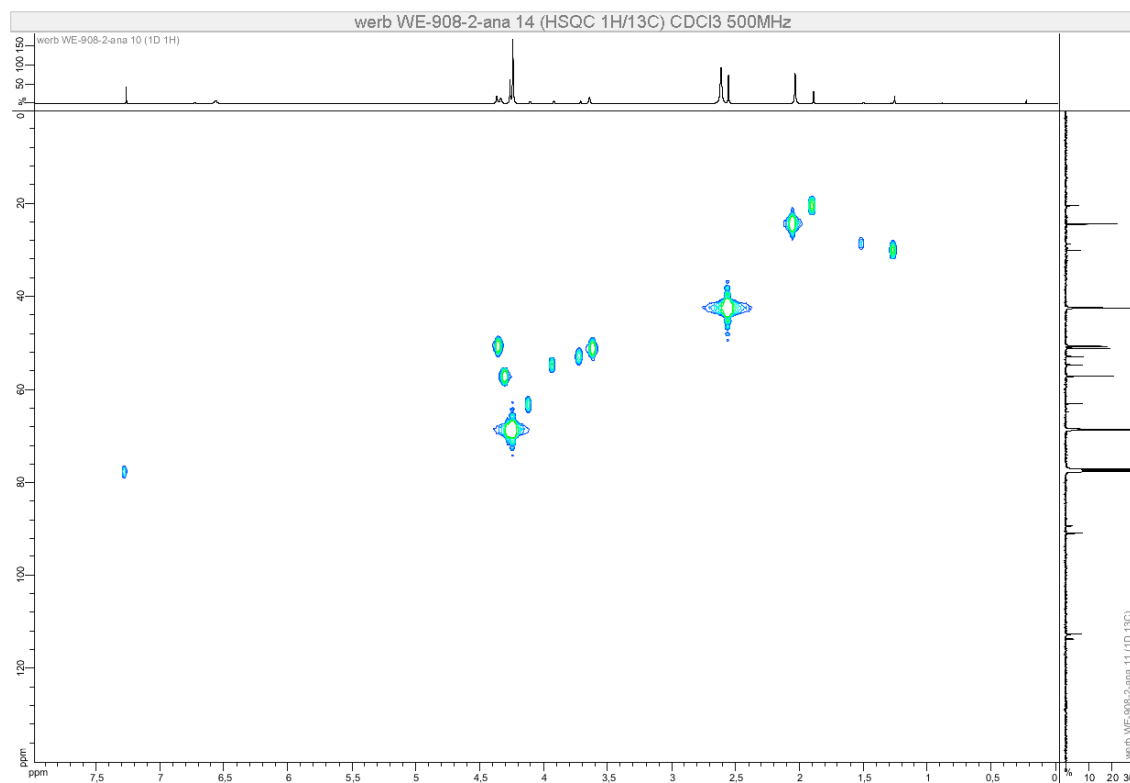
DEPT 135 (126 MHz, CDCl₃)



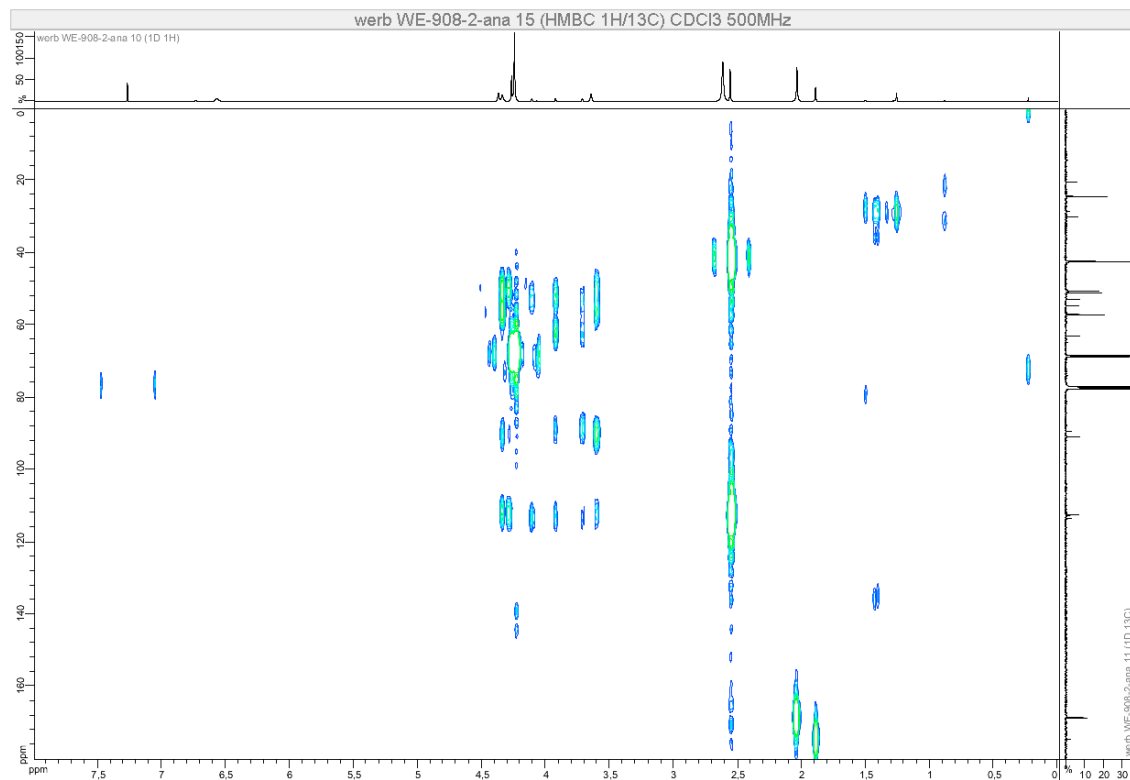
COSY (500 MHz, CDCl₃)



HSQC (500 MHz, CDCl₃)

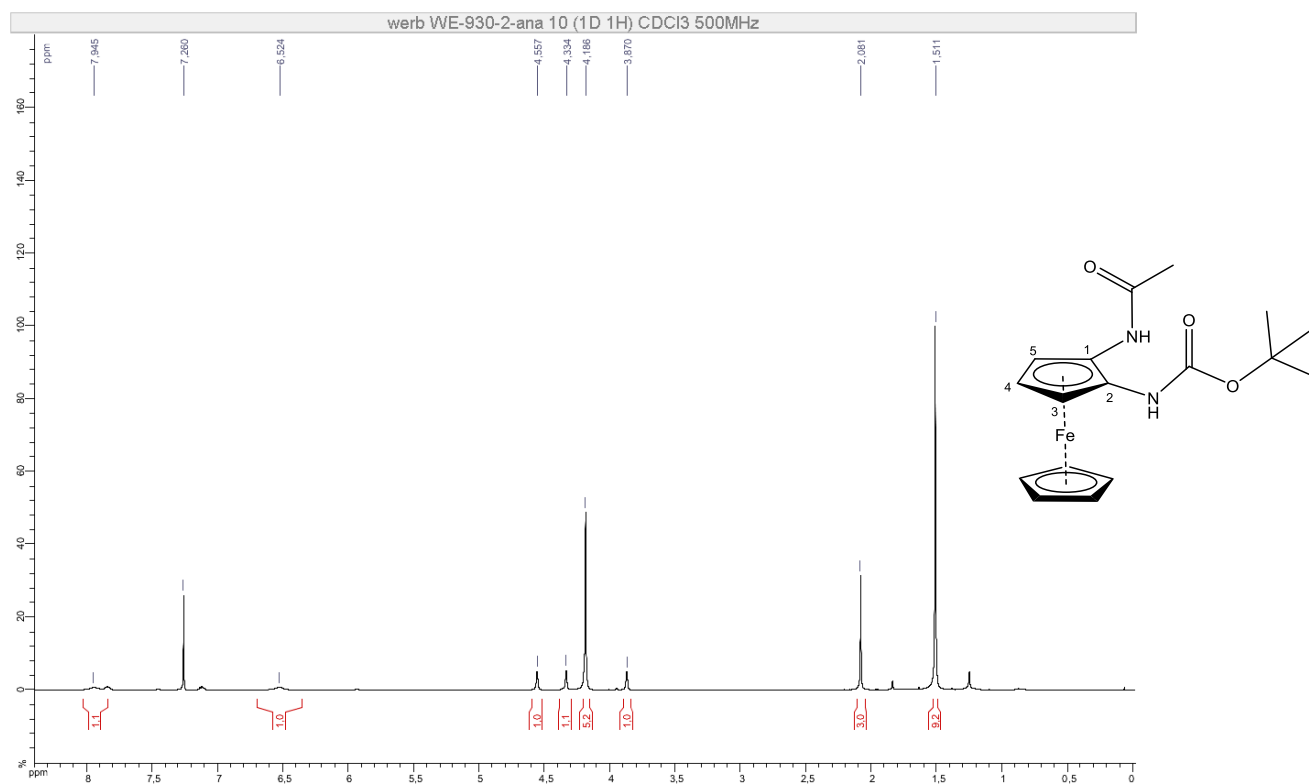


HMBC (500 MHz, CDCl₃)

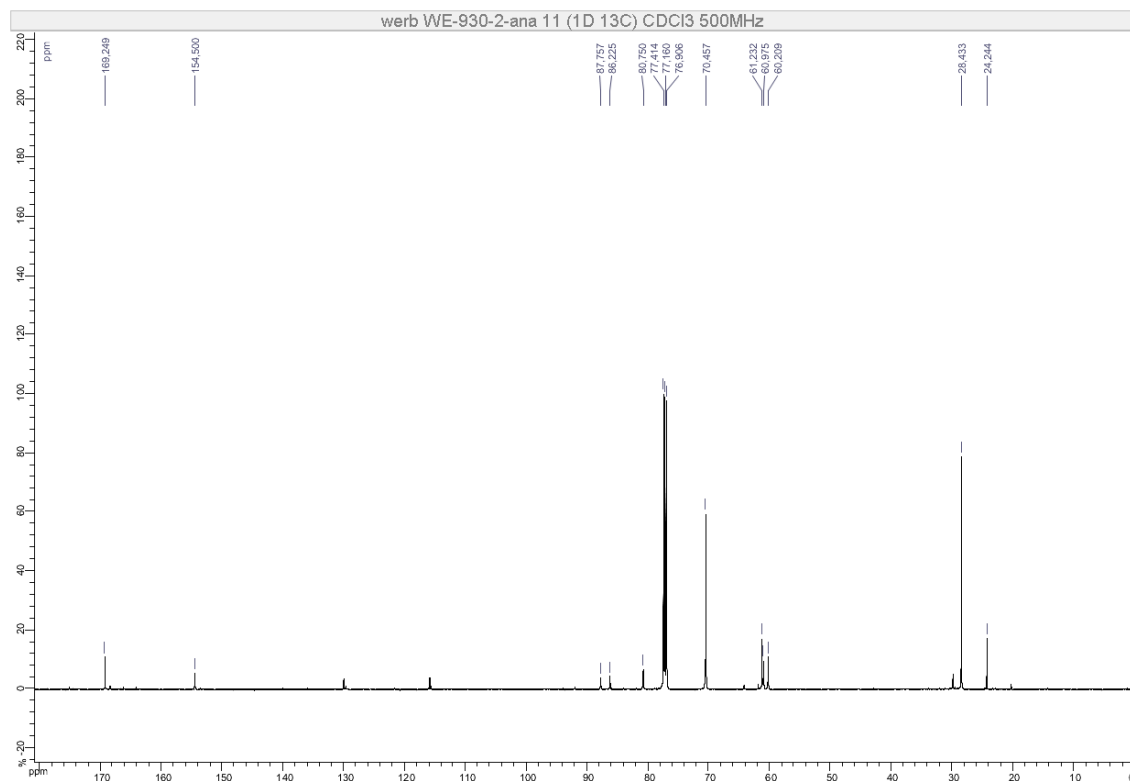


***N*-(2-(*tert*-Butoxycarbonylamino)ferrocenyl)acetamide (2l, racemic mixture)**

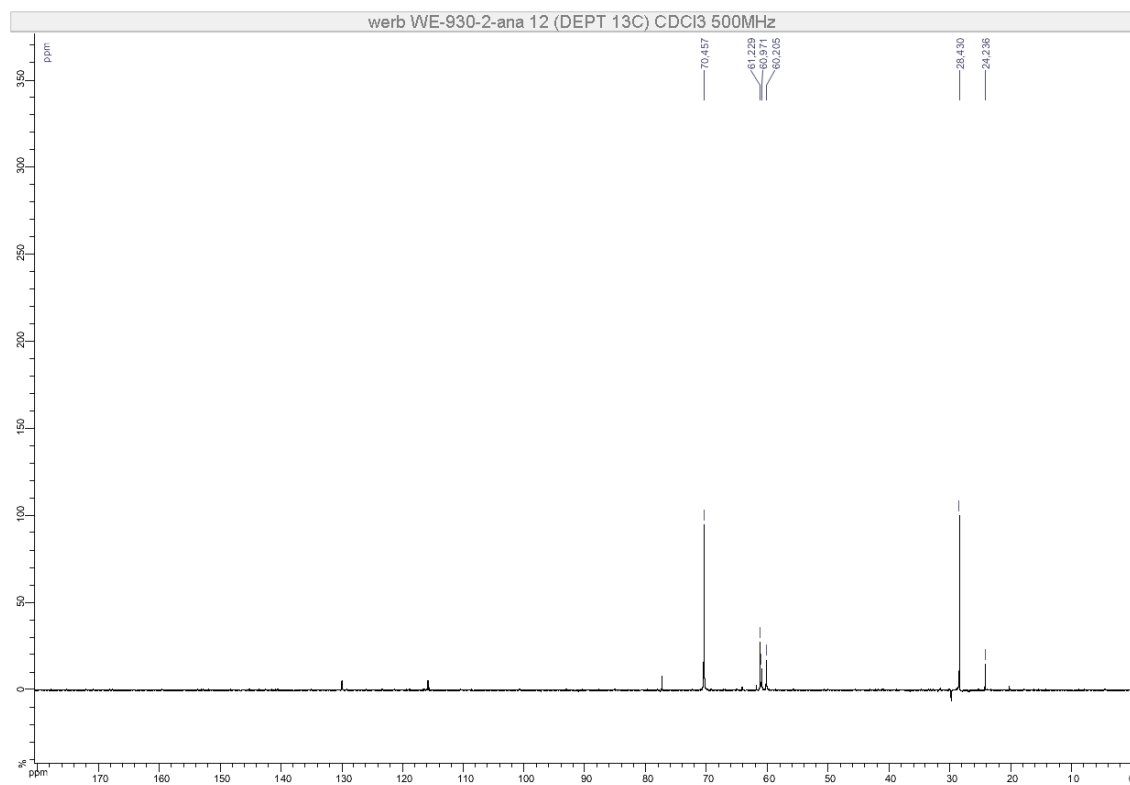
¹H NMR (500 MHz, CDCl₃)



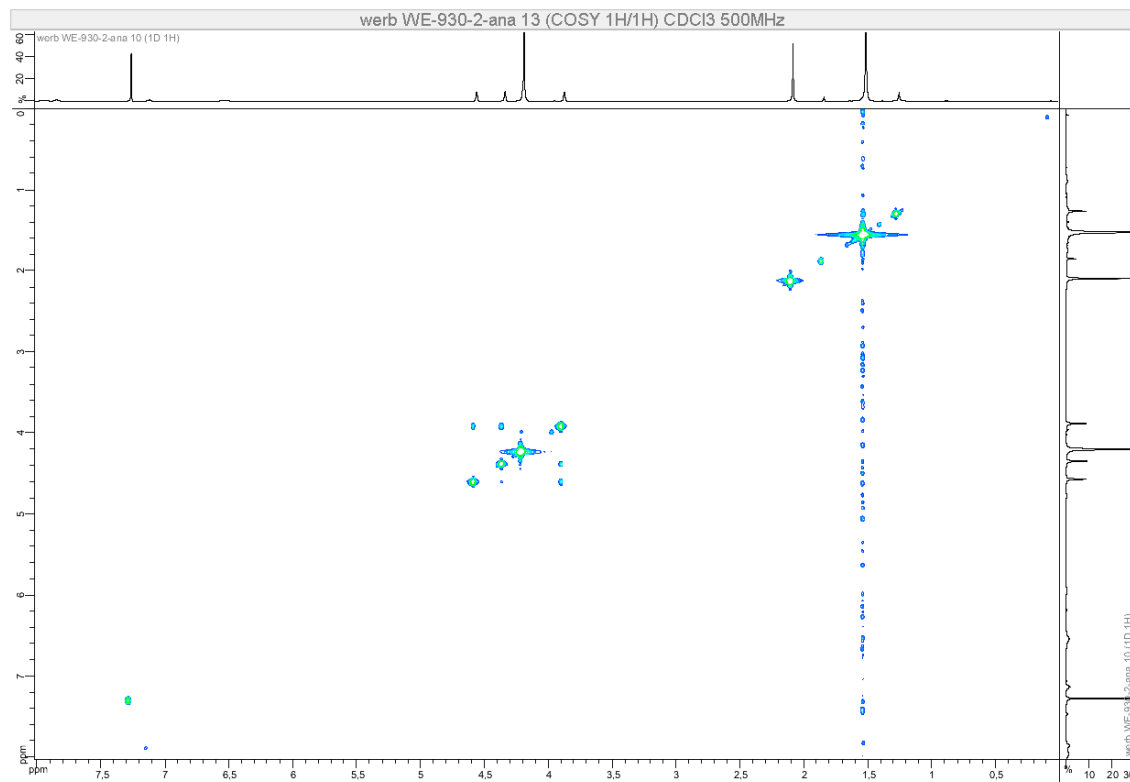
¹³C NMR (126 MHz, CDCl₃)



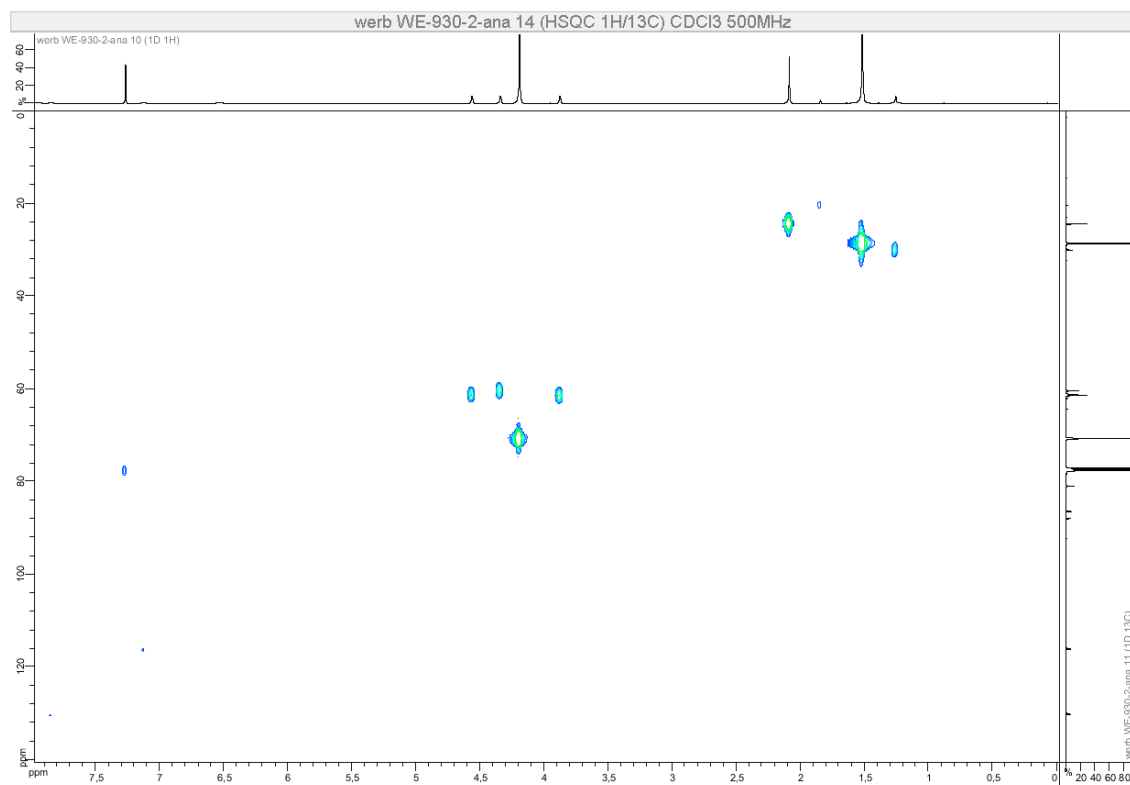
DEPT 135 (126 MHz, CDCl₃)



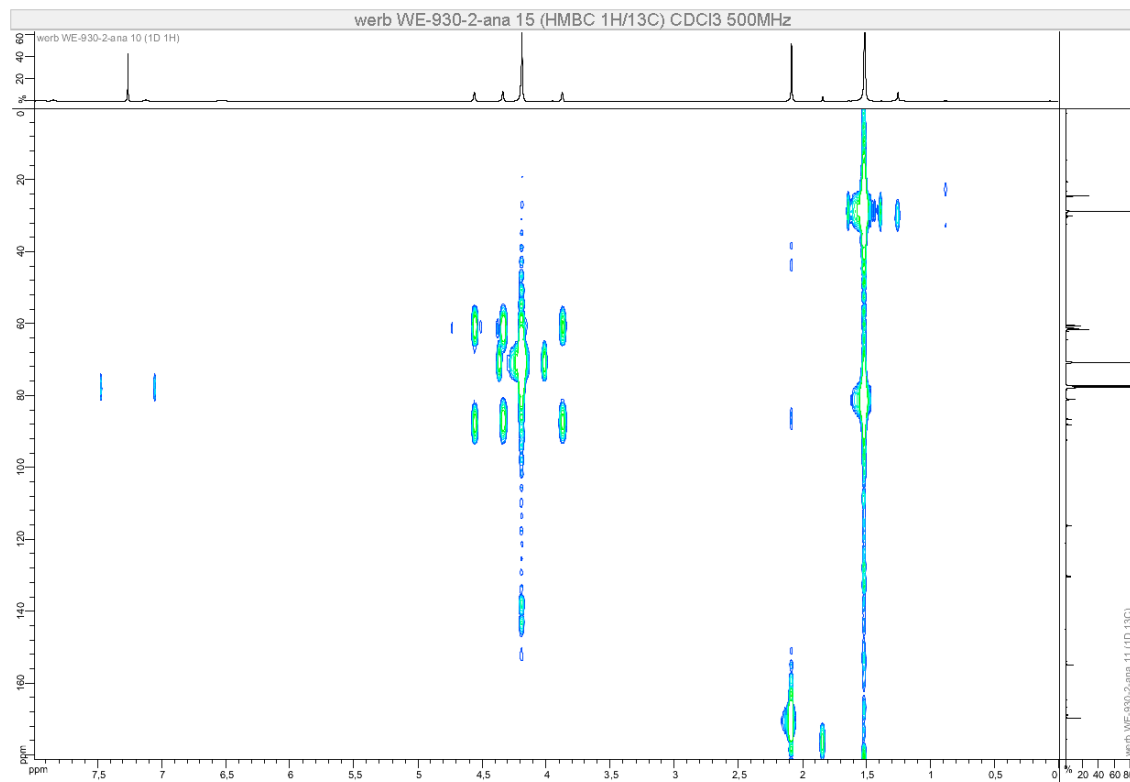
COSY (500 MHz, CDCl₃)



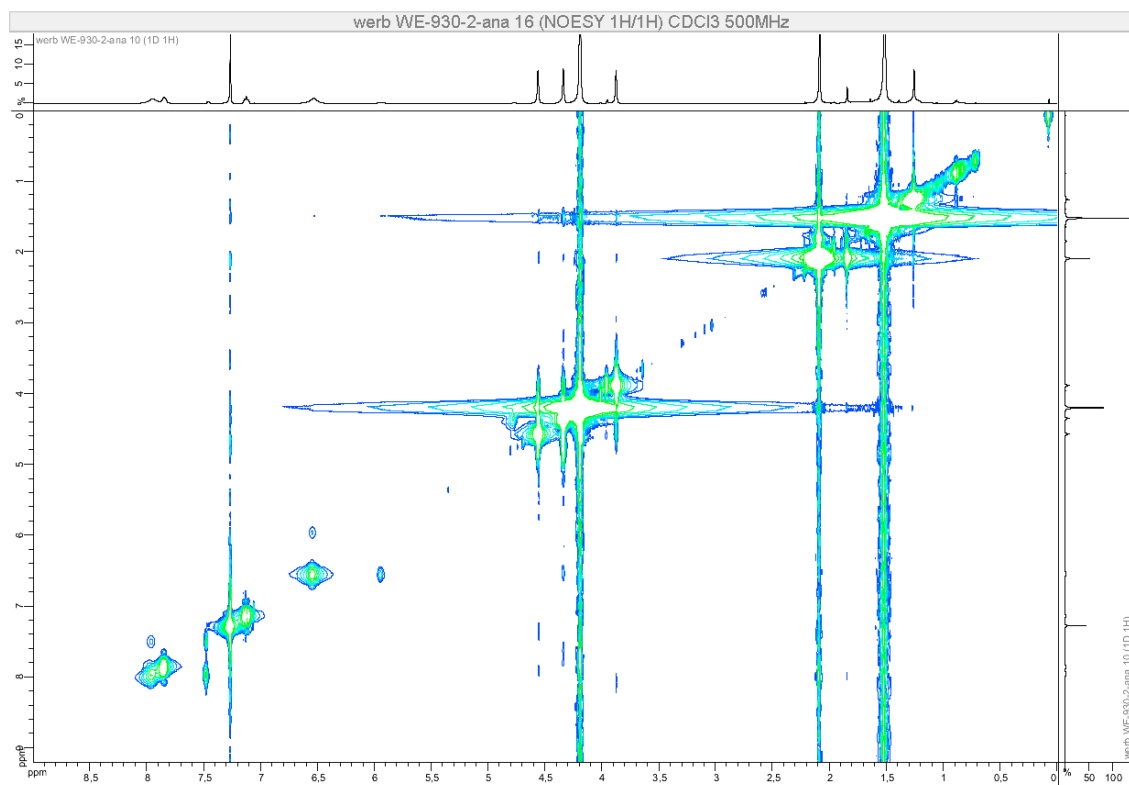
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

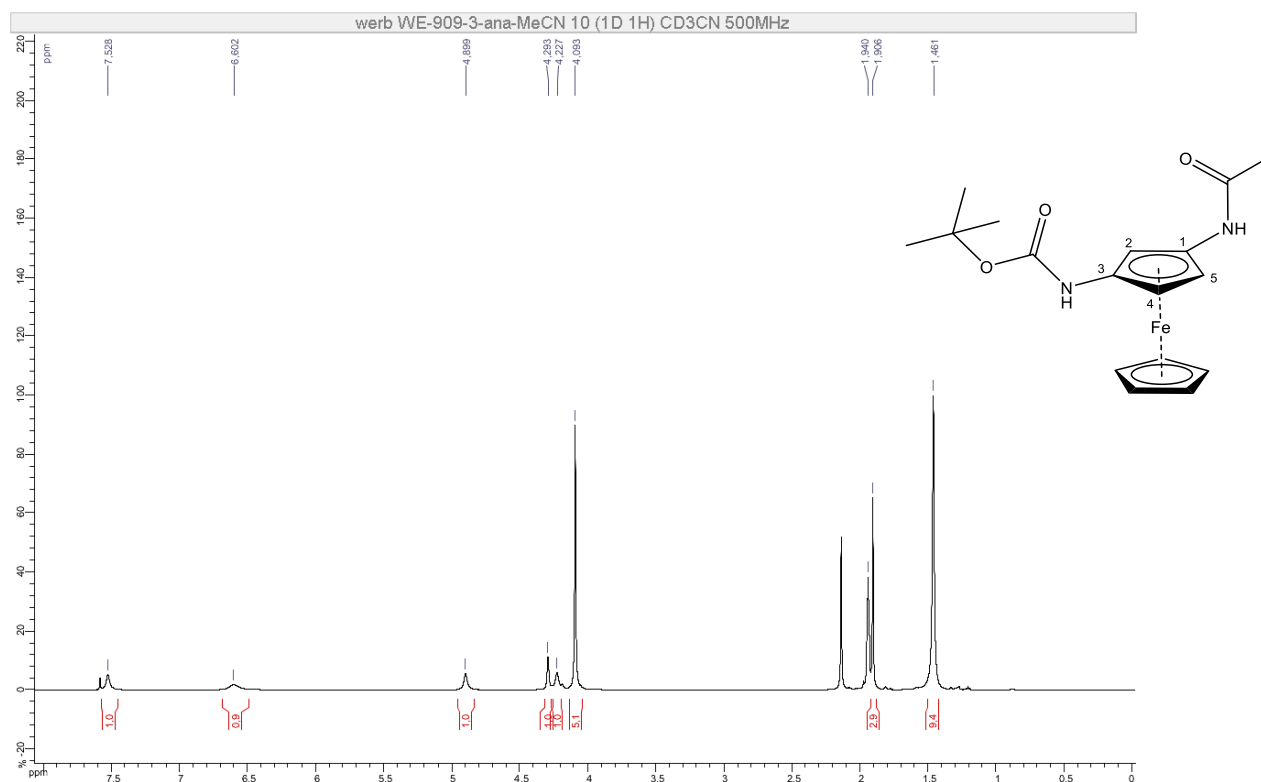


NOESY (500 MHz, CDCl₃)

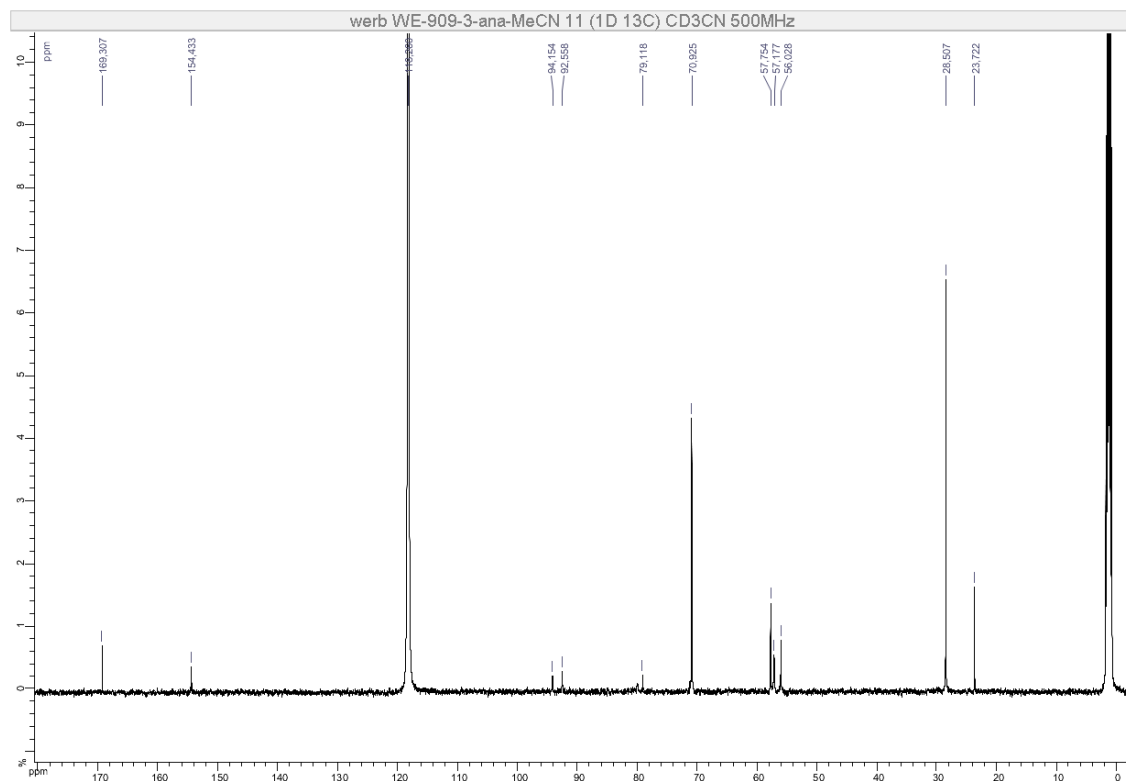


***N*-(3-(*tert*-Butoxycarbonylamino)ferrocenyl)acetamide (4I, racemic mixture)**

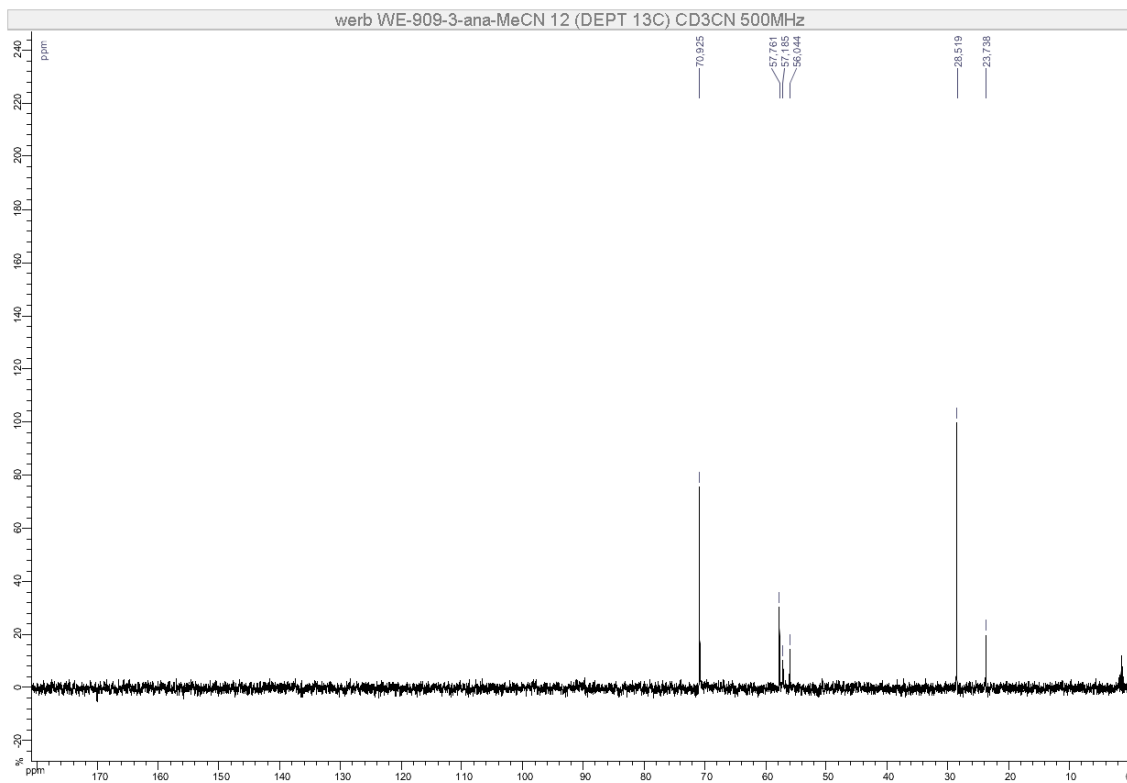
¹H NMR (500 MHz, CD₃CN)



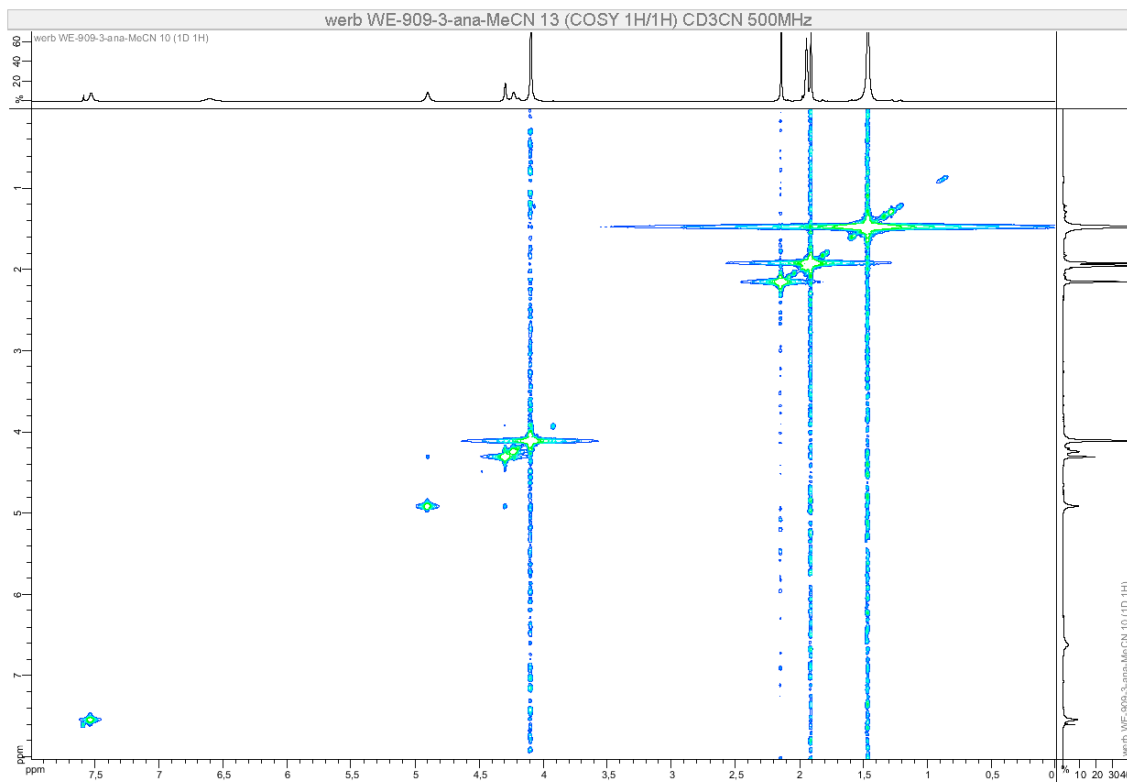
¹³C NMR (126 MHz, CD₃CN)



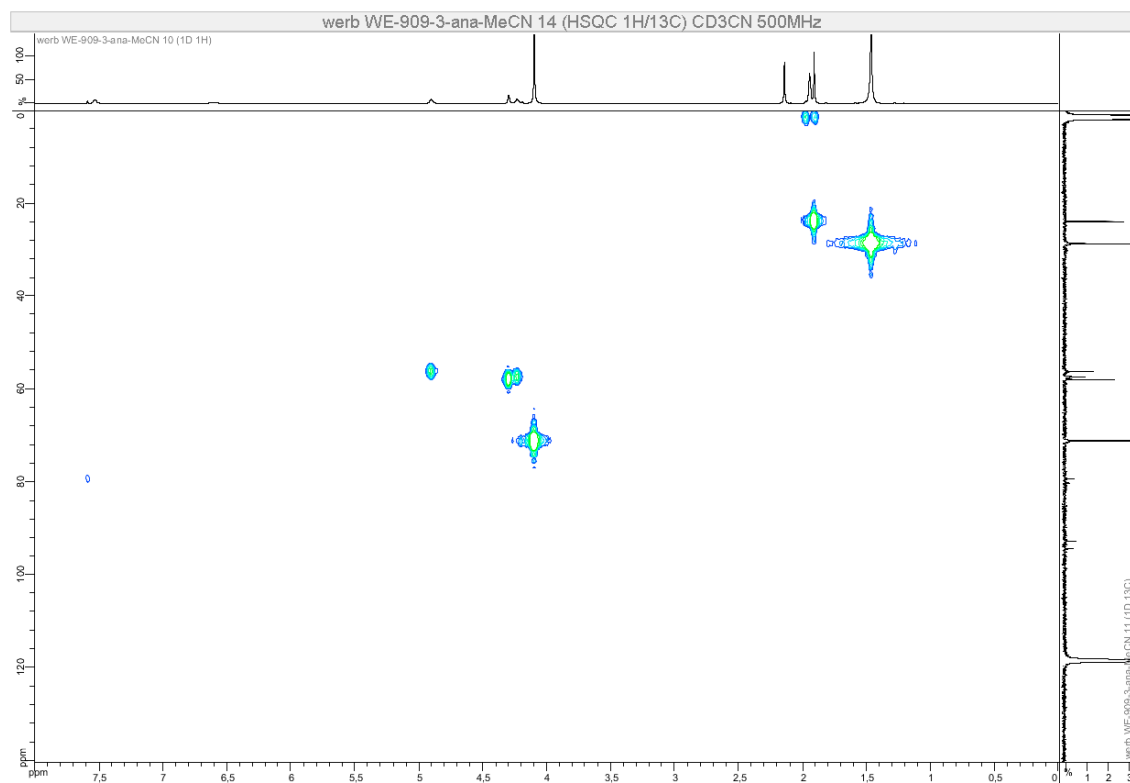
DEPT 135 (126 MHz, CD₃CN)



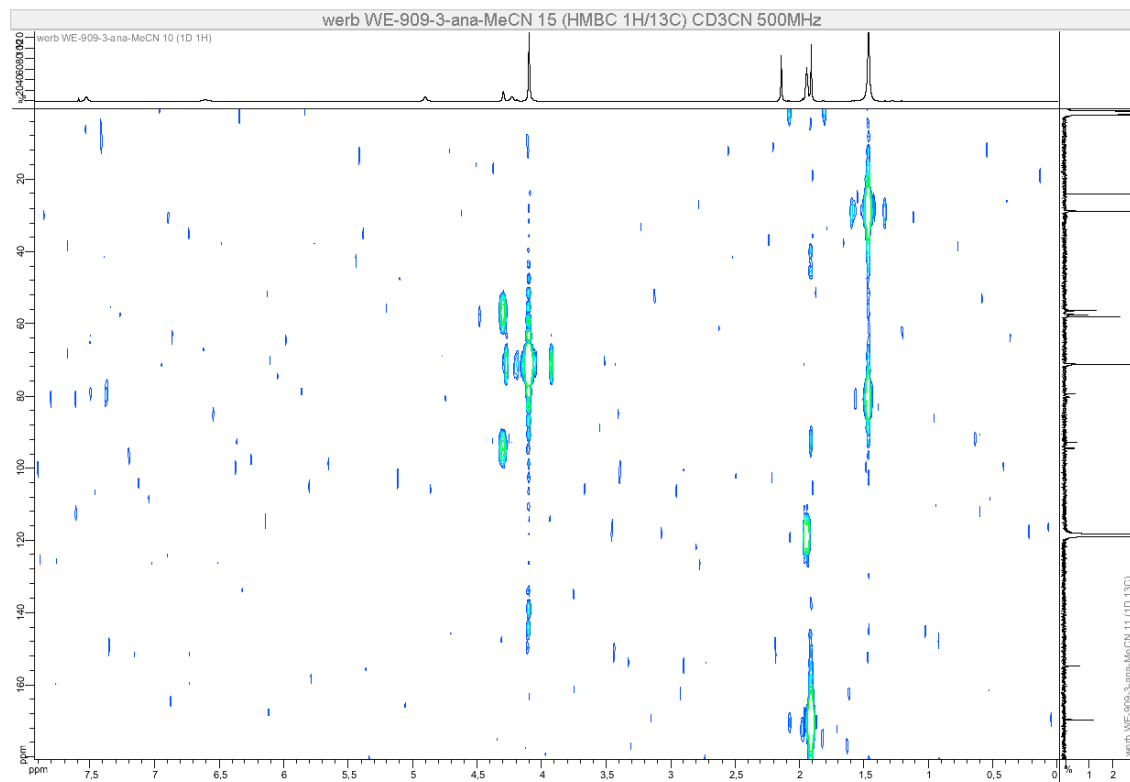
COSY (500 MHz, CD₃CN)



HSQC (500 MHz, CD₃CN)

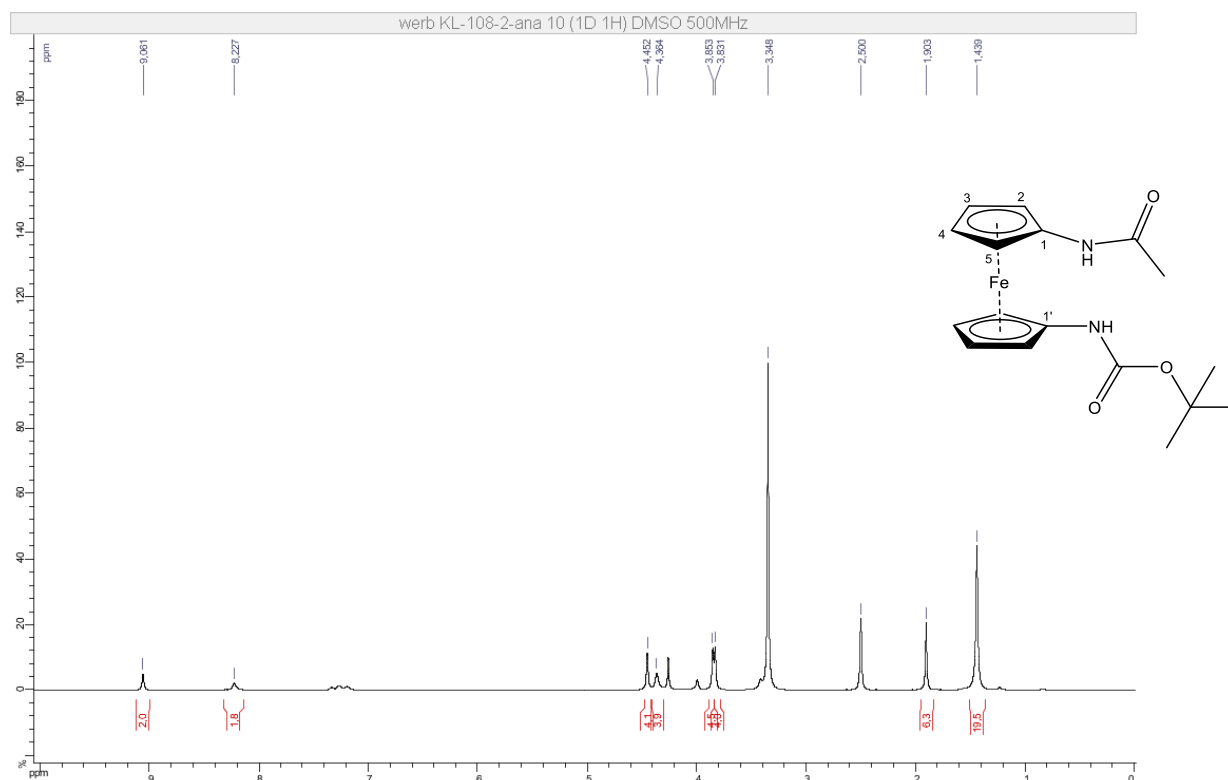


HMBC (500 MHz, CD₃CN)

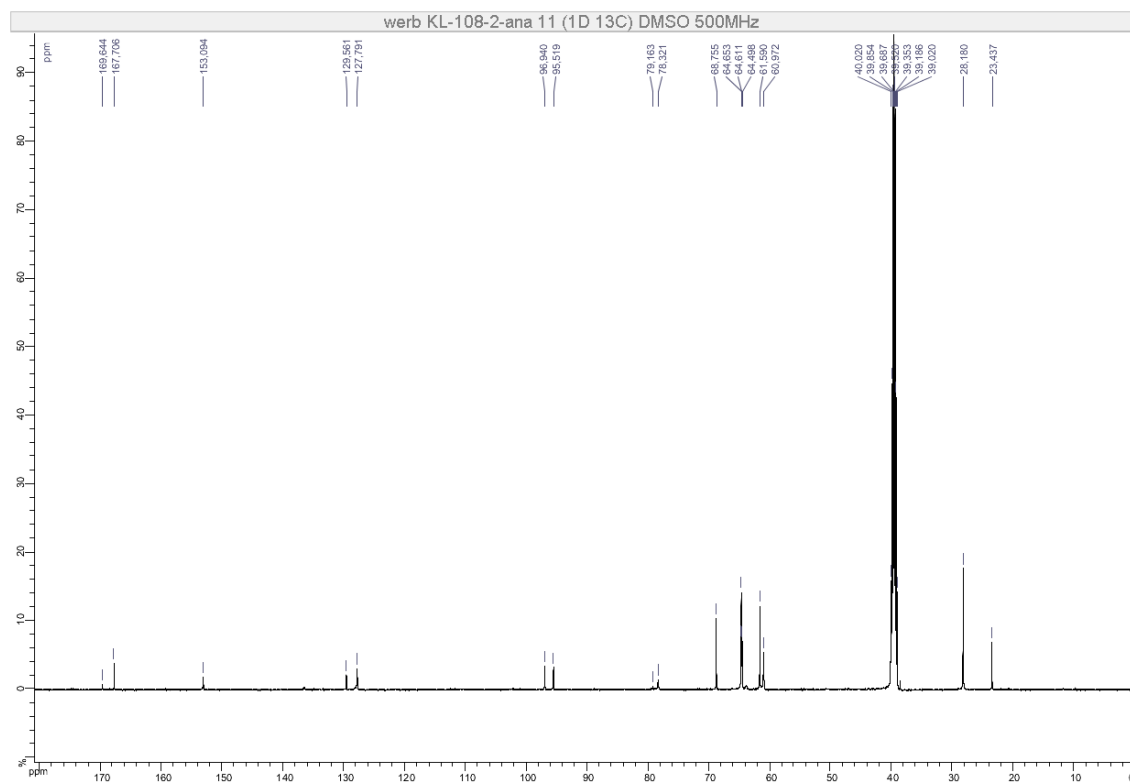


N-(1'-(*tert*-Butoxycarbonylamino)ferrocenyl)acetamide (6l)

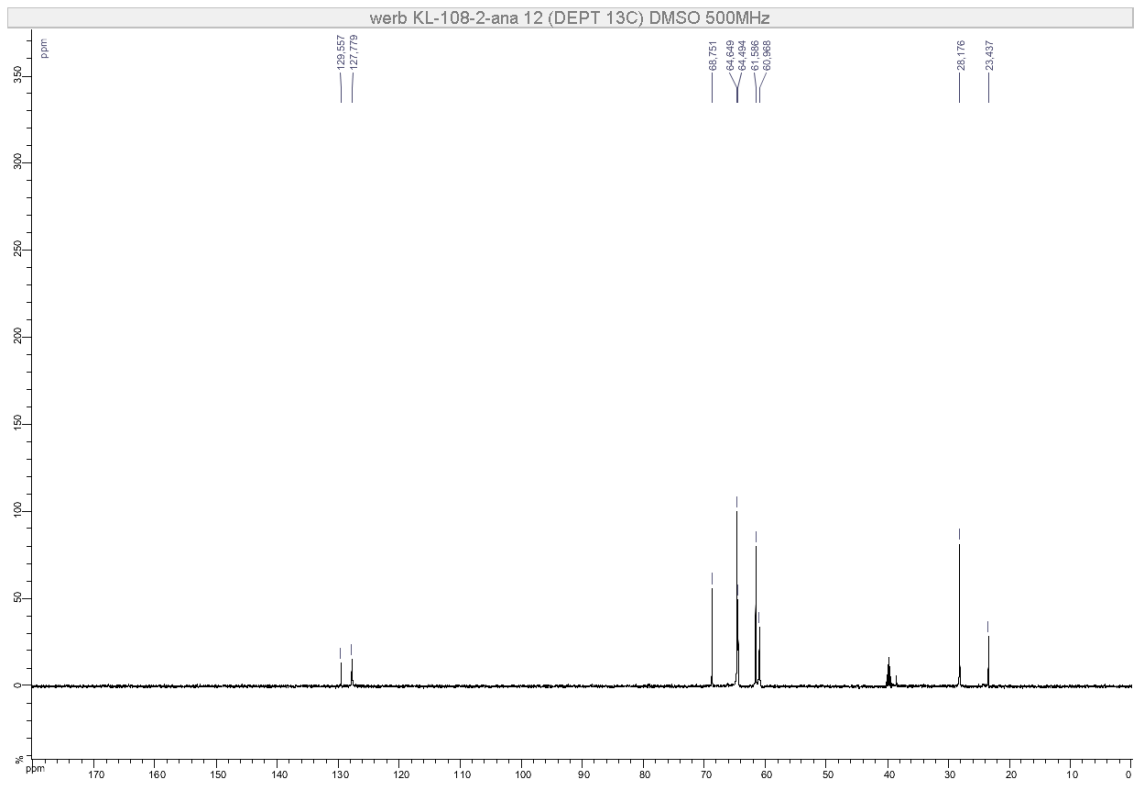
^1H NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$) – presence of an inseparable impurity



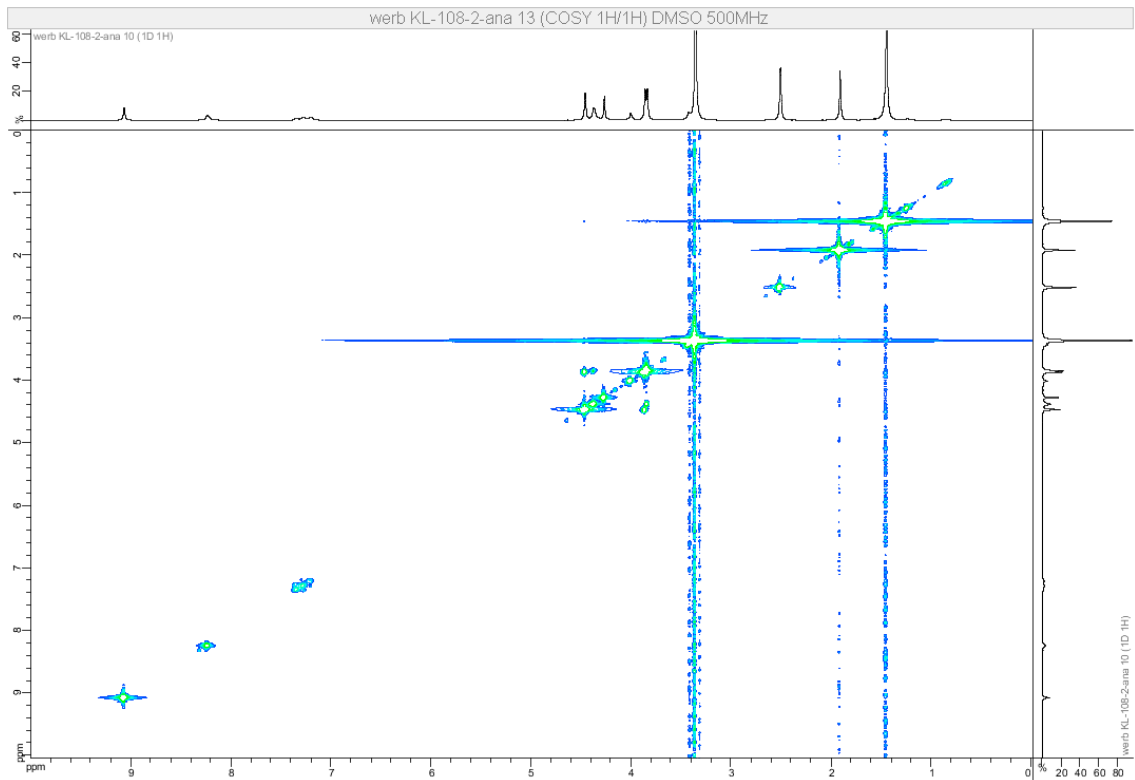
^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{SO}$)



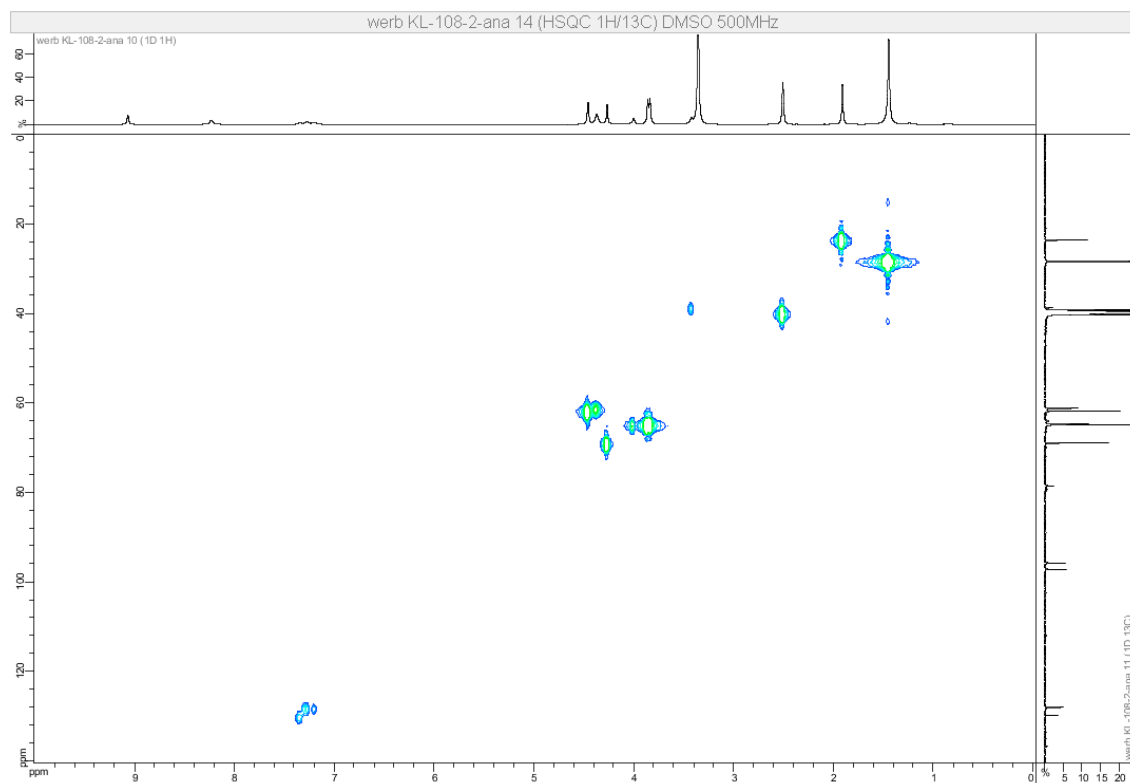
DEPT 135 (126 MHz, (CD₃)₂SO)



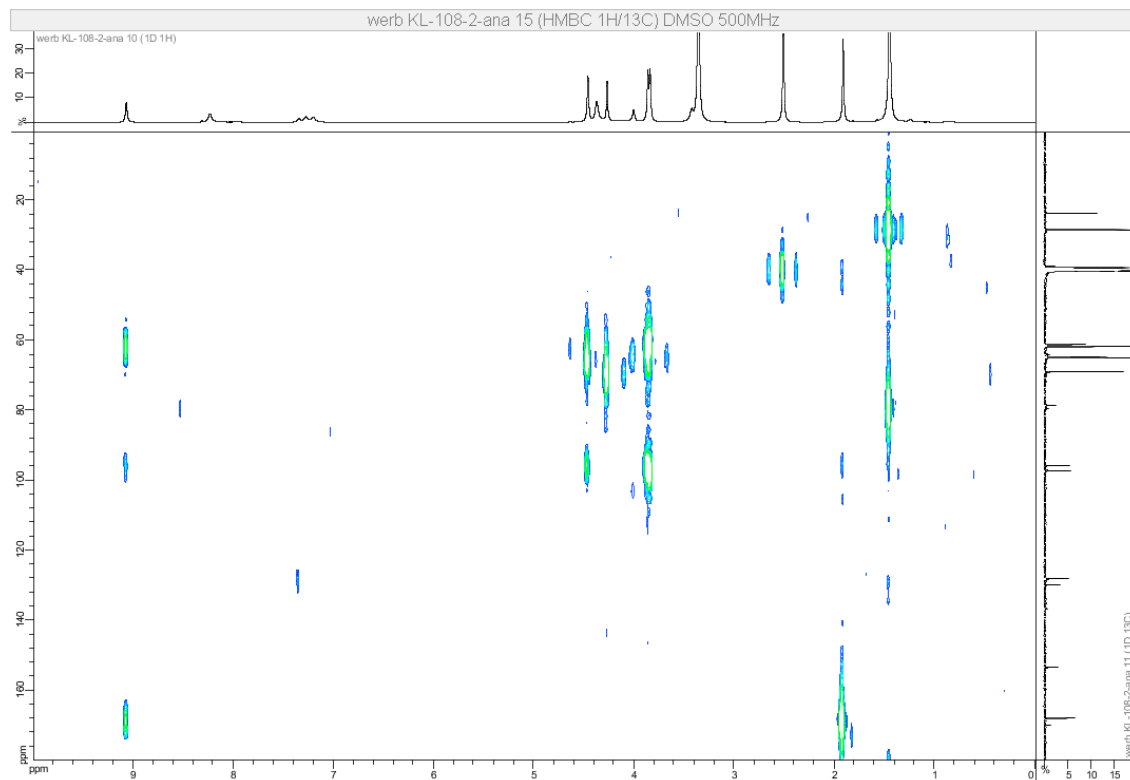
COSY (500 MHz, (CD₃)₂SO)



HSQC (500 MHz, (CD₃)₂SO)

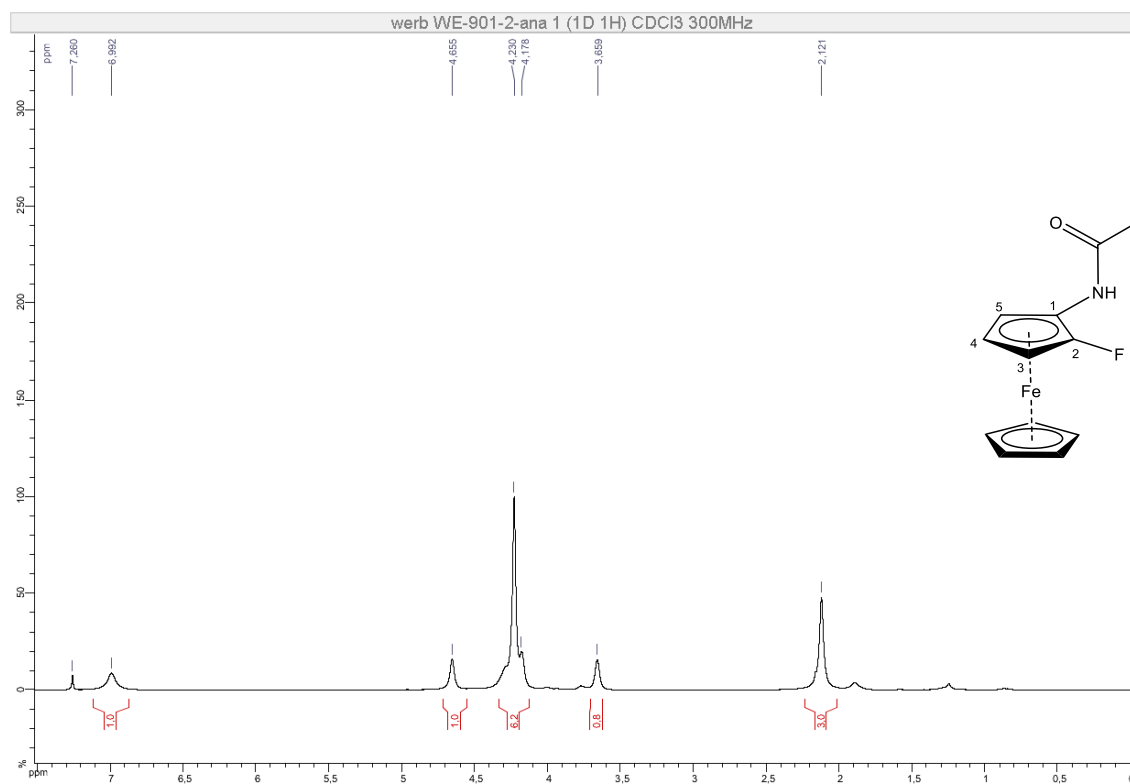


HMBC (500 MHz, (CD₃)₂SO)

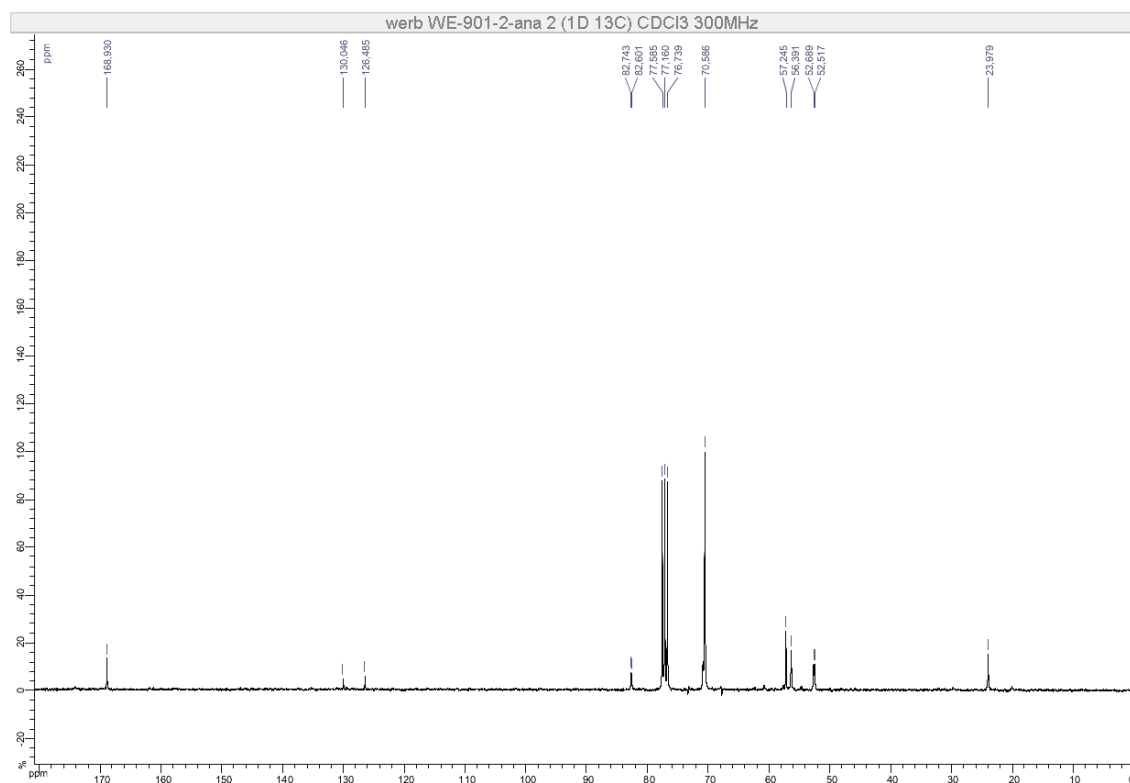


N-(2-Fluoroferrocenyl)acetamide (**2m**, racemic mixture)

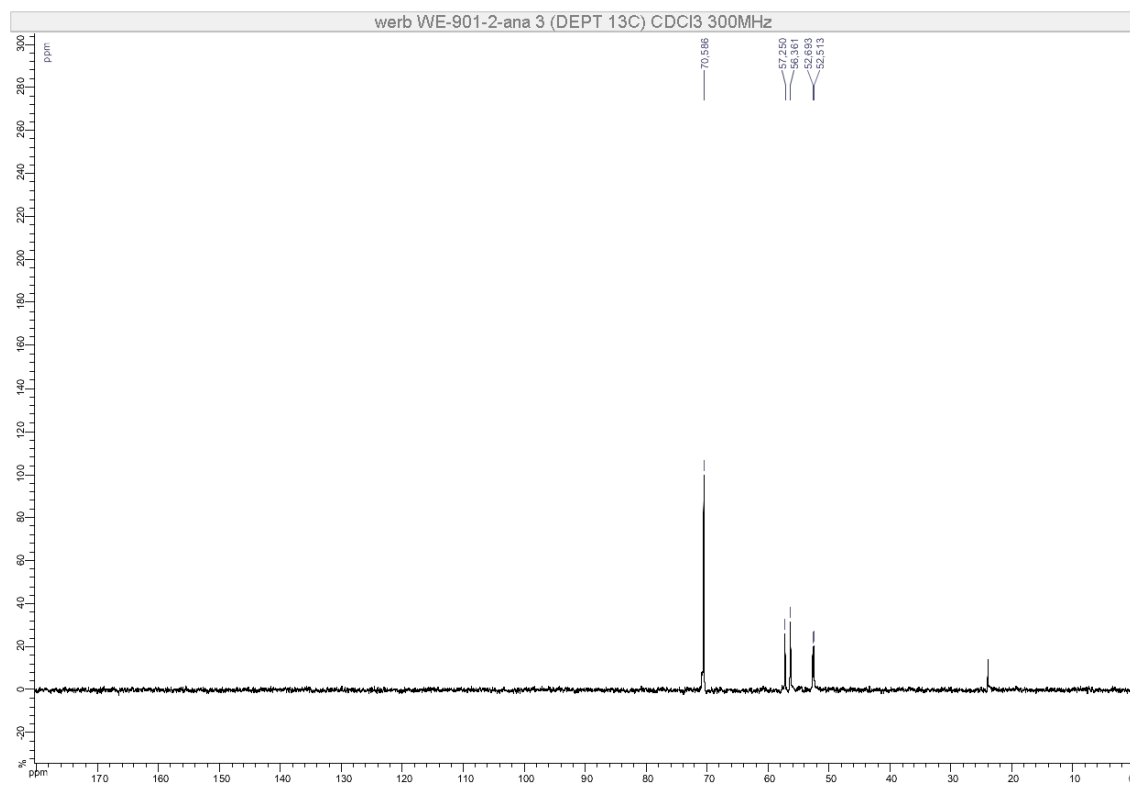
^1H NMR (300 MHz, CDCl_3)



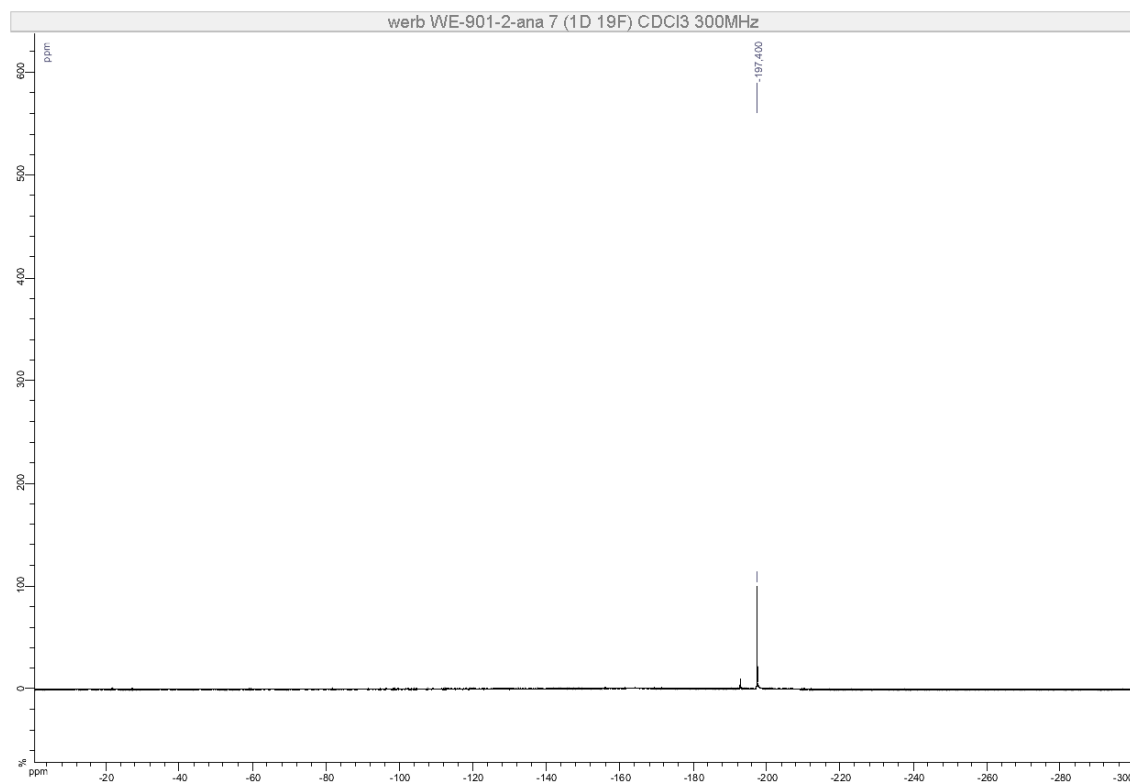
^{13}C NMR (75 MHz, CDCl_3)



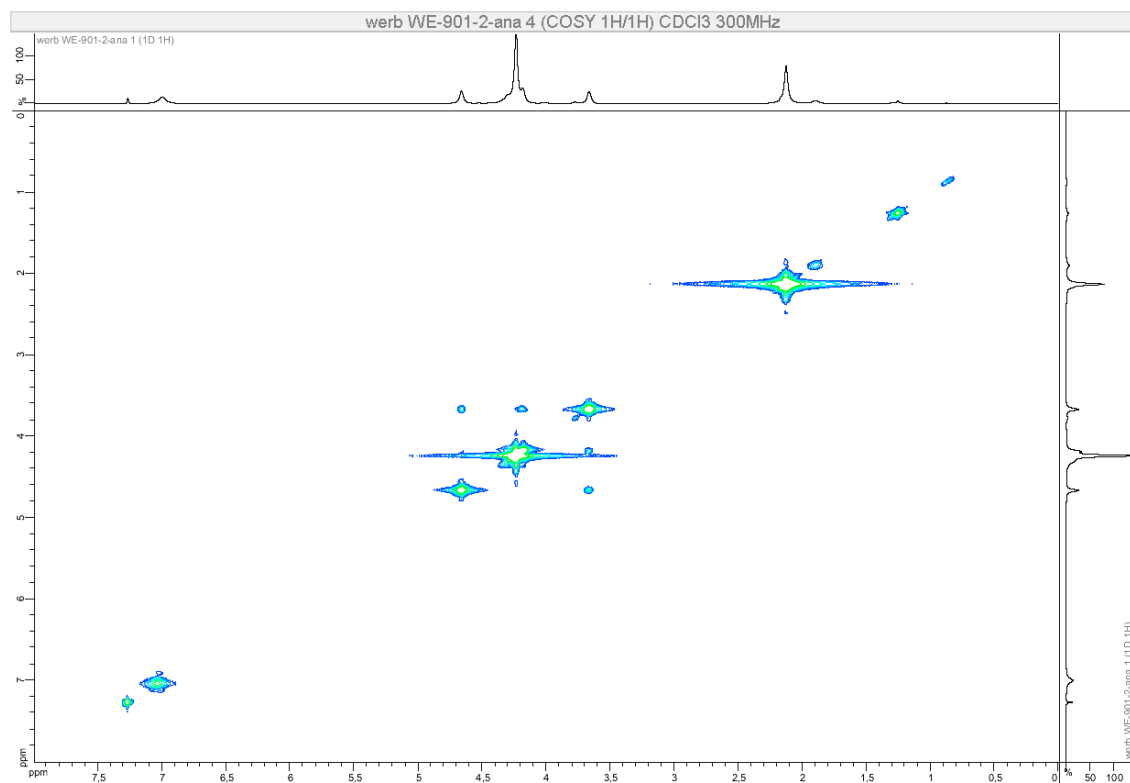
DEPT 135 (75 MHz, CDCl₃)



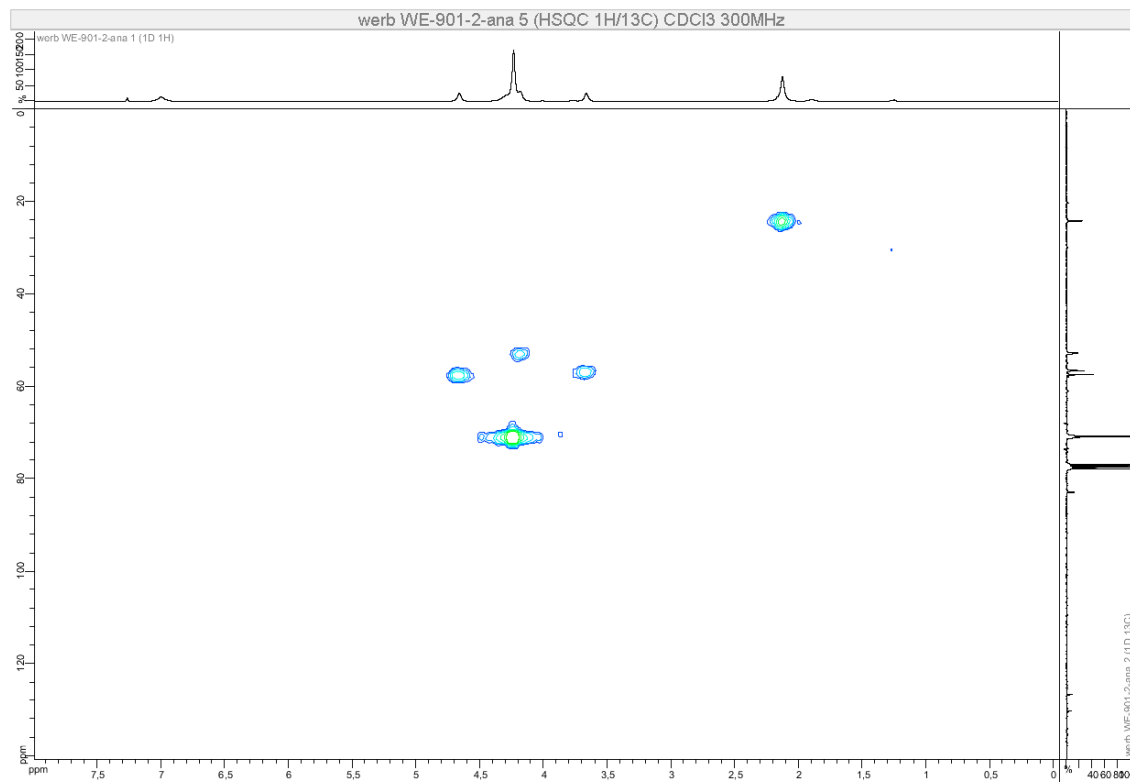
¹⁹F NMR (282 MHz, CDCl₃)



COSY (300 MHz, CDCl₃)

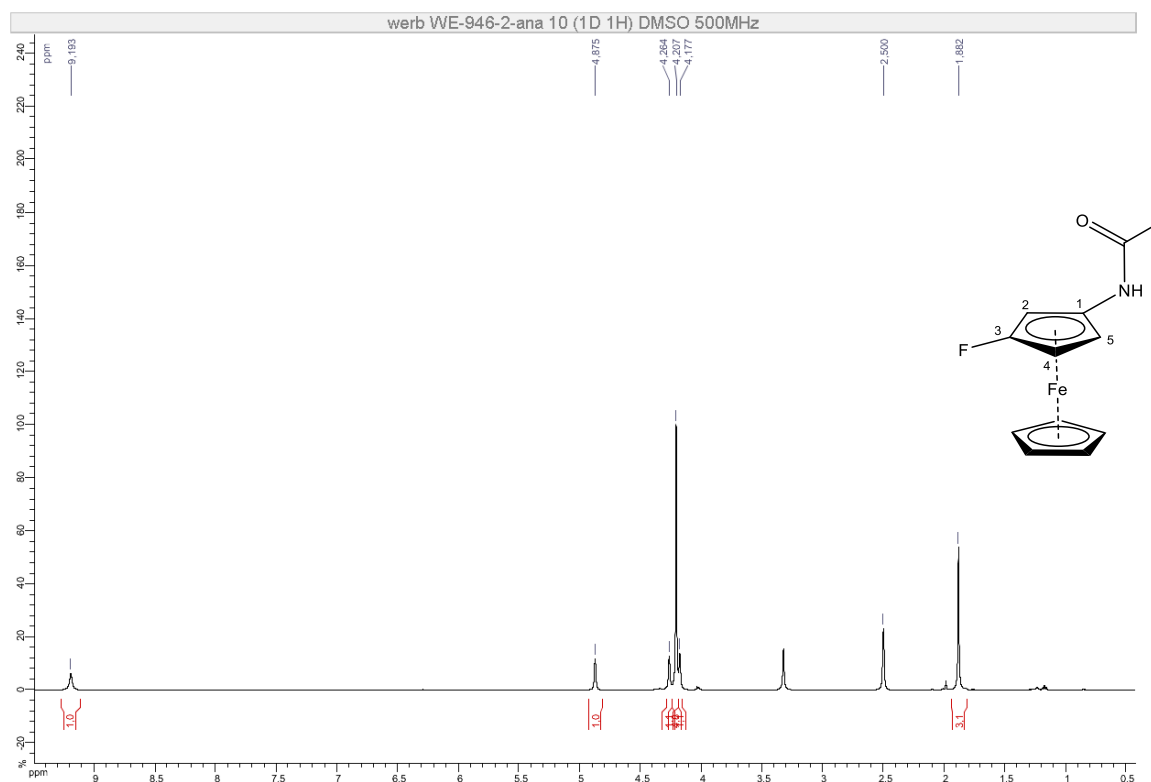


HSQC (300 MHz, CDCl₃)

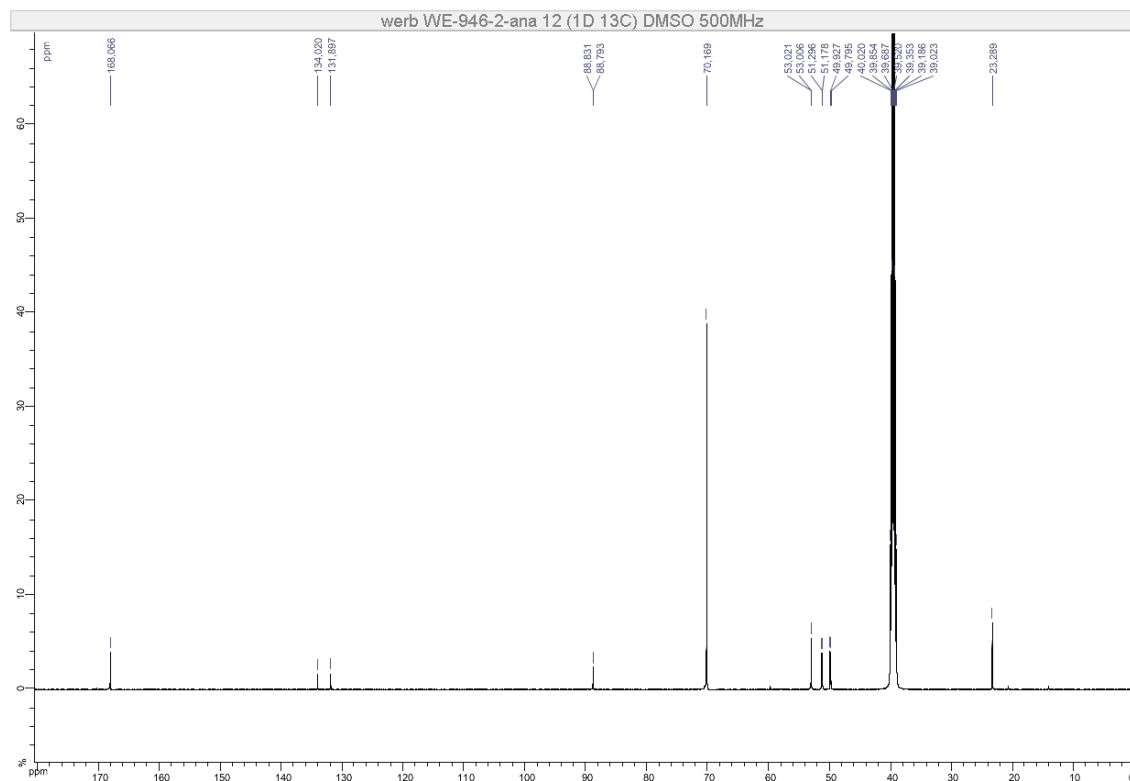


N-(3-Fluorofenyl)acetamide (4m, racemic mixture)

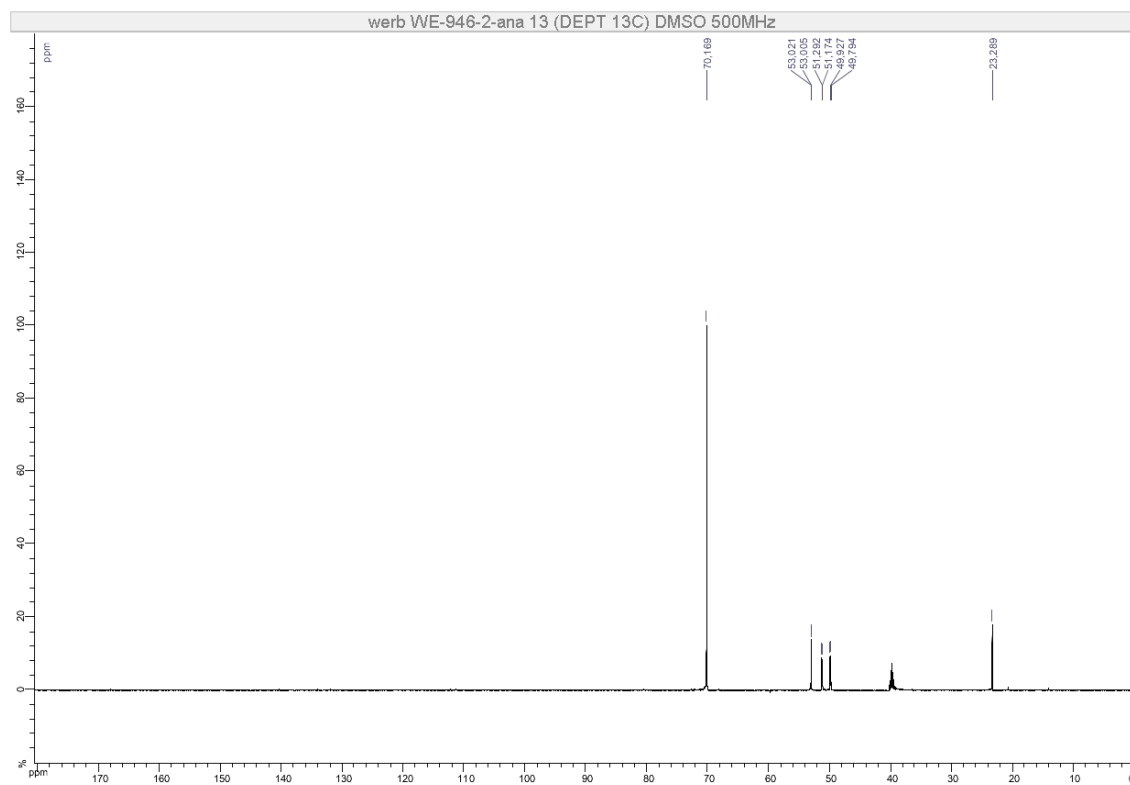
^1H NMR (500 MHz, $(\text{CD}_3)_2\text{SO}$)



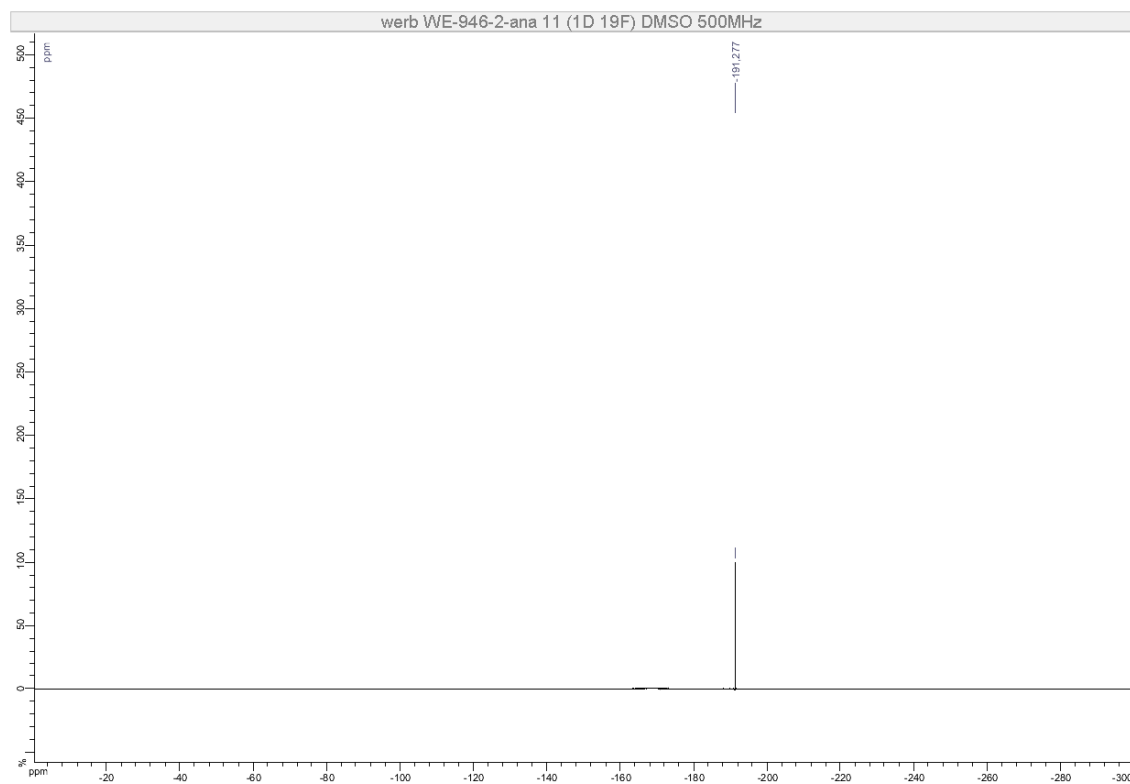
^{13}C NMR (126 MHz, $(\text{CD}_3)_2\text{SO}$)



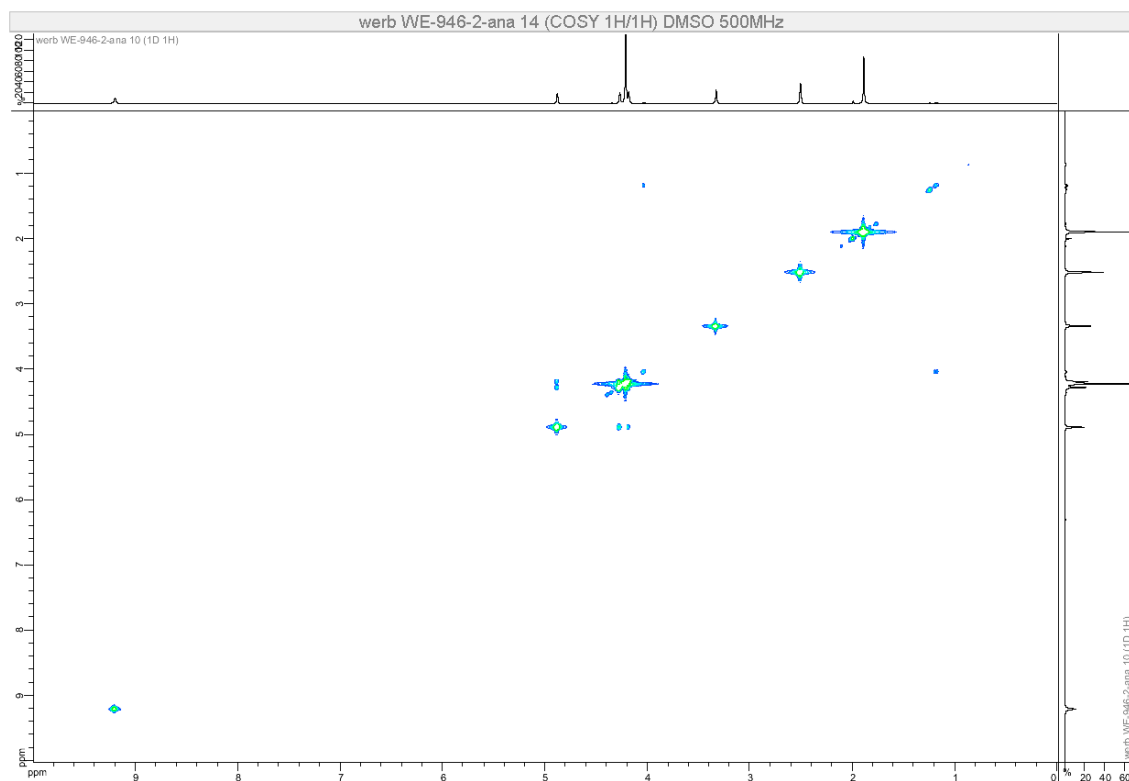
DEPT 135 (126 MHz, (CD₃)₂SO)



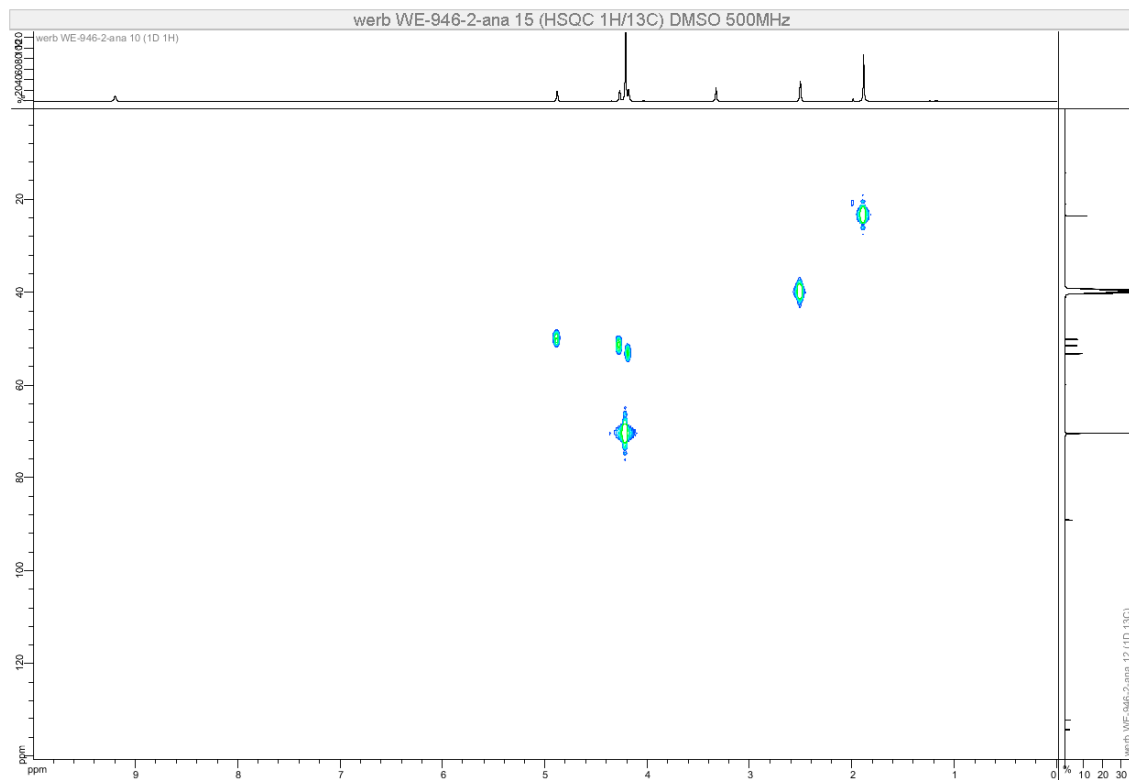
¹⁹F NMR (470 MHz, (CD₃)₂SO)



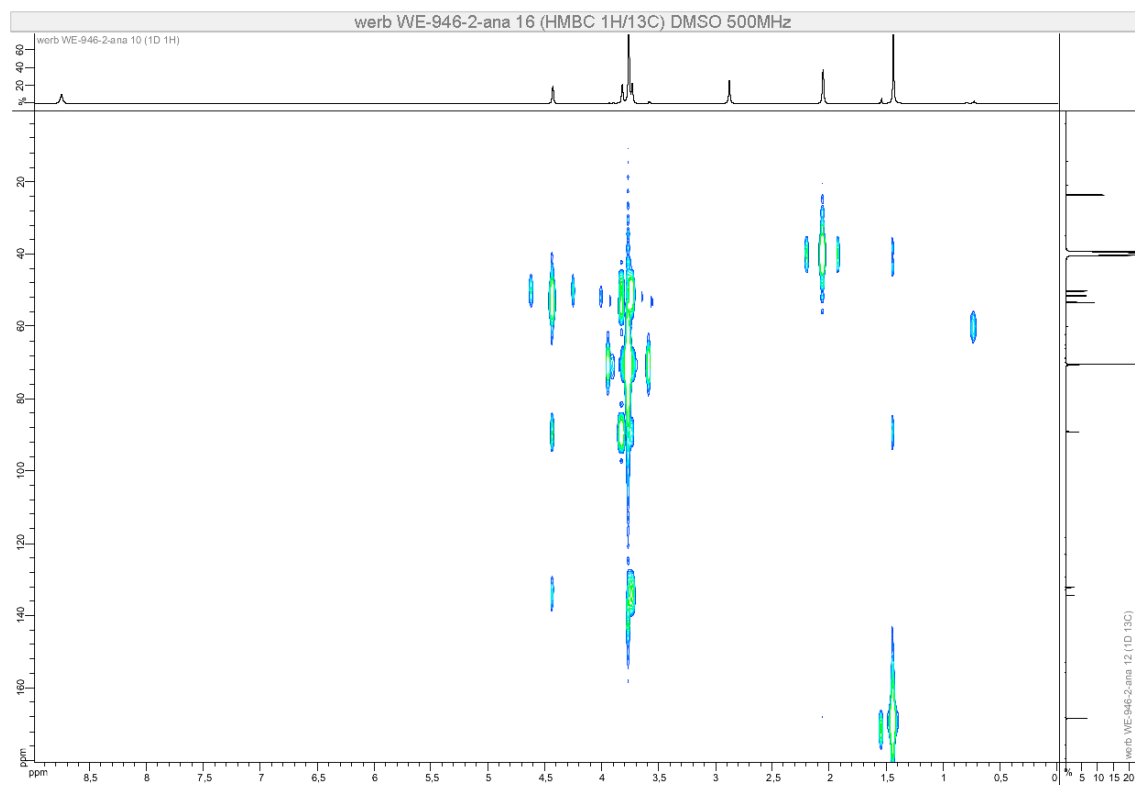
COSY (500 MHz, (CD₃)₂SO)



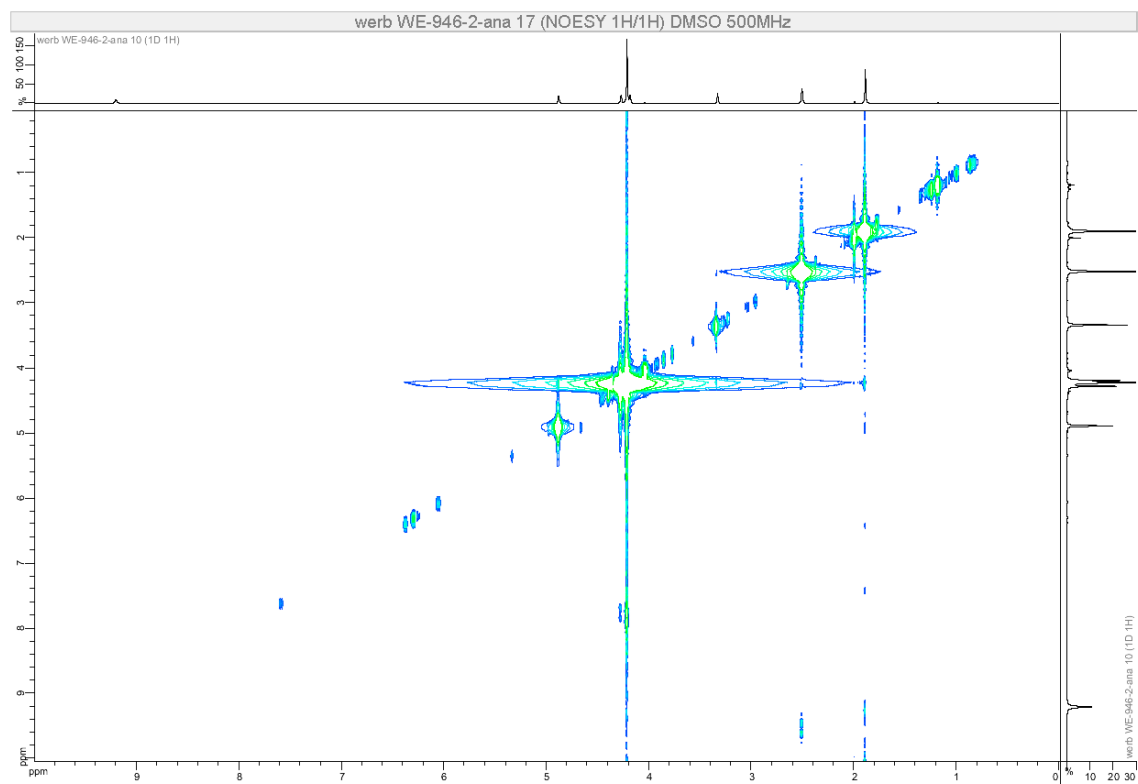
HSQC (500 MHz, (CD₃)₂SO)



HMBC (500 MHz, (CD₃)₂SO)

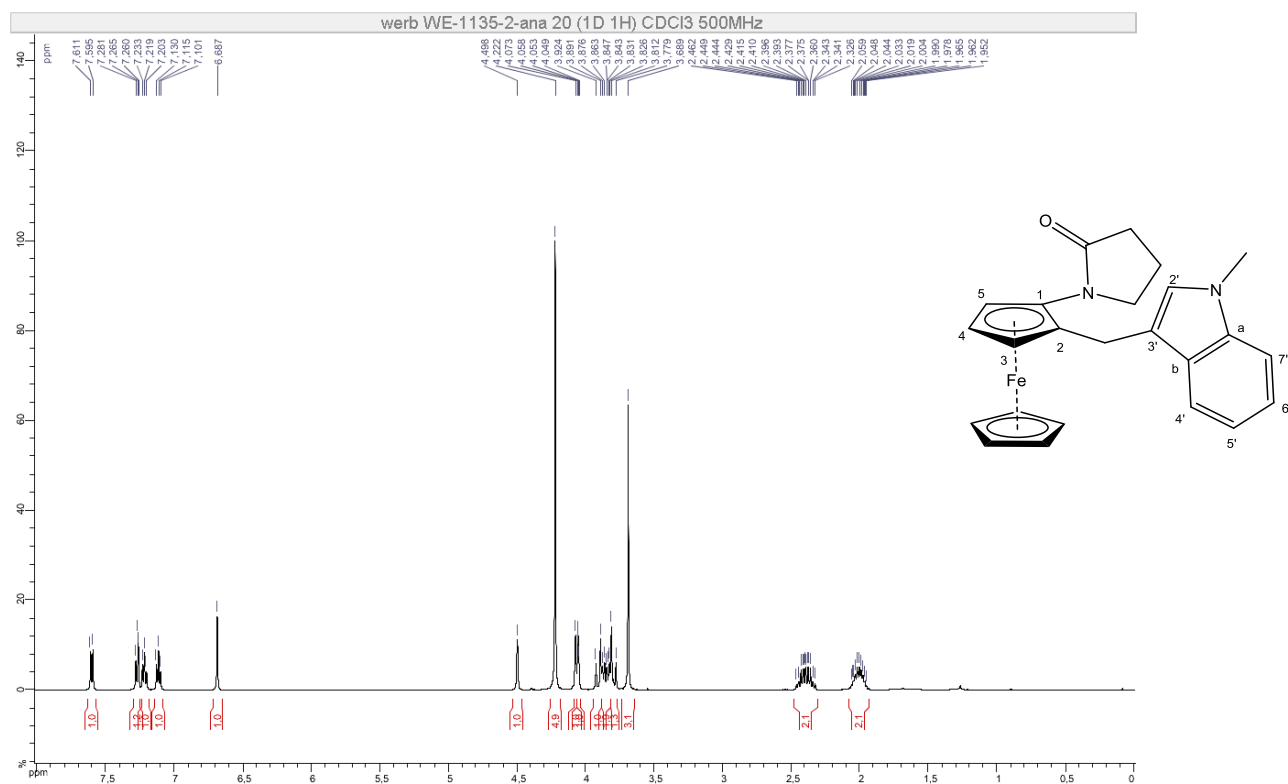


NOESY (500 MHz, (CD₃)₂SO)

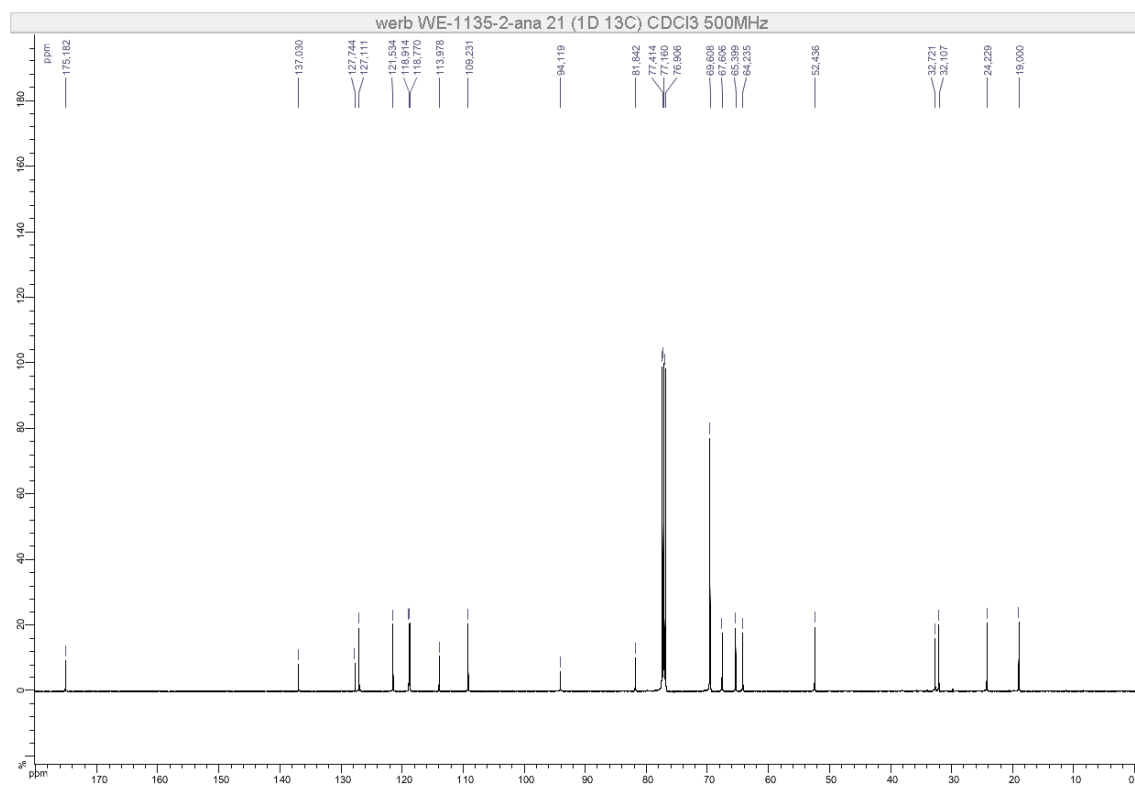


N-(2-(*N*-Methyl-3-indolylmethyl)ferrocenyl)-2-pyrrolidone (4n, racemic mixture)

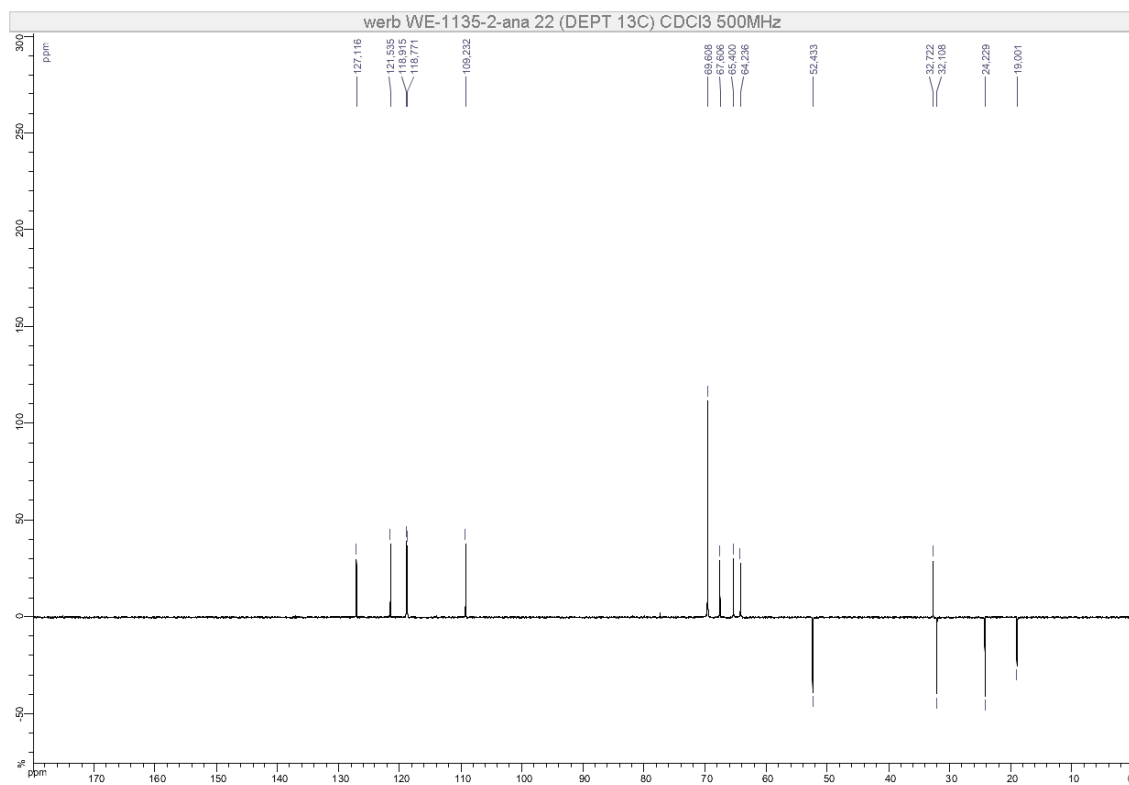
^1H NMR (500 MHz, CDCl_3)



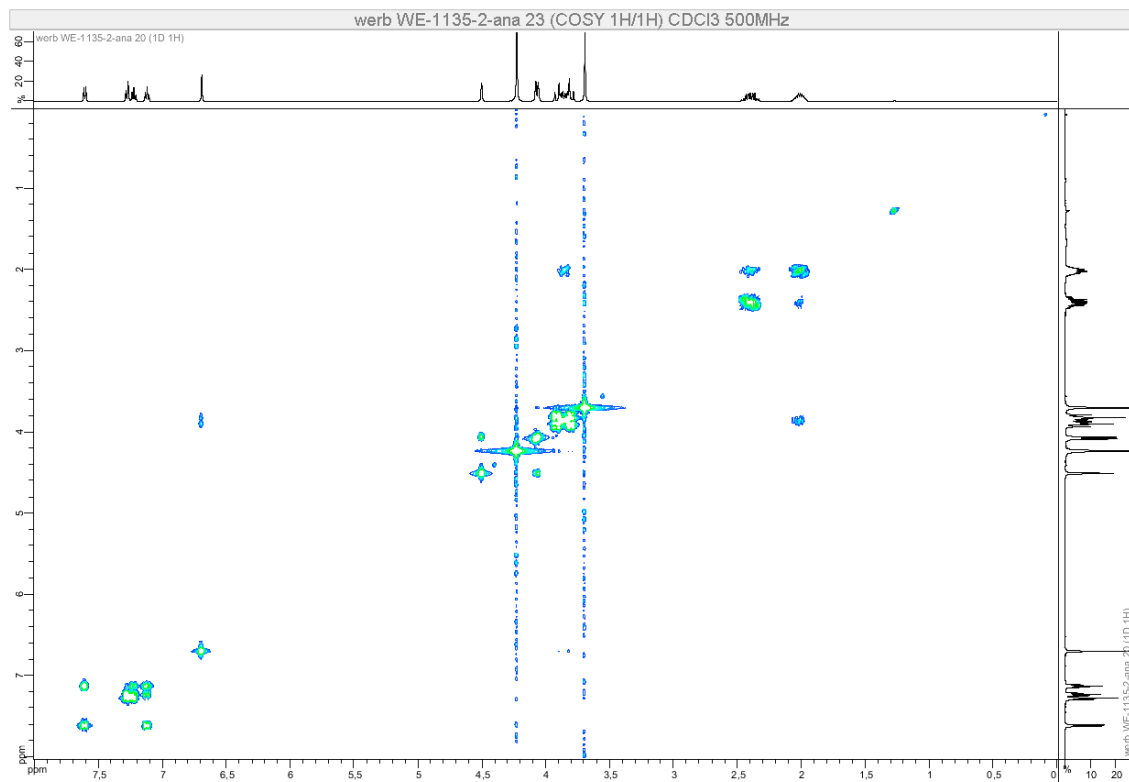
^{13}C NMR (126 MHz, CDCl_3)



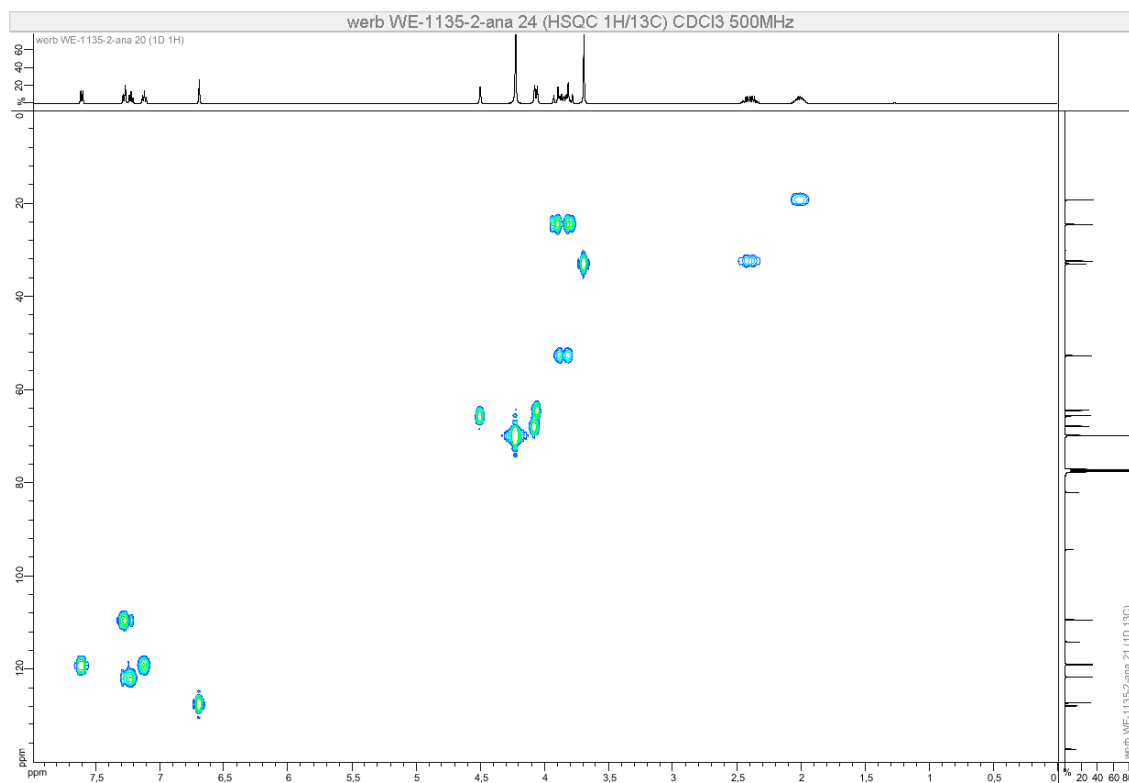
DEPT 135 (126 MHz, CDCl₃)



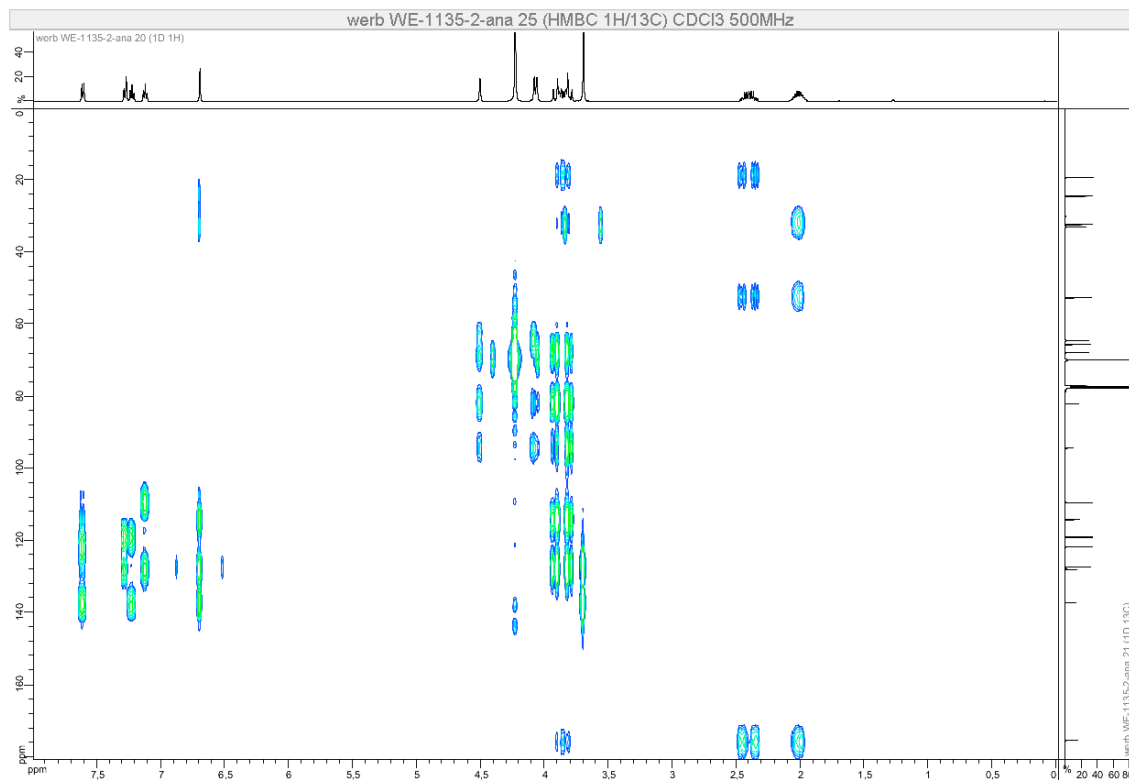
COSY (500 MHz, CDCl₃)



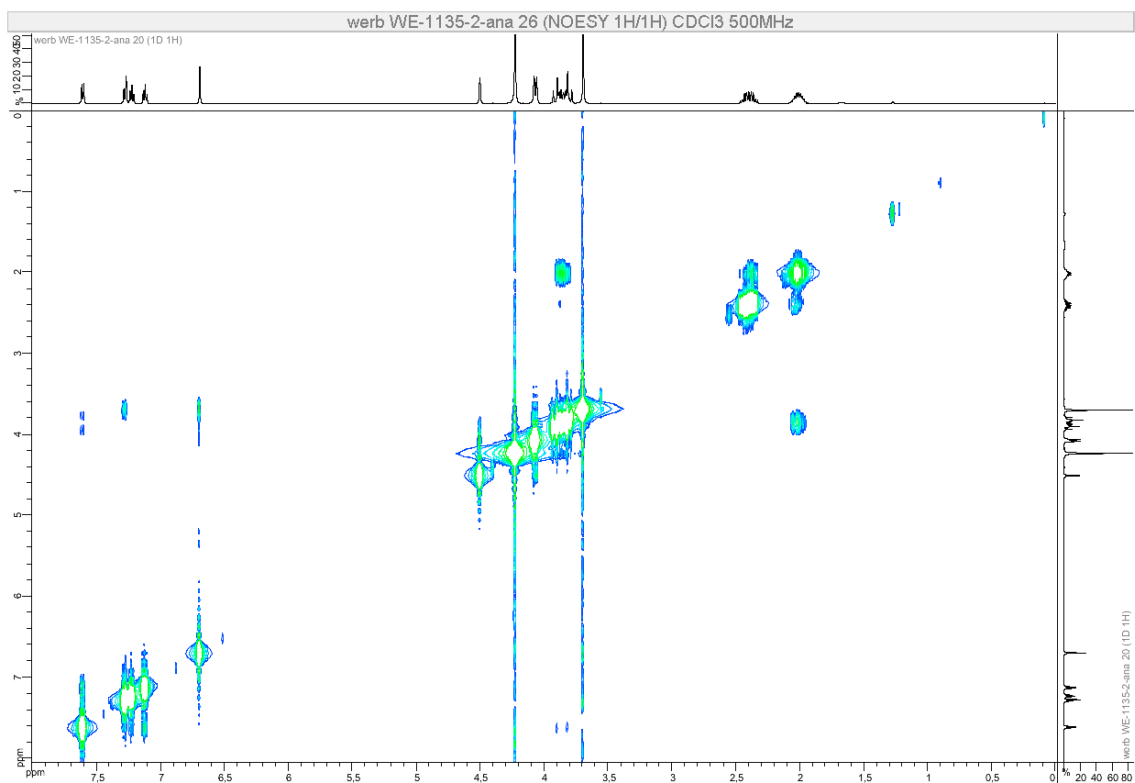
HSQC (500 MHz, CDCl₃)



HMBC (500 MHz, CDCl₃)

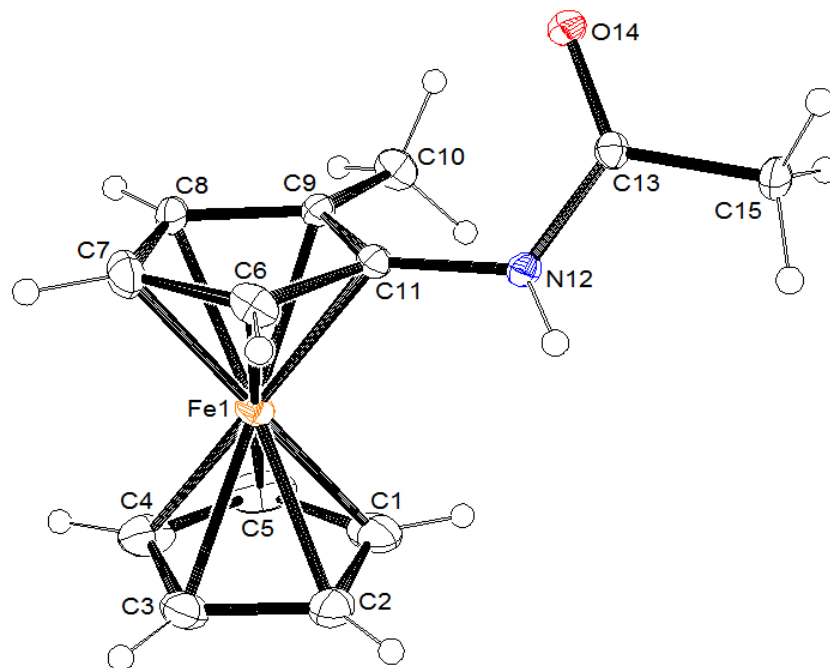


NOESY (500 MHz, CDCl₃)

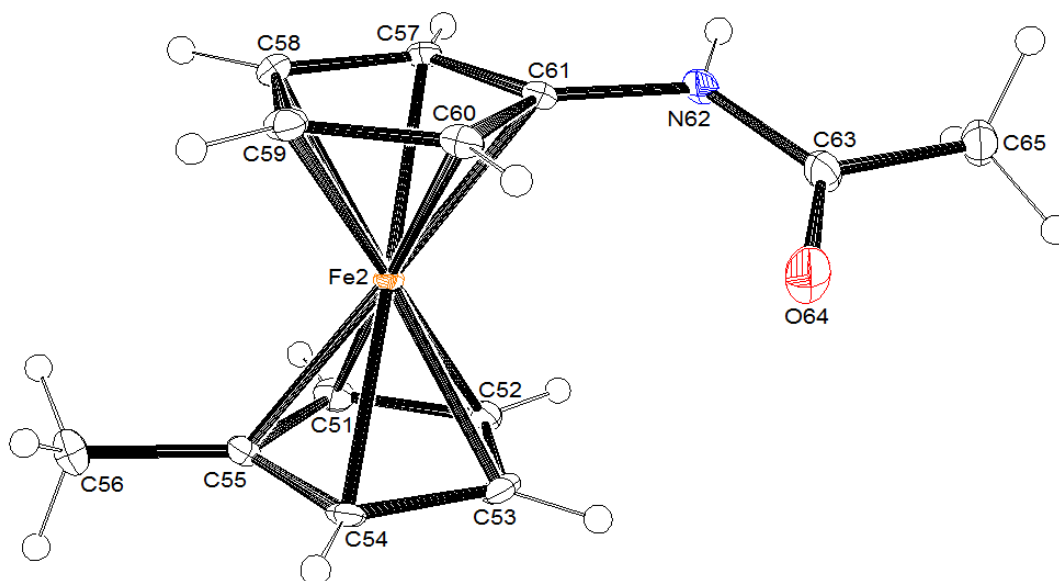


ORTEP Diagrams (30% probability)

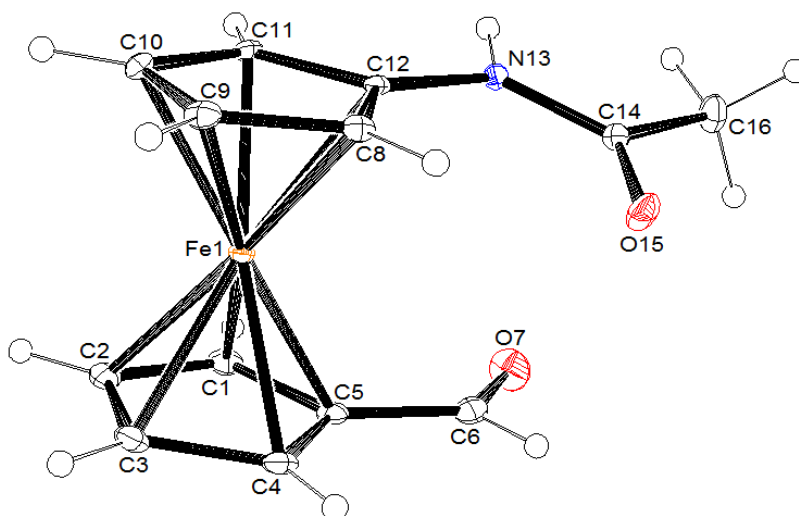
N-(2-Methylferrocenyl)acetamide (**2b**, stereoisomeric mixture due to rotamers)



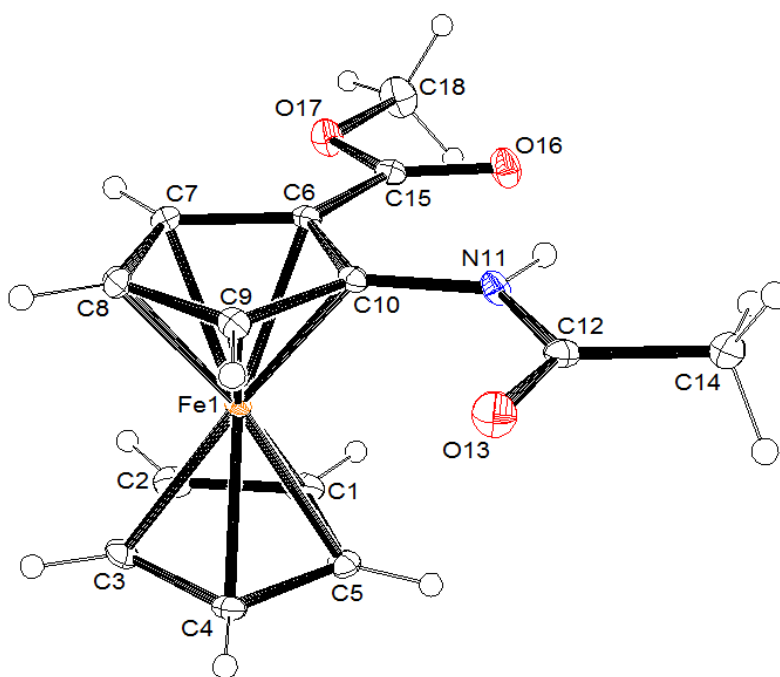
N-(1'-Methylferrocenyl)acetamide (**6b**)



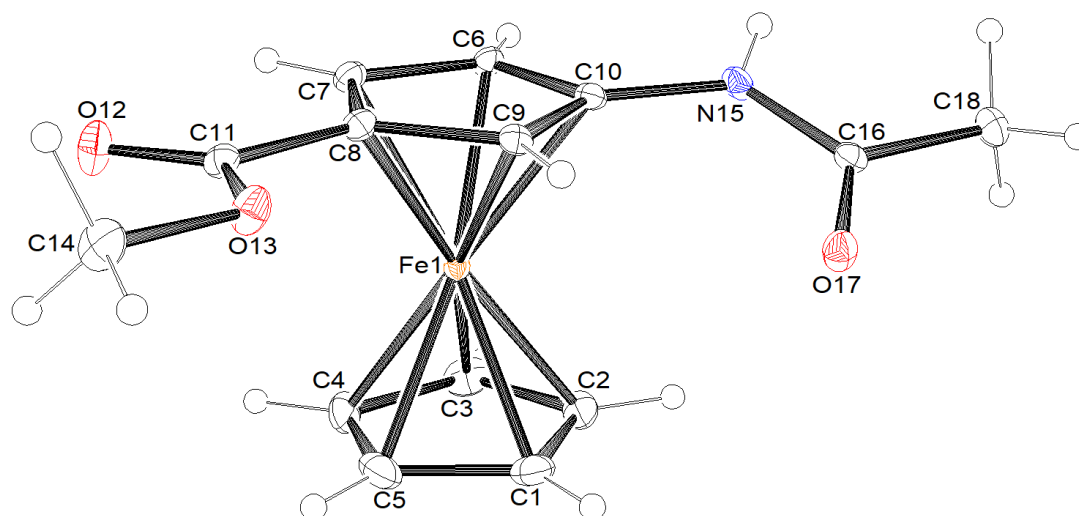
***N*-(1'-Formylferrocenyl)acetamide (6f)**



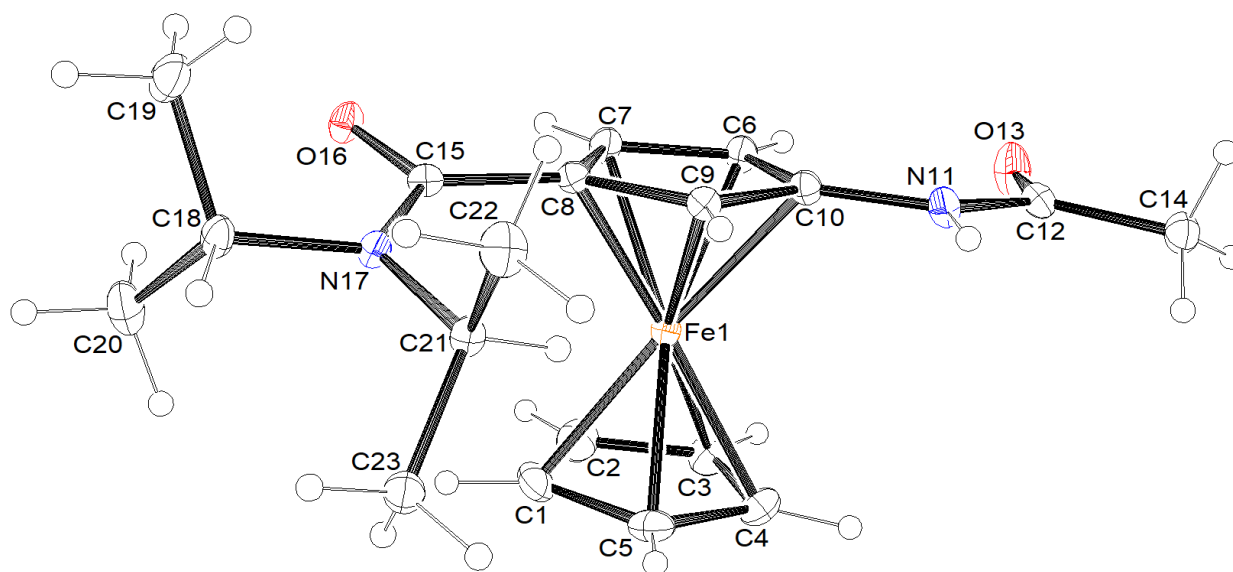
***N*-(2-(Methoxycarbonyl)ferrocenyl)acetamide (2i, racemic mixture)**



***N*-3-(Methoxycarbonyl)ferrocenyl)acetamide (4i, racemic mixture)**



***N*-3-(Diisopropylaminocarbonyl)ferrocenyl)acetamide (4j, racemic mixture)**



N-(1'-(Diisopropylaminocarbonyl)ferrocenyl)acetamide (**6j**, racemic mixture)

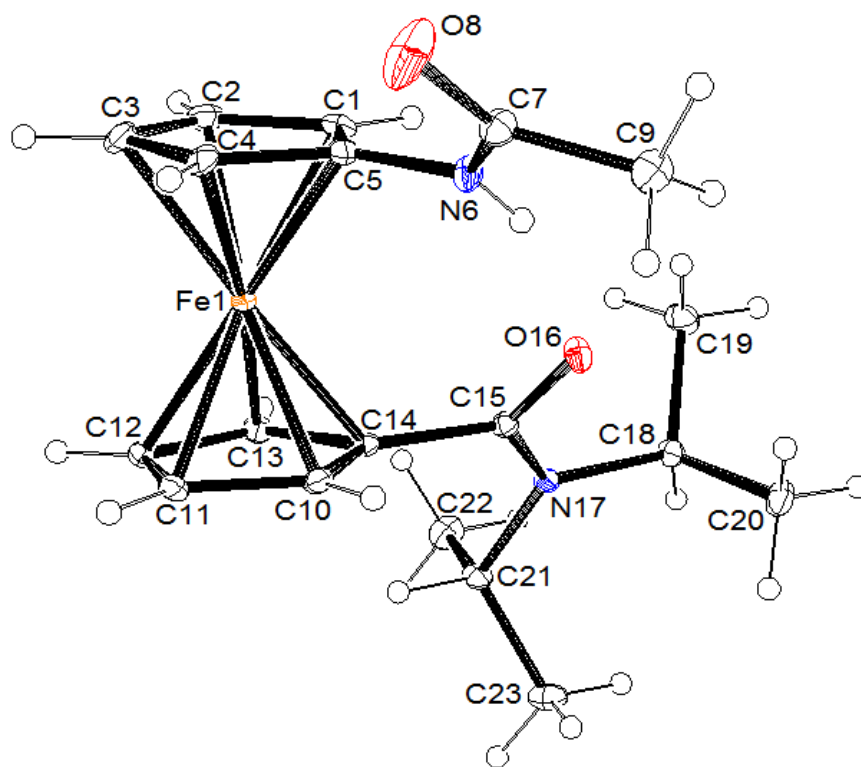


Table S1. Calculated values of the CDFT molecular structure descriptors^a for the deiodinated ferrocenes corresponding to selected substrates involved.

		Descriptor ^b																		
		Global					Local													
Subst	C at	χ	η	ω	Nu	E_{HOMO}	E_{LUMO}	q_M	q_{APT}	q_{NBO}	q_H	f^-	f^+	f_0	ω^{loc}	Nu^{loc}	s^-	s^+	s_0	s_T
a		2.97	8.28	0.534	3.81	-0.1950	-0.0005	-0.134	0.039	-0.241	-0.0576	0.0504	0.0512	0.0508	0.0273	0.1922	0.1657	0.1683	0.1670	1.016
b	2	2.91	8.17	0.517	3.88	-0.1927	0.0015	-0.152	0.019	-0.233	-0.0620	0.0471	0.0573	0.0522	0.0296	0.1828	0.1571	0.1908	0.1739	1.215
	3	2.91	8.17	0.517	3.88	-0.1927	0.0015	-0.133	0.035	-0.237	-0.0589	0.0498	0.0500	0.0499	0.0259	0.1930	0.1658	0.1667	0.1662	1.005
	1'	2.91	8.17	0.517	3.88	-0.1927	0.0015	-0.138	0.037	-0.245	-0.0592	0.0472	0.0436	0.0454	0.0225	0.1832	0.1573	0.1453	0.1513	0.924
c	2	2.95	7.91	0.550	3.92	-0.1913	-0.0009	-0.137	0.036	-0.228	-0.0581	0.0419	0.0413	0.0416	0.0227	0.1640	0.1440	0.1420	0.1431	0.986
	3	2.95	7.91	0.550	3.92	-0.1913	-0.0009	-0.133	0.036	-0.236	-0.0583	0.0453	0.0511	0.0482	0.0282	0.1773	0.1557	0.1760	0.1659	1.130
	1'	2.95	7.91	0.550	3.92	-0.1913	-0.0009	-0.138	0.039	-0.244	-0.0589	0.0434	0.0569	0.0501	0.0313	0.1698	0.1492	0.1956	0.1724	1.311
d	2	2.87	8.11	0.506	3.91	-0.1915	0.0027	-0.146	0.032	-0.228	-0.0600	0.0467	0.0570	0.0519	0.0289	0.1825	0.1565	0.1912	0.1739	1.222
	3	2.87	8.11	0.506	3.91	-0.1915	0.0027	-0.135	0.034	-0.238	-0.0584	0.0486	0.0493	0.0489	0.0249	0.1899	0.1629	0.1651	0.1640	1.013
	1'	2.87	8.11	0.506	3.91	-0.1915	0.0027	-0.132	0.034	-0.237	-0.0563	0.0479	0.0439	0.0459	0.0222	0.1874	0.1607	0.1471	0.1539	0.915
f	2	3.61	7.75	0.840	3.34	-0.2181	-0.0317	-0.156	0.104	-0.210	-0.0475	0.0442	0.0363	0.0402	0.0304	0.1473	0.1550	0.1272	0.1411	0.821
	3	3.61	7.75	0.840	3.34	-0.2181	-0.0317	-0.125	0.027	-0.230	-0.0479	0.0470	0.0422	0.0446	0.0354	0.1567	0.1649	0.1482	0.1566	0.898
	1'	3.61	7.75	0.840	3.34	-0.2181	-0.0317	-0.134	0.058	-0.230	-0.0487	0.0478	0.0512	0.0495	0.0430	0.1596	0.1680	0.1799	0.1739	1.071
g	2	3.60	7.21	0.898	3.52	-0.2059	-0.0548	-0.156	0.107	-0.214	-0.0515	0.0424	0.0235	0.0330	0.0211	0.1492	0.1599	0.0888	0.1243	0.556
	3	3.60	7.21	0.898	3.52	-0.2059	-0.0548	-0.128	0.021	-0.233	-0.0514	0.0453	0.0283	0.0368	0.0254	0.1593	0.1708	0.1067	0.1387	0.625
	1'	3.60	7.21	0.898	3.52	-0.2059	-0.0548	-0.134	0.059	-0.229	-0.0498	0.0463	0.0273	0.0368	0.0245	0.1629	0.1746	0.1031	0.1389	0.590
h	2	3.68	7.94	0.851	3.19	-0.2126	-0.0431	-0.121	0.100	-0.201	-0.0427	0.0440	0.0397	0.0419	0.0338	0.1402	0.1508	0.1359	0.1434	0.901
	3	3.68	7.94	0.851	3.19	-0.2126	-0.0431	-0.127	0.027	-0.233	-0.0467	0.0469	0.0474	0.0472	0.0404	0.1493	0.1606	0.1625	0.1615	1.012
	1'	3.68	7.94	0.851	3.19	-0.2126	-0.0431	-0.133	0.050	-0.228	-0.0471	0.0483	0.0579	0.0531	0.0493	0.1539	0.1655	0.1985	0.1820	1.199
i	2	3.39	7.81	0.738	3.50	-0.2064	-0.0261	-0.141	0.098	-0.204	-0.0485	0.0446	0.0371	0.0408	0.0274	0.1561	0.1552	0.1293	0.1423	0.833
	3	3.39	7.81	0.738	3.50	-0.2064	-0.0261	-0.129	0.023	-0.234	-0.0506	0.0471	0.0440	0.0456	0.0324	0.1651	0.1641	0.1533	0.1587	0.934
	1'	3.39	7.81	0.738	3.50	-0.2064	-0.0261	-0.135	0.055	-0.233	-0.0513	0.0477	0.0535	0.0506	0.0394	0.1673	0.1663	0.1864	0.1764	1.121
m	2	3.16	8.29	0.602	3.65	-0.2009	-0.0069	-0.190	-0.029	-0.297	-0.0658	0.0497	0.0607	0.0552	0.0365	0.1816	0.1632	0.1992	0.1812	1.221
	2	3.16	8.29	0.602	3.65	-0.2009	-0.0069	-0.135	0.050	-0.238	-0.0556	0.0505	0.0507	0.0506	0.0305	0.1847	0.1659	0.1665	0.1662	1.004
	1'	3.16	8.29	0.602	3.65	-0.2009	-0.0069	-0.139	0.028	-0.244	-0.0573	0.0487	0.0451	0.0469	0.0272	0.1778	0.1597	0.1481	0.1539	0.927

^a See section Computational Details for the detailed descriptor meaning. Recall that all investigated structures have ferrocene part in an eclipsed conformation. In addition, only bare ferrocene and prototypes of **b**, **h** and **m** have vertical plane of symmetry; hence, for the rest of the structures, the local descriptors of the carbons corresponding to the substituted ring were averaged (C2 with C5, C3 with C4). ^b Atomic charges and f 's are in elementary charge units (e), orbital energies are in Hartree, other global descriptors are in eV, s 's are in e-Hartree, ω^{loc} and Nu^{loc} e-eV.

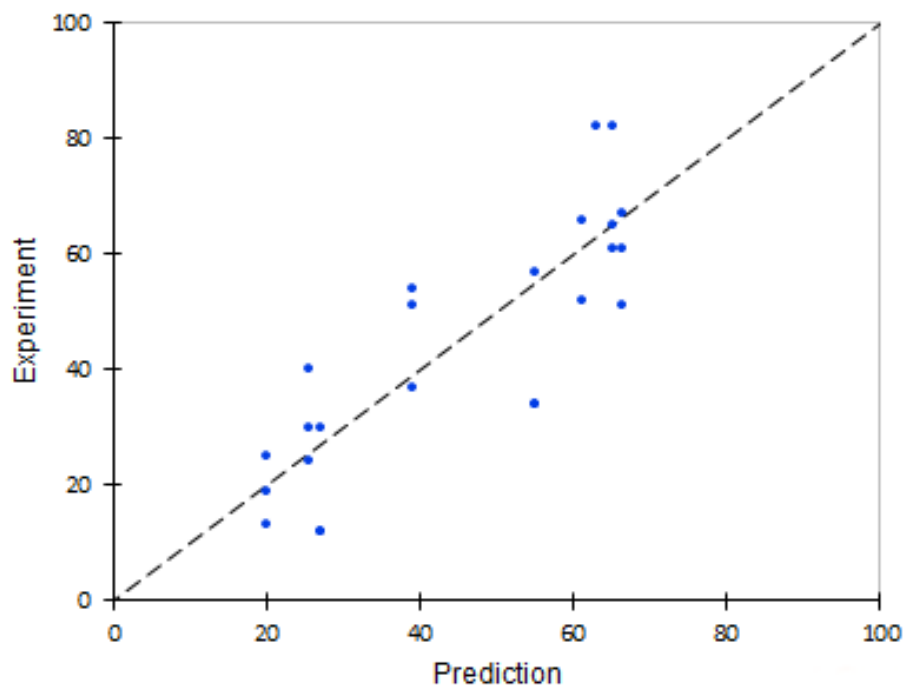


Figure S1. Predicted vs experimental yield for substituted iodoferrocenes reacted with acetamide.

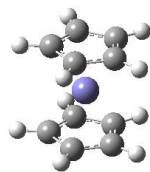
Table S2. Yield averaged over positions of parent ferrocenes.

Prototype	Yield, %
a	82
b	69
c	39
d	60
f	18
g	19
h	31
i	47
m	46

Cartesian coordinates of DFT optimized structures

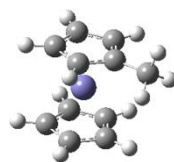
a

atom	X	Y	Z
Fe	0.00000	0.00000	0.00000
C	0.00000	1.21480	1.68740
H	0.00000	2.29660	1.66030
C	1.15540	0.37540	1.68740
H	2.18420	0.70970	1.66030
C	0.71400	-0.98280	1.68740
H	1.34990	-1.85800	1.66030
C	-0.71400	-0.98280	1.68740
H	-1.34990	-1.85800	1.66030
C	-1.15540	0.37540	1.68740
H	-2.18420	0.70970	1.66030
C	1.15540	0.37540	-1.68740
H	2.18420	0.70970	-1.66030
C	0.71400	-0.98280	-1.68740
H	1.34990	-1.85800	-1.66030
C	-0.71400	-0.98280	-1.68740
H	-1.34990	-1.85800	-1.66030
C	-1.15540	0.37540	-1.68740
H	-2.18420	0.70970	-1.66030
C	0.00000	1.21480	-1.68740
H	0.00000	2.29660	-1.66030



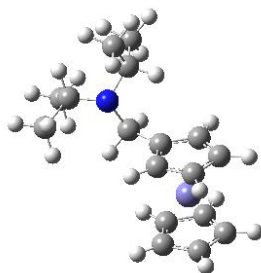
b

atom	X	Y	Z
Fe	0.20442	-0.16345	0.00004
C	-1.50772	-0.40270	-1.15078
C	-1.80741	0.39466	-0.00011
C	-1.50774	-0.40252	1.15070
C	-1.02686	-1.67411	0.71374
C	-1.02686	-1.67421	-0.71360
C	1.65161	0.78854	-1.15084
C	1.36307	1.56210	0.01449
C	1.66126	0.76265	1.15977
C	2.13316	-0.50510	0.70222
C	2.12727	-0.48908	-0.72577
H	-1.60036	-0.07712	2.17942
H	-0.68823	-2.48022	1.35135
H	-0.68820	-2.48043	-1.35106
H	1.50512	1.10372	-2.17564
H	0.96112	2.56691	0.02744
H	1.52353	1.05498	2.19255
H	2.41443	-1.34221	1.32769
H	2.40344	-1.31187	-1.37215
H	-1.60040	-0.07759	-2.17958
C	-2.38188	1.78195	-0.00003
H	-2.06669	2.34343	-0.88601
H	-3.47993	1.75356	0.00043
H	-2.06594	2.34347	0.88566



c

atom	X	Y	Z
Fe	-2.04360	-0.15514	0.04321
C	-0.52260	-0.60400	1.39054
C	0.01350	-0.50947	0.06688
C	-0.65701	-1.49255	-0.73025
C	-1.59956	-2.18045	0.09252
C	-1.51305	-1.63041	1.40772
C	-2.92296	1.64804	0.59404
C	-2.39147	1.74523	-0.72777
C	-3.03733	0.76139	-1.53715
C	-3.96839	0.05680	-0.71566
C	-3.89738	0.60395	0.60140
H	-0.49724	-1.65572	-1.78892
H	-2.28071	-2.95696	-0.23023
H	-2.12060	-1.91479	2.25711
H	-2.62030	2.24034	1.44772
H	-1.61605	2.42635	-1.05337
H	-2.83460	0.56483	-2.58177
H	-4.59212	-0.77054	-1.02791
H	-4.46041	0.26653	1.46174
H	-0.23291	0.01764	2.22784
C	1.10720	0.42912	-0.38307
H	1.10287	0.47112	-1.48872
H	0.86335	1.43866	-0.04011
N	2.41685	0.08196	0.17505
C	2.96675	-1.19841	-0.30505
C	3.88373	-1.84105	0.74699
C	3.65471	-1.15365	-1.68621
H	2.09651	-1.85802	-0.39918
H	3.37045	-1.89862	1.71187
H	4.16413	-2.85507	0.43817
H	4.81404	-1.27723	0.88743
H	3.00665	-0.70248	-2.44652
H	4.59034	-0.58235	-1.65407
H	3.90185	-2.16817	-2.02195
C	3.35617	1.21015	0.32522
C	3.04640	1.99439	1.61233
C	3.45661	2.17030	-0.88094
H	4.34586	0.75996	0.45866
H	3.05032	1.32366	2.47690
H	3.78827	2.78549	1.77686



H	2.06125	2.47507	1.56225
H	3.68519	1.63870	-1.80917
H	2.52577	2.72920	-1.03267
H	4.25173	2.90601	-0.70989

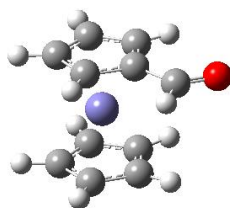
d

atom	X	Y	Z
Fe	0.79583	0.11429	-0.00917
C	-0.07761	1.61433	1.12401
C	-1.03154	1.07547	0.20174
C	-0.51997	1.28386	-1.11725
C	0.74428	1.93705	-1.00820
C	1.01706	2.14542	0.37774
C	1.39152	-1.42560	1.25299
C	0.48832	-1.92115	0.26361
C	1.06540	-1.67894	-1.01951
C	2.32553	-1.03585	-0.82396
C	2.52686	-0.87784	0.58085
H	-0.99579	0.95303	-2.02993
H	1.39824	2.19503	-1.83094
H	1.91207	2.59060	0.79206
H	1.23079	-1.43334	2.32322
H	-0.48862	-2.34803	0.44401
H	0.60731	-1.90554	-1.97303
H	2.99351	-0.69437	-1.60404
H	3.37524	-0.39906	1.05237
H	-0.16134	1.59188	2.20335
C	-2.35913	0.48350	0.56244
H	-3.13914	1.26648	0.52635
H	-2.33496	0.10312	1.59788
O	-2.69566	-0.55374	-0.34230
C	-3.98973	-1.06874	-0.11583
H	-4.76480	-0.29385	-0.23399
H	-4.15811	-1.85526	-0.85596
H	-4.08652	-1.50142	0.89356



f

atom	X	Y	Z
Fe	-0.40035	0.19025	0.00051
C	1.26999	0.75520	-1.09996
C	1.65921	0.26981	0.19446
C	1.03419	1.10885	1.18243
C	0.28317	2.10375	0.49898
C	0.42921	1.88445	-0.90775
C	-1.43911	-1.23959	-1.09550
C	-1.03476	-1.78652	0.15870
C	-1.62020	-0.99805	1.19599
C	-2.39052	0.03535	0.58112
C	-2.27816	-0.11316	-0.83431
H	1.11408	0.98898	2.25538
H	-0.32356	2.87135	0.96114
H	-0.05379	2.45648	-1.68907
H	-1.13298	-1.59447	-2.07054
H	-0.36452	-2.62503	0.29578
H	-1.48249	-1.14250	2.25945
H	-2.93386	0.81596	1.09706
H	-2.72175	0.53523	-1.57836
H	1.56025	0.31089	-2.04164
C	2.46204	-0.92684	0.46587
O	2.99114	-1.61840	-0.38608
H	2.56835	-1.17556	1.54608



g

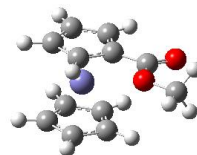
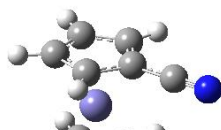
atom	X	Y	Z
Fe	-1.72237	0.09379	-0.13101
O	0.98924	-0.51557	2.20808
C	0.01105	0.94082	0.63694
C	-0.23801	1.42611	-0.69667
C	-1.49727	2.08965	-0.69791
C	-2.04057	2.01792	0.62256
C	-1.12560	1.30229	1.44058
C	-1.52747	-1.97434	-0.09638
C	-1.70962	-1.52311	-1.43917
C	-2.96554	-0.84642	-1.50868
C	-3.55697	-0.87909	-0.20963
C	-2.66746	-1.57714	0.66376
C	1.12239	0.10333	1.15542
C	2.41445	0.00712	0.39585
C	3.17646	-1.16200	0.55236
C	4.39766	-1.30359	-0.10048
C	4.88855	-0.26531	-0.89870
C	4.15325	0.91311	-1.03675
C	2.91892	1.04797	-0.39851
H	0.39681	1.27494	-1.55794
H	-1.97712	2.53561	-1.55942
H	-3.00201	2.40487	0.93379
H	-1.24215	1.04695	2.48413
H	-0.65412	-2.47877	0.29499
H	-1.00470	-1.64238	-2.25142
H	-3.38040	-0.36300	-2.38354
H	-4.49762	-0.42419	0.07207
H	-2.81089	-1.74132	1.72334
H	2.79168	-1.94624	1.19647
H	4.97196	-2.21873	0.01637
H	4.54155	1.73054	-1.63837
H	2.36447	1.97595	-0.49242
H	5.84485	-0.37226	-1.40392



h

atom	X	Y	Z
Fe	-0.18402	-0.36659	0.00000
C	1.49730	-0.00929	1.16366
C	1.49367	0.83770	0.00000
C	1.49730	-0.00929	-1.16366
C	1.51146	-1.35832	-0.71436
C	1.51146	-1.35832	0.71436
C	-1.87074	0.00886	1.15513
C	-1.87135	0.84747	0.00000
C	-1.87074	0.00886	-1.15513
C	-1.87074	-1.34978	-0.71379
C	-1.87074	-1.34978	0.71379
H	1.47856	0.33544	-2.18812
H	1.49099	-2.23428	-1.34877
H	1.49099	-2.23428	1.34877
H	-1.84207	0.34486	2.18316
H	-1.82533	1.92881	0.00000
H	-1.84207	0.34486	-2.18316
H	-1.84151	-2.22506	-1.34944
H	-1.84151	-2.22506	1.34944
H	1.47856	0.33544	2.18812
C	1.47262	2.26186	0.00000
N	1.46587	3.42584	0.00000

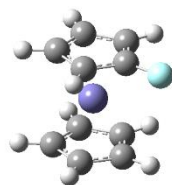
i



atom	X	Y	Z
Fe	0.94155	0.11936	-0.03822
C	-0.95591	0.93288	0.08424
C	-0.10812	1.51562	1.08394
C	0.97179	2.15736	0.41824
C	0.80256	1.97313	-0.99046
C	-0.38379	1.21720	-1.20163
C	0.82130	-1.93524	0.25810
C	1.66064	-1.34459	1.25017
C	2.74704	-0.70257	0.58114
C	2.57719	-0.89542	-0.82322
C	1.38566	-1.65728	-1.02360
H	-0.27262	1.44738	2.14999
H	1.79959	2.66466	0.89586
H	1.48005	2.31766	-1.76078
H	-0.78181	0.88969	-2.15129
H	-0.10310	-2.46579	0.44572
H	1.48358	-1.35215	2.31740
H	3.53969	-0.13719	1.05332
H	3.22006	-0.50371	-1.60064
H	0.96803	-1.94642	-1.97895
C	-2.16943	0.15342	0.38676
O	-2.58537	-0.08095	1.50523
O	-2.79421	-0.26676	-0.74182
C	-3.99677	-1.01790	-0.52747
H	-4.37519	-1.25511	-1.52251
H	-3.78726	-1.93473	0.03107
H	-4.72759	-0.42558	0.03006

m

atom	X	Y	Z
Fe	-0.15926	0.18492	0.00000
C	-0.26553	-1.53675	1.16456
C	0.51271	-1.77762	0.00000
C	-0.26553	-1.53675	-1.16456
C	-1.56878	-1.15518	-0.71416
C	-1.56878	-1.15518	0.71416
C	0.68997	1.68666	1.15474
C	1.49331	1.43905	0.00000
C	0.68997	1.68666	-1.15474
C	-0.60805	2.08650	-0.71408
C	-0.60805	2.08650	0.71408
H	0.07778	-1.61998	-2.18627
H	-2.40198	-0.88643	-1.34963
H	-2.40198	-0.88643	1.34963
H	1.00071	1.55918	2.18346
H	2.51661	1.08705	0.00000
H	1.00071	1.55918	-2.18346
H	-1.45240	2.31767	-1.35021
H	-1.45240	2.31767	1.35021
H	0.07778	-1.61998	2.18627
F	1.79648	-2.17547	0.00000



benzene

atom	X	Y	Z
C	-1.06282	-0.90591	0.00001
C	0.25327	-1.37325	0.00007
C	1.31599	-0.46745	-0.00006
C	1.06275	0.90600	0.00001
C	-0.25315	1.37327	0.00006
C	-1.31603	0.46735	-0.00006
H	-1.88970	-1.61101	-0.00007
H	0.45015	-2.44198	0.00008
H	2.34004	-0.83108	-0.00015
H	1.88980	1.61089	0.00001
H	-0.45029	2.44195	0.00002
H	-2.34000	0.83123	-0.00006

toluene

atom	X	Y	Z
C	-1.20130	-1.20536	0.00220
C	0.19423	-1.20235	-0.00902
C	0.91390	-0.00006	-0.01142
C	0.19429	1.20232	-0.00902
C	-1.20120	1.20542	0.00220
C	-1.90512	0.00003	0.00852
H	-1.73879	-2.15030	0.00155
H	0.73440	-2.14681	-0.01795
H	0.73454	2.14673	-0.01795
H	-1.73867	2.15036	0.00155
H	-2.99187	0.00009	0.01400
C	2.42554	-0.00002	0.00942
H	2.80995	0.00244	1.03850
H	2.83420	-0.88728	-0.48638
H	2.83423	0.88490	-0.49055

fluorobenzene

atom	X	Y	Z
C	-1.13556	-1.20860	0.00000
C	0.26042	-1.21759	0.00001
C	0.93164	-0.00002	-0.00002
C	0.26043	1.21758	-0.00001
C	-1.13553	1.20862	0.00002
C	-1.83593	0.00000	-0.00001
H	-1.67510	-2.15172	0.00001
H	0.82861	-2.14204	0.00001
H	0.82867	2.14200	-0.00001
H	-1.67509	2.15172	0.00002
H	-2.92196	0.00003	-0.00002
F	2.28245	0.00000	0.00001

benzaldehyde

atom	X	Y	Z
C	1.73594	1.06060	-0.00003
C	0.36107	1.29211	0.00003
C	-0.53394	0.21447	-0.00008
C	-0.04515	-1.10115	-0.00004
C	1.32630	-1.33125	0.00005
C	2.21684	-0.25075	0.00000
H	2.43026	1.89616	0.00000
H	-0.02499	2.30955	0.00013
H	-0.75906	-1.91924	-0.00012
H	1.70793	-2.34855	0.00014
H	3.28824	-0.43329	0.00003
C	-1.99224	0.46870	0.00002
O	-2.84767	-0.39584	0.00003
H	-2.27395	1.54572	0.00001

benzonitrile

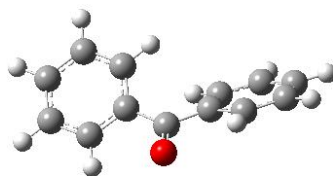
atom	X	Y	Z
C	-1.48402	-1.21087	0.00000
C	-0.09146	-1.21746	0.00002
C	0.61028	-0.00003	0.00000
C	-0.09144	1.21745	0.00001
C	-1.48397	1.21090	0.00001
C	-2.18066	0.00001	-0.00001
H	-2.02615	-2.15196	-0.00002
H	0.45875	-2.15283	0.00001
H	0.45885	2.15278	0.00000
H	-2.02611	2.15198	0.00000
H	-3.26704	0.00005	-0.00001
C	2.04504	-0.00001	-0.00001
N	3.20844	0.00000	0.00000

methyl benzoate

atom	X	Y	Z
C	-2.13367	-1.37526	-0.00001
C	-0.75335	-1.18141	-0.00002
C	-0.23043	0.11928	-0.00002
C	-1.09879	1.21943	0.00001
C	-2.47708	1.02127	0.00002
C	-2.99610	-0.27627	0.00001
H	-2.53711	-2.38413	-0.00002
H	-0.07798	-2.02953	-0.00003
H	-0.67269	2.21732	0.00001
H	-3.14733	1.87642	0.00004
H	-4.07193	-0.43076	0.00002
C	1.23485	0.39138	-0.00002
O	1.73017	1.50164	-0.00011
O	1.97305	-0.74381	0.00007
C	3.39466	-0.54780	0.00005
H	3.70653	0.00654	0.88934
H	3.82770	-1.54867	0.00013
H	3.70653	0.00640	-0.88932

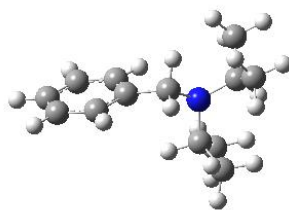
benzophenone

atom	X	Y	Z
C	2.70884	-1.53456	0.67034
C	1.45426	-0.92580	0.61752
C	1.30393	0.33724	0.02442
C	2.43422	0.98342	-0.50186
C	3.68087	0.36657	-0.46635
C	3.82077	-0.89497	0.12061
H	2.81722	-2.50668	1.14362
H	0.59661	-1.42137	1.06101
H	2.31034	1.97170	-0.93276
H	4.54667	0.86916	-0.88899
H	4.79570	-1.37411	0.15465
C	0.00003	1.08038	-0.00017
O	0.00003	2.30675	-0.00039
C	-1.30391	0.33728	-0.02449
C	-1.45444	-0.92559	-0.61793
C	-2.43402	0.98331	0.50232
C	-2.70906	-1.53427	-0.67063
H	-0.59690	-1.42105	-1.06176
C	-3.68071	0.36649	0.46698
H	-2.31003	1.97148	0.93347
C	-3.82081	-0.89483	-0.12037
H	-2.81762	-2.50622	-1.14422
H	-4.54635	0.86898	0.89006
H	-4.79576	-1.37394	-0.15431



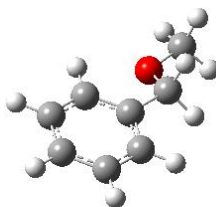
diisopropylaminomethylbenzene

atom	X	Y	Z
C	-3.08043	-0.48126	1.26031
C	-1.74594	-0.61797	0.88049
C	-1.34011	-0.31901	-0.42725
C	-2.30177	0.12480	-1.34156
C	-3.64047	0.26019	-0.96607
C	-4.03407	-0.04313	0.33733
H	-3.37847	-0.71703	2.27905
H	-0.99819	-0.94555	1.59697
H	-1.99943	0.36821	-2.35833
H	-4.37233	0.60899	-1.69034
H	-5.07407	0.06462	0.63432
C	0.10399	-0.52620	-0.86228
H	0.26220	-1.60183	-1.00760
H	0.24067	-0.06830	-1.86012
N	1.08107	-0.06707	0.11967
C	1.11522	1.39871	0.29090
C	1.92618	2.17497	-0.76745
C	1.55215	1.78424	1.71163
H	0.06931	1.71210	0.19053
H	1.62098	1.91015	-1.78618
H	1.77263	3.25408	-0.64676
H	3.00182	1.98435	-0.67303
H	0.94156	1.26038	2.45348
H	2.60432	1.54138	1.90171
H	1.43686	2.86367	1.86465
C	2.37202	-0.78361	0.11839
C	3.00367	-1.03143	-1.26919
C	2.24779	-2.10423	0.89630
H	3.06785	-0.14880	0.67795
H	3.11024	-0.10640	-1.84315
H	4.00148	-1.47125	-1.15383
H	2.40796	-1.73193	-1.86591
H	1.88755	-1.91689	1.91250
H	1.54406	-2.79143	0.41043
H	3.21623	-2.61545	0.95673



methoxymethylbenzene

atom	X	Y	Z
C	-1.85941	1.36948	0.03613
C	-0.50384	1.04953	0.12260
C	-0.08936	-0.28665	0.09417
C	-1.05362	-1.29414	-0.02310
C	-2.40991	-0.97578	-0.10058
C	-2.81697	0.35924	-0.07187
H	-2.16818	2.41168	0.05319
H	0.24393	1.83187	0.19878
H	-0.74137	-2.33617	-0.05751
H	-3.14668	-1.76963	-0.19275
H	-3.87233	0.61028	-0.13845
C	1.37115	-0.65119	0.23620
H	1.61230	-0.83452	1.30008
H	1.58001	-1.59389	-0.29879
O	2.18603	0.39237	-0.26179
C	3.56176	0.14252	-0.07377
H	3.88754	-0.76785	-0.60274
H	4.10320	1.00093	-0.47961
H	3.81458	0.03024	0.99337

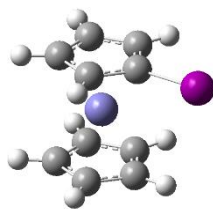


iodobenzene (in 1,4-dioxane)

atom	X	Y	Z
C	0.00000	1.20790	-2.65046
C	0.00000	1.21692	-1.25304
C	0.00000	0.00000	-0.56801
C	0.00000	-1.21692	-1.25304
C	0.00000	-1.20790	-2.65046
C	0.00000	0.00000	-3.35076
H	0.00000	2.15243	-3.18754
H	0.00000	2.15711	-0.71227
H	0.00000	-2.15711	-0.71227
H	0.00000	-2.15243	-3.18754
H	0.00000	0.00000	-4.43693
I	0.00000	0.00000	1.55832

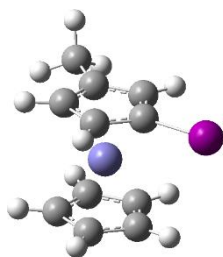
1a (in 1,4-dioxane)

atom	X	Y	Z
Fe	1.15914	-0.62320	0.00000
C	0.79559	1.04803	1.16327
C	-0.03586	1.04559	0.00000
C	0.79559	1.04803	-1.16327
C	2.15043	1.05297	-0.71413
C	2.15043	1.05297	0.71413
C	0.79167	-2.30388	1.15550
C	-0.04696	-2.30734	0.00000
C	0.79167	-2.30388	-1.15550
C	2.15043	-2.29834	-0.71411
C	2.15043	-2.29834	0.71411
H	0.45333	1.03091	-2.18869
H	3.02566	1.02514	-1.35006
H	3.02566	1.02514	1.35006
H	0.45624	-2.27514	2.18396
H	-1.12845	-2.26821	0.00000
H	0.45624	-2.27514	-2.18396
H	3.02569	-2.26350	-1.34970
H	3.02569	-2.26350	1.34970
H	0.45333	1.03091	2.18869
I	-2.13380	1.15135	0.00000



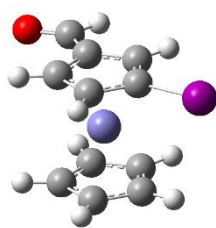
3b (in 1,4-dioxane)

atom	X	Y	Z
Fe	-1.17164	-0.17886	0.12272
C	-0.15070	1.38915	-0.75195
C	0.65554	0.73932	0.23389
C	-0.00537	0.82660	1.49744
C	-1.22509	1.53652	1.28271
C	-1.32380	1.88813	-0.10159
C	-1.69883	-1.52117	-1.36643
C	-0.88685	-2.16815	-0.38661
C	-1.55340	-2.07452	0.87246
C	-2.77902	-1.36889	0.67106
C	-2.86902	-1.02635	-0.71268
H	0.34744	0.41126	2.43126
H	-1.97403	1.74431	2.03696
H	-1.45406	-1.39780	-2.41336
H	0.08699	-2.60764	-0.55864
H	-1.17878	-2.44230	1.81878
H	-3.49632	-1.10820	1.43846
H	-3.66632	-0.46049	-1.17709
H	0.07917	1.47187	-1.80584
I	2.55581	-0.09445	-0.09765
C	-2.42833	2.67637	-0.74580
H	-2.21149	3.75213	-0.71278
H	-2.55678	2.39655	-1.79658
H	-3.38165	2.51443	-0.23175



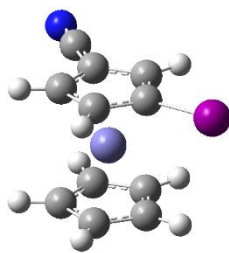
3f (in 1,4-dioxane)

atom	X	Y	Z
Fe	1.00252	0.41423	0.11740
C	0.17756	-1.25998	-0.75827
C	-0.70937	-0.74305	0.22681
C	-0.04606	-0.74183	1.49674
C	1.25901	-1.26623	1.30181
C	1.40537	-1.59861	-0.08834
C	1.35309	1.83268	-1.35468
C	0.45179	2.34946	-0.37541
C	1.11457	2.33305	0.88849
C	2.42831	1.80623	0.69192
C	2.57539	1.49984	-0.69422
H	-0.46374	-0.37886	2.42563
H	2.02807	-1.37871	2.05338
H	1.13772	1.69122	-2.40561
H	-0.57263	2.65071	-0.55115
H	0.68325	2.63054	1.83529
H	3.16835	1.63339	1.46205
H	3.44672	1.05176	-1.15389
H	-0.03299	-1.37801	-1.81260
I	-2.69893	-0.16517	-0.10332
C	2.62486	-2.09199	-0.73664
O	3.65253	-2.38255	-0.14722
H	2.55547	-2.19500	-1.84120



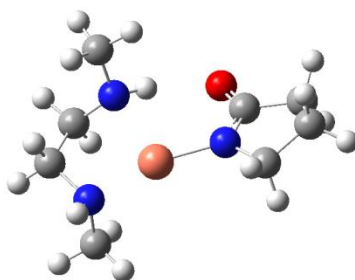
3h (in 1,4-dioxane)

atom	X	Y	Z
Fe	1.05207	0.38432	0.15959
C	0.21007	-1.33509	-0.60591
C	-0.69319	-0.71477	0.30311
C	-0.07412	-0.62078	1.58918
C	1.22435	-1.18980	1.48993
C	1.40610	-1.64154	0.13521
C	1.49718	1.64137	-1.42689
C	0.58234	2.27922	-0.53497
C	1.20264	2.36627	0.74742
C	2.50291	1.78199	0.64917
C	2.68415	1.33511	-0.69450
H	-0.51131	-0.17475	2.47139
H	1.95916	-1.26211	2.27987
H	1.31055	1.40066	-2.46514
H	-0.42467	2.59382	-0.77575
H	0.75169	2.76885	1.64494
H	3.21159	1.66498	1.45848
H	3.54883	0.80846	-1.07729
H	0.03750	-1.54488	-1.65158
I	-2.65290	-0.12443	-0.14855
C	2.57441	-2.26268	-0.39094
N	3.52361	-2.78408	-0.81800



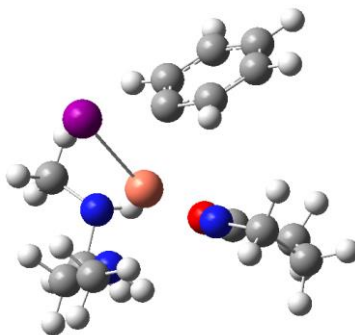
[(dmeda)Cu(pyrr)] complex (in 1,4-dioxane)

atom	X	Y	Z
Cu	0.31953	-0.58895	-0.31231
N	1.22366	1.49727	0.01671
N	2.25487	-1.20707	-0.22196
N	-1.55509	-0.40753	-0.15302
C	2.51084	1.13759	0.59600
C	3.14239	-0.00967	-0.21035
C	-2.05711	0.59521	0.59236
C	-2.62315	-1.29654	-0.61642
C	-3.59088	0.49140	0.65647
C	-3.92612	-0.47349	-0.48614
O	-1.41388	1.48823	1.18747
C	1.25562	2.51798	-1.02560
H	0.48566	1.69911	0.69871
H	2.45070	-1.73923	-1.06827
C	2.49254	-2.10796	0.93193
H	3.21982	1.98169	0.62429
H	2.35370	0.81770	1.63260
H	4.13388	-0.26783	0.18806
H	3.27240	0.31066	-1.24900
H	0.22910	2.72475	-1.34033
H	1.71681	3.46253	-0.69026
H	1.81246	2.16489	-1.90217
H	3.54479	-2.42040	0.99010
H	2.22611	-1.59597	1.85921
H	1.85563	-2.98954	0.83372
H	-2.44087	-1.62894	-1.64528
H	-2.67220	-2.20483	0.00826
H	-3.87186	0.08258	1.63736
H	-4.05167	1.47999	0.57295
H	-4.10199	0.08895	-1.41129
H	-4.80664	-1.09826	-0.30293



transition state for iodobenzene (in 1,4-dioxane)

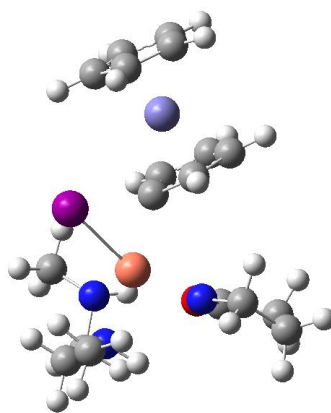
atom	X	Y	Z
Cu	0.08747	-0.41232	-0.13834
N	0.67020	-2.34233	-1.09316
N	0.29565	-1.64498	1.73107
N	-1.88168	-0.68114	-0.46248
C	1.18189	-3.18994	-0.00383
C	0.30354	-3.03129	1.23876
C	-2.75049	-0.88498	0.53933
C	-2.59395	-0.32104	-1.68833
C	-4.19903	-0.73953	0.04105
C	-4.04894	-0.80581	-1.48246
O	-2.47585	-1.14904	1.73463
I	2.33989	0.93641	-0.30772
C	0.15983	1.72155	0.06748
C	-0.15997	2.06645	1.38773
C	-1.13348	3.04115	1.61459
C	-1.74254	3.70044	0.54334
C	-1.37440	3.38271	-0.76732
C	-0.40914	2.40561	-1.01622
H	0.32465	1.57490	2.22323
H	-1.40547	3.28968	2.63688
H	-2.48678	4.46927	0.72920
H	-1.83173	3.90199	-1.60553
H	-0.11298	2.17435	-2.03366
C	1.49724	-2.38858	-2.30429
H	-0.28051	-2.63556	-1.31782
H	-0.66562	-1.42292	2.03314
C	1.27765	-1.38799	2.78530
H	1.22786	-4.25086	-0.29985
H	2.20748	-2.86614	0.21232
H	0.64118	-3.73564	2.01484
H	-0.73022	-3.29658	0.98804
H	1.15193	-0.36894	3.16247
H	1.17813	-2.08444	3.63362
H	2.29600	-1.47253	2.39015
H	1.01000	-1.81547	-3.09809
H	2.46742	-1.92637	-2.09607
H	1.66975	-3.41549	-2.66176
H	-4.84453	-1.50871	0.47513
H	-4.58241	0.23506	0.37413
H	-4.77948	-0.20408	-2.03335



H	-4.14583	-1.84386	-1.82426
H	-2.56702	0.76963	-1.84851
H	-2.12422	-0.78057	-2.56907

transition state for **1a** (in 1,4-dioxane)

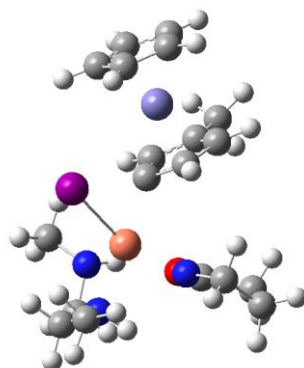
atom	X	Y	Z
Cu	-1.29614	-0.23681	-0.16166
N	-3.17192	-1.20139	-0.76488
N	-2.15616	-0.64905	1.91270
N	-2.09123	1.59191	-0.43281
C	-3.70234	-1.89252	0.42283
C	-3.56125	-0.99374	1.65266
C	-2.33916	2.43698	0.58041
C	-2.08955	2.30933	-1.70889
C	-2.61489	3.85351	0.04600
C	-2.87186	3.61781	-1.44625
O	-2.34853	2.16554	1.80381
I	0.41091	-2.10188	-0.54242
C	-3.22489	-2.01522	-1.98547
H	-3.69481	-0.33659	-0.90477
H	-2.11678	0.34546	2.17798
C	-1.50479	-1.51510	2.89517
H	-4.75607	-2.18313	0.28359
H	-3.12159	-2.81363	0.55479
H	-4.02816	-1.48719	2.51907
H	-4.10557	-0.05749	1.48138
H	-0.48534	-1.16244	3.07726
H	-2.04028	-1.54218	3.85818
H	-1.43450	-2.53936	2.51273
H	-2.91270	-1.40790	-2.83953
H	-2.52843	-2.85409	-1.88898
H	-4.23147	-2.41483	-2.18023
H	-3.43987	4.32579	0.58731
H	-1.71840	4.46602	0.21582
H	-2.55189	4.44096	-2.09360
H	-3.94216	3.45163	-1.62121
H	-1.05851	2.53081	-2.03008
H	-2.54564	1.70438	-2.50452
C	0.68638	0.33766	-0.11094
C	1.02687	0.95164	1.13704
C	1.22442	1.12710	-1.17481
C	1.65203	2.20122	0.83164
C	1.77797	2.30696	-0.58667
H	1.17470	0.89200	-2.22858
H	2.00337	2.92150	1.55949
H	2.24923	3.11912	-1.12572



Fe	2.79297	0.65016	0.10088
C	4.26068	-0.04155	1.39888
C	4.76278	1.03944	0.61206
C	3.86690	-1.08608	0.51050
H	4.16188	-0.05153	2.47663
C	4.67824	0.66115	-0.76271
H	5.10502	1.99487	0.98854
C	4.12190	-0.65271	-0.82480
H	3.40622	-2.02198	0.79591
H	4.94982	1.27863	-1.60916
H	3.89543	-1.20667	-1.72629
H	0.78599	0.58084	2.12199

transition state for **3b** (in 1,4-dioxane)

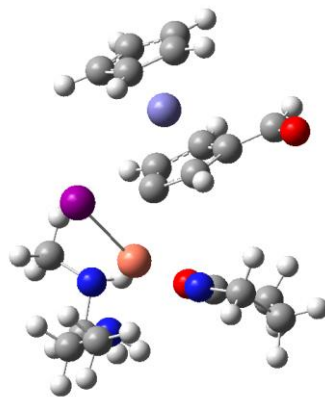
atom	X	Y	Z
Cu	-1.37168	-0.25938	-0.15870
N	-3.31437	-1.15433	-0.64759
N	-2.21823	-0.42237	1.95542
N	-2.06968	1.58289	-0.58371
C	-3.86534	-1.69603	0.60645
C	-3.64667	-0.69604	1.74317
C	-2.25223	2.53154	0.34813
C	-2.05307	2.17628	-1.92172
C	-2.46181	3.90516	-0.31393
C	-2.75772	3.54557	-1.77391
O	-2.25347	2.37724	1.59193
I	0.20403	-2.25787	-0.39765
C	-3.44029	-2.07367	-1.78516
H	-3.78507	-0.27492	-0.86190
H	-2.11167	0.58727	2.12851
C	-1.60823	-1.23601	3.00678
H	-4.93737	-1.93104	0.50768
H	-3.34035	-2.63548	0.81833
H	-4.13150	-1.07216	2.65736
H	-4.12975	0.25427	1.48732
H	-0.56548	-0.93570	3.14524
H	-2.12881	-1.13980	3.97360
H	-1.61034	-2.29342	2.72004
H	-3.10932	-1.56900	-2.69704
H	-2.79356	-2.94111	-1.62014
H	-4.47284	-2.42660	-1.92695
H	-3.25107	4.46976	0.19114
H	-1.53151	4.48172	-0.21409
H	-2.40484	4.28528	-2.50009
H	-3.83845	3.42417	-1.91882
H	-1.01769	2.30802	-2.27648
H	-2.55644	1.52590	-2.65019
C	0.63336	0.20318	-0.18692
C	1.05993	0.87489	1.00246
C	1.19103	0.87555	-1.31752
C	1.75945	2.06201	0.60461
C	1.83787	2.05220	-0.82428
H	1.09531	0.57383	-2.35094
Fe	2.76045	0.37720	-0.06164
C	4.28969	-0.20525	1.21911



C	4.79506	0.66888	0.20934
C	3.73444	-1.35007	0.57231
H	4.29376	-0.01561	2.28475
C	4.55279	0.06233	-1.06132
H	5.24321	1.64020	0.37524
C	3.89658	-1.18498	-0.83552
H	3.23193	-2.17440	1.06003
H	4.78921	0.49215	-2.02619
H	3.53841	-1.86299	-1.59878
H	0.82980	0.58870	2.01847
H	2.34470	2.79368	-1.43047
C	2.26783	3.13589	1.52285
H	1.48357	3.87575	1.72817
H	2.58857	2.71952	2.48357
H	3.11910	3.66406	1.07930

transition state for **3f** (in 1,4-dioxane)

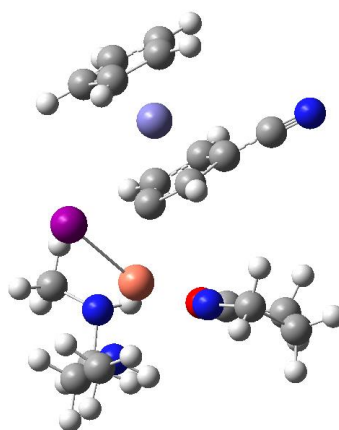
atom	X	Y	Z
Cu	-1.48172	-0.16428	-0.17284
N	-3.42383	-0.73876	-1.00180
N	-2.52928	-0.69428	1.77713
N	-1.93741	1.78618	-0.22360
C	-4.13830	-1.47408	0.05672
C	-3.94866	-0.76616	1.39957
C	-2.11183	2.52197	0.88562
C	-1.75421	2.65097	-1.39123
C	-2.13700	4.02048	0.53906
C	-2.33876	4.02312	-0.98036
O	-2.23175	2.09817	2.05902
I	-0.02633	-2.21125	-0.69498
C	-3.50483	-1.38537	-2.31821
H	-3.80616	0.20528	-1.06145
H	-2.35221	0.23790	2.17884
C	-2.09743	-1.77275	2.66645
H	-5.21114	-1.57172	-0.17372
H	-3.71652	-2.48574	0.09656
H	-4.55008	-1.27593	2.16785
H	-4.32376	0.26129	1.32380
H	-1.05291	-1.61697	2.95203
H	-2.70286	-1.83211	3.58532
H	-2.15770	-2.73863	2.15288
H	-3.04084	-0.73901	-3.06818
H	-2.95237	-2.32977	-2.29062
H	-4.54216	-1.59427	-2.61923
H	-2.91102	4.54350	1.10826
H	-1.16967	4.45667	0.82493
H	-1.85724	4.85991	-1.49631
H	-3.40966	4.05565	-1.21647
H	-0.68593	2.74389	-1.64586
H	-2.25459	2.23353	-2.27546
C	0.56558	0.06333	0.03452
C	0.94629	0.41161	1.37358
C	1.27320	0.89483	-0.87696
C	1.76741	1.57066	1.29515
C	1.96843	1.88449	-0.09551
H	1.24334	0.85018	-1.95562
Fe	2.71908	0.02838	0.33800
C	4.10174	-0.92810	1.56058



C	4.74612	0.06573	0.76515
C	3.49573	-1.87268	0.67895
H	4.04437	-0.93892	2.64131
C	4.54072	-0.26771	-0.61064
H	5.26546	0.93976	1.13650
C	3.77015	-1.46572	-0.66134
H	2.89239	-2.72083	0.97319
H	4.86977	0.31479	-1.46137
H	3.40647	-1.94960	-1.55799
H	0.61169	-0.07406	2.27813
H	2.18081	2.11431	2.13564
C	2.82010	2.95453	-0.61666
O	2.97718	3.21091	-1.80011
H	3.33556	3.55385	0.16567

transition state for **3h** (in 1,4-dioxane)

atom	X	Y	Z
Cu	-1.47827	-0.15373	-0.17584
N	-3.43639	-0.73970	-0.95640
N	-2.48798	-0.62907	1.80400
N	-1.91179	1.79871	-0.26926
C	-4.13505	-1.44099	0.13561
C	-3.91488	-0.69857	1.45494
C	-2.05085	2.56151	0.82716
C	-1.75427	2.63478	-1.46076
C	-2.07245	4.05154	0.44721
C	-2.31496	4.02154	-1.06601
O	-2.14282	2.16417	2.01211
I	-0.03507	-2.22016	-0.66883
C	-3.54446	-1.42390	-2.25176
H	-3.81645	0.20374	-1.03669
H	-2.29530	0.31096	2.17962
C	-2.04763	-1.68944	2.71102
H	-5.21260	-1.53735	-0.07166
H	-3.71907	-2.45410	0.19488
H	-4.50580	-1.18222	2.24777
H	-4.28297	0.32965	1.35824
H	-0.99768	-1.53349	2.97600
H	-2.63804	-1.72344	3.64074
H	-2.12204	-2.66654	2.22108
H	-3.09152	-0.80195	-3.02864
H	-2.99621	-2.37012	-2.20663
H	-4.58804	-1.63614	-2.52761
H	-2.82681	4.59431	1.02418
H	-1.09440	4.48570	0.69712
H	-1.83974	4.84174	-1.61332
H	-3.39139	4.05871	-1.27453
H	-0.69230	2.71302	-1.74703
H	-2.28187	2.20185	-2.32143
C	0.58372	0.05117	-0.00761
C	0.97224	0.45588	1.31056
C	1.28405	0.84862	-0.95791
C	1.79608	1.61042	1.18713
C	1.99052	1.86523	-0.21604
H	1.23820	0.76529	-2.03388
H	2.21575	2.19045	1.99795
Fe	2.73015	0.02677	0.27702



C	4.08129	-0.94008	1.52553
C	4.74060	0.07459	0.76838
C	3.51387	-1.87496	0.60911
H	3.98930	-0.97037	2.60346
C	4.58233	-0.23669	-0.61758
H	5.23469	0.95006	1.16942
C	3.82386	-1.44089	-0.71459
H	2.90973	-2.73340	0.86986
H	4.93522	0.36431	-1.44566
H	3.49804	-1.91560	-1.63062
H	0.64457	0.01059	2.23783
C	2.76465	2.91823	-0.77912
N	3.38210	3.78920	-1.24460