



Supporting Information

for

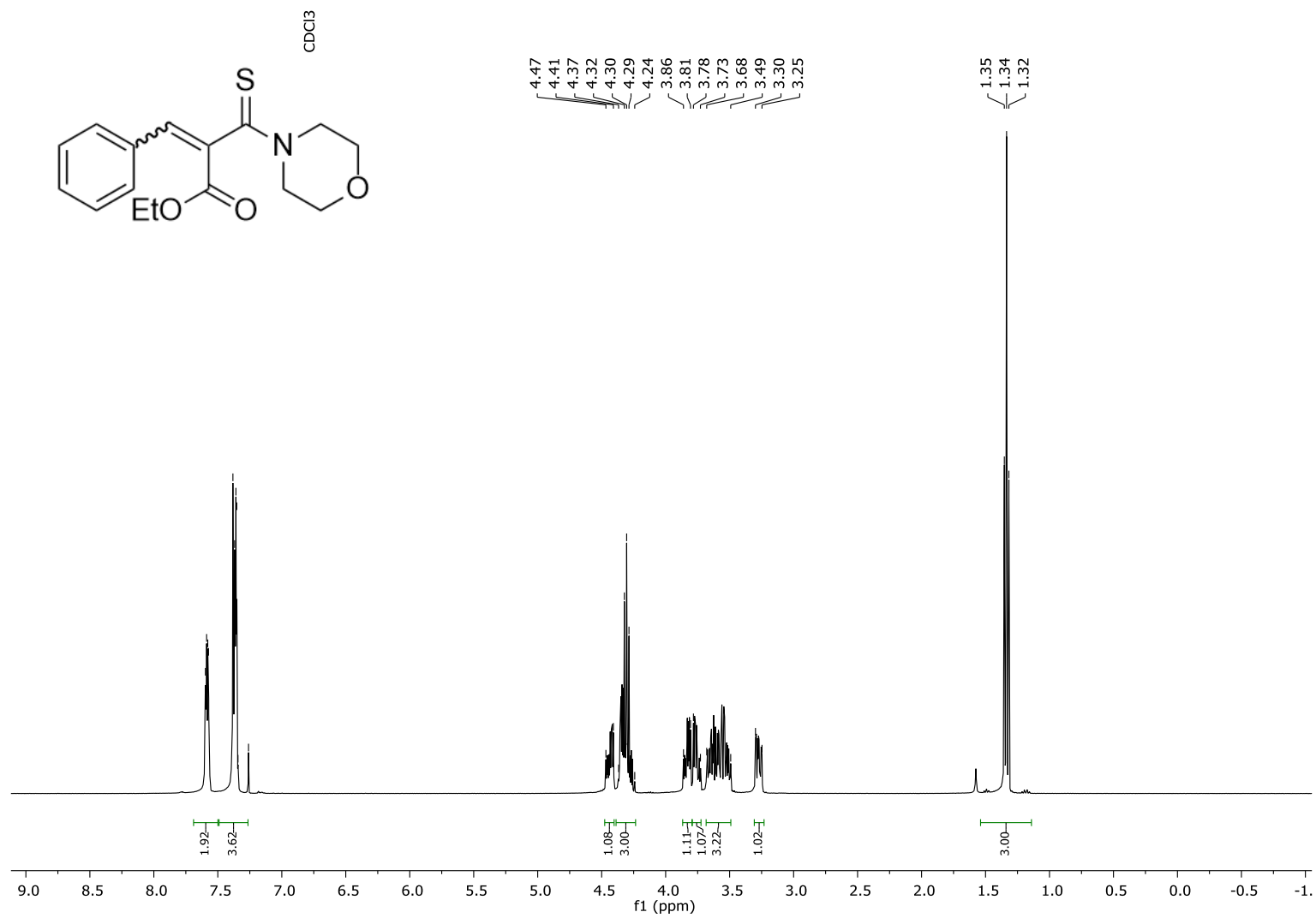
Reactions of acryl thioamides with iminoiodinanes as a one-step synthesis of *N*-sulfonyl-2,3-dihydro-1,2-thiazoles

Vladimir G. Ilkin, Pavel S. Silaichev, Valeriy O. Filimonov, Tetyana V. Beryozkina, Margarita D. Likhacheva, Pavel A. Slepukhin, Wim Dehaen and Vasiliy A. Bakulev

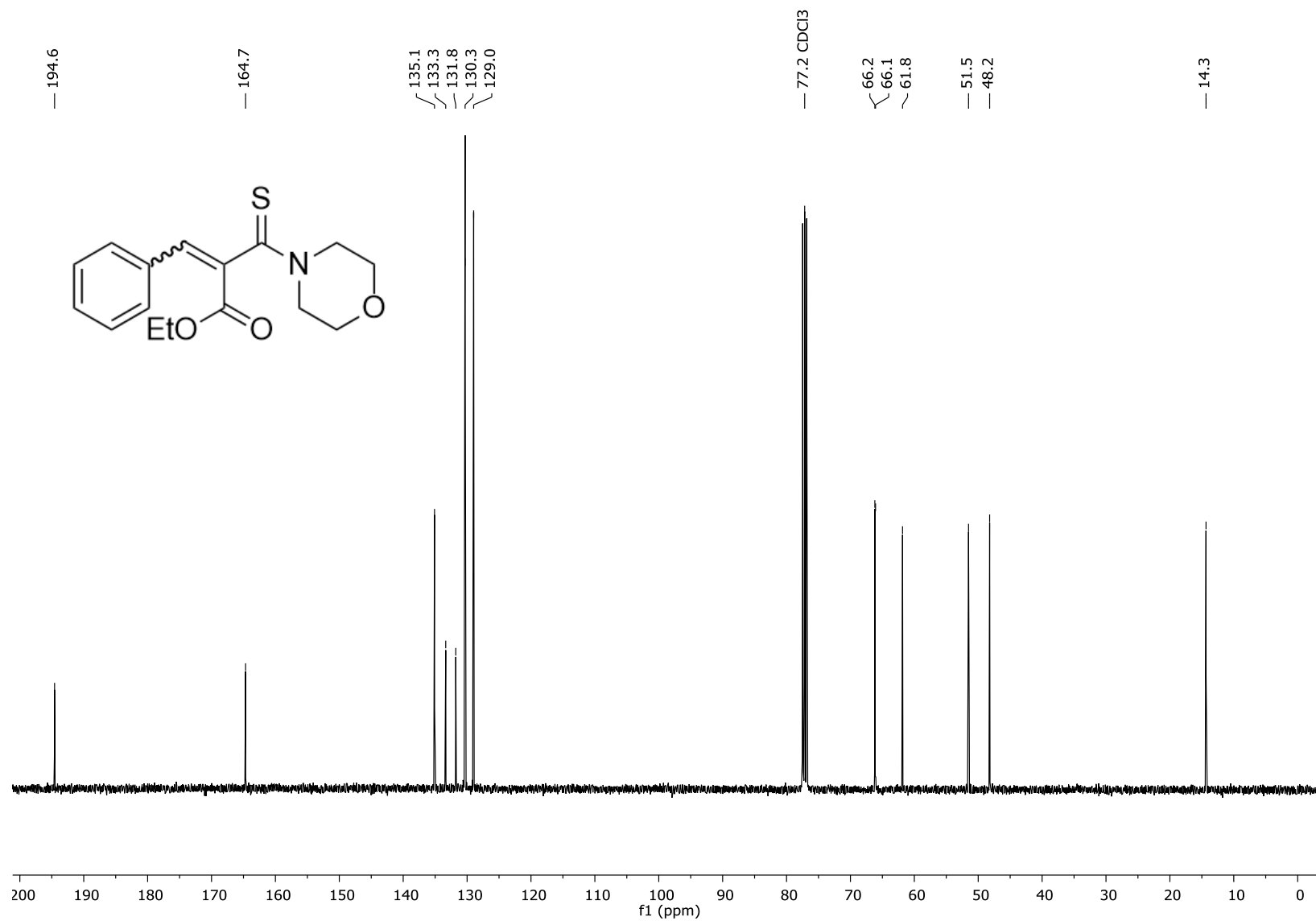
Beilstein J. Org. Chem. **2025**, 21, 1397–1403. doi:10.3762/bjoc.21.104

Copies of NMR and HRMS spectra of all new compounds

¹H NMR (CDCl₃) spectrum of **1h**

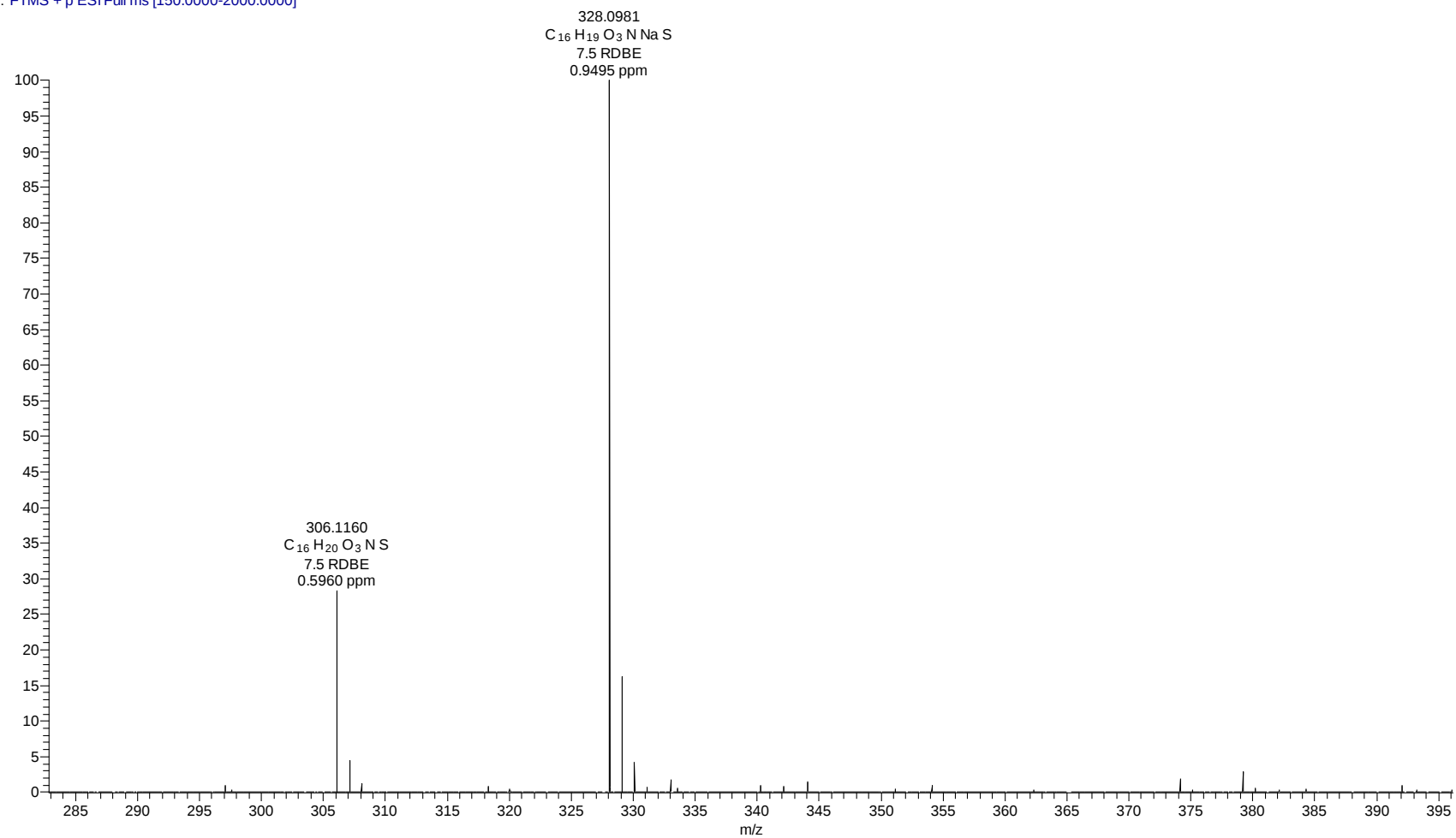


^{13}C NMR (CDCl_3) spectrum of **1h**

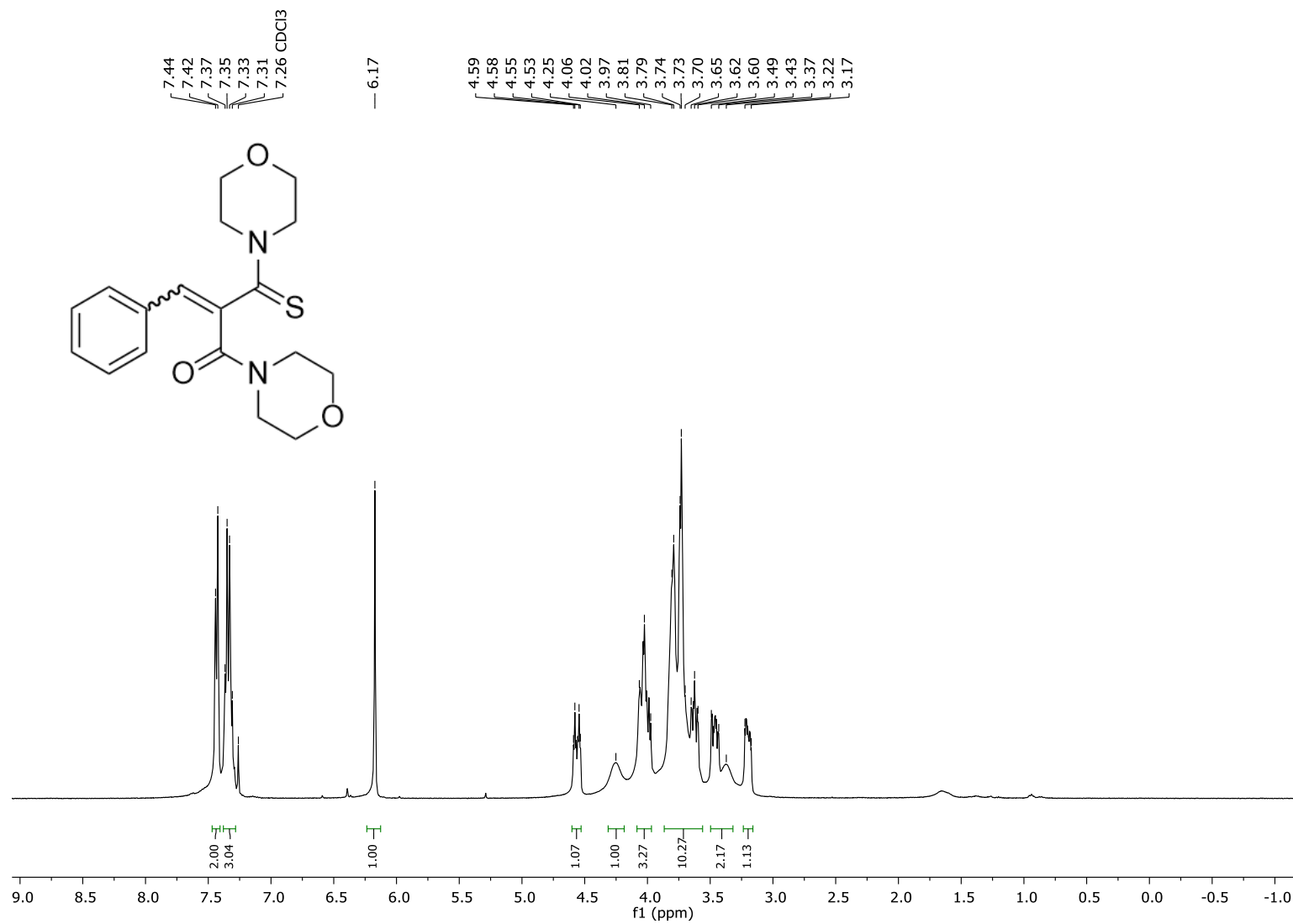


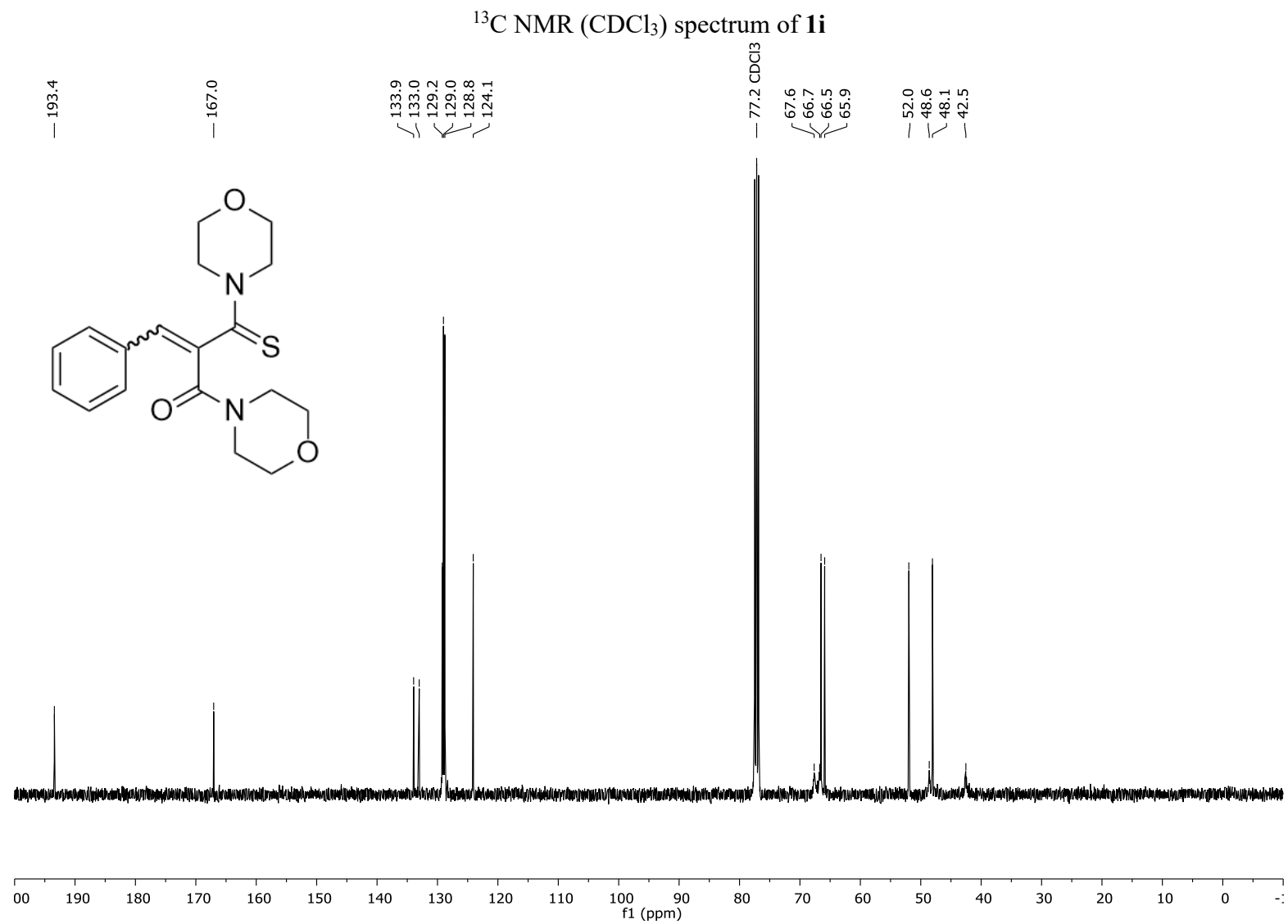
HRMS of 1h

6B-19_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11, 0.83-0.95 NL: 1.04E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]

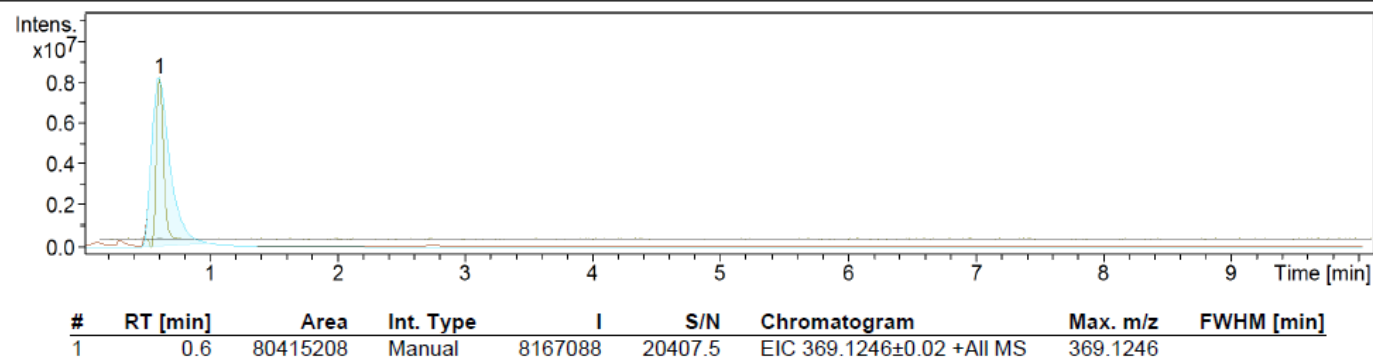


¹H NMR (CDCl₃) spectrum of **1i**

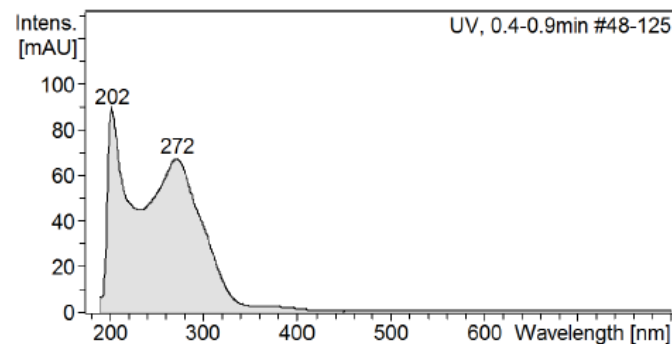




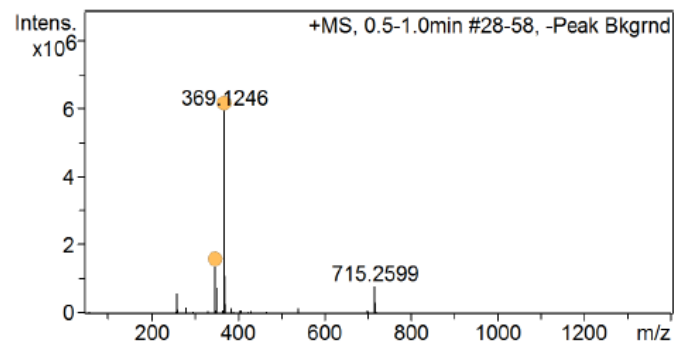
HRMS of 1i



Cmpd 1, 0.6 min

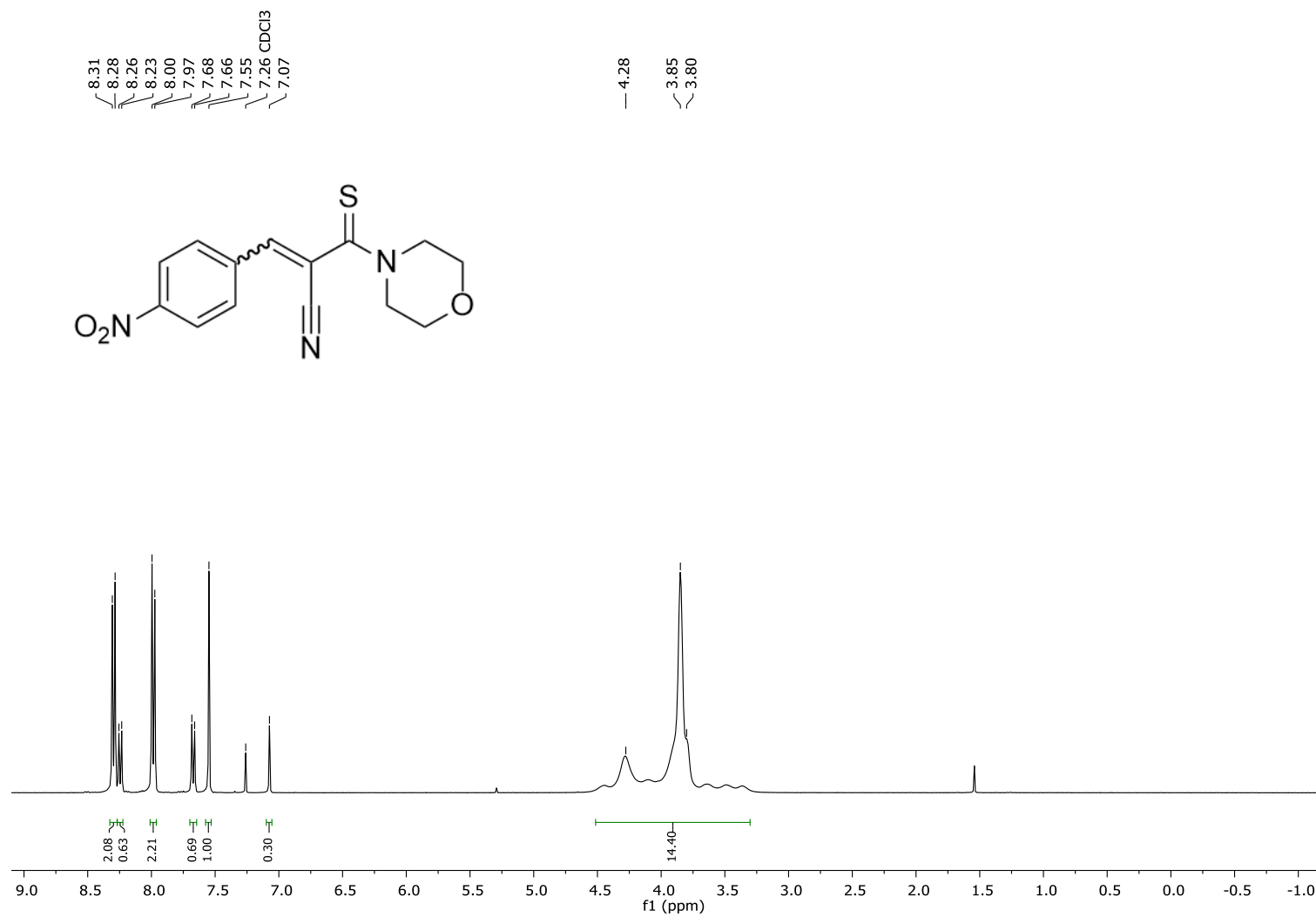


#	Wavelength	Intensity
0	202	88.5
1	272	67.2

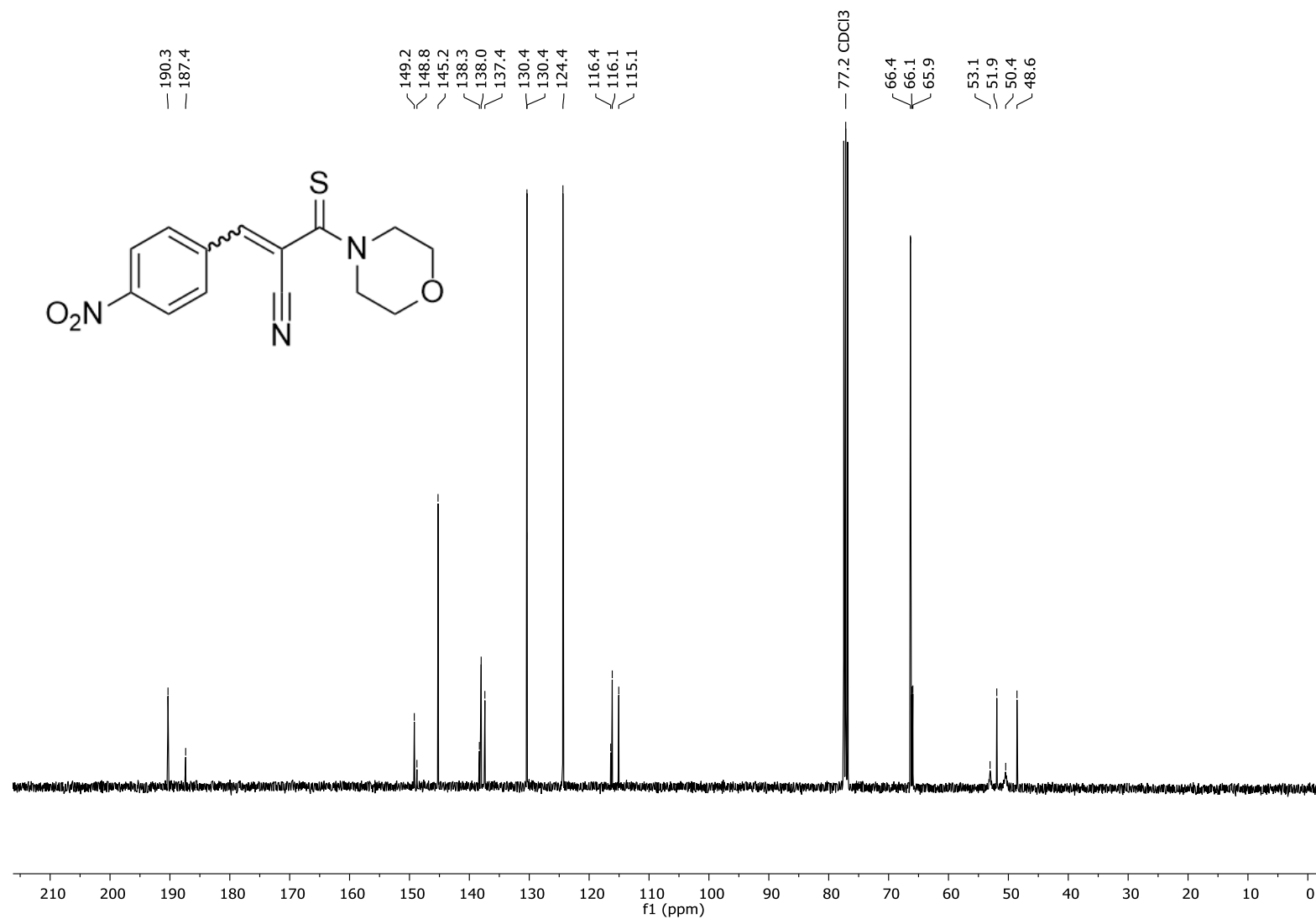


#	m/z	Res.	S/N	I	I %	FWHM
1	260.0741	25358	180831264.0	566339	9.6	0.0103
2	280.1306	21792	48452780.0	151748	2.6	0.0129
3	347.1425	30459	432144384.0	1353419	22.9	0.0114
4	348.1453	22287	86193560.0	269947	4.6	0.0156
5	353.1474	32516	235000608.0	735991	12.4	0.0109
6	369.1246	39171	1890813184.0	5921775	100.0	0.0094
7	370.1274	30763	345250080.0	1081277	18.3	0.0120
8	371.1235	19195	86247744.0	270116	4.6	0.0193
9	715.2599	38524	245509232.0	768902	13.0	0.0186
10	716.2626	29051	93640208.0	293269	5.0	0.0247

^1H NMR (CDCl_3) spectrum of **1k**

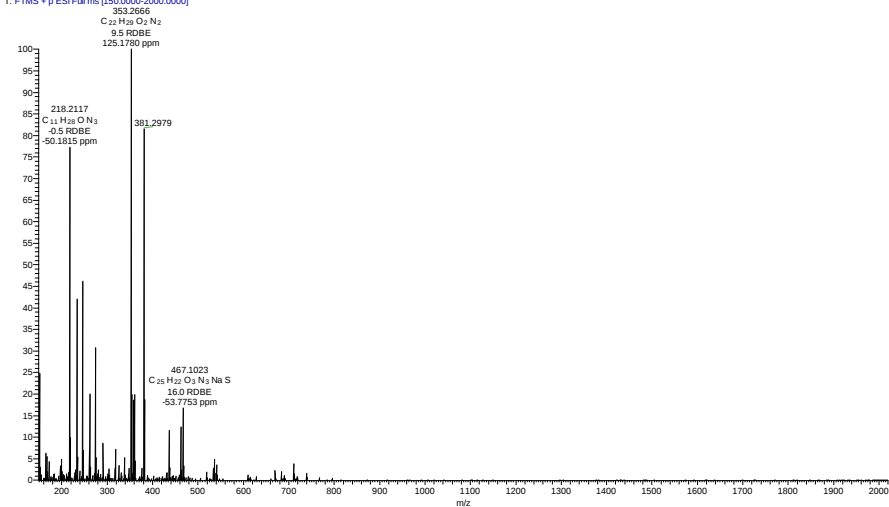


^{13}C NMR (CDCl_3) spectrum of **1k**

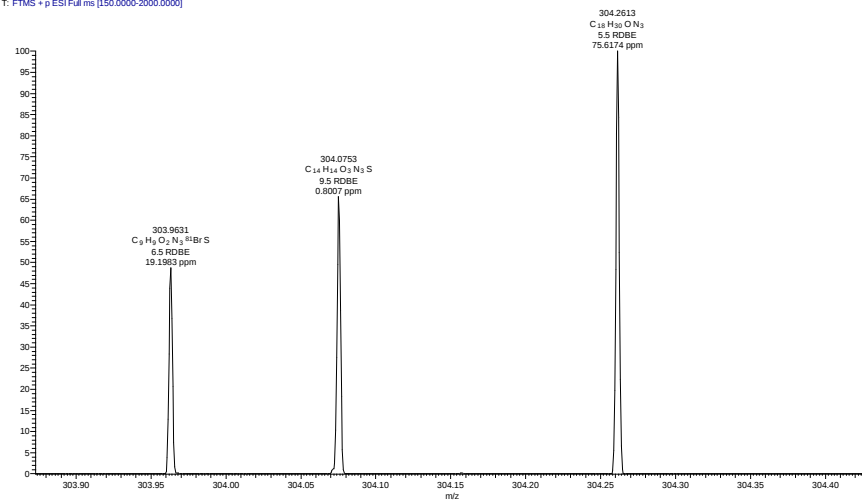


HRMS of 1k

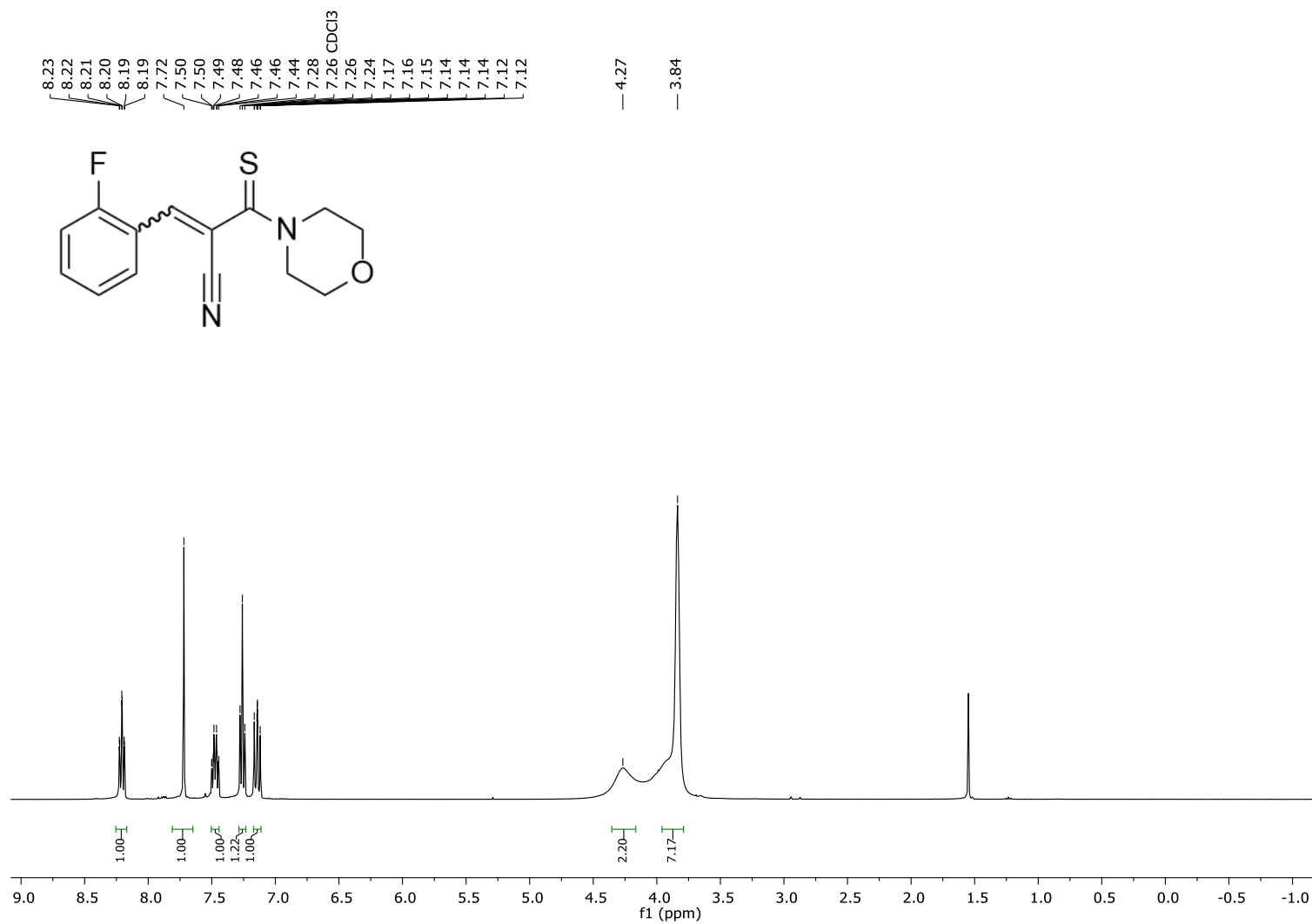
VF-70 Pos 240213111646 #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11, 0.83-0.95 NL: 1.32E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



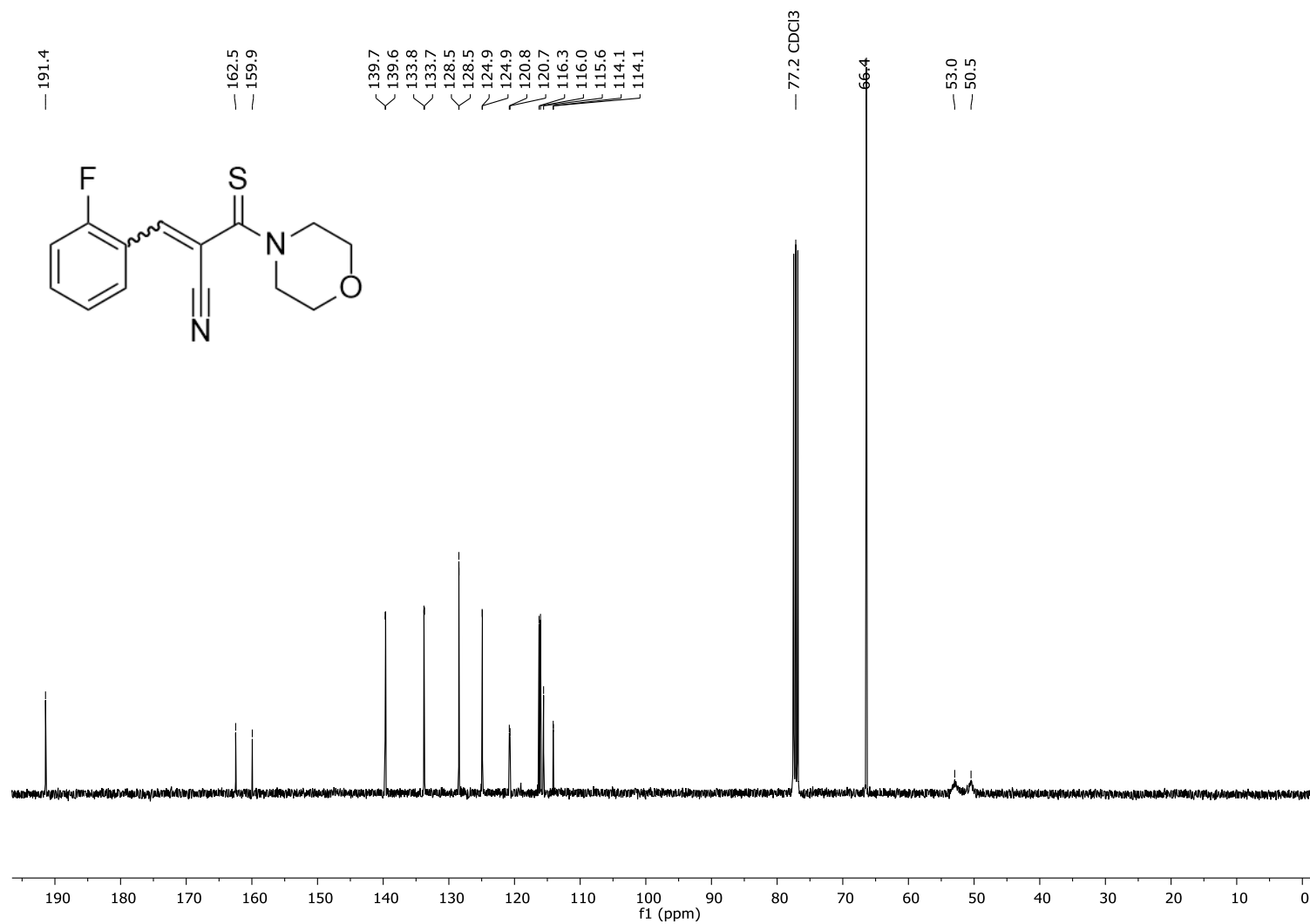
VF-70 Pos 240213111646 #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11, 0.83-0.95 NL: 3.54E5
T: FTMS + p ESI Full ms [150.0000-2000.0000]



^1H NMR (CDCl_3) spectrum of **1n**



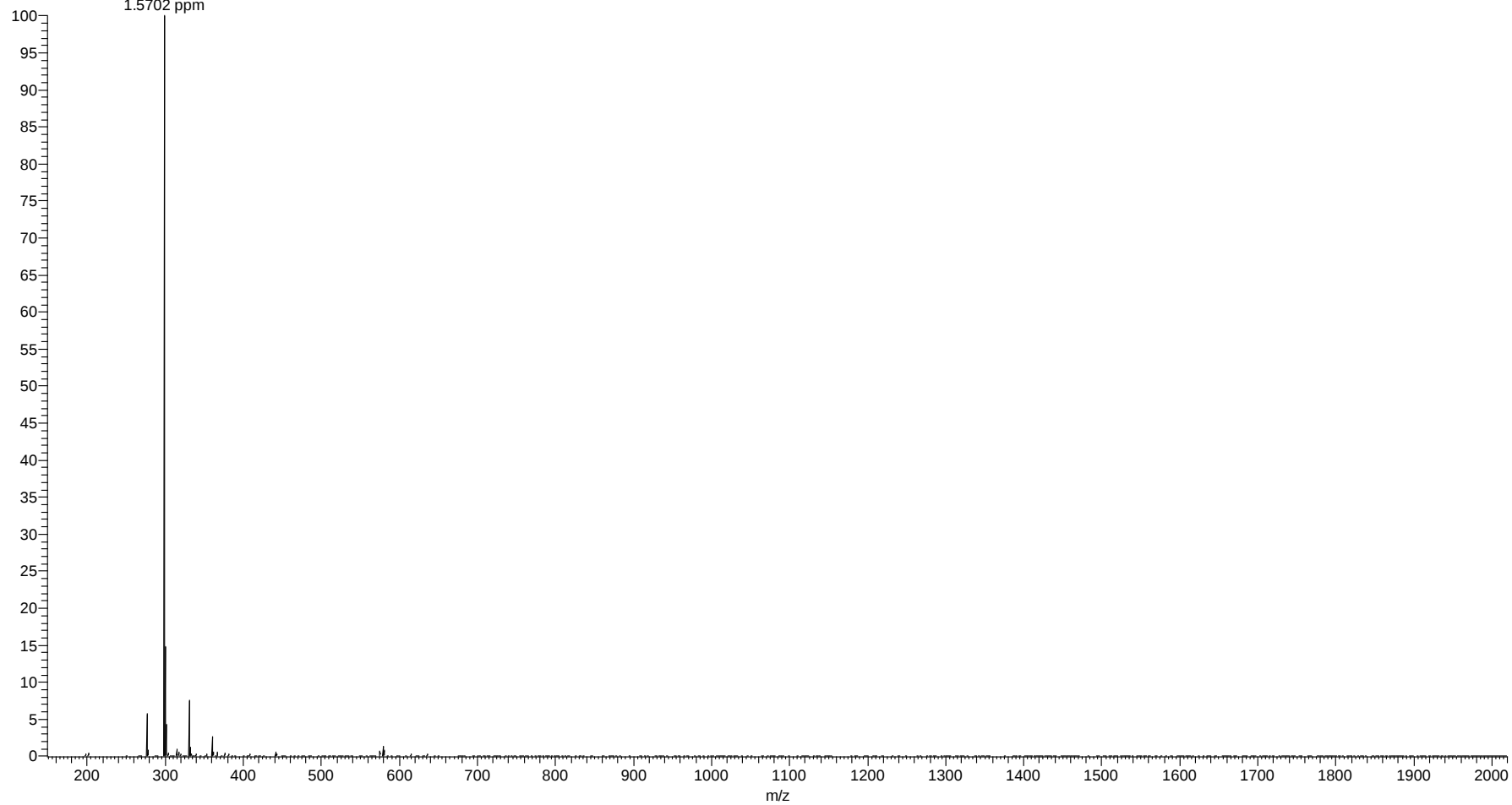
^{13}C NMR (CDCl_3) spectrum of **1n**



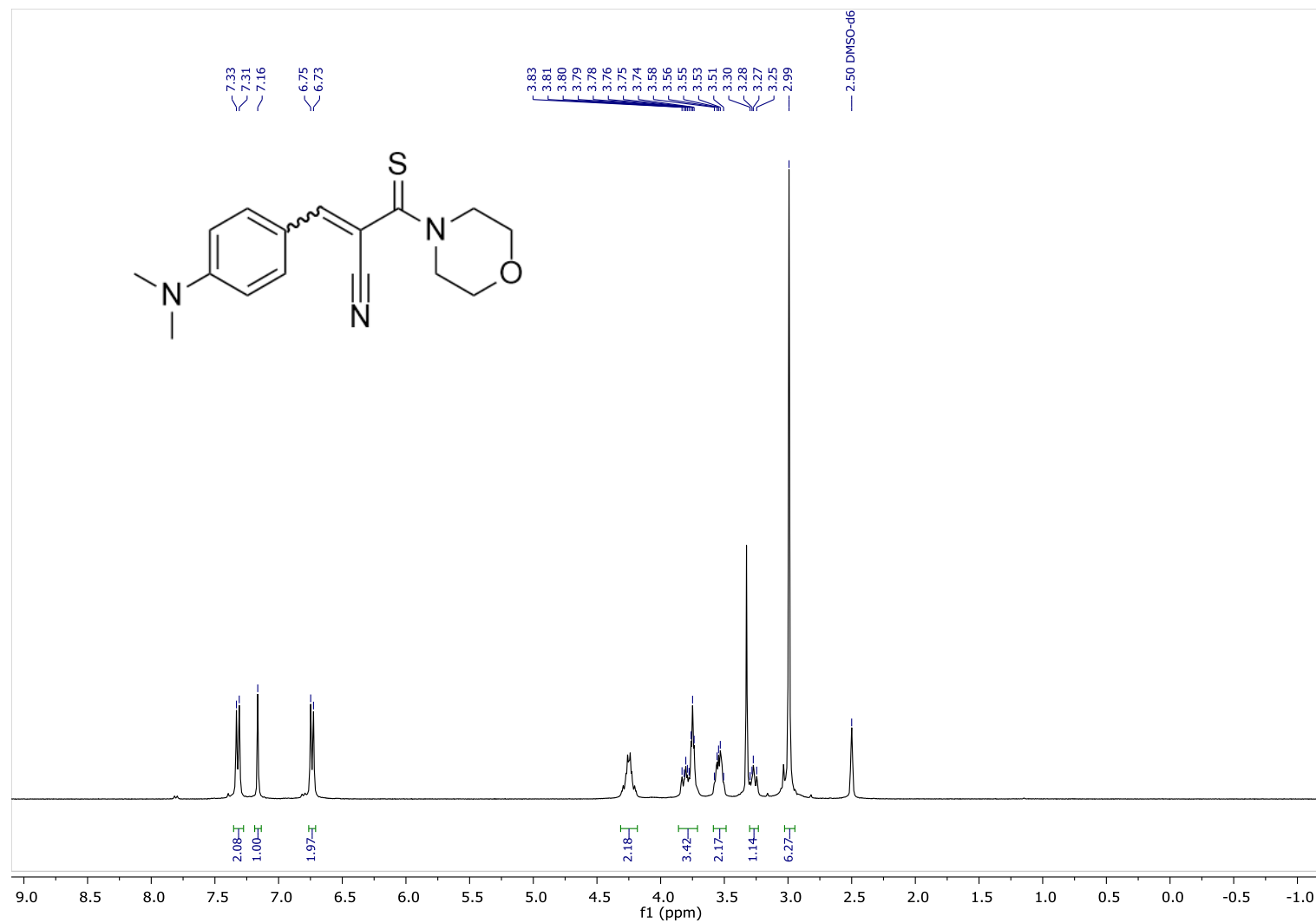
HRMS **1n**

PSG94 #51-102 RT: 0.23-0.45 AV: 52 SB: 54 0.07-0.15 , 0.83-0.97 NL: 3.04E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]

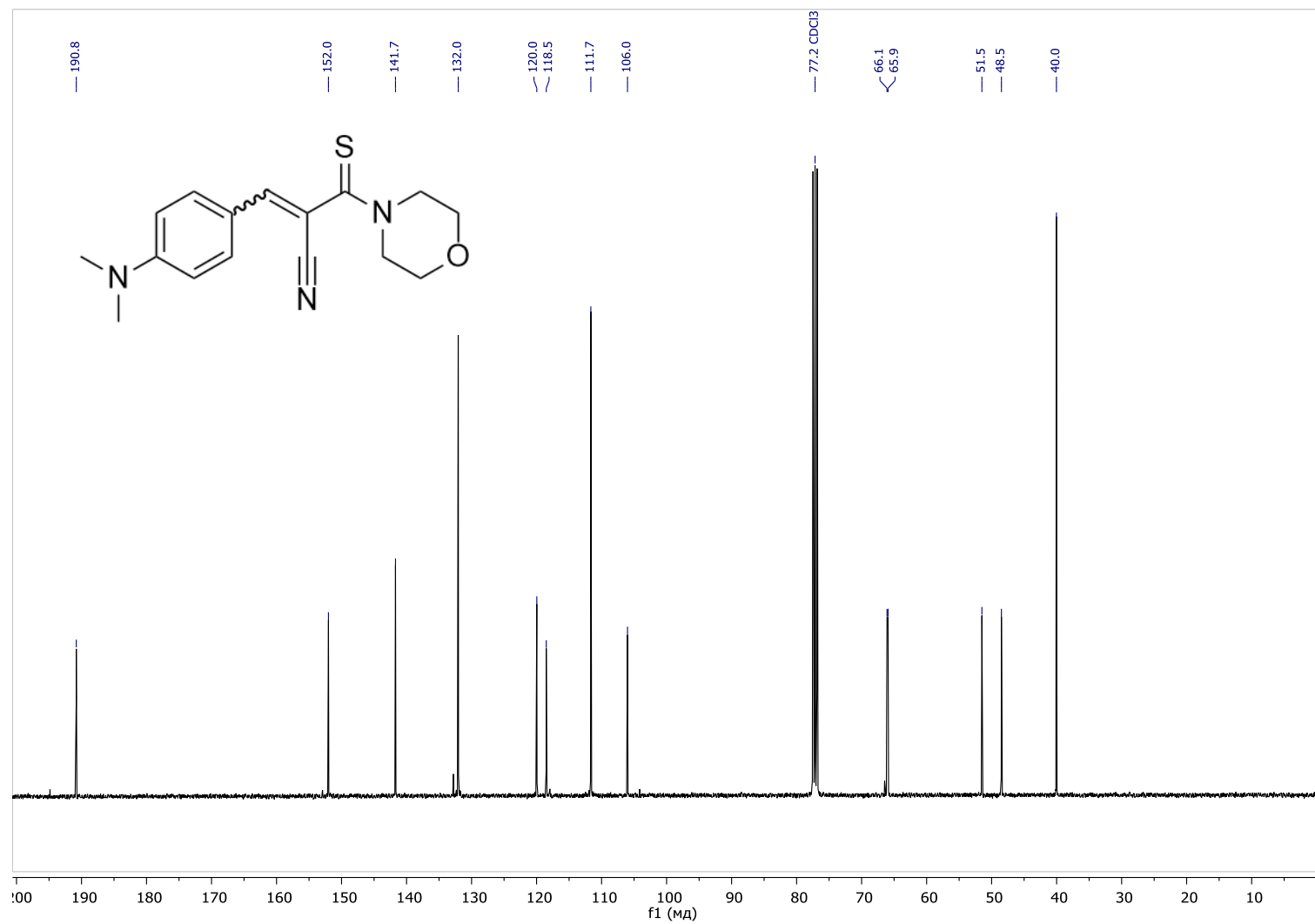
299.0630
C₁₄ H₁₃ O N₂ F Na S
8.5 RDBE
1.5702 ppm



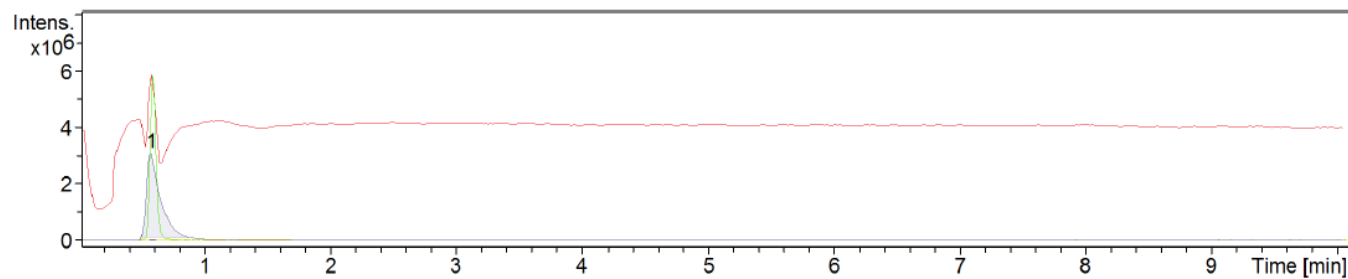
^1H NMR (CDCl_3) spectrum of **1o**



^{13}C NMR (CDCl_3) spectrum of **1o**

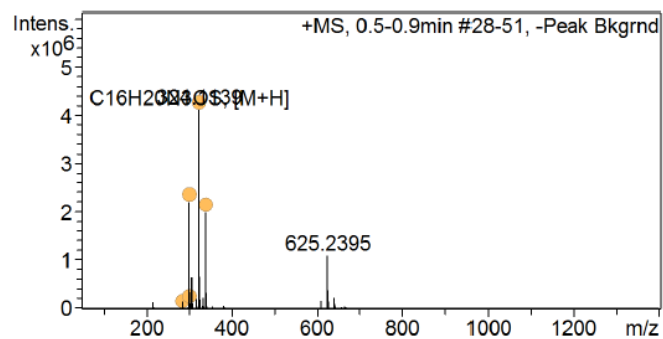


HRMS of 1o



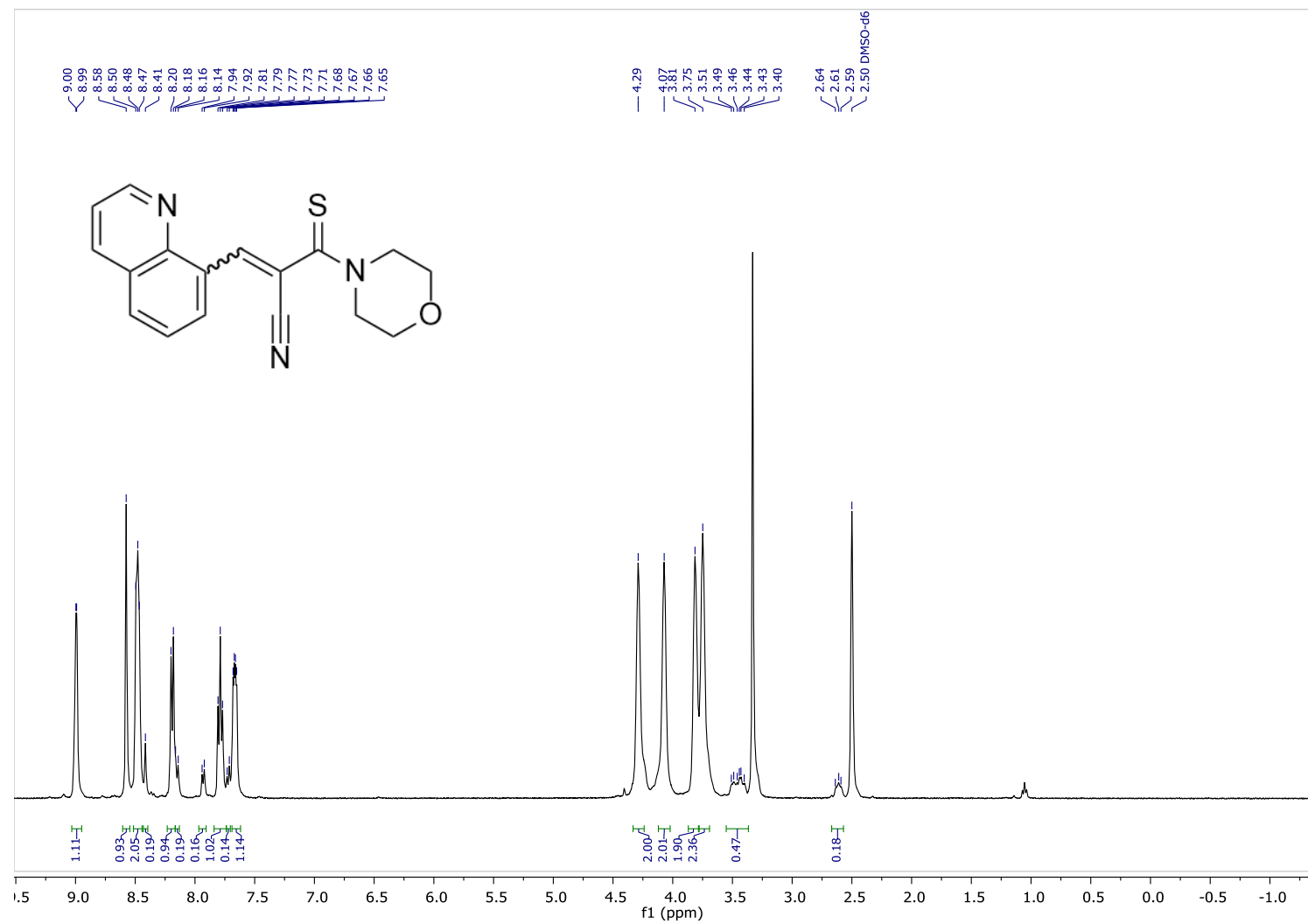
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	22423718	Manual	3086967	1362.7	EIC 302.1321 +All MS	324.1139	

Cmpd 1, 0.6 min

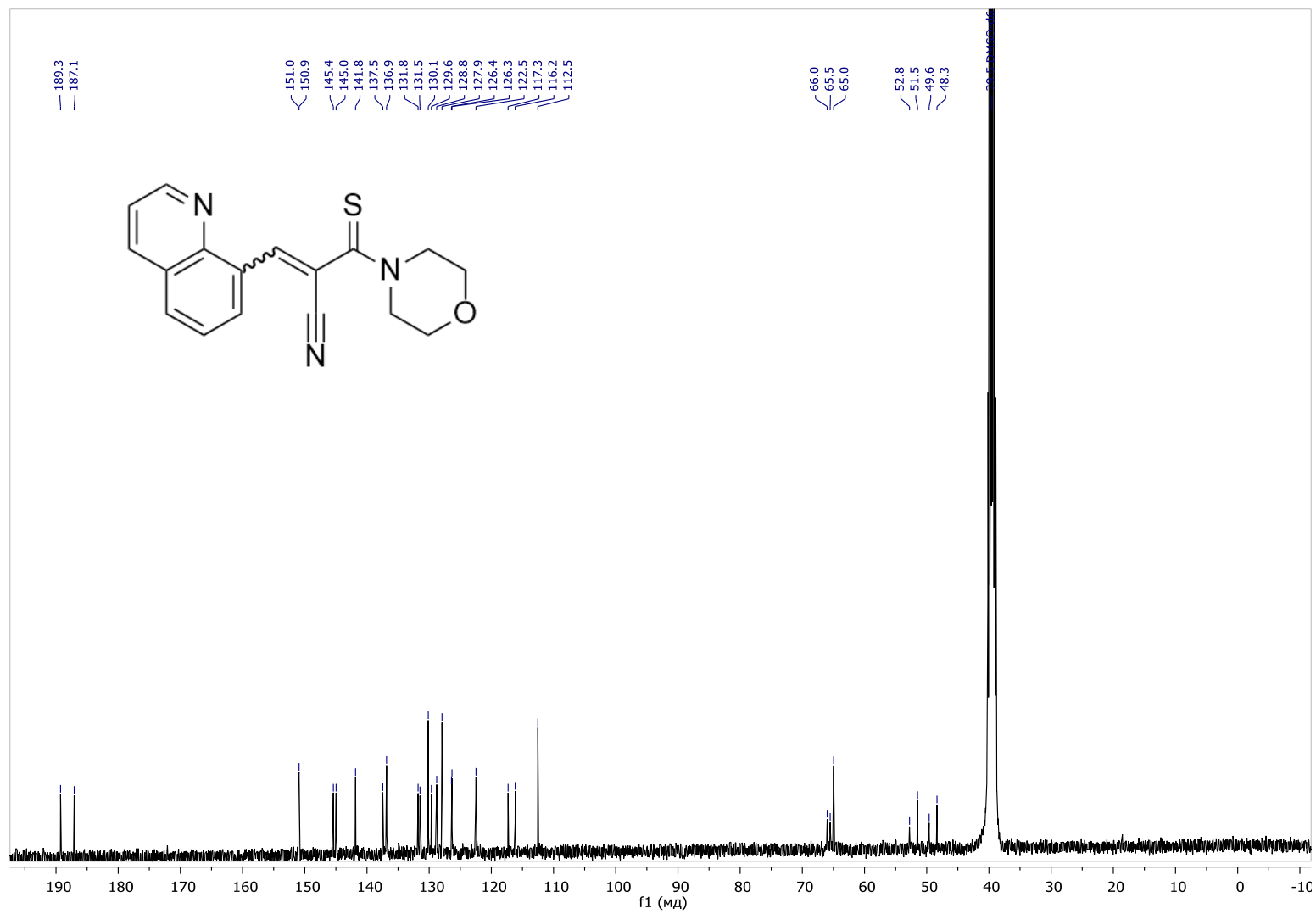


#	m/z	Res.	S/N	I	I %	FWHM
1	302.1321	31816	433271232.0	2194917	53.5	0.0095
2	303.1347	21914	66431592.0	336537	8.2	0.0138
3	308.1364	25284	125473632.0	635639	15.5	0.0122
4	324.1139	34370	809106240.0	4098866	100.0	0.0094
5	325.1166	26225	129311816.0	655083	16.0	0.0124
6	340.0884	30338	393768992.0	1994801	48.7	0.0112
7	341.0909	21635	65457388.0	331602	8.1	0.0158
8	342.0859	19429	44935800.0	227641	5.6	0.0176
9	625.2395	34626	216216320.0	1095334	26.7	0.0181
10	626.2421	26293	74780872.0	378834	9.2	0.0238

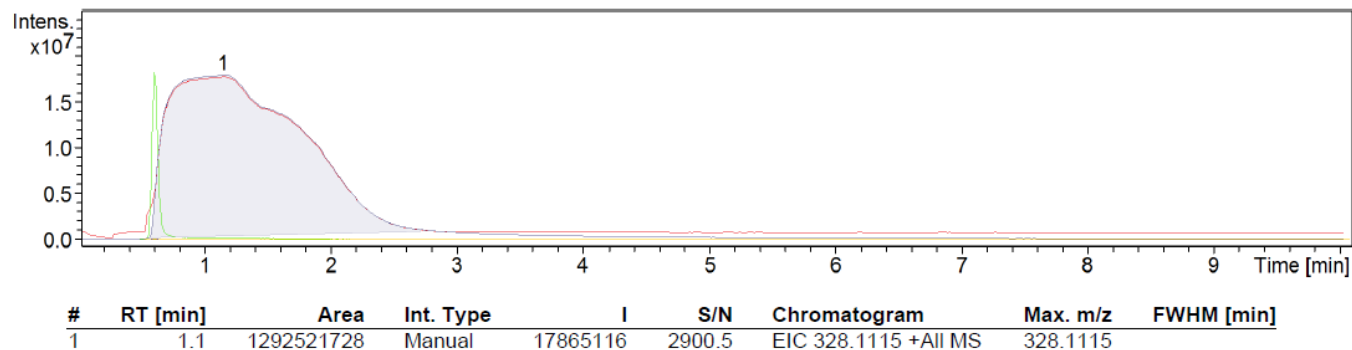
¹H NMR (CDCl₃) spectrum of **1s**



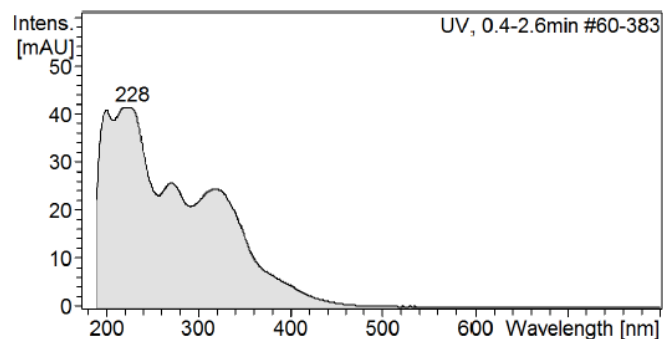
^{13}C NMR (CDCl_3) spectrum of **1s**



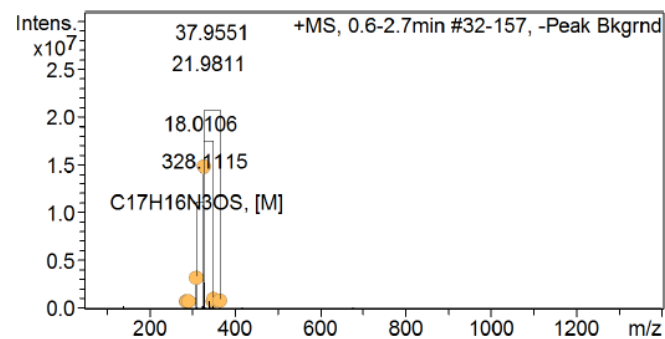
HRMS of 1s



Cmpd 1, 1.1 min

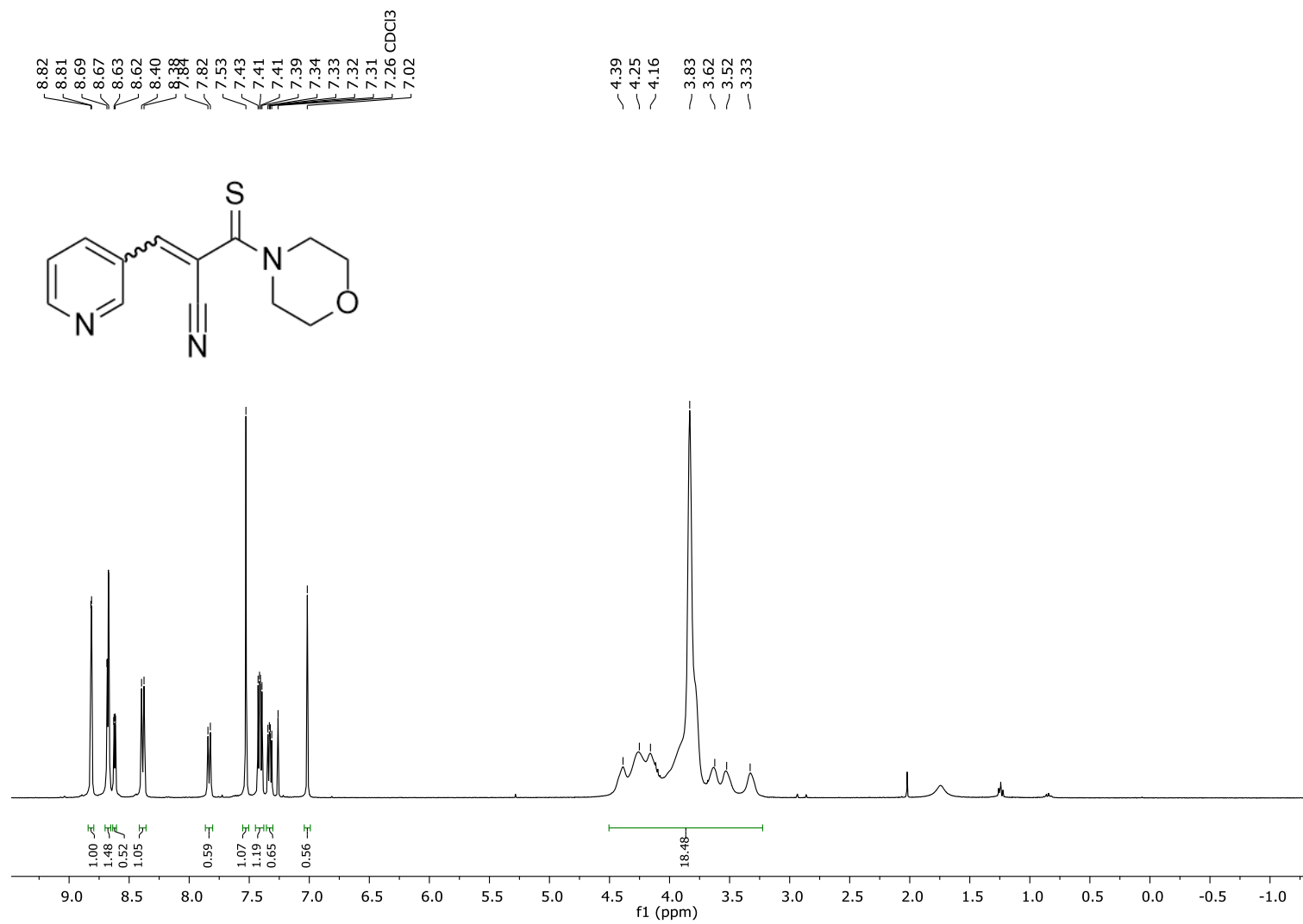


#	Wavelength	Intensity
0	228	41.2

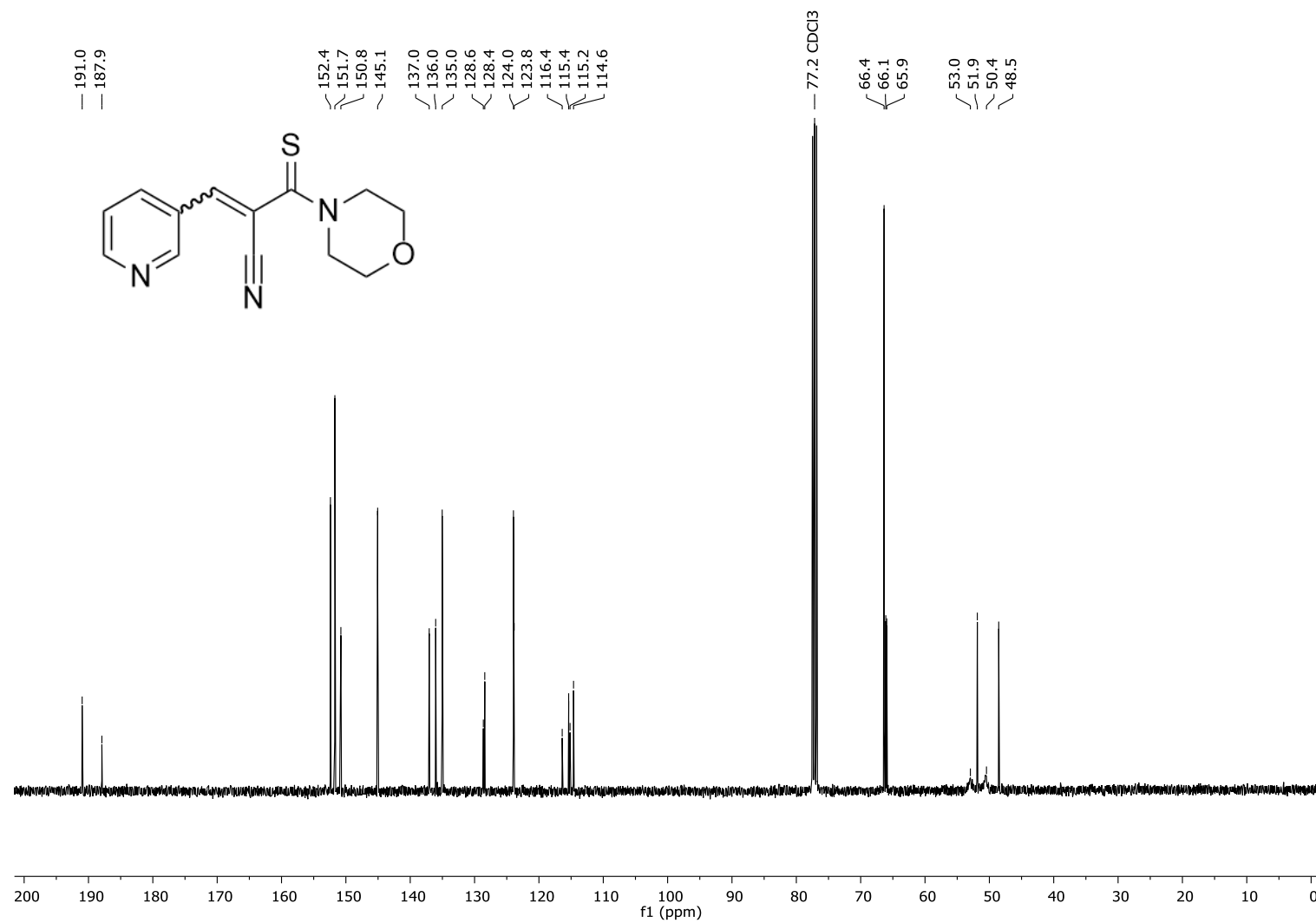


#	m/z	Res.	S/N	I	I %	FWHM
1	139.1226	18943	101209912.0	259449	1.9	0.0073
2	310.1009	32536	947761536.0	2429565	17.4	0.0095
3	311.1035	24608	168408576.0	431711	3.1	0.0126
4	326.0951	21429	101091328.0	259145	1.9	0.0152
5	328.1115	25741	5457144320.0	13989262	100.0	0.0127
6	329.1142	31533	1050522944.0	2692991	19.3	0.0104
7	330.1100	19140	249405584.0	639345	4.6	0.0172
8	342.1267	25349	319576032.0	819226	5.9	0.0135
9	343.1292	20143	64647076.0	165721	1.2	0.0170
10	350.0926	21255	92324624.0	236672	1.7	0.0165

^1H NMR (CDCl_3) spectrum of **1t**

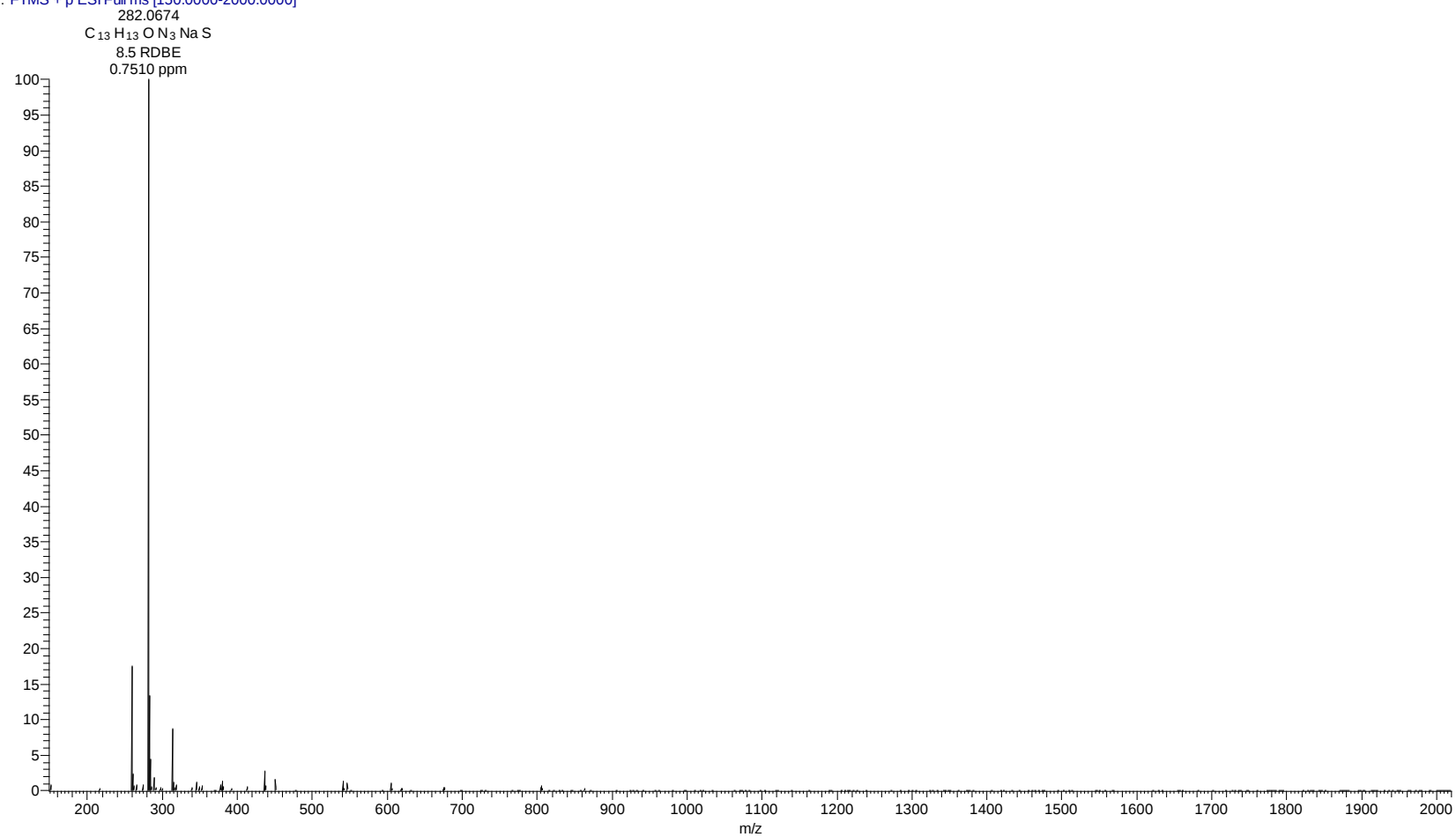


^{13}C NMR (CDCl_3) spectrum of **1t**

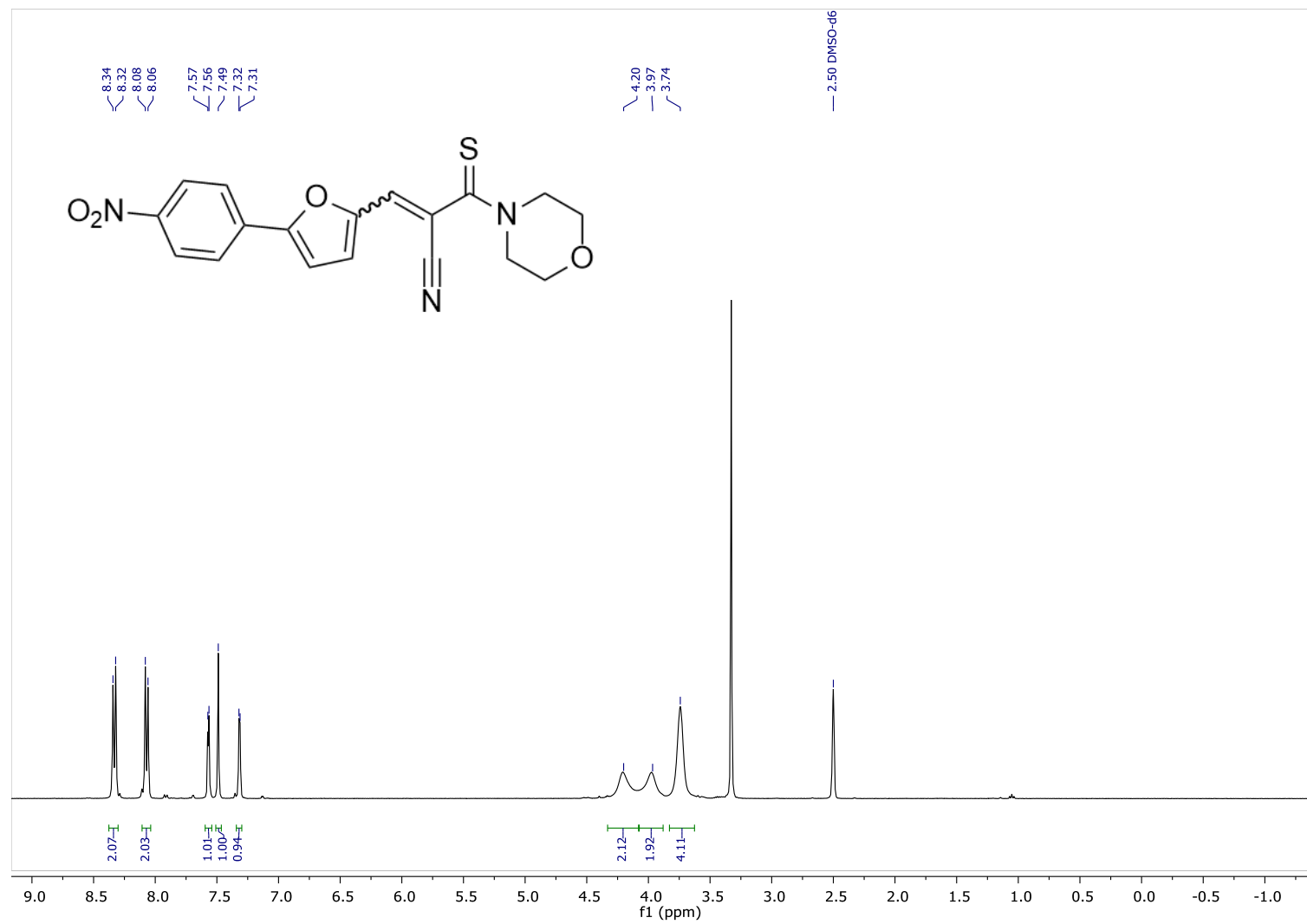


HRMS of 1t

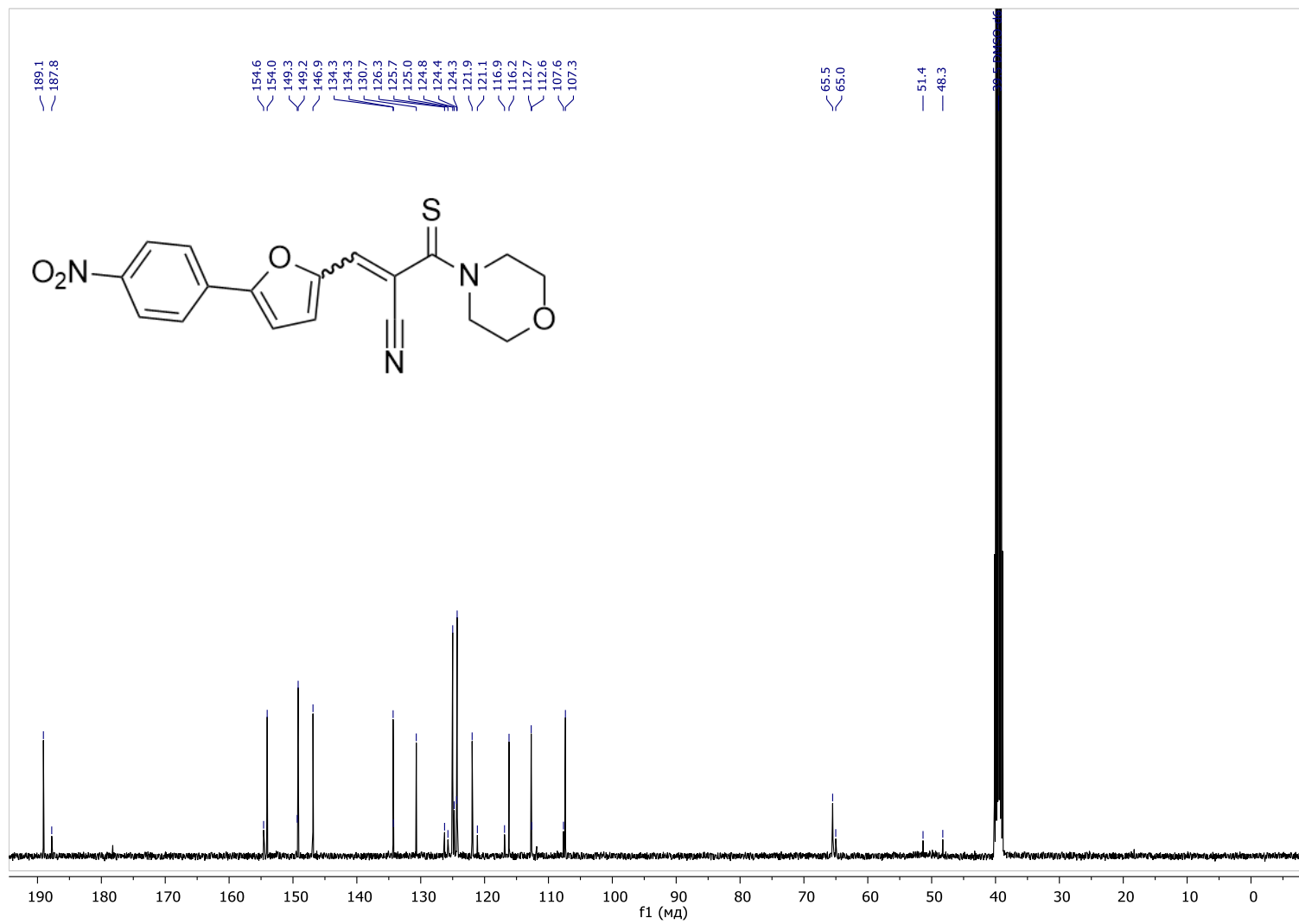
VF-101_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 1.69E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]



^1H NMR (DMSO- d_6) spectrum of **1v**

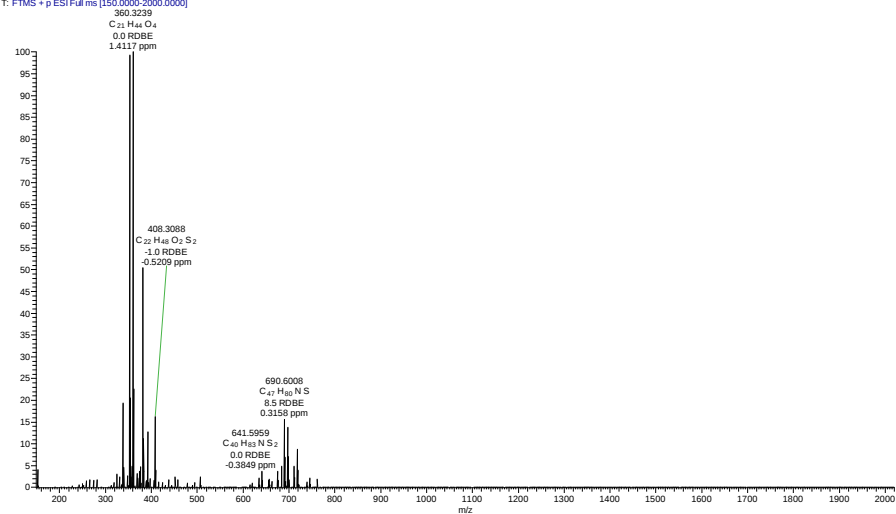


^{13}C NMR (DMSO- d_6) spectrum of **1v**

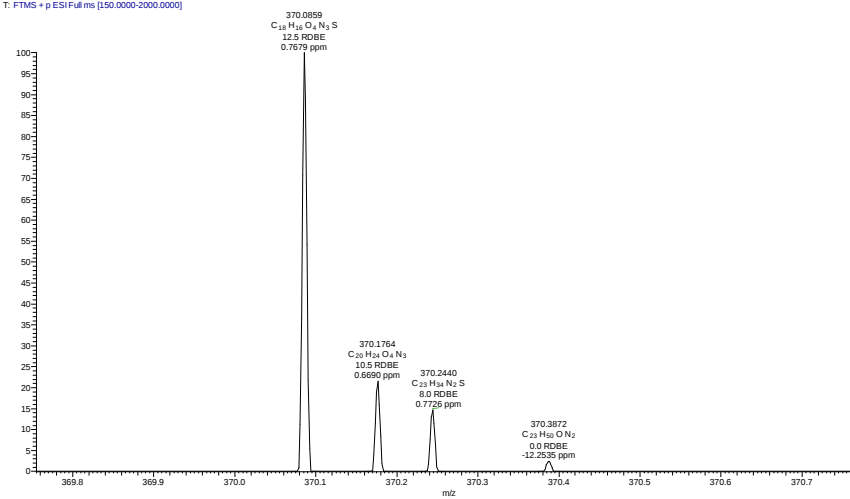


HRMS of 1v

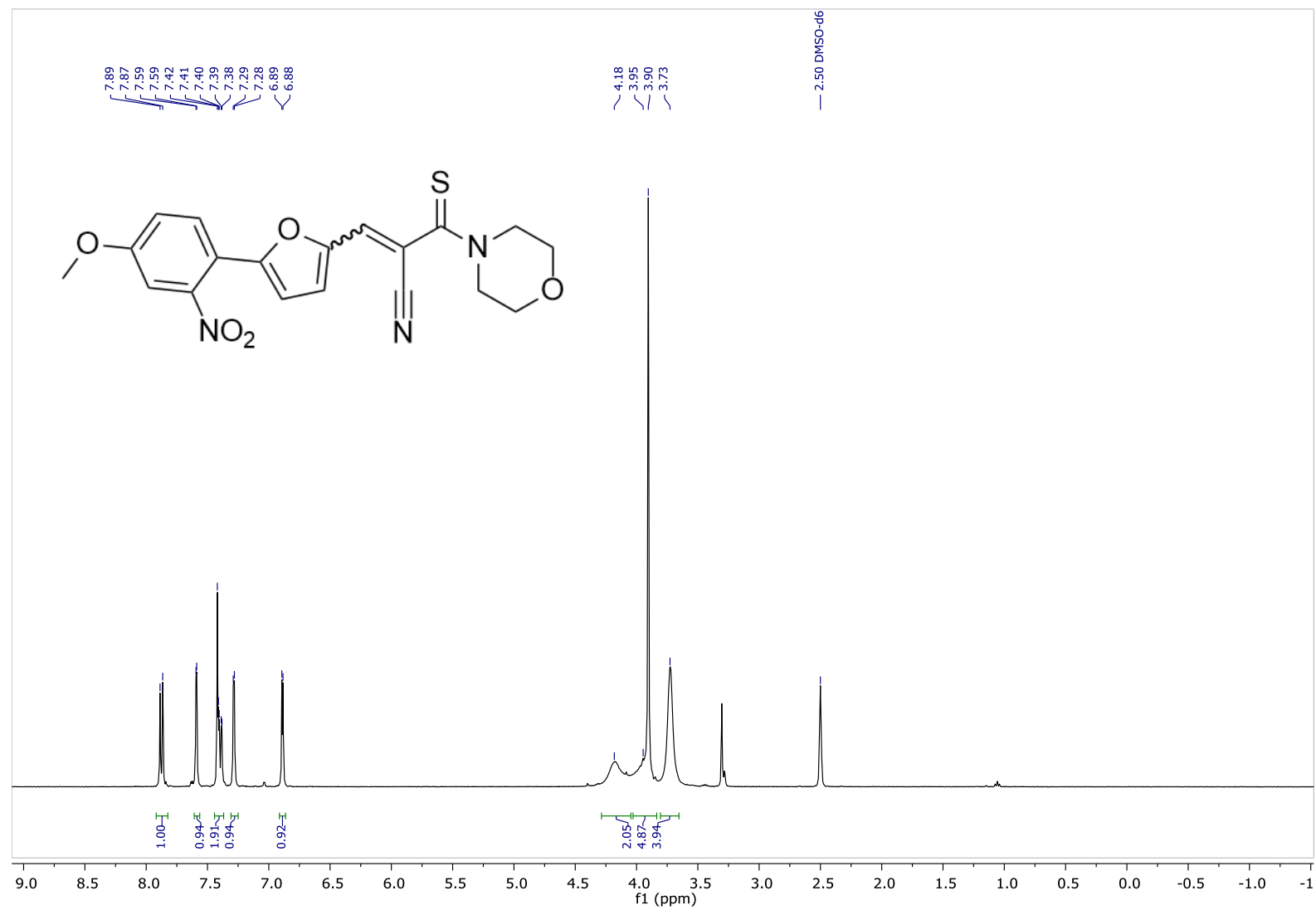
AT7 ESI Pos 240731182600 #52-86 RT: 0.23-0.38 AV: 35 SB: 43 0.06-0.13 0.79-0.90 NL: 1.09E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]



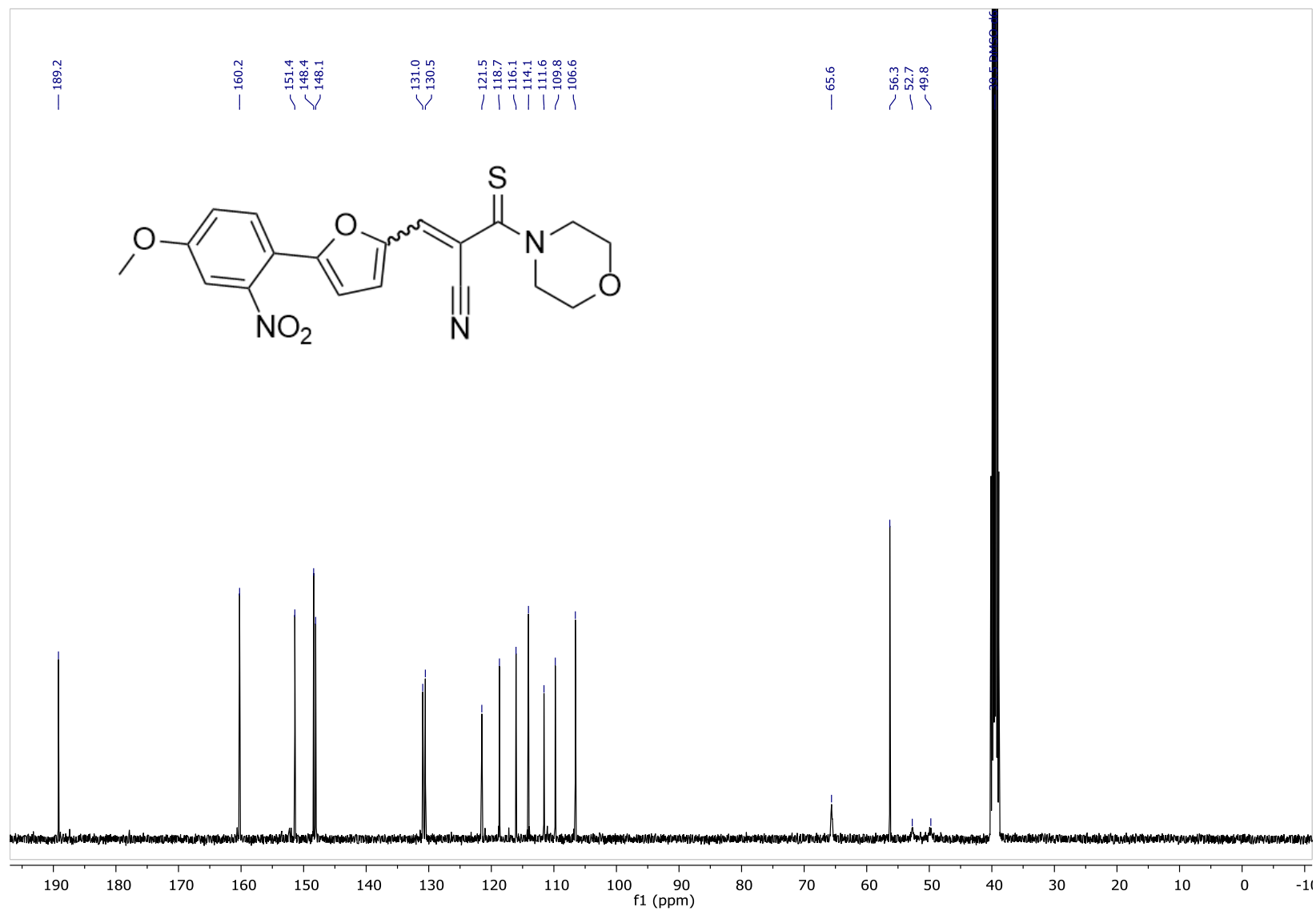
AT7 ESI Pos 240731182600 #52-86 RT: 0.23-0.38 AV: 35 SB: 43 0.06-0.13 0.79-0.90 NL: 2.28E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (DMSO-d₆) spectrum of **1w**

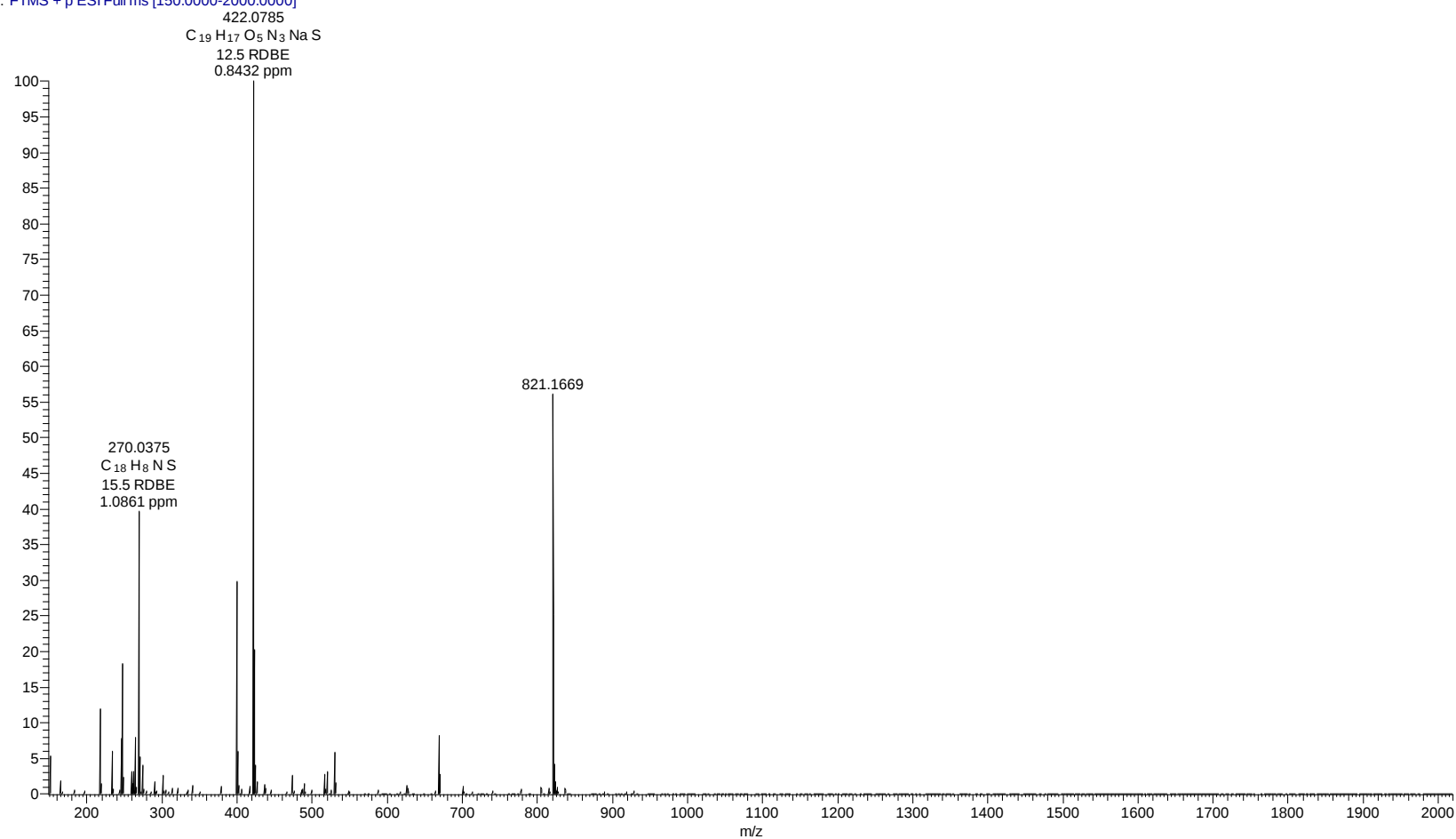


^{13}C NMR (DMSO- d_6) spectrum of **1w**

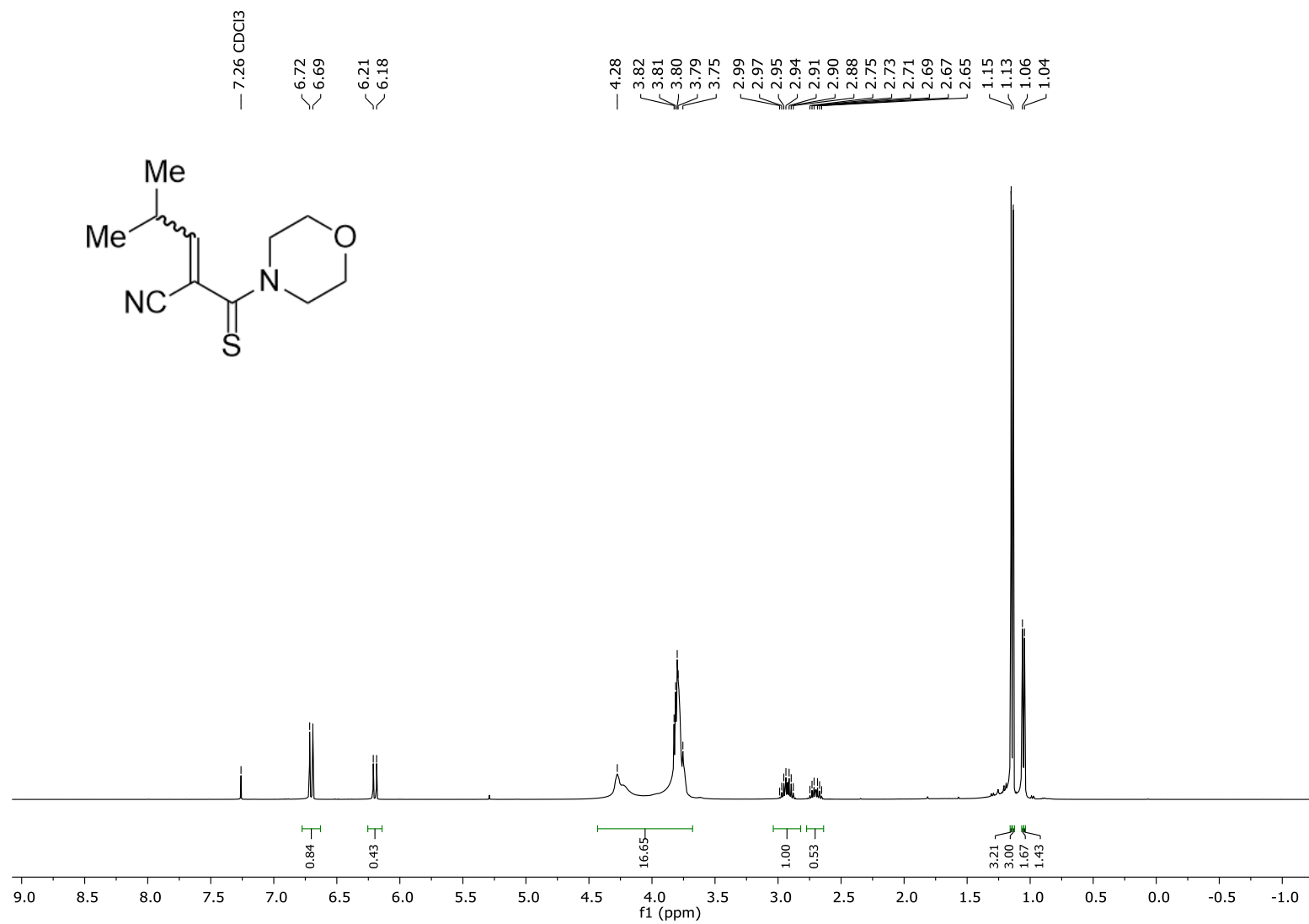


HRMS of 1w

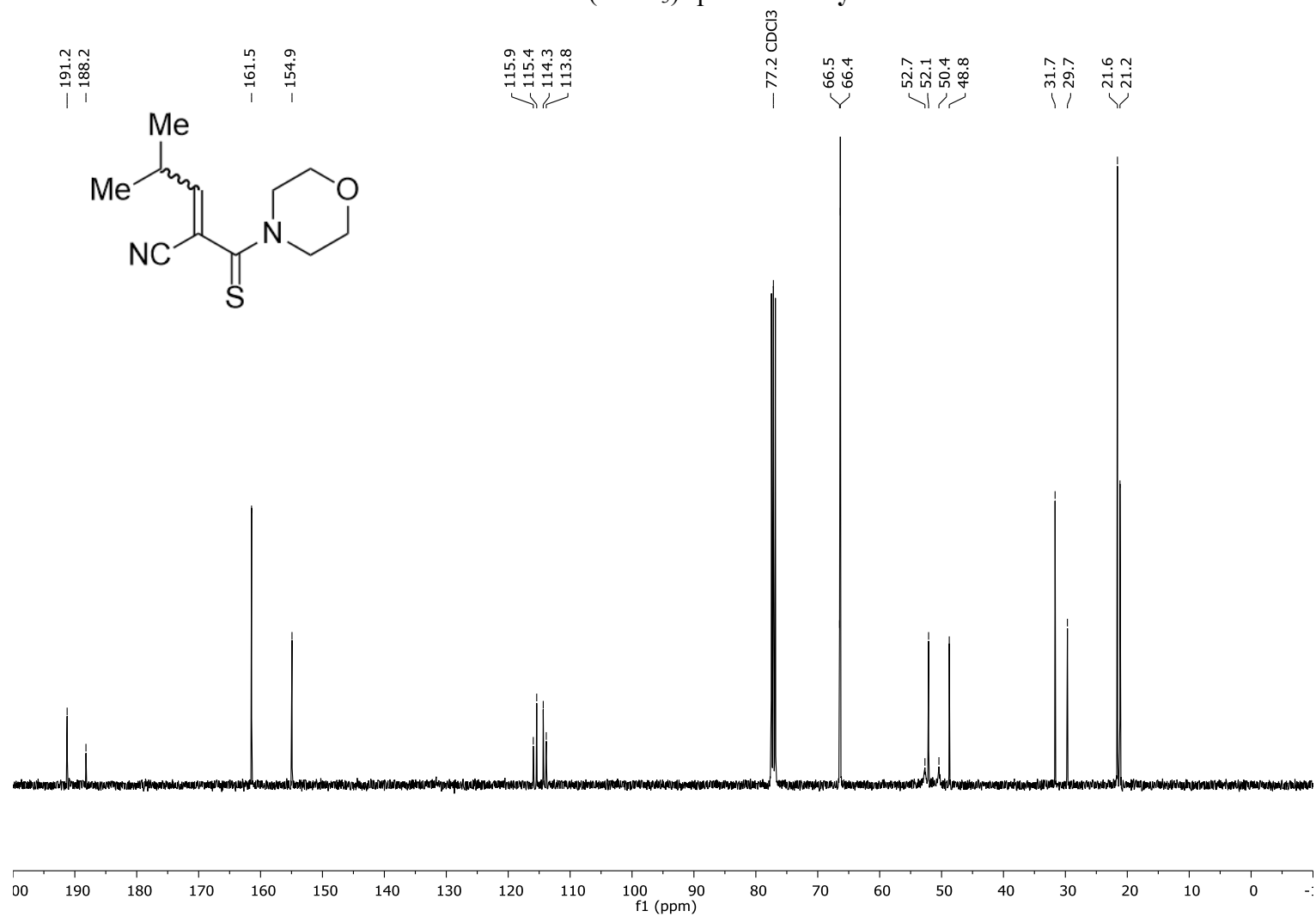
TR10_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 6.50E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



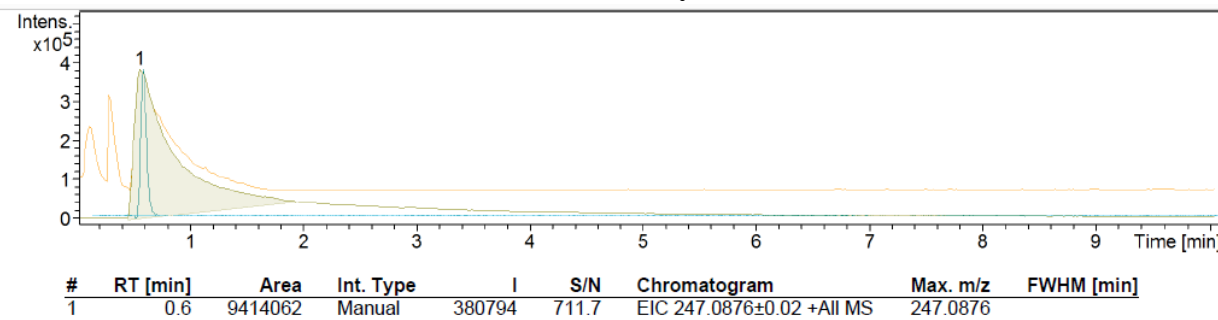
¹H NMR (CDCl₃) spectrum of **1y**



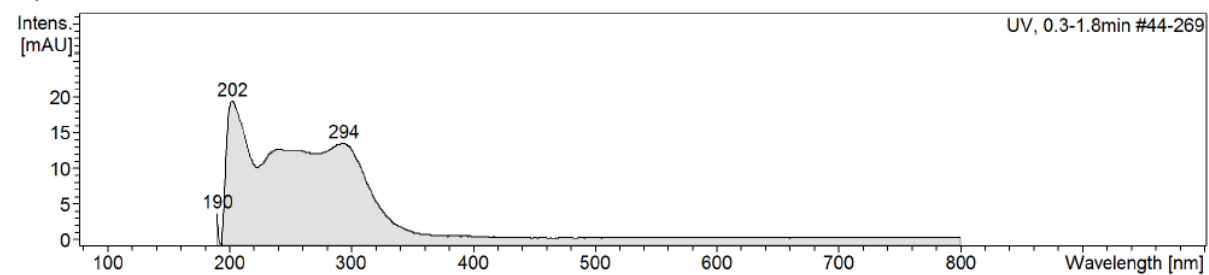
^{13}C NMR (CDCl_3) spectrum of **1y**



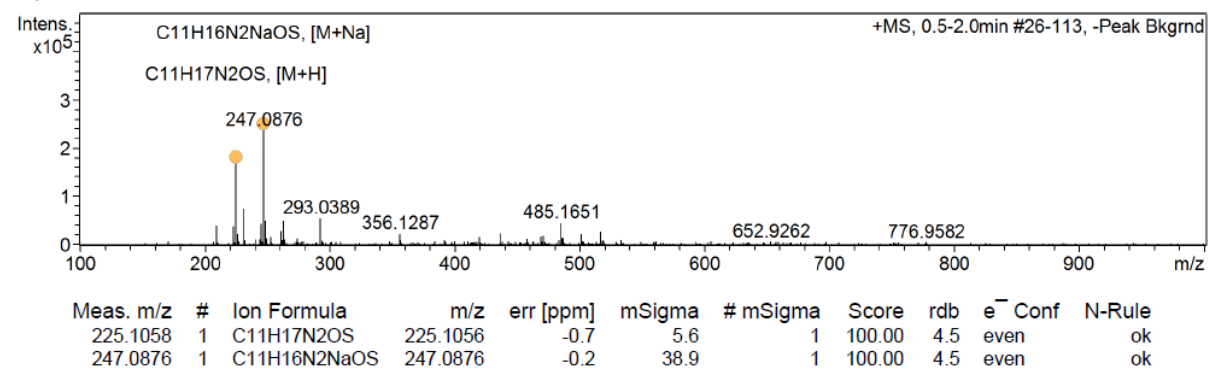
HRMS of 1y



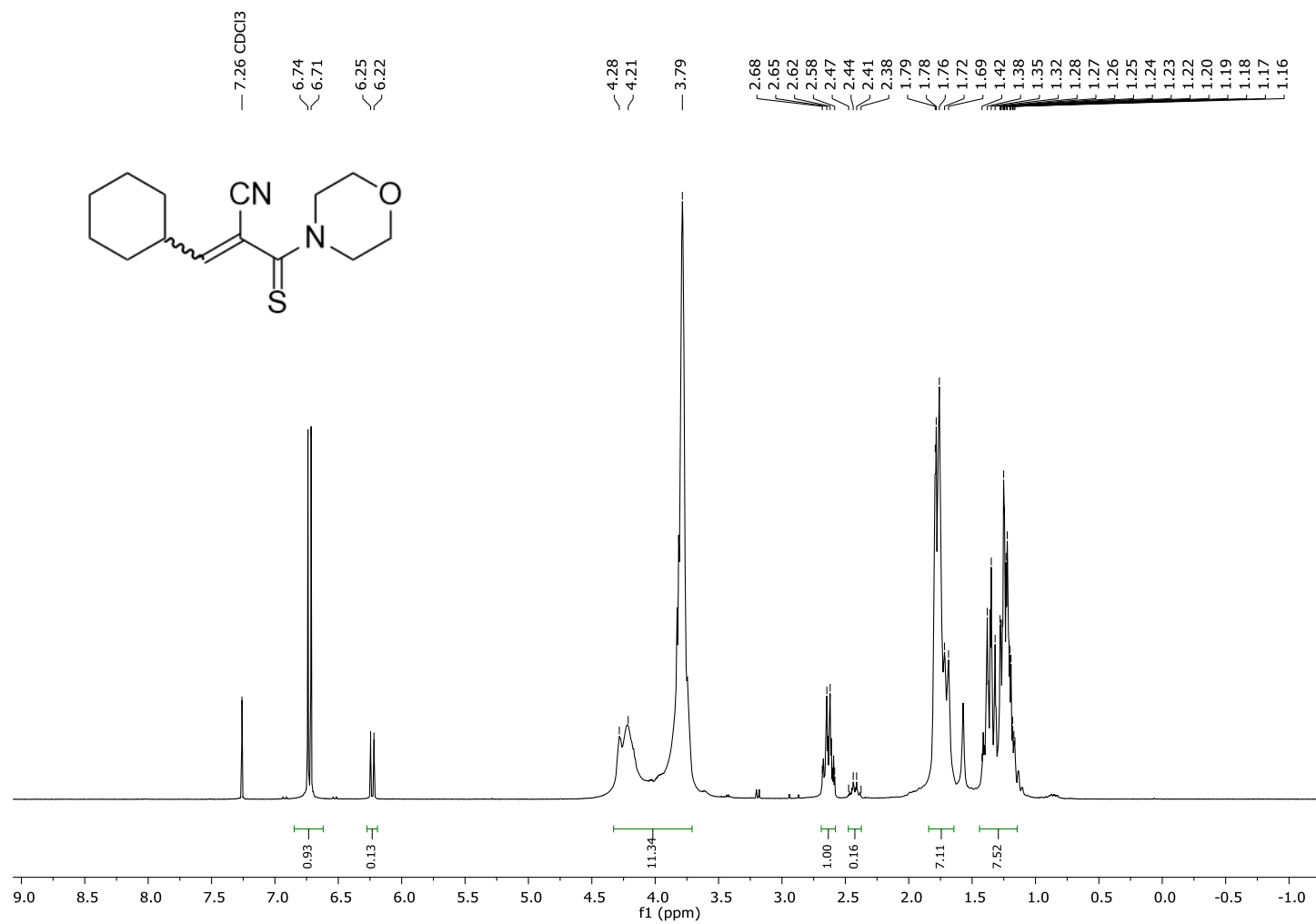
Cmpd 1, 0.6 min



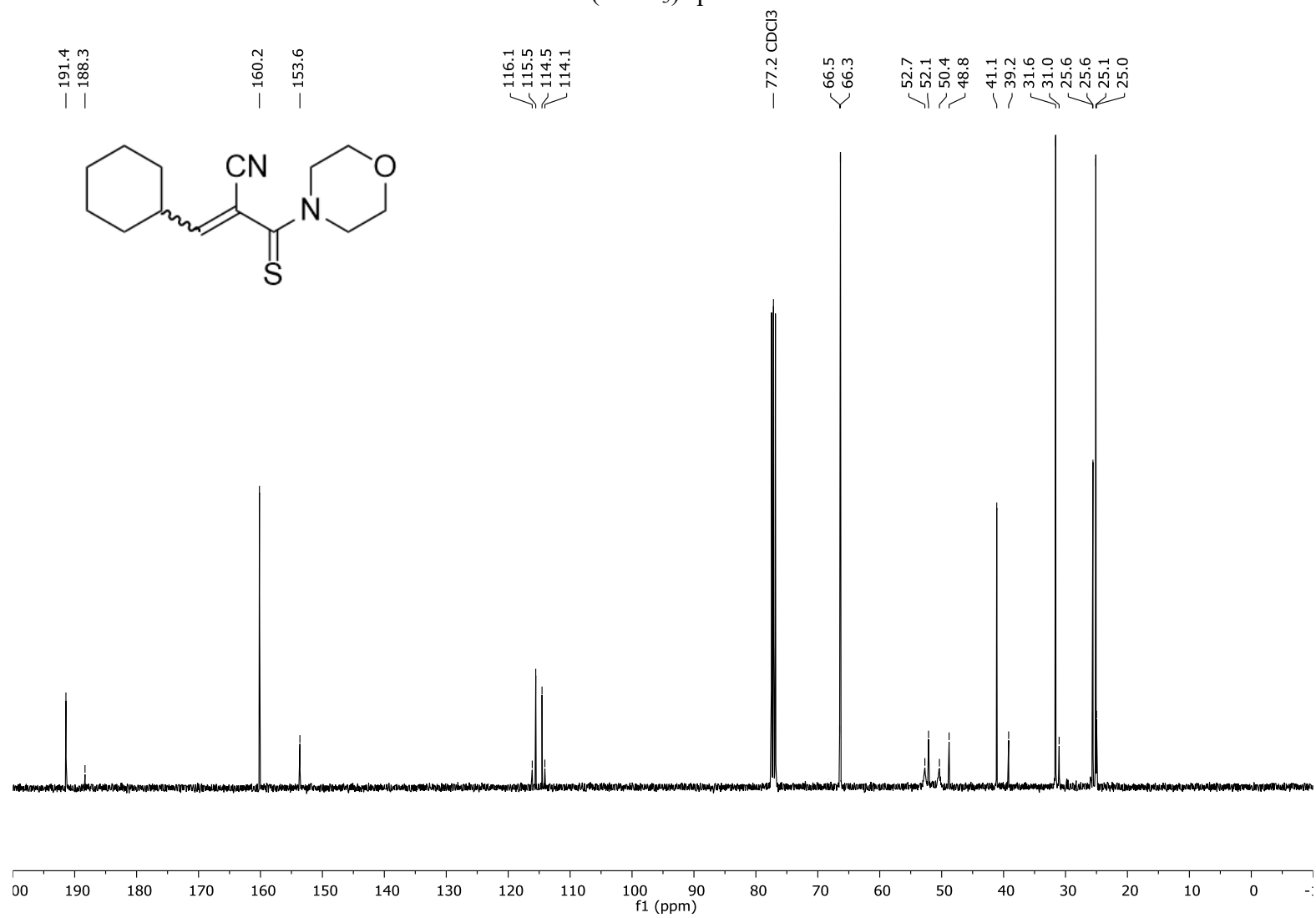
Cmpd 1, 0.6 min



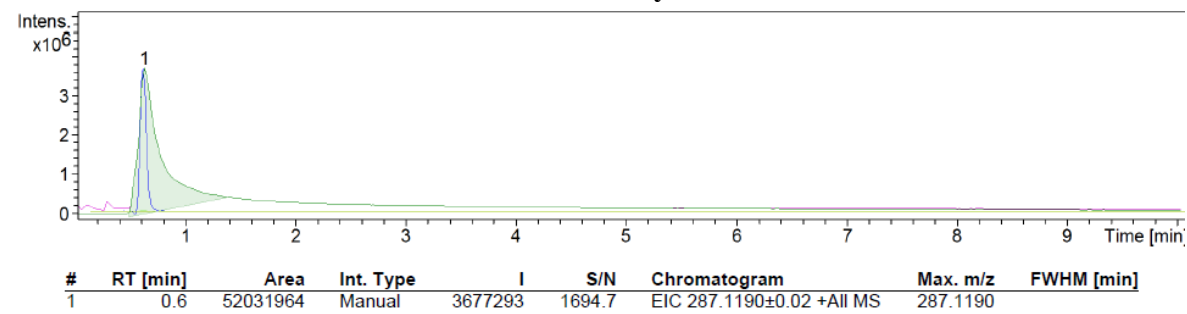
¹H NMR (CDCl₃) spectrum of **1z**



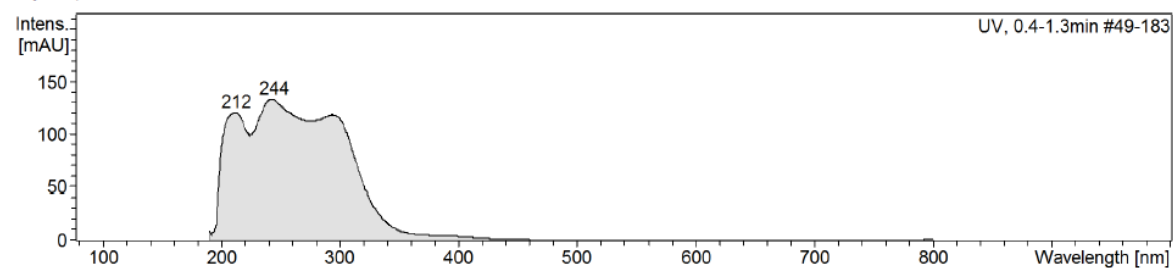
^{13}C NMR (CDCl_3) spectrum of **1z**



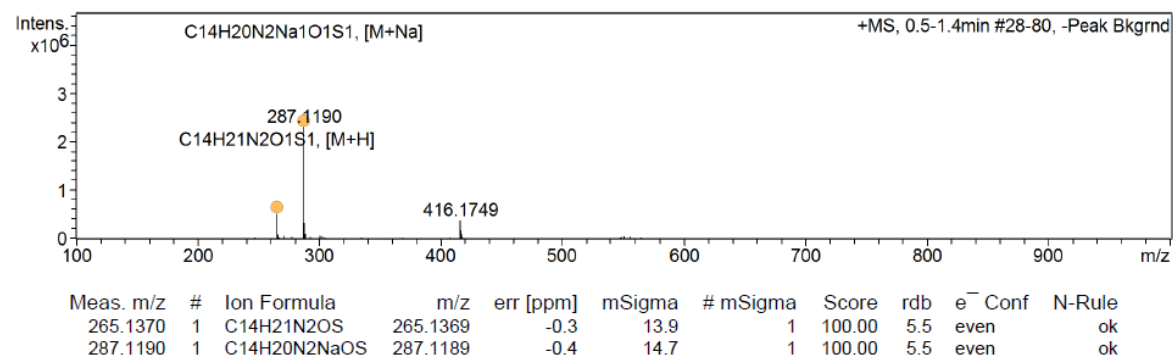
HRMS of 1y



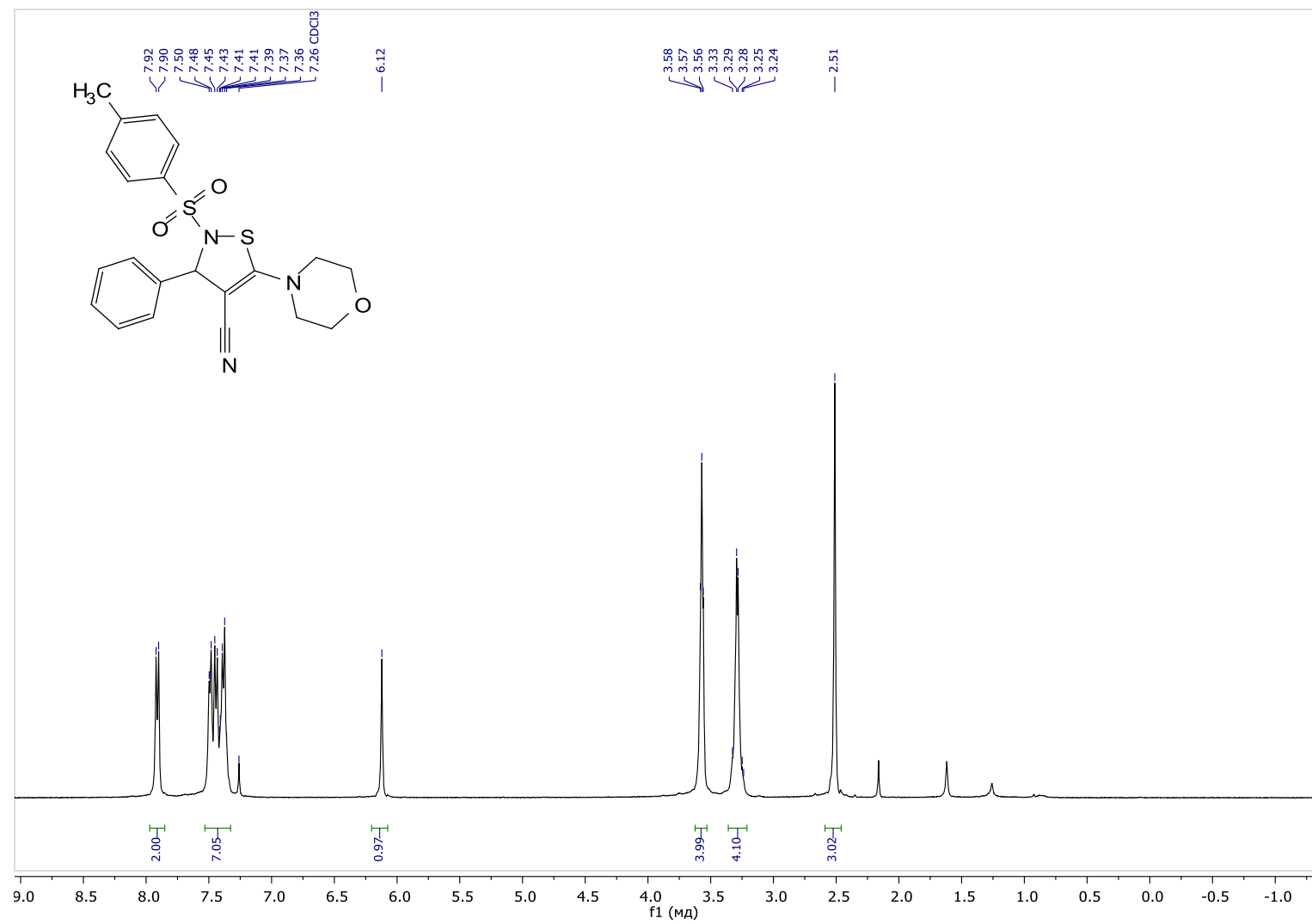
Cmpd 1, 0.6 min



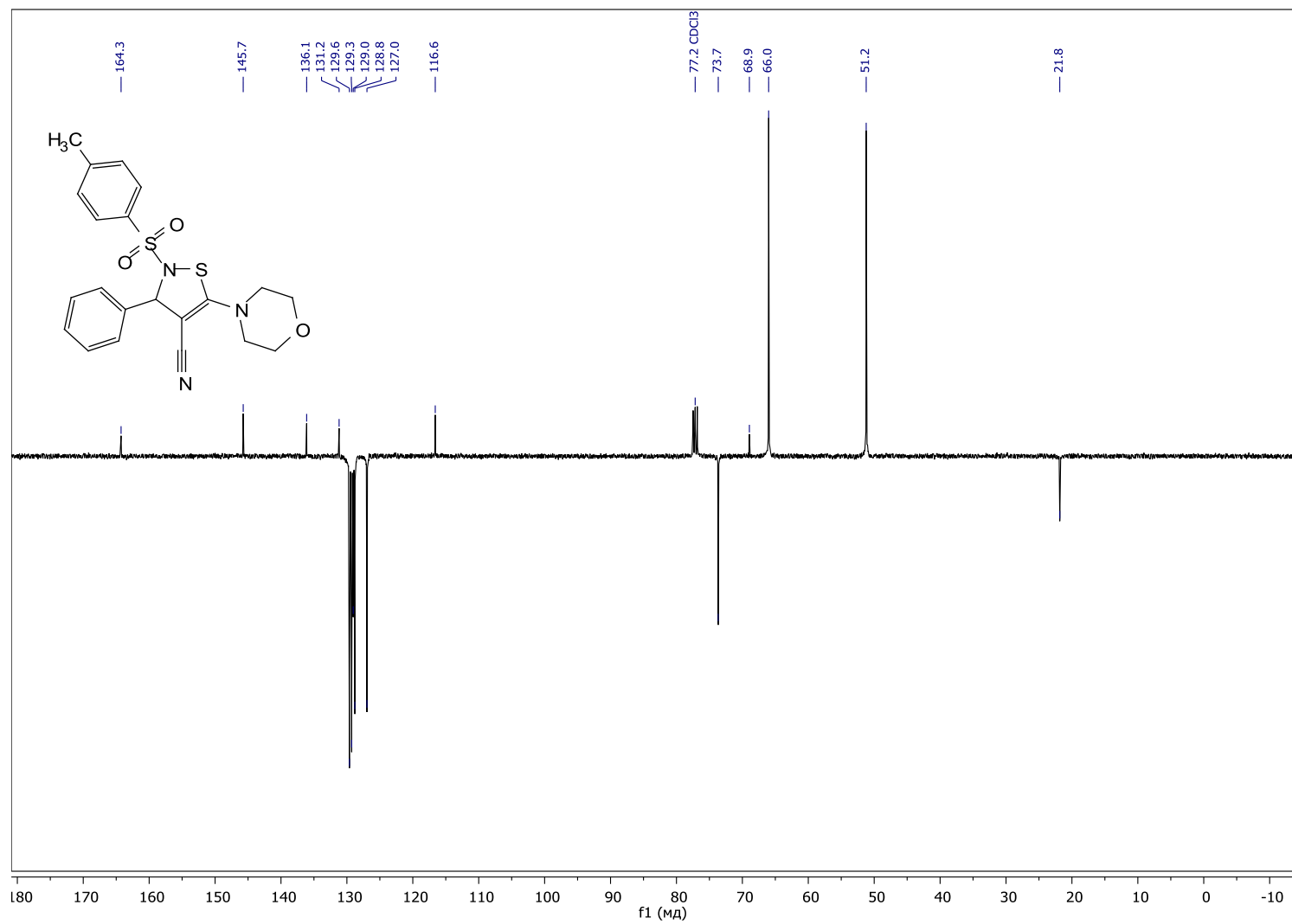
Cmpd 1, 0.6 min



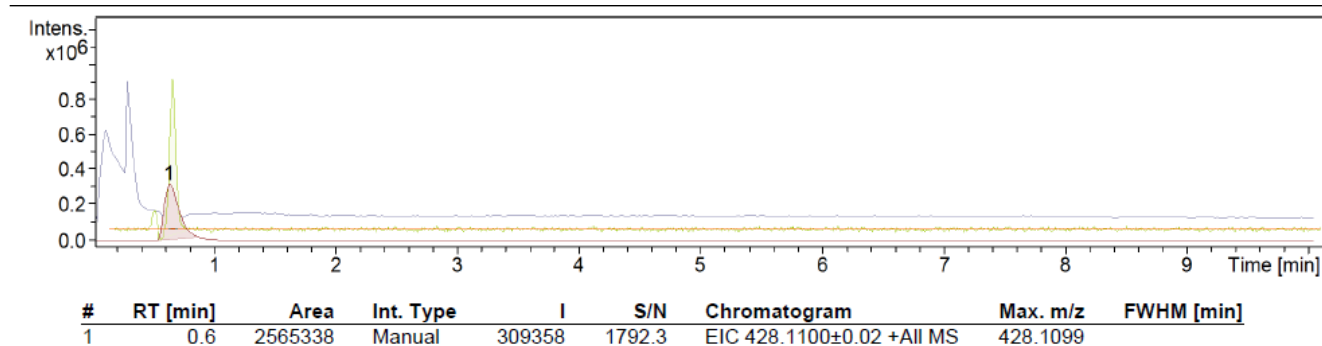
^1H NMR (CDCl_3) spectrum of **3aa**



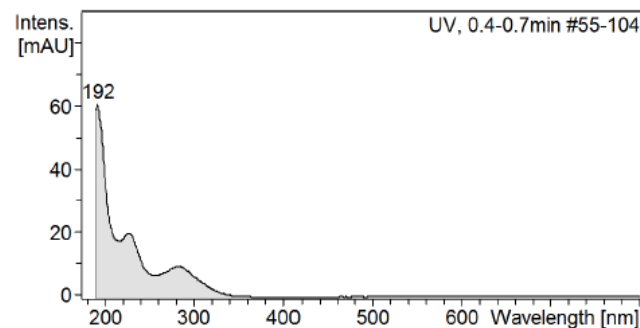
^{13}C NMR (CDCl_3) spectrum of **3aa**



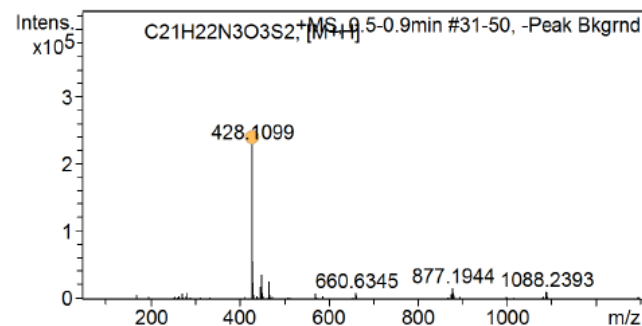
HRMS of **3aa**



Cmpd 1, 0.6 min

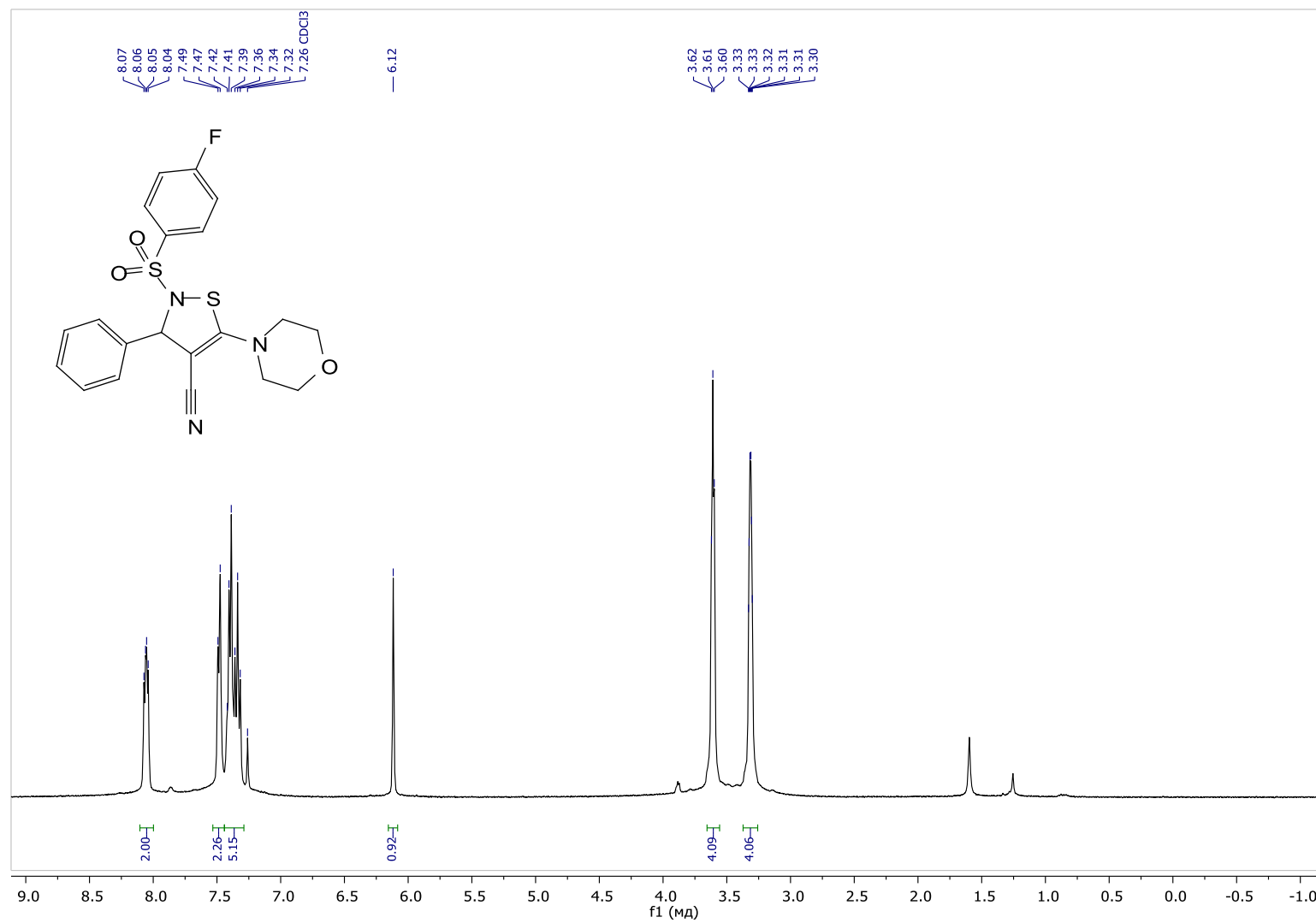


#	Wavelength	Intensity
0	192	60.4

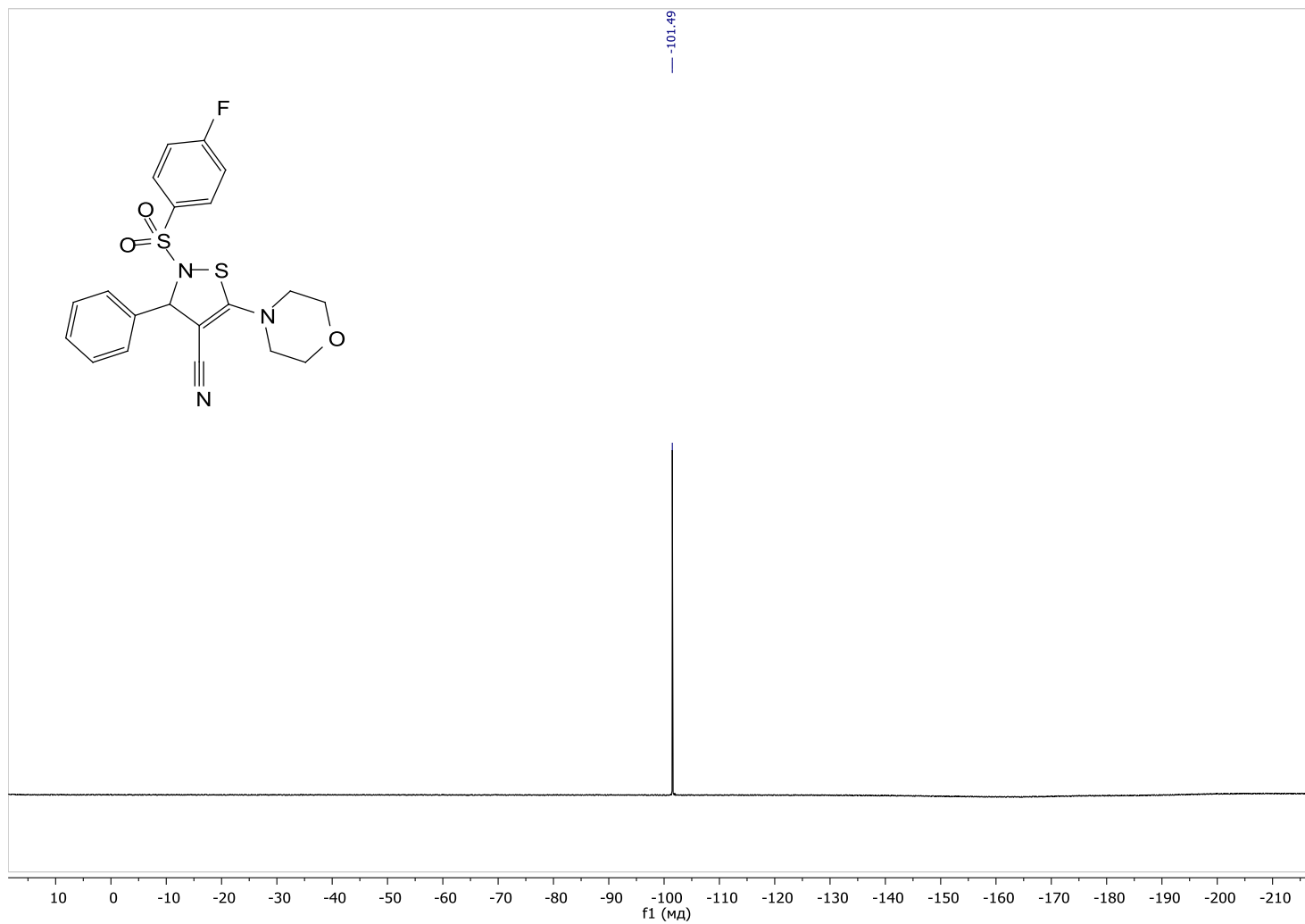


#	m/z	Res.	S/N	I	I %	FWHM
1	428.1099	23016	128879464.0	228119	100.0	0.0186
2	429.1125	19976	30610454.0	54181	23.8	0.0215
3	430.1079	17574	13124928.0	23231	10.2	0.0245
4	447.0837	20913	9885801.0	17498	7.7	0.0214
5	447.5843	20398	4946705.5	8756	3.8	0.0219
6	450.0914	20401	19882364.0	35192	15.4	0.0221
7	466.0654	20919	14484337.0	25638	11.2	0.0223
8	877.1944	22742	8865959.0	15693	6.9	0.0386
9	1088.2393	25762	5895925.0	10436	4.6	0.0422
10	1088.7391	24706	5371830.0	9508	4.2	0.0441

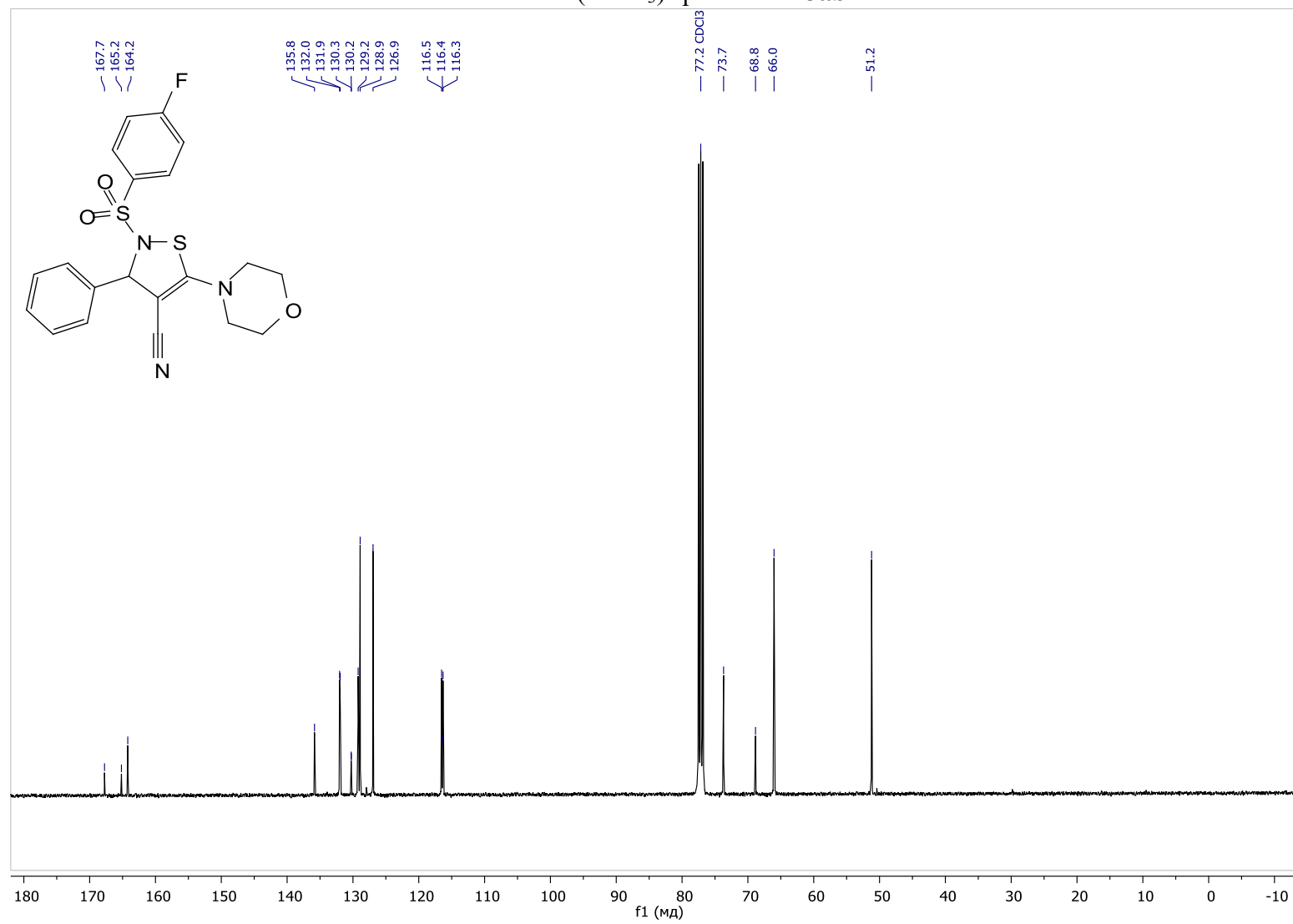
¹H NMR (CDCl₃) spectrum of **3ab**



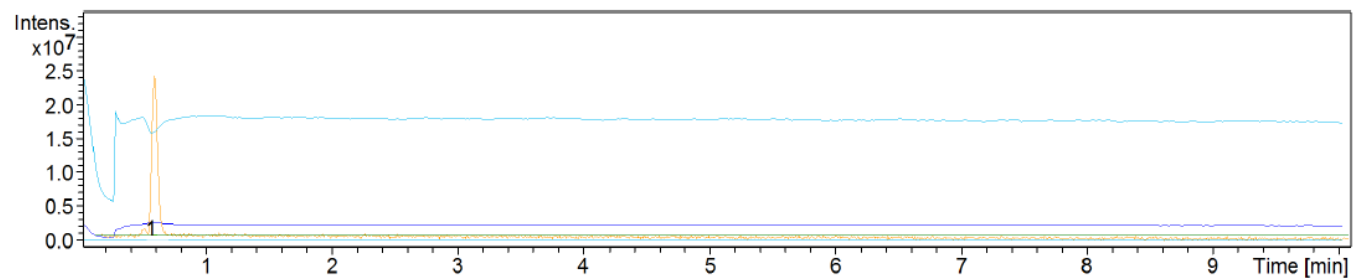
^{19}F NMR (CDCl_3) spectrum of **3ab**



^{13}C NMR (CDCl_3) spectrum of **3ab**

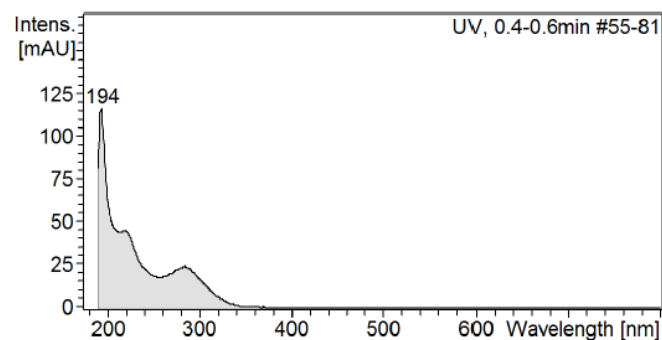


HRMS of **3ab**

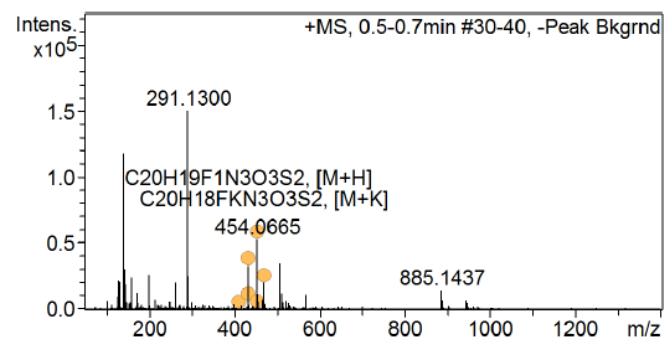


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	203380	Manual	77368	12.4	EIC C ₂₀ H ₁₈ FN ₃ O ₃ S ₂ [M+H], M+NH ₄ ⁺	432.0846; 449.1112	All MS 291.1300

Cmpd 1, 0.6 min

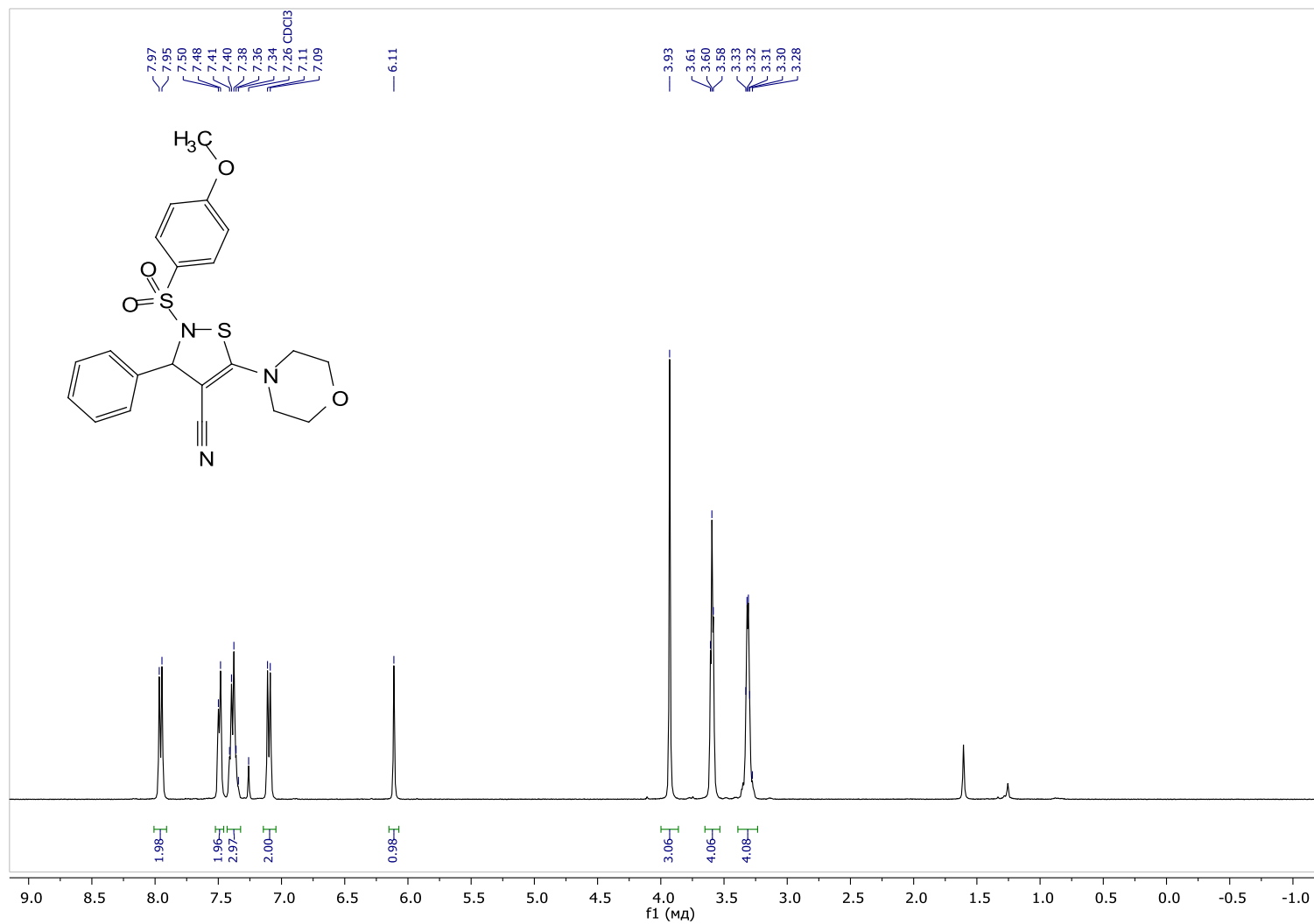


#	Wavelength	Intensity
0	194	115.5

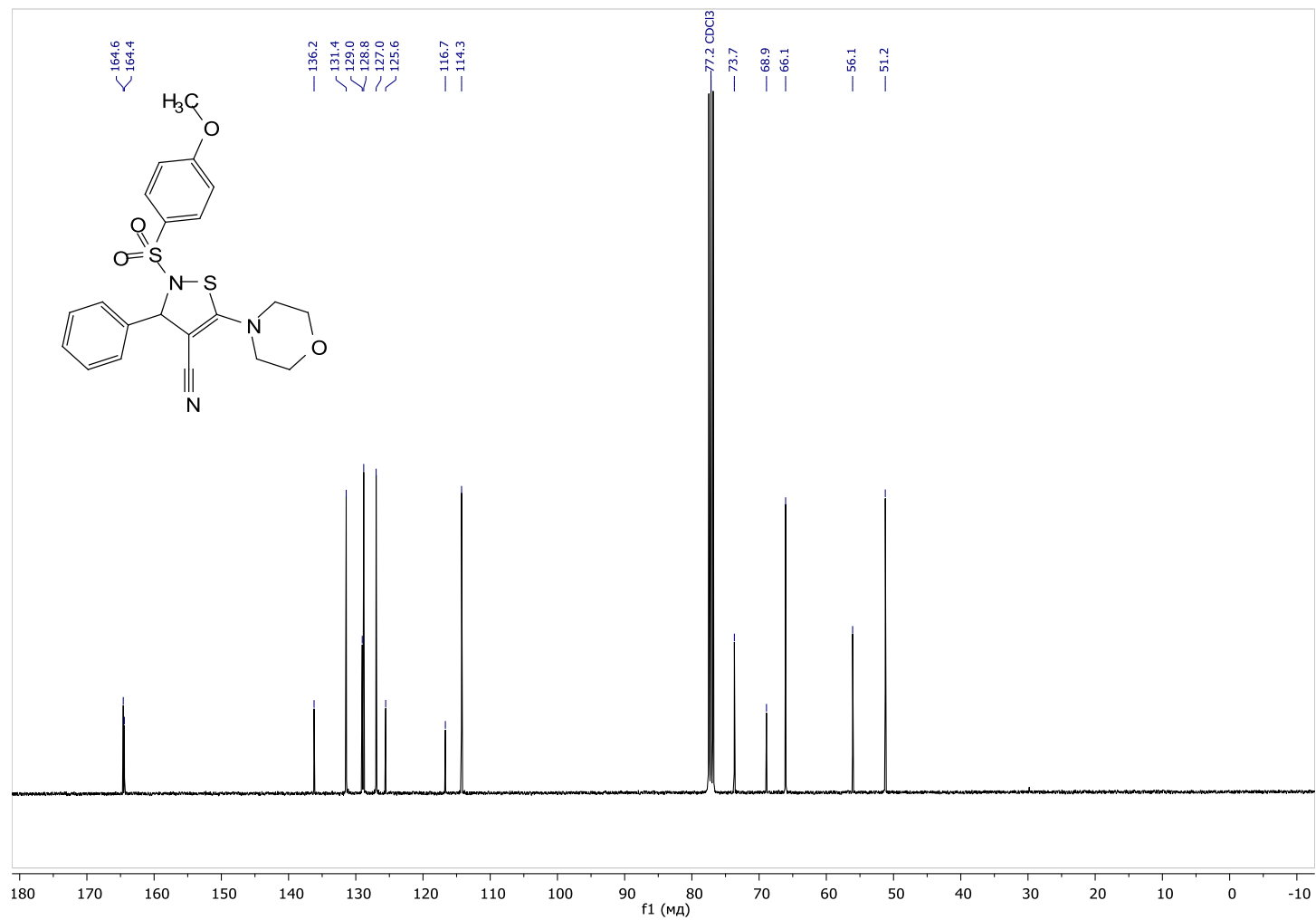


#	m/z	Res.	S/N	I	I %	FWHM
1	128.1434	17366	1741176.0	21421	14.3	0.0074
2	139.1231	20703	9553919.0	117536	78.5	0.0067
3	142.1589	18244	2498196.8	30734	20.5	0.0078
4	158.1537	18186	1960475.1	24119	16.1	0.0087
5	199.1439	19525	2093463.8	25755	17.2	0.0102
6	291.1300	29033	12170005.0	149720	100.0	0.0100
7	292.1329	21848	2008376.1	24708	16.5	0.0134
8	432.0844	20308	2672344.0	32876	22.0	0.0213
9	454.0665	20988	4325999.5	53220	35.5	0.0216
10	507.3282	19672	2838541.3	34921	23.3	0.0258

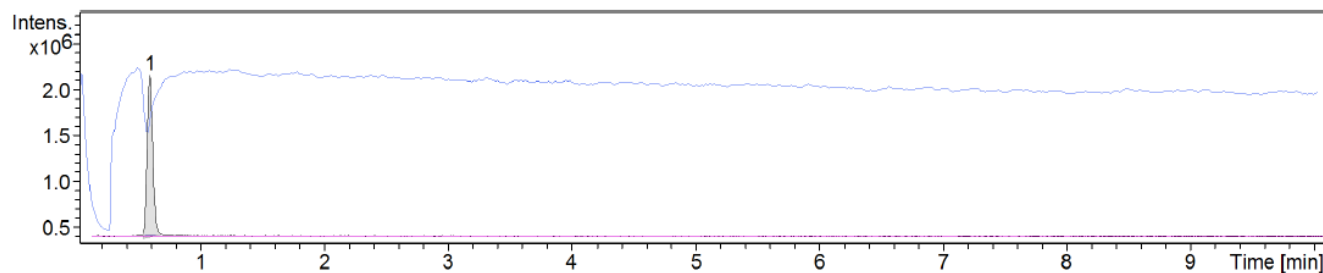
^1H NMR (CDCl_3) spectrum of **3ac**



^{13}C NMR (CDCl_3) spectrum of **3ac**

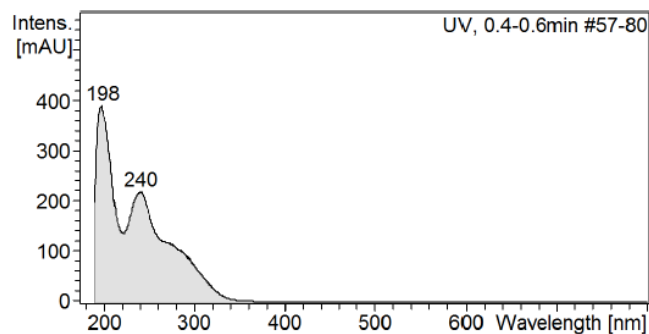


HRMS of 3ac

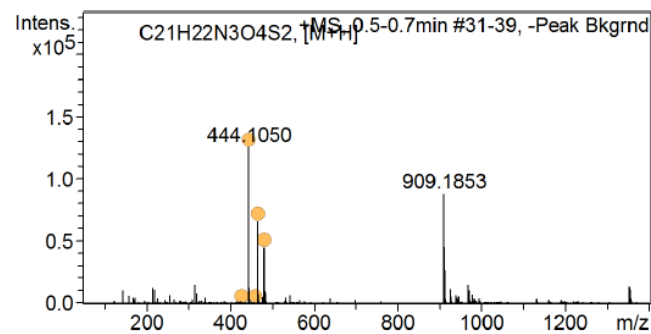


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	403660	Manual	121236	282.9	UV Chromatogram, 190-800 nm	444.1050	

Cmpd 1, 0.6 min

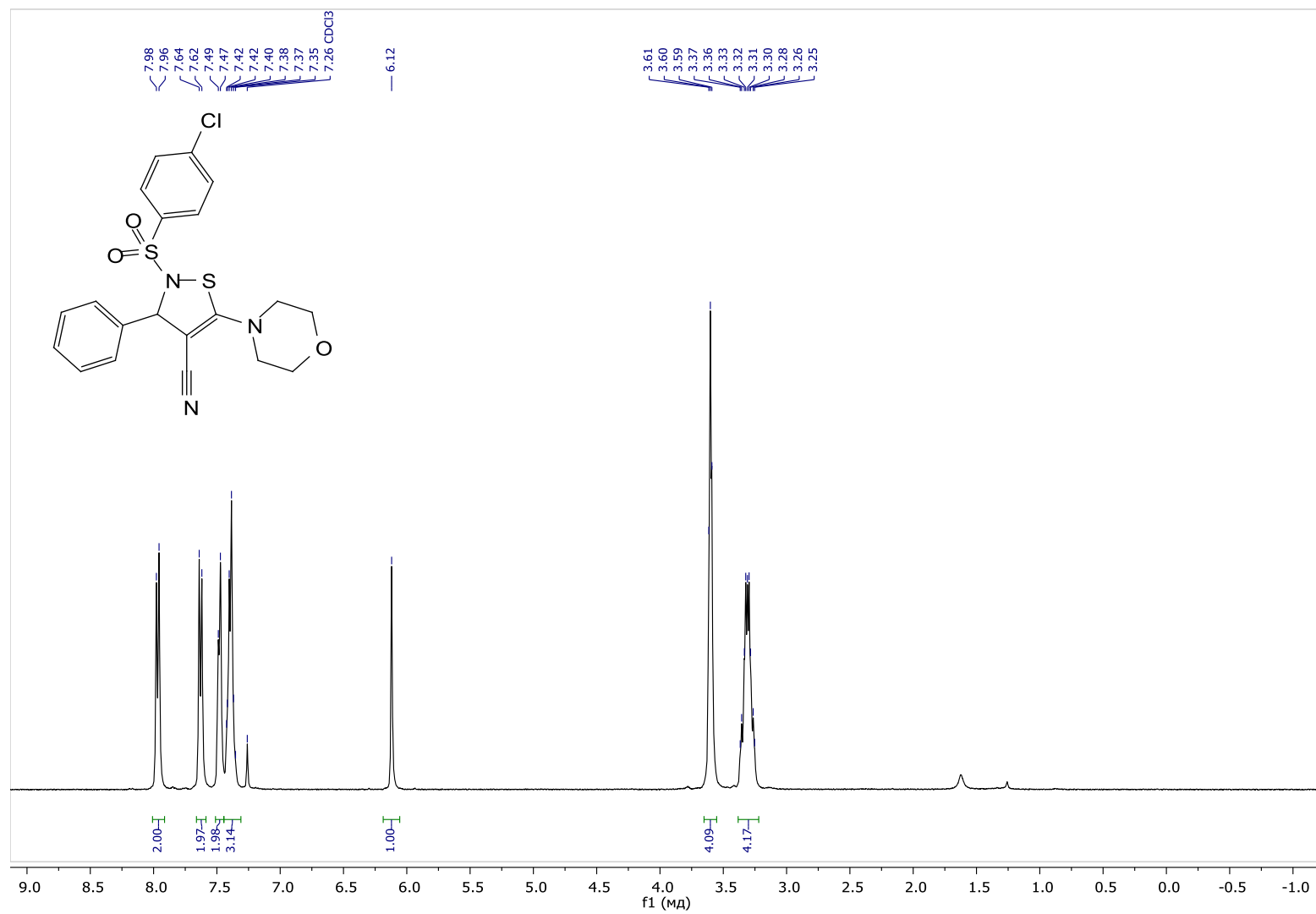


#	Wavelength	Intensity
0	198	387.5
1	240	217.0

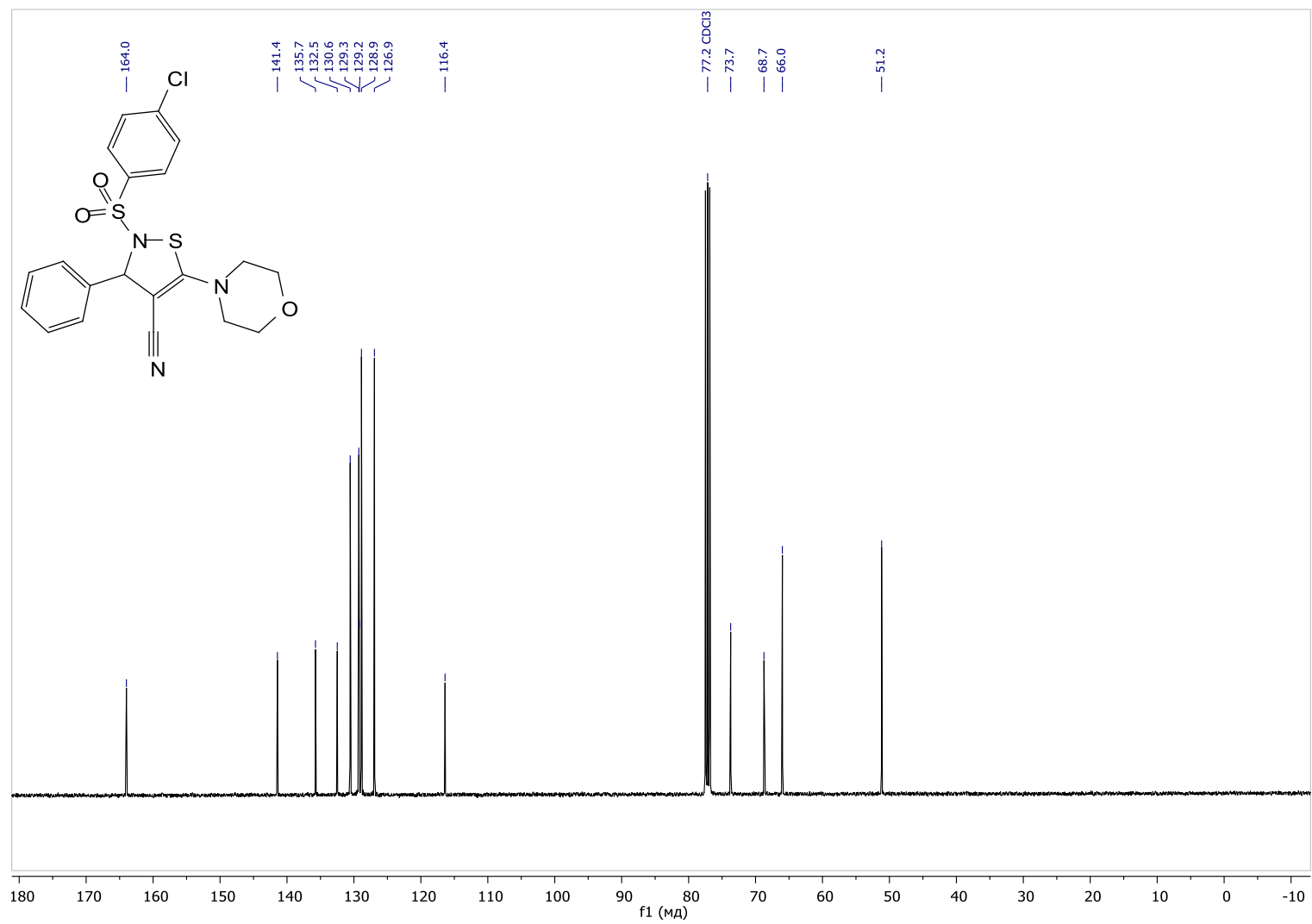


#	m/z	Res.	S/N	I	I %	FWHM
1	316.3203	20538	1227602.0	14843	11.9	0.0154
2	444.1050	22934	10334461.0	124951	100.0	0.0194
3	445.1076	20293	2541050.0	30723	24.6	0.0219
4	466.0864	21282	5452649.0	65926	52.8	0.0219
5	467.0891	19810	1410503.0	17054	13.6	0.0236
6	482.0603	20799	3710549.0	44863	35.9	0.0232
7	909.1853	25666	7262980.0	87814	70.3	0.0354
8	910.1874	23292	3765613.3	45529	36.4	0.0391
9	911.1845	21354	2179008.3	26346	21.1	0.0427
10	967.1430	21640	1259315.4	15226	12.2	0.0447

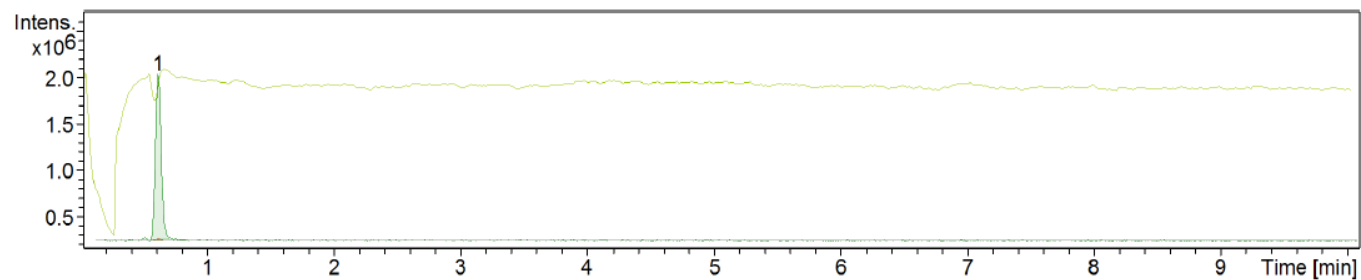
^1H NMR (CDCl_3) spectrum of **3ad**



^{13}C NMR (CDCl_3) spectrum of **3ad**

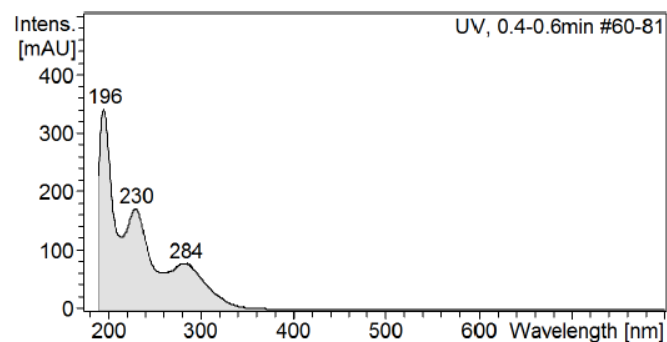


HRMS of **3ad**

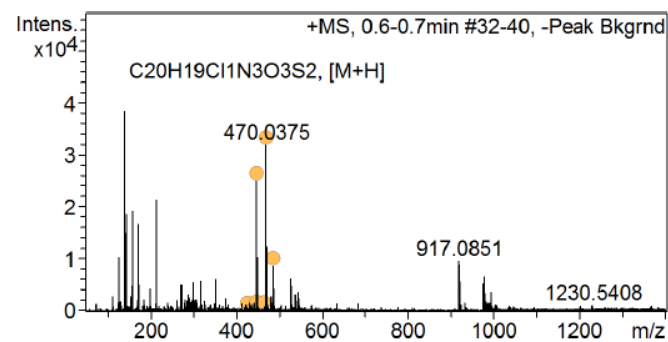


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	257070	Manual	78451	184.4	UV Chromatogram, 190-800 nm	139.1232	

Cmpd 1, 0.6 min

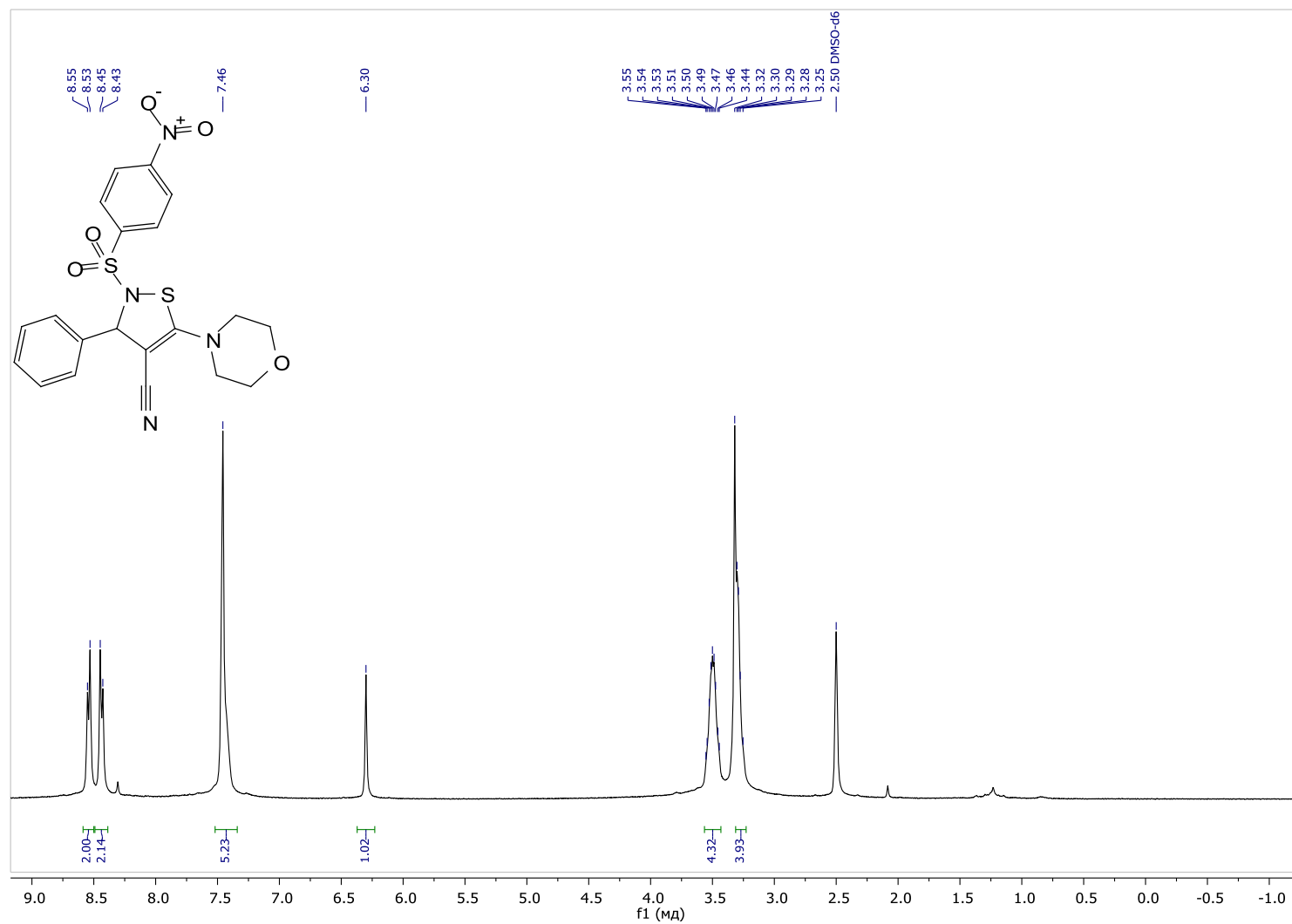


#	Wavelength	Intensity
0	196	340.3
1	230	171.5
2	284	78.1

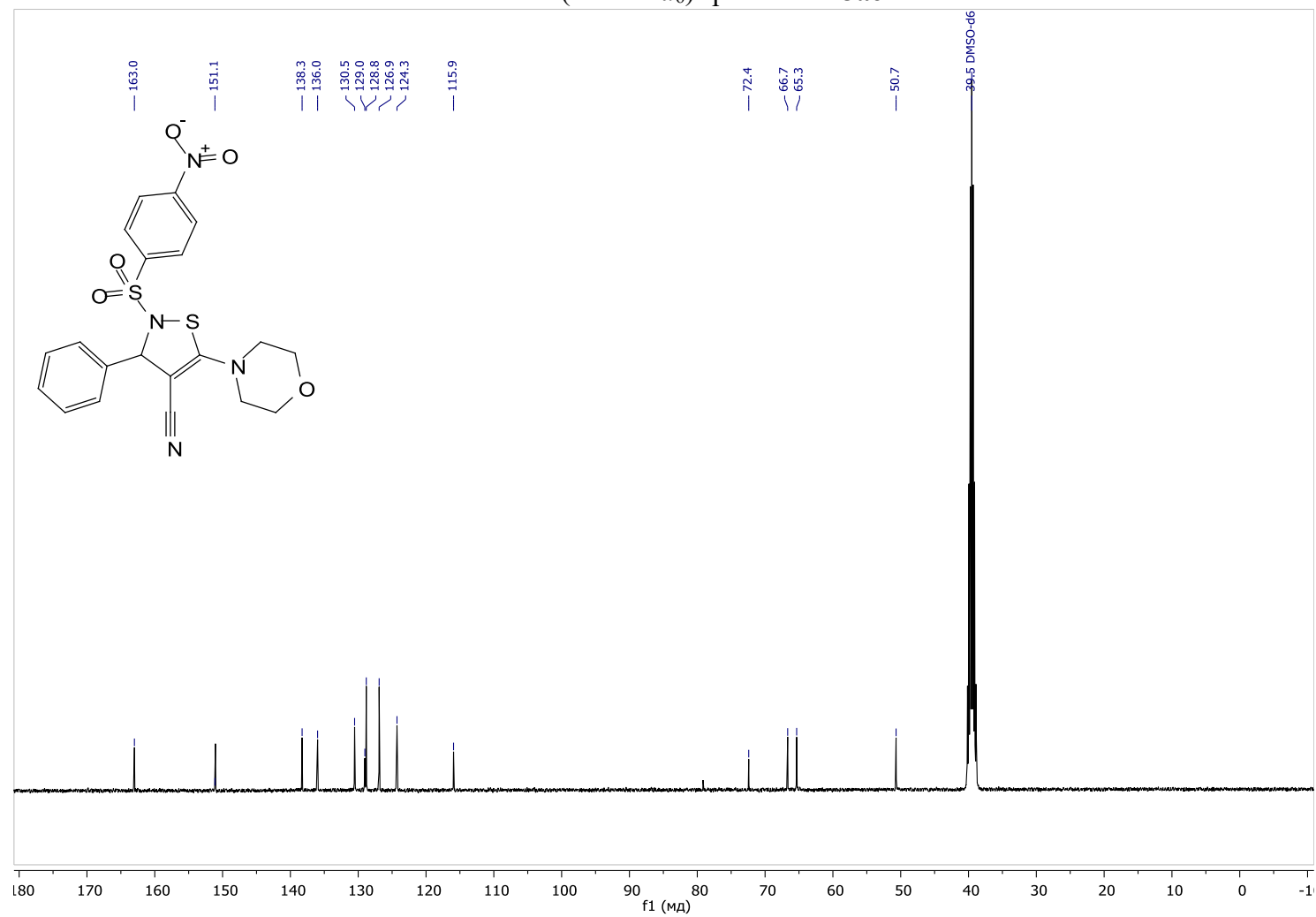


#	m/z	Res.	S/N	I	I %	FWHM
1	139.1232	19729	5283883.0	38297	100.0	0.0071
2	142.1590	18635	2081020.3	15083	39.4	0.0076
3	143.1181	16569	2571527.0	18638	48.7	0.0086
4	158.1538	18410	2645341.3	19173	50.1	0.0086
5	172.1331	17904	2317819.8	16799	43.9	0.0096
6	213.1227	17851	2956544.0	21429	56.0	0.0119
7	448.0551	20718	3446639.5	24981	65.2	0.0216
8	450.0528	19281	1437743.1	10421	27.2	0.0233
9	470.0375	21134	4386319.0	31792	83.0	0.0222
10	472.0346	19605	1726835.1	12516	32.7	0.0241

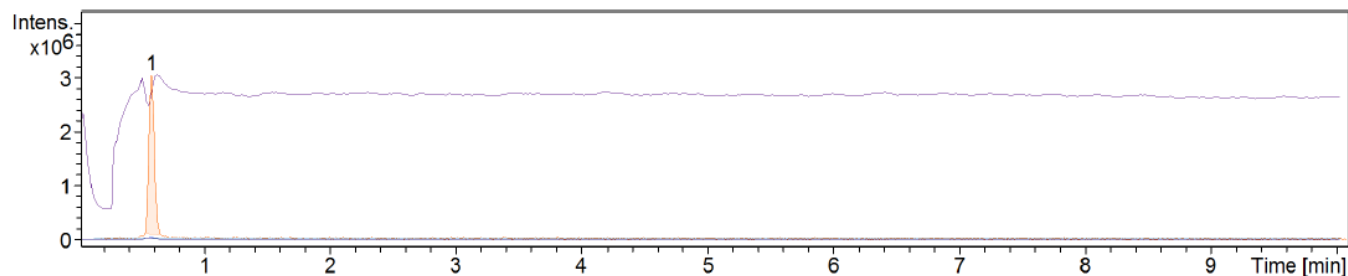
^1H NMR ($\text{DMSO-}d_6$) spectrum of **3ae**



^{13}C NMR (DMSO- d_6) spectrum of **3ae**

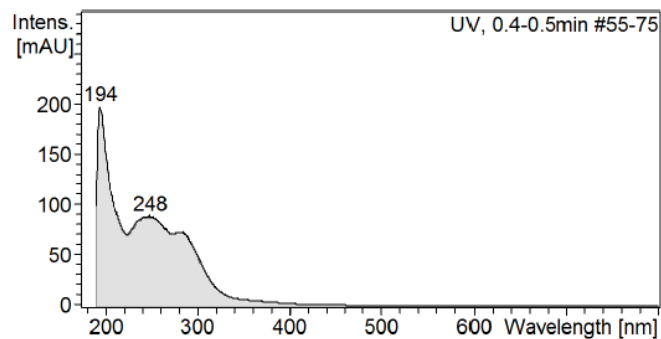


HRMS of **3ae**

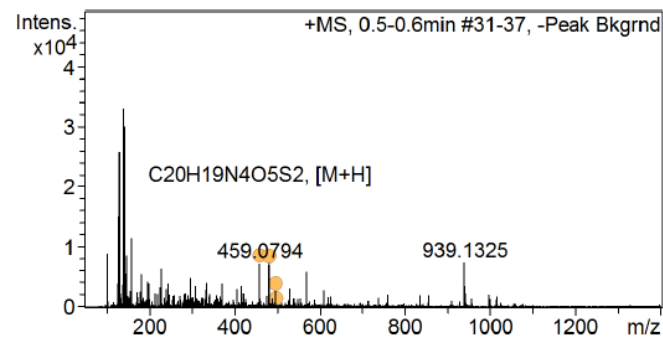


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	172609	Manual	56511	122.5	UV Chromatogram, 190-800 nm	139.1230	

Cmpd 1, 0.6 min

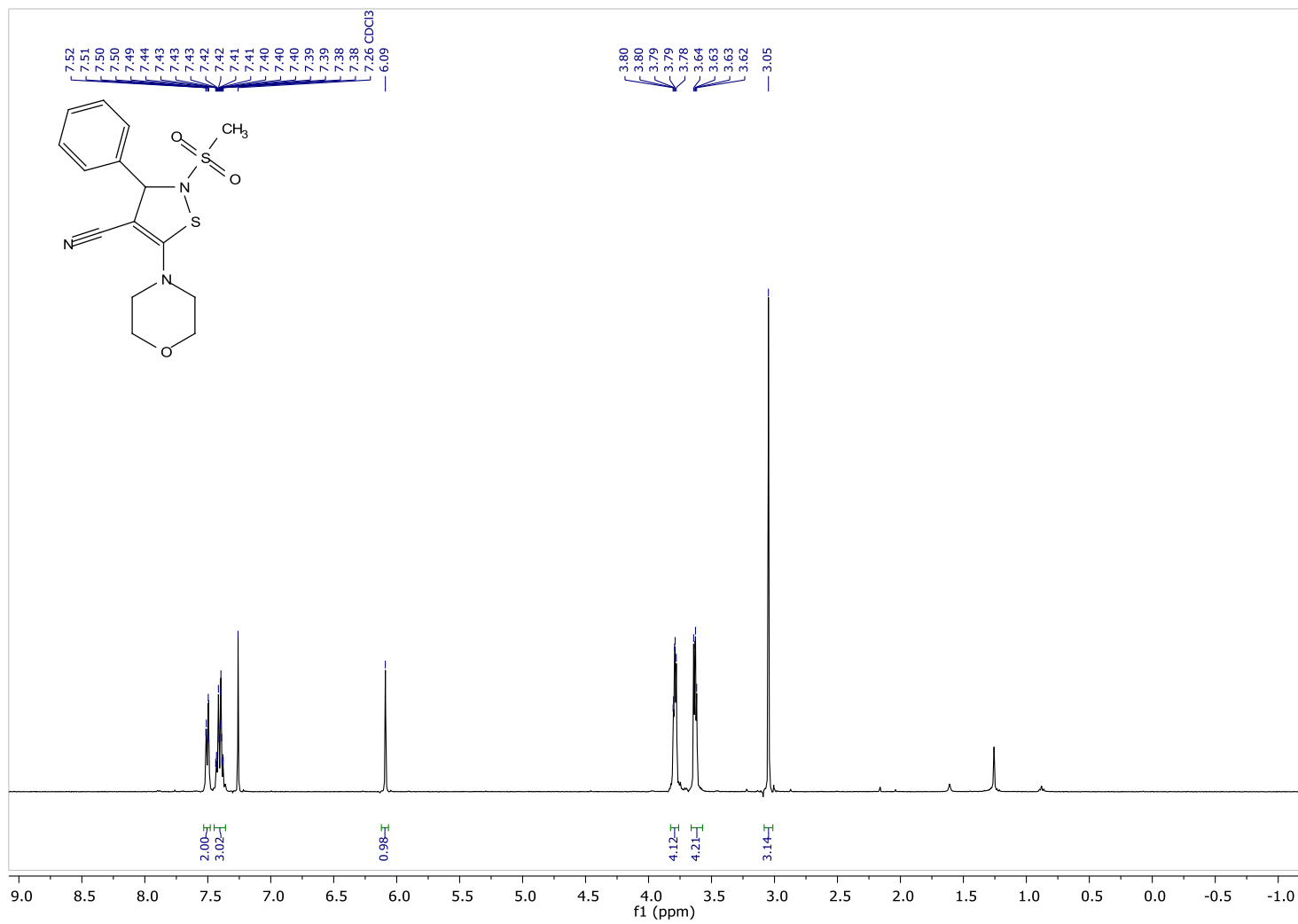


#	Wavelength	Intensity
0	194	196.8
1	248	88.1

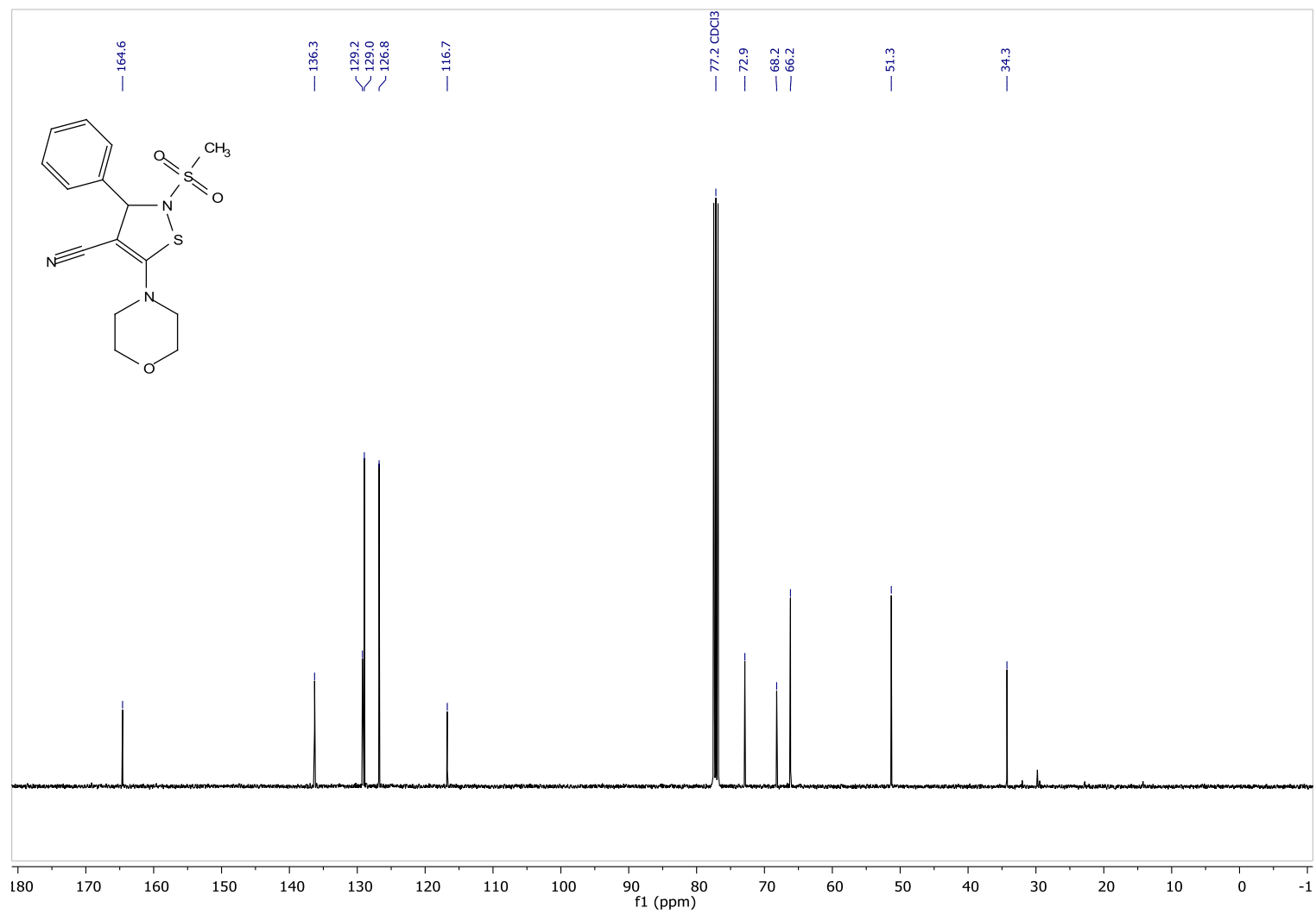


#	m/z	Res.	S/N	I	I %	FWHM
1	102.1275	17196	3022350.3	8918	27.1	0.0059
2	128.1434	18031	5108408.5	15073	45.8	0.0071
3	130.1591	18518	8719433.0	25728	78.1	0.0070
4	139.1230	19362	11164568.0	32943	100.0	0.0072
5	142.1590	19005	10164604.0	29992	91.0	0.0075
6	146.1536	17303	2929789.0	8645	26.2	0.0084
7	158.1537	17964	3890437.5	11479	34.8	0.0088
8	459.0794	20841	2510372.0	7407	22.5	0.0220
9	481.0612	20302	2467577.3	7281	22.1	0.0237
10	939.1325	22608	2525650.8	7452	22.6	0.0415

^1H NMR (CDCl_3) spectrum of **3af**

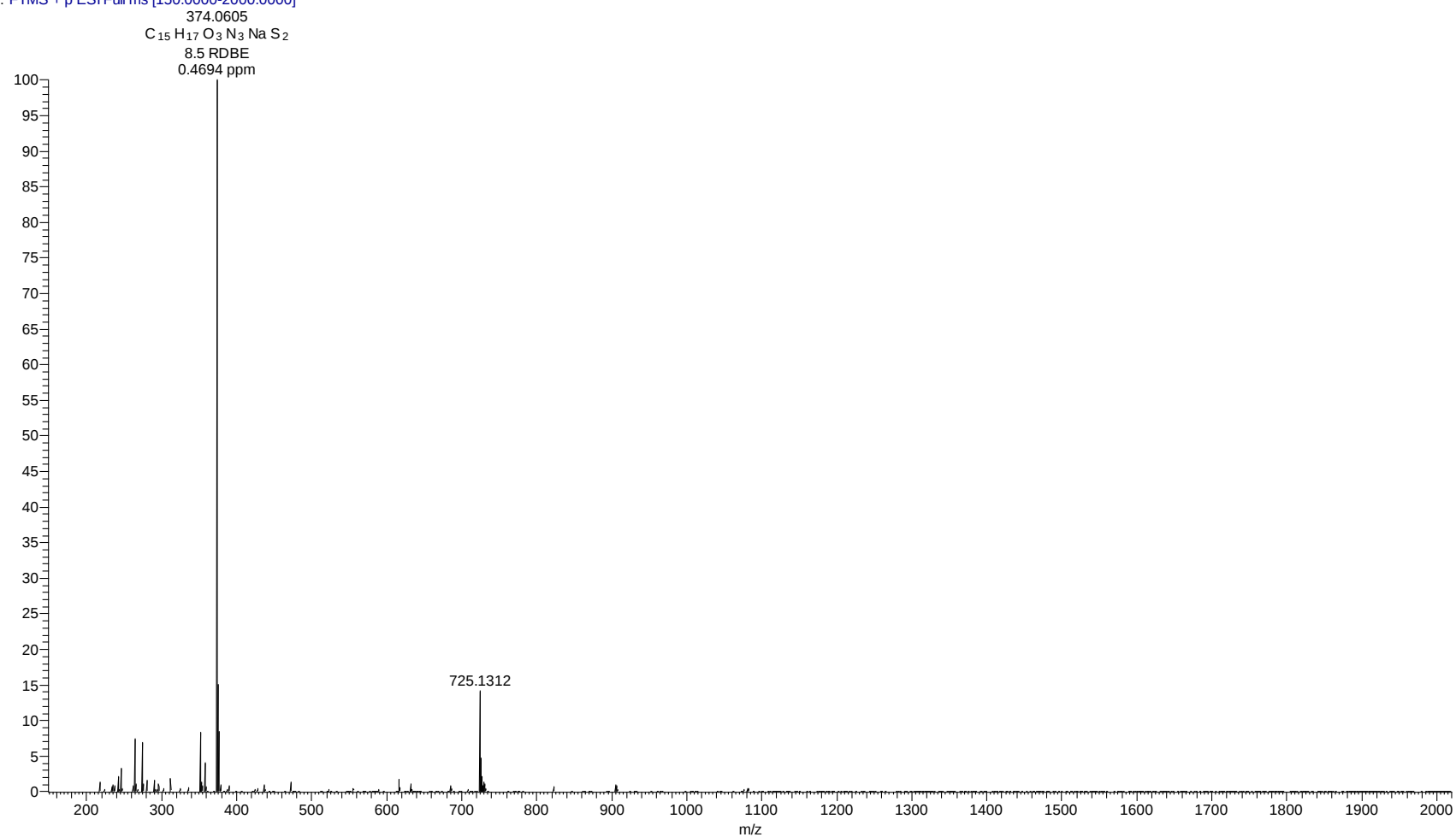


^{13}C NMR (CDCl_3) spectrum of **3af**

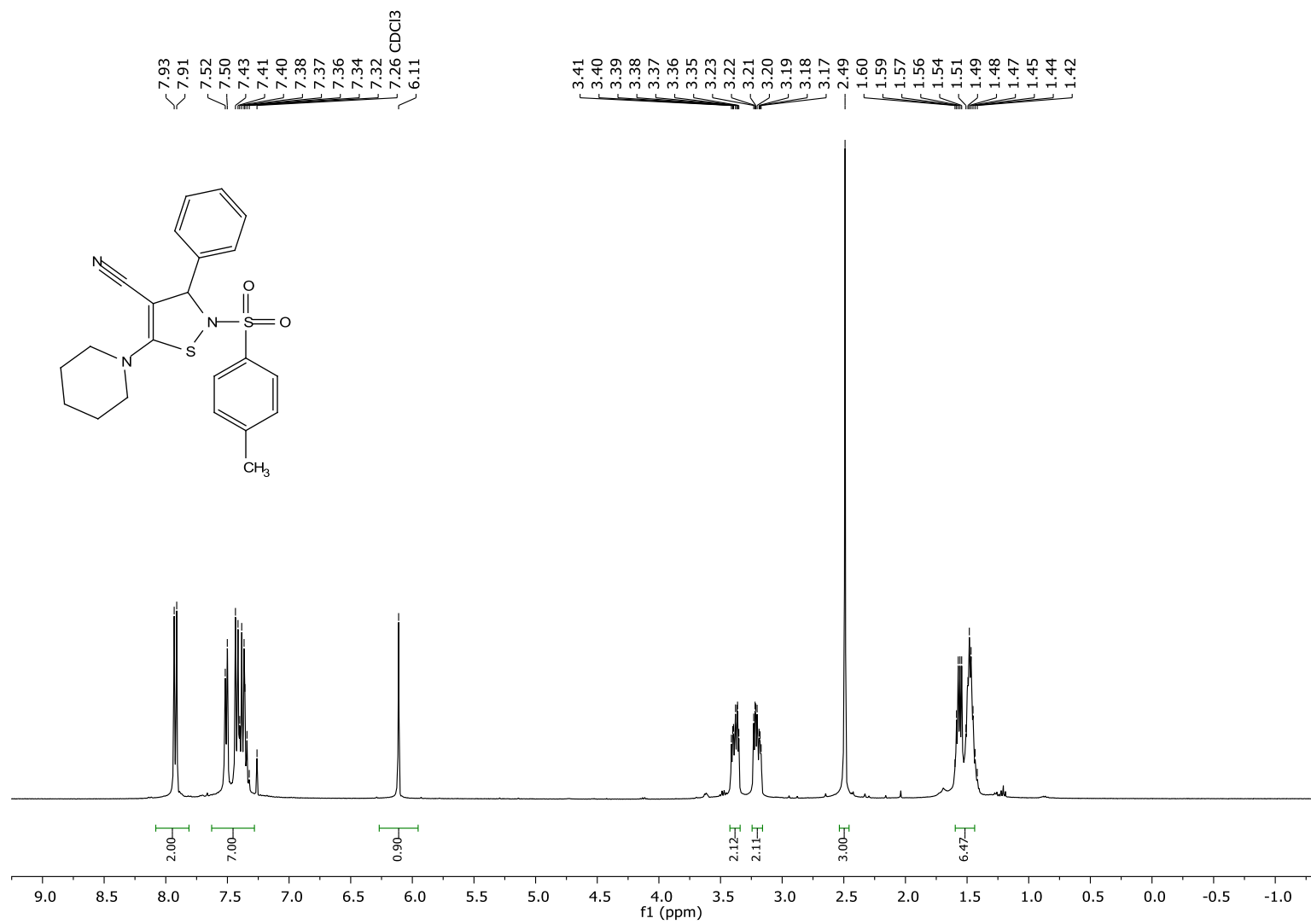


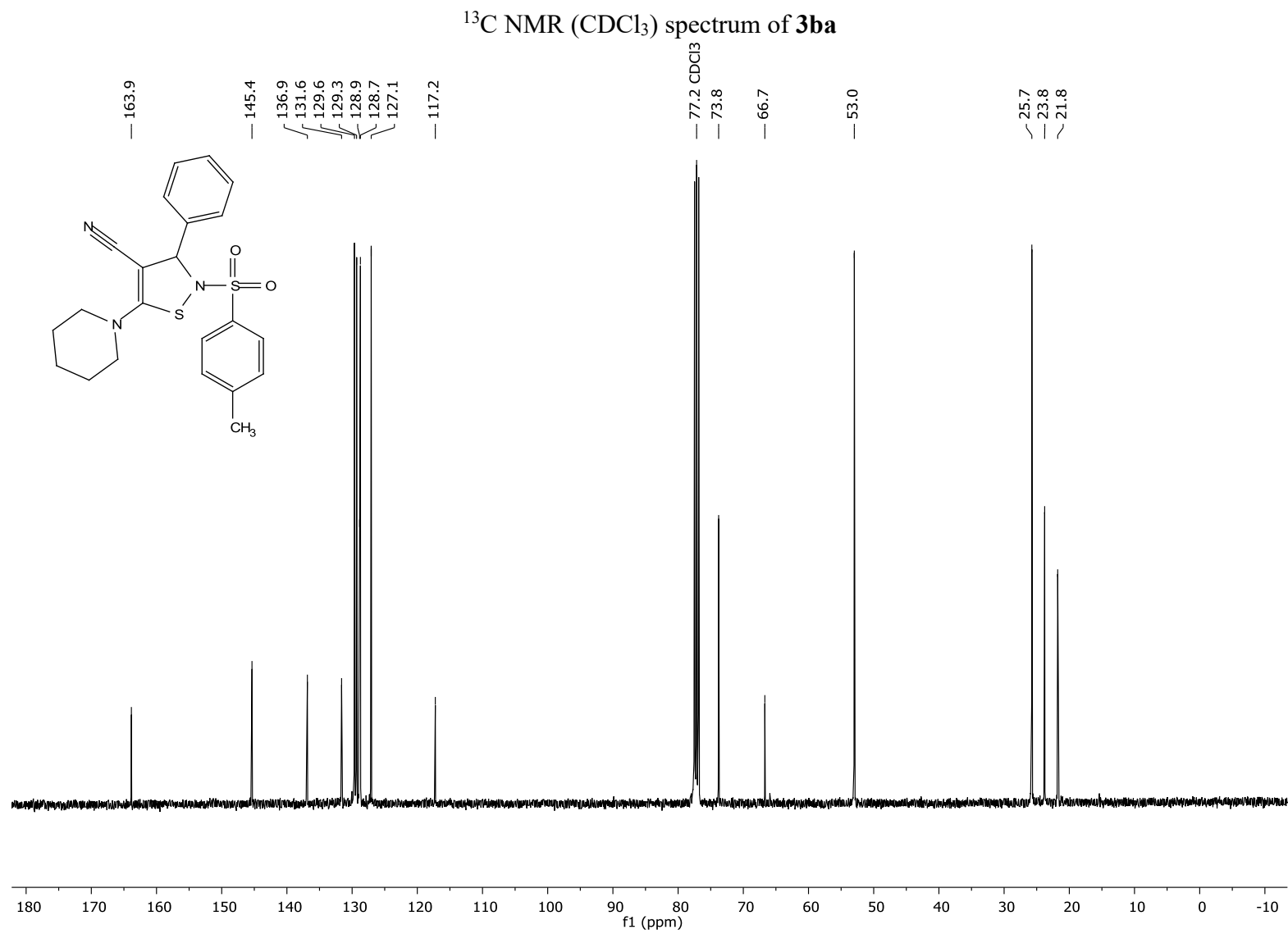
HRMS of 3af

O6A_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 7.54E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



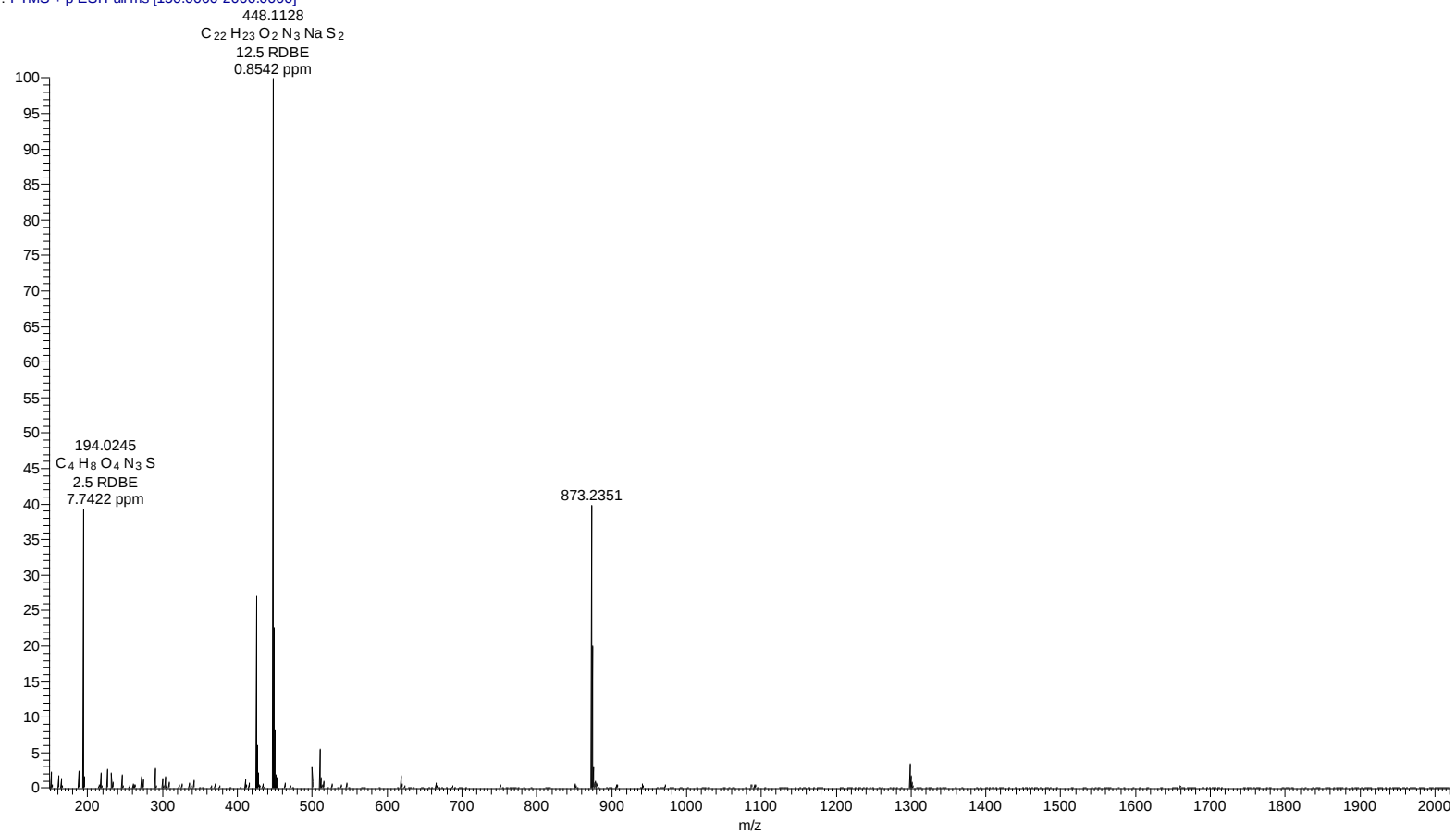
^1H NMR (CDCl_3) spectrum of **3ba**

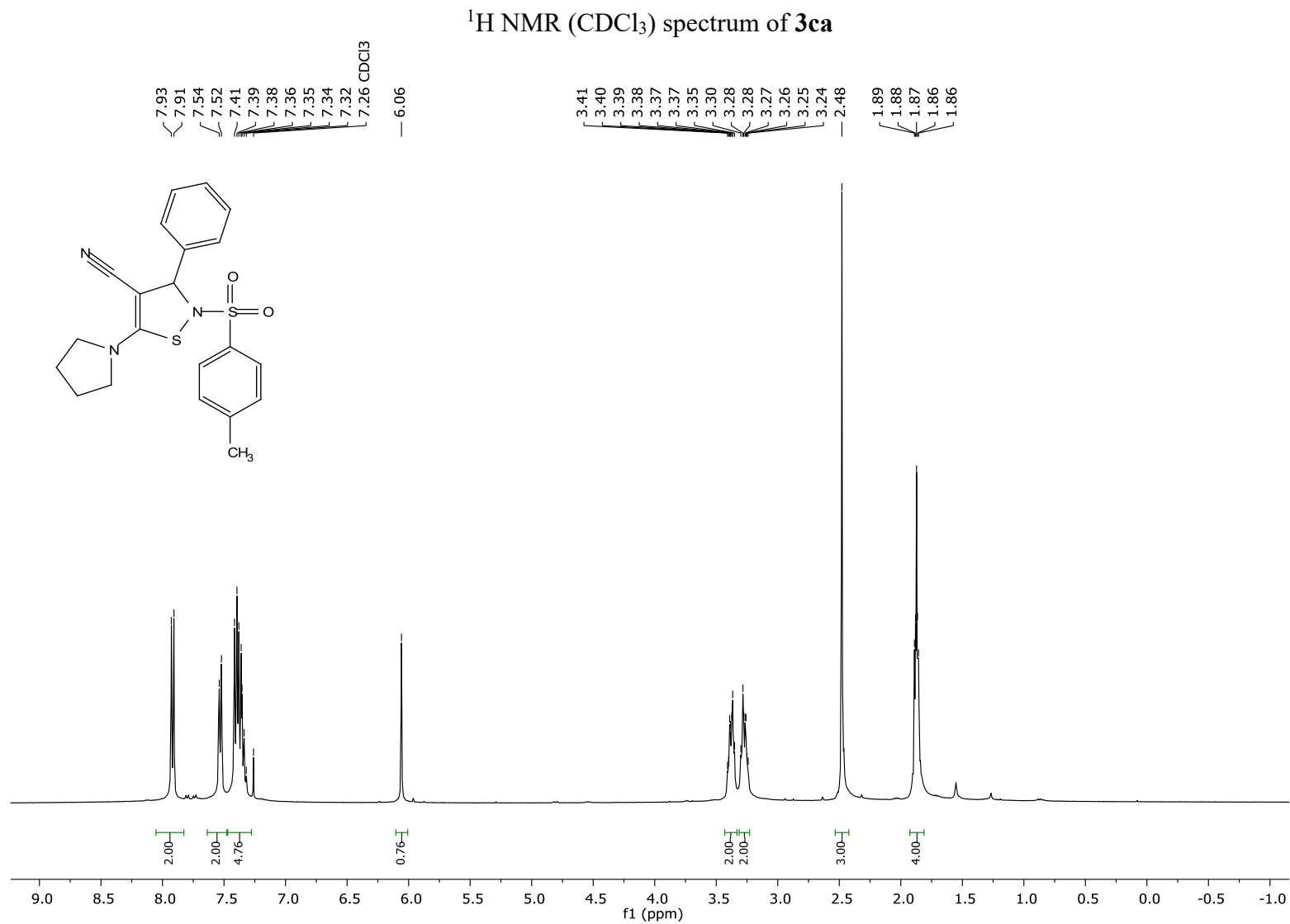




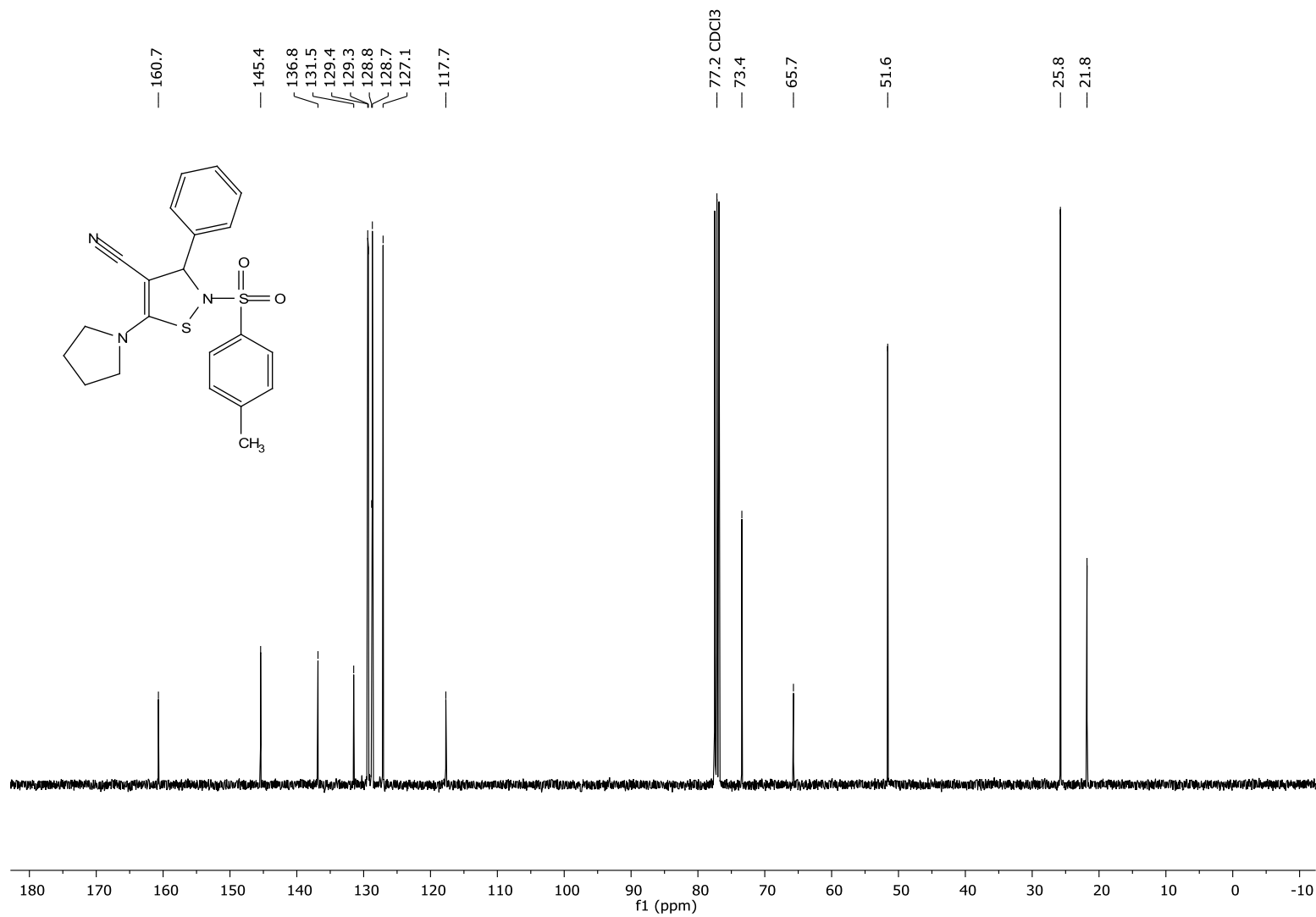
HRMS of **3ba**

VF-182_1_Pos_240213125547 #29-53 RT: 0.25-0.45 AV: 25 SB: 8 0.06-0.11, 0.83 NL: 1.22E8
T: FTMS +p ESI Full ms [150.0000-2000.0000]



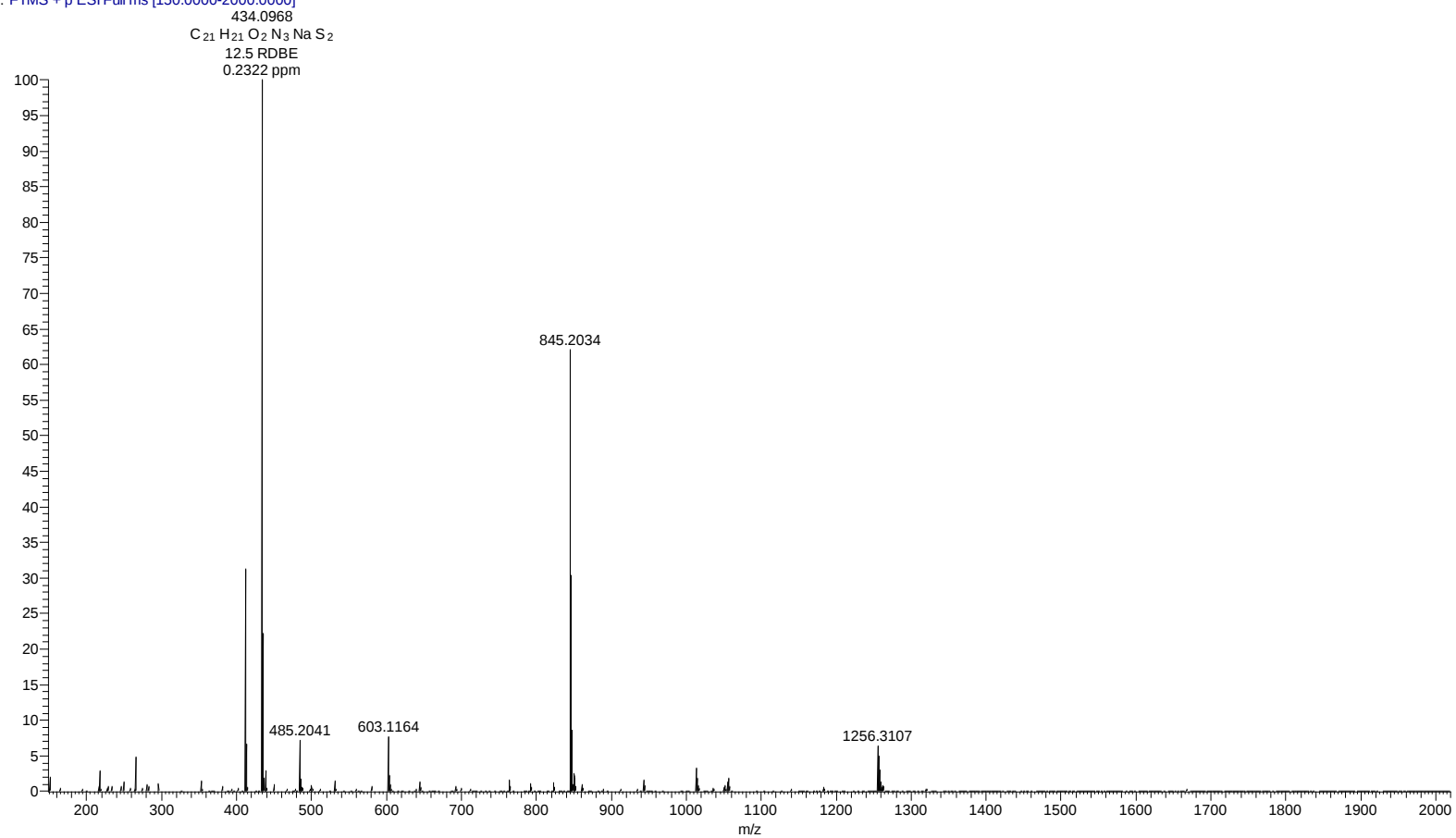


^{13}C NMR (CDCl_3) spectrum of **3ca**

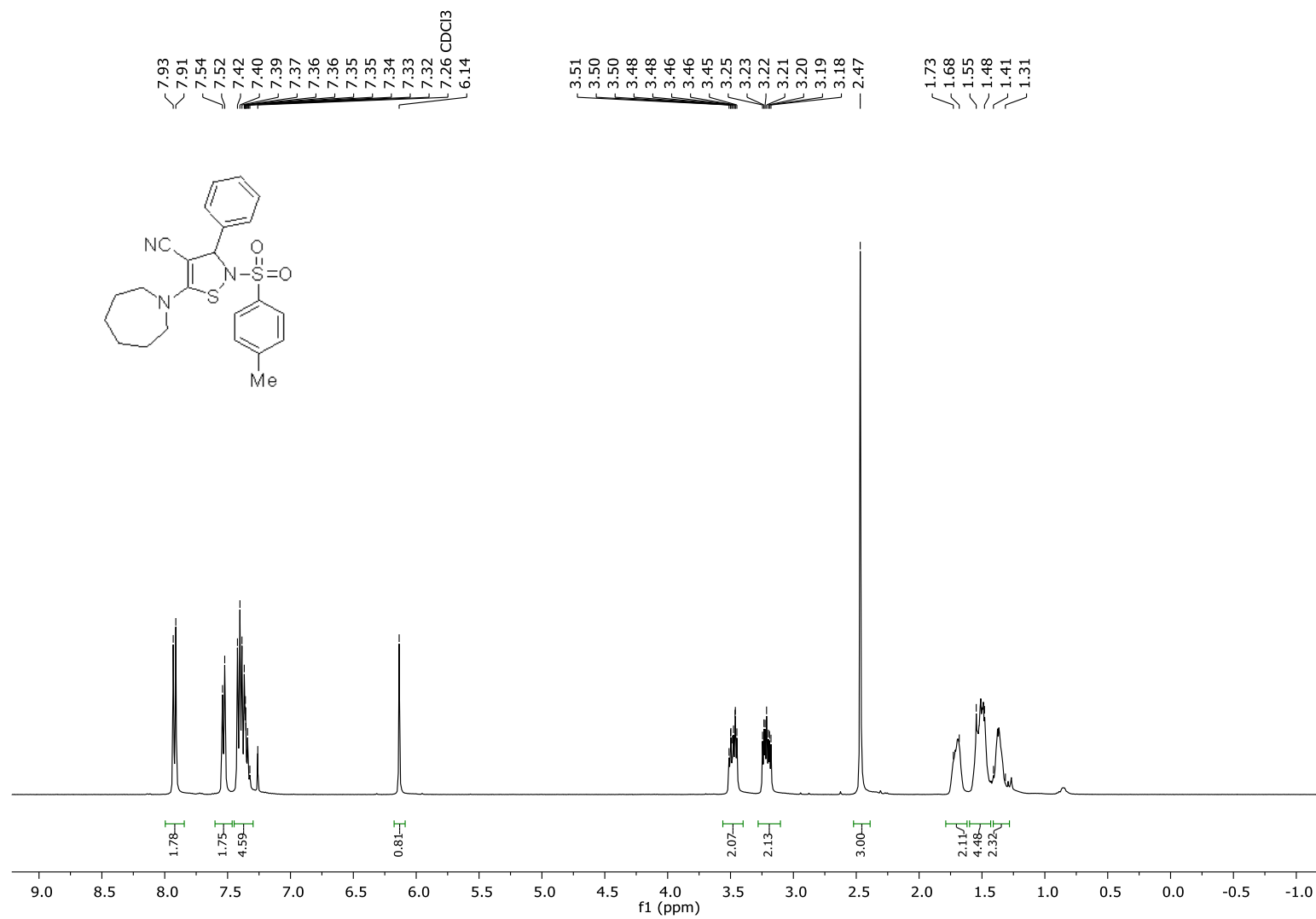


HRMS of 3ca

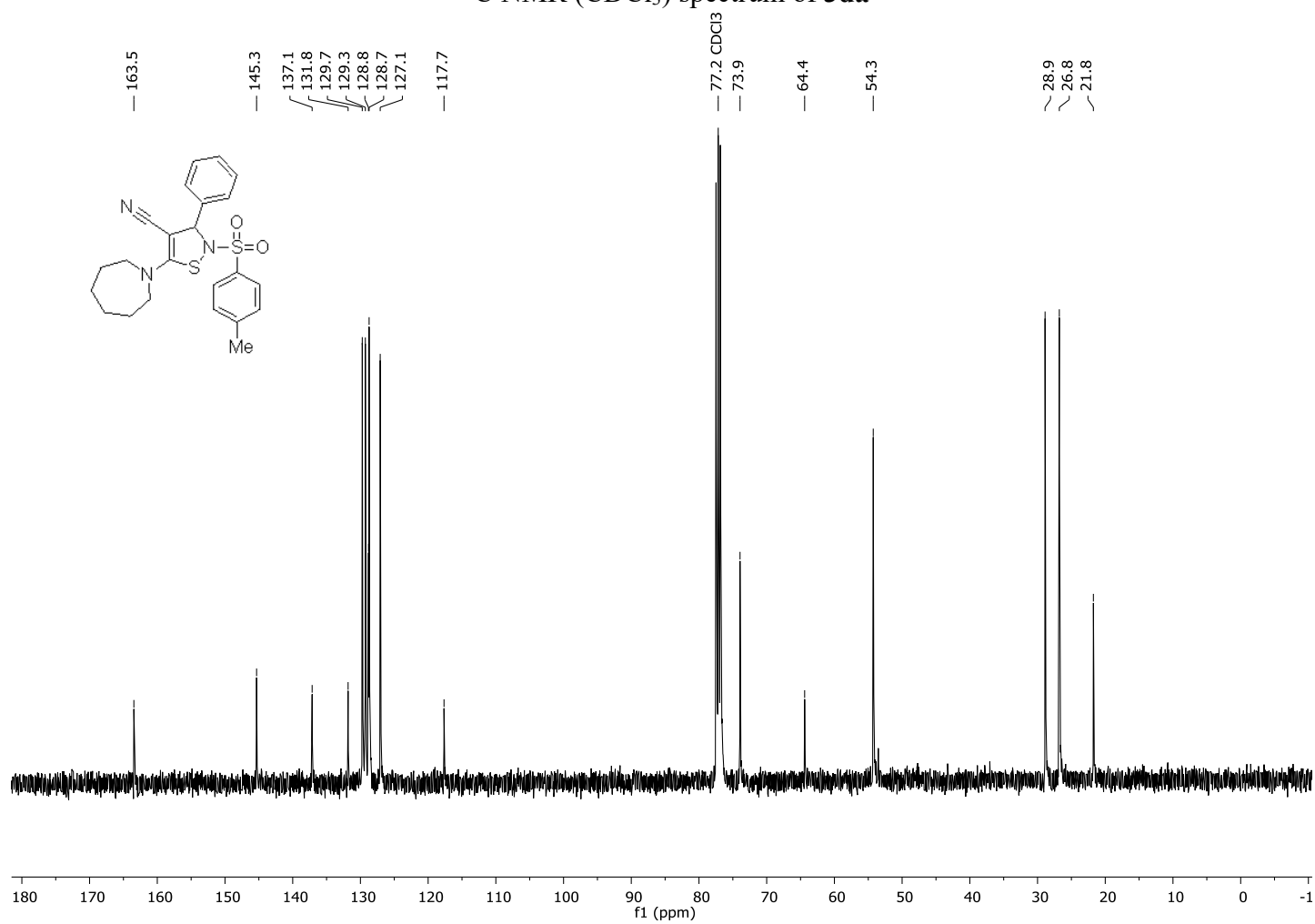
VF-135_Pos_240213100538 #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 5.06E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



^1H NMR (CDCl_3) spectrum of **3da**

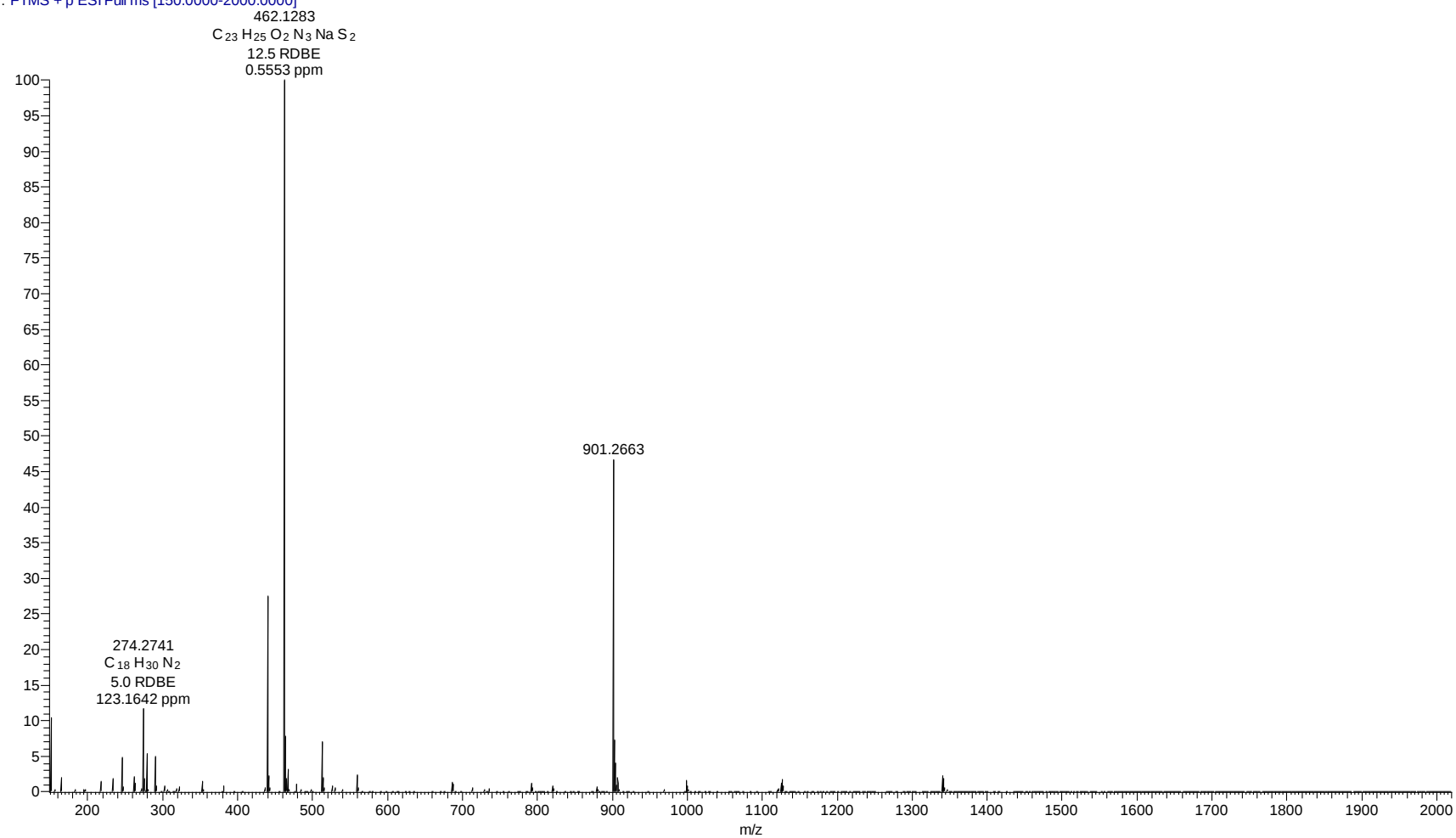


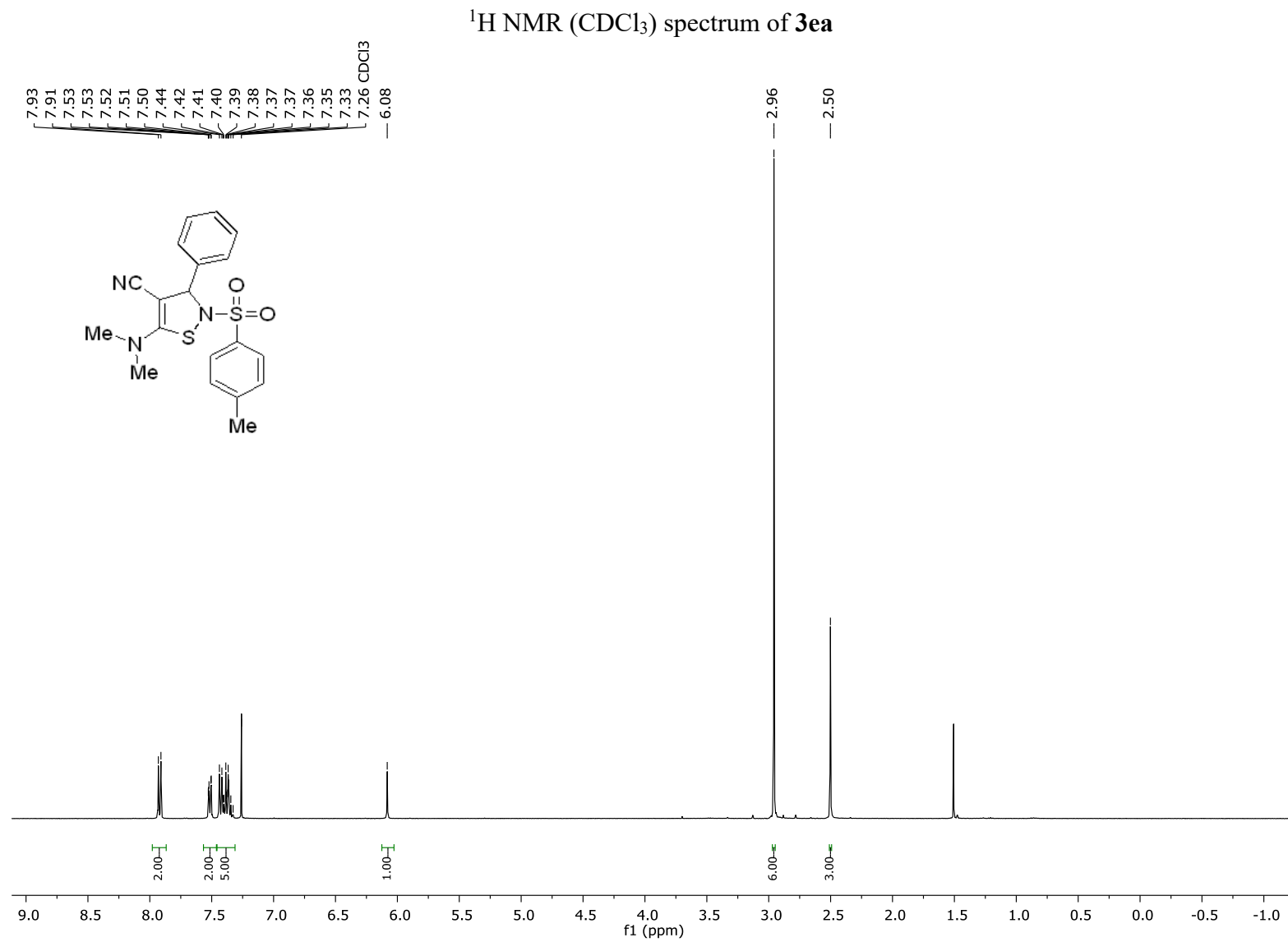
¹³C NMR (CDCl₃) spectrum of **3da**



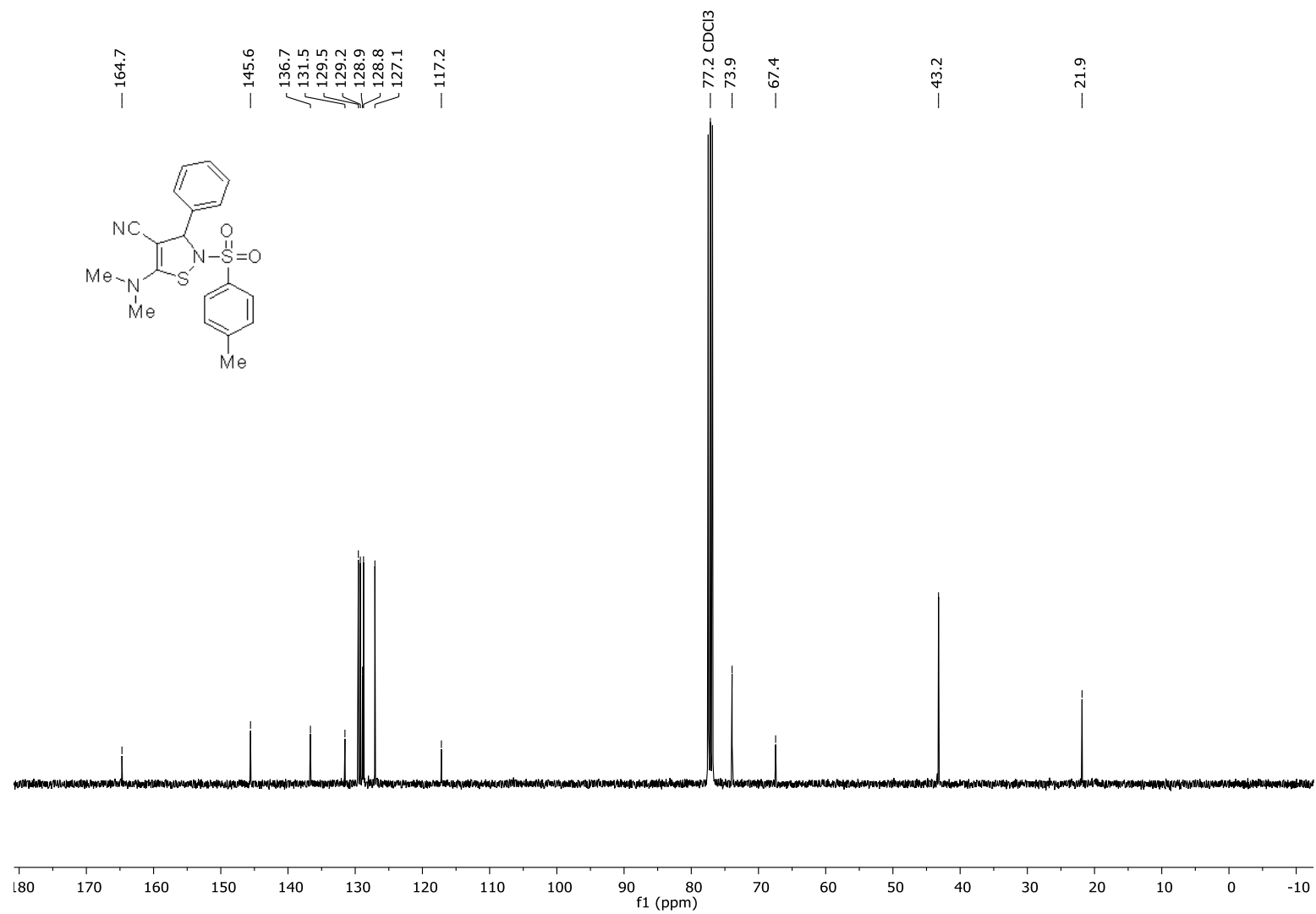
HRMS of **3da**

VF-141_Pos_240213101357 #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 4.85E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



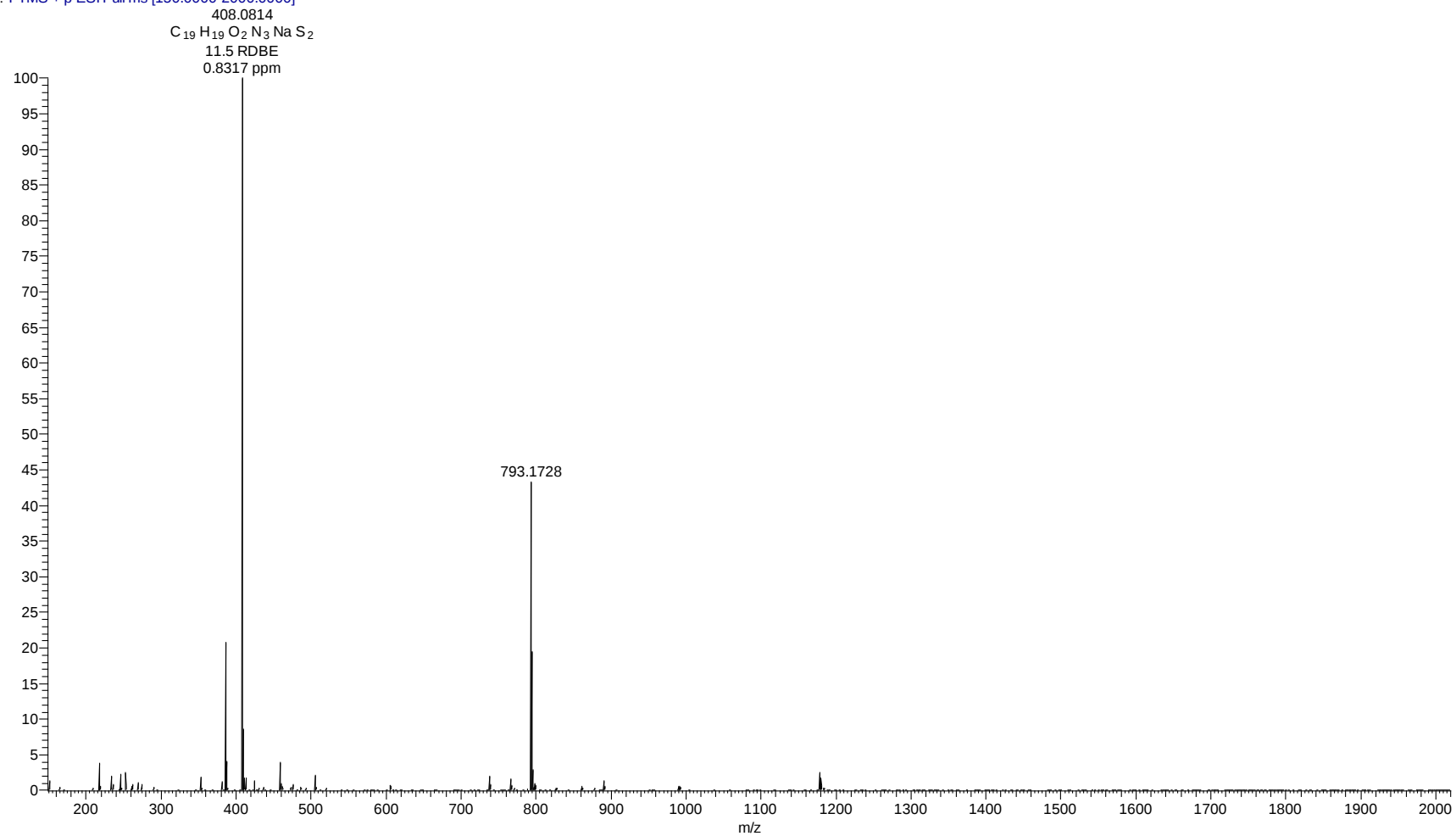


^{13}C NMR (CDCl_3) spectrum of **3ea**

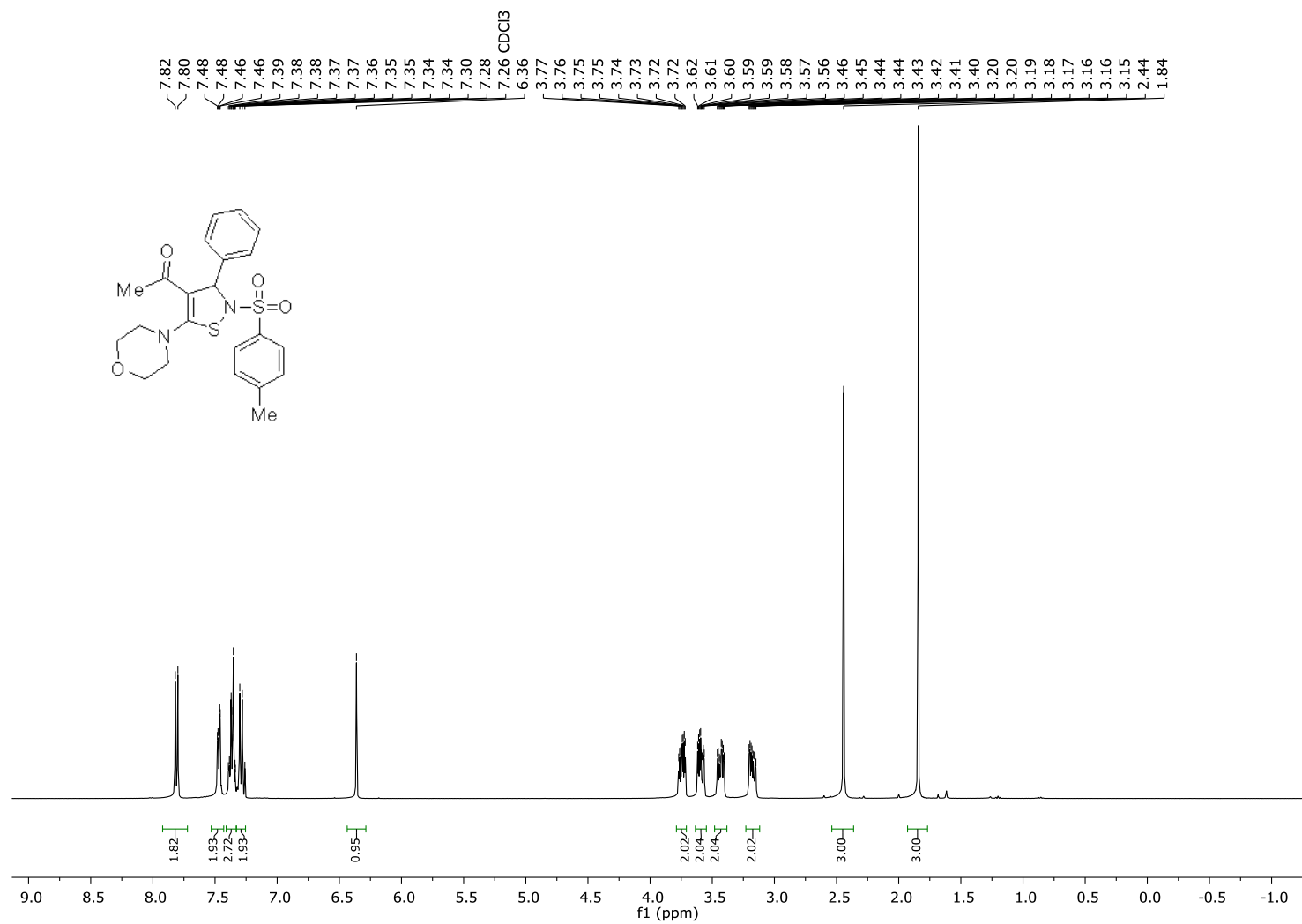


HRMS of **3ea**

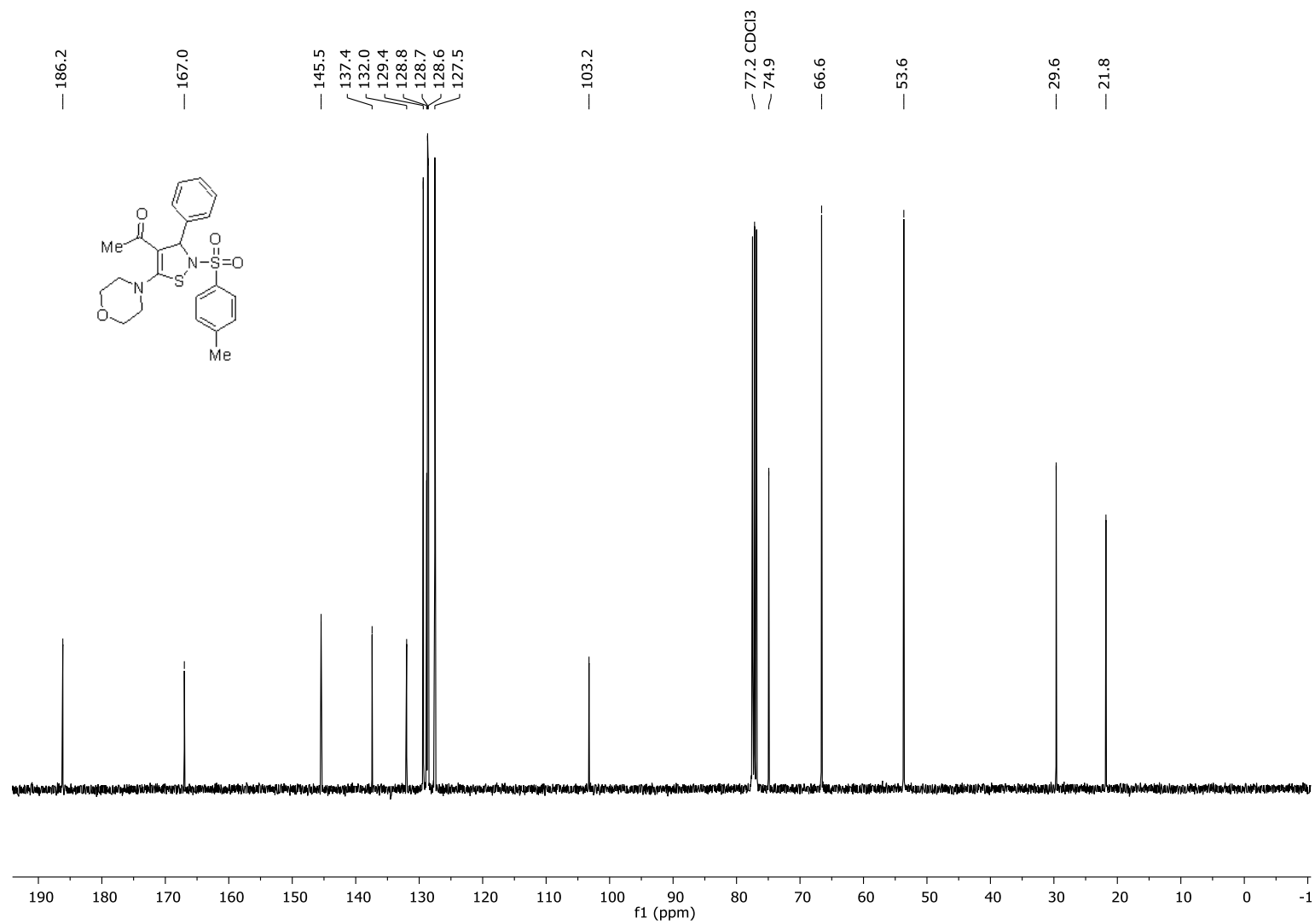
VF-169_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 1.24E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (CDCl₃) spectrum of **3fa**

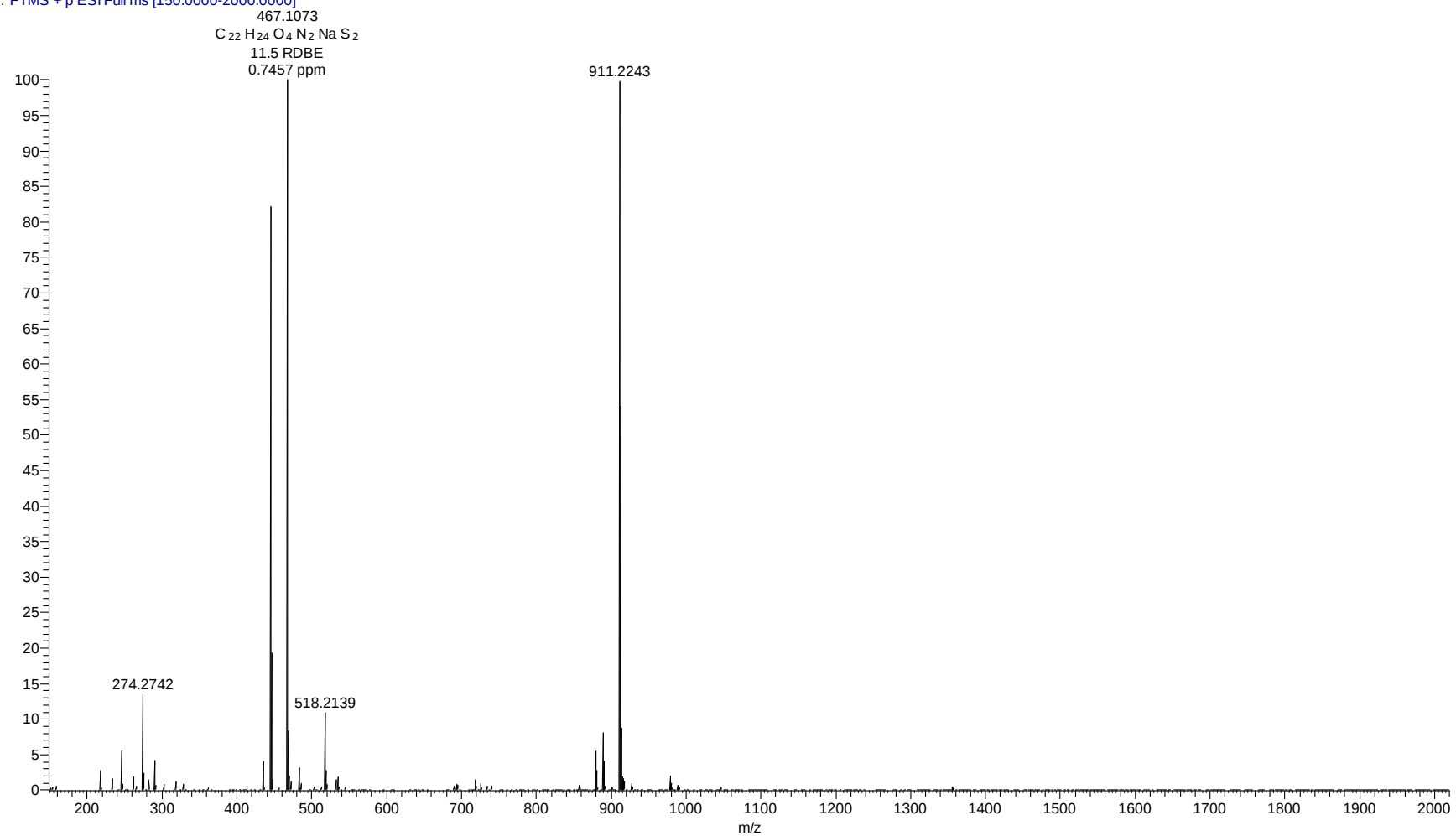


^{13}C NMR (CDCl_3) spectrum of **3fa**

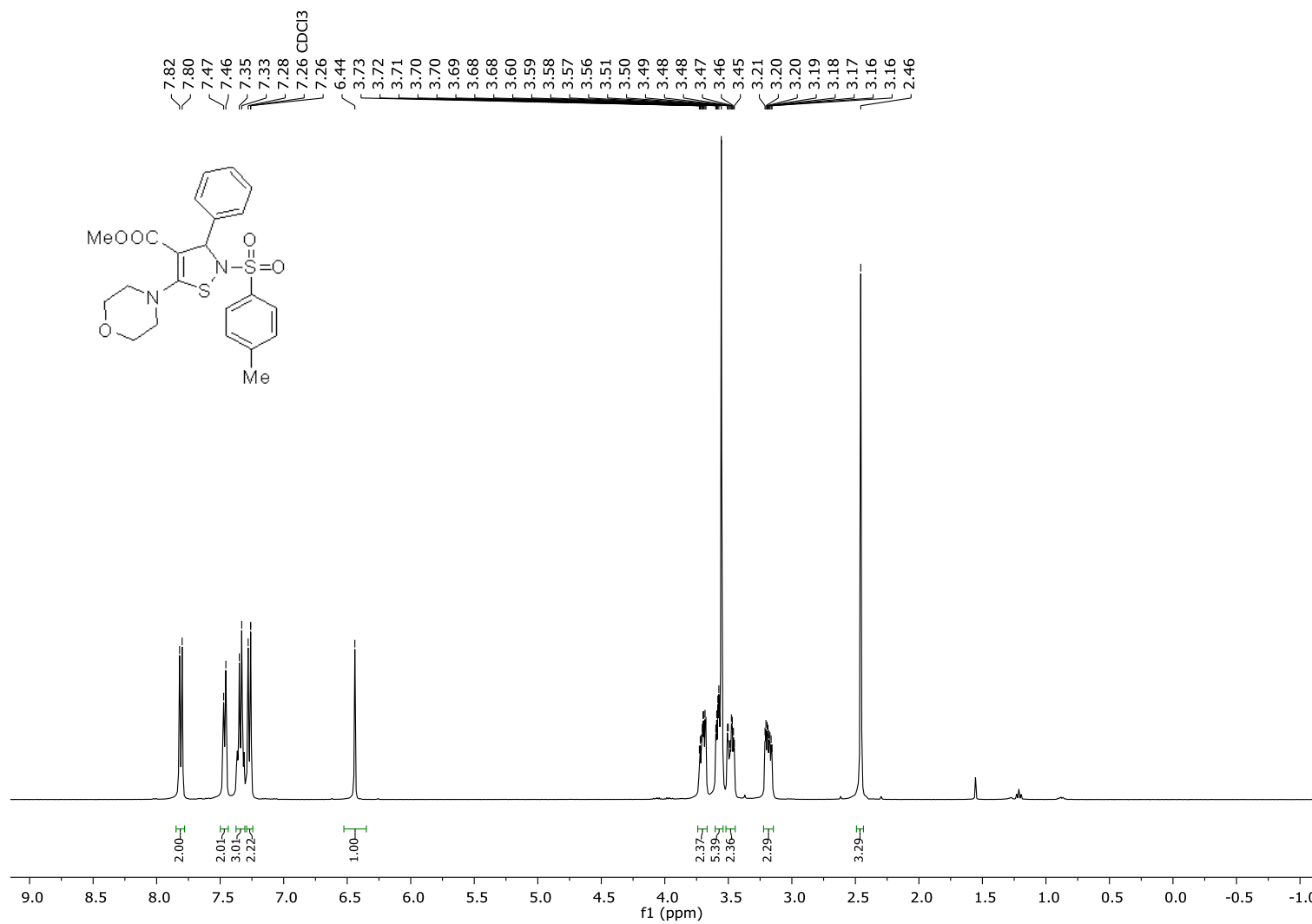


HRMS of 3fa

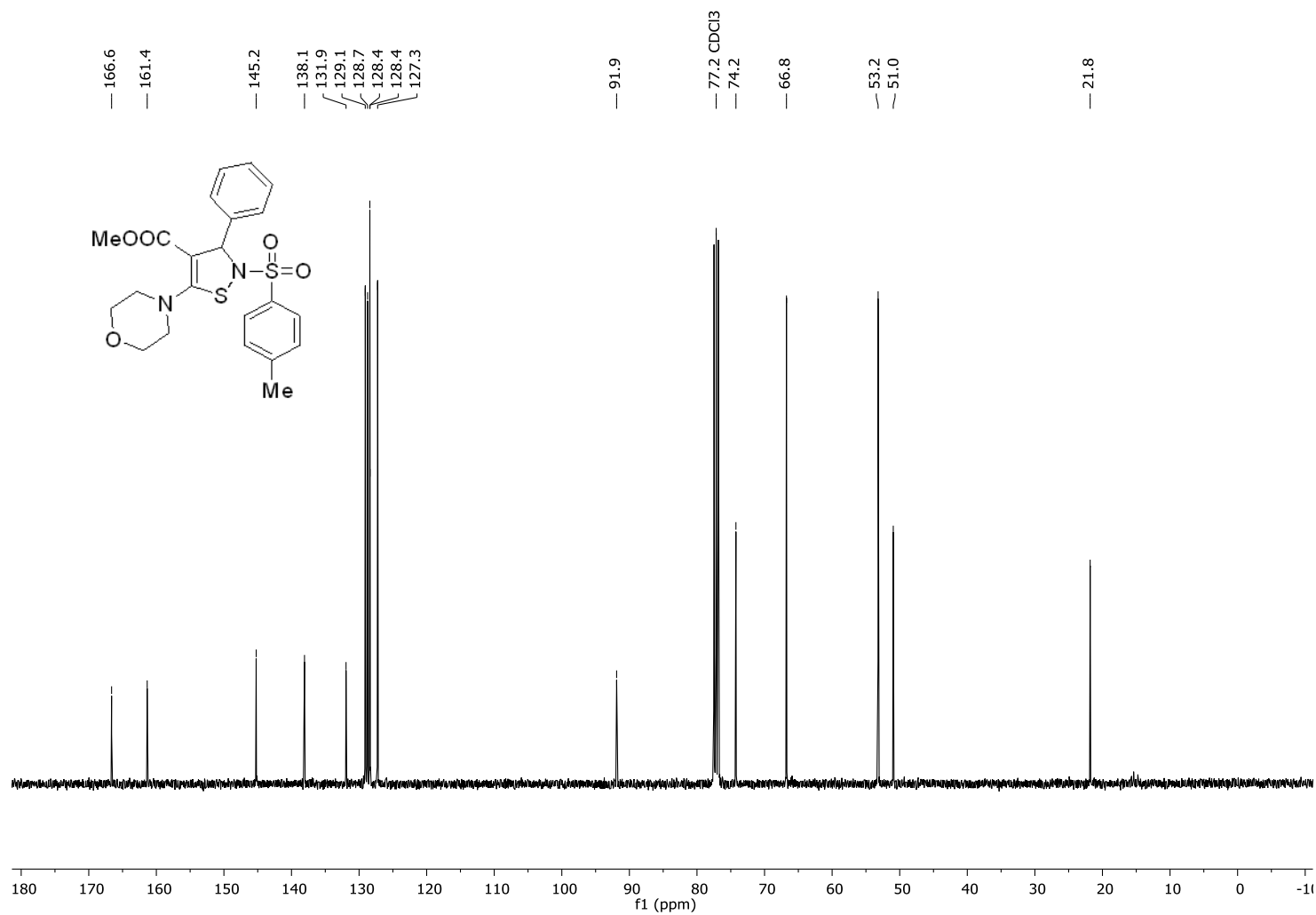
VF-225_Pos_240213124810 #29-53 RT: 0.25-0.45 AV: 25 SB: 7 0.06-0.11 , 0.72 NL: 7.16E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



^1H NMR (CDCl_3) spectrum of **3ga**

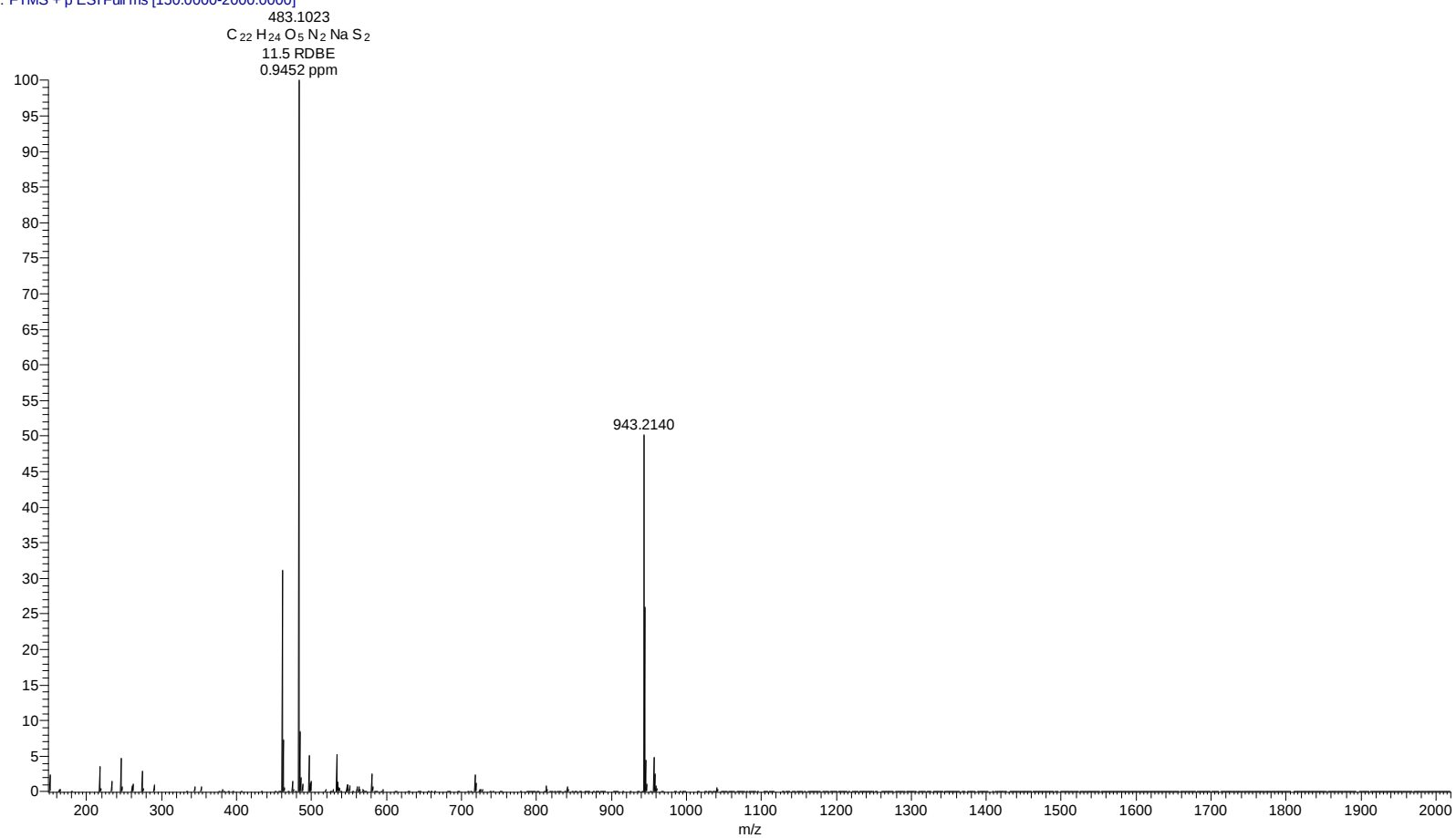


^{13}C NMR (CDCl_3) spectrum of **3ga**

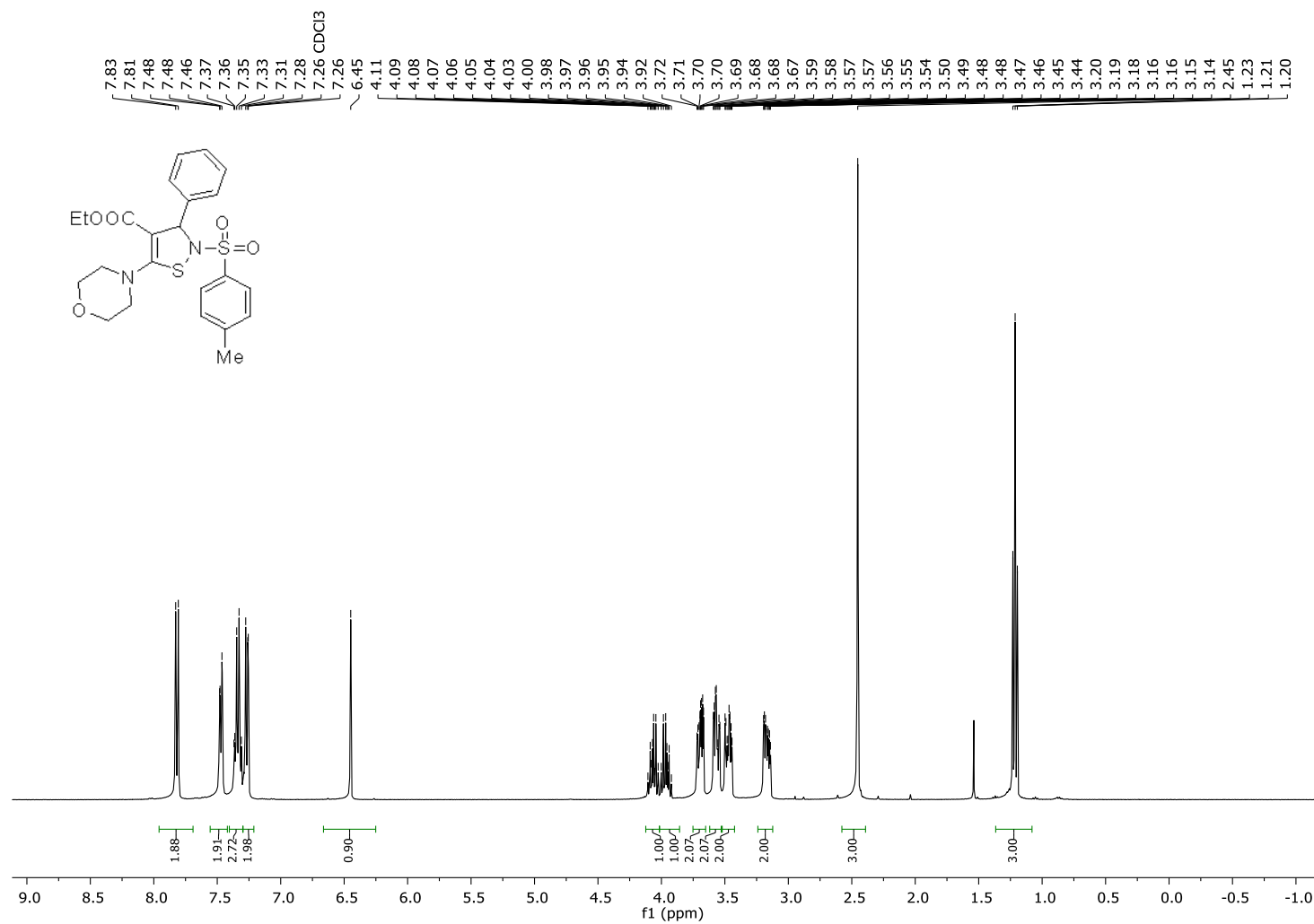


HRMS of **3ga**

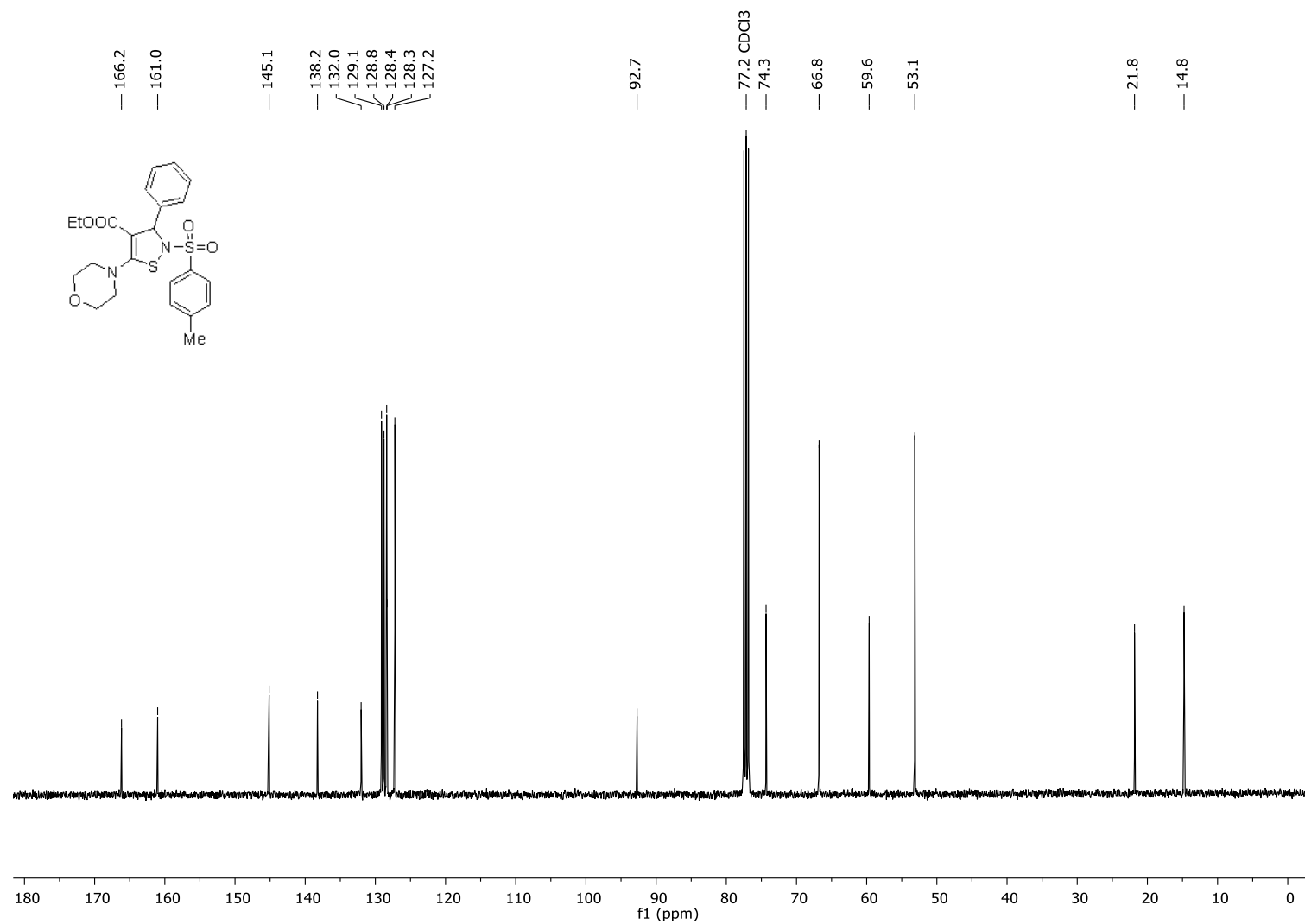
VF-226_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 1.52E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (CDCl₃) spectrum of **3ha**

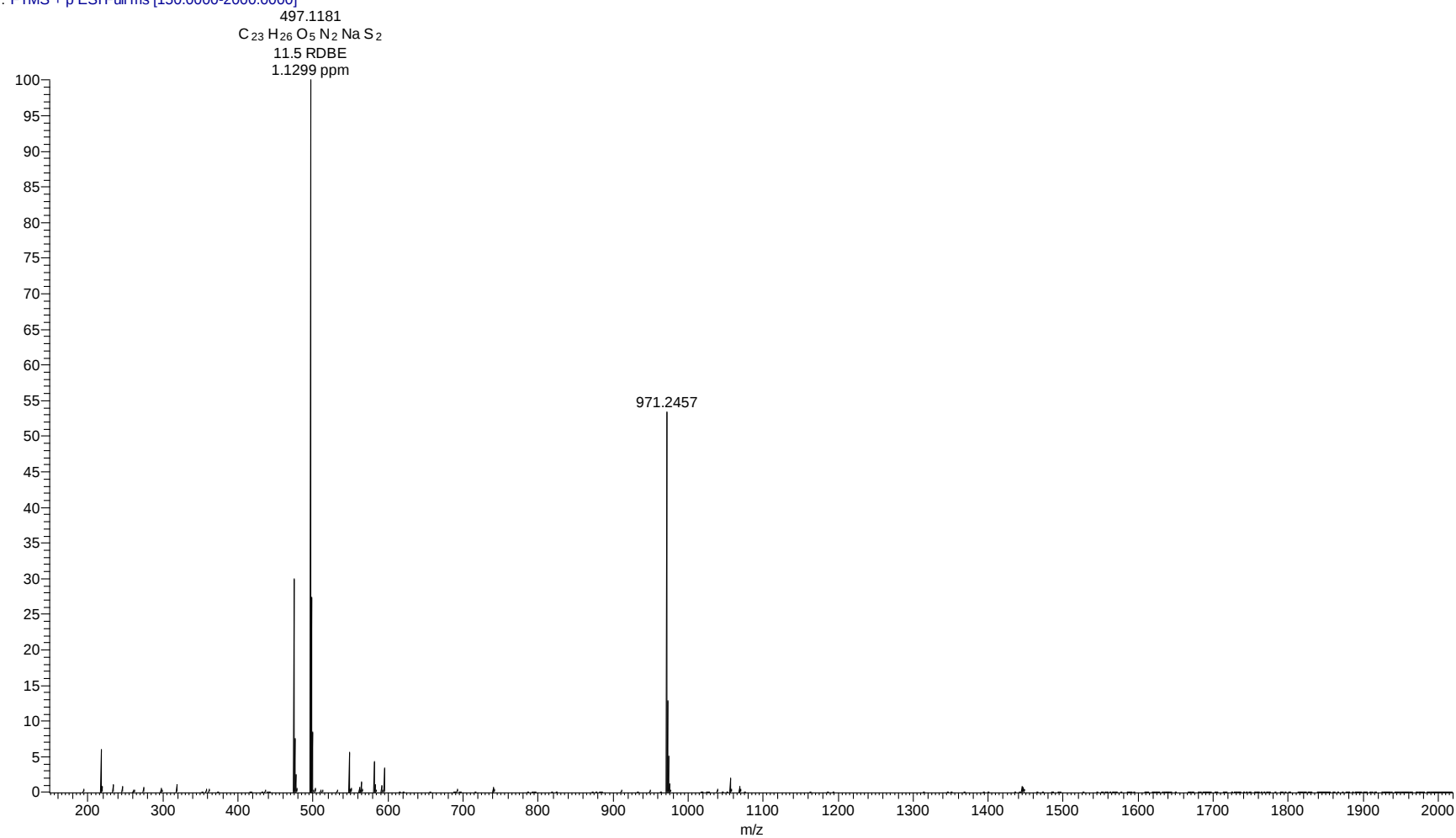


^{13}C NMR (CDCl_3) spectrum of **3ha**

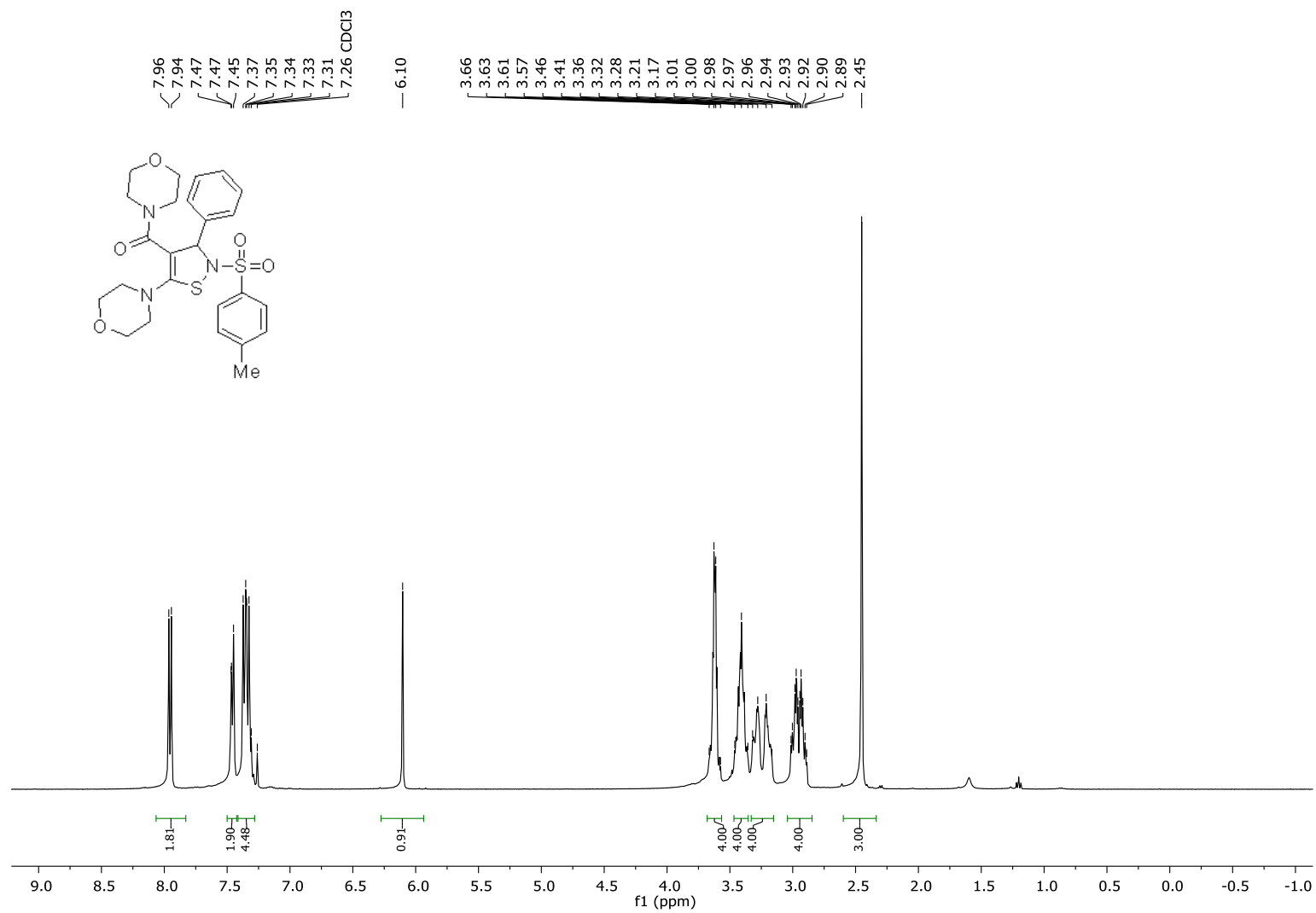


HRMS of **3ha**

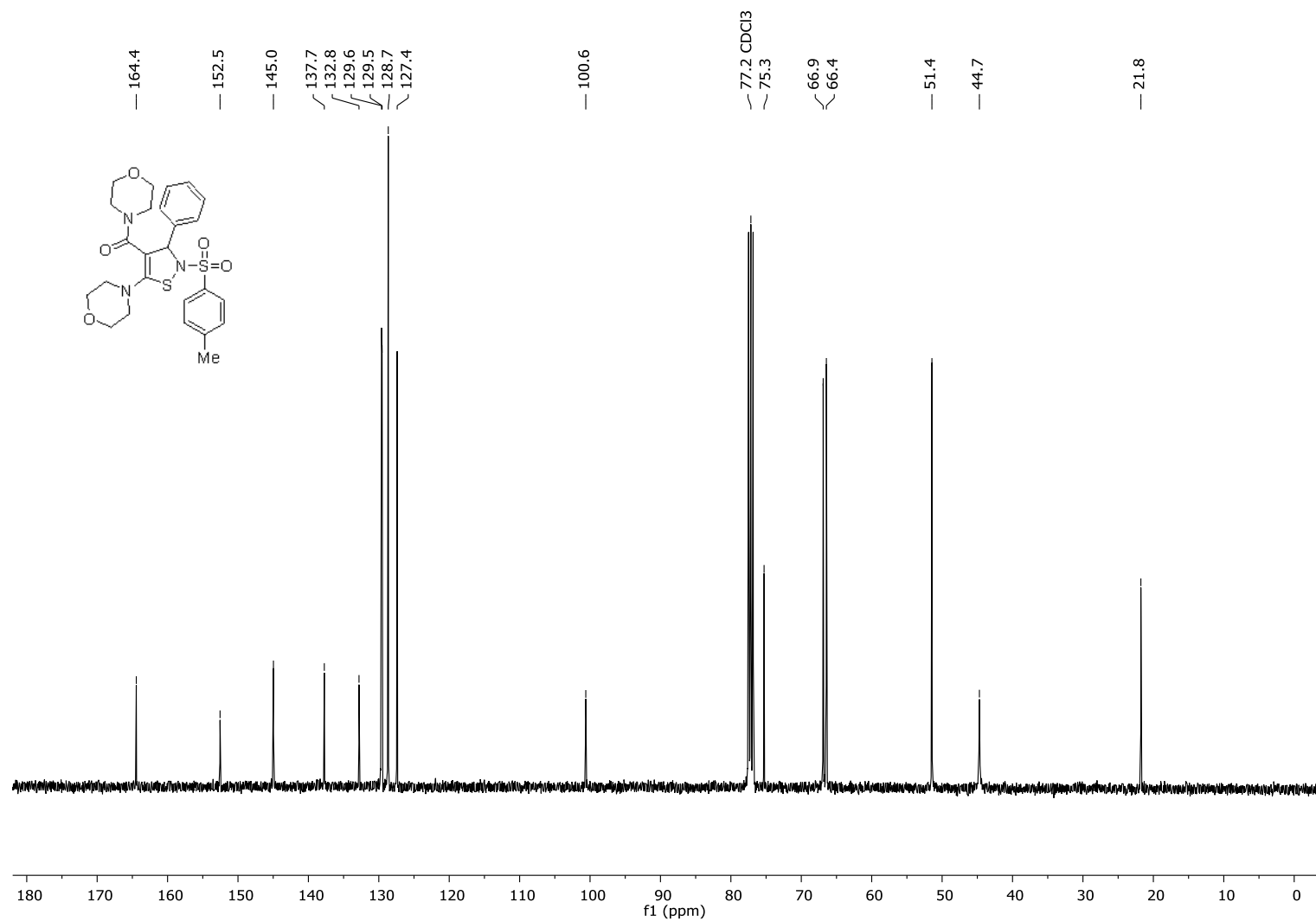
VF-207_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 2.50E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (CDCl₃) spectrum of **3ia**

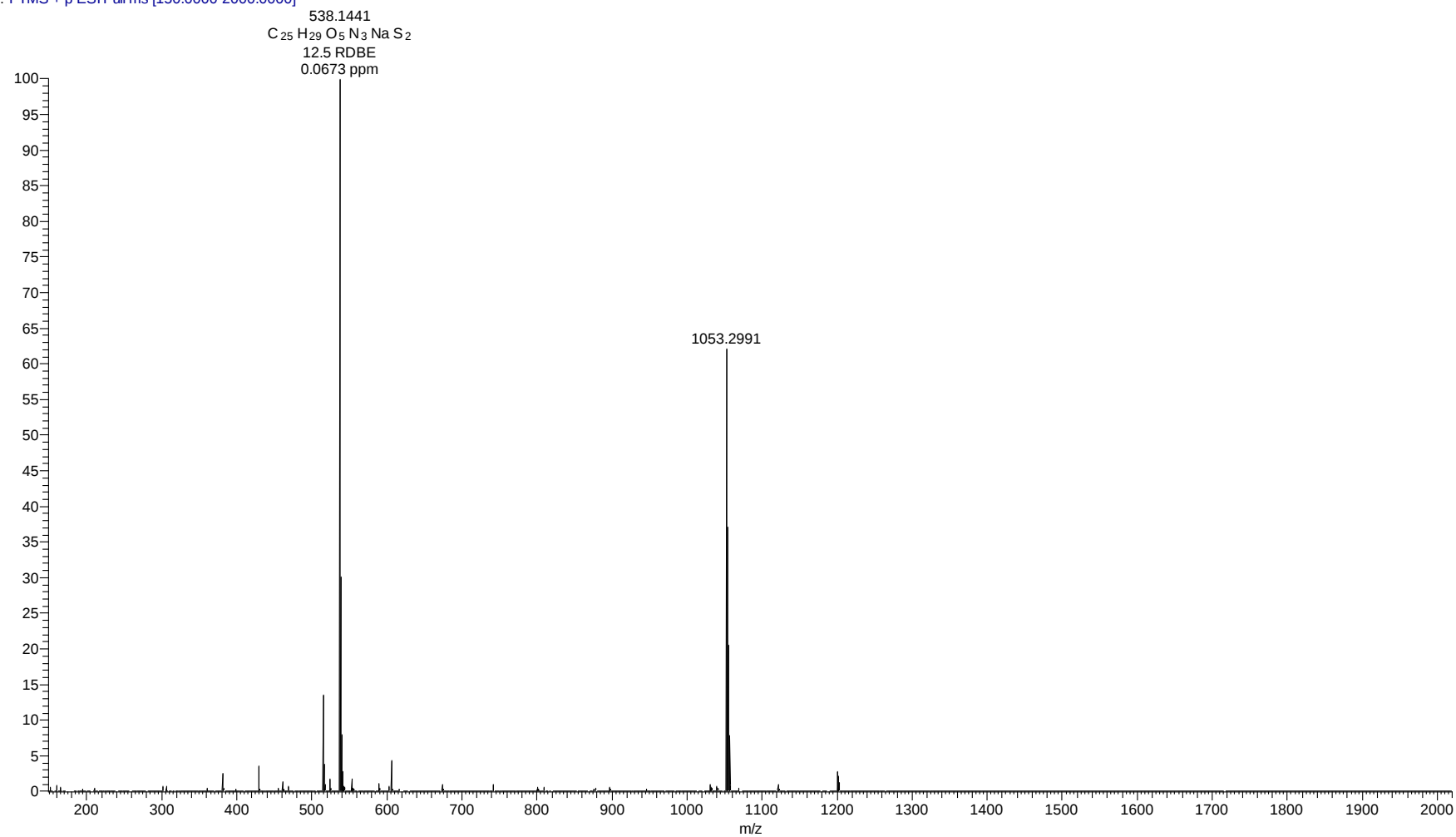


¹³C NMR (CDCl₃) spectrum of **3ia**

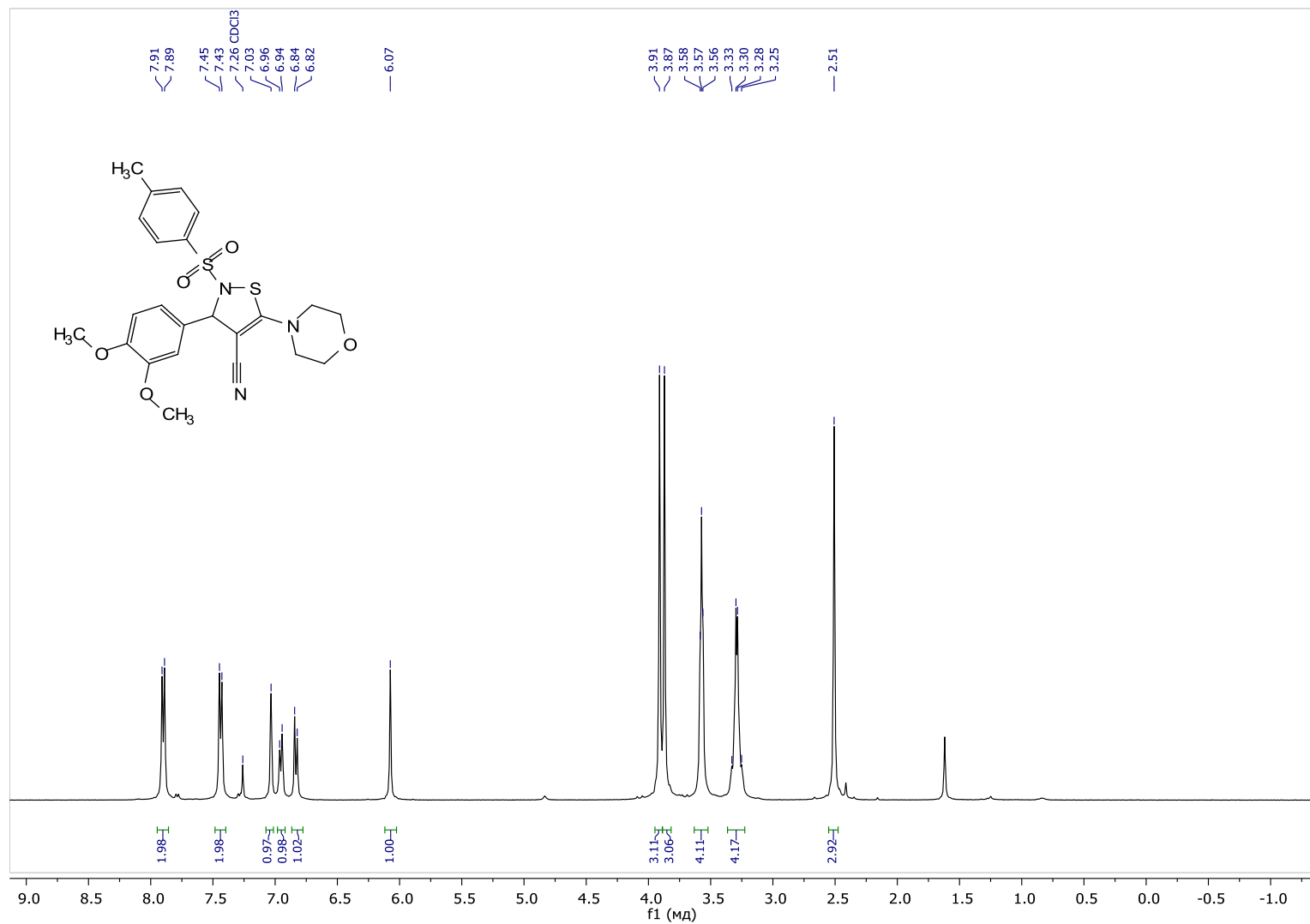


HRMS of **3ia**

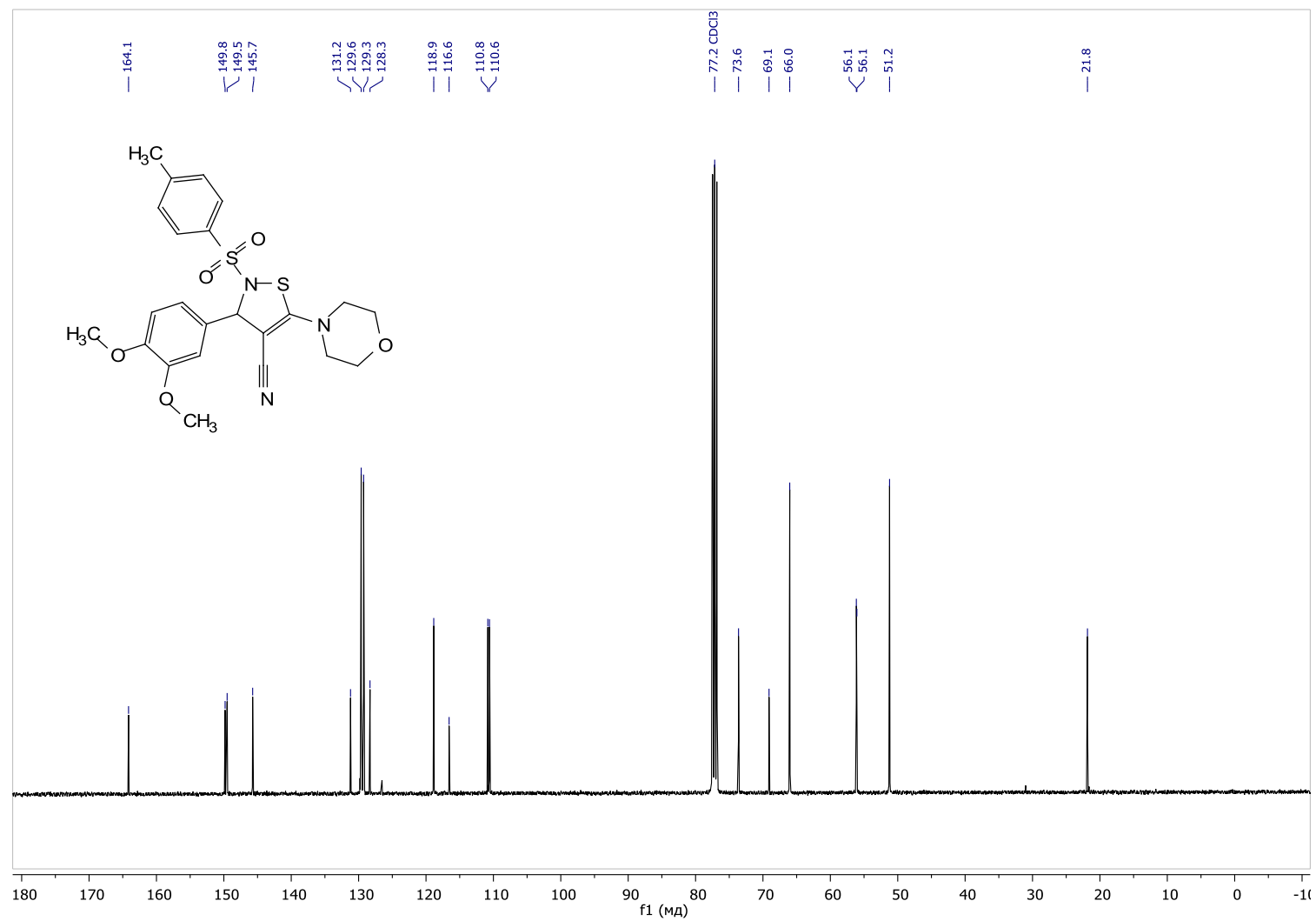
PSG76 #68 RT: 0.30 AV: 1 SB: 54 0.07-0.15 , 0.83-0.97 NL: 1.17E8
T: FTMS + p ESI Full ms [150.0000-2000.0000]



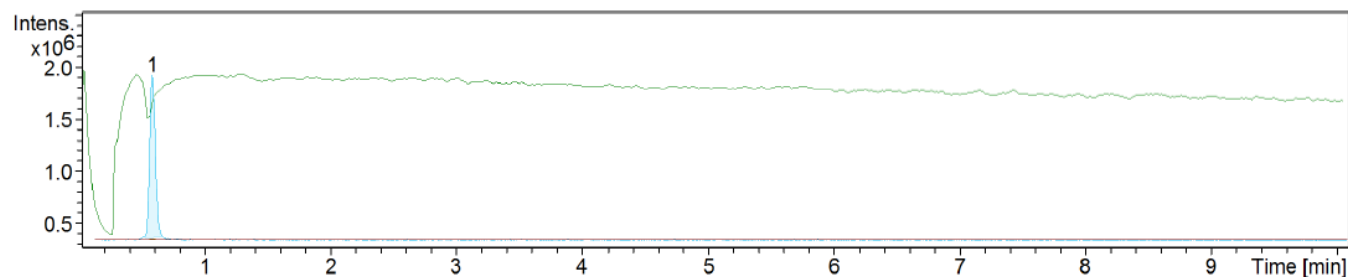
¹H NMR (CDCl₃) spectrum of **3ja**



^{13}C NMR (CDCl_3) spectrum of **3ja**

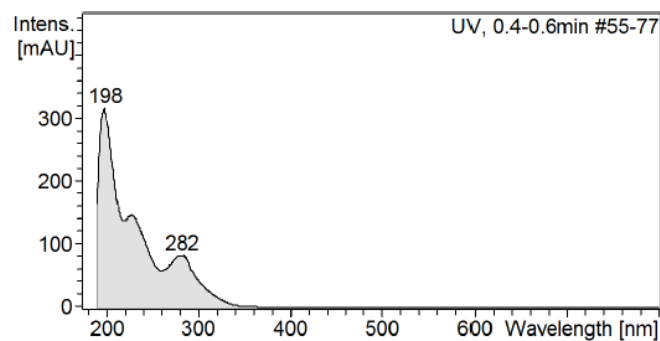


HRMS of 3ja

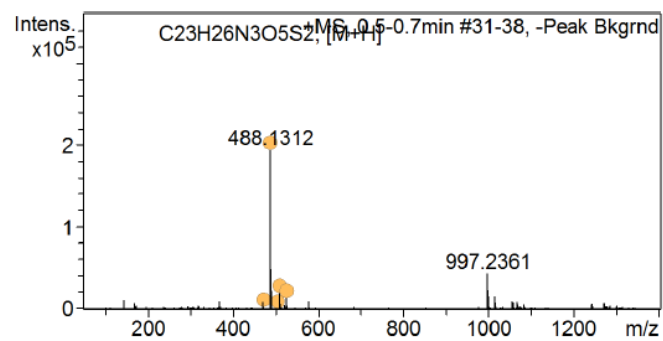


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	257715	Manual	80426	193.0	UV Chromatogram, 190-800 nm	488.1312	

Cmpd 1, 0.6 min

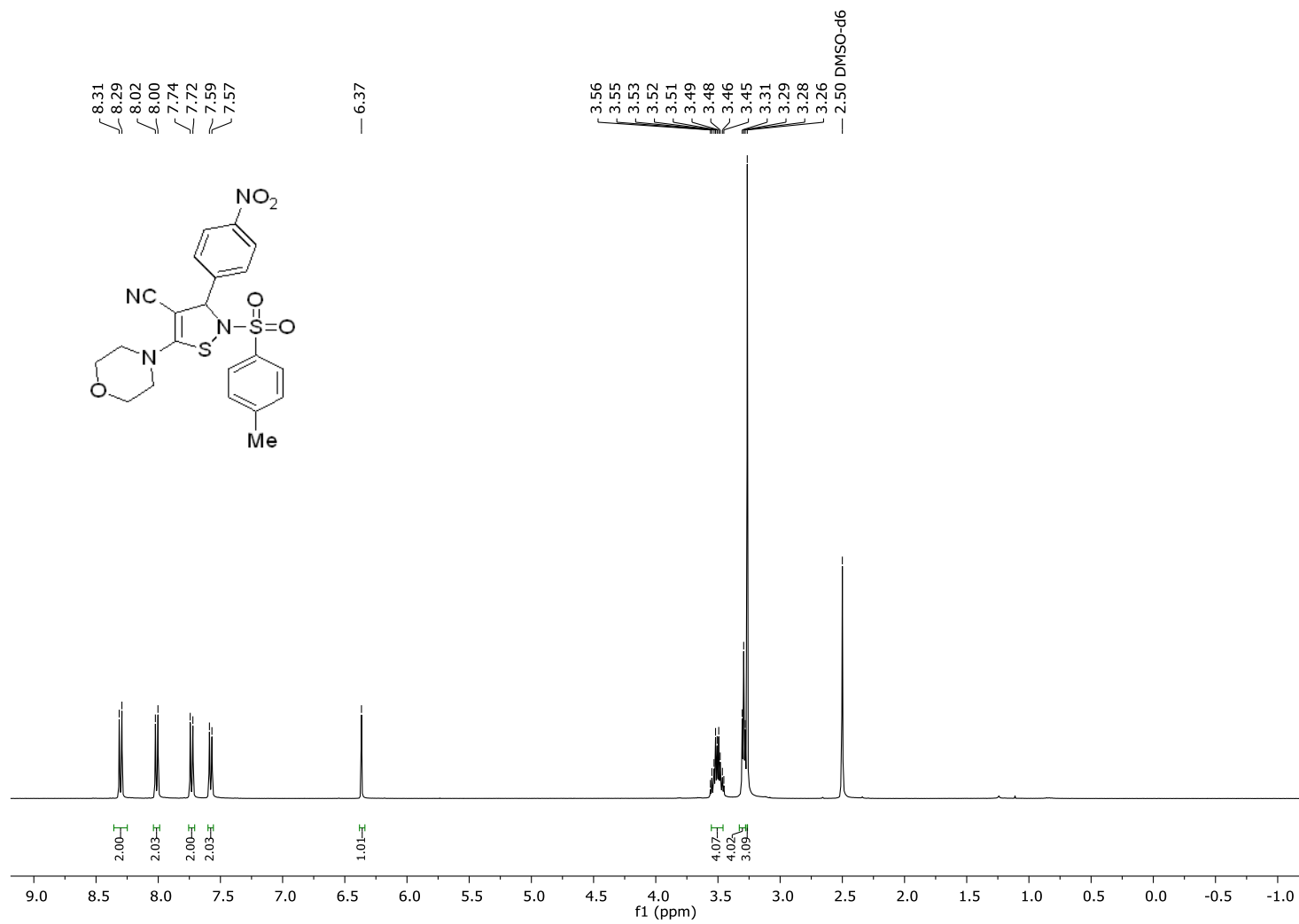


#	Wavelength	Intensity
0	198	314.3
1	282	82.4

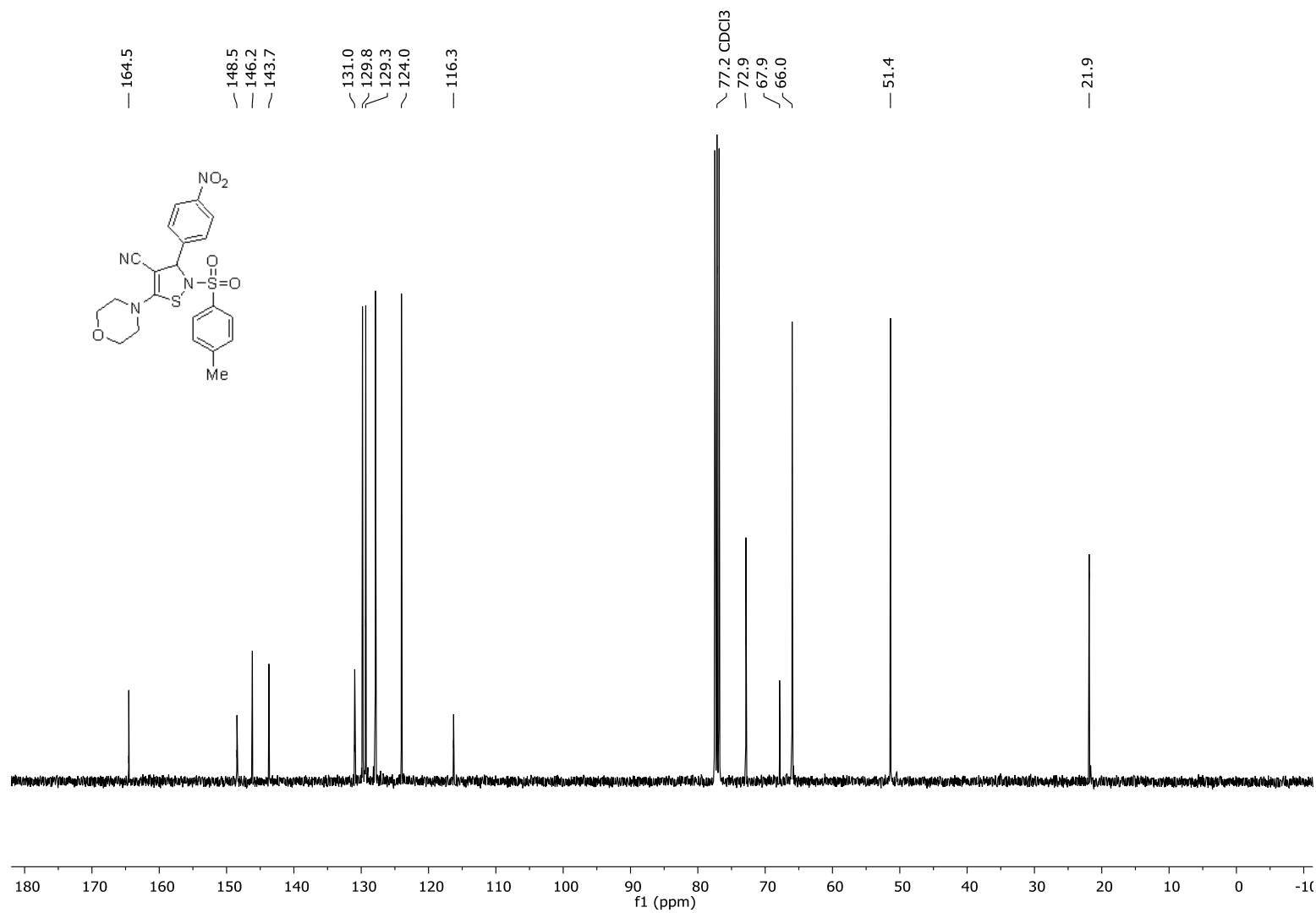


#	m/z	Res.	S/N	I	I %	FWHM
1	143.1180	16781	3880511.5	11032	5.7	0.0085
2	488.1312	25807	68036504.0	193421	100.0	0.0189
3	489.1337	21515	17491142.0	49726	25.7	0.0227
4	490.1294	19151	7984089.0	22698	11.7	0.0256
5	510.1122	20146	6707280.5	19068	9.9	0.0253
6	526.0862	20197	4741428.5	13479	7.0	0.0260
7	997.2361	24204	15259904.0	43382	22.4	0.0412
8	998.2388	22076	8146493.5	23160	12.0	0.0452
9	999.2365	22085	5331550.5	15157	7.8	0.0452
10	1013.2098	22014	5355012.5	15224	7.9	0.0460

¹H NMR (DMSO-*d*₆) spectrum of **3ka**

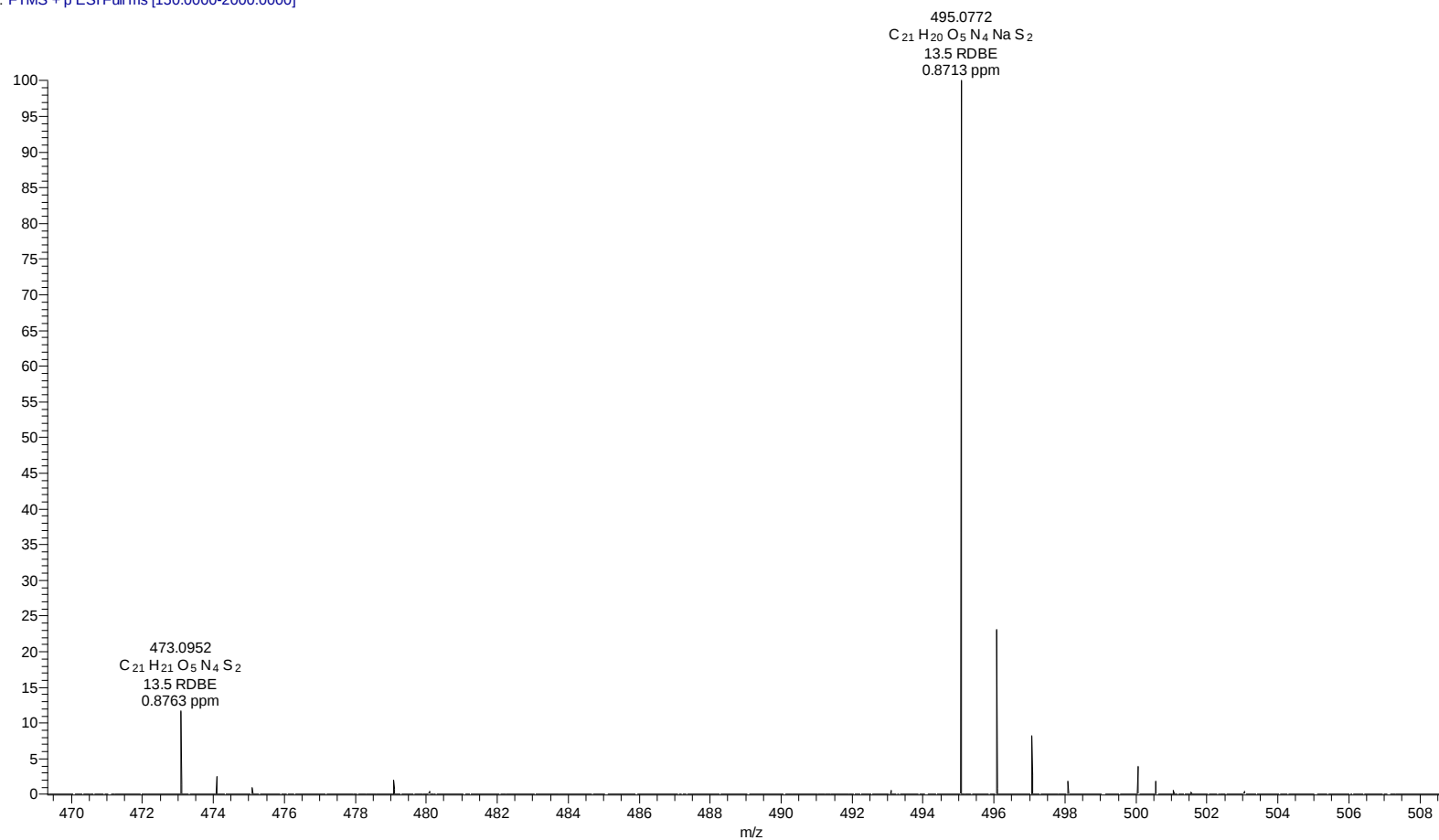


^{13}C NMR (CDCl_3) spectrum of **3ka**

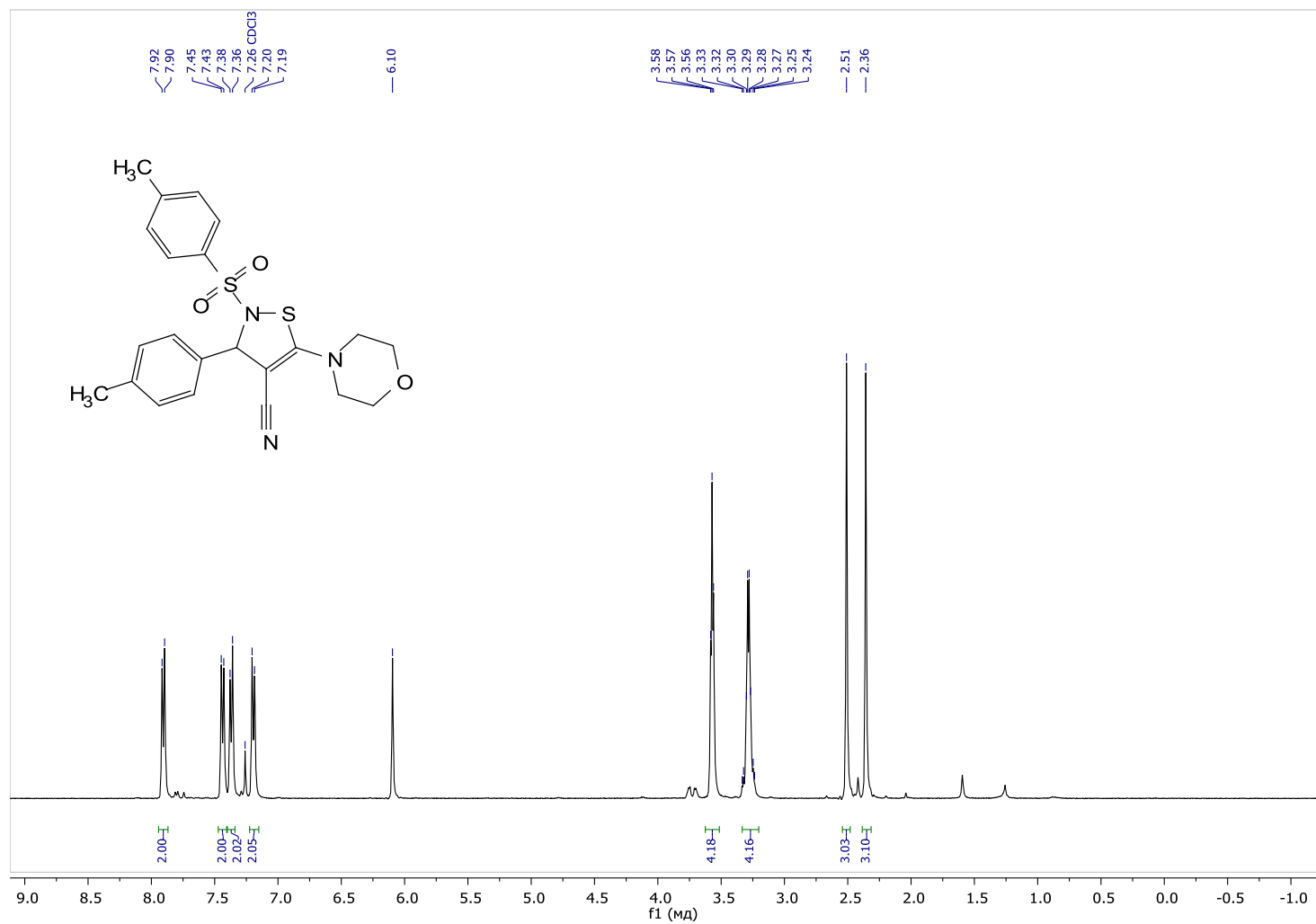


HRMS of **3ka**

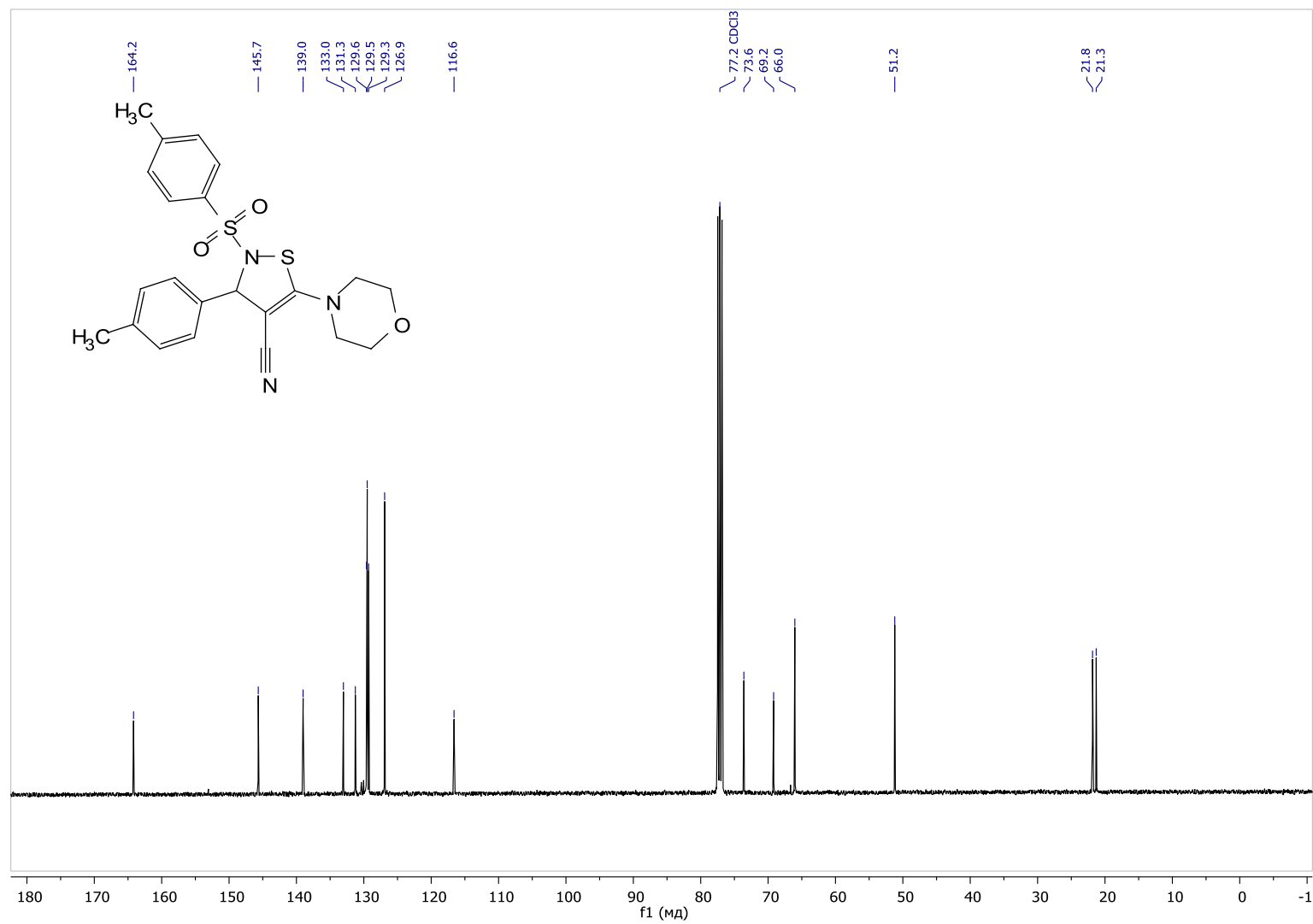
VF-87_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 1.44E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



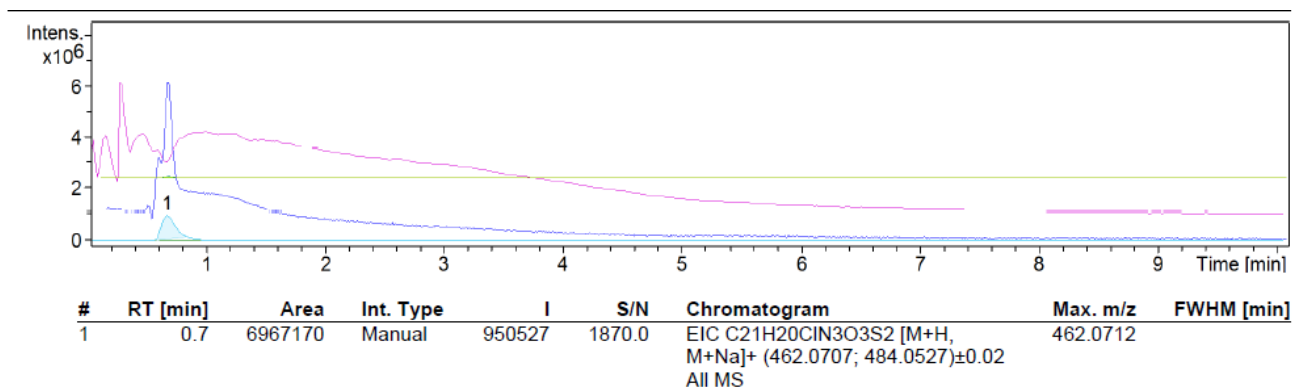
^1H NMR (CDCl_3) spectrum of **3la**



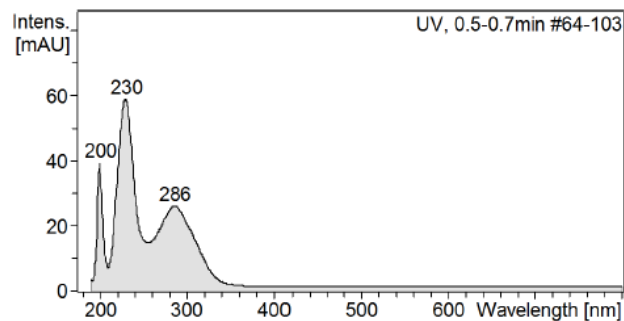
^{13}C NMR (CDCl_3) spectrum of **3la**



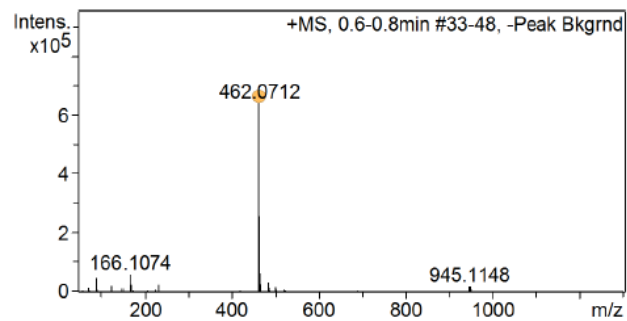
HRMS of 3la



Cmpd 1, 0.7 min

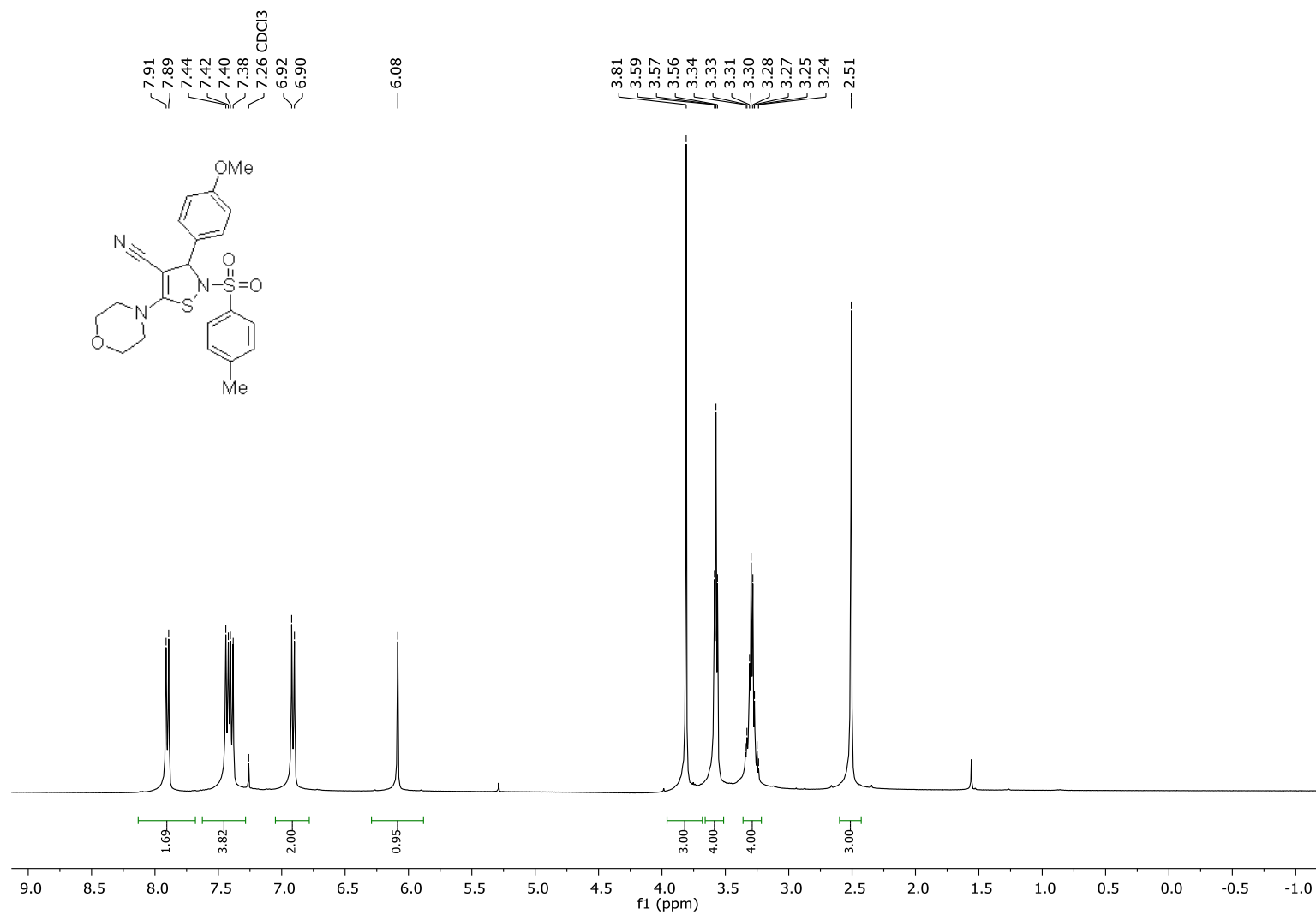


#	Wavelength	Intensity
0	200	39.3
1	230	58.8
2	286	26.2

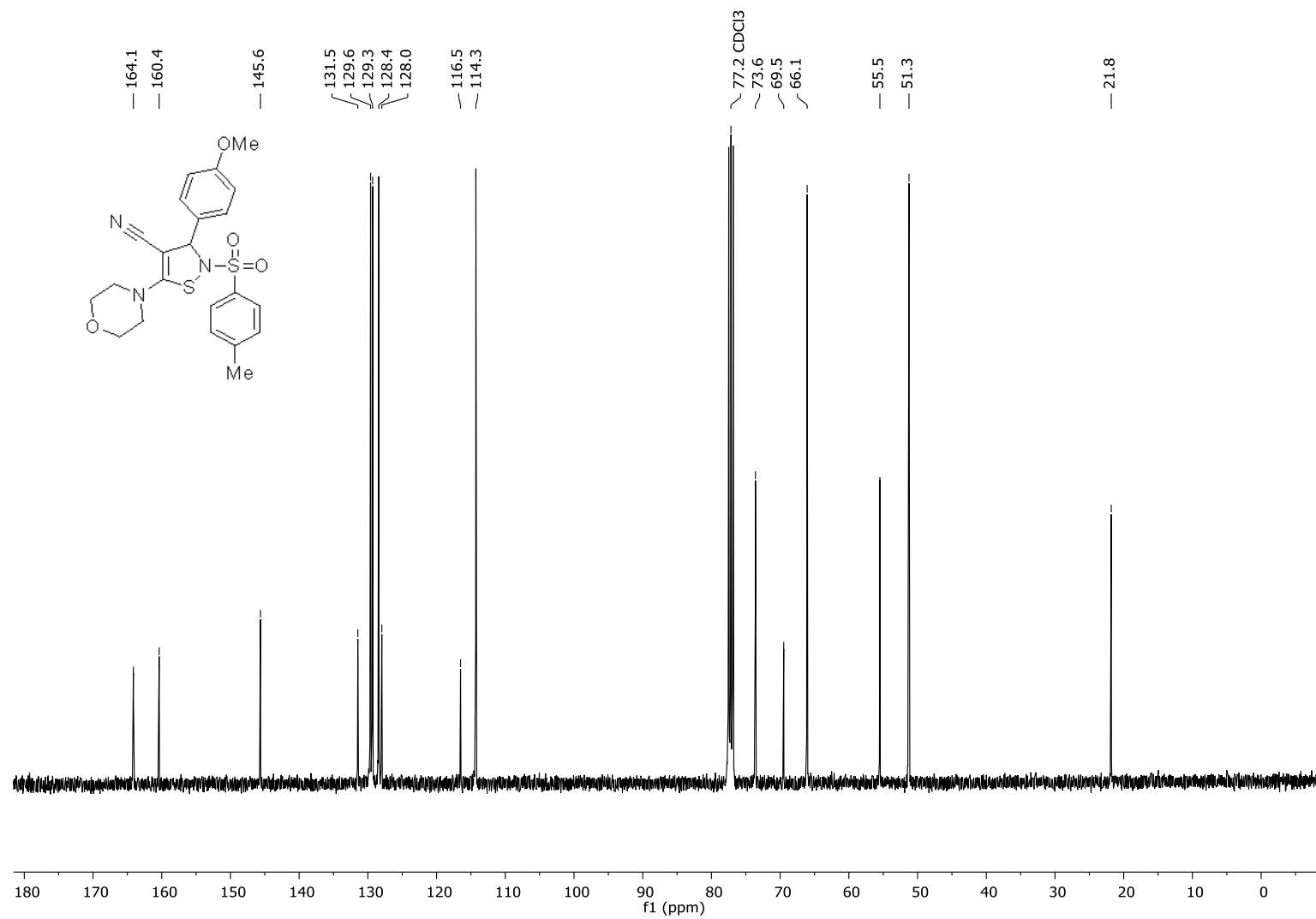


#	m/z	Res.	S/N	I	I %	FWHM
1	91.0393	18339	23848024.0	44213	6.9	0.0050
2	166.1074	20910	30936734.0	57355	9.0	0.0079
3	169.0427	17541	12486836.0	23150	3.6	0.0096
4	231.0835	17801	12487251.0	23151	3.6	0.0130
5	462.0712	28467	344354048.0	638413	100.0	0.0162
6	463.0736	21407	80385752.0	149031	23.3	0.0216
7	464.0683	22912	138767184.0	257266	40.3	0.0203
8	465.0703	19740	32930016.0	61050	9.6	0.0236
9	466.0663	17751	12733924.0	23608	3.7	0.0263
10	484.0521	19481	16335288.0	30285	4.7	0.0248

^1H NMR (CDCl_3) spectrum of **3ma**

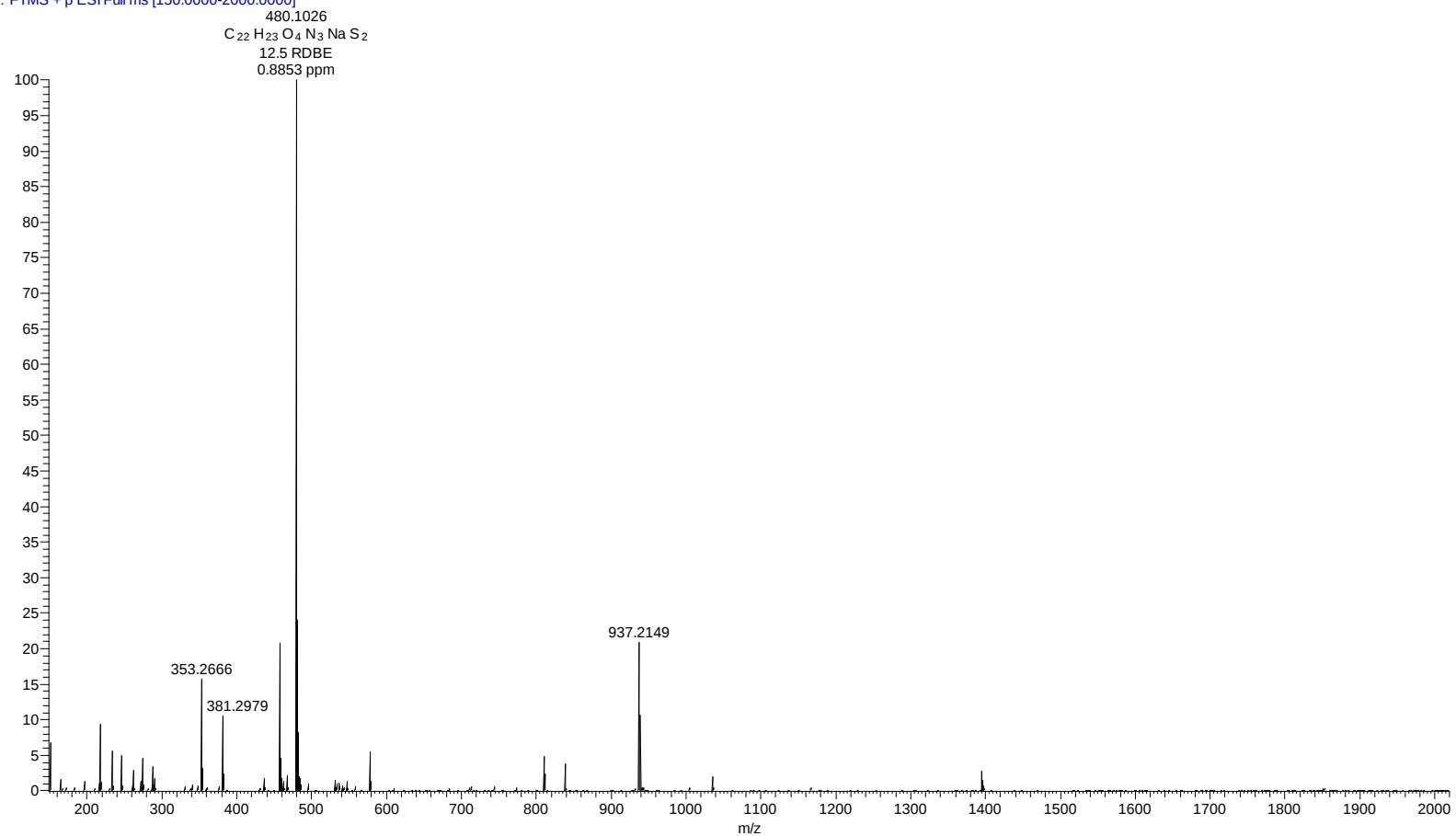


^{13}C NMR (CDCl_3) spectrum of **3ma**

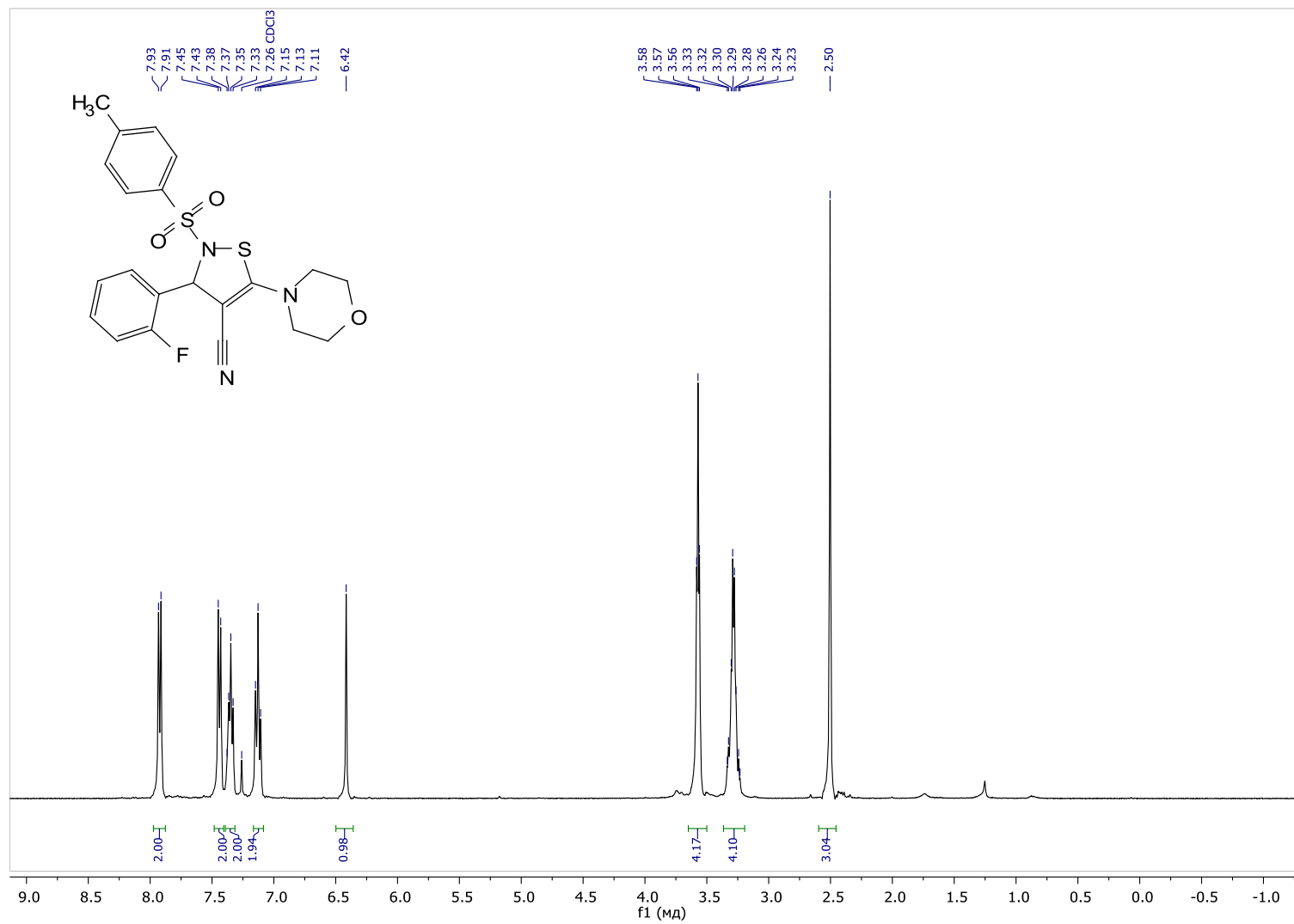


HRMS of 3ma

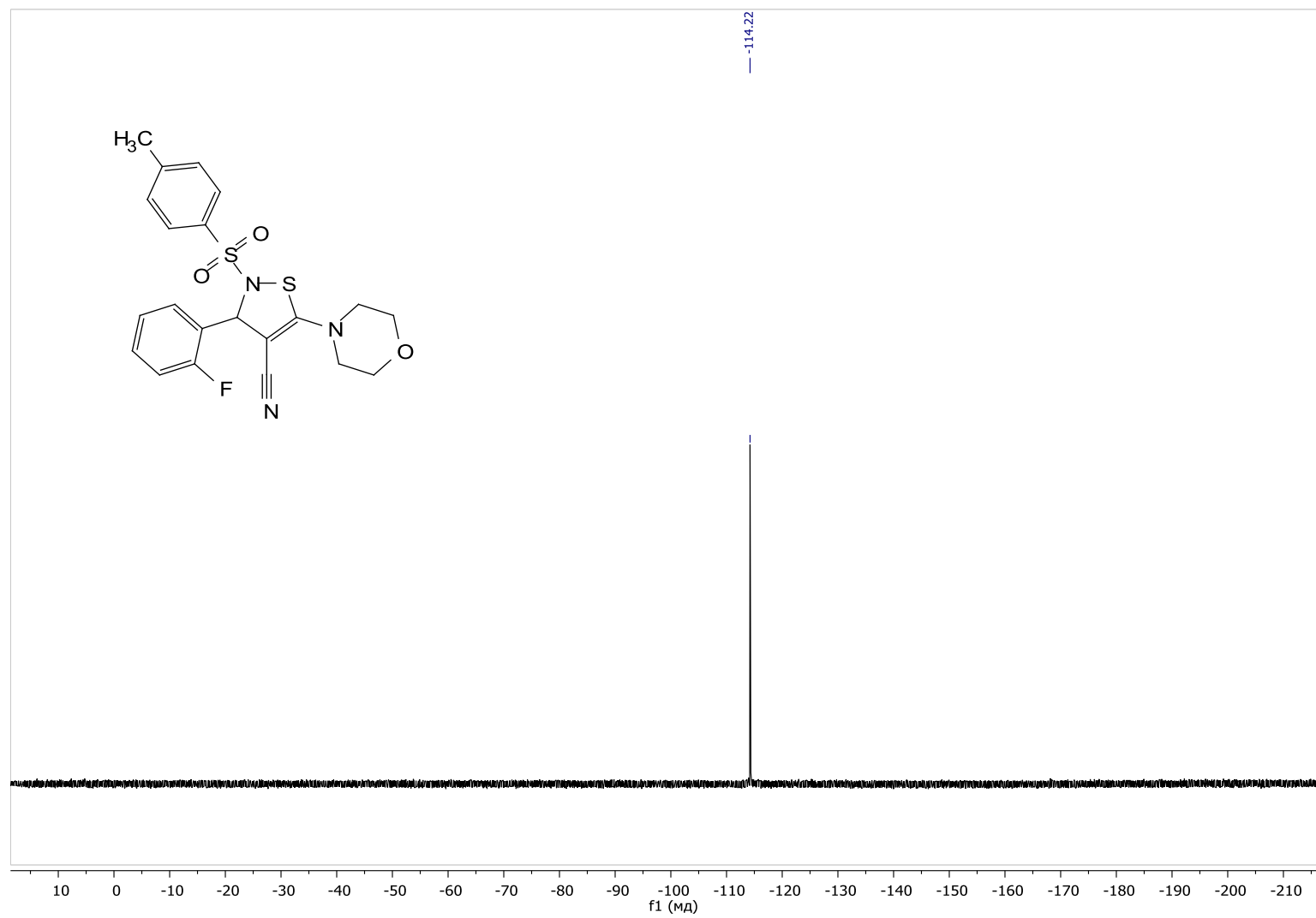
VF-134_Pos_240213100050 #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 4.47E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



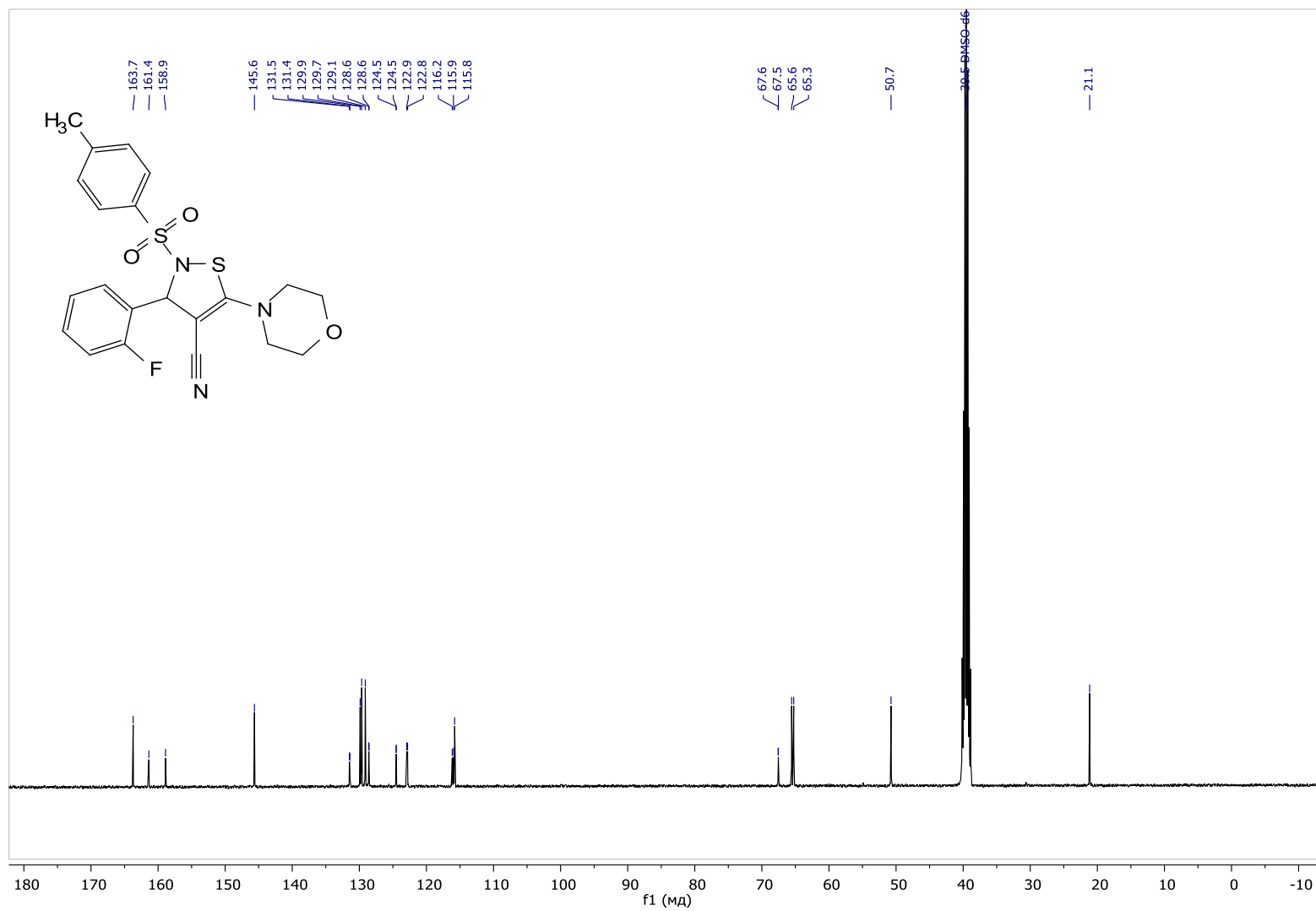
^1H NMR (CDCl_3) spectrum of **3na**



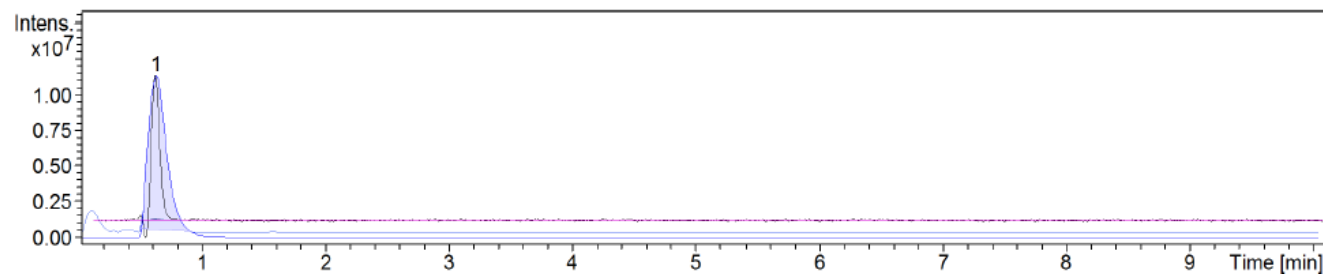
^{19}F NMR (CDCl_3) spectrum of **3na**



^{13}C NMR (DMSO- d_6) spectrum of **3na**

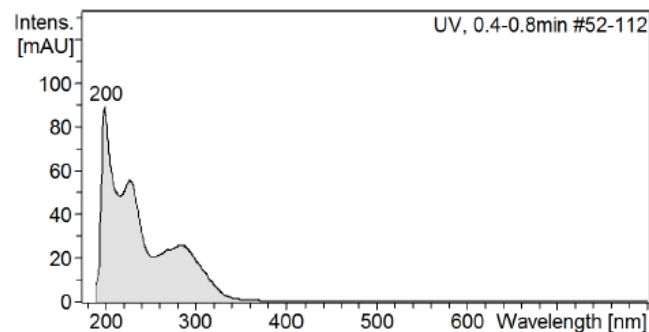


HRMS of **3na**

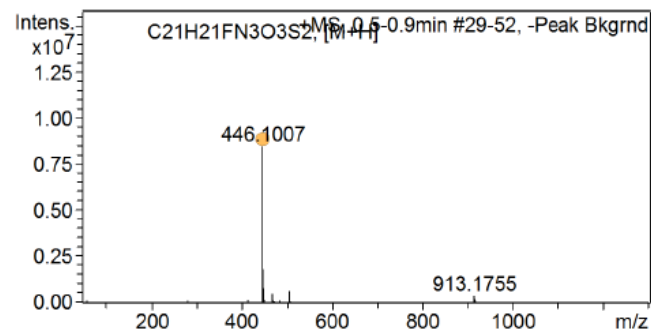


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	108223808	Manual	11257631	31118.0	EIC 446.0987±0.02 +All MS	446.1007	

Cmpd 1, 0.6 min

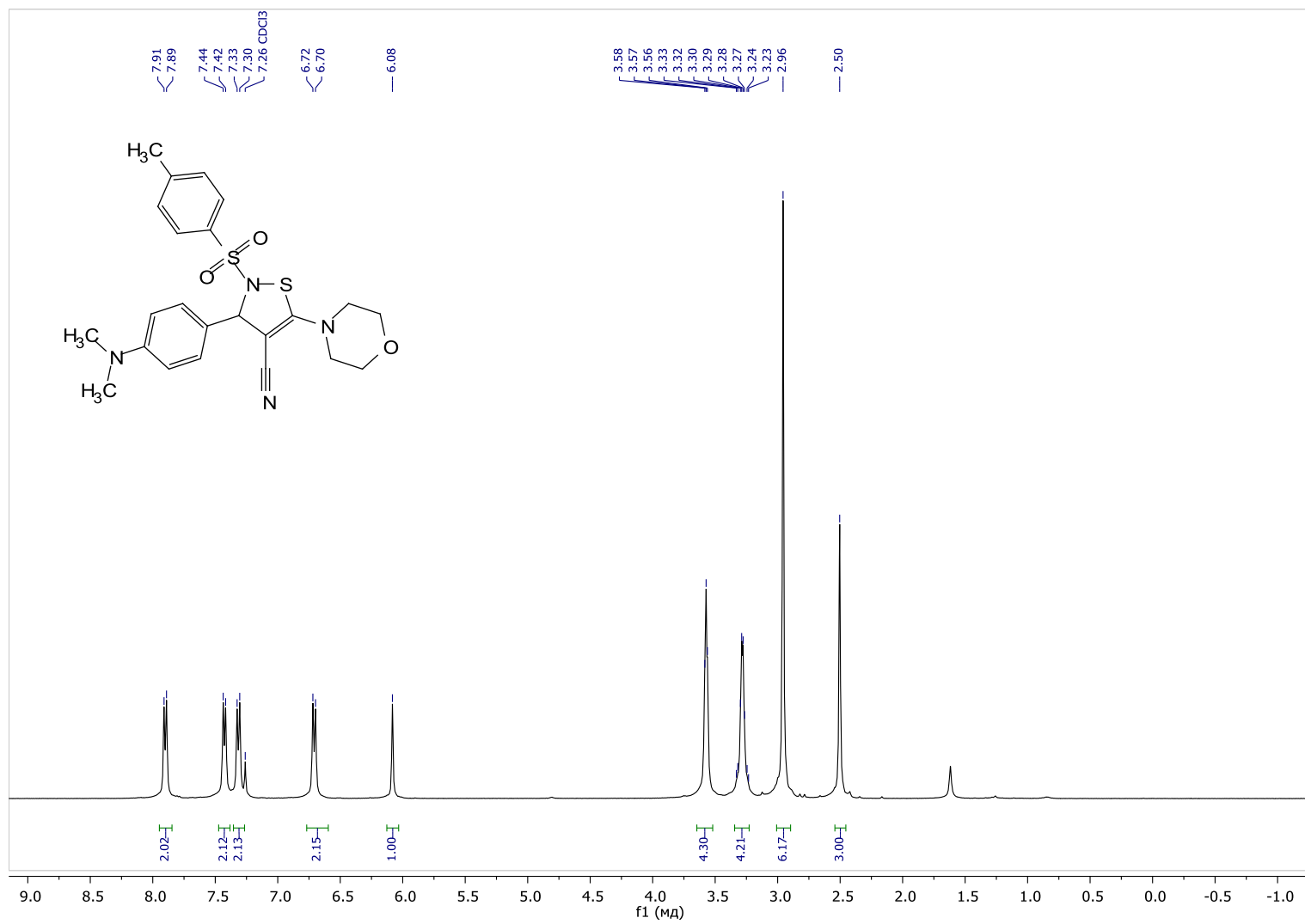


#	Wavelength	Intensity
0	200	89.1

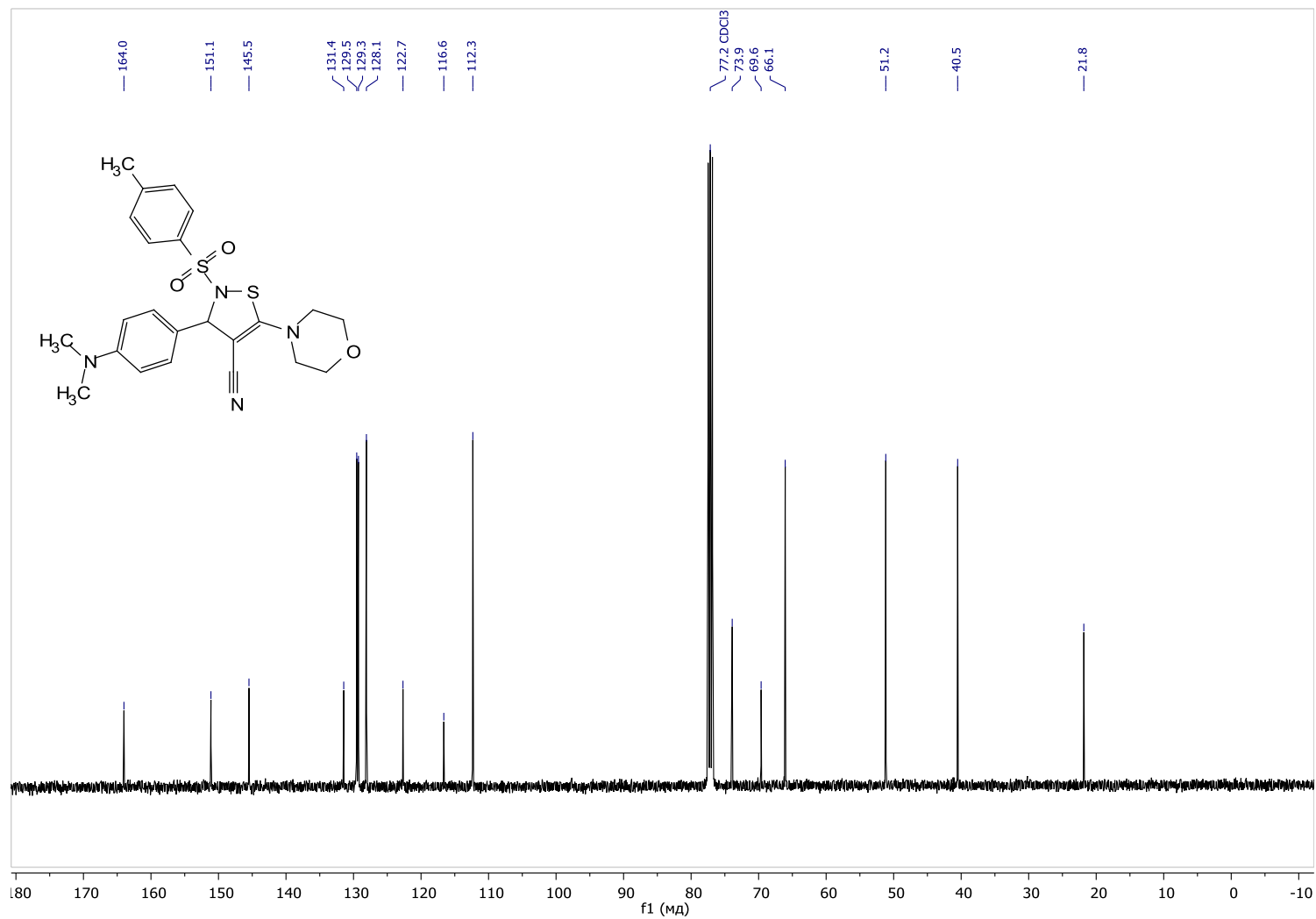


#	m/z	Res.	S/N	I	I %	FWHM
1	414.1263	21333	19514274.0	146872	1.7	0.0194
2	446.1007	39592	1120244096.0	8431403	100.0	0.0113
3	447.1037	32163	238496928.0	1795023	21.3	0.0139
4	448.0992	24305	96361864.0	725258	8.6	0.0184
5	449.1003	19451	18586732.0	139891	1.7	0.0231
6	468.0823	25387	64444732.0	485037	5.8	0.0184
7	504.1536	27257	80141016.0	603173	7.2	0.0185
8	505.1559	21139	20727910.0	156007	1.9	0.0239
9	913.1755	30914	44036976.0	331440	3.9	0.0295
10	914.1780	26238	21774960.0	163887	1.9	0.0348

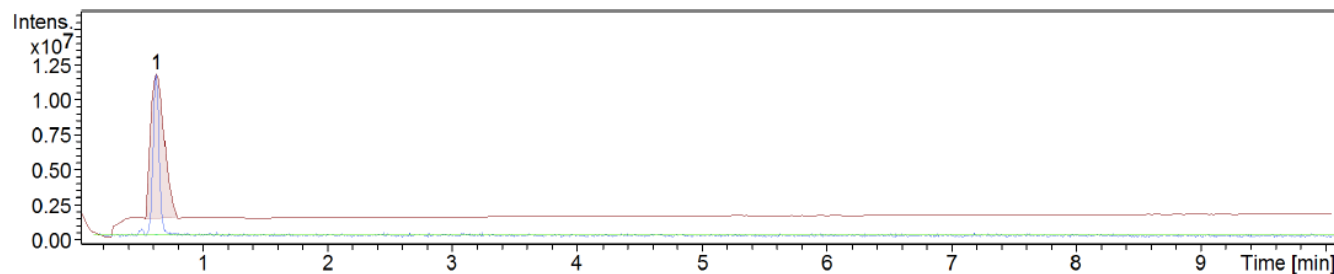
¹H NMR (CDCl₃) spectrum of **30a**



^{13}C NMR (CDCl_3) spectrum of **3oa**

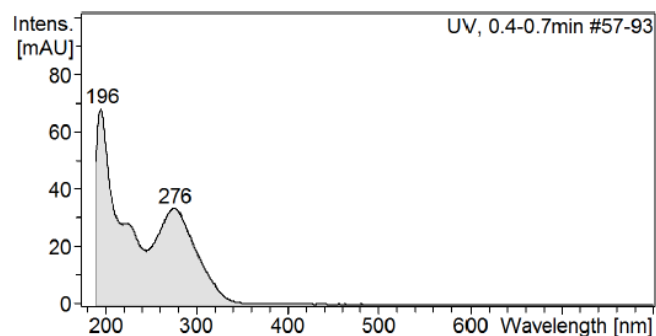


HRMS of **30a**

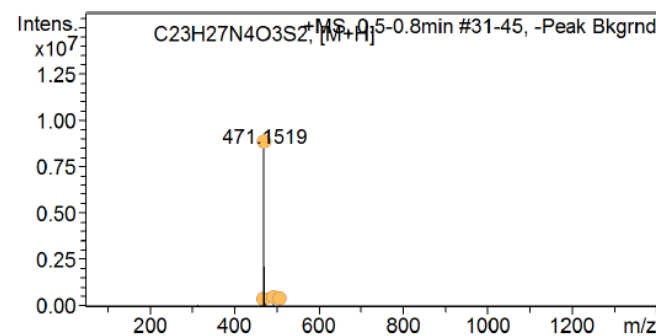


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	77795384	Manual	11749728	508.0	BPC +All MS	471.1519	

Cmpd 1, 0.6 min

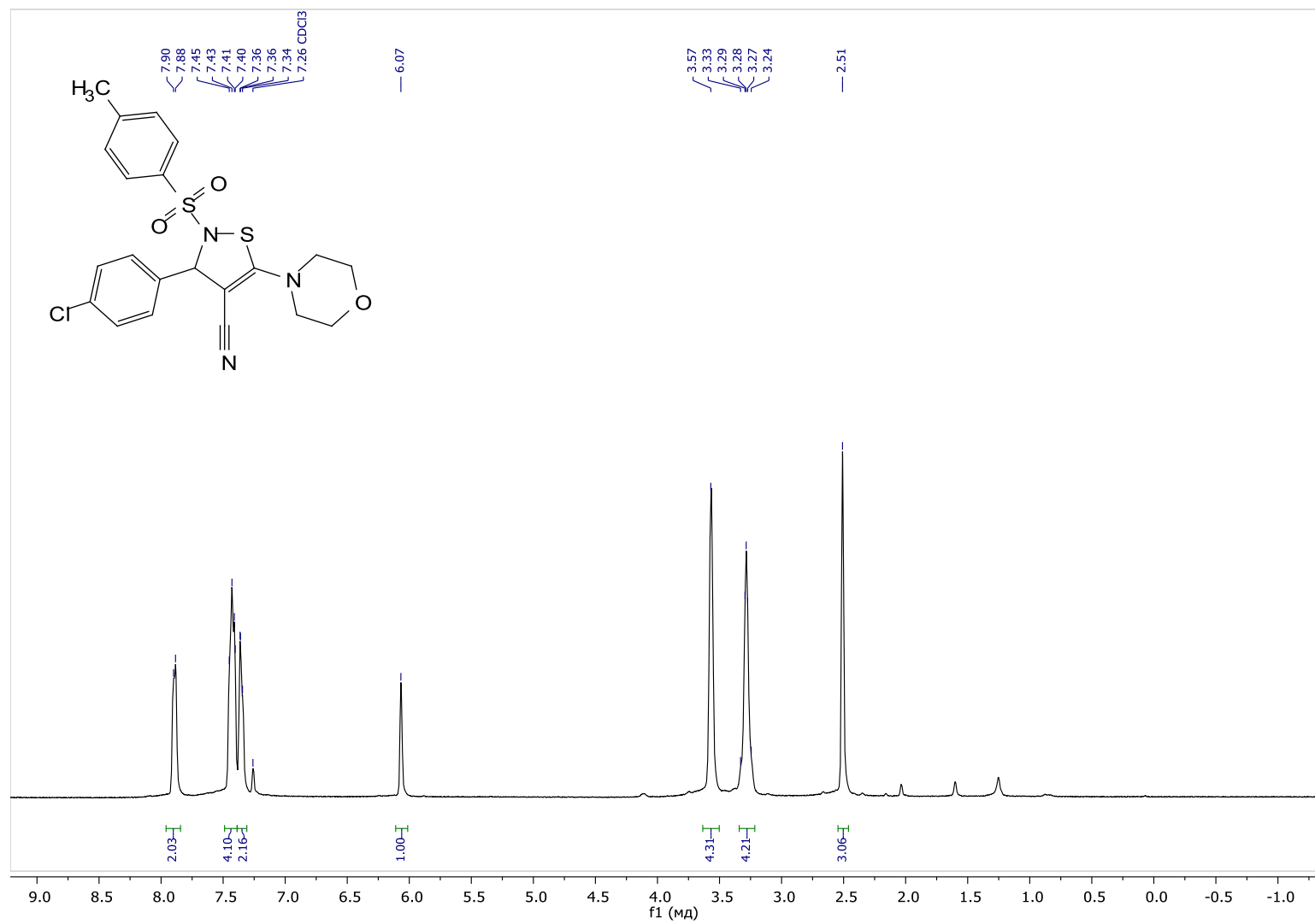


#	Wavelength	Intensity
0	196	67.7
1	276	33.3

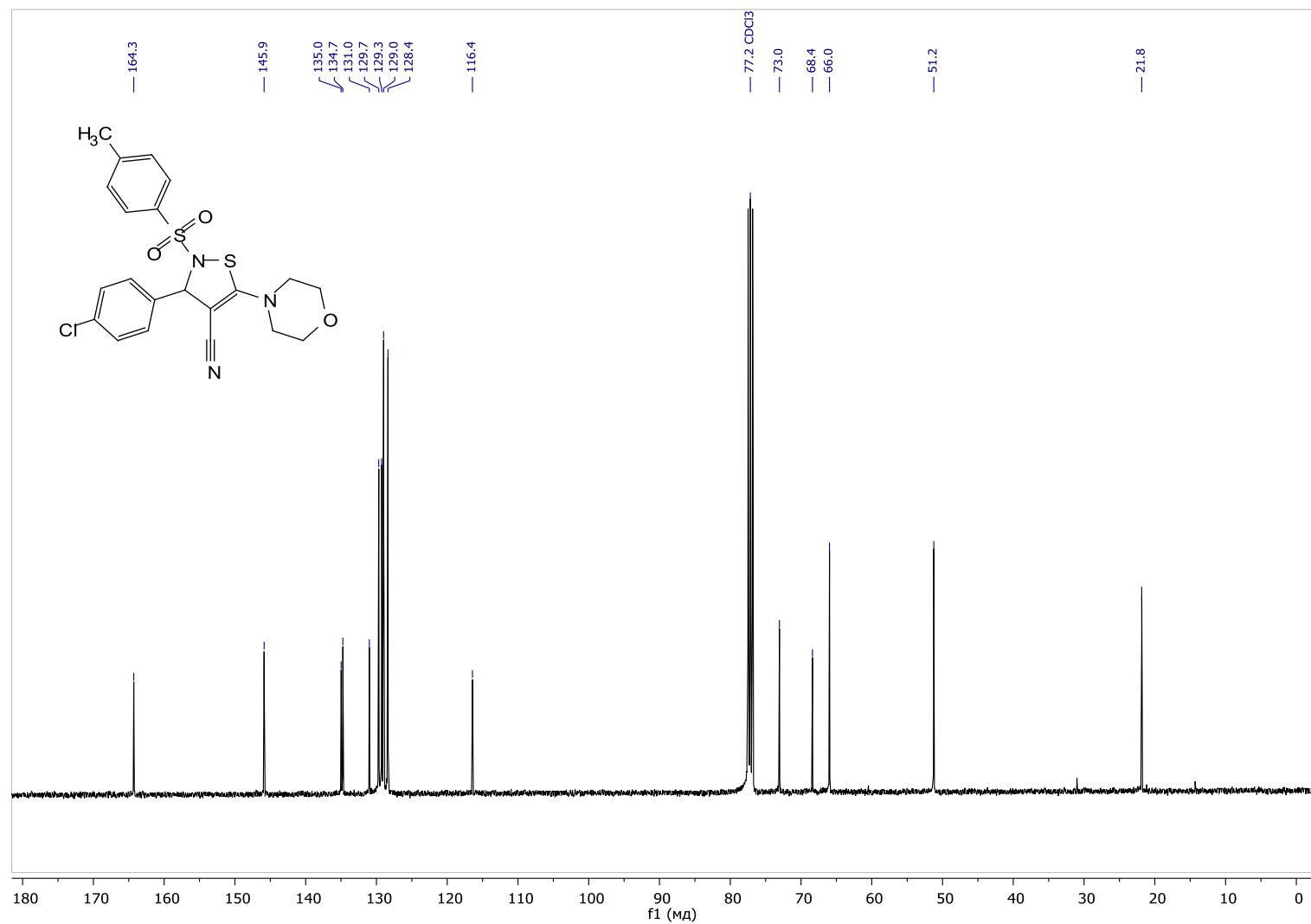


#	m/z	Res.	S/N	I	I %	FWHM
1	315.1266	19351	3658764.5	72284	0.9	0.0163
2	471.1519	30538	425545344.0	8407209	100.0	0.0154
3	471.5521	17796	1992938.8	39373	0.5	0.0265
4	472.1545	34456	108452792.0	2142628	25.5	0.0137
5	473.1504	25053	40309732.0	796372	9.5	0.0189
6	474.1510	20093	8637641.0	170648	2.0	0.0236
7	475.1492	15902	1846111.5	36472	0.4	0.0299
8	493.1325	20663	4803625.5	94902	1.1	0.0239
9	509.1063	19020	1972855.4	38976	0.5	0.0268
10	551.0909	20404	1952696.3	38578	0.5	0.0270

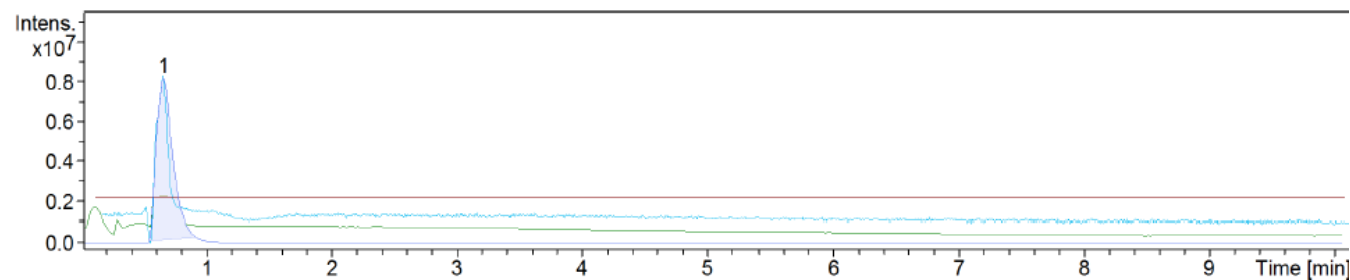
^1H NMR (CDCl_3) spectrum of **3pa**



^{13}C NMR (CDCl_3) spectrum of **3pa**

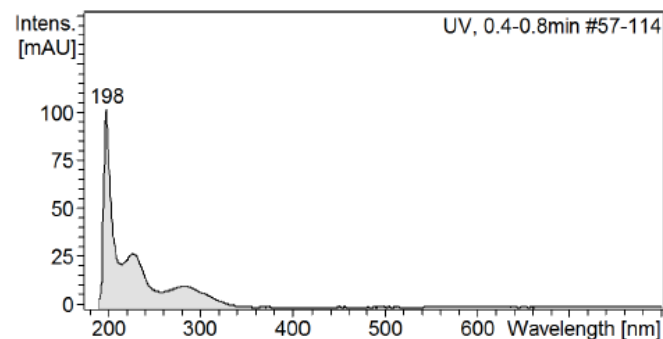


HRMS of 3pa

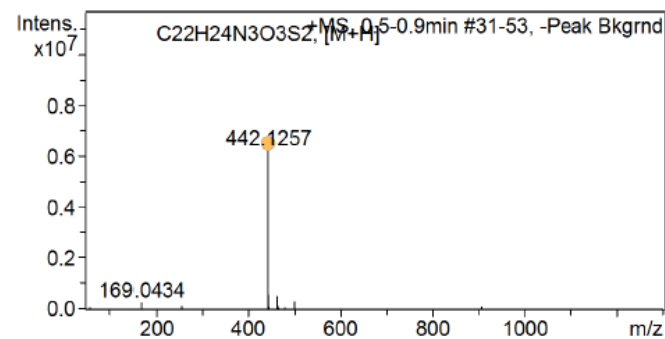


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.7	72452992	Manual	8179648	40750.3	EIC 442.1233±0.02 +All MS	442.1257	

Cmpd 1, 0.7 min

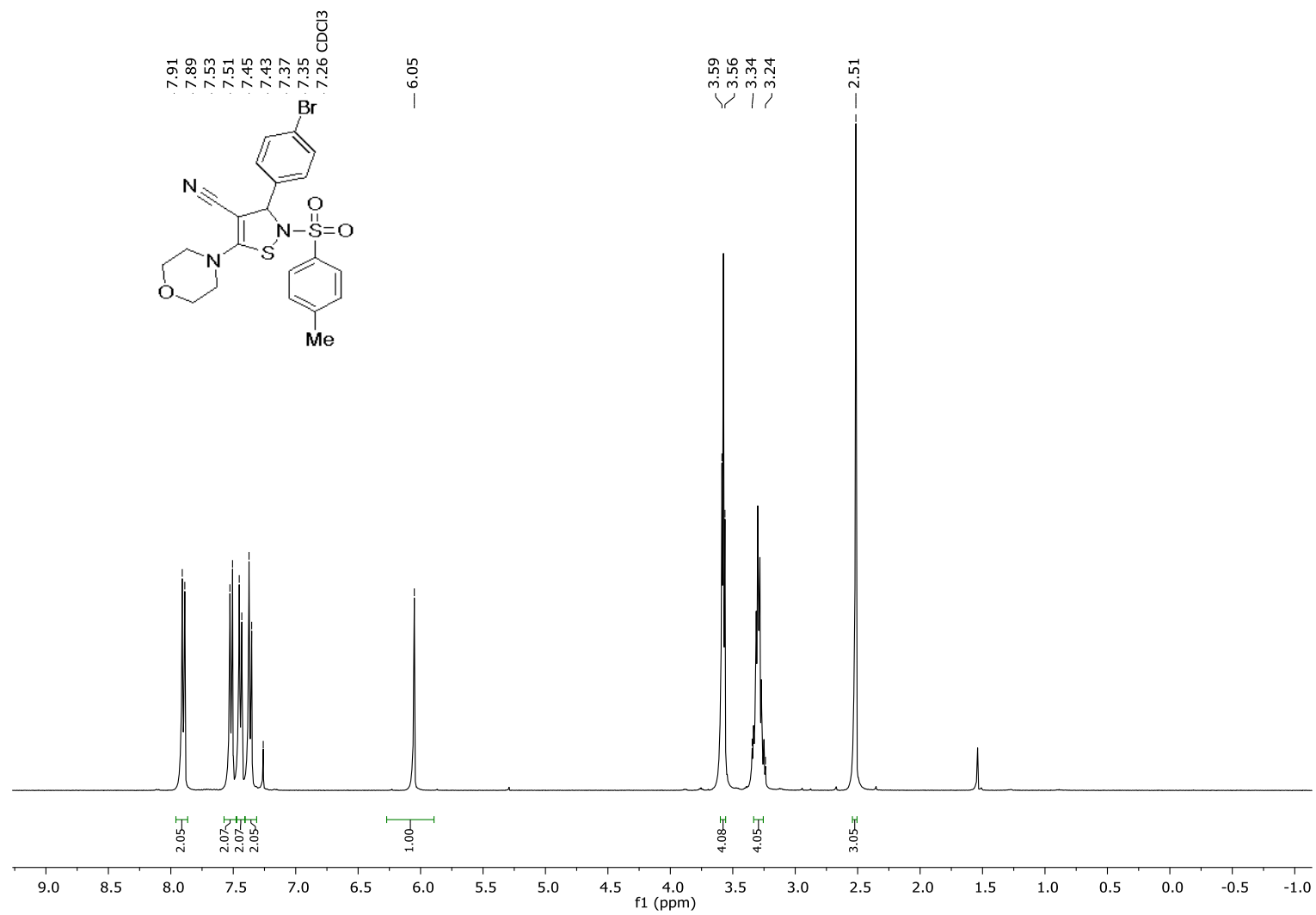


#	Wavelength	Intensity
0	198	101.4

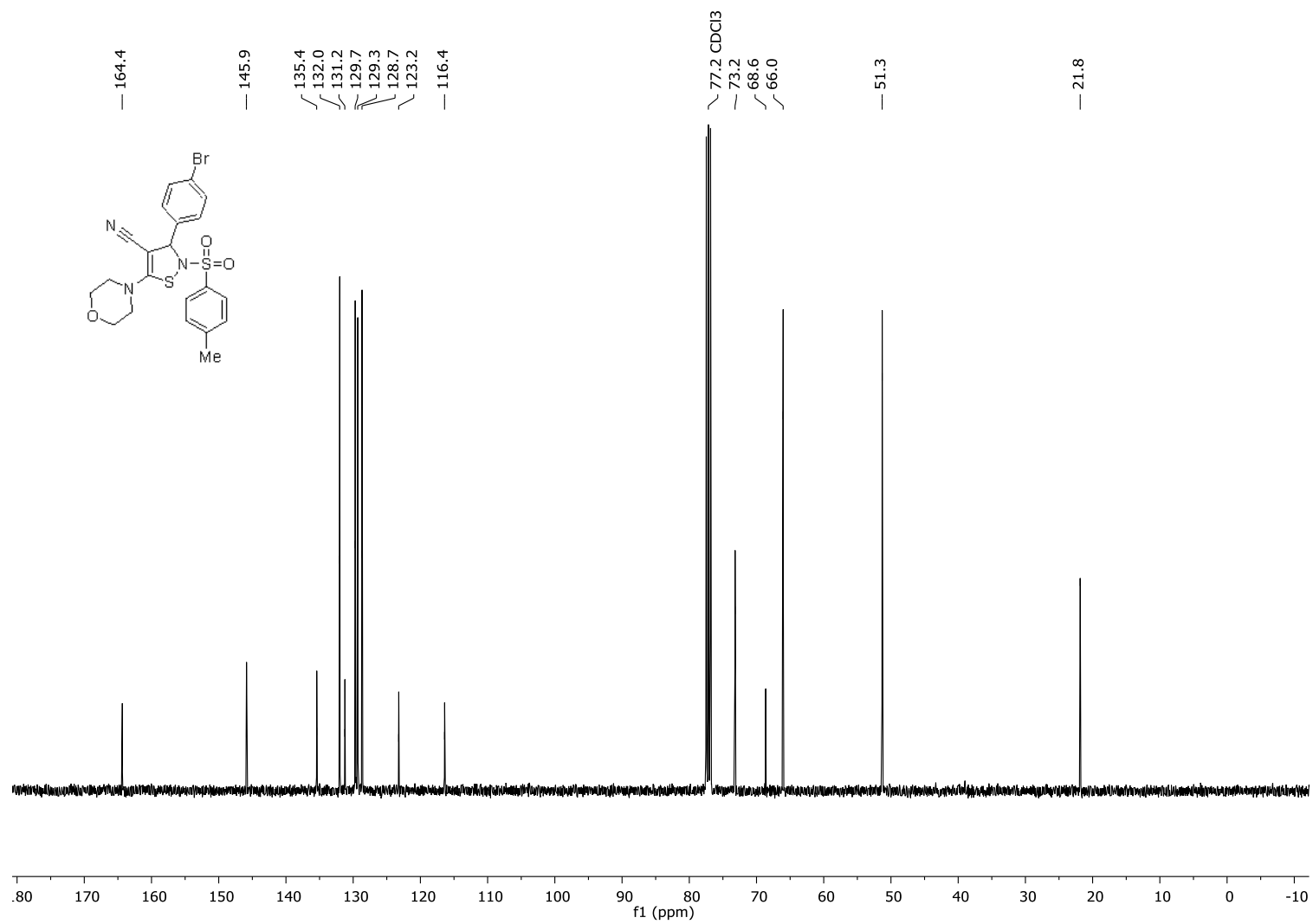


#	m/z	Res.	S/N	I	I %	FWHM
1	169.0434	20831	31916674.0	259728	4.2	0.0081
2	257.1646	20920	14570147.0	118568	1.9	0.0123
3	442.1257	40945	763024832.0	6209270	100.0	0.0108
4	443.1288	31605	173096464.0	1408608	22.7	0.0140
5	444.1243	22423	65815572.0	535588	8.6	0.0198
6	445.1249	19097	13757497.0	111954	1.8	0.0233
7	464.1075	25271	61675796.0	501899	8.1	0.0184
8	465.1099	20233	15876154.0	129195	2.1	0.0230
9	500.1787	23353	36161592.0	294272	4.7	0.0214
10	905.2246	24564	12844662.0	104526	1.7	0.0369

^1H NMR (CDCl_3) spectrum of **3qa**

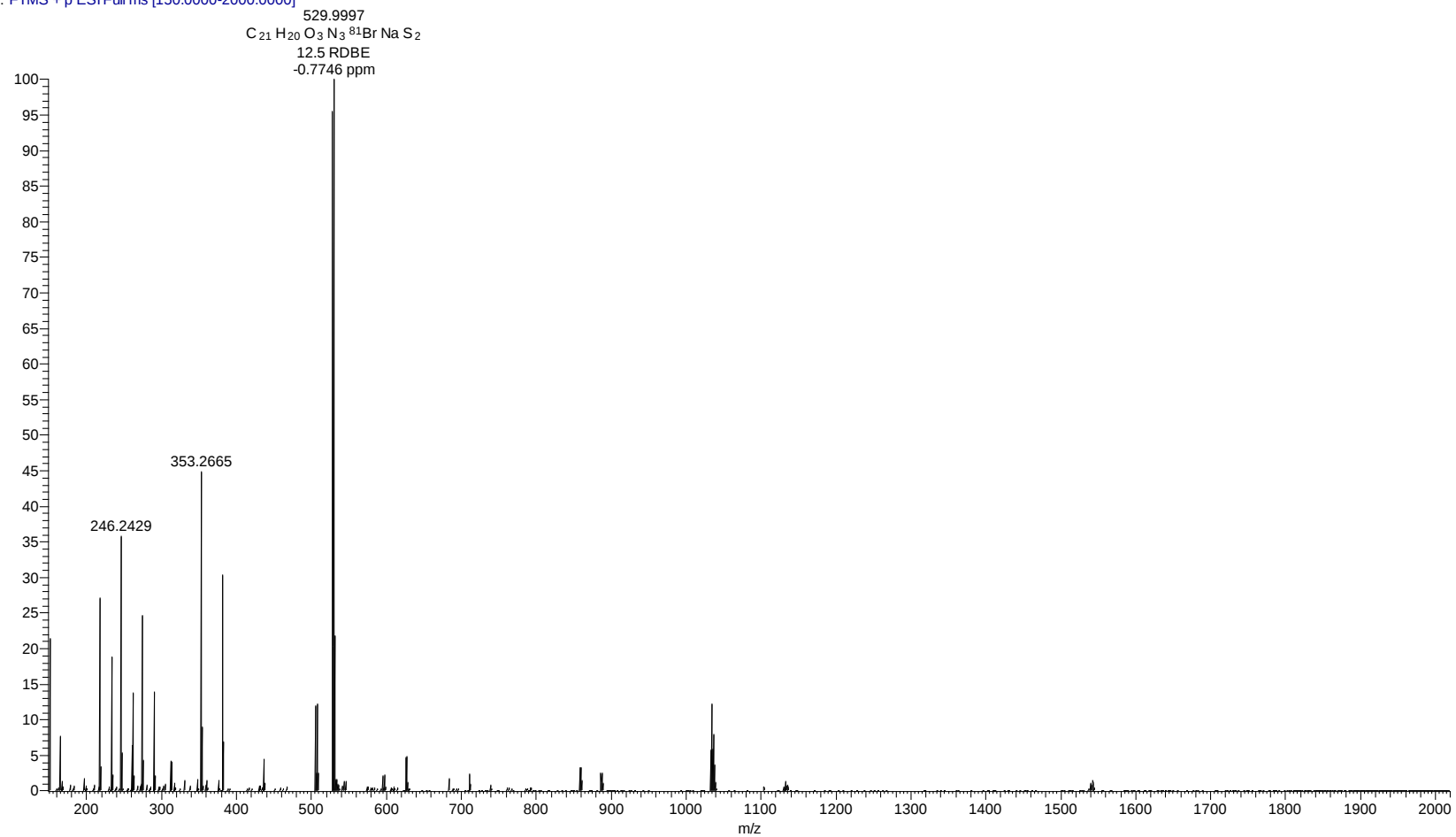


^{13}C NMR (CDCl_3) spectrum of **3qa**

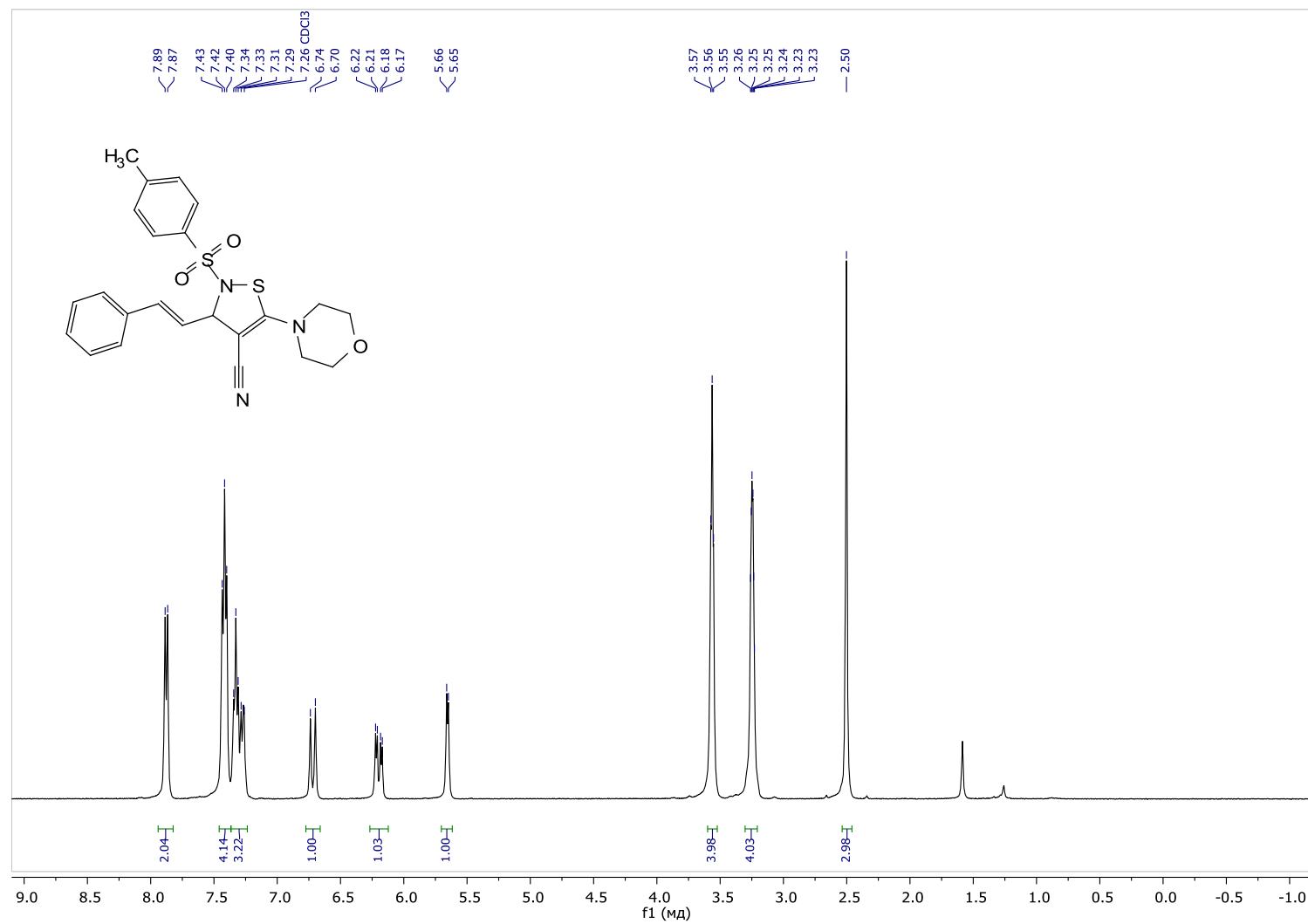


HRMS of **3qa**

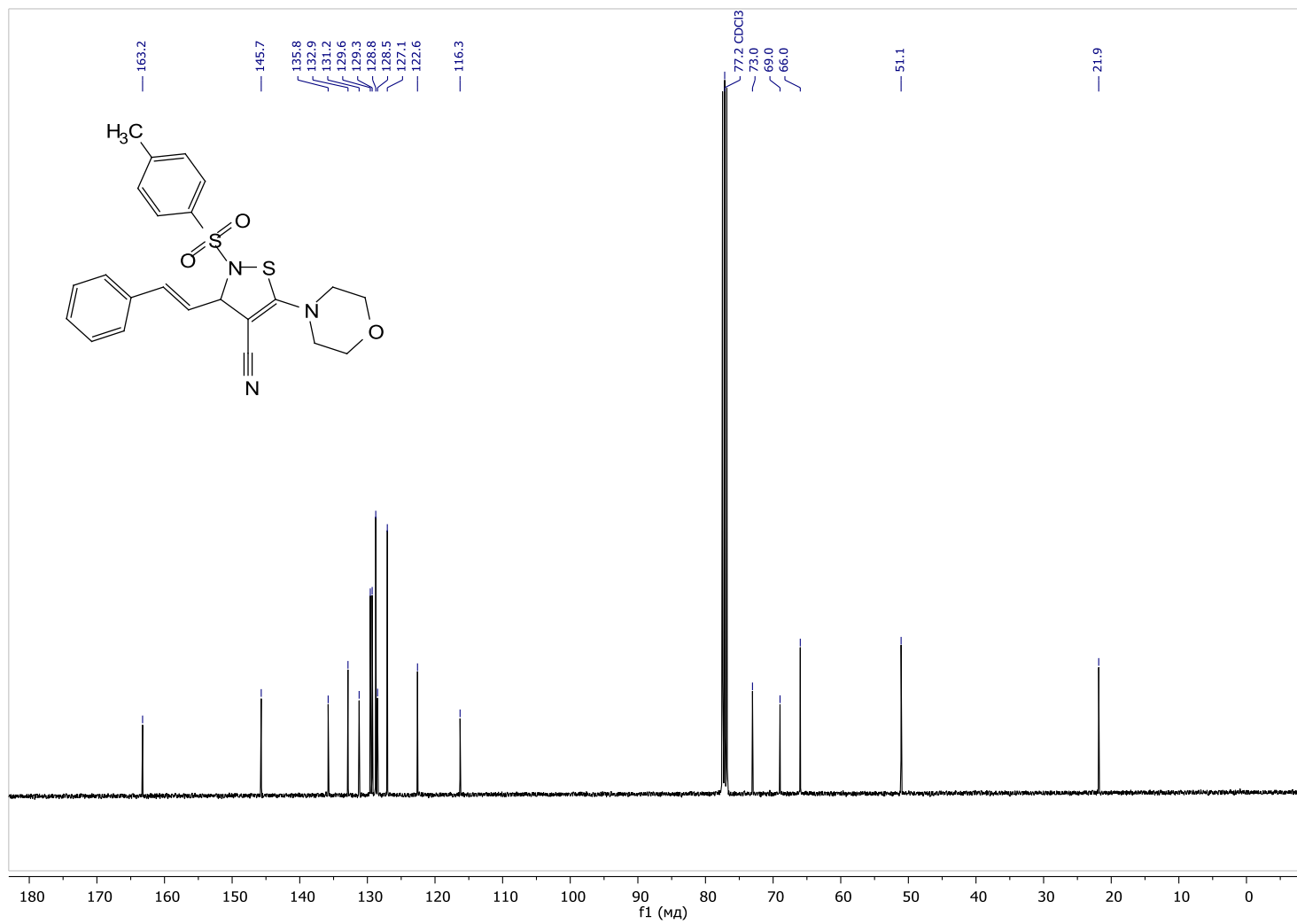
VF-93_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 2.21E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



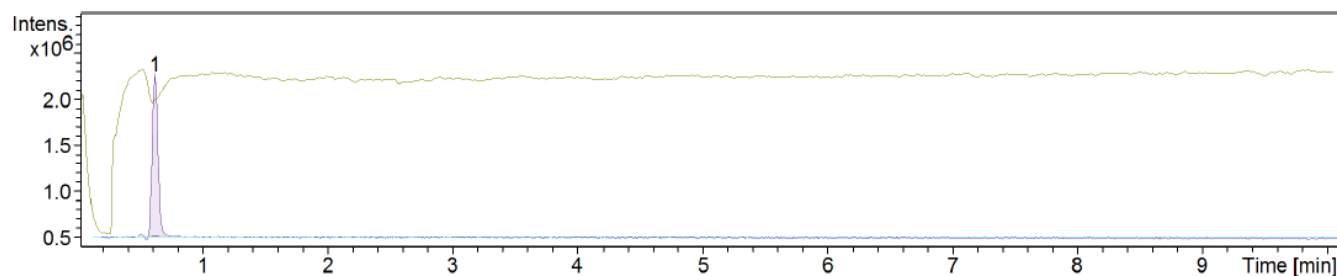
¹H NMR (CDCl₃) spectrum of **3ra**



^{13}C NMR (CDCl_3) spectrum of **3ra**

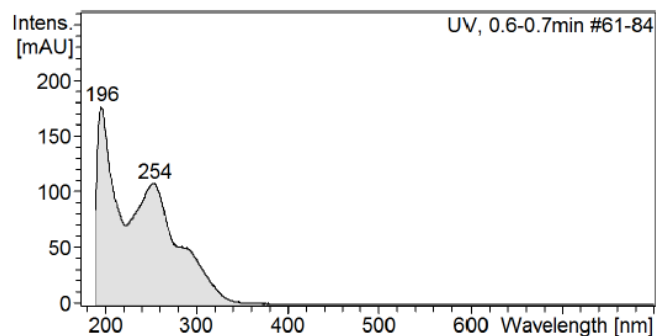


HRMS of 3ra

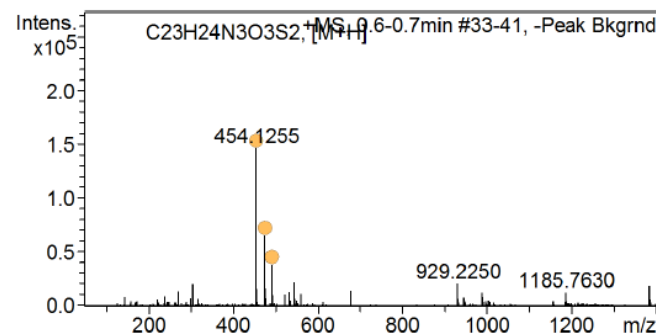


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	194073	Manual	60477	148.0	UV Chromatogram, 190-800 nm	454.1255	

Cmpd 1, 0.6 min

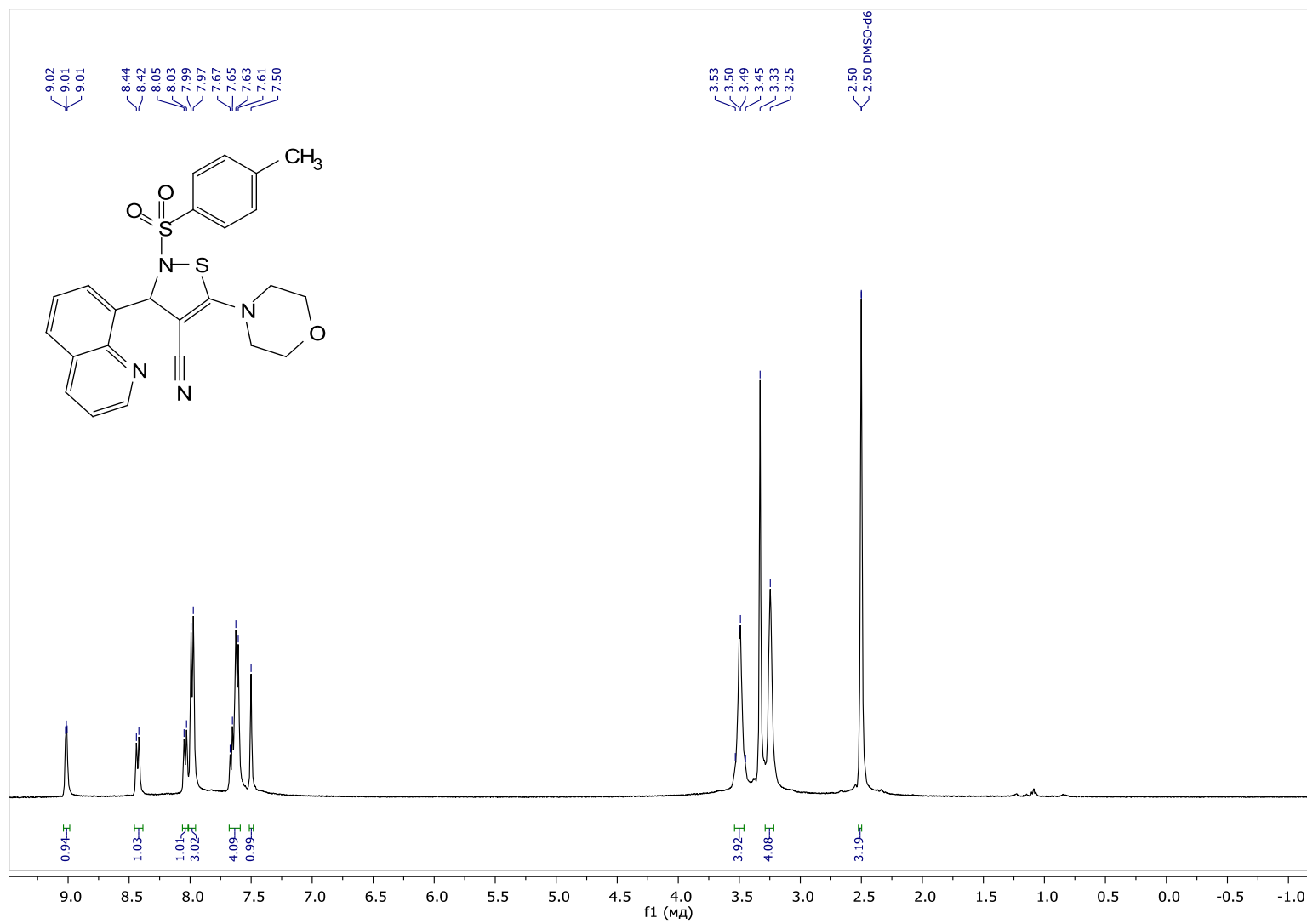


#	Wavelength	Intensity
0	196	175.8
1	254	107.3

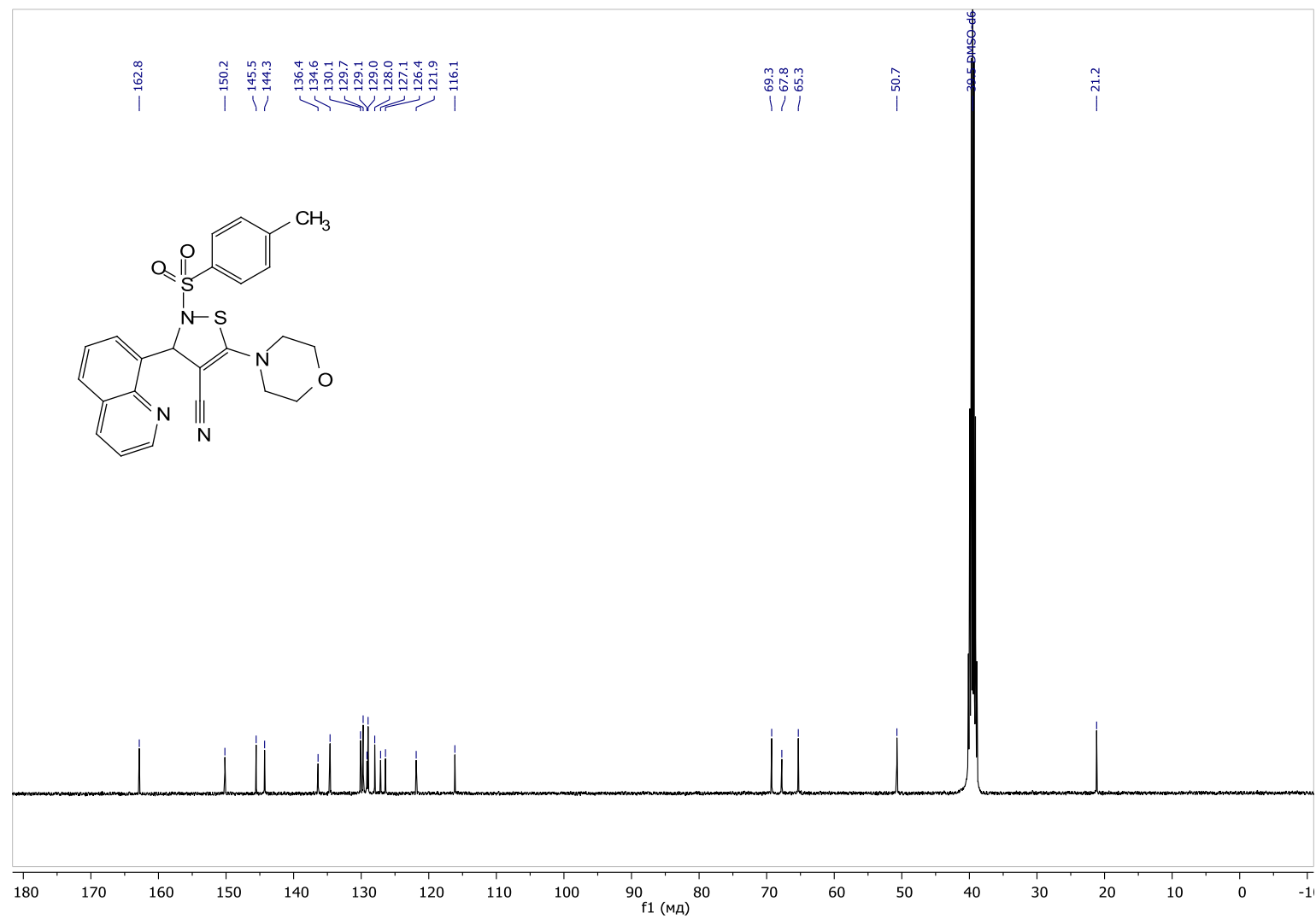


#	m/z	Res.	S/N	I	I %	FWHM
1	305.3022	19665	4065745.3	20023	13.7	0.0155
2	454.1255	23848	29686678.0	146200	100.0	0.0190
3	455.1280	20462	7653192.0	37690	25.8	0.0222
4	476.1067	21291	13292856.0	65464	44.8	0.0224
5	477.1098	18720	3275426.3	16131	11.0	0.0255
6	492.0807	20734	7795246.5	38390	26.3	0.0237
7	544.0940	20268	4413087.0	21733	14.9	0.0268
8	929.2250	23177	4174060.3	20556	14.1	0.0401
9	1382.3414	23228	3737368.5	18406	12.6	0.0595
10	1383.3436	24091	3807002.0	18749	12.8	0.0574

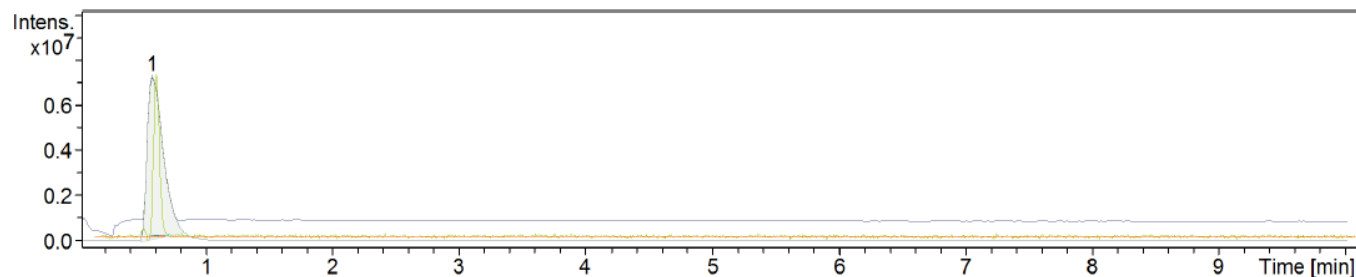
^1H NMR ($\text{DMSO-}d_6$) spectrum of **3sa**



^{13}C NMR (DMSO- d_6) spectrum of **3sa**

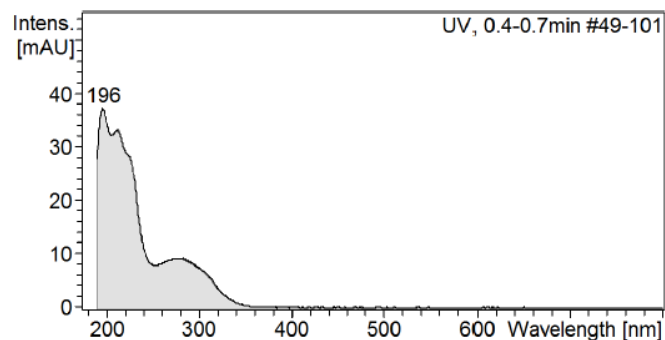


HRMS of 3sa

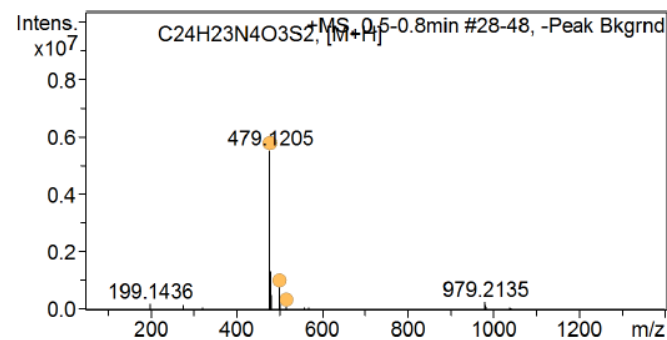


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	63860744	Manual	7268343	3732.9	EIC 479.1205 +All MS	479.1205	

Cmpd 1, 0.6 min

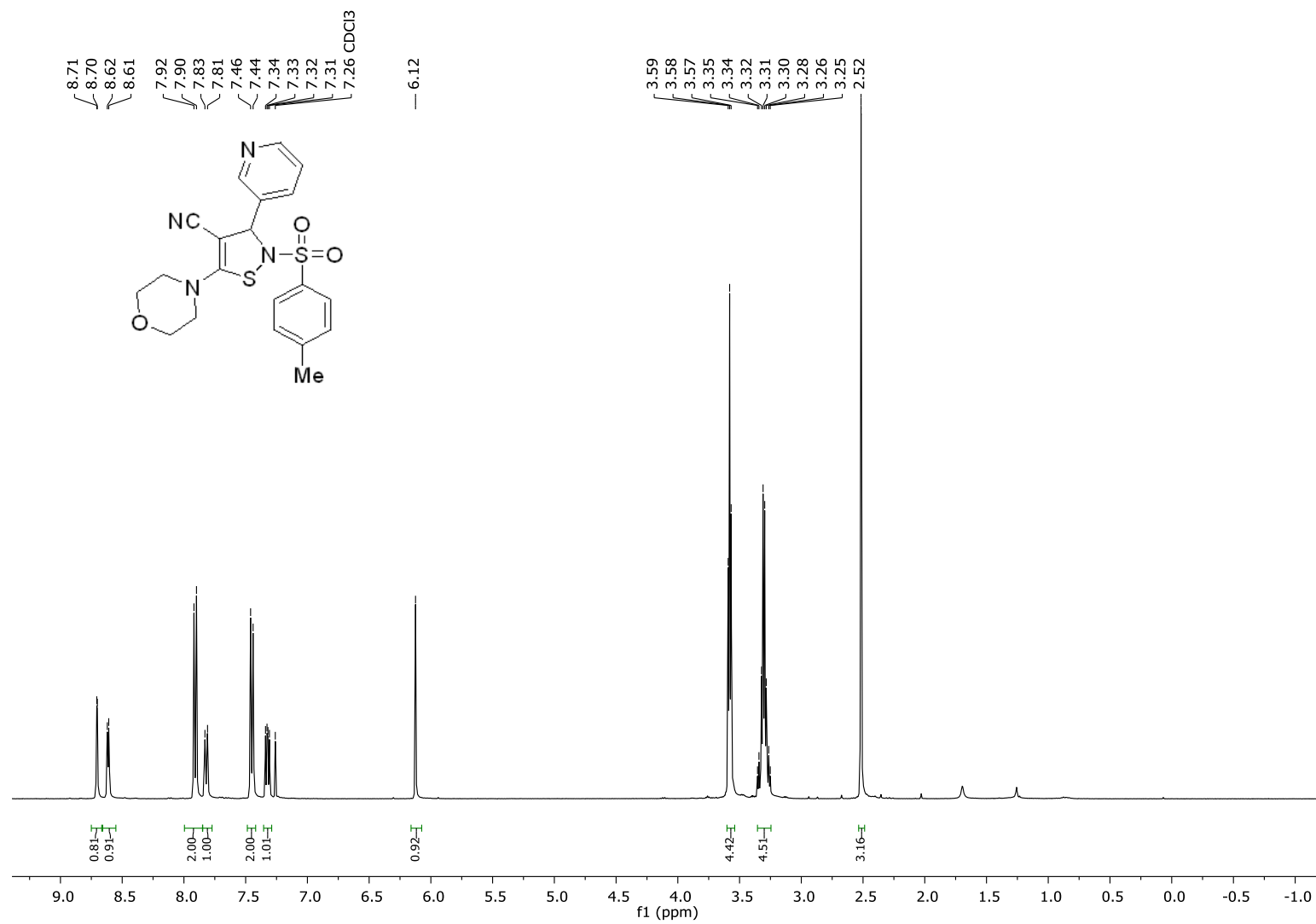


#	Wavelength	Intensity
0	196	37.2

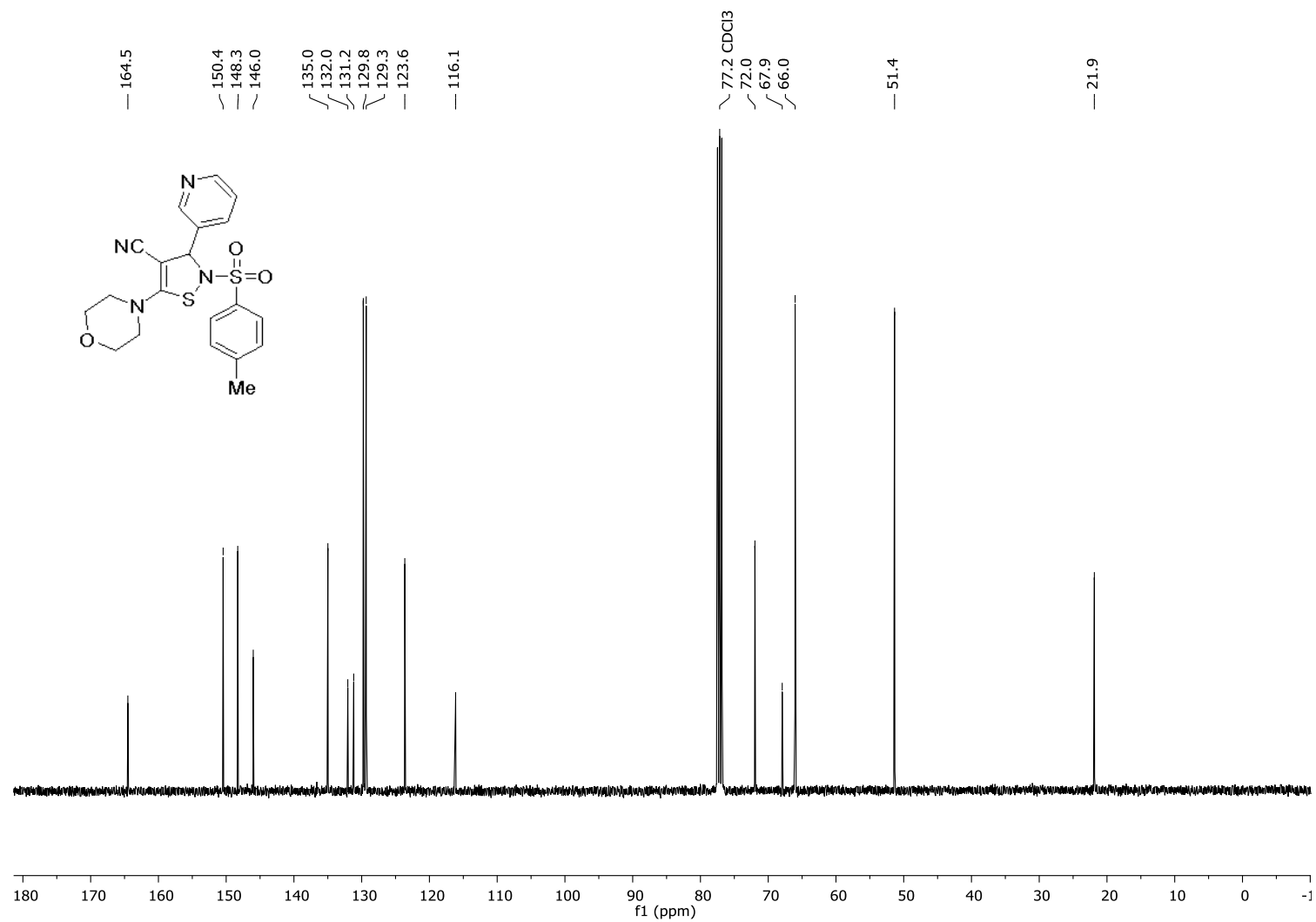


#	m/z	Res.	S/N	I	I %	FWHM
1	199.1436	18758	8568632.0	203115	3.7	0.0106
2	277.1201	20394	6395646.5	151606	2.8	0.0136
3	479.1205	39483	231824176.0	5495283	100.0	0.0121
4	480.1233	30727	55933656.0	1325881	24.1	0.0156
5	481.1192	22353	21274806.0	504309	9.2	0.0215
6	482.1200	18624	4666859.0	110626	2.0	0.0259
7	501.1019	27211	31876052.0	755607	13.8	0.0184
8	502.1043	21451	8504620.0	201598	3.7	0.0234
9	979.2135	31310	10958886.0	259775	4.7	0.0313
10	980.2160	26529	6093268.0	144438	2.6	0.0369

¹H NMR (CDCl₃) spectrum of **3ta**

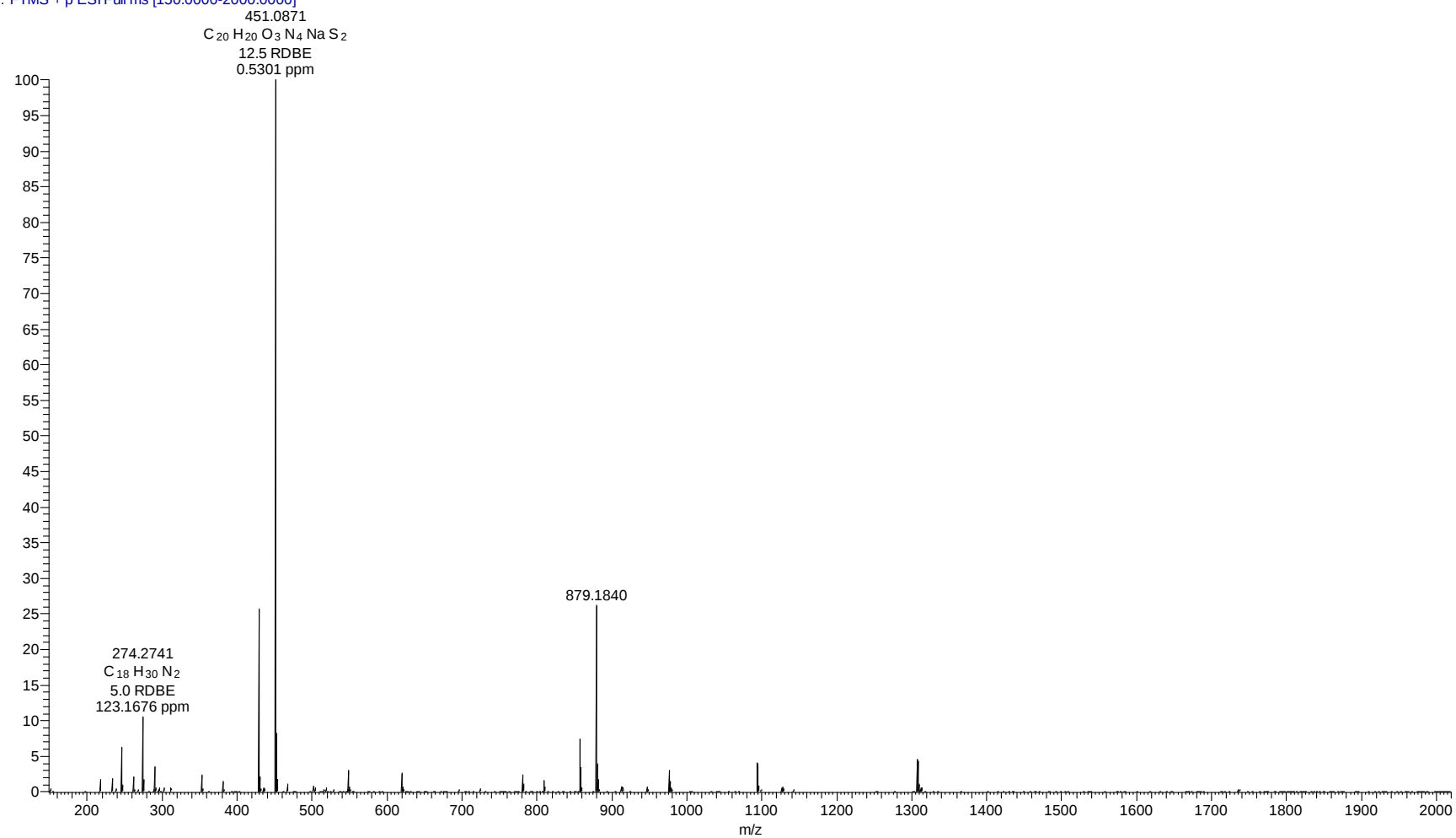


^{13}C NMR (CDCl_3) spectrum of **3ta**

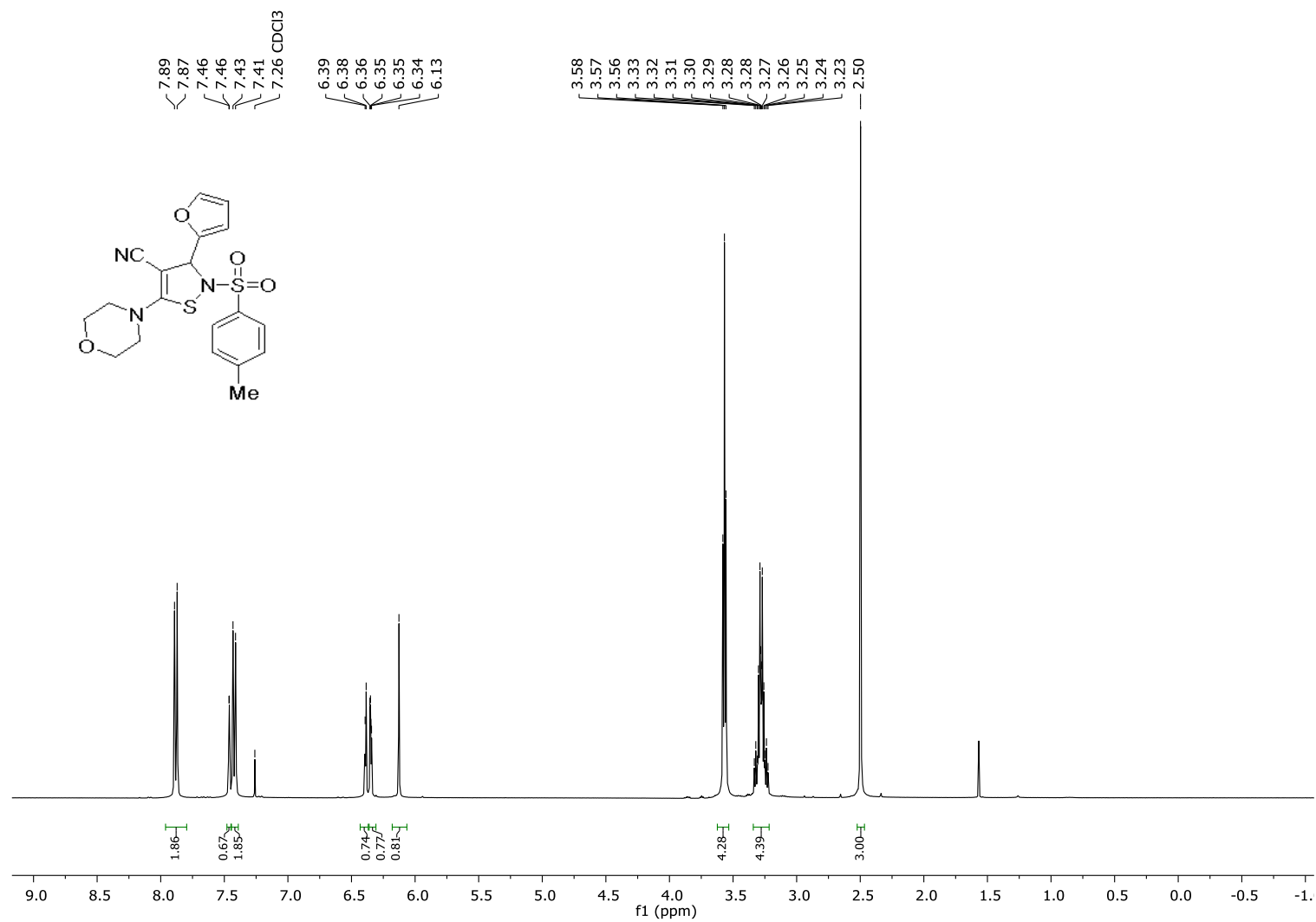


HRMS of **3ta**

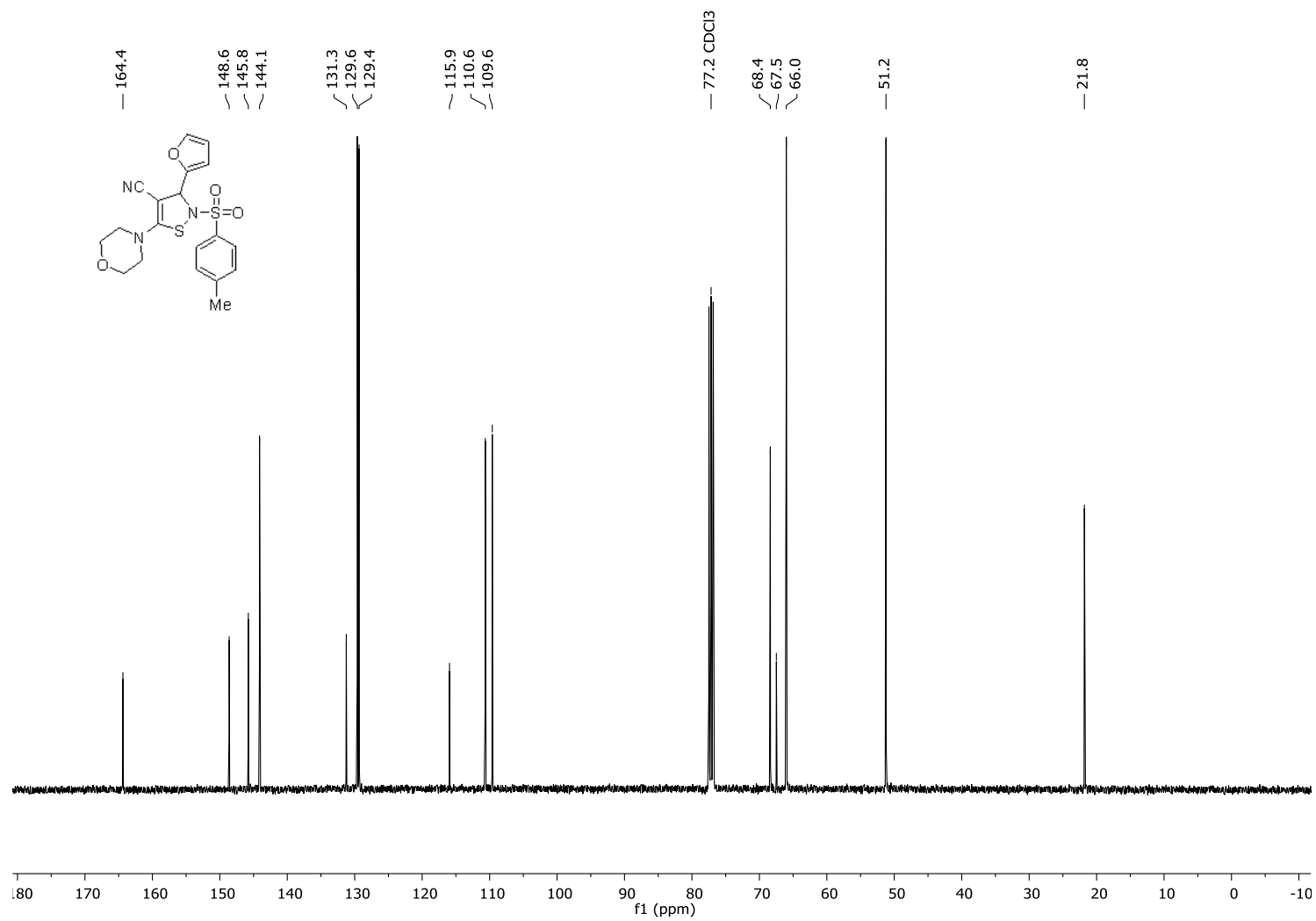
VF-136_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 6.10E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (CDCl₃) spectrum of **3ua**

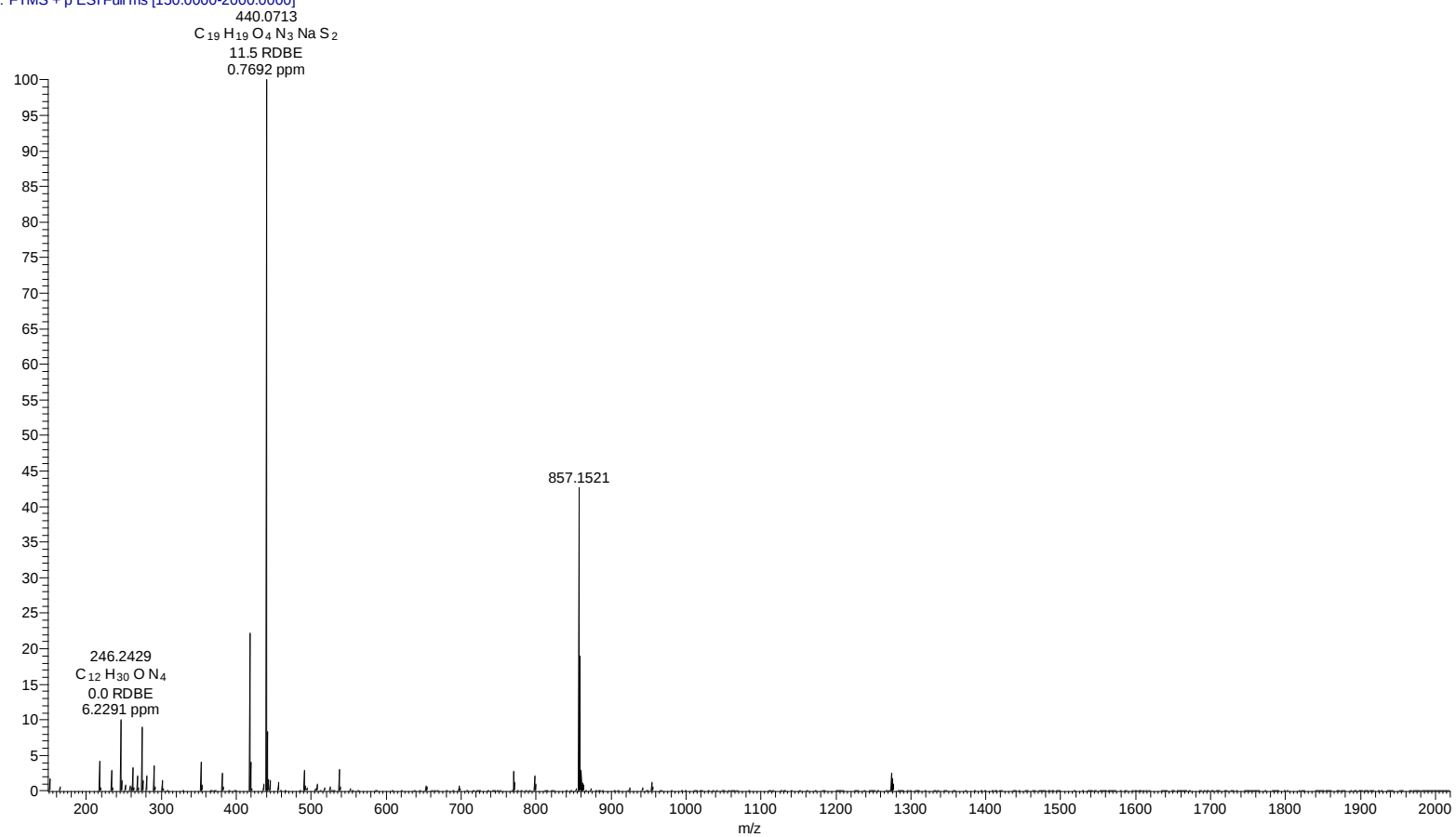


^{13}C NMR (CDCl_3) spectrum of **3ua**

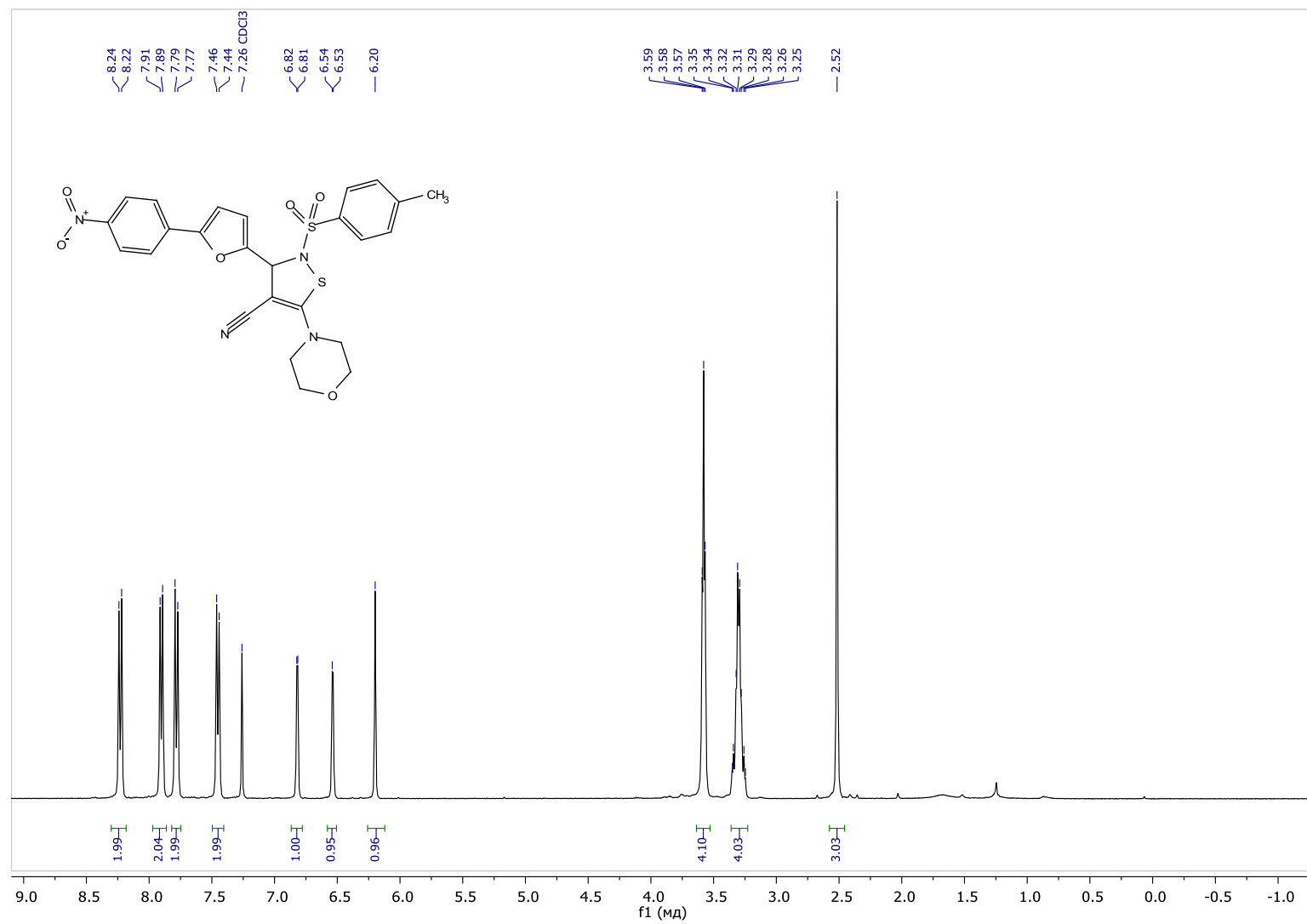


HRMS of **3ua**

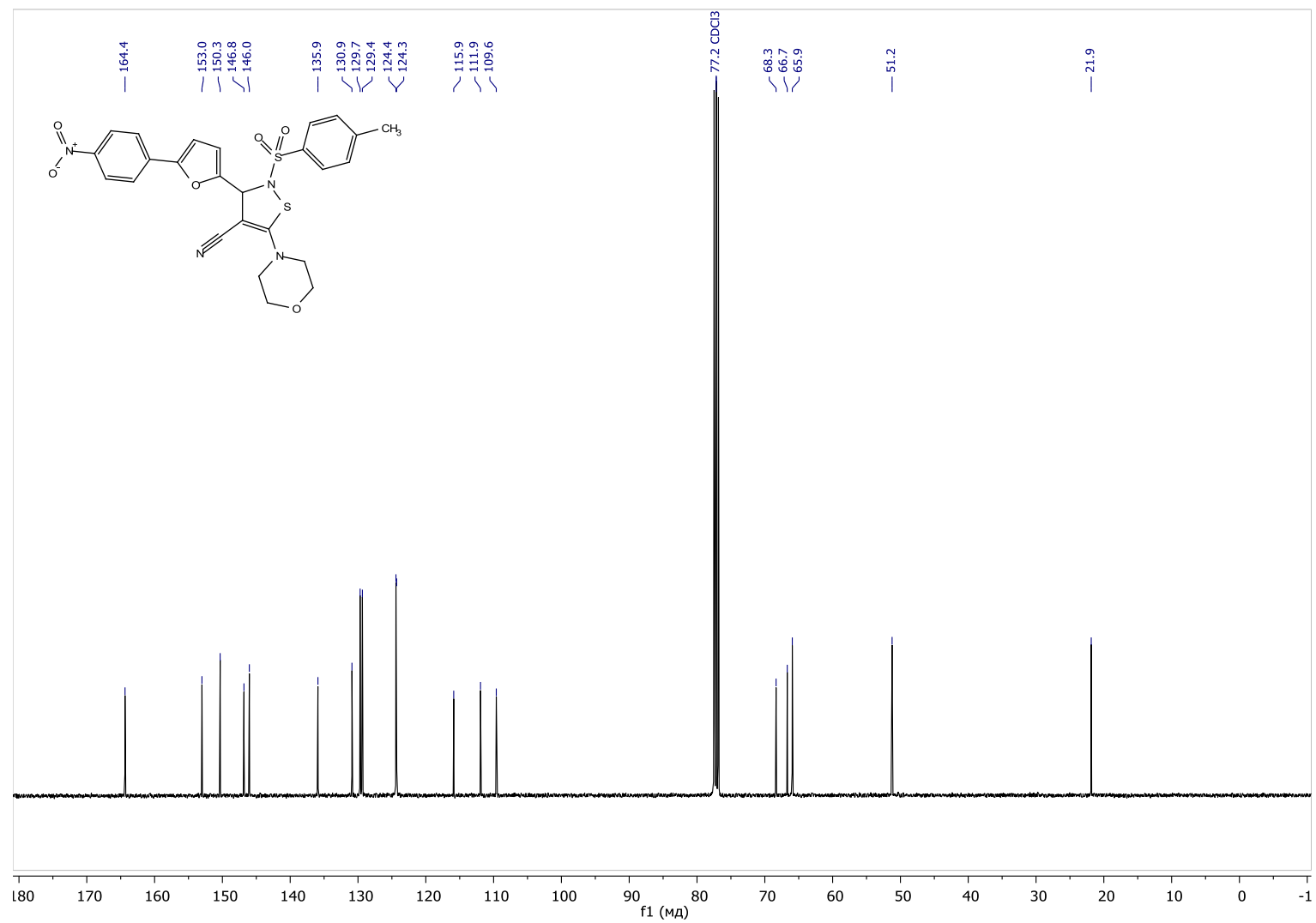
VF-96_Pos #29-53 RT: 0.25-0.45 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 9.47E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



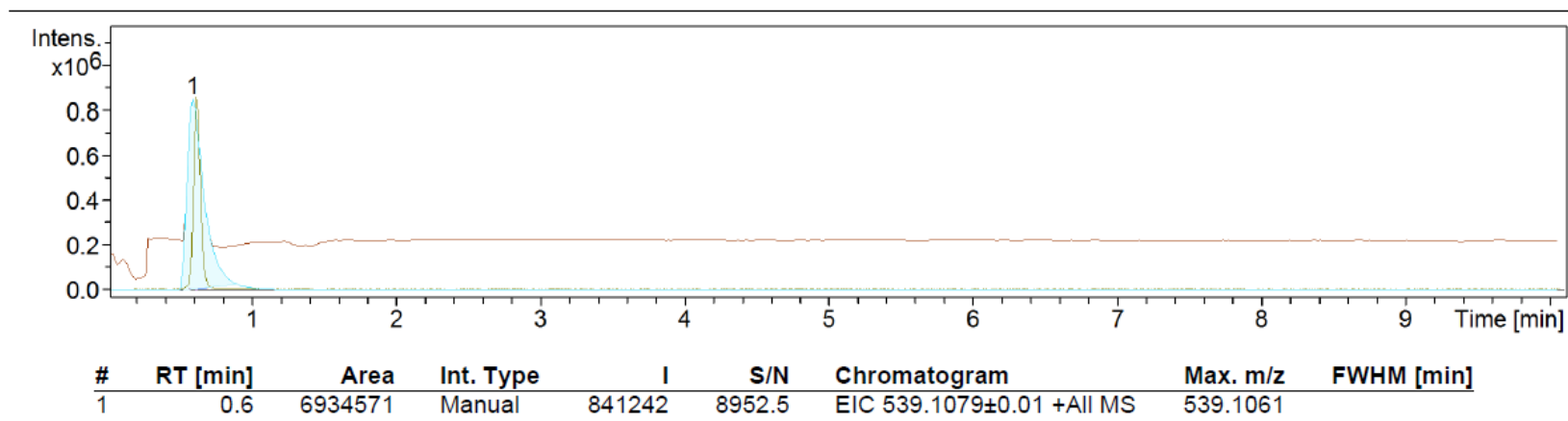
^1H NMR (CDCl_3) spectrum of **3va**



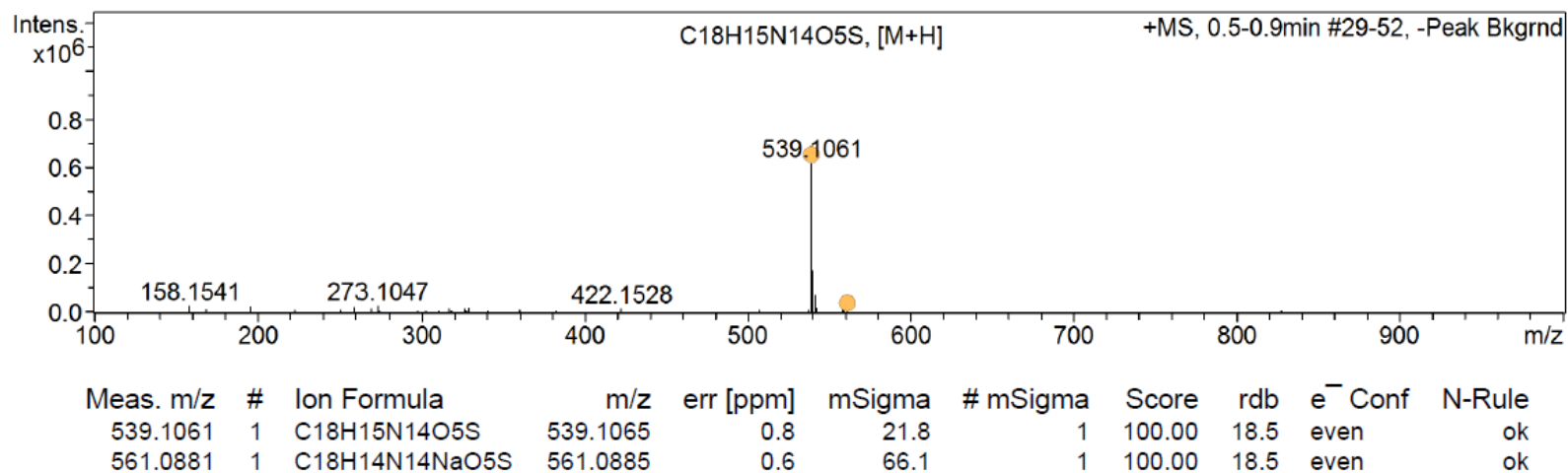
^{13}C NMR (CDCl_3) spectrum of **3va**



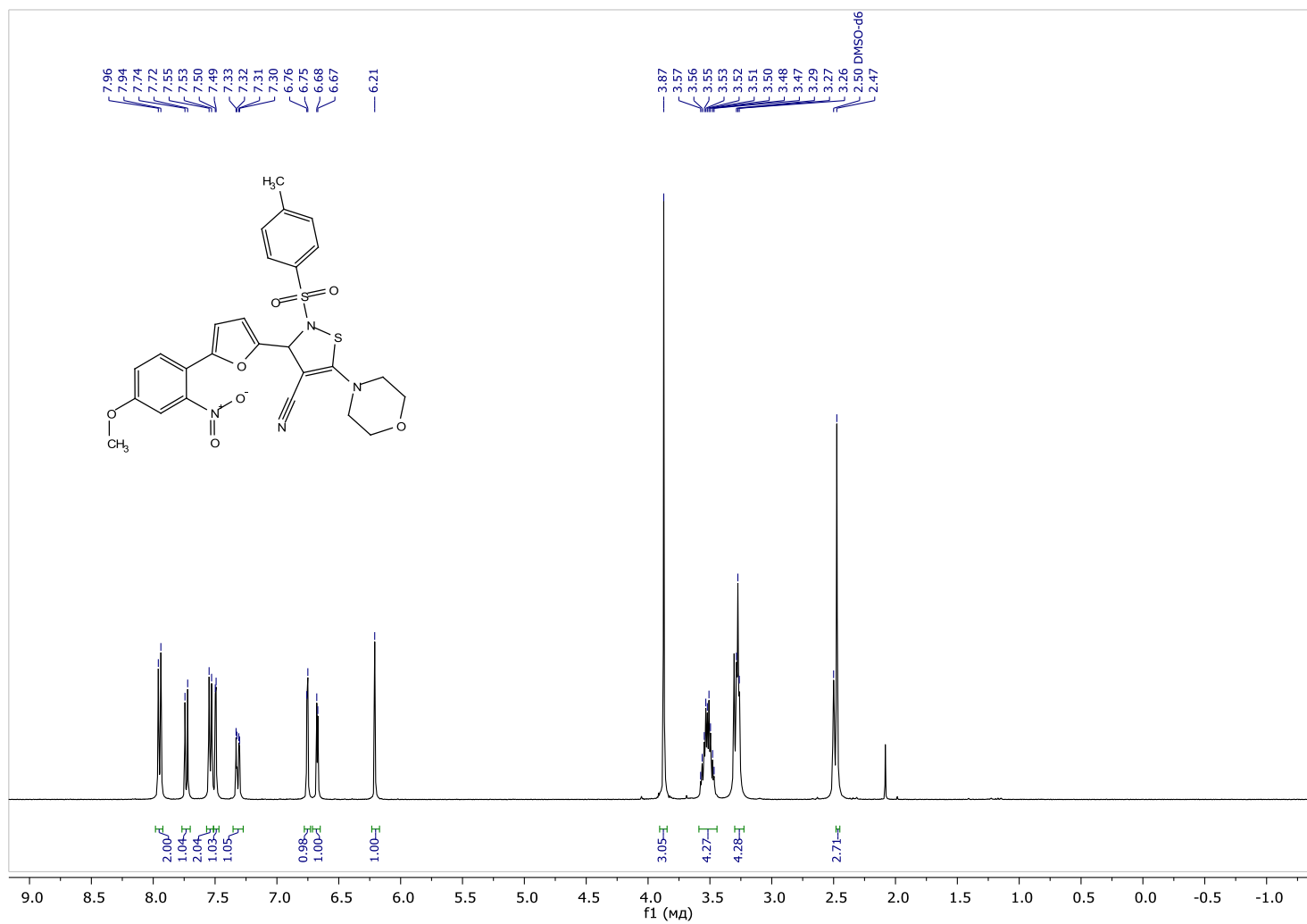
HRMS of 3va



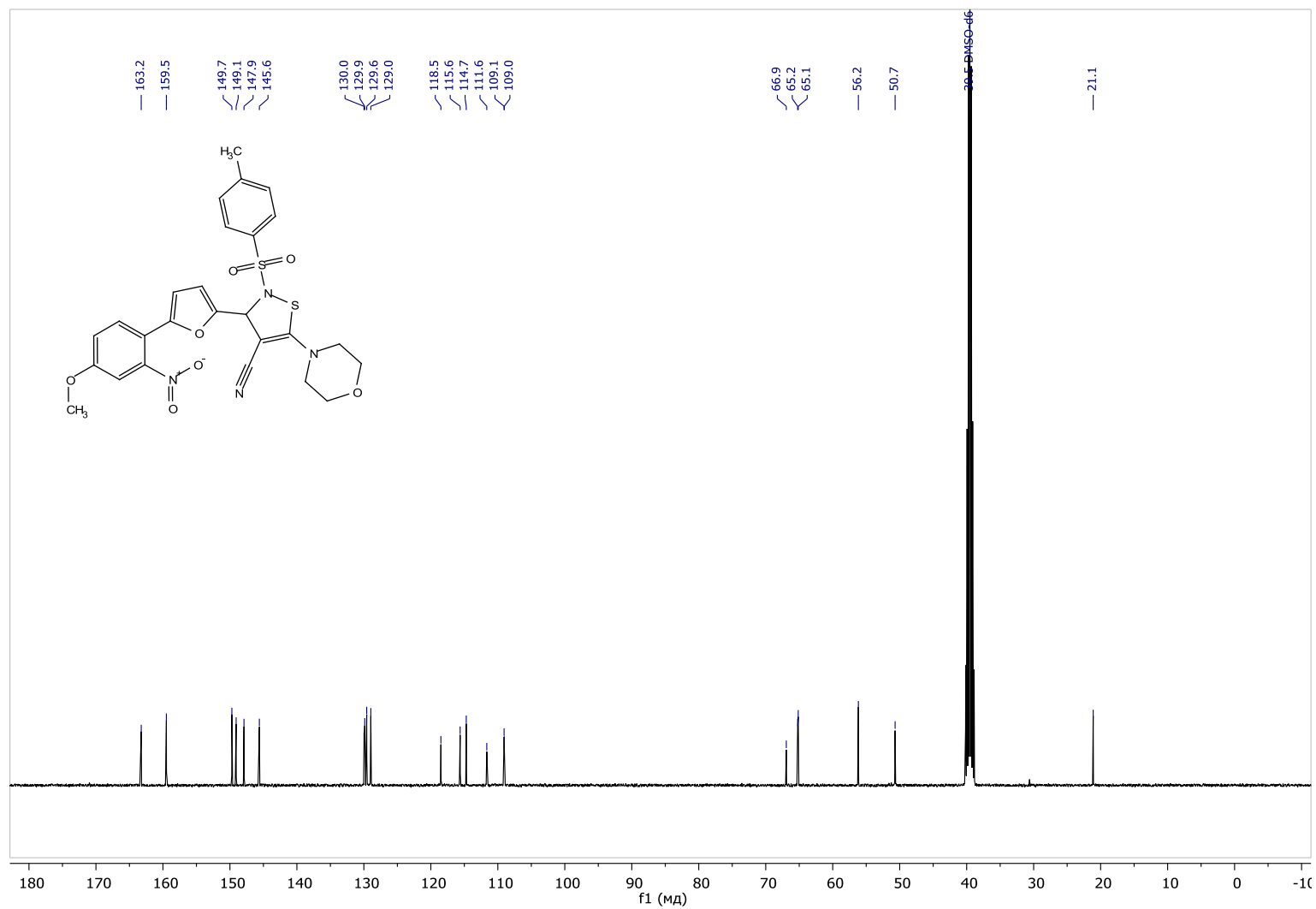
Cmpd 1, 0.6 min



¹H NMR (DMSO-*d*₆) spectrum of **3wa**

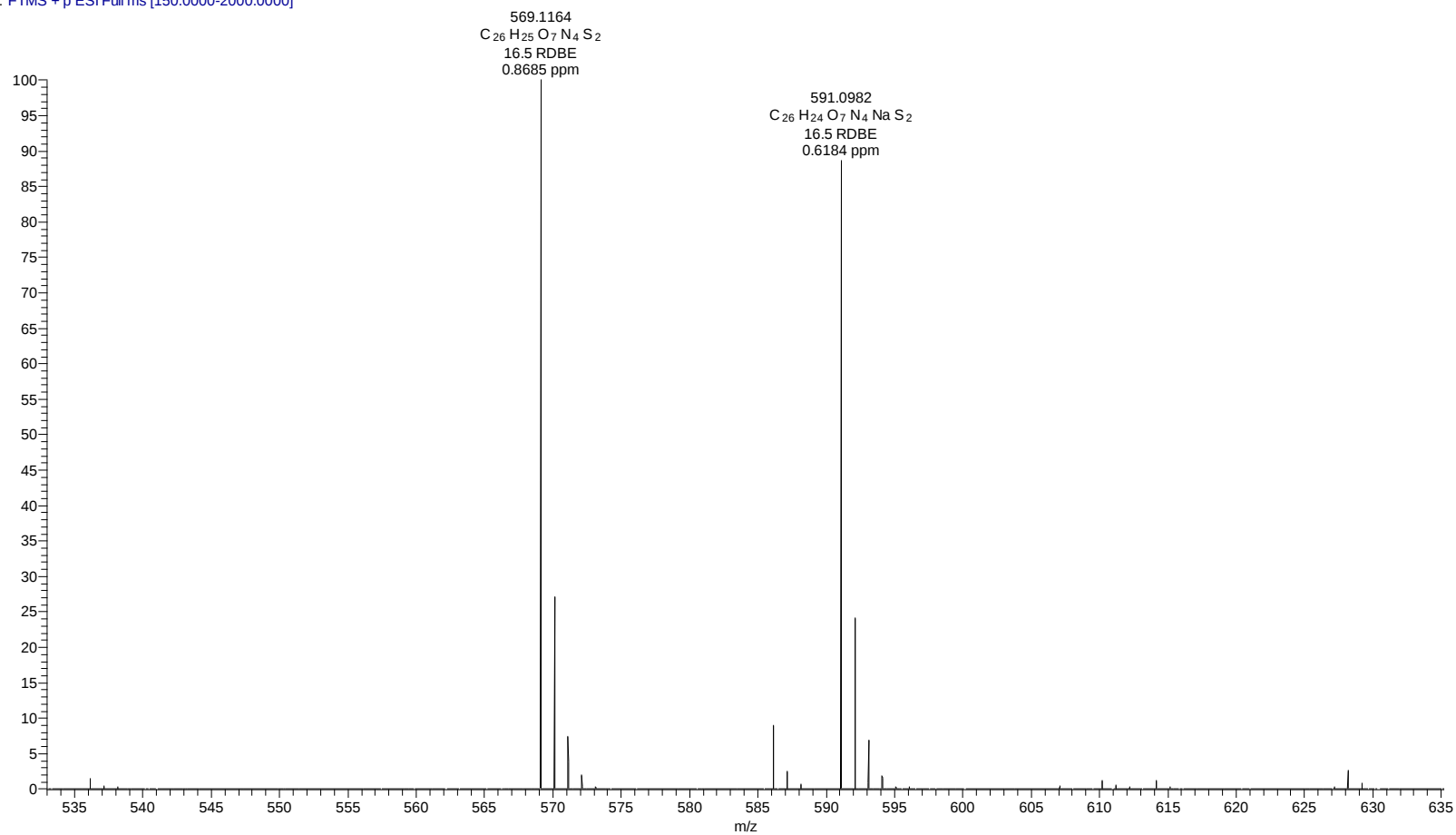


^{13}C NMR (DMSO- d_6) spectrum of **3wa**

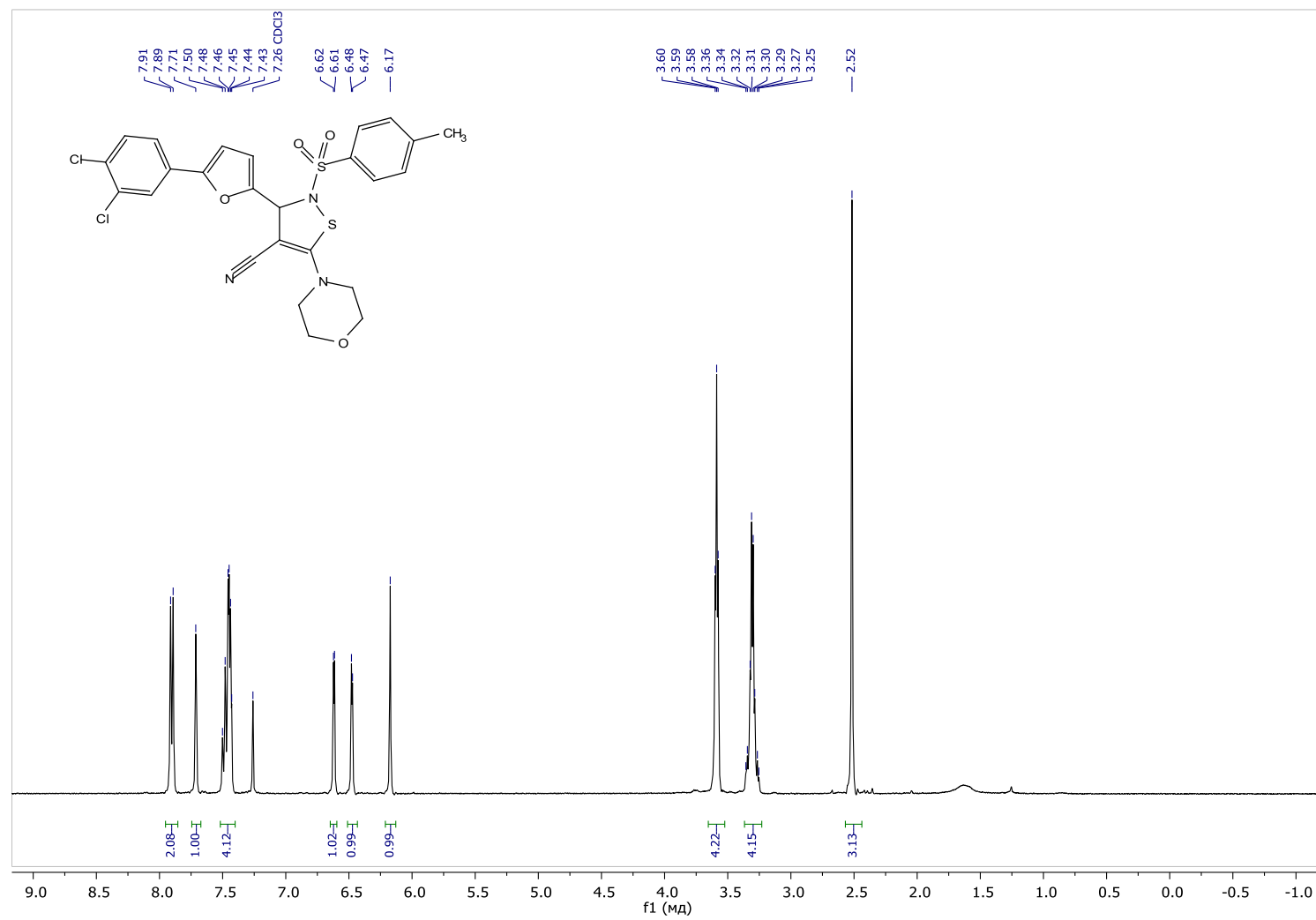


HRMS of **3wa**

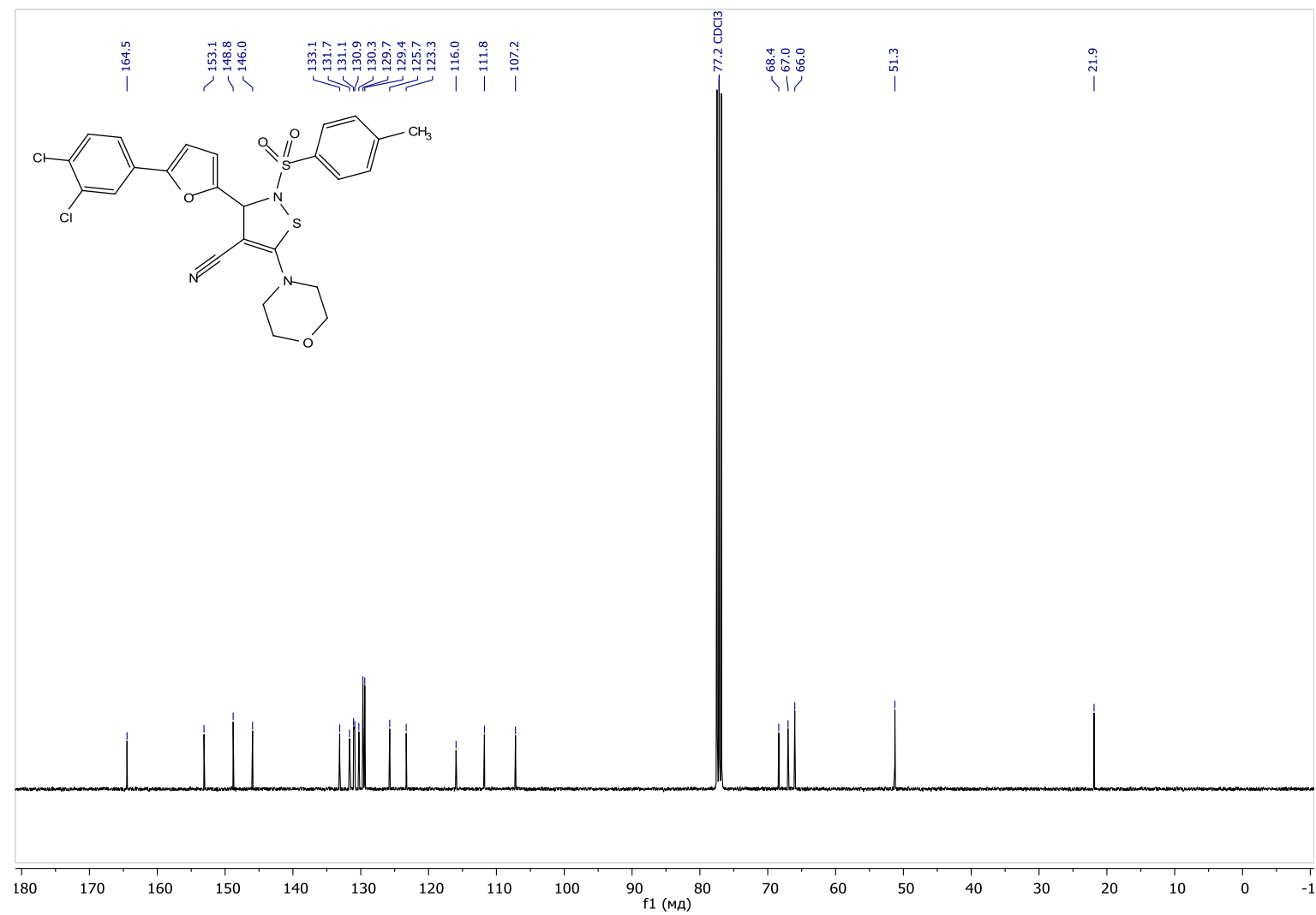
N-21_Pos #29-45 RT: 0.25-0.39 AV: 17 SB: 24 0.05-0.12 , 0.76-0.88 NL: 2.93E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (CDCl₃) spectrum of **3xa**

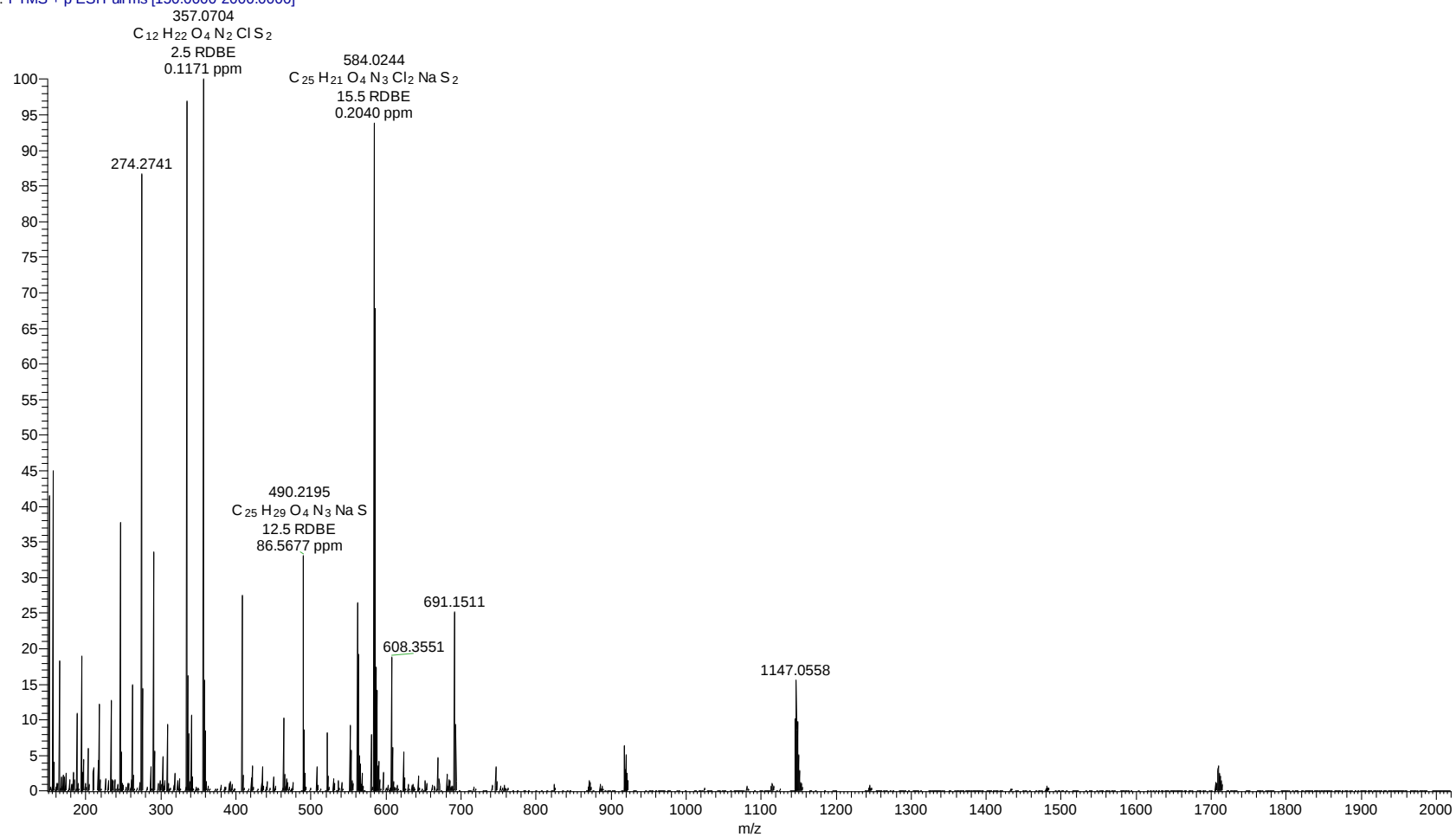


^{13}C NMR (CDCl_3) spectrum of **3xa**

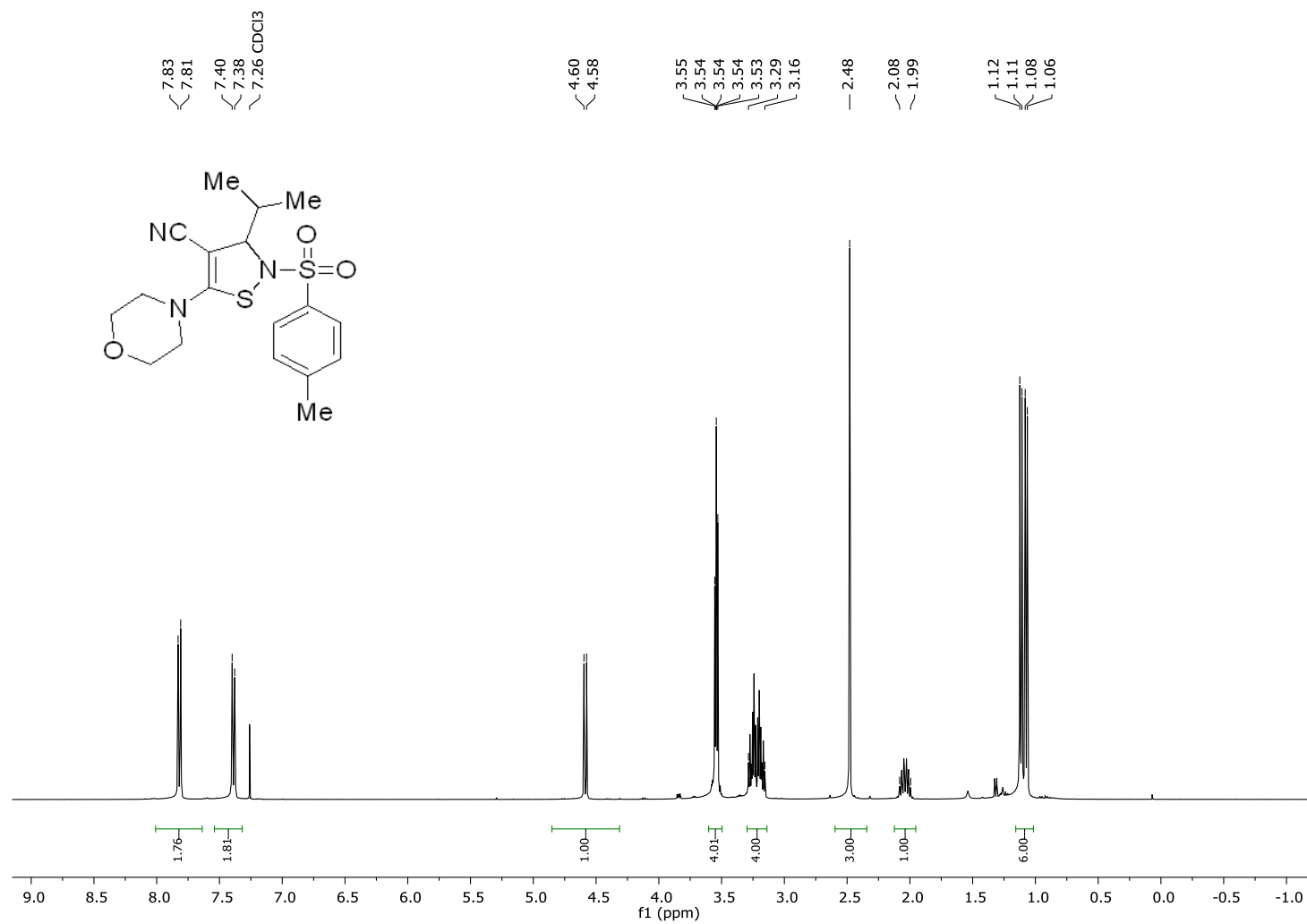


HRMS of **3xa**

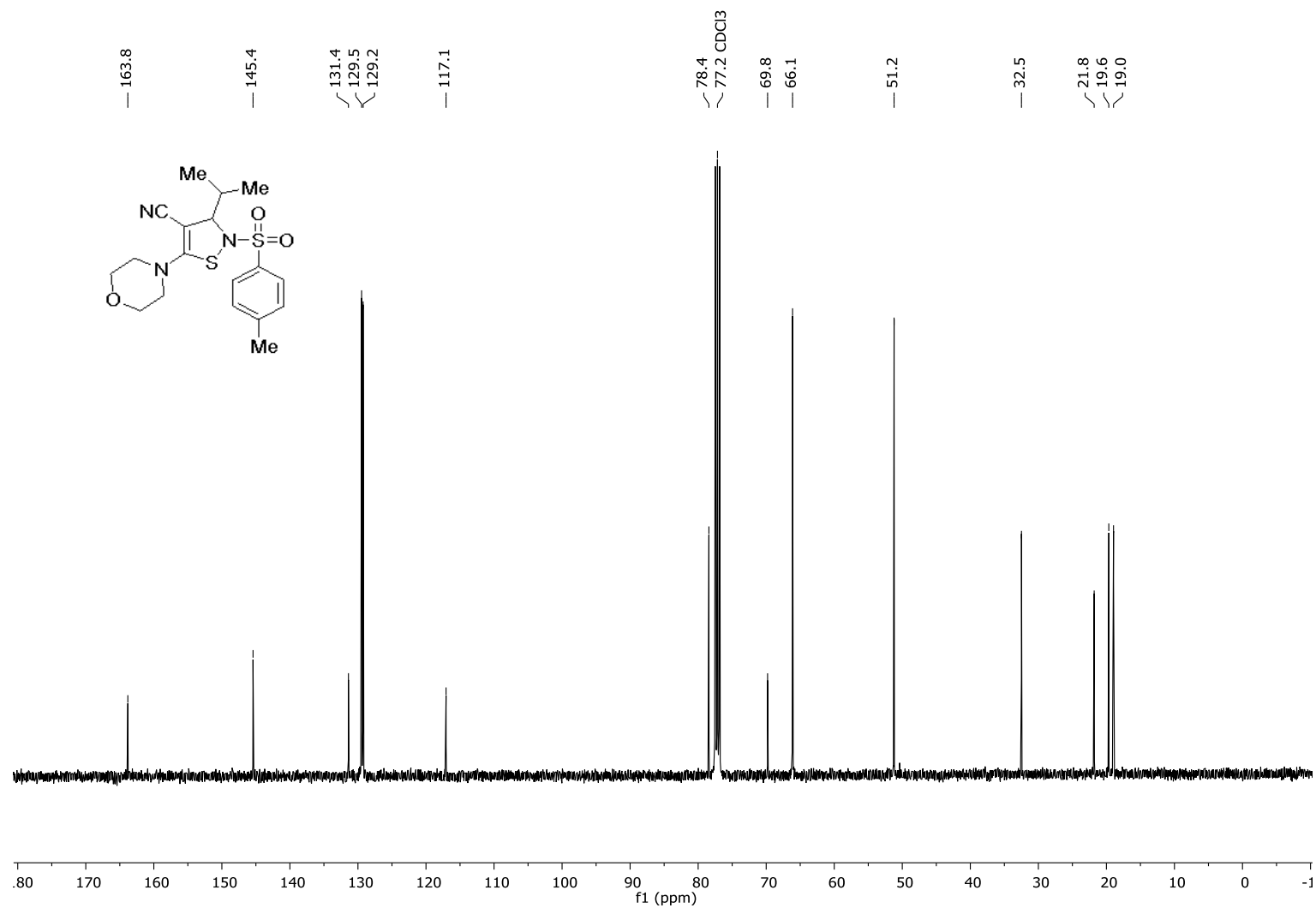
N20_Pos #30-54 RT: 0.26-0.46 AV: 25 SB: 21 0.06-0.11 , 0.83-0.95 NL: 1.24E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]



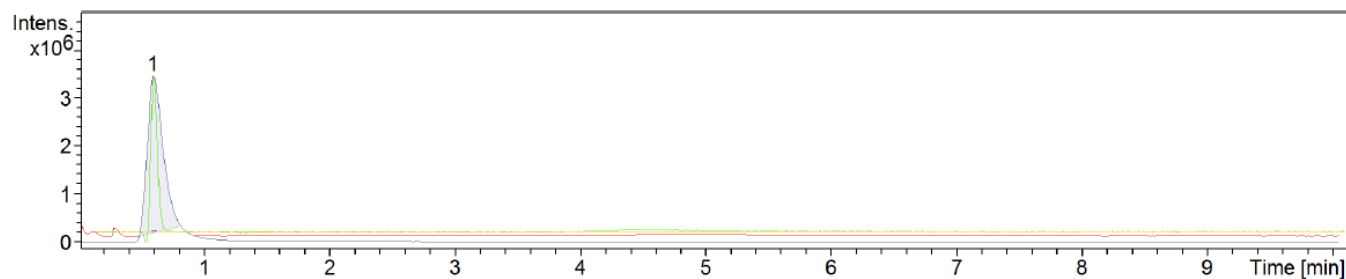
¹H NMR (CDCl₃) spectrum of **3ya**



^{13}C NMR (CDCl_3) spectrum of **3ya**

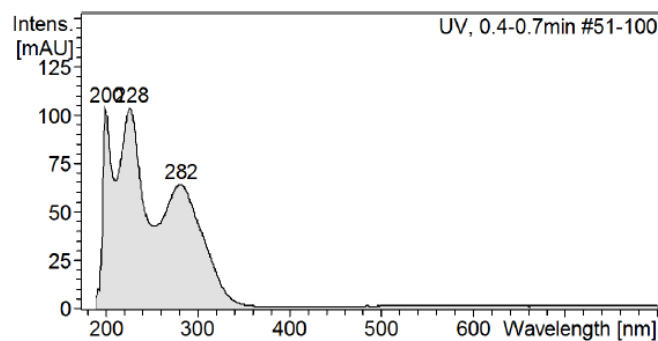


HRMS of 3ya

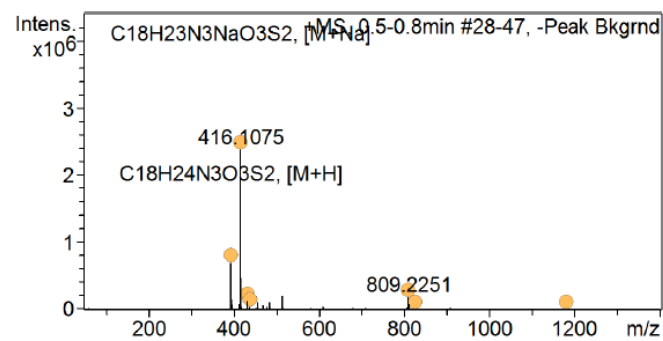


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	28001498	Manual	3441882	10956.4	EIC 416.1075±0.02 +All MS	416.1075	

Cmpd 1, 0.6 min

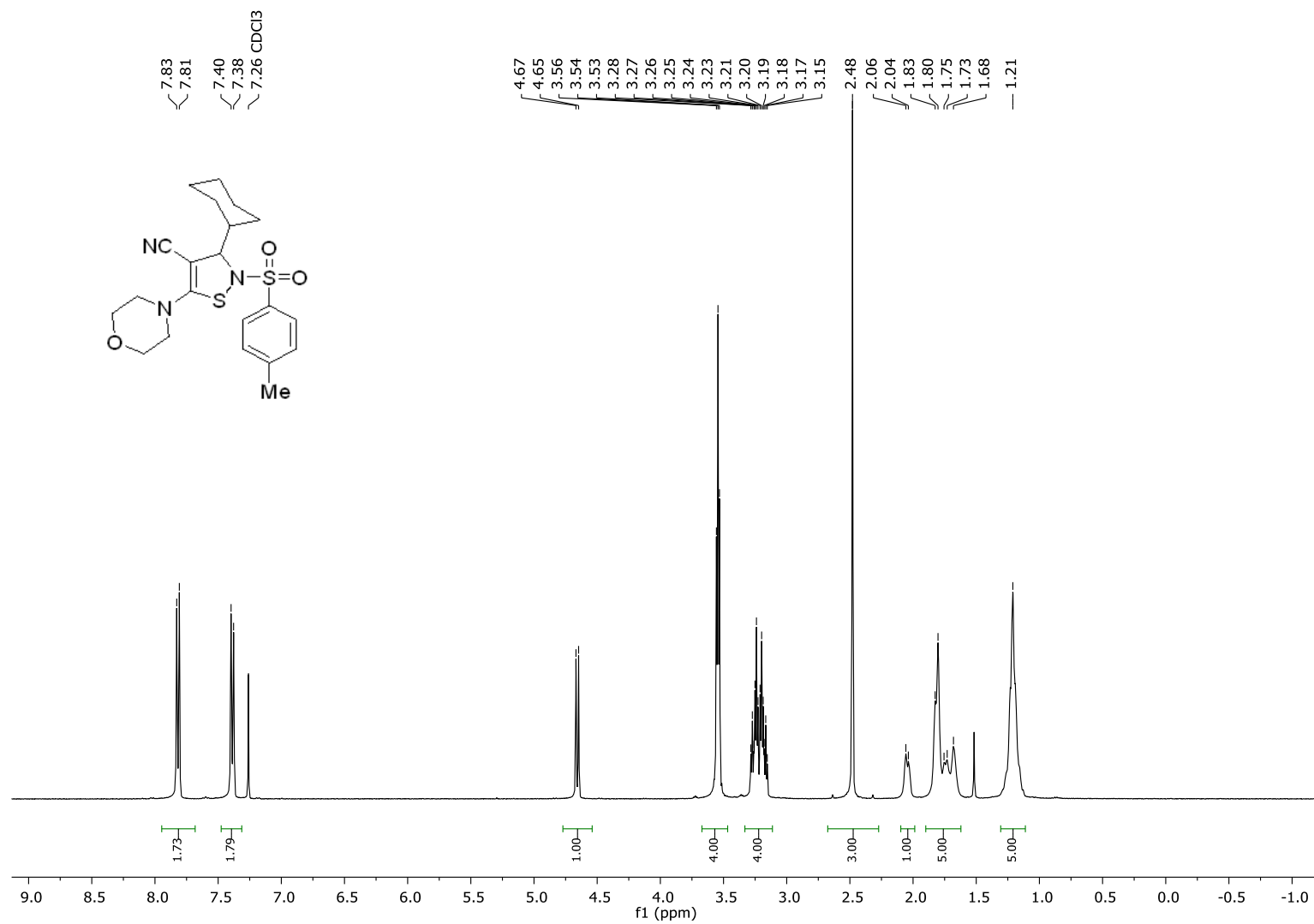


#	Wavelength	Intensity
0	200	103.4
1	228	103.4
2	282	64.3

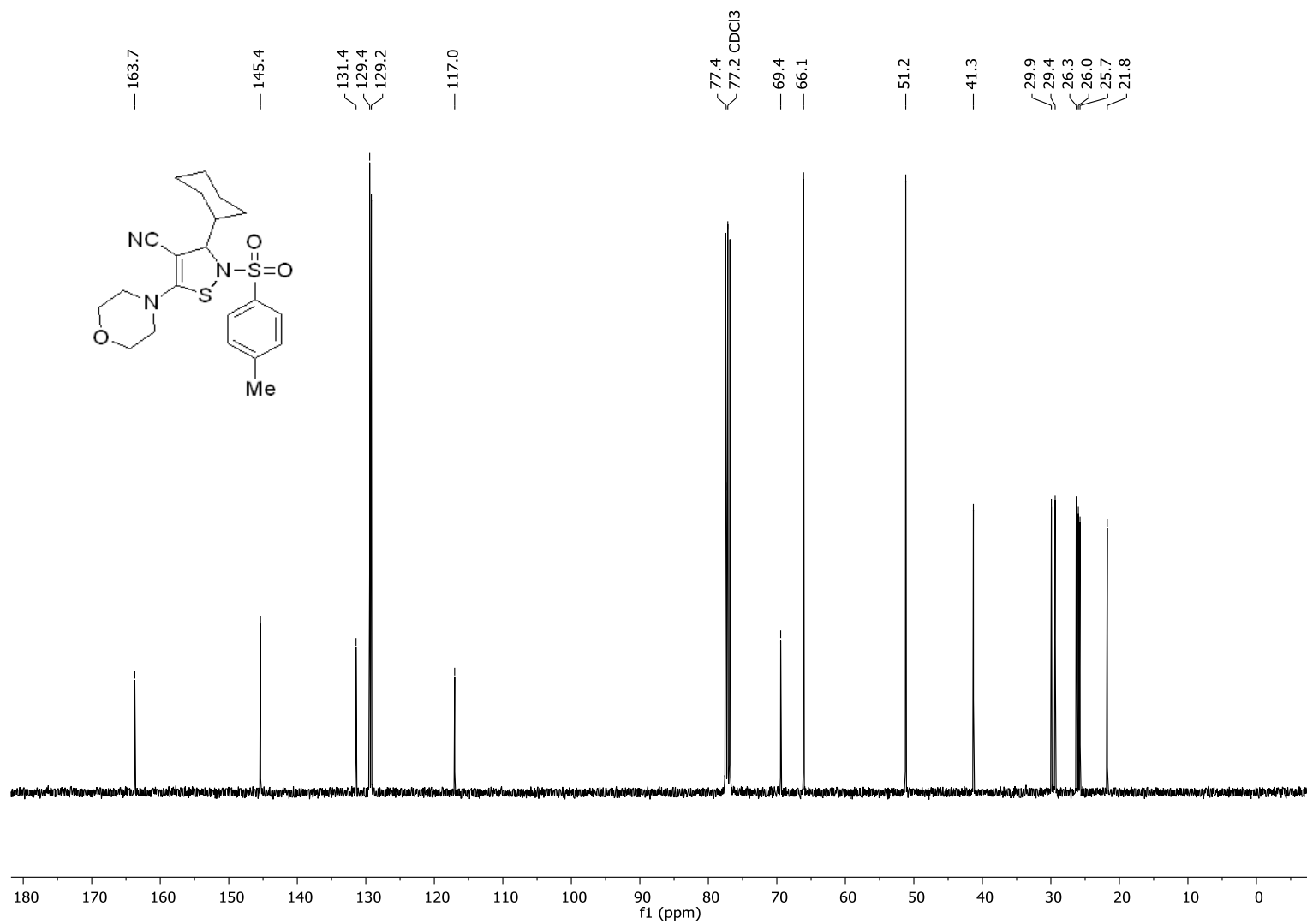


#	m/z	Res.	S/N	I	I %	FWHM
1	394.1253	28045	533429088.0	696943	29.4	0.0141
2	395.1280	20363	114767552.0	149948	6.3	0.0194
3	416.1075	36261	1811445504.0	2366715	100.0	0.0115
4	417.1099	24977	351598240.0	459375	19.4	0.0167
5	418.1046	19490	162584656.0	212422	9.0	0.0215
6	432.0810	19893	95236416.0	124430	5.3	0.0217
7	456.0993	19770	76034040.0	99341	4.2	0.0231
8	484.0944	19878	81571528.0	106576	4.5	0.0244
9	514.1048	21448	153495024.0	200546	8.5	0.0240
10	809.2251	27488	137441984.0	179573	7.6	0.0294

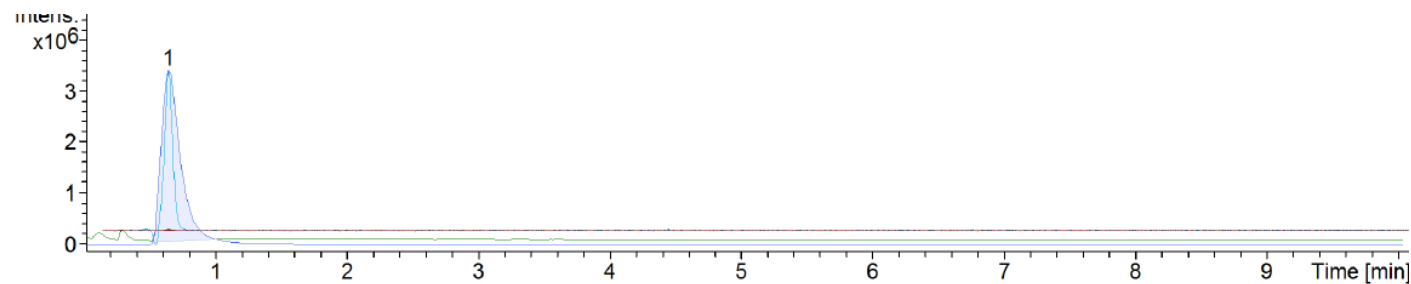
¹H NMR (CDCl₃) spectrum of **3za**



^{13}C NMR (CDCl_3) spectrum of **3za**

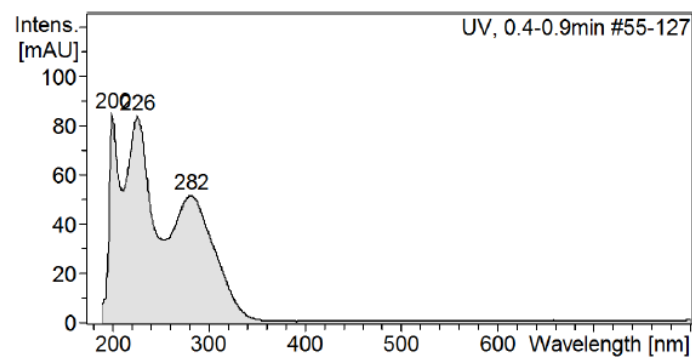


HRMS of **3za**

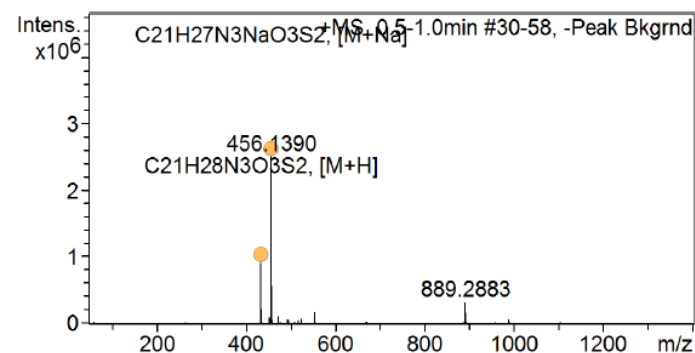


#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.6	33195916	Manual	3386411	17067.4	EIC 456.1390±0.02 +All MS	456.1390	

Cmpd 1, 0.6 min



#	Wavelength	Intensity
0	200	84.4
1	226	83.6
2	282	51.9



#	m/z	Res.	S/N	I	I %	FWHM
1	434.1568	29792	34548200.0	920691	36.9	0.0146
2	435.1593	21144	8284613.0	220781	8.8	0.0206
3	436.1548	17322	3654905.5	97401	3.9	0.0252
4	456.1390	37563	93632856.0	2495267	100.0	0.0121
5	457.1416	26687	20877188.0	556366	22.3	0.0171
6	458.1370	19834	9099524.0	242498	9.7	0.0231
7	472.1124	19770	4194104.8	111771	4.5	0.0239
8	554.1365	20978	6182741.0	164767	6.6	0.0264
9	889.2883	32375	11791003.0	314224	12.6	0.0275
10	890.2909	25962	5869462.0	156418	6.3	0.0343