

Structure-Activity Relationship Studies on the Inhibition of the Bacterial Translation of Novel Odilorhabdins Analogues

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Docking studies of peptides **1** (NOSO-95179), **50** and **53**

The *Autodock Vina* software¹ was used to perform docking studies of peptide **1** (NOSO-95179) and its analogues **50** and **53** in the *Thermus thermophilus* 70S ribosome (6CAE)². An active region of 6CAE residues within 12 Å around the ligands was used for the docking studies. The conformations of the ligand **1**, **50** and **53** structures were based on biologically active conformation of NOSO-95179. Rotation of amide bonds was restricted in ligands **50** and **53**.

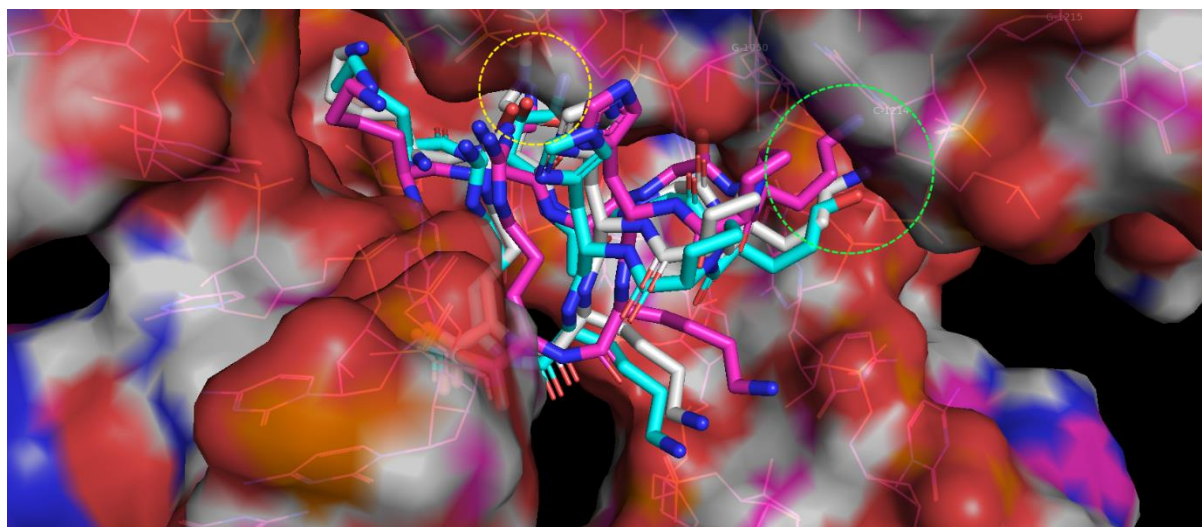


Figure S1. Overlay of **1** (NOSO-95179; magenta), **50** (gray) and **53** (cyan) in primary binding site of Bacterial Ribosome decoding center. Orientation of γ -aminopropyl sidechain of D-Orn (for **1** and **50**) and that of γ -hydroxypropyl residue (for **53**) is marked by green-colored dotted circle (right-hand site). Positioning of Dab(β OH sidechain (for **1** and **53**) and that of N-methyl analog in **50** is marked by yellow-colored dotted circle (middle).

(1) Trott, O.; Olson, A., J. AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J. Comput. Chem.* **2010**, *31*, 455–461.

doi:[10.1002/jcc.21334](https://doi.org/10.1002/jcc.21334)

(2) PDB ID: 6CAE; See <https://www.rcsb.org/structure/6CAE>

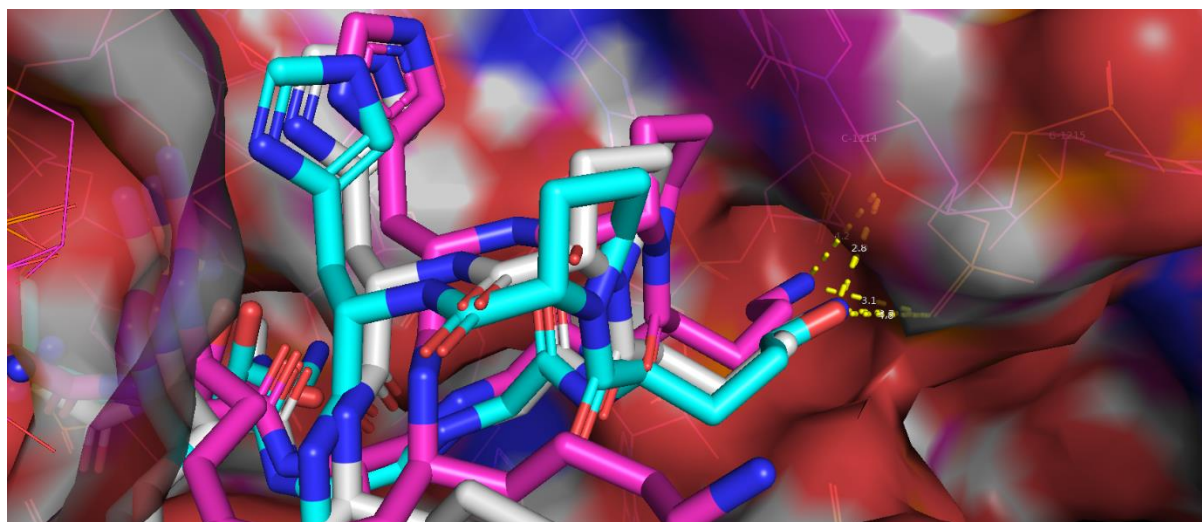


Figure S2. Calculated distances in Å for the hydrogen bonding between peptides **1**, **53** and sugar-phosphate backbone atoms of 16S rRNA helices 31, 32, and 34

Interacting moieties	Ribose oxygen O4' of 16S rRNA residue C1214	Oxygen of phosphate (P=O) between 16S residues C1214 and G1215
D-Orn residue of 1 (NOSO-95179)	4.2 Å	3.1 Å
γ -Hydroxypropyl residue of 53	2.8 Å	4.8 Å

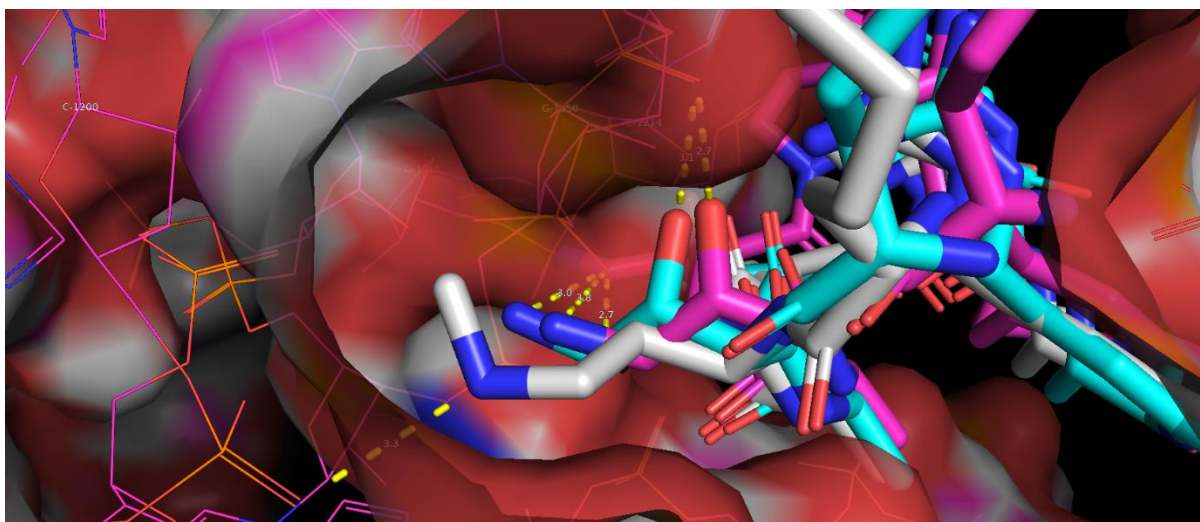


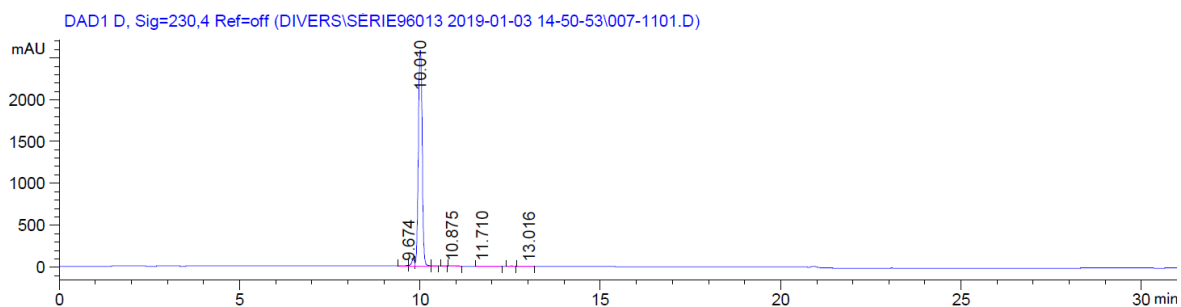
Figure S3. Calculated distances in Å for the hydrogen bonding between peptides **1**, **50** and sugar-phosphate backbone atoms of 16S rRNA helices 31, 32, and 34

Interacting moieties	Oxygen of phosphate (P=O) between 16S residues G1050 and C1051	Oxygen of phosphate (P=O) between 16S residues C1051 and U1052	Oxygen of phosphate (P=O) between 16S residues U-1199 and C-1200
Dab(β OH) residue of 1	3.8 Å (for NH ₂)	2.7 Å (for OH)	-
<i>N</i> -methyl Dab(β OH) residue of 50	5.0 Å (for NHMe) 2.7 Å (for OH)	-	3.3 Å (for NHMe)

LC-MS Spectra of analogues 40-59

40

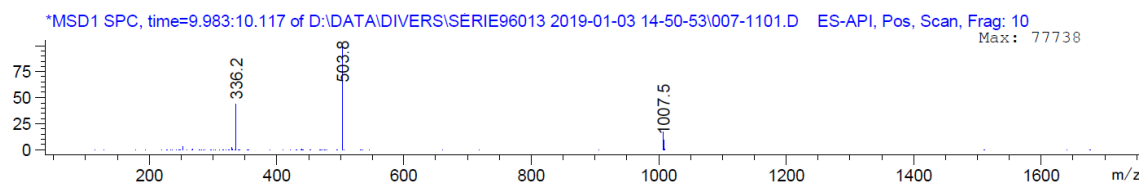
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

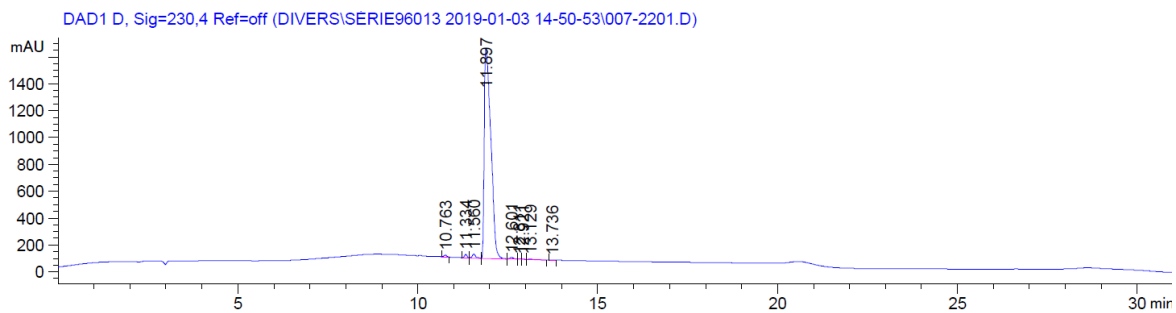
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.674	BV	0.0721	42.17771	8.76833	0.2174
2	9.811	VV	0.0832	426.32272	78.71645	2.1974
3	10.010	VB	0.1174	1.88536e4	2576.44214	97.1755
4	10.359	BB	0.0742	8.24217	1.77321	0.0425
5	10.657	BB	0.0802	5.81694	1.12650	0.0300
6	10.875	BB	0.1372	12.90220	1.30684	0.0665
7	11.710	BB	0.1688	12.74033	1.02655	0.0657
8	12.538	BB	0.0827	16.02421	2.97928	0.0826
9	13.016	BB	0.2040	23.78063	1.69207	0.1226

Totals : 1.94016e4 2673.83136



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.054	1546864	1006.45 I
		503.75 I
		336.20 I

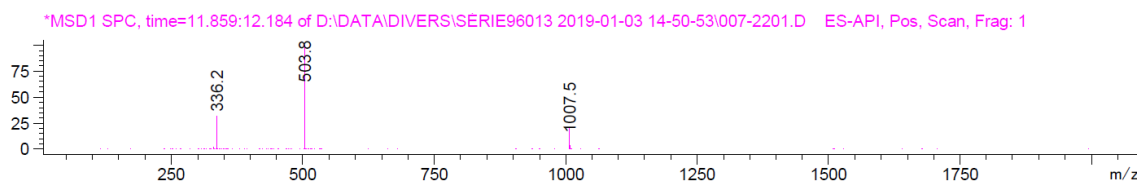
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.763	MM	0.0968	75.97897	13.08061	0.3721
2	11.334	BV	0.0762	124.42718	25.81097	0.6094
3	11.560	VB	0.0980	201.65620	30.15701	0.9876
4	11.897	BB	0.2224	1.98699e4	1562.52869	97.3079
5	12.601	BV	0.1028	85.01138	12.59321	0.4163
6	12.811	VV	0.0770	8.98535	1.71812	0.0440
7	12.921	VB	0.0704	8.79136	1.95805	0.0431
8	13.129	BB	0.1258	33.24395	3.81106	0.1628
9	13.736	BB	0.0900	11.61539	2.05413	0.0569

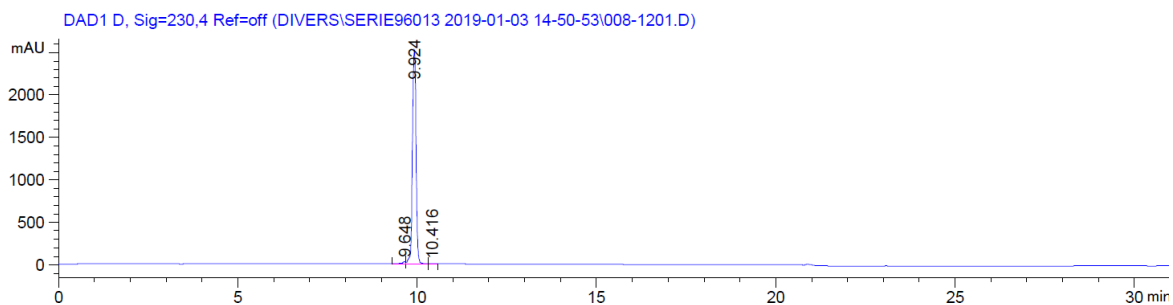
Totals : 2.04196e4 1653.71185



Retention Time (MS)	MS Area	Mol. Weight or Ion
11.925	5042406	1007.45 I
		1006.40 I
		503.80 I
		336.20 I

41

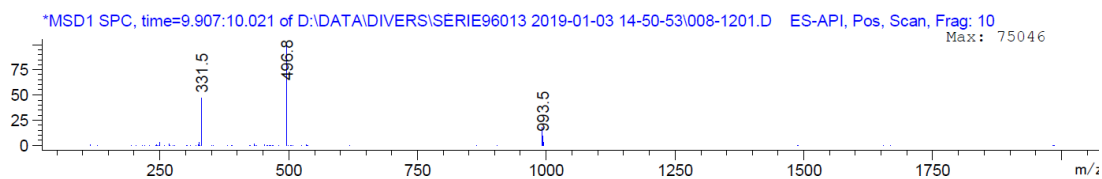
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

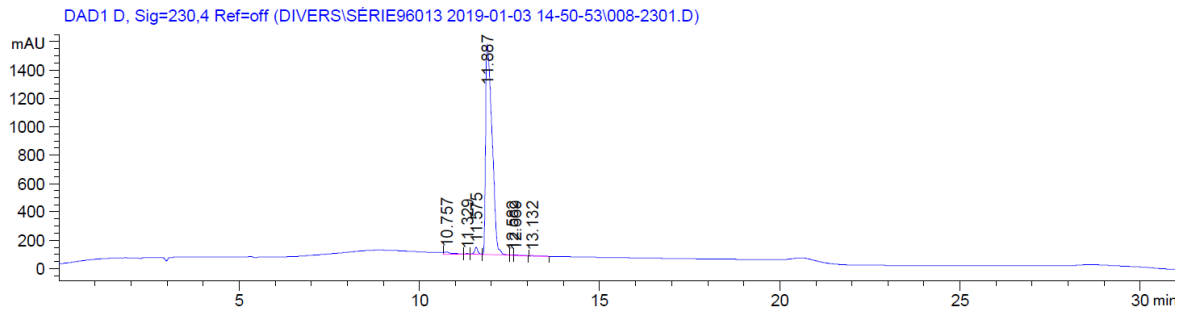
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.648	BV	0.0966	152.59465	22.64439	0.8494
2	9.924	VV	0.1122	1.77832e4	2522.99902	98.9894
3	10.416	VB	0.1059	28.95081	4.22573	0.1612

Totals : 1.79648e4 2549.86913



Retention Time (MS)	MS Area	Mol. Weight or Ion
9.969	1515525	992.40 I
		496.80 I
		331.50 I

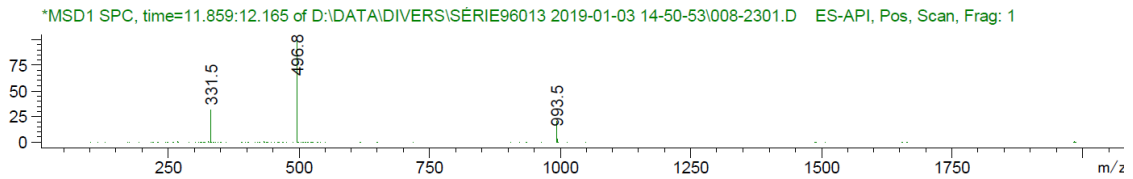
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.757	VB	0.1573	199.69034	16.97110	1.0513
2	11.329	BV	0.0829	14.16445	2.62610	0.0746
3	11.575	VV	0.0954	304.91779	48.45715	1.6053
4	11.887	VV	0.2176	1.84094e4	1474.84961	96.9208
5	12.582	VV	0.0857	23.37090	4.02872	0.1230
6	12.669	VB	0.1042	34.46262	4.66546	0.1814
7	13.132	BB	0.1174	8.26960	1.07901	0.0435

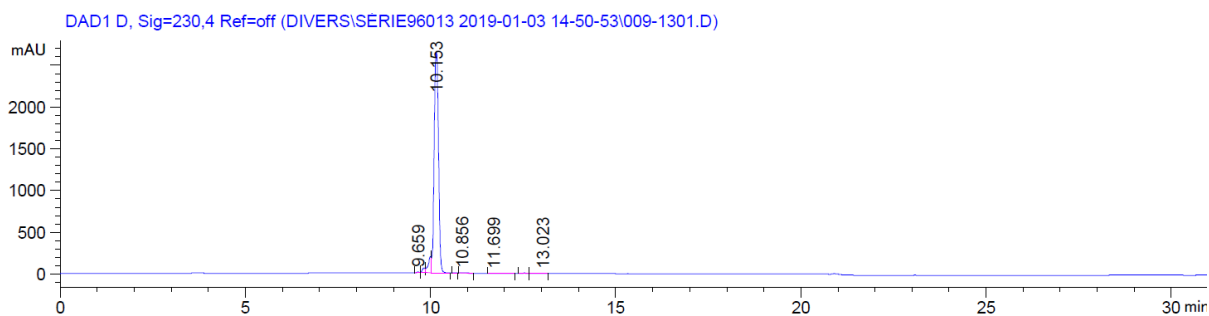
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Retention Time (MS)	MS Area	Mol. Weight or Ion
12.010	5222094	993.45 I
		992.45 I
		496.80 I
		331.55 I

42

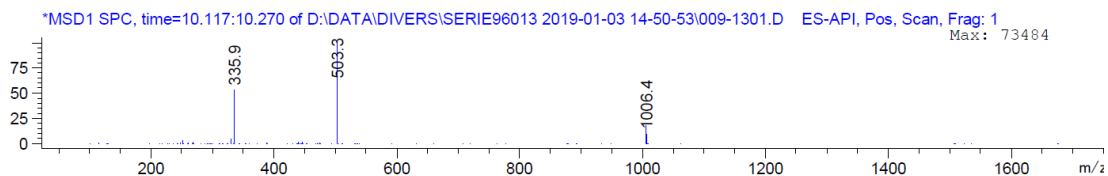
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

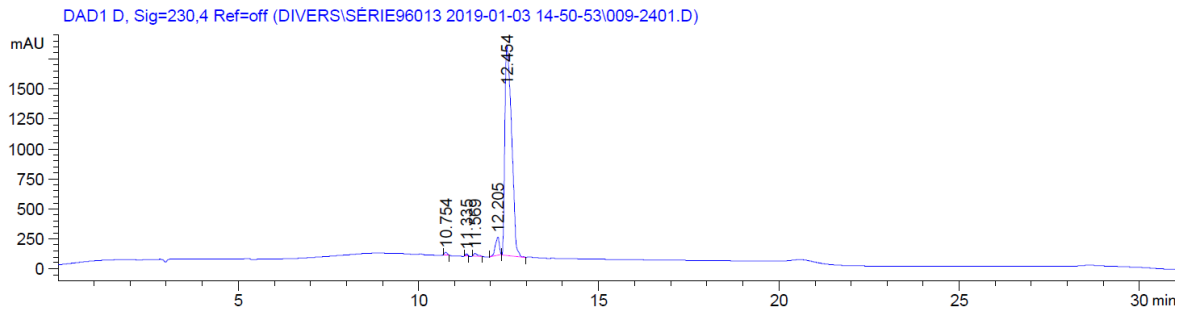
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.659	BB	0.0675	34.10287	8.38100	0.1482
2	9.820	BV	0.0780	286.02124	55.61639	1.2431
3	9.997	VV	0.0816	1123.03625	193.73082	4.8809
4	10.153	VB	0.1326	2.14699e4	2649.09302	93.3124
5	10.648	BB	0.0755	6.93689	1.45933	0.0301
6	10.856	BB	0.1338	17.18402	1.79266	0.0747
7	11.699	BB	0.2001	17.71755	1.18757	0.0770
8	12.532	BB	0.0826	20.01781	3.72893	0.0870
9	13.023	BB	0.1715	33.70819	2.70253	0.1465

Totals : 2.30087e4 2917.69225



Retention Time (MS)	MS Area	Mol. Weight or Ion
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		503.30 I
		335.85 I

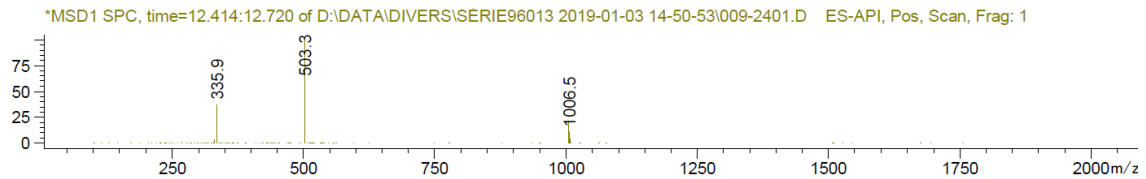
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.754	MM	0.0881	119.94674	22.68241	0.4960
2	11.335	MM	0.0673	66.23920	16.41135	0.2739
3	11.569	MM	0.1216	155.85890	21.36598	0.6445
4	12.205	MM	0.1257	1149.32813	152.42255	4.7530
5	12.454	MM	0.2158	2.26899e4	1752.73450	93.8325

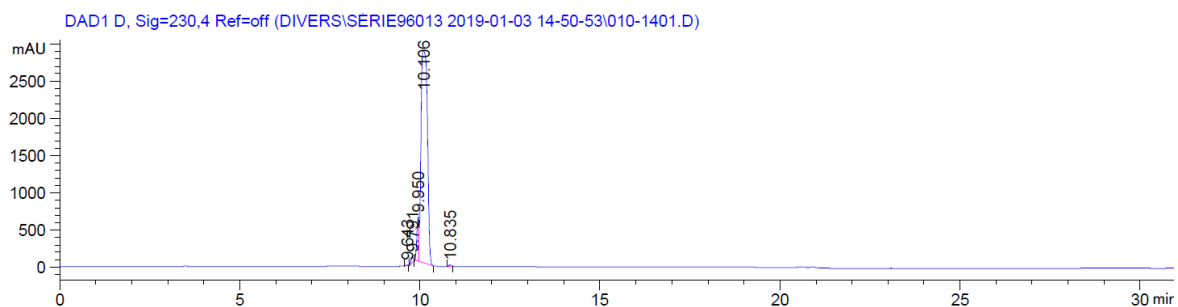
Totals : 2.41812e4 1965.61679



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.489	5821027	1006.45 I
		1005.45 I
		503.30 I
		335.85 I

43

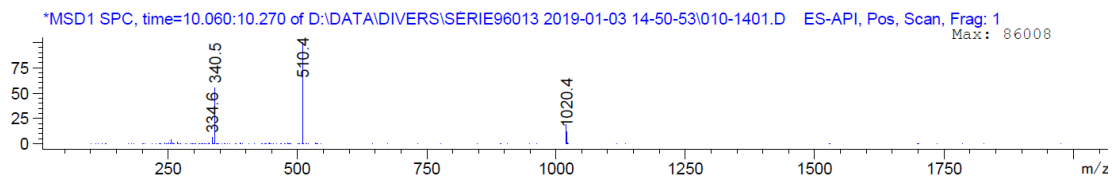
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

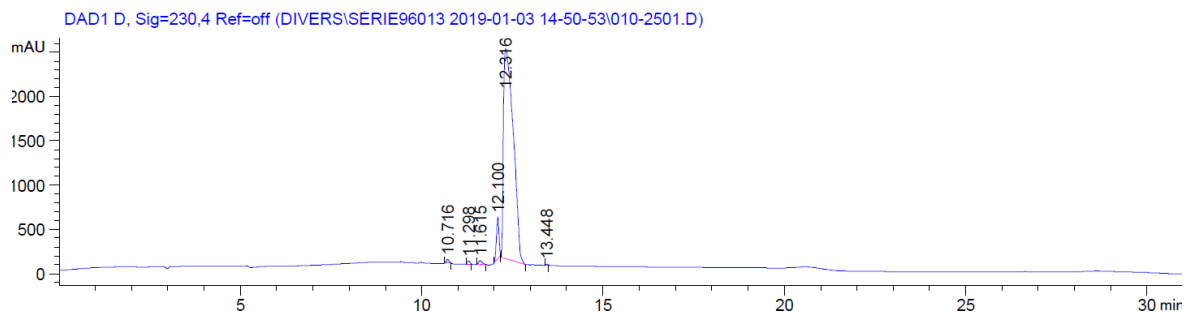
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.643	MM	0.0704	54.02478	12.78527	0.1416
2	9.791	MM	0.0680	331.00214	81.11092	0.8675
3	9.950	MF	0.0694	2459.40234	590.61194	6.4459
4	10.106	FM	0.2062	3.52299e4	2847.33398	92.3346
5	10.835	MM	0.0757	80.26951	17.67154	0.2104

Totals : 3.81546e4 3549.51365



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.147	3627443	1020.40 I
		1019.45 I
		510.35 I
		340.55 I

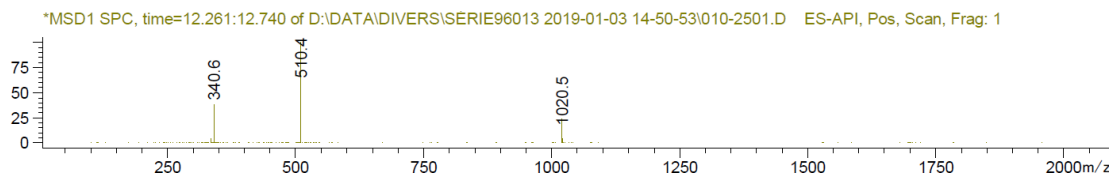
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.716	MM	0.0960	233.44279	40.54294	0.4915
2	11.298	MM	0.0746	156.24905	34.90910	0.3289
3	11.615	MM	0.1056	246.75500	38.92963	0.5195
4	12.100	MM	0.0837	2346.08496	467.38135	4.9391
5	12.316	MM	0.3129	4.44650e4	2368.78052	93.6106
6	13.448	MM	0.0644	52.44215	13.56448	0.1104

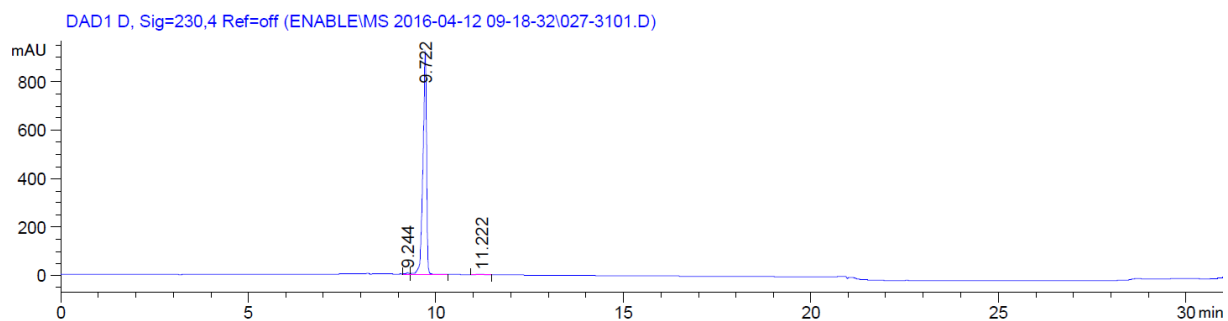
Totals : 4.75000e4 2964.10801



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.387	8633108	1020.50 I
		1019.50 I
		510.40 I
		340.60 I

44

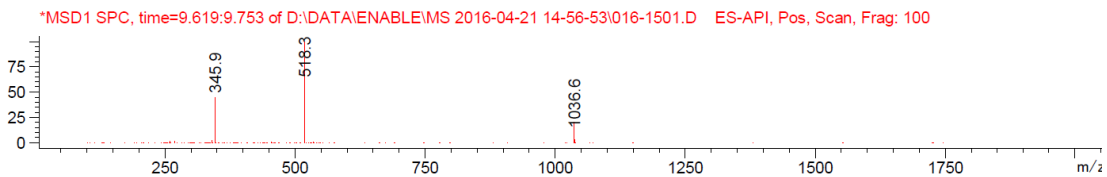
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

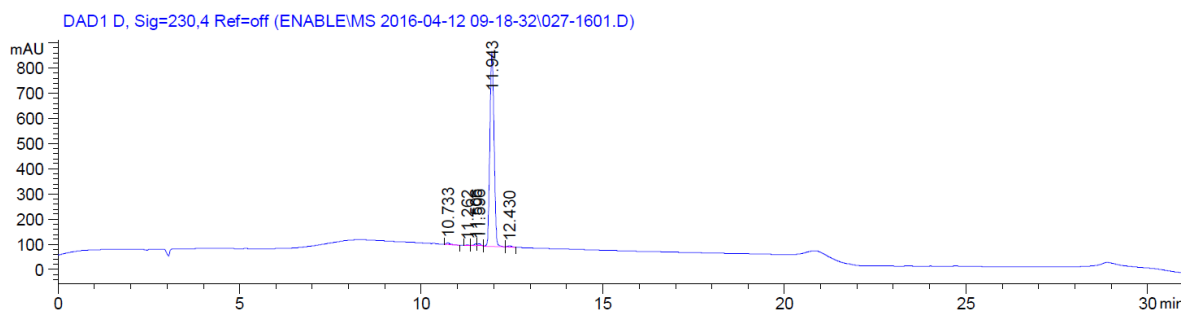
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1	9.244	BV	0.0795	28.57822	5.41783	0.4630
2	9.722	VB	0.0978	6117.25781	917.42657	99.1156
3	11.222	BB	0.1418	26.00842	2.62094	0.4214

Totals : 6171.84445 925.46535



Retention Time (MS)	MS Area	Mol. Weight or Ion
9.697	3291688	1035.50 I
		518.35 I
		345.90 I

Method B

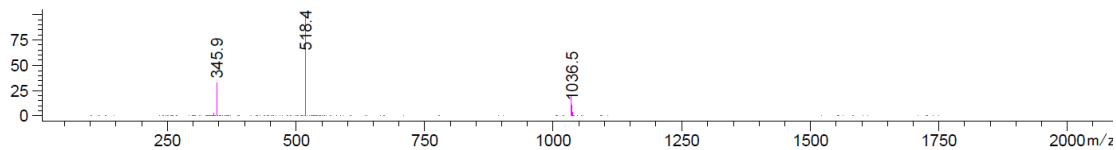


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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.733	BB	0.0976	48.55537	7.29567	0.7699
2	11.262	BB	0.0800	12.75155	2.56682	0.2022
3	11.506	BV	0.0911	42.54167	6.98167	0.6745
4	11.596	VB	0.0858	50.60494	8.96791	0.8024
5	11.943	BV	0.1259	6115.27588	776.06909	96.9632
6	12.430	VB	0.1029	37.07299	5.48166	0.5878

Totals : 6306.80240 807.36283

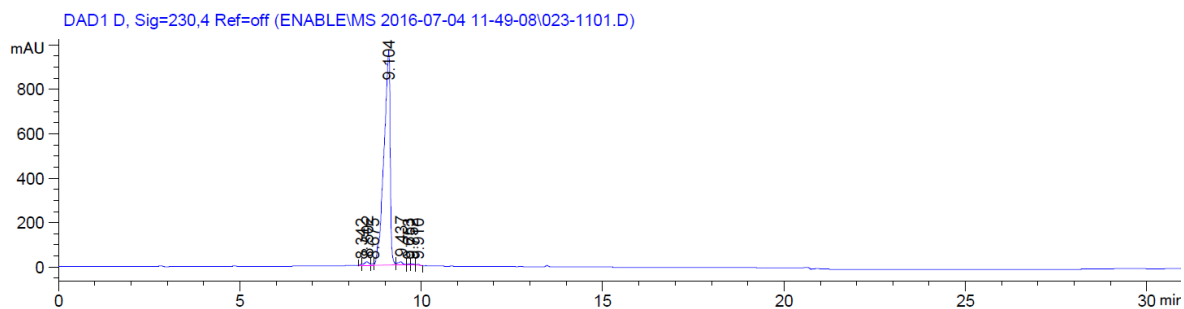
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Retention Time (MS)	MS Area	Mol. Weight or Ion
11.892	6233766	1036.50 I
		1035.50 I
		518.40 I
		345.90 I

45

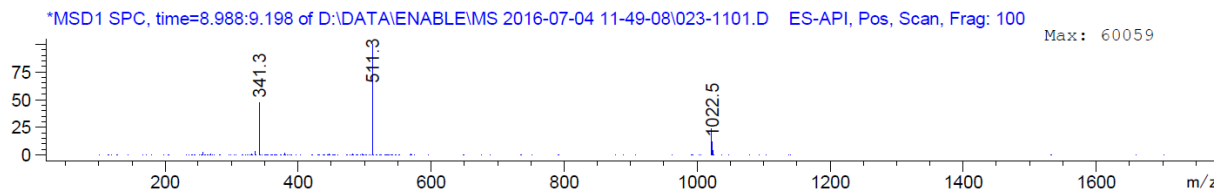
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

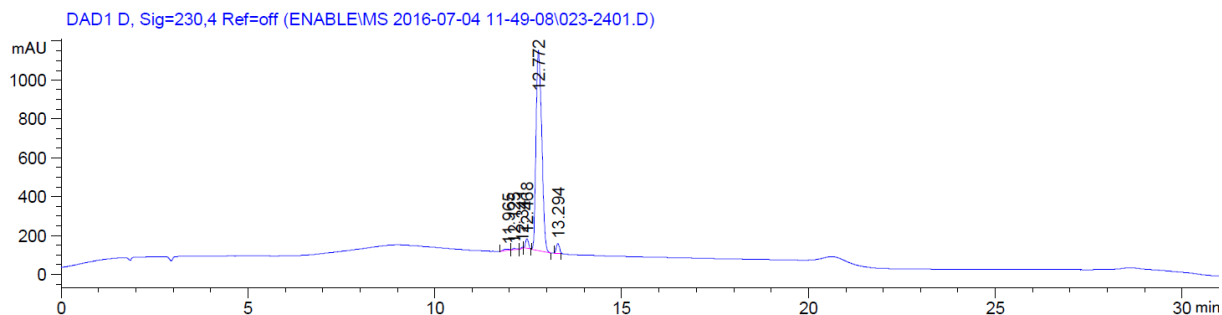
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.342	BV	0.0605	19.99083	5.23677	0.1668
2	8.502	VV	0.1343	156.84450	16.58382	1.3083
3	8.675	VV	0.0584	27.54270	6.92721	0.2297
4	9.104	VV	0.1639	1.15987e4	967.15839	96.7508
5	9.437	VB	0.1258	126.22858	13.66347	1.0529
6	9.653	BV	0.0612	16.78866	4.15315	0.1400
7	9.752	VB	0.0953	24.08353	4.17539	0.2009
8	9.910	BB	0.0722	18.04328	3.74815	0.1505

Totals : 1.19883e4 1021.64634



Retention Time (MS)	MS Area	Mol. Weight or Ion
9.151	2442426	1022.50 I
		1021.60 I
		511.30 I
		341.25 I

Method B

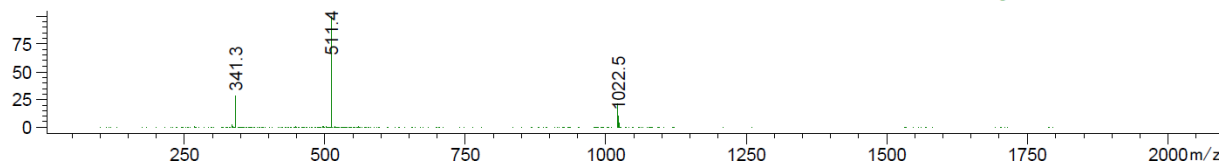


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.965	MM	0.2057	75.71786	6.13467	0.6518
2	12.125	MM	0.1187	52.15832	7.32470	0.4490
3	12.341	MM	0.0566	16.24432	4.78654	0.1398
4	12.468	MM	0.0882	265.14740	50.12386	2.2824
5	12.772	BB	0.1735	1.09385e4	1033.58630	94.1603
6	13.294	MM	0.0937	269.12027	47.88817	2.3166

Totals : 1.16169e4 1149.84424

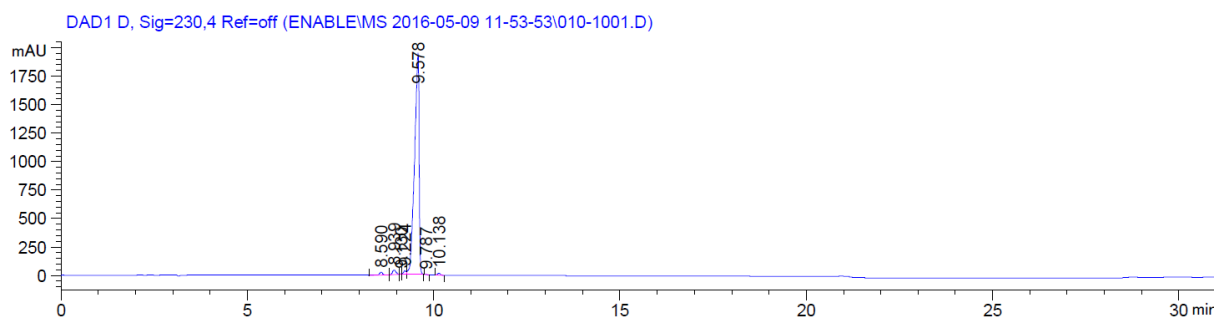
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Retention Time (MS)	MS Area	Mol. Weight or Ion
12.828	4960191	1022.50 I
		1021.50 I
		511.35 I
		341.30 I

46

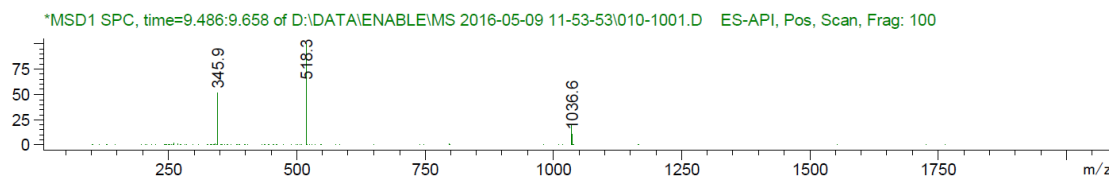
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

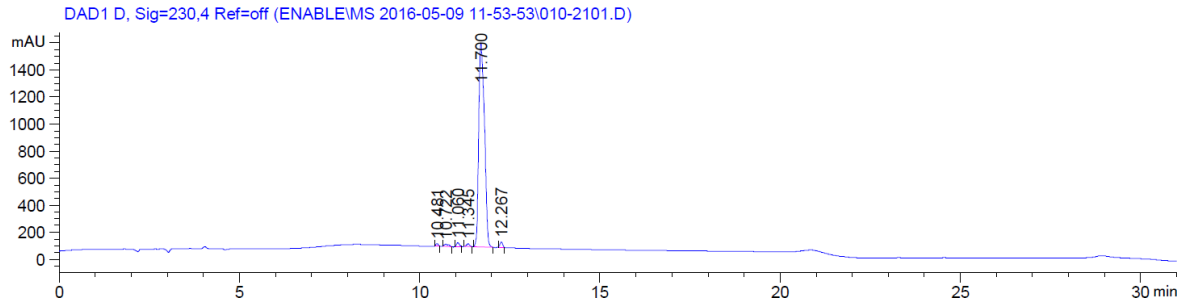
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.590	BB	0.0980	166.18126	25.51121	0.9664
2	8.939	BB	0.0961	253.16490	39.85386	1.4722
3	9.130	BV	0.0503	19.91481	6.40641	0.1158
4	9.224	VV	0.0679	141.71313	30.68143	0.8241
5	9.578	VB	0.1191	1.65188e4	1944.39868	96.0578
6	9.787	BB	0.0680	10.76864	2.61777	0.0626
7	10.138	BB	0.0722	86.18295	18.55128	0.5012

Totals : 1.71967e4 2068.02063



Retention Time (MS)	MS Area	Mol. Weight or Ion
9.602	1921076	1036.55 I
		1035.55 I
		518.35 I
		345.90 I

Method B

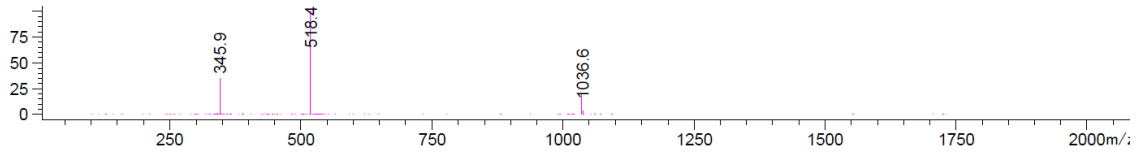


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.481	MM	0.0763	82.45522	18.00970	0.4735
2	10.722	PM	0.1484	140.44057	15.77632	0.8066
3	11.060	PM	0.0877	146.46281	27.84579	0.8412
4	11.345	MM	0.0957	123.14696	21.44285	0.7072
5	11.700	MM	0.1848	1.67211e4	1507.81958	96.0307
6	12.267	MM	0.0848	198.63551	39.02130	1.1408

Totals : 1.74122e4 1629.91553

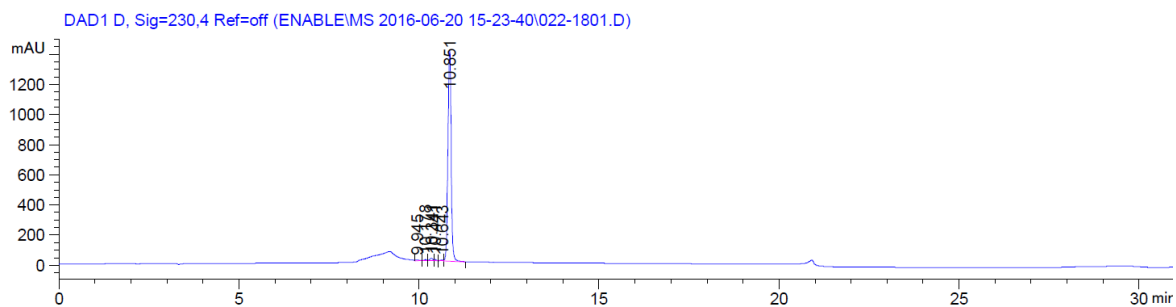
*MSD1 SPC, time=11.629:11.917 of D:\DATA\ENABLEIMS 2016-05-09 11-53-53\010-2101.D ES-API, Pos, Scan, Frag: 100



Retention Time (MS)	MS Area	Mol. Weight or Ion
11.728	6423115	1036.55 I
		1035.55 I
		518.40 I
		345.90 I

47

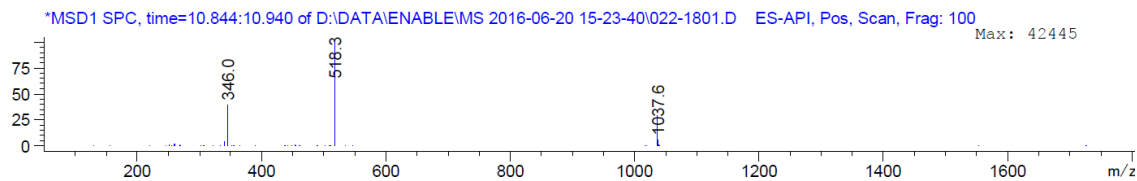
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

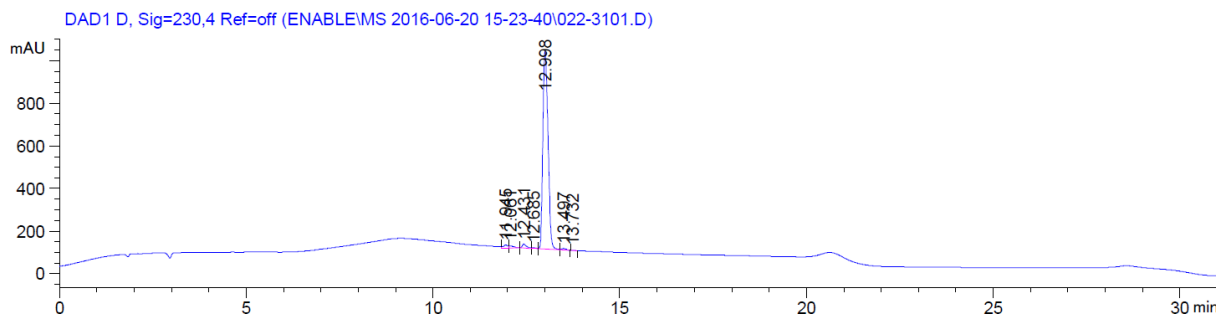
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.945	VB	0.1003	41.24303	5.99061	0.4655
2	10.178	BB	0.0761	24.50549	5.28858	0.2766
3	10.341	BV	0.0769	74.42452	14.73945	0.8400
4	10.441	VB	0.0654	29.67697	7.01384	0.3350
5	10.643	BV	0.0775	35.52905	6.96859	0.4010
6	10.851	VB	0.0959	8654.46094	1404.53125	97.6819

Totals : 8859.84000 1444.53233



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.891	905506	1036.50 I
		1035.55 I
		518.35 I
		346.00 I

Method B

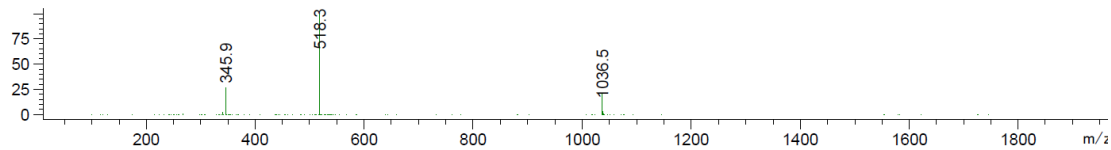


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.945	VV	0.1182	122.44259	14.55062	1.3124
2	12.061	VB	0.1186	85.98064	9.41406	0.9216
3	12.431	BV	0.1160	154.41937	19.16538	1.6552
4	12.685	VV	0.0930	25.14604	3.90905	0.2695
5	12.998	VV	0.1547	8880.58008	935.56238	95.1886
6	13.497	VB	0.1172	55.00299	7.19225	0.5896
7	13.732	BB	0.0886	5.88832	1.06273	0.0631

Totals : 9329.46004 990.85646

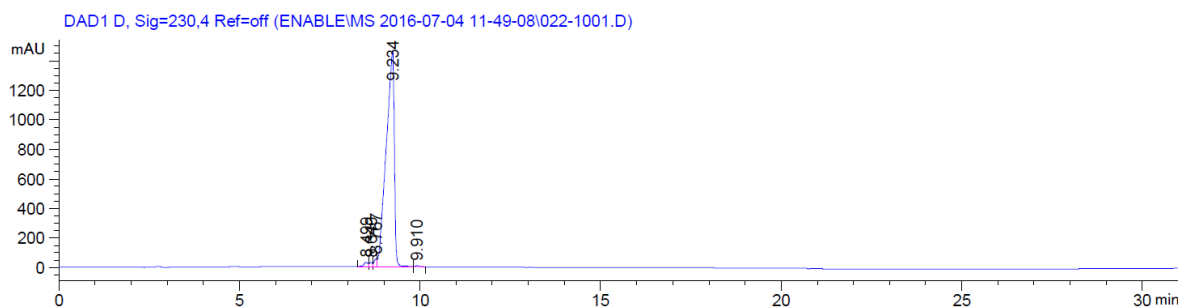
*MSD1 SPC, time=12.950:13.180 of D:\DATA\ENABLEIMS 2016-06-20 15-23-40\022-3101.D ES-API, Pos, Scan, Frag: 100



Retention Time (MS)	MS Area	Mol. Weight or Ion
13.054	5616837	1036.50 I
		1035.55 I
		518.35 I
		345.90 I

48

Method A

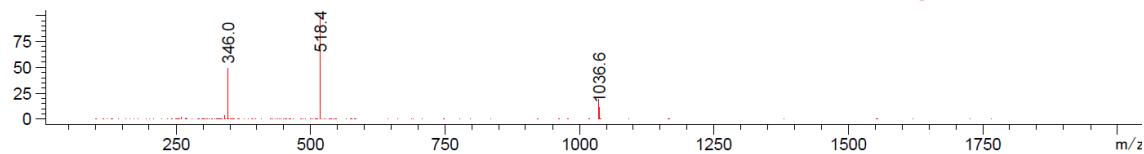


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.499	BV	0.1246	249.76675	29.54174	1.0569
2	8.640	VV	0.0869	177.98502	30.14559	0.7531
3	8.767	VV	0.0756	264.97946	51.87306	1.1212
4	9.234	VB	0.2245	2.28976e4	1463.59705	96.8879
5	9.910	BB	0.0835	42.75761	7.61523	0.1809

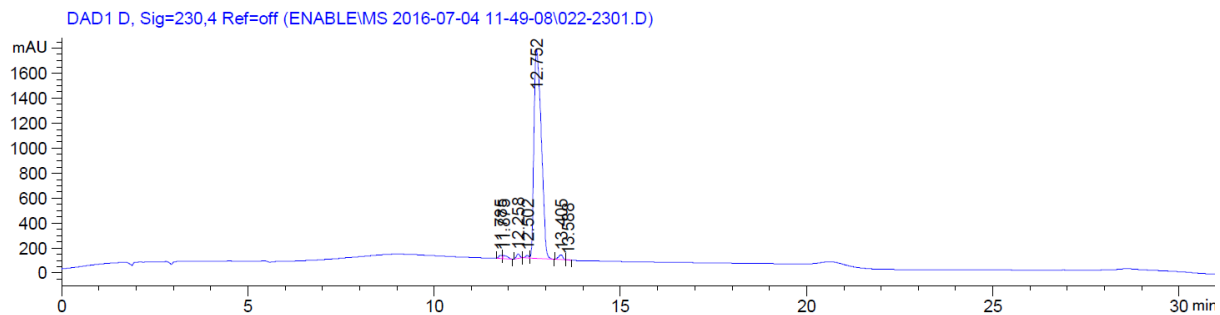
Totals : 2.36331e4 1582.77267

*MSD1 SPC, time=9.026:9.351 of D:\DATA\ENABLEIMS 2016-07-04 11-49-08\022-1001.D ES-API, Pos, Scan, Frag: 100



Retention Time (MS)	MS Area	Mol. Weight or Ion
9.257	4583736	1036.55 I
		1035.55 I
		518.40 I
		345.95 I

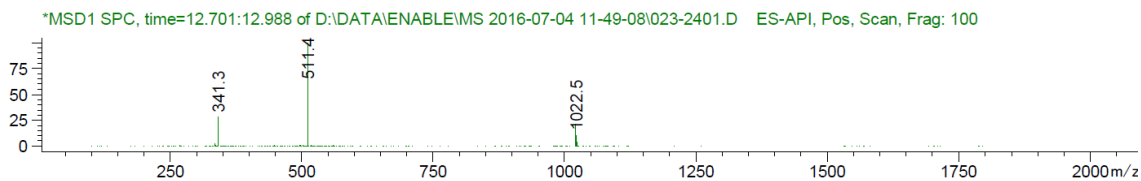
Method B



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.785	BV	0.0907	149.49118	24.68218	0.6290
2	11.875	VB	0.1209	213.75029	23.32694	0.8993
3	12.258	BB	0.0977	217.21559	35.36412	0.9139
4	12.502	BV	0.0909	128.60890	21.78367	0.5411
5	12.752	VB	0.2342	2.27557e4	1677.87732	95.7424
6	13.405	BB	0.1145	294.40036	38.80049	1.2387
7	13.588	BB	0.0749	8.45444	1.79655	0.0356

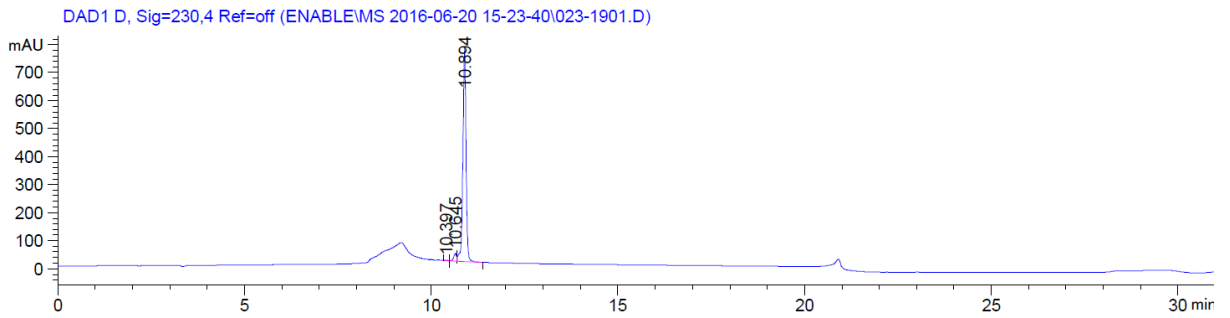
Totals : 2.37677e4 1823.63128



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.846	8704919	1036.50 I
		1035.55 I
		518.30 I
		345.95 I

49

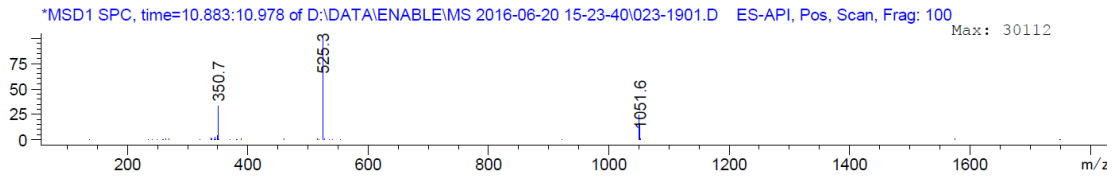
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

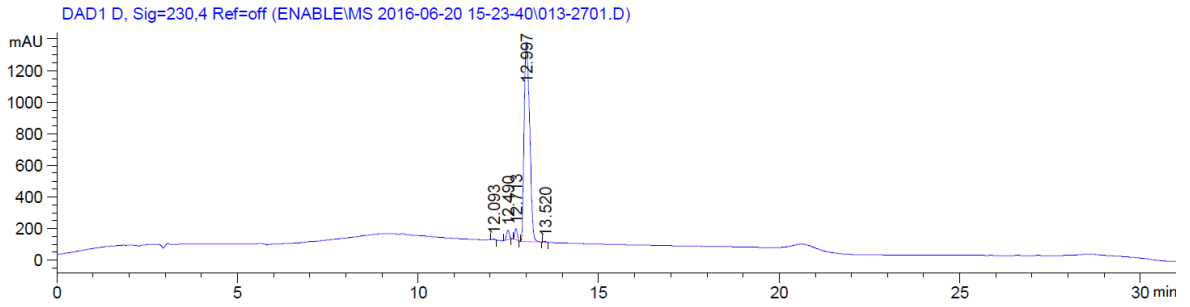
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.397	BB	0.0736	7.09362	1.60518	0.1508
2	10.645	BV	0.0808	144.94875	26.92311	3.0823
3	10.894	VB	0.0913	4550.60010	766.09430	96.7669

Totals : 4702.64246 794.62259



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.928	495061	1050.60 I
		1049.55 I
		525.30 I
		350.70 I

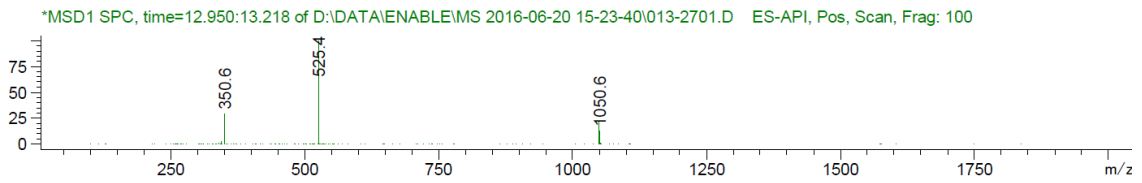
Method B



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.093	MM	0.0818	27.91074	5.68846	0.1988
2	12.490	MM	0.0851	307.09311	60.11841	2.1874
3	12.713	MM	0.0809	332.93707	68.55609	2.3715
4	12.997	MM	0.1770	1.33524e4	1256.98633	95.1087
5	13.520	MM	0.0777	18.75299	4.02183	0.1336

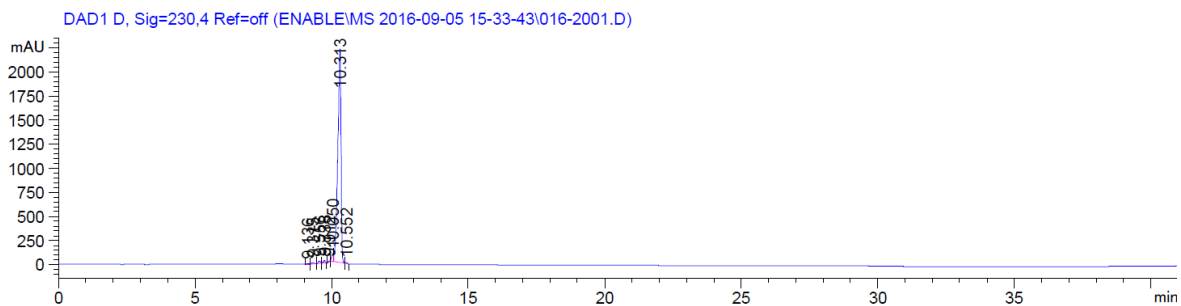
Totals : 1.40391e4 1395.37111



Retention Time (MS)	MS Area	Mol. Weight or Ion
13.048	6112523	1050.60 I
		1049.60 I
		525.40 I
		350.60 I

50

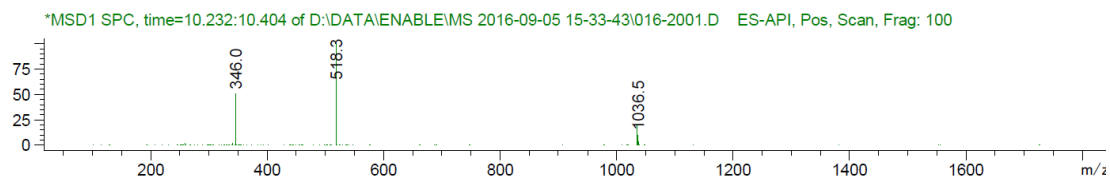
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

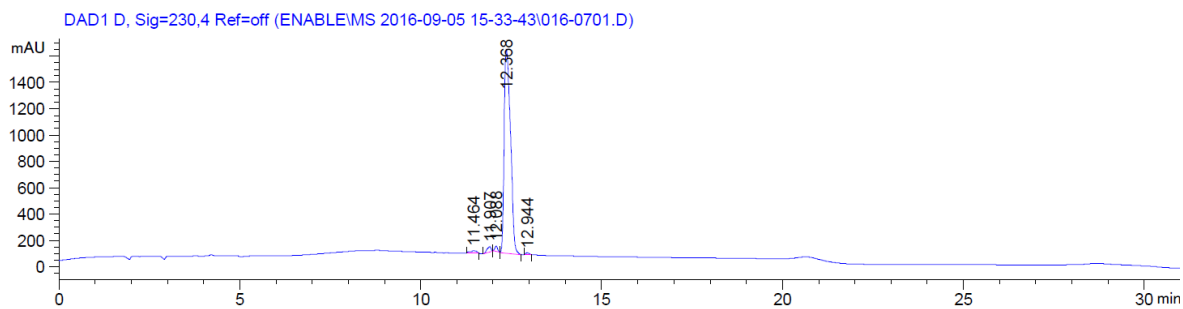
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.136	BV	0.0995	9.28975	1.60489	0.0494
2	9.315	VB	0.0875	87.63902	15.60359	0.4659
3	9.556	BV	0.0926	149.80009	26.24298	0.7963
4	9.738	VB	0.0884	132.50914	24.00226	0.7044
5	9.912	MM	0.0698	29.74391	7.10507	0.1581
6	10.050	MF	0.0787	398.78909	84.47592	2.1199
7	10.313	FM	0.1345	1.79633e4	2225.95410	95.4921
8	10.552	BB	0.0639	40.21887	10.22766	0.2138

Totals : 1.88113e4 2395.21648



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.348	2666095	1035.55 I
		518.35 I
		345.95 I

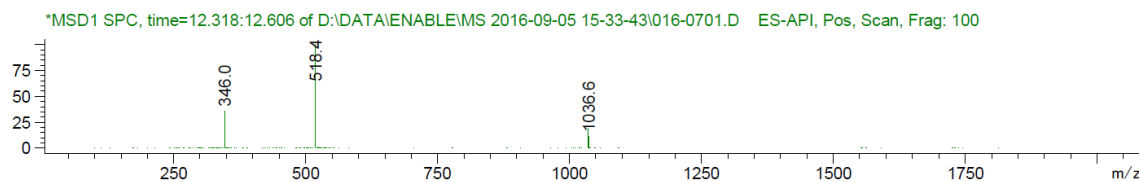
Method B



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.464	MM	0.2130	271.19586	21.21706	1.3727
2	11.907	MM	0.1312	311.21216	39.52490	1.5752
3	12.088	MM	0.0897	221.19272	41.10050	1.1196
4	12.368	MM	0.2030	1.88655e4	1548.58398	95.4907
5	12.944	MM	0.1126	87.27248	12.91544	0.4417

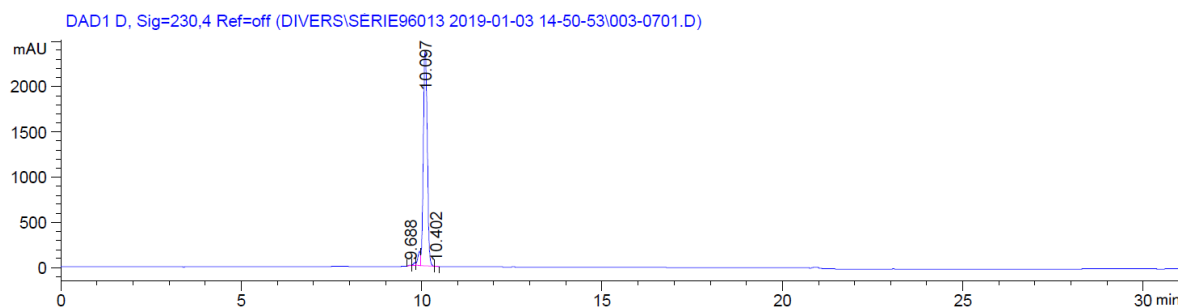
Totals : 1.97564e4 1663.34189



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.430	6291380	1036.55 I
		1035.55 I
		518.40 I
		345.95 I

51

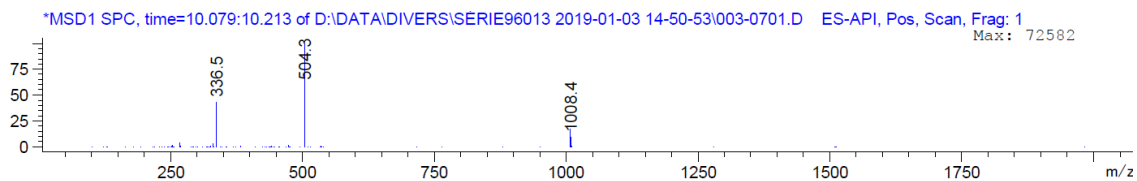
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

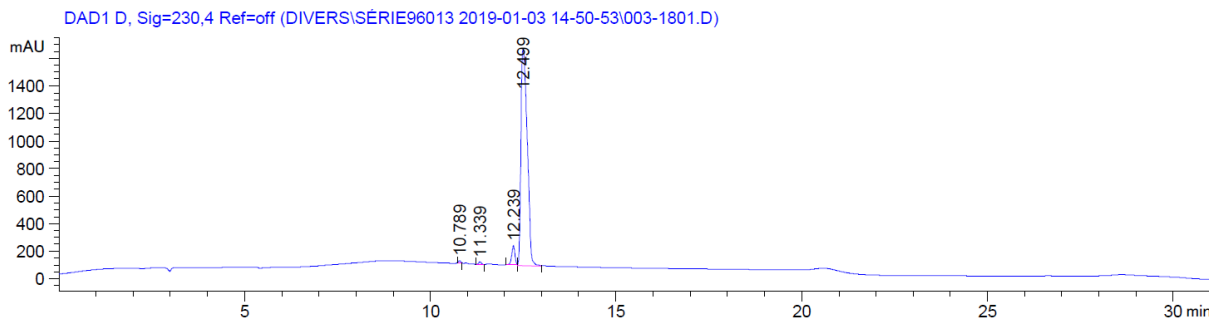
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.688	BB	0.0765	32.01066	6.84626	0.1664
2	9.810	BV	0.0629	112.64354	28.02790	0.5857
3	9.938	VV	0.0755	791.56036	155.26288	4.1157
4	10.097	VB	0.1237	1.82835e4	2377.23462	95.0652
5	10.402	BB	0.0724	12.87137	2.86530	0.0669

Totals : 1.92326e4 2570.23695



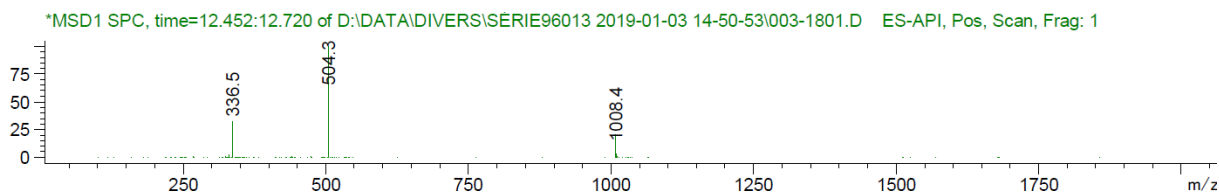
Retention Time (MS)	MS Area	Mol. Weight or Ion
10.139	1750790	1007.40 I
		504.30 I
		336.55 I

Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

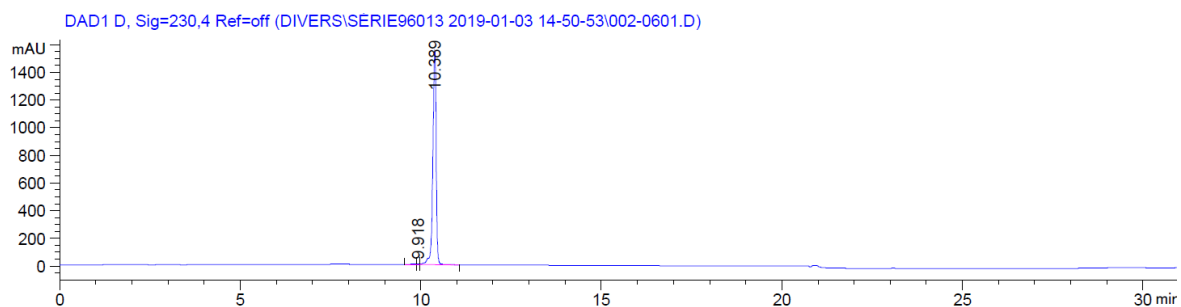
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.789	MM	0.0821	87.02290	17.67191	0.4482
2	11.339	BB	0.0733	87.30430	18.40888	0.4496
3	12.239	MM	0.0962	785.40546	136.10315	4.0451
4	12.499	VV	0.2027	1.84564e4	1575.71155	95.0570



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.542	5285188	1008.40 I
		1007.45 I
		504.30 I
		336.55 I

52

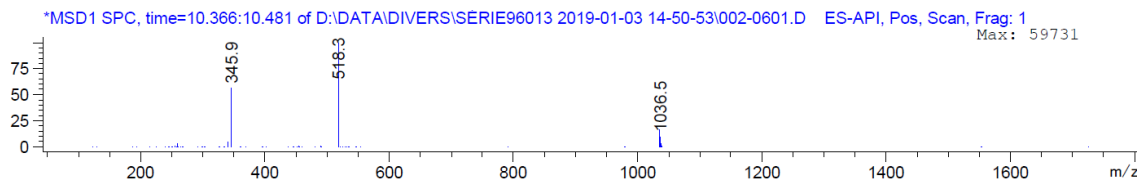
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

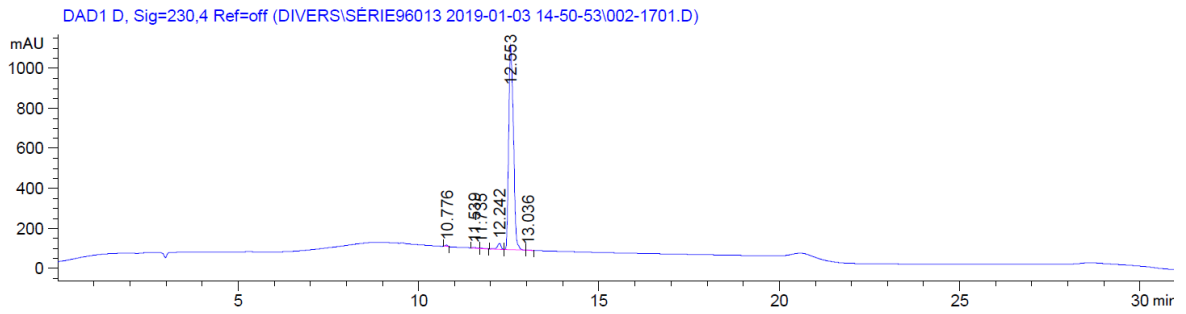
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.814	BV	0.1323	40.30087	4.50948	0.4012
2	9.918	VV	0.0820	18.10246	3.20202	0.1802
3	10.389	VB	0.0972	9985.84473	1548.74011	99.4185

Totals : 1.00442e4 1556.45161



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.426	1280823	1035.40 I
		518.25 I
		345.85 I

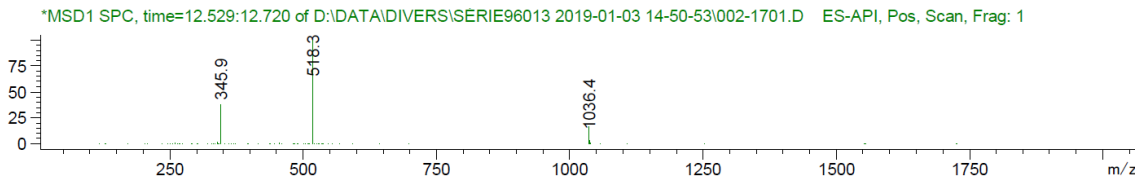
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.776	MM	0.0848	33.11284	6.50768	0.3449
2	11.539	BV	0.1075	21.76361	3.04224	0.2267
3	11.735	VB	0.0869	11.41854	1.99245	0.1189
4	12.242	BB	0.1094	208.24982	29.14622	2.1689
5	12.553	BV	0.1485	9318.10840	1020.97742	97.0476
6	13.036	VB	0.1021	8.93161	1.33501	0.0930

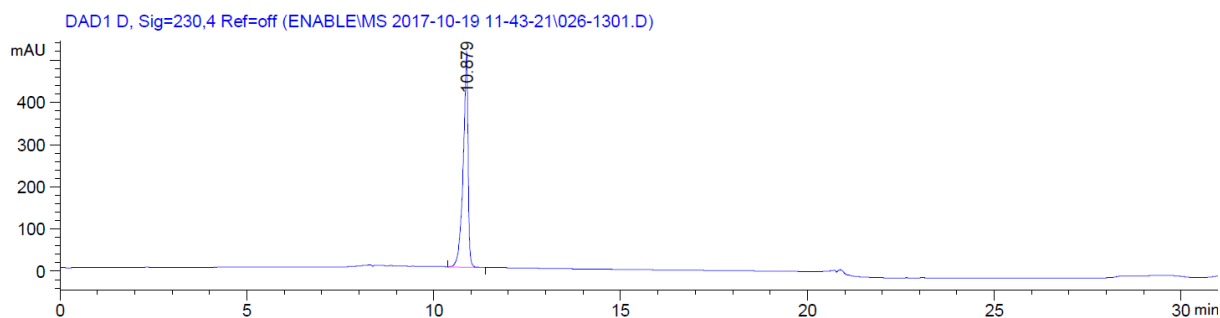
Totals : 9601.58481 1063.00101



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.610	3524989	1035.45 I
		518.35 I
		345.90 I

53

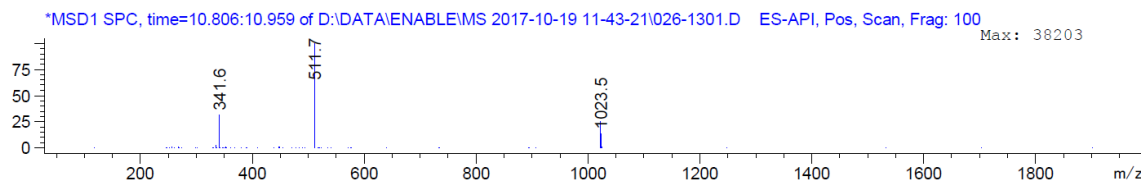
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.879	BB	0.1261	4630.67432	509.19025	100.0000

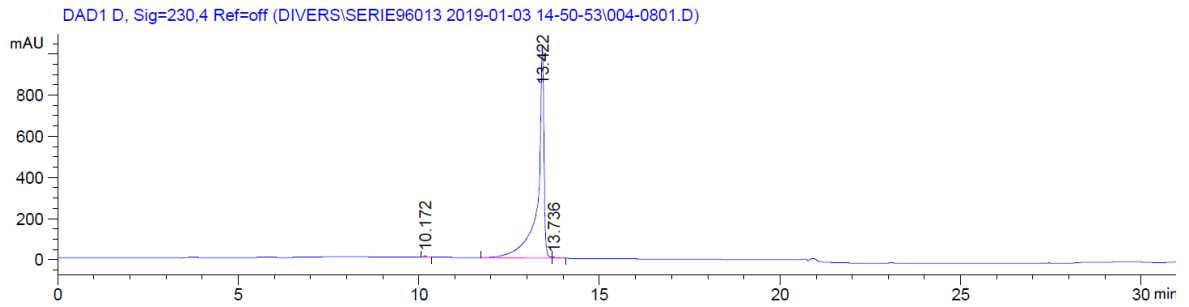
Totals : 4630.67432 509.19025



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.913	830372	1023.50 I
		1022.55 I
		511.70 I
		341.60 I

54

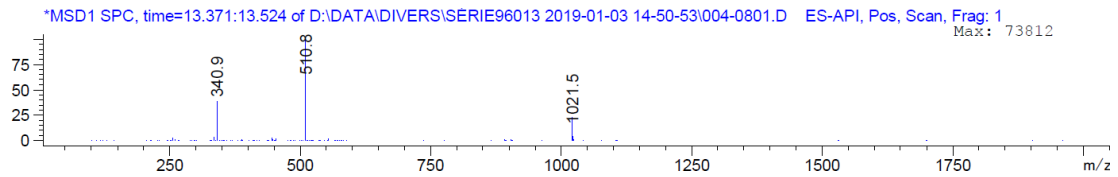
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

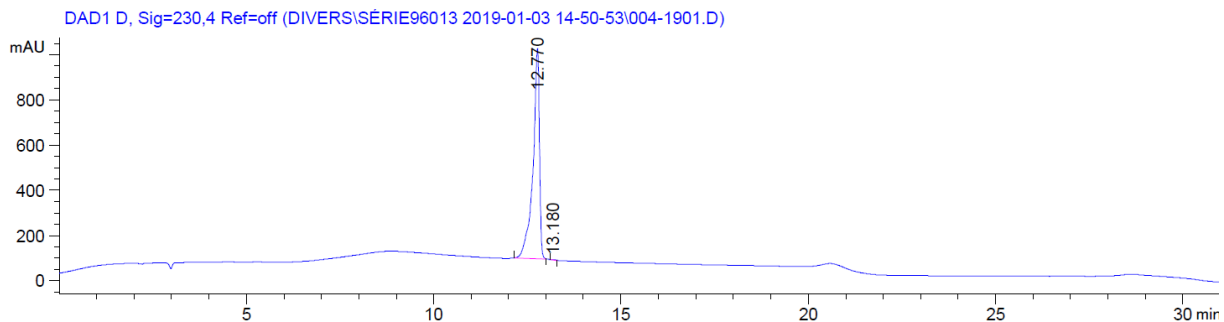
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.172	BB	0.0832	38.01067	7.01340	0.3097
2	13.422	BV	0.1593	1.21965e4	1036.25818	99.3701
3	13.736	VB	0.1137	39.30333	4.69415	0.3202

Totals : 1.22738e4 1047.96574



Retention Time (MS)	MS Area	Mol. Weight or Ion
13.453	2372656	1021.45 I
		1020.45 I
		510.80 I
		340.85 I

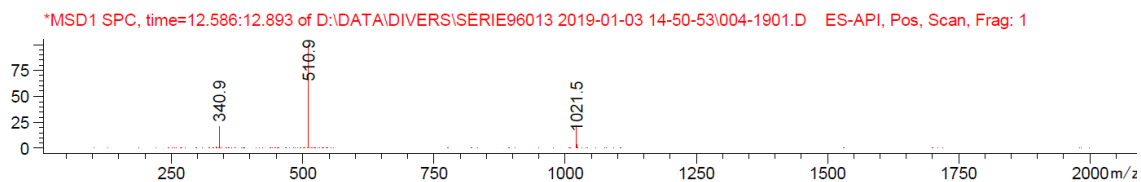
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.770	MM	0.2003	1.11650e4	929.03534	99.8233
2	13.180	MM	0.1487	19.75928	2.21432	0.1767

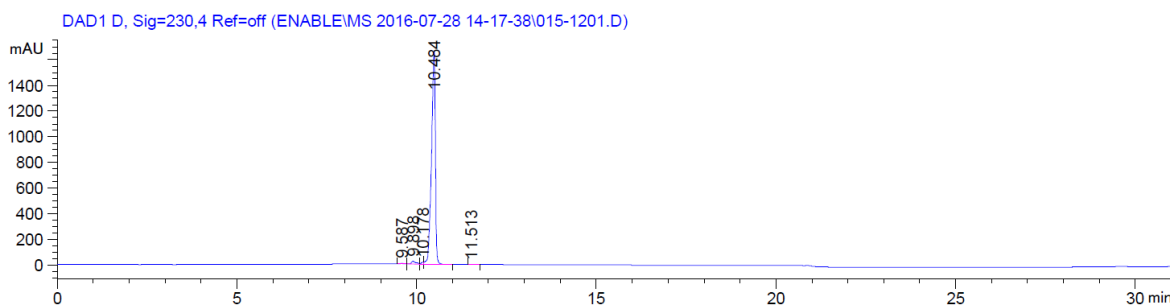
Totals : 1.11847e4 931.24966



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.815	5556733	1021.45 I
		1020.40 I
		510.85 I
		340.90 I

55

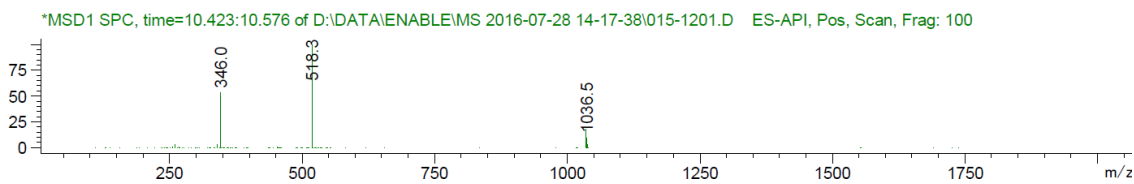
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

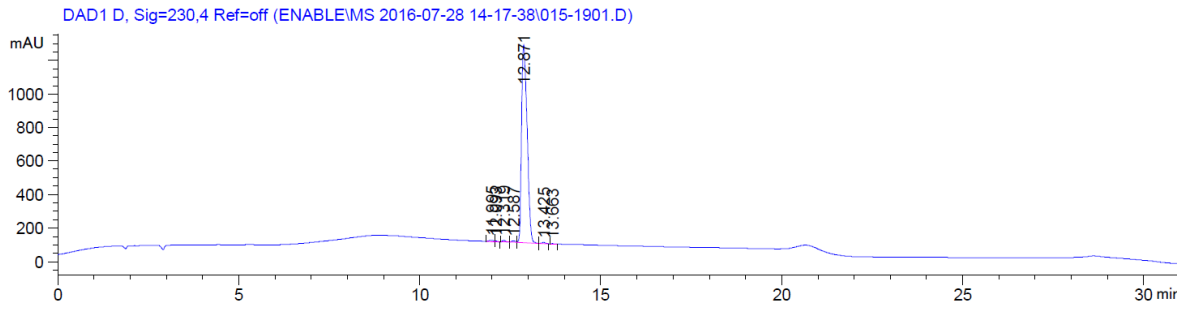
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.587	BB	0.0917	32.35168	5.57783	0.2549
2	9.898	BV	0.1262	187.51689	21.40194	1.4775
3	10.178	VV	0.0685	68.11547	15.14725	0.5367
4	10.484	VB	0.1068	1.23964e4	1665.70691	97.6716
5	11.513	BB	0.0865	7.53375	1.32243	0.0594

Totals : 1.26919e4 1709.15636



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.514	2292536	1035.55 I
		518.30 I
		345.95 I

Method B

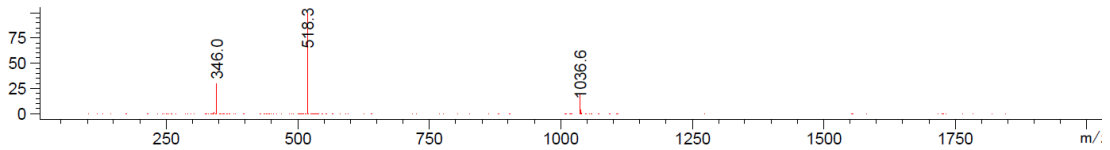


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.995	BV	0.1151	65.05975	7.65542	0.5039
2	12.093	VB	0.0731	23.99856	5.08276	0.1859
3	12.319	BB	0.0937	64.40707	10.77756	0.4988
4	12.587	BV	0.1144	68.32314	9.01267	0.5292
5	12.871	VB	0.1750	1.26443e4	1180.25964	97.9313
6	13.425	BB	0.1091	38.90525	5.59867	0.3013
7	13.663	BB	0.0902	6.40112	1.12746	0.0496

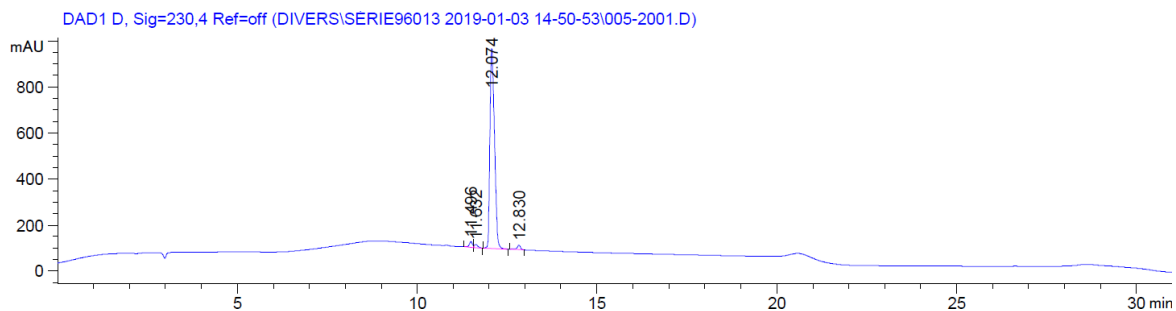
Totals : 1.29114e4 1219.51419

*MSD1 SPC, time=12.816:13.084 of D:\DATA\ENABLEMS 2016-07-28 14-17-38\015-1901.D ES-API, Pos, Scan, Frag: 100



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.944	6916874	1036.60 I
		1035.60 I
		518.35 I
		346.00 I

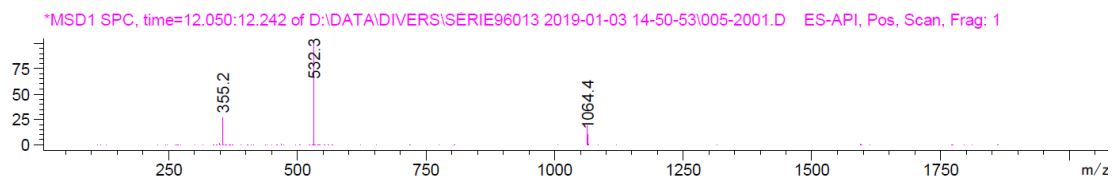
Method B



Signal 5: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.496	BV	0.0913	154.31429	25.23747	1.9159
2	11.632	VB	0.0950	84.10658	13.44915	1.0442
3	12.074	BB	0.1412	7683.54883	868.76624	95.3959
4	12.830	BB	0.1014	132.41014	19.44880	1.6440

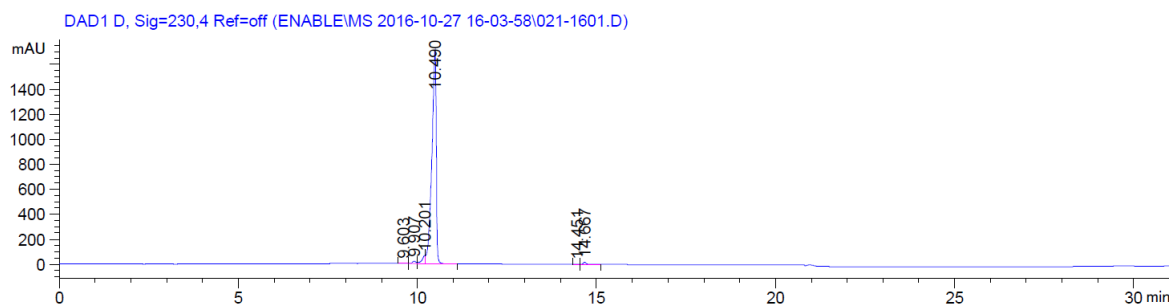
Totals : 8054.37983 926.90165



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.106	2931279	1064.40 I
		1063.45 I
		532.30 I
		355.20 I

57

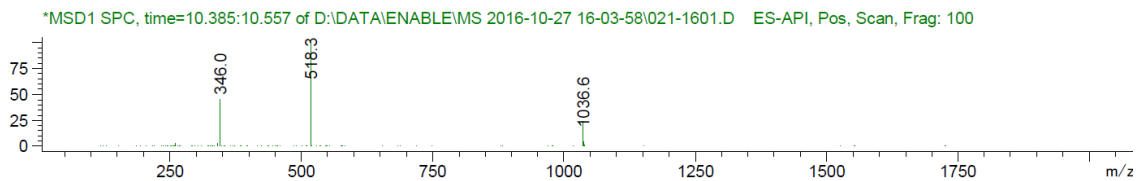
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

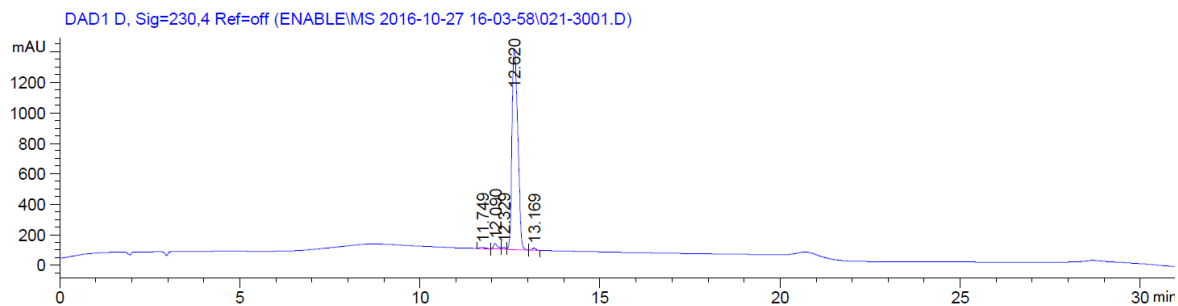
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.603	BB	0.0971	19.60659	3.12754	0.1293
2	9.907	BV	0.0945	121.45603	19.54083	0.8010
3	10.201	VV	0.0889	393.50620	62.96568	2.5953
4	10.490	VB	0.1213	1.45267e4	1706.55835	95.8076
5	14.451	BV	0.0871	5.78539	1.03623	0.0382
6	14.667	VB	0.0889	95.31788	16.61053	0.6286

Totals : 1.51623e4 1809.83914



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.517	2315031	1036.55 I
		1035.60 I
		518.35 I
		345.95 I

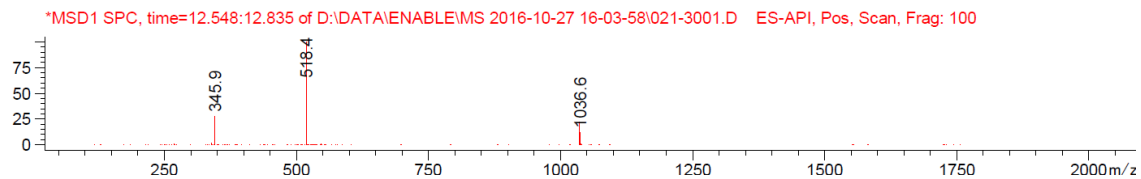
Method B



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.749	VB	0.1508	86.32375	7.47232	0.5629
2	12.090	BV	0.1118	294.30505	38.22289	1.9191
3	12.329	VV	0.1014	73.57627	10.80943	0.4798
4	12.620	VB	0.1887	1.47848e4	1319.32666	96.4075
5	13.169	BB	0.1053	96.72965	14.23028	0.6307

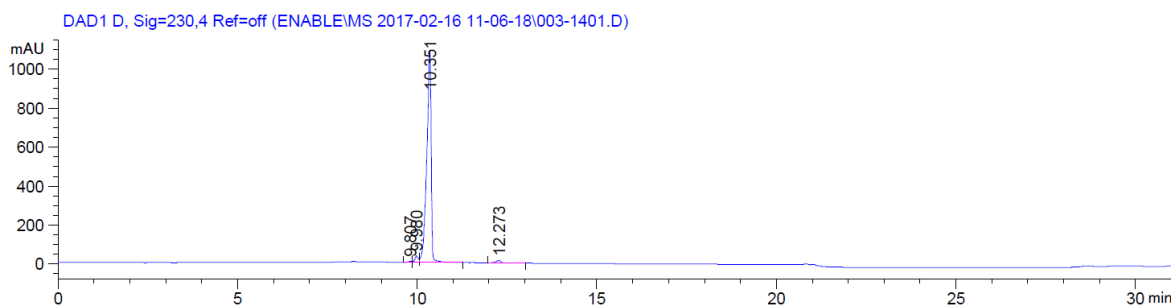
Totals : 1.53357e4 1390.06158



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.645	5839972	1036.55 I
		1035.55 I
		518.40 I
		345.90 I

58

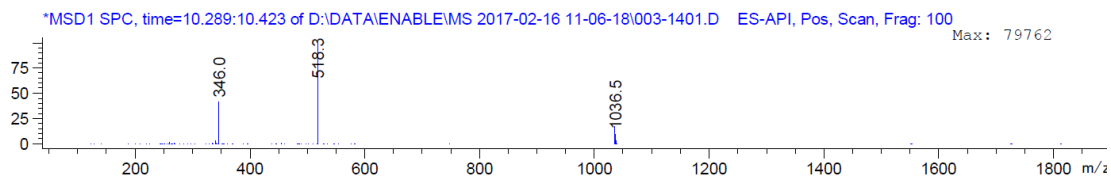
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

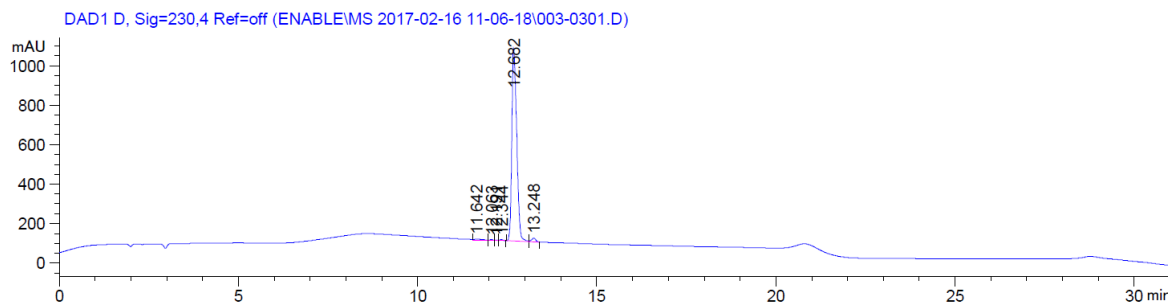
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.807	BV	0.1061	32.13961	4.35652	0.3358
2	9.980	VV	0.0923	208.87387	33.71469	2.1824
3	10.351	VB	0.1203	9207.07520	1092.20117	96.1996
4	12.273	BB	0.1403	122.71976	12.97631	1.2822

Totals : 9570.80844 1143.24869



Retention Time (MS)	MS Area	Mol. Weight or Ion
10.375	1745101	1035.50 I
		518.35 I
		346.00 I

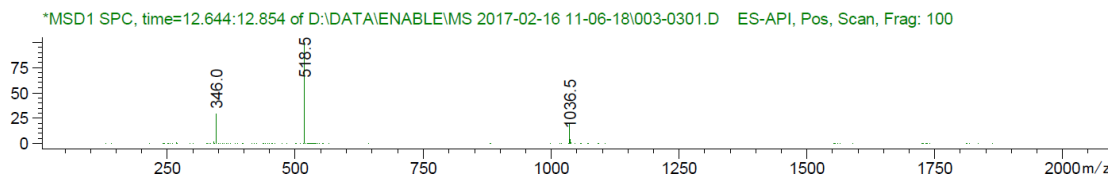
Method B



Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.642	VB	0.1876	60.87515	4.18690	0.6362
2	12.063	BV	0.0908	16.34480	2.77052	0.1708
3	12.191	VV	0.0851	15.26792	2.65583	0.1596
4	12.344	VB	0.1056	31.73701	4.77126	0.3317
5	12.682	BV	0.1510	9289.55566	976.37860	97.0833
6	13.248	VB	0.1214	154.86755	19.35061	1.6185

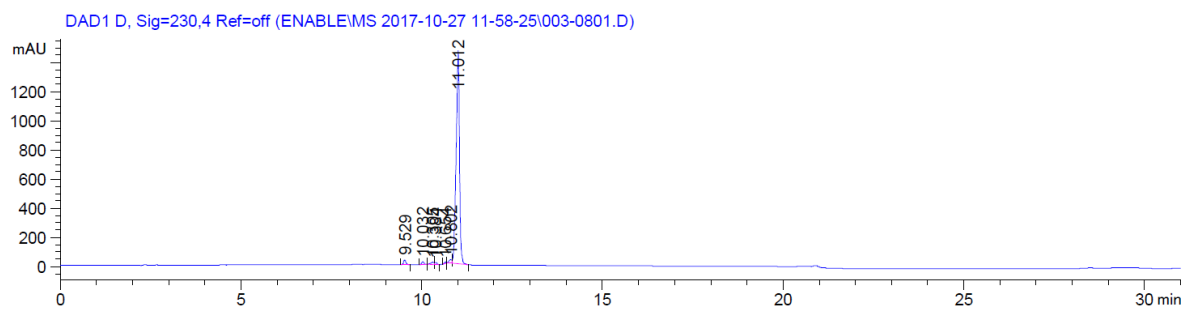
Totals : 9568.64810 1010.11371



Retention Time (MS)	MS Area	Mol. Weight or Ion
12.715	4712490	1036.50 I
		1035.50 I
		518.45 I
		346.00 I

59

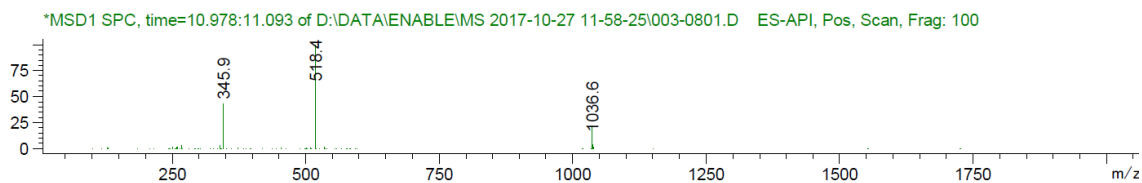
Method A



Signal 3: DAD1 D, Sig=230,4 Ref=off

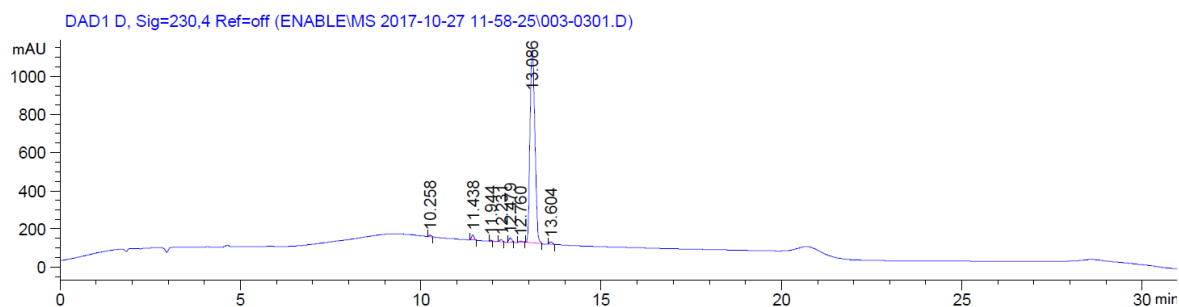
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.529	BV	0.0710	142.82413	31.43040	1.4085
2	10.032	BB	0.0713	85.62523	18.74433	0.8444
3	10.305	BV	0.0897	98.05633	15.11749	0.9670
4	10.384	VB	0.0672	62.36259	14.20648	0.6150
5	10.654	BB	0.0568	27.38220	7.82821	0.2700
6	10.802	BV	0.0880	128.21124	24.94132	1.2644
7	11.012	VB	0.0962	9595.89453	1468.57446	94.6307

Totals : 1.01404e4 1580.84269



Retention Time (MS)	MS Area	Mol. Weight or Ion
11.048	1519901	1036.60 I
		1035.55 I
		518.40 I
		345.90 I

Method B

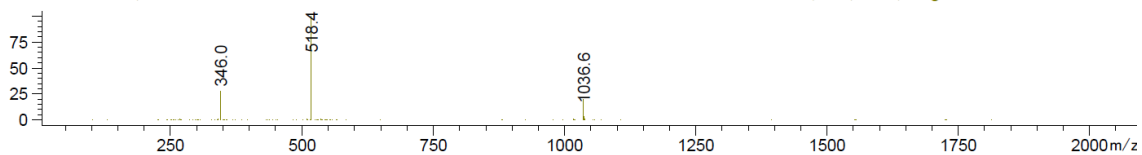


Signal 3: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.258	MM	0.0859	45.35149	8.79884	0.4558
2	11.438	MM	0.0805	126.29135	26.15914	1.2692
3	11.944	MM	0.0710	21.63646	5.08214	0.2174
4	12.231	MM	0.0800	54.42853	11.34539	0.5470
5	12.479	MM	0.0901	117.06335	21.65335	1.1765
6	12.760	MM	0.1303	41.89608	5.35731	0.4211
7	13.086	MM	0.1566	9462.63379	1007.05878	95.0995
8	13.604	PM	0.1063	80.94316	12.69617	0.8135

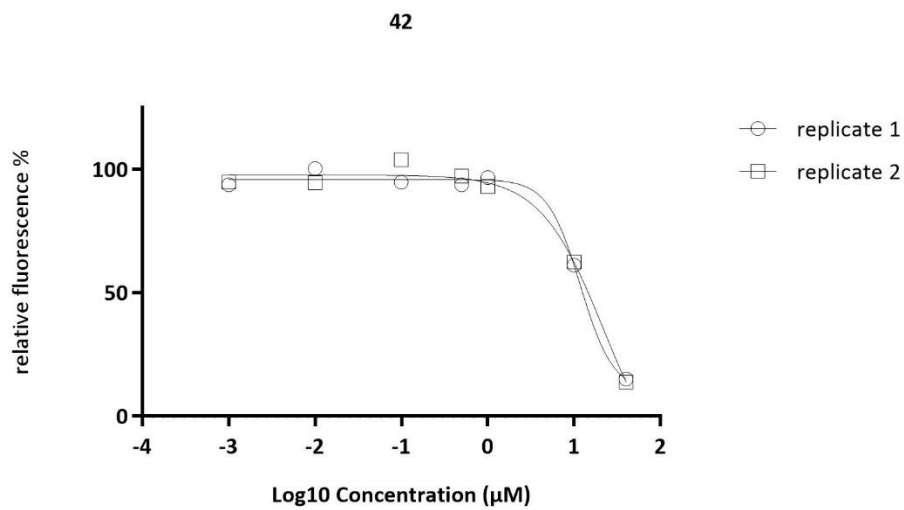
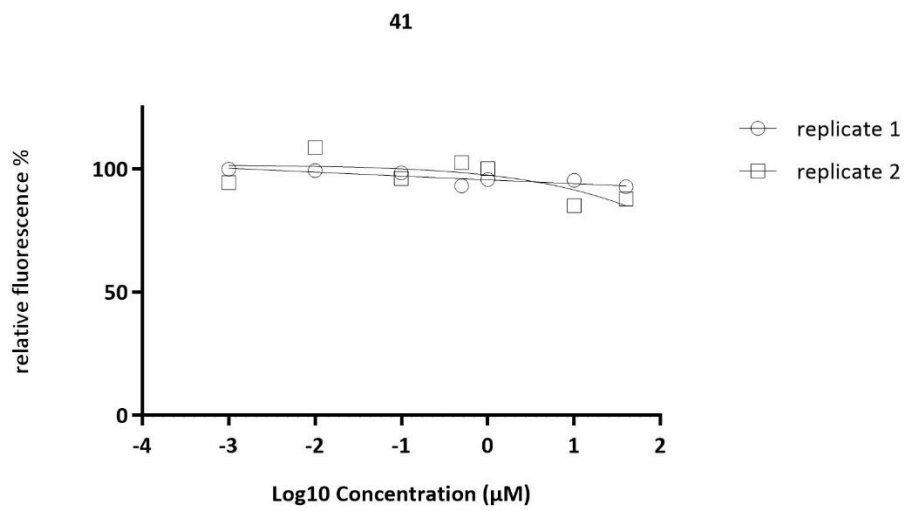
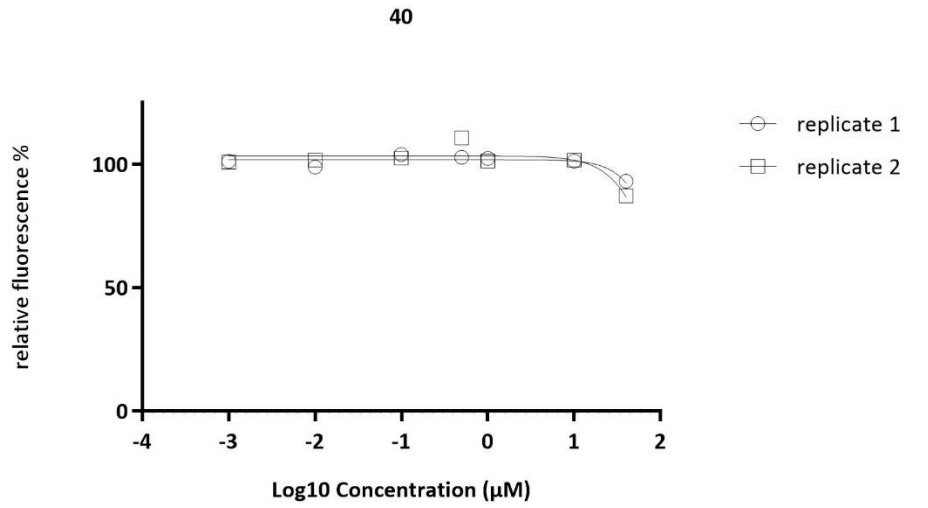
Totals : 9950.24421 1098.15111

*MSD1 SPC, time=13.027:13.256 of D:\DATA\ENABLEMS 2017-10-27 11-58-25\003-0301.D ES-API, Pos, Scan, Frag: 100

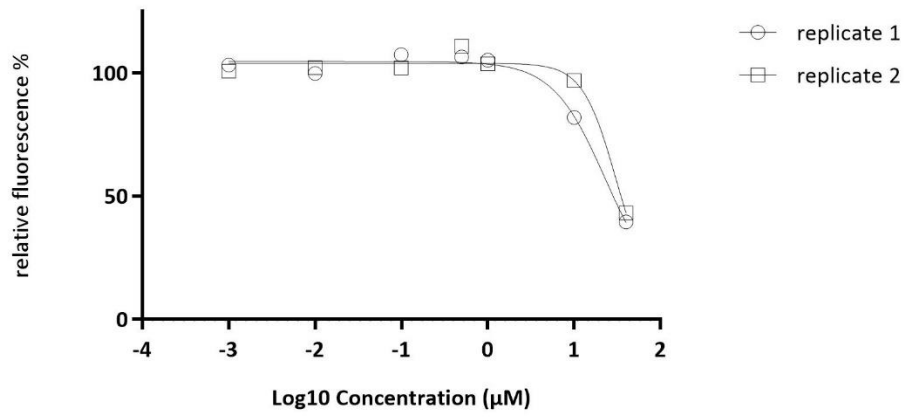


Retention Time (MS)	MS Area	Mol. Weight or Ion
13.122	4607709	1036.55 I
		1035.55 I
		518.40 I
		345.95 I

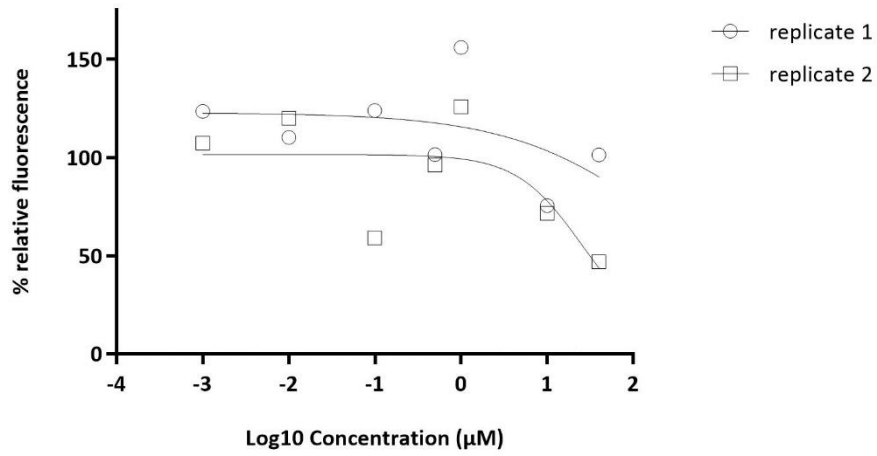
Inhibition of the bacterial translation for analogues 40-59



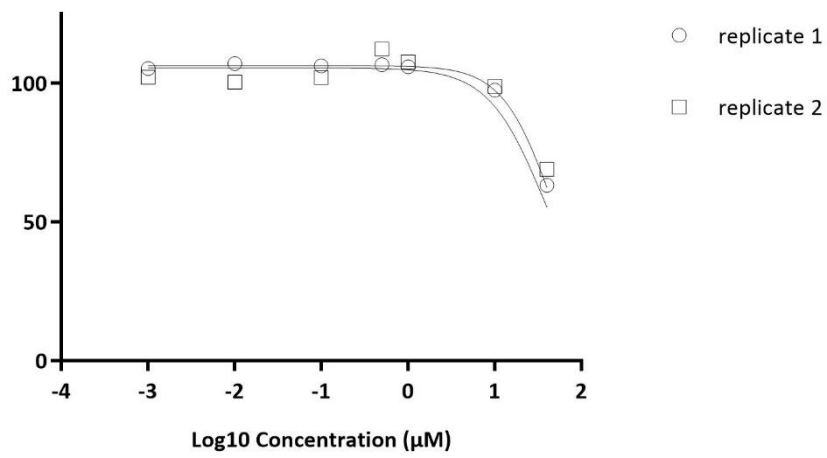
43

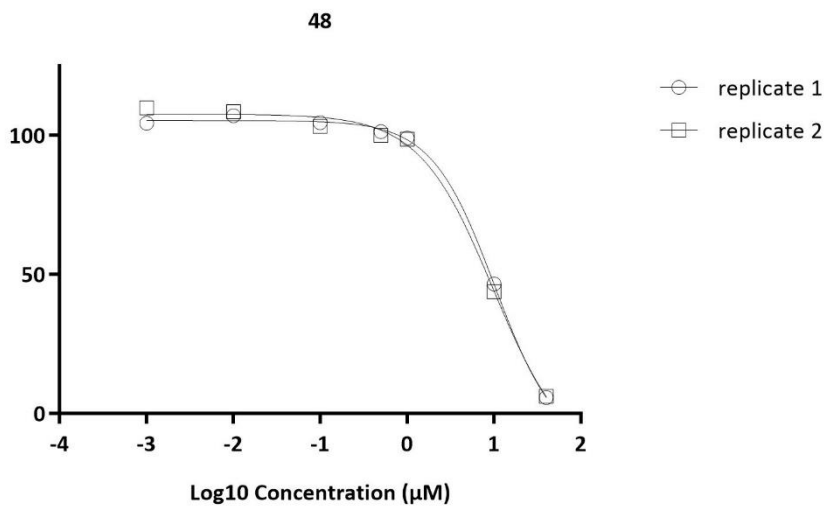
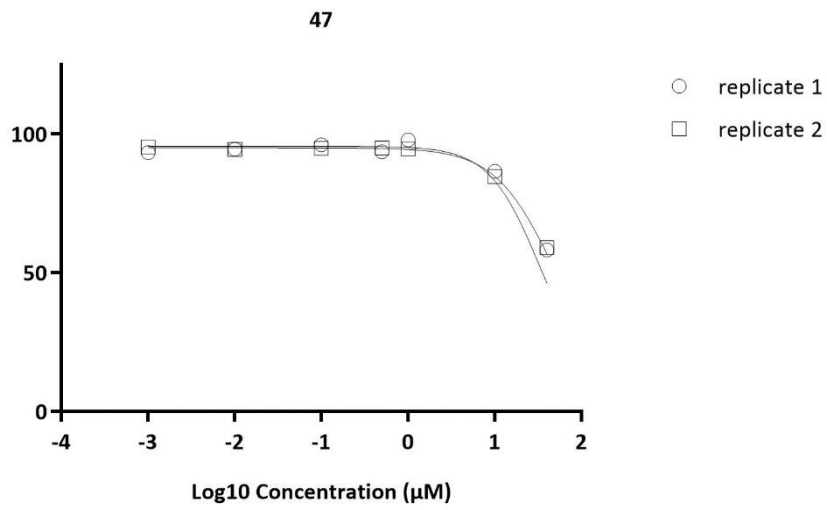
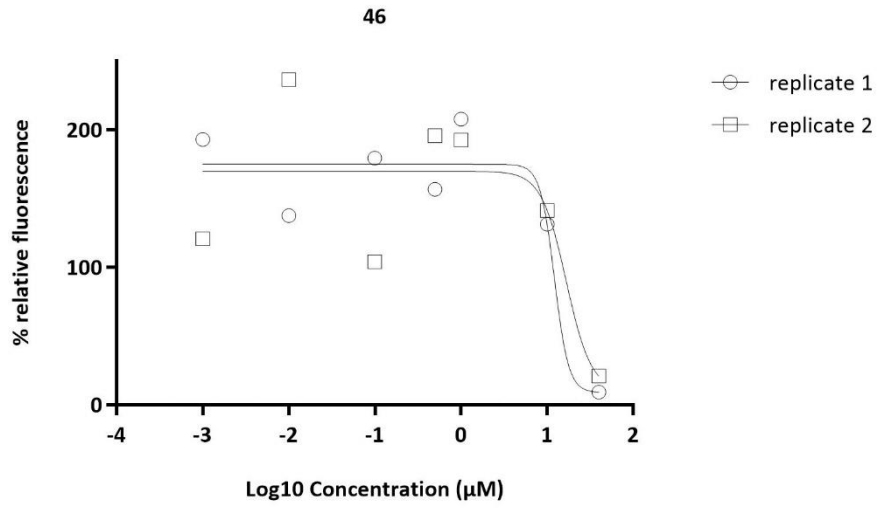


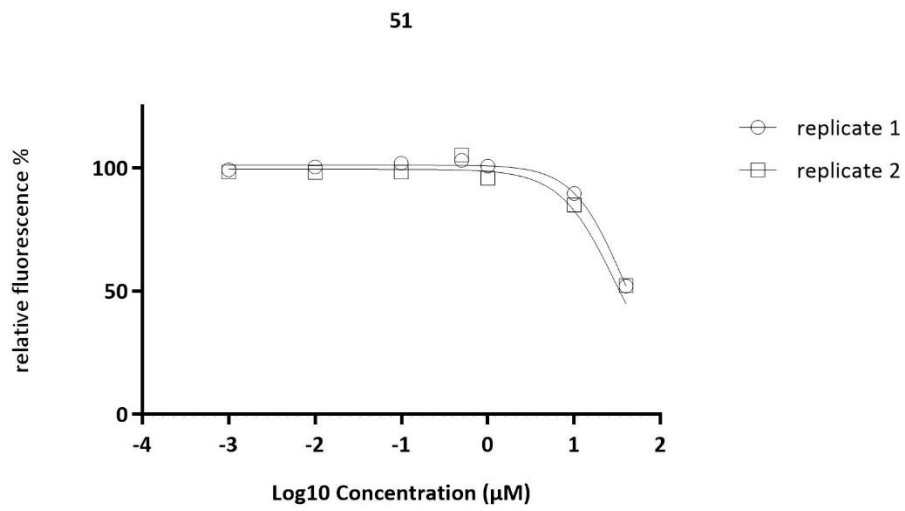
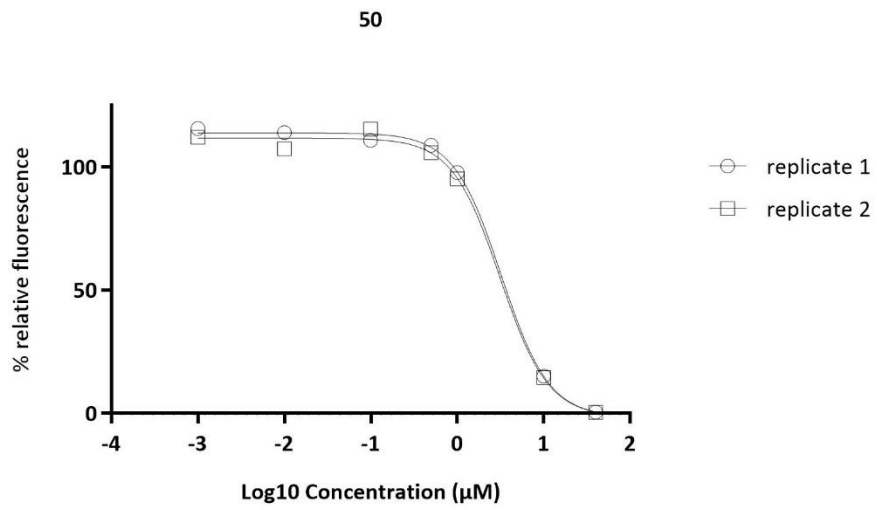
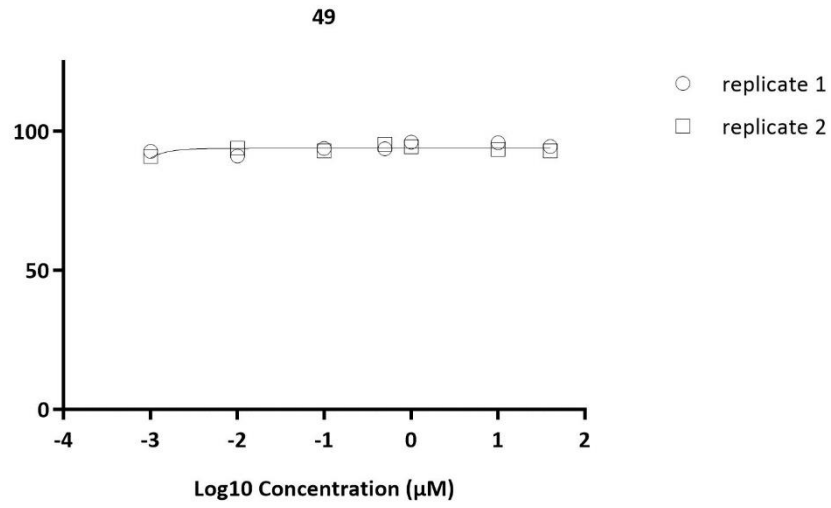
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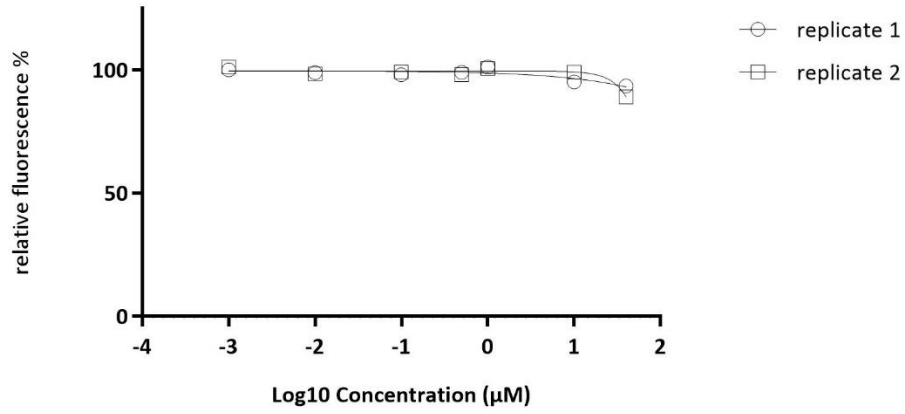
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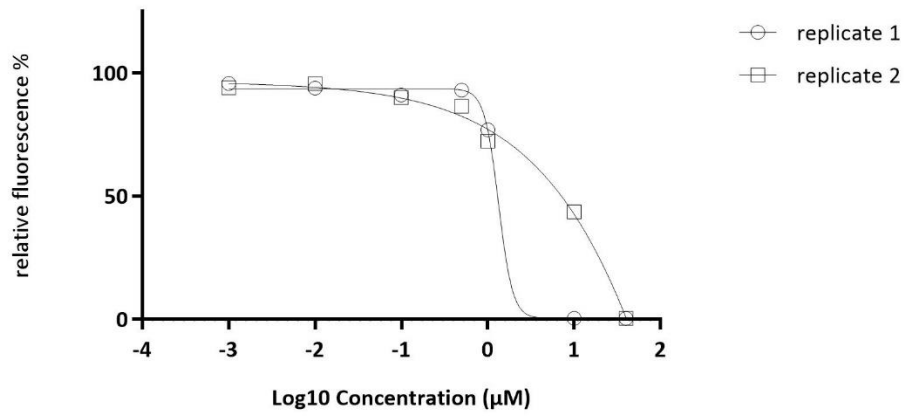




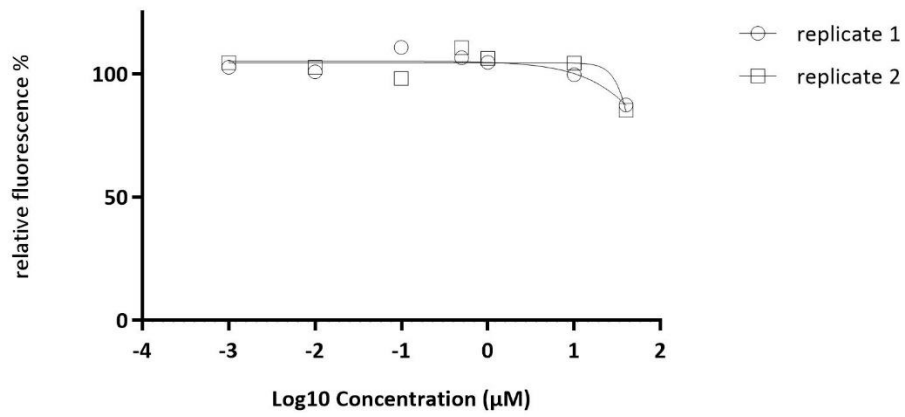
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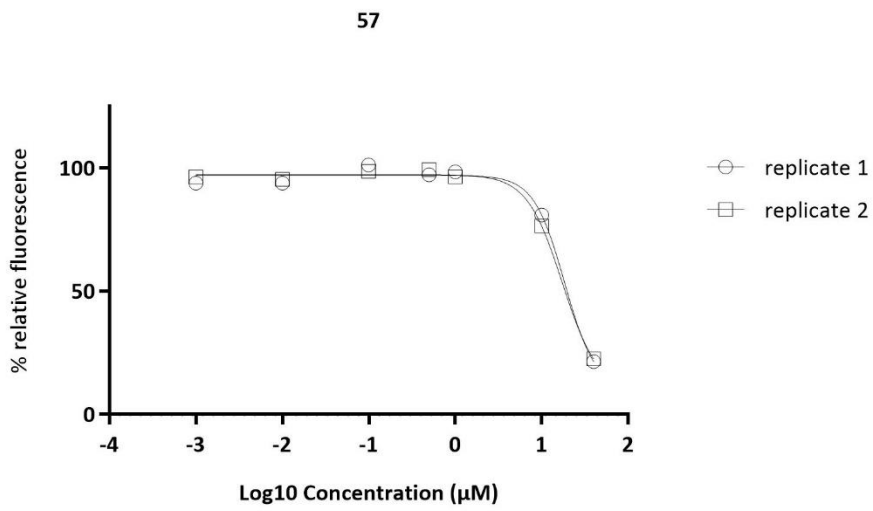
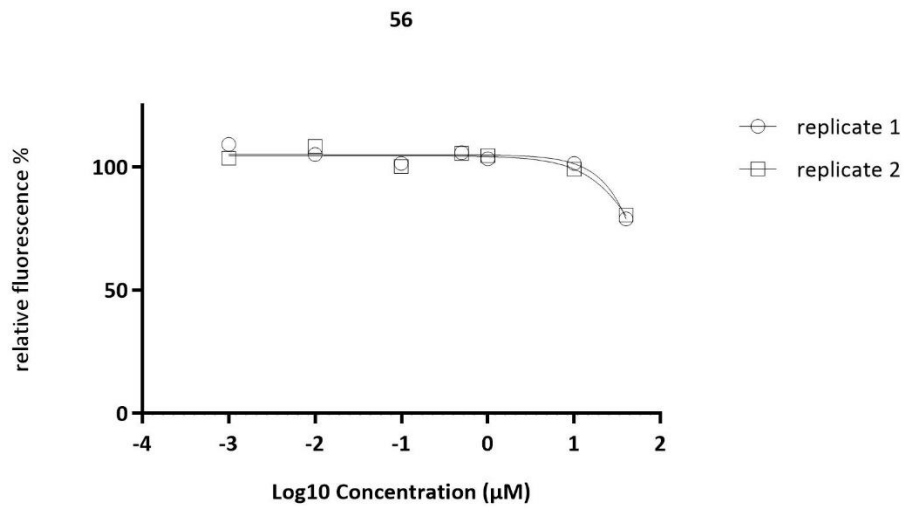
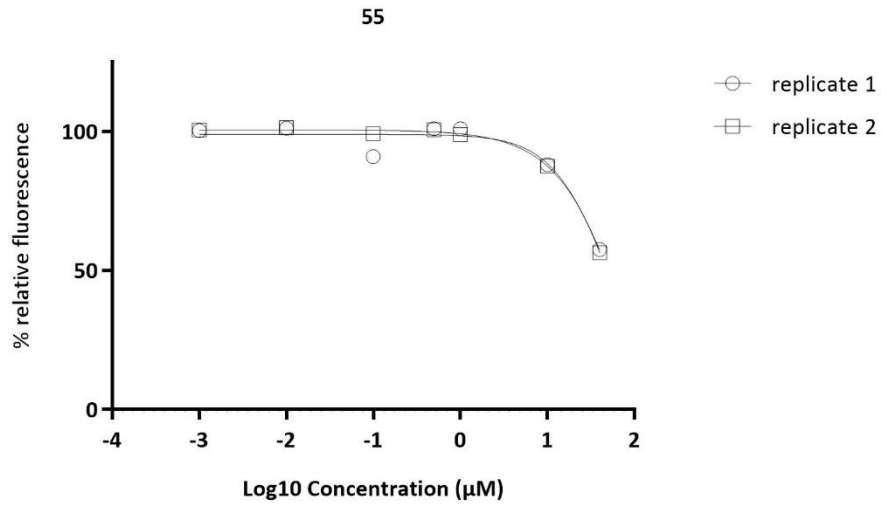


53

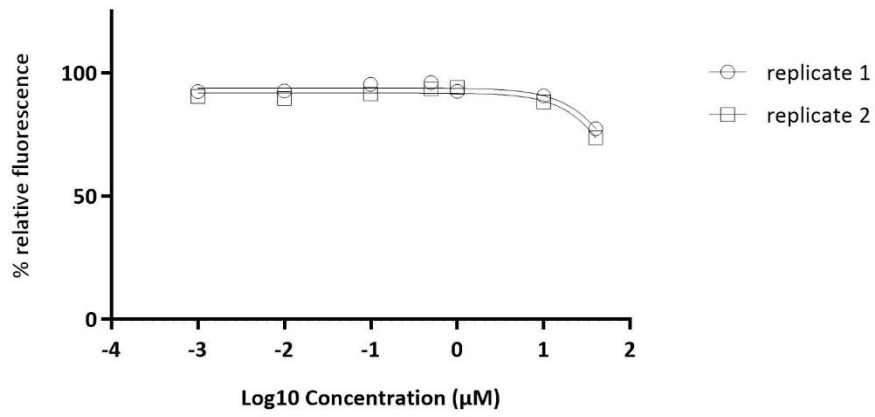


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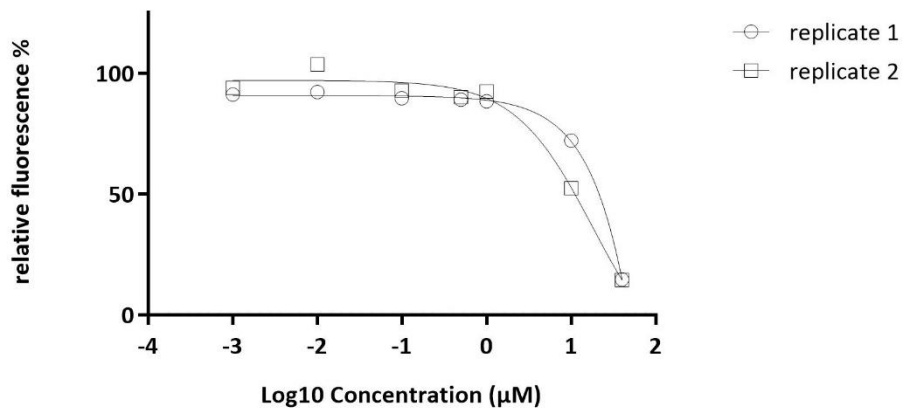




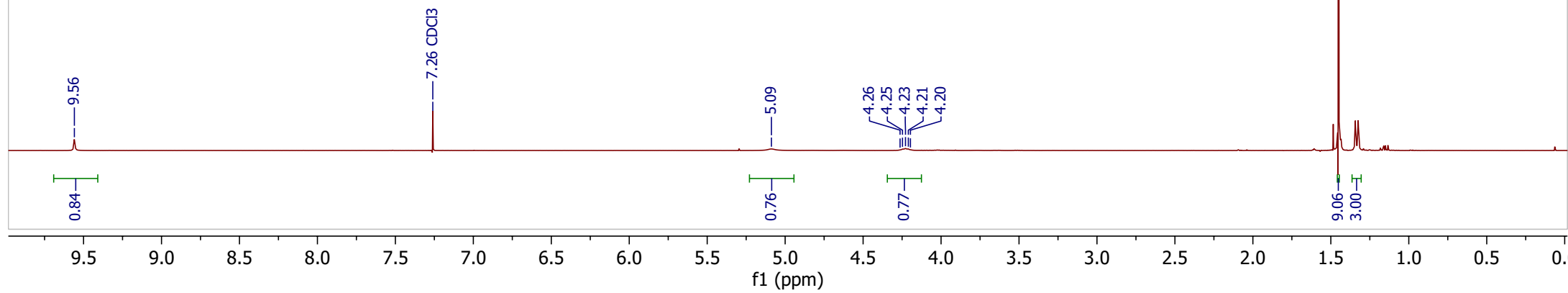
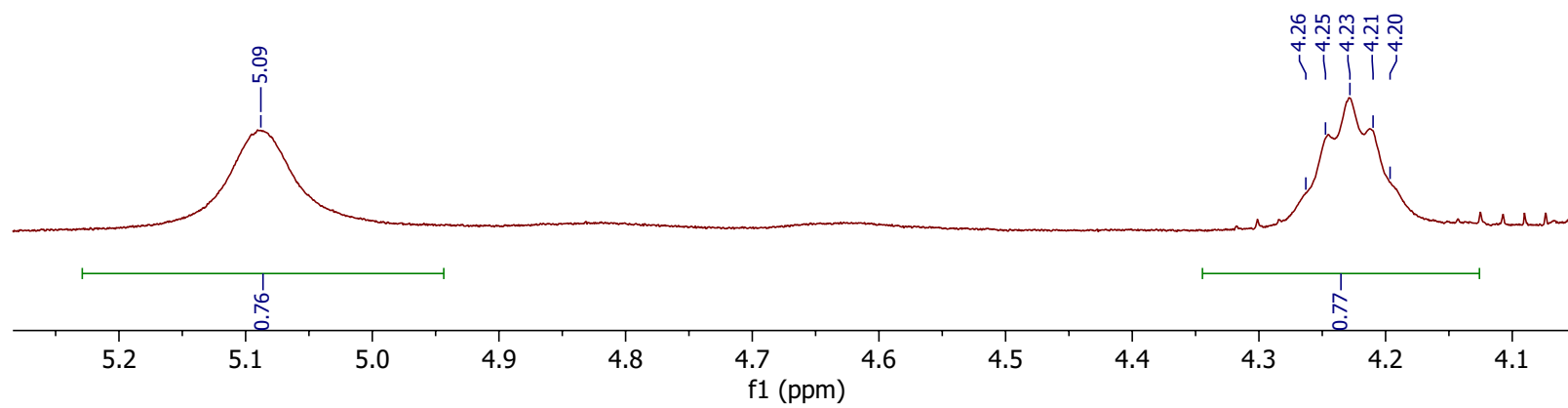
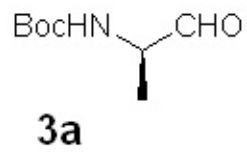
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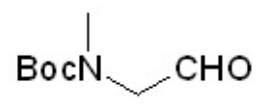


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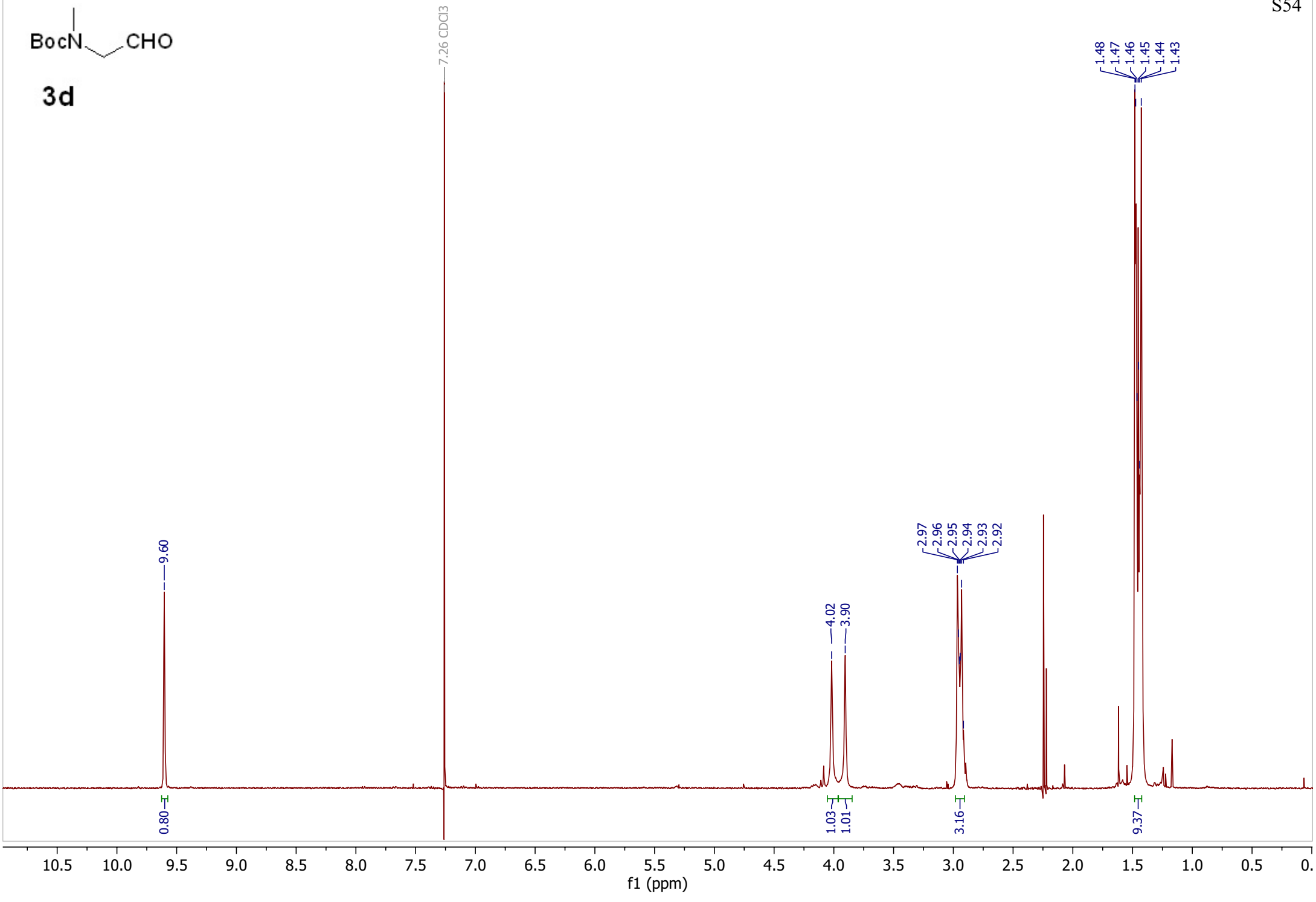


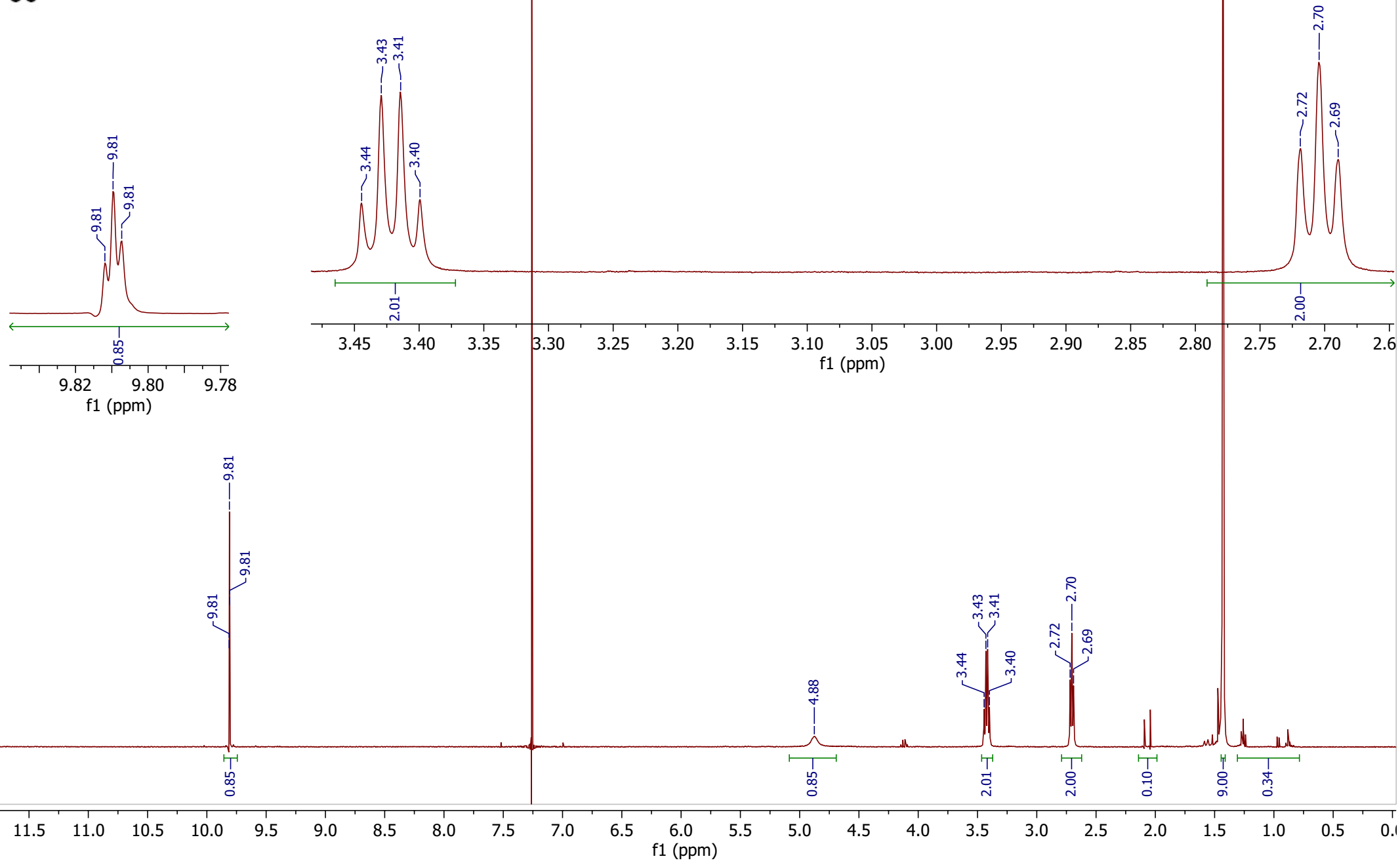
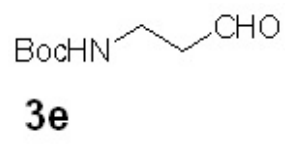
^1H and ^{13}C NMR Spectra

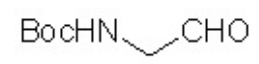




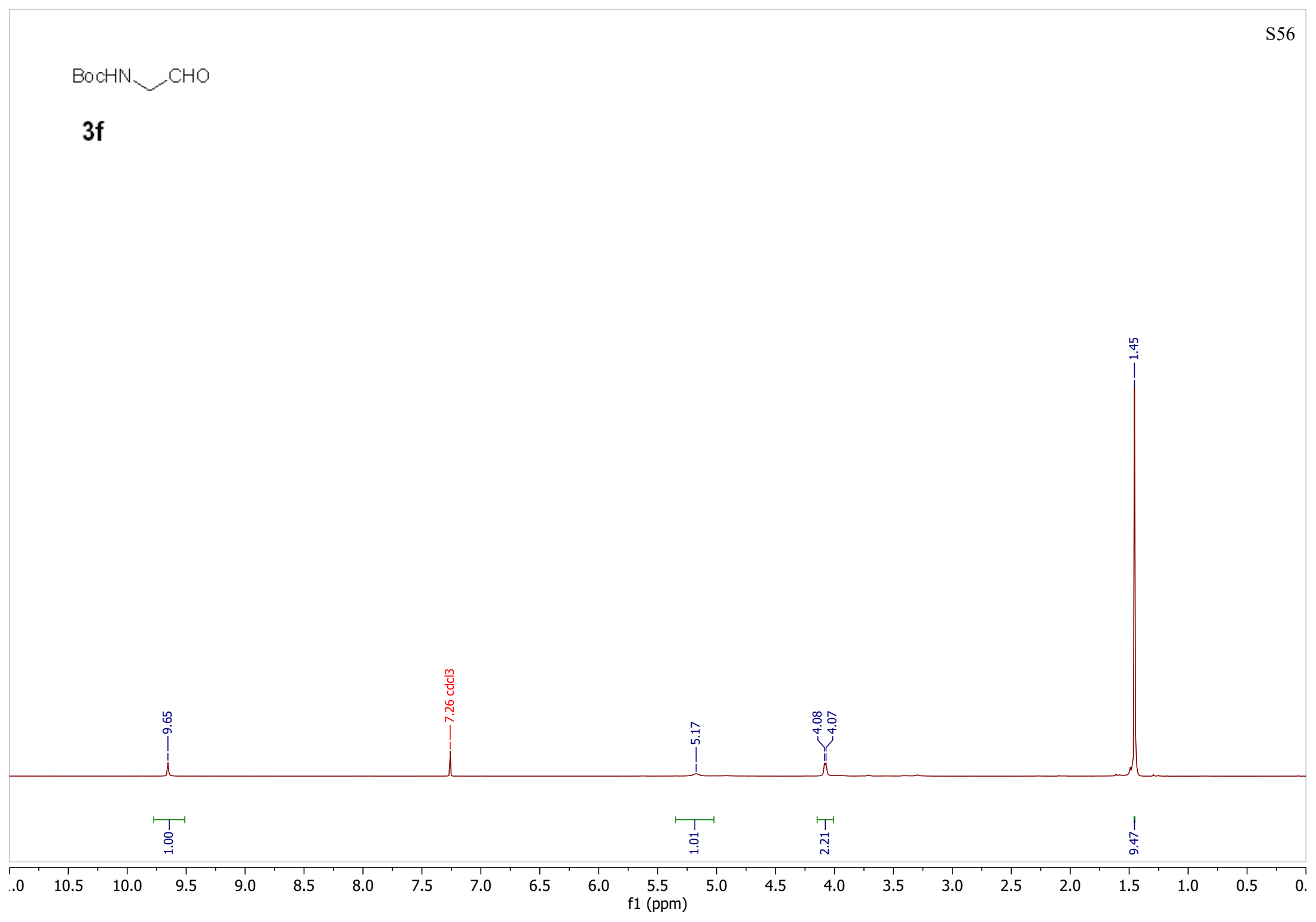
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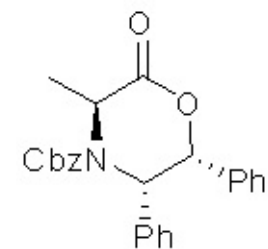
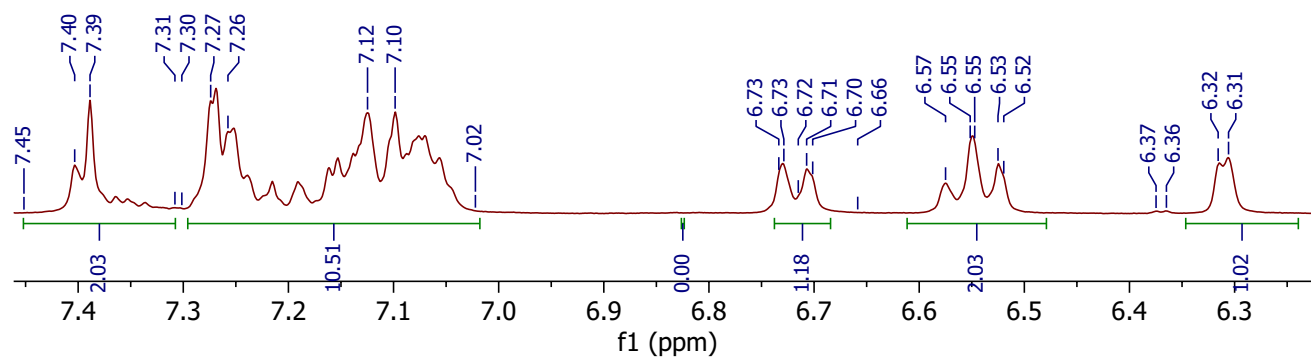




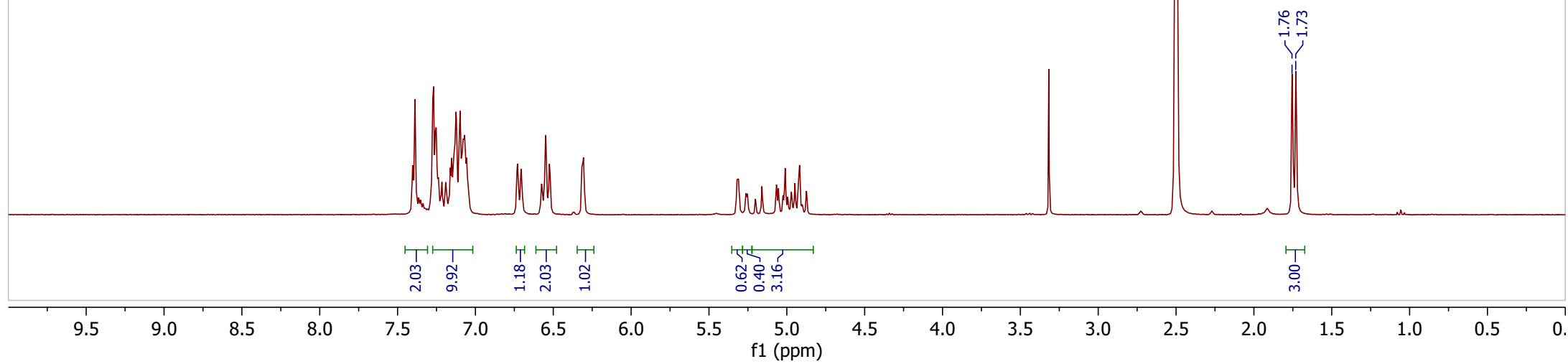
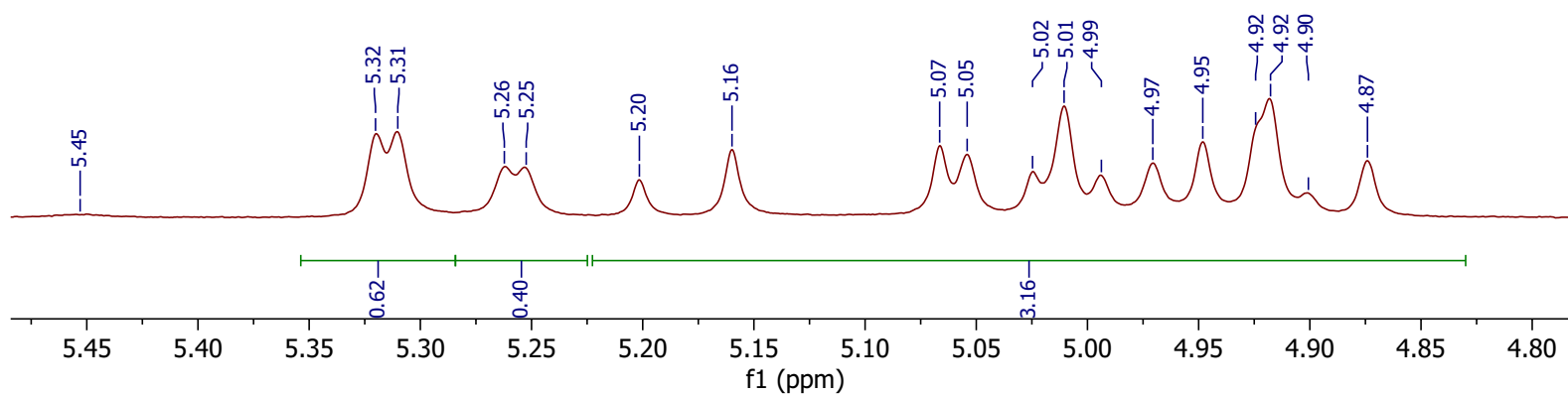


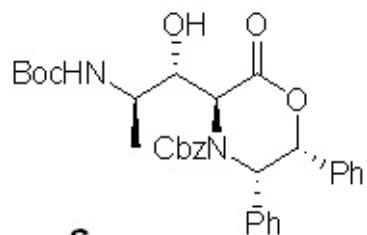
3f



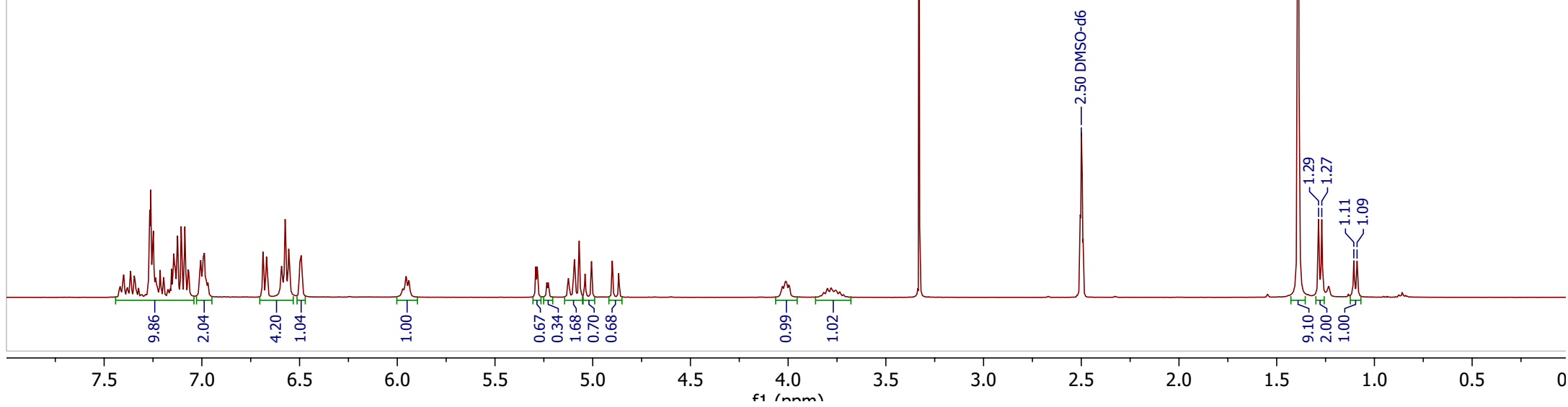
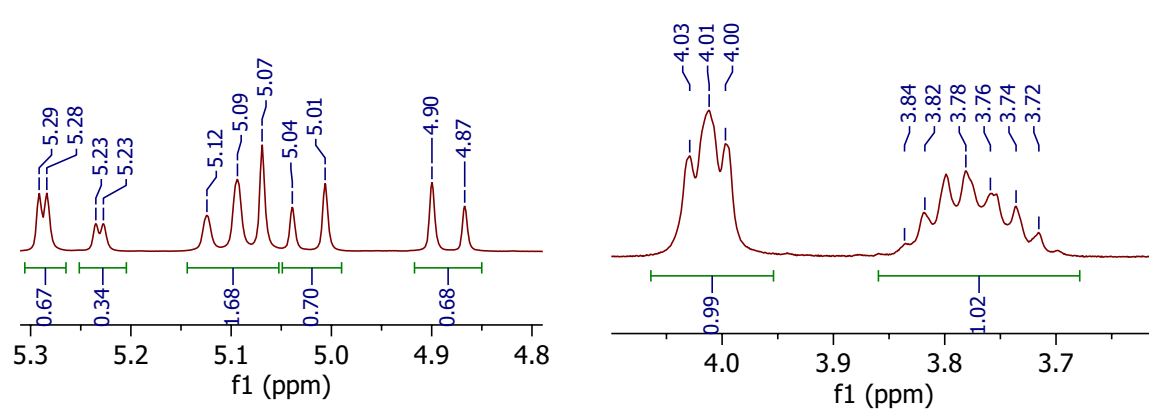
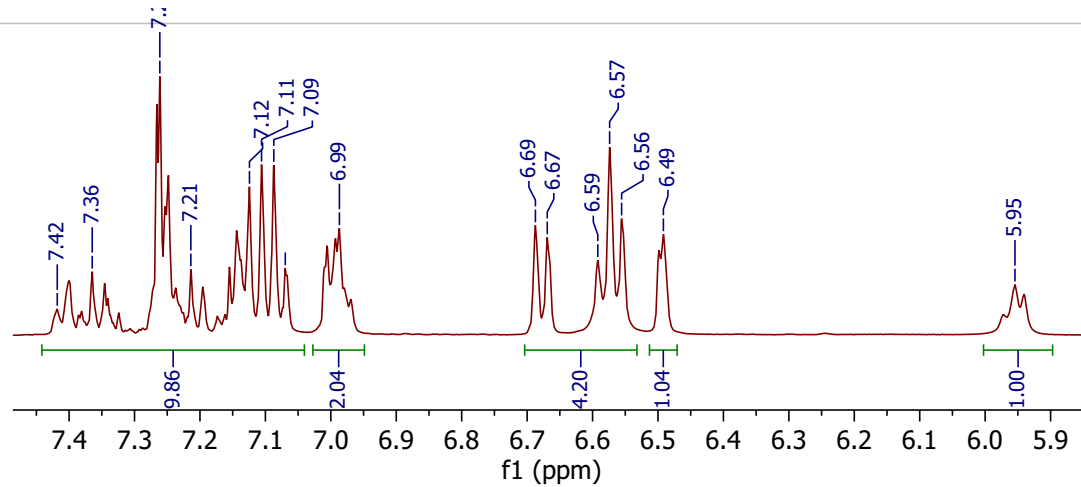


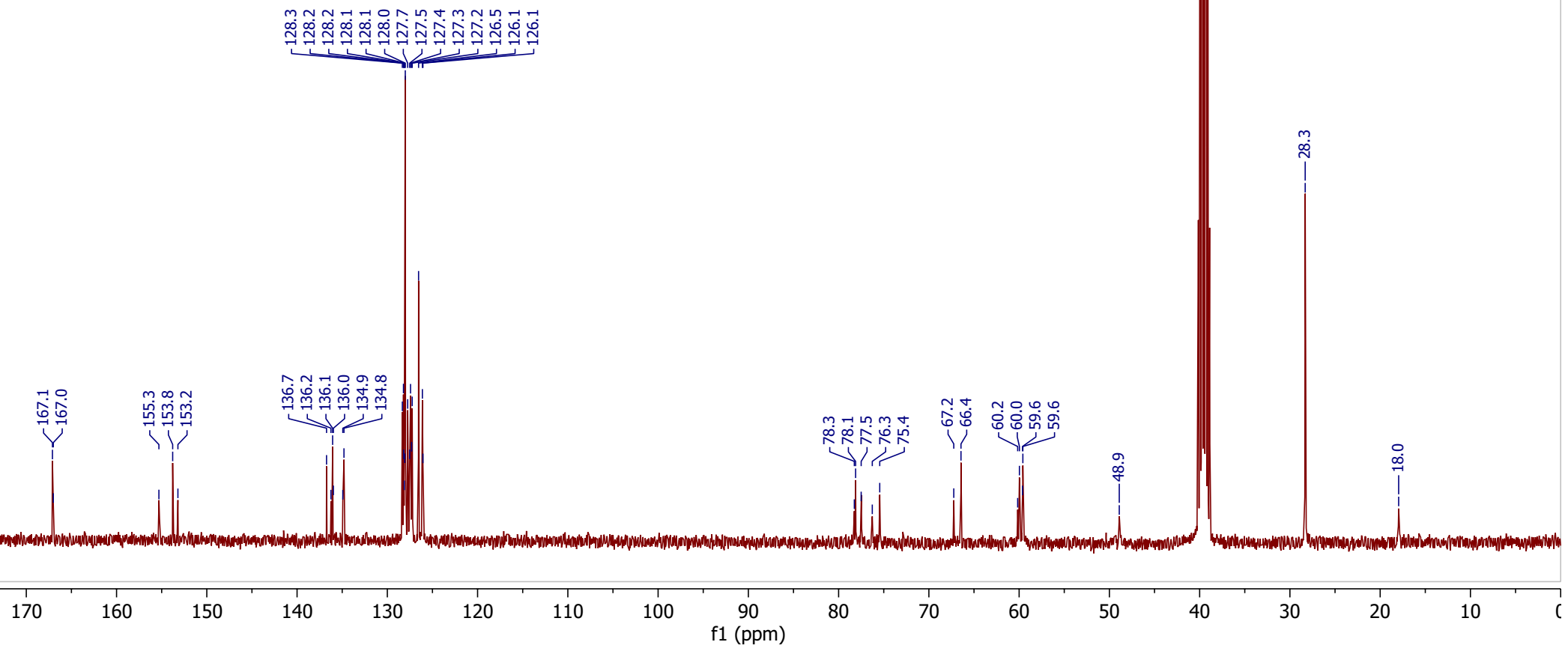
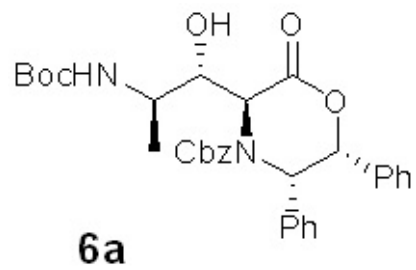
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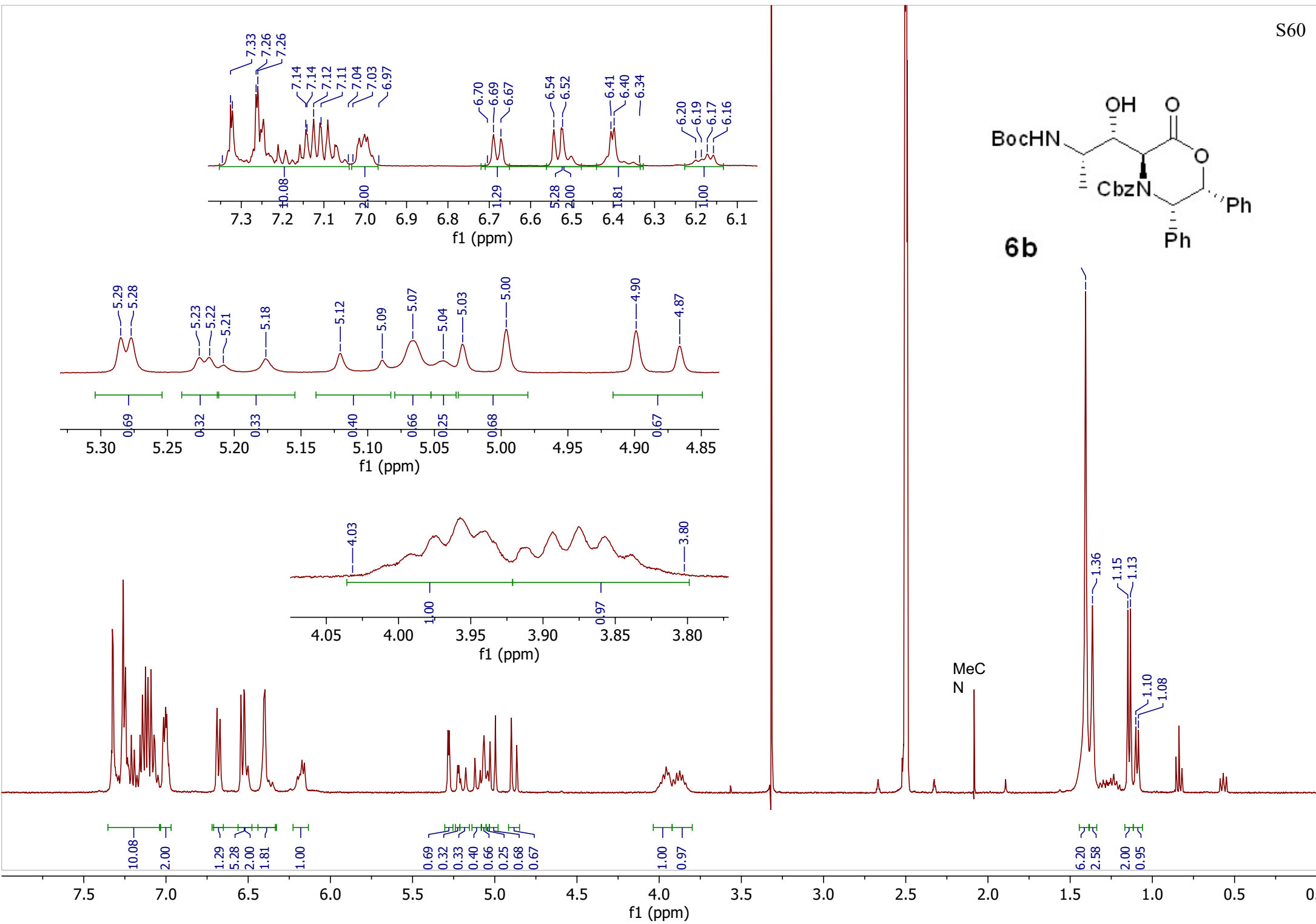


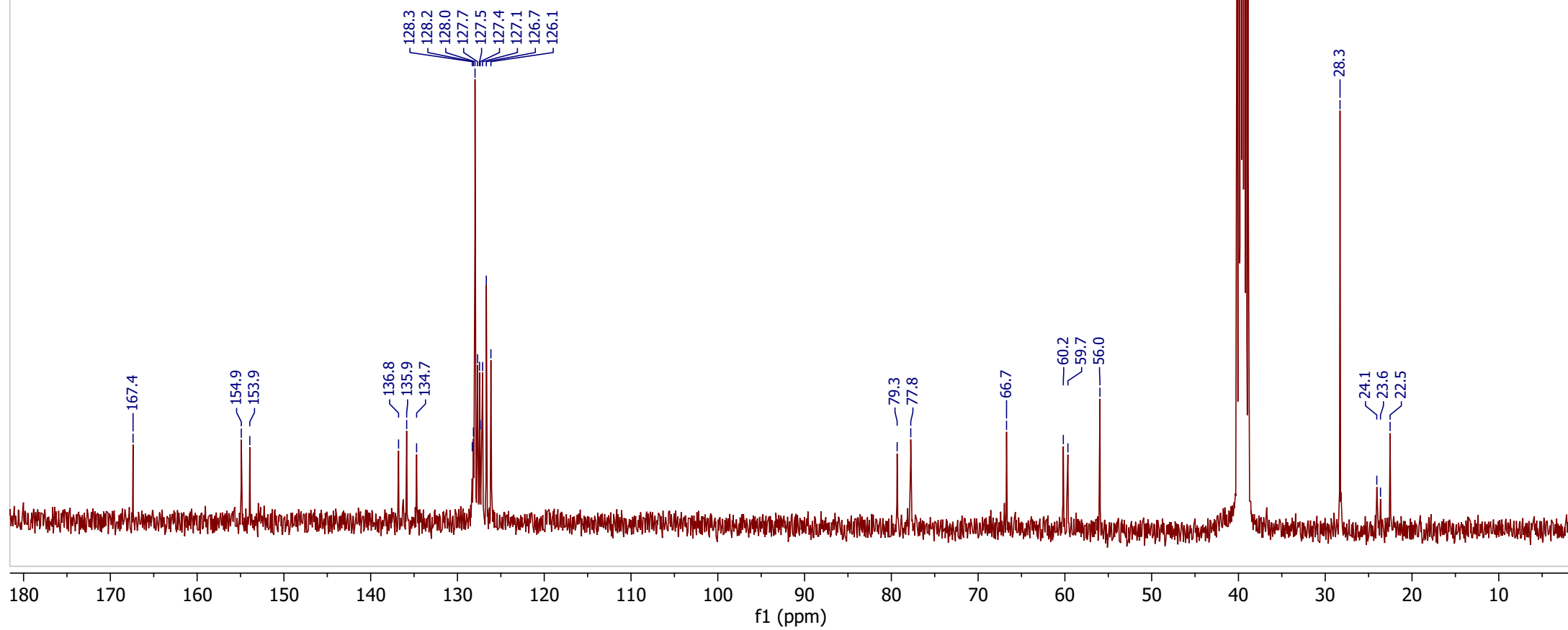
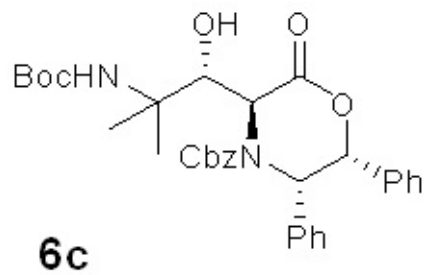


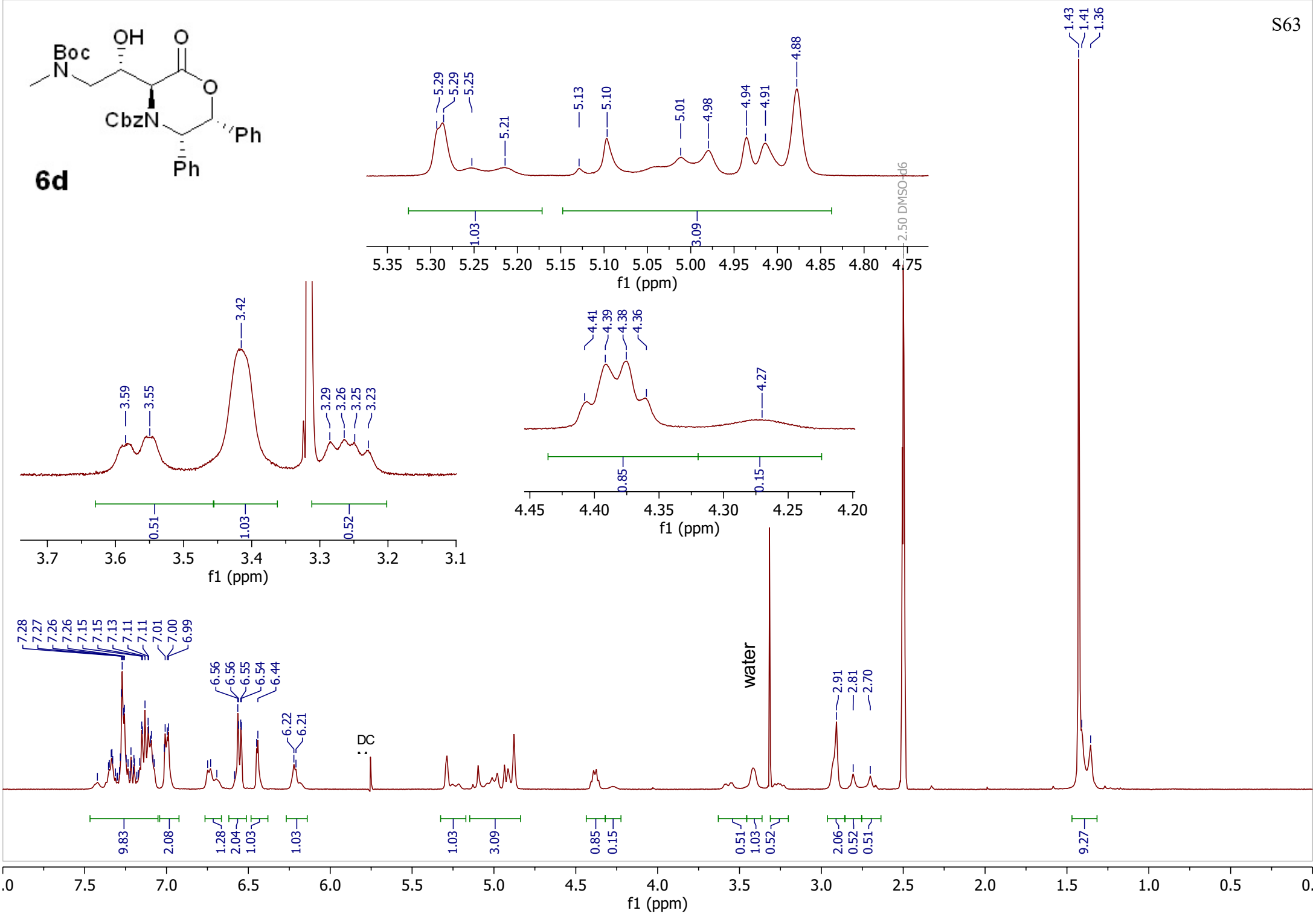
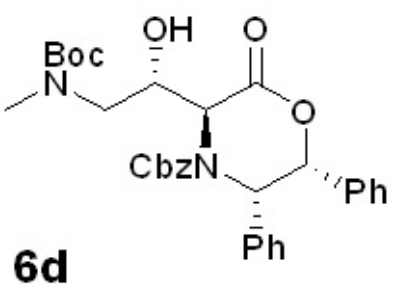
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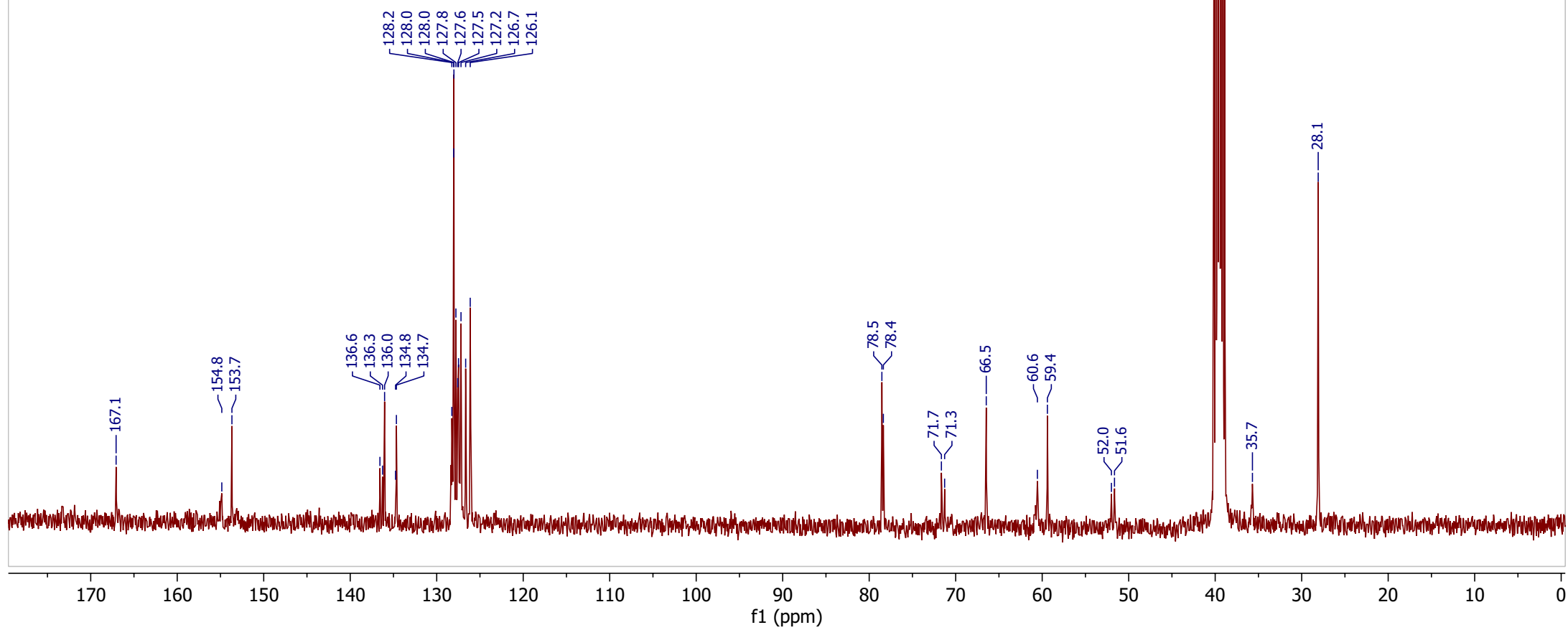
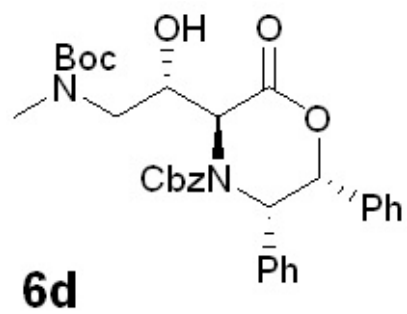


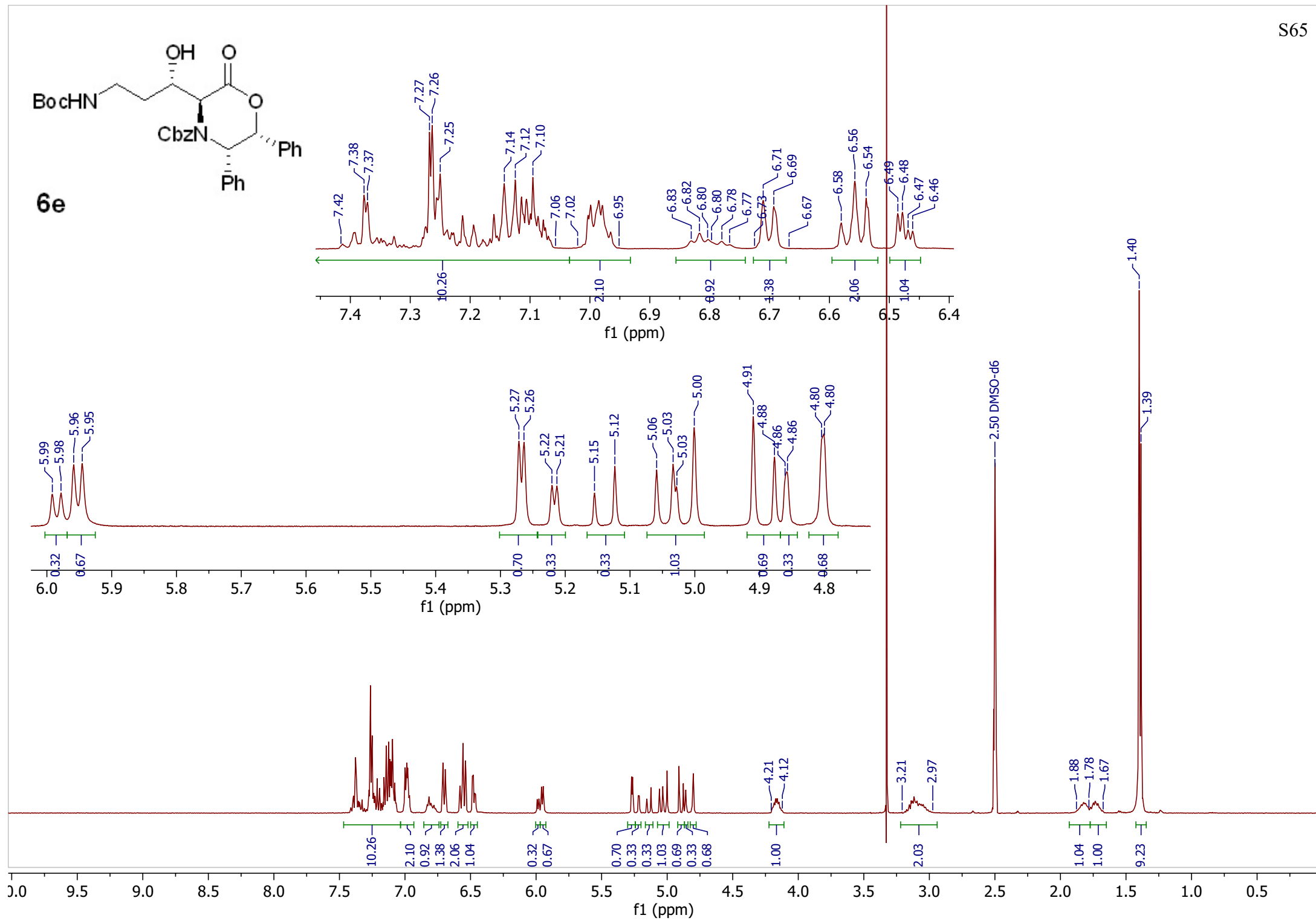


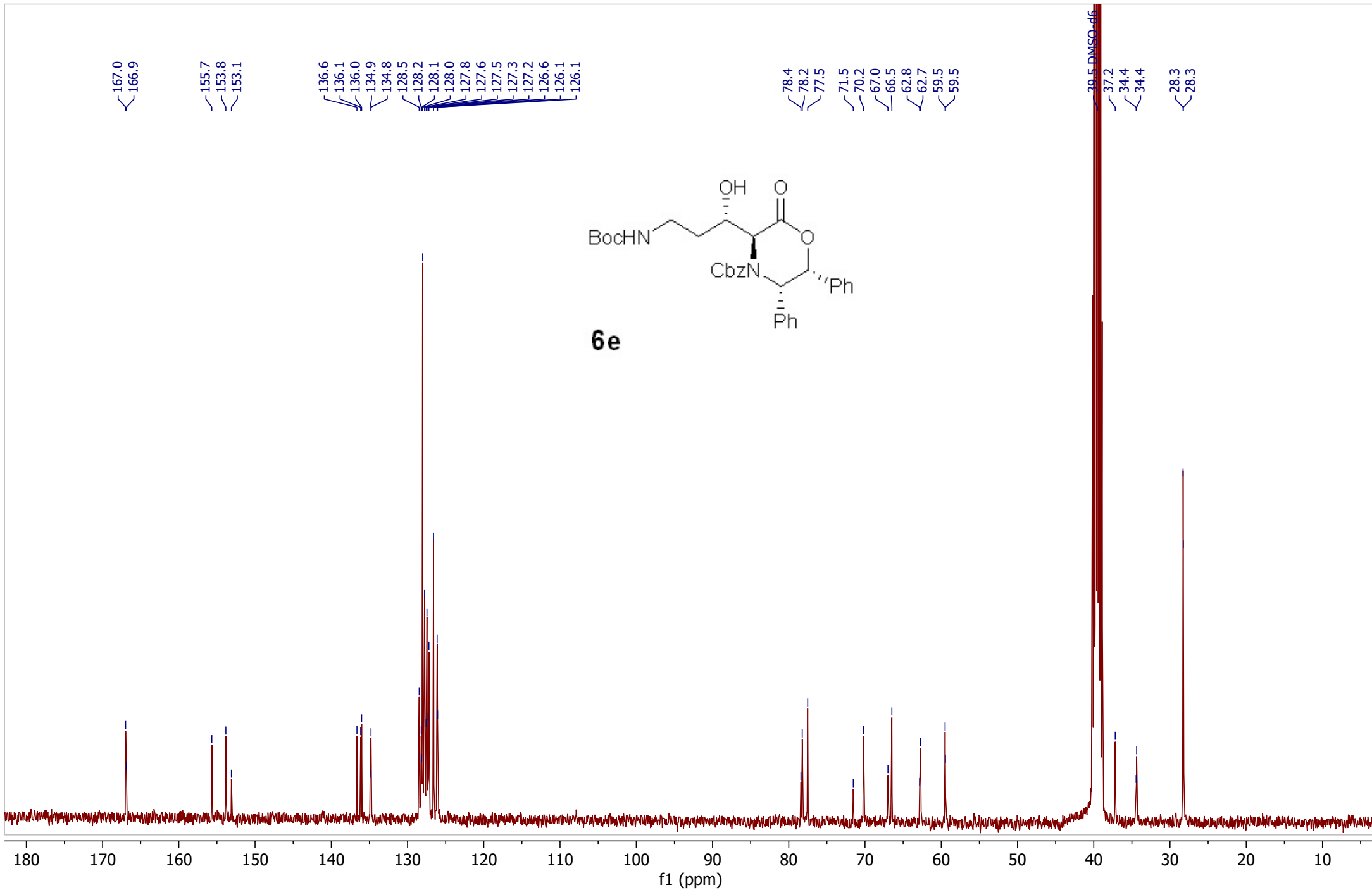


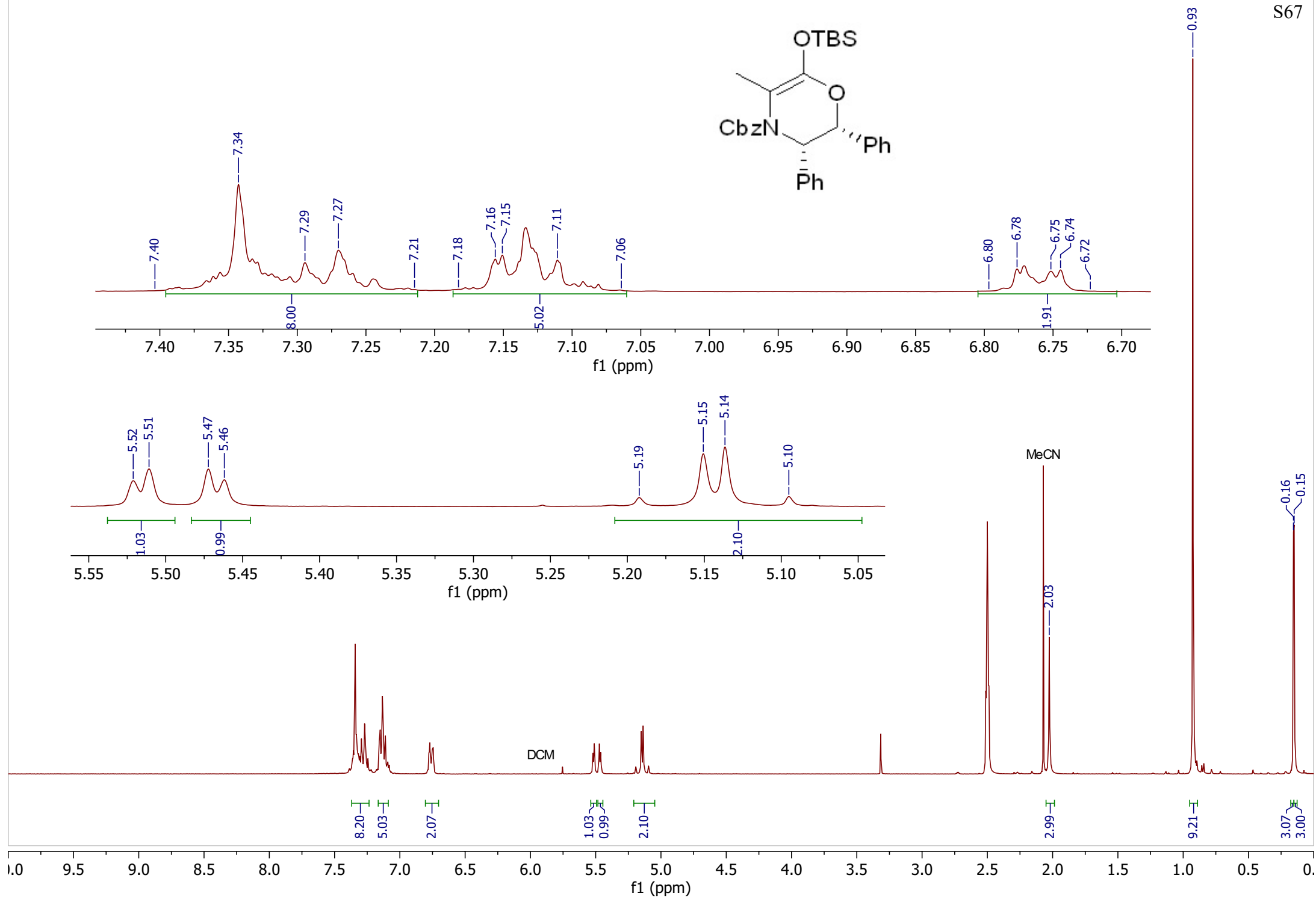
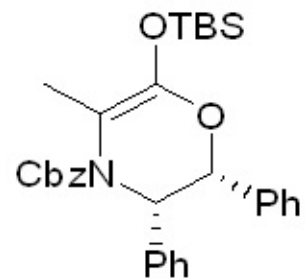


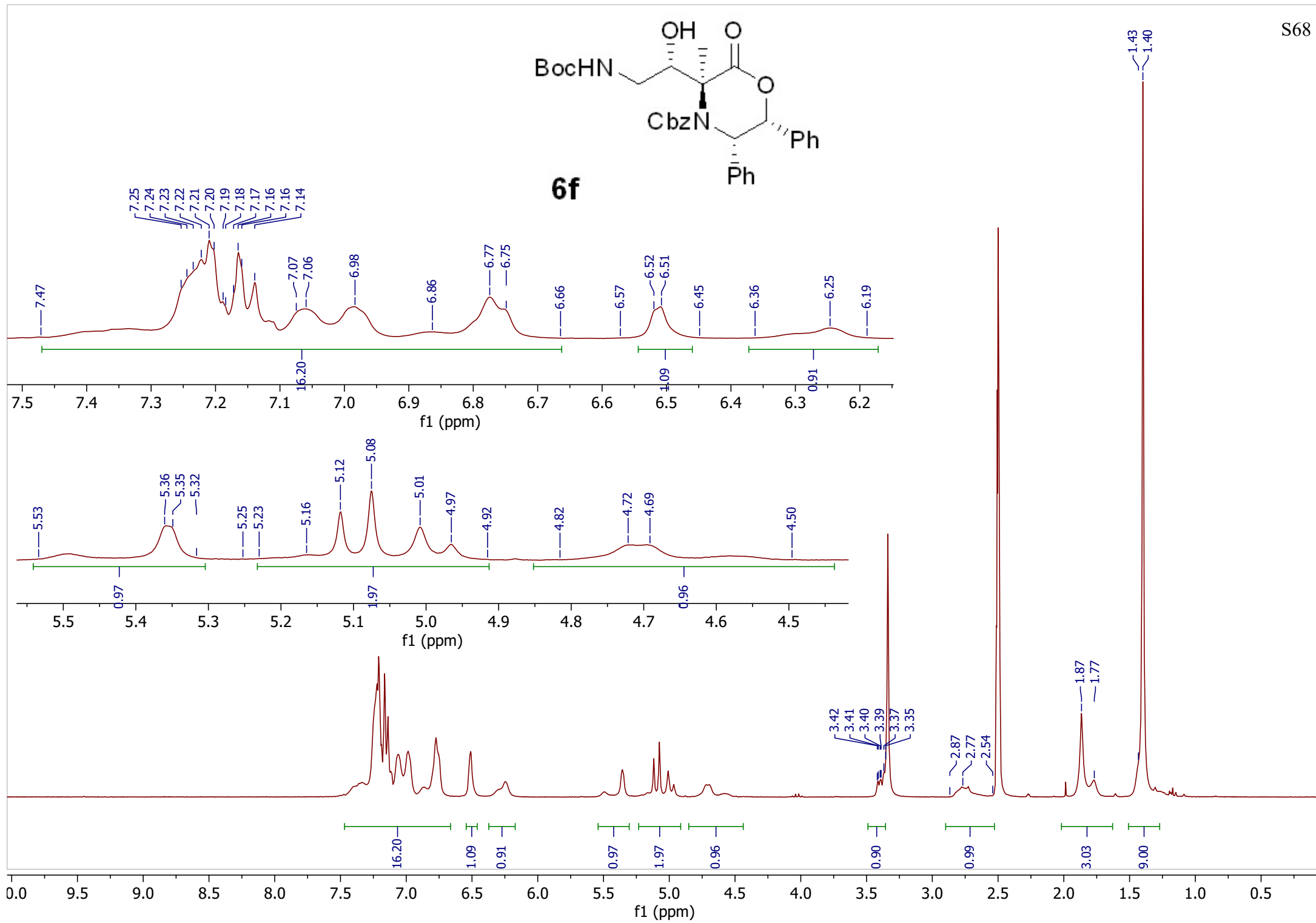


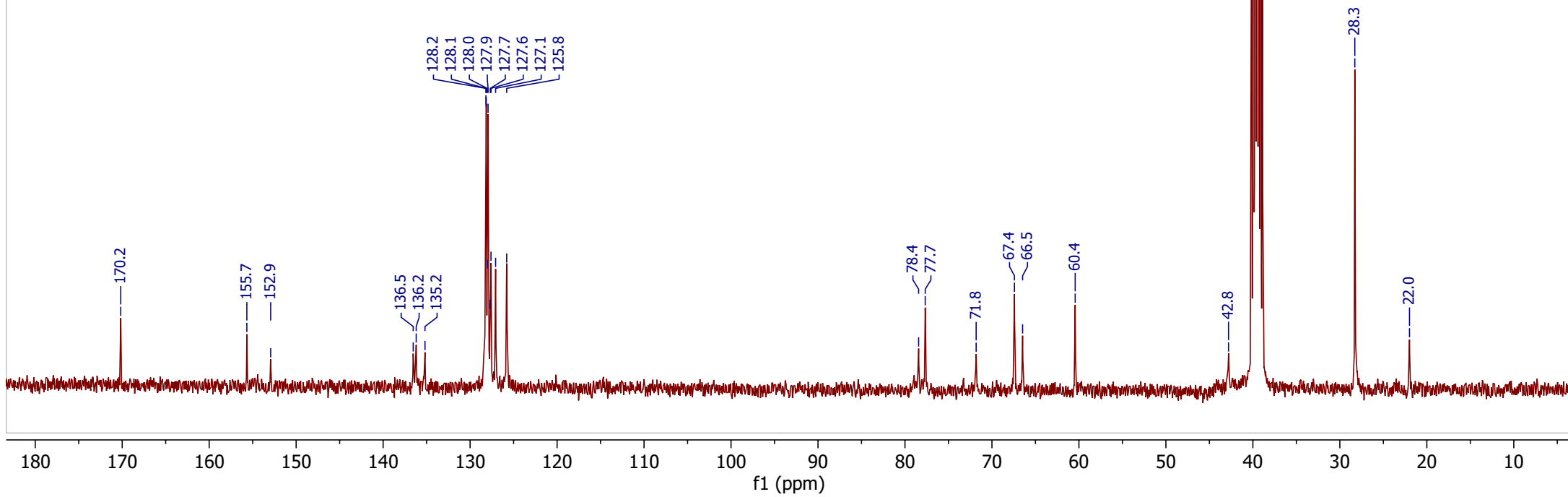
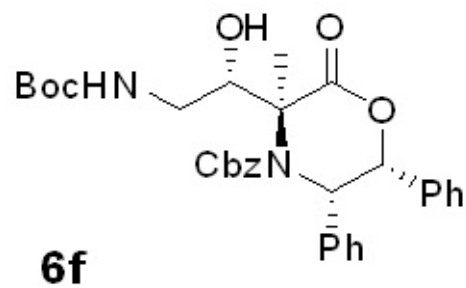


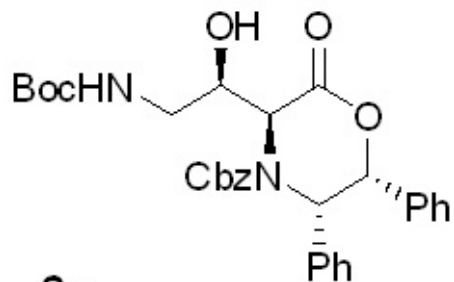




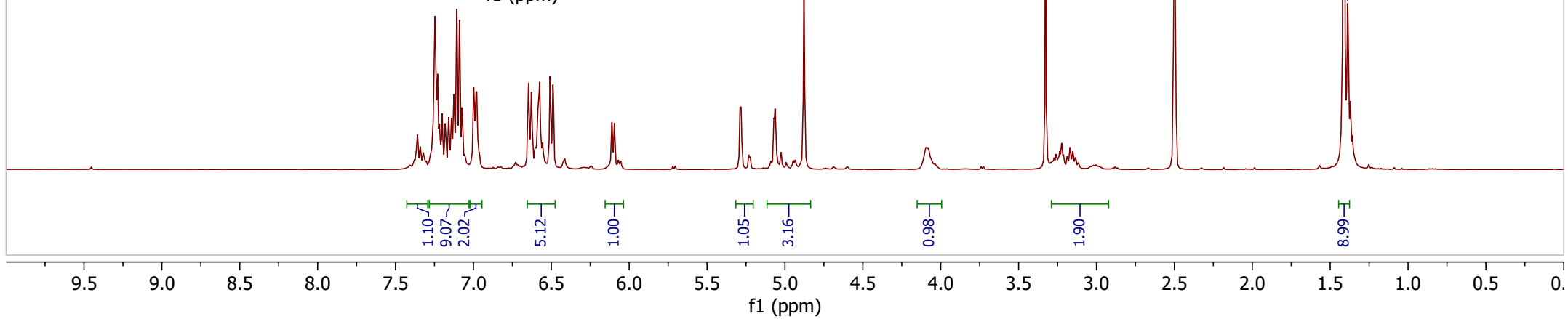
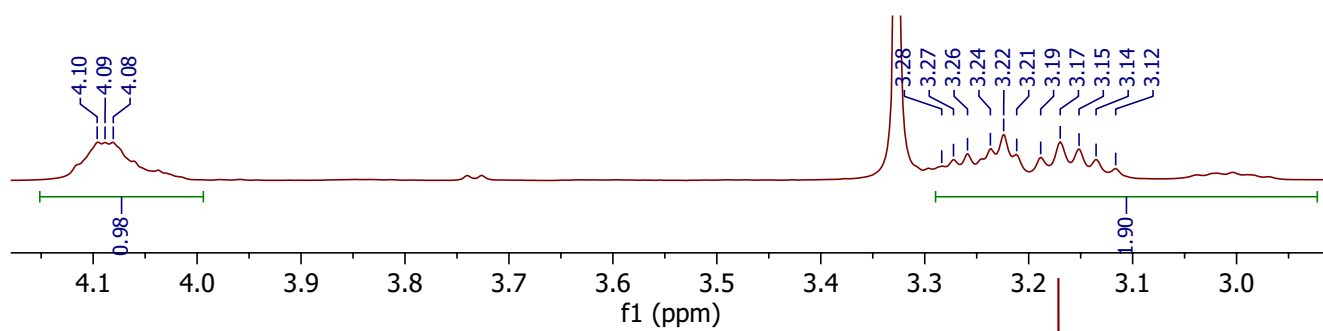
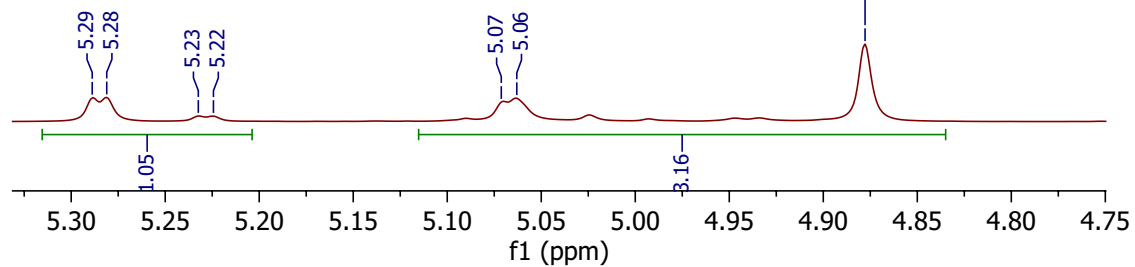
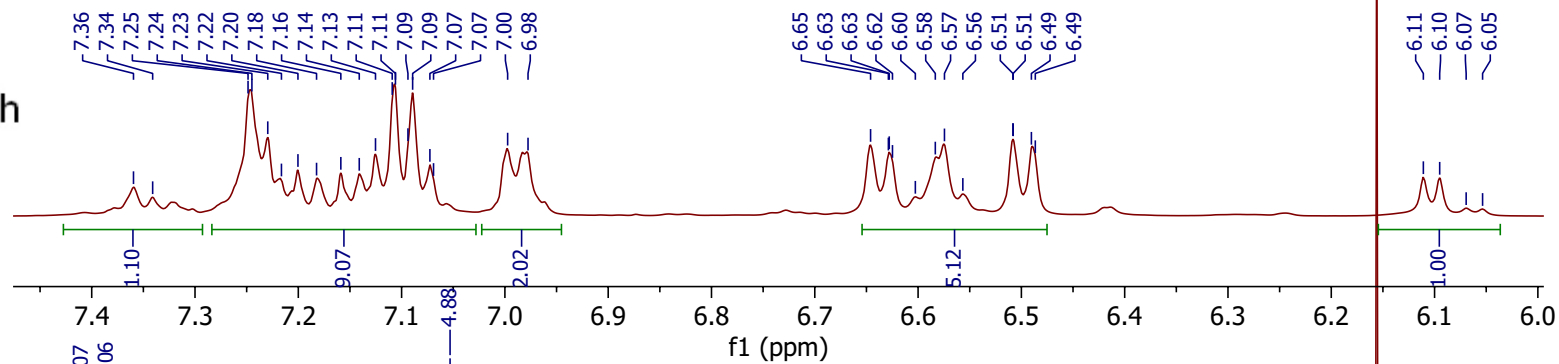


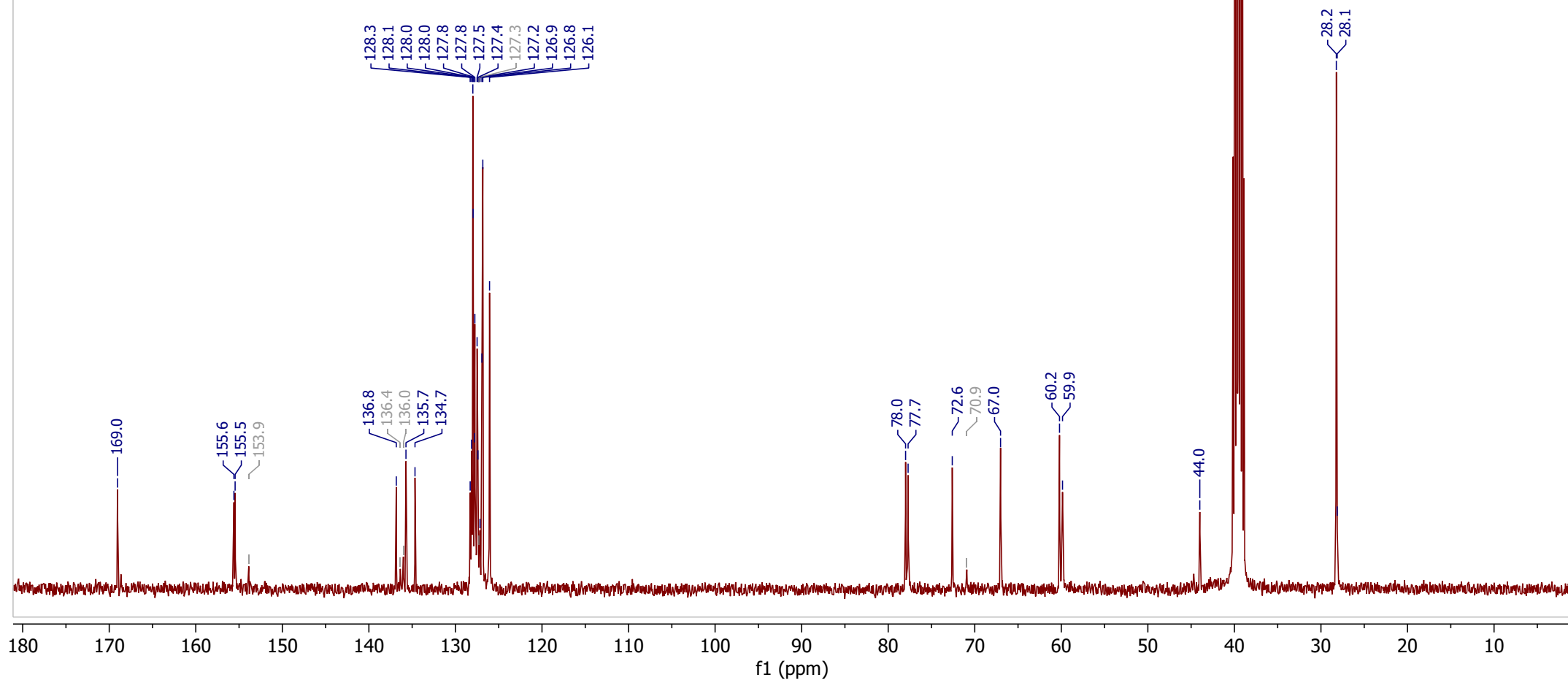
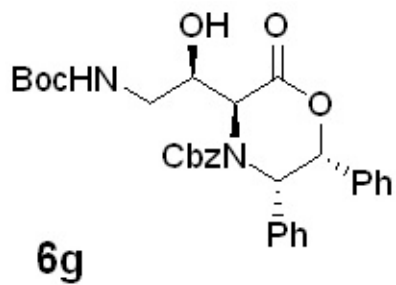


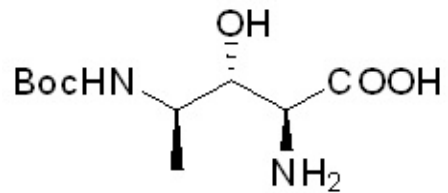




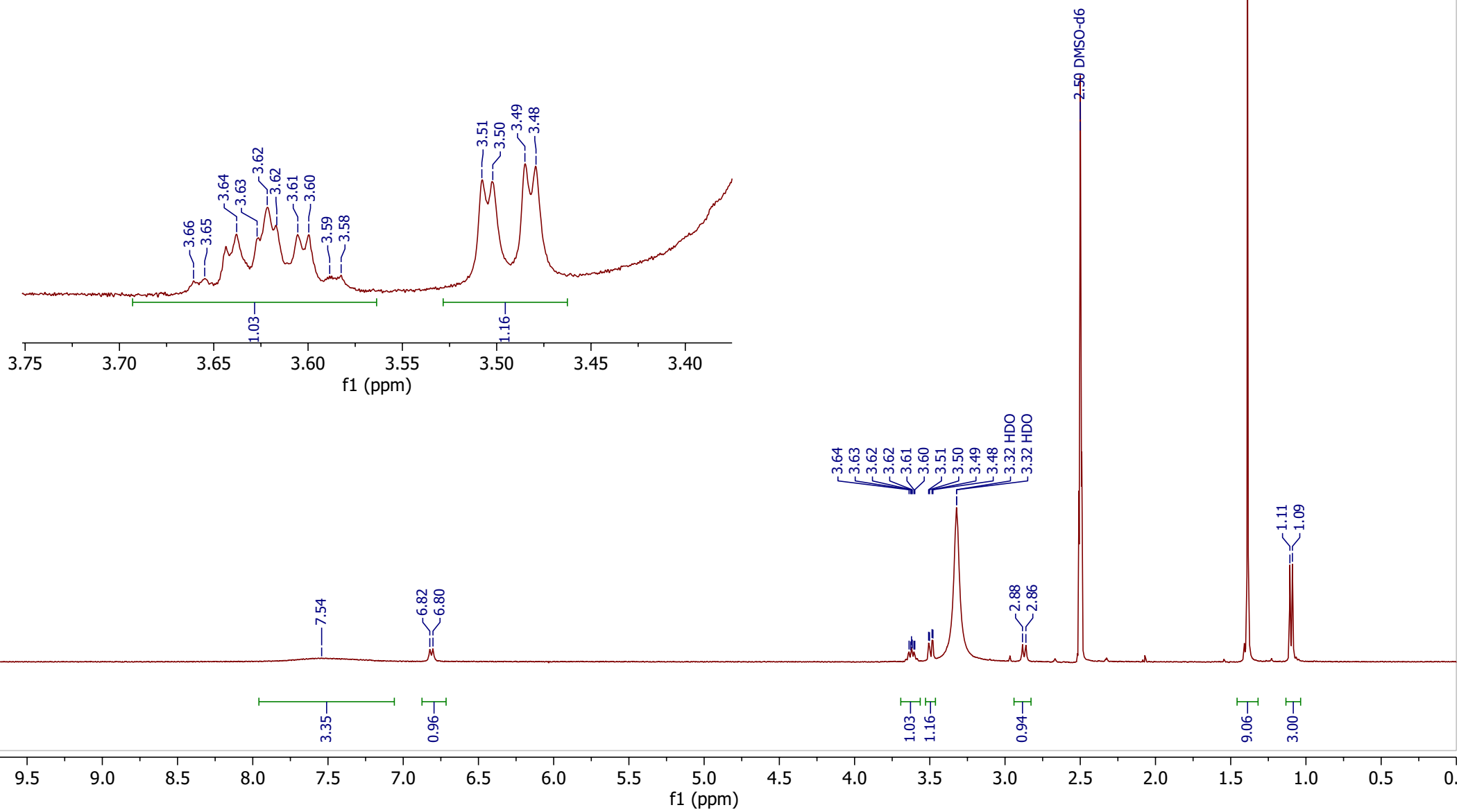
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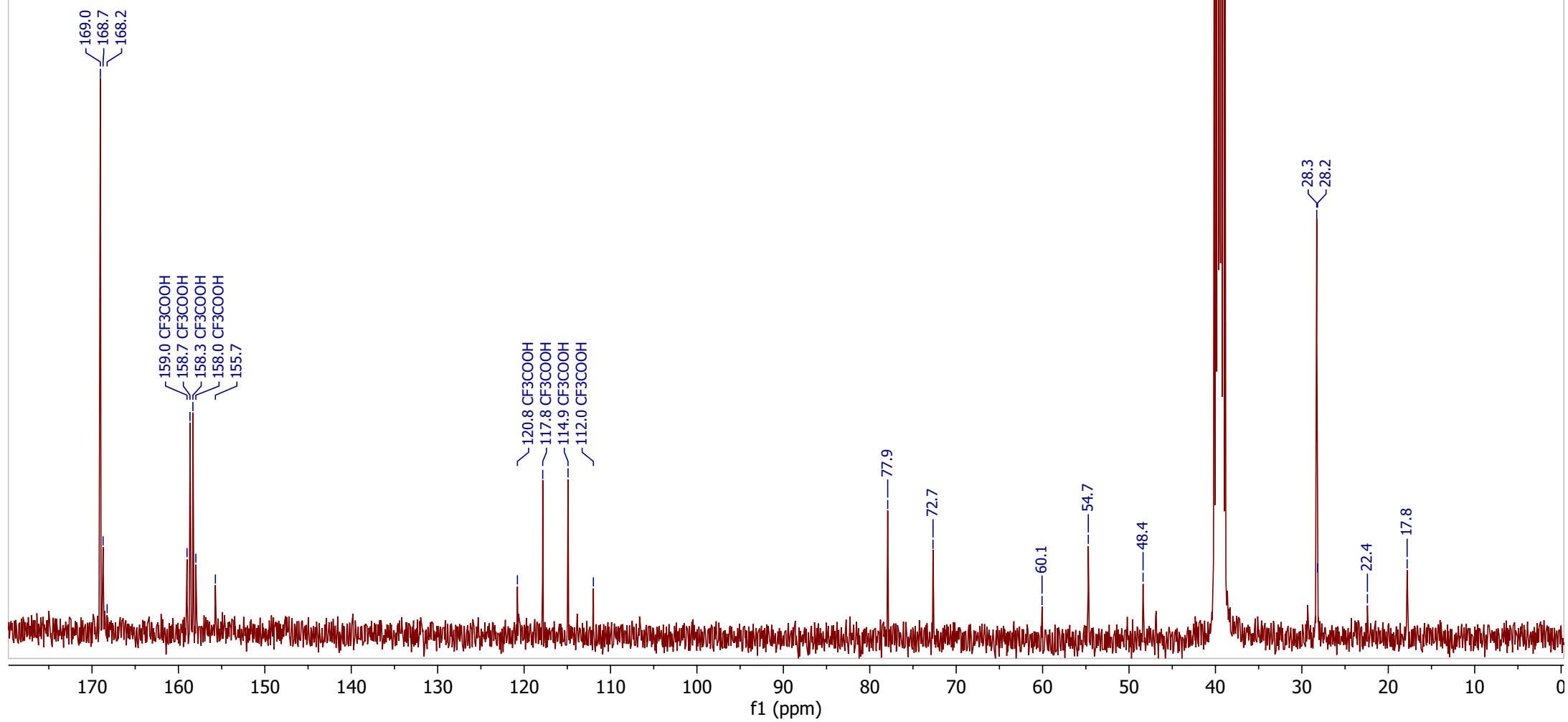
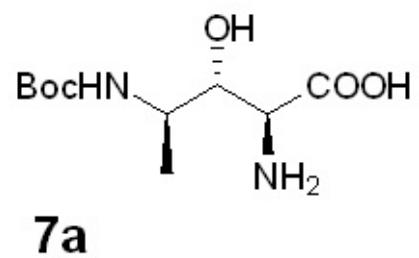


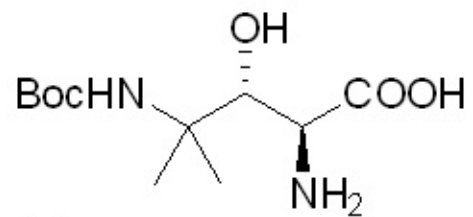




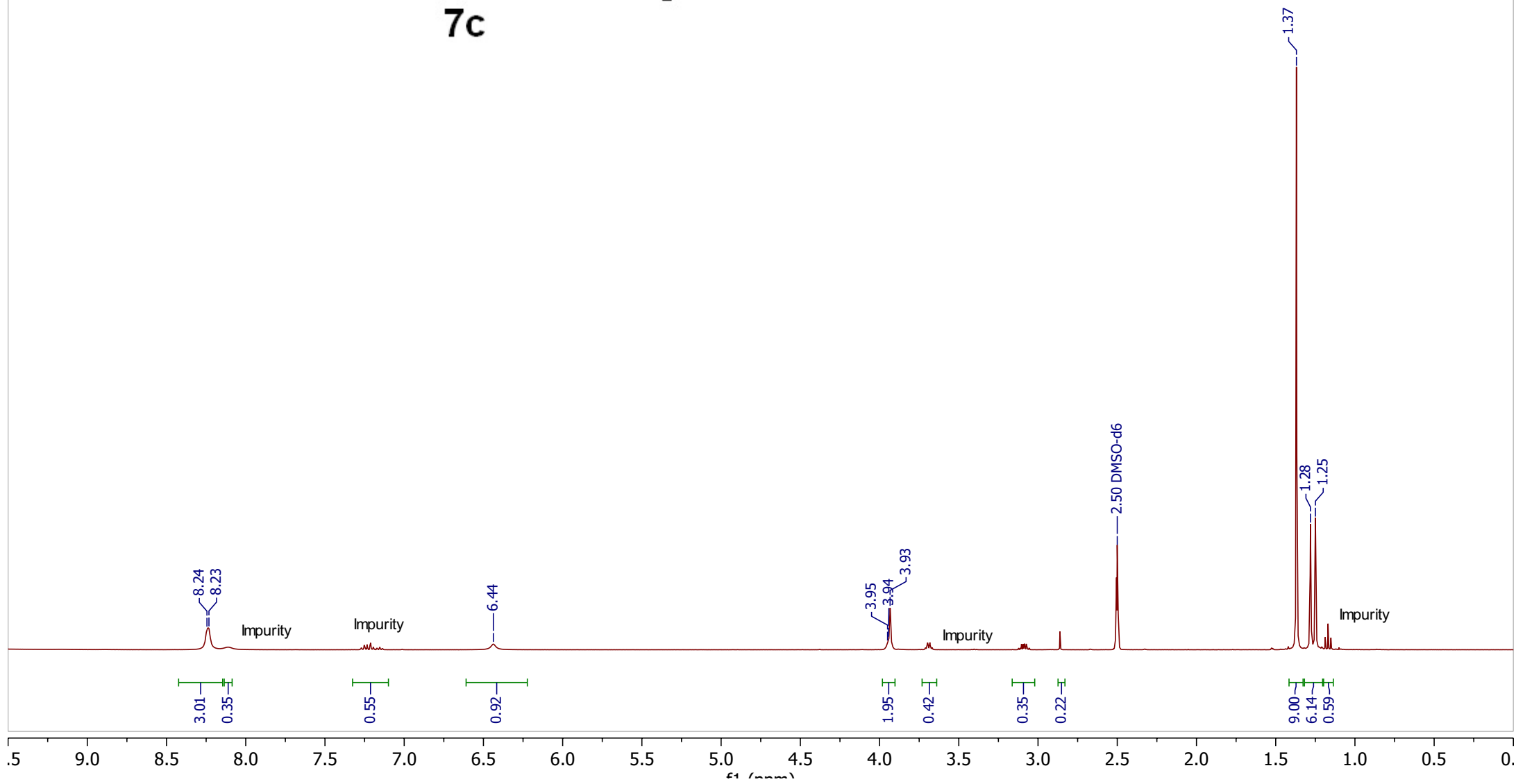
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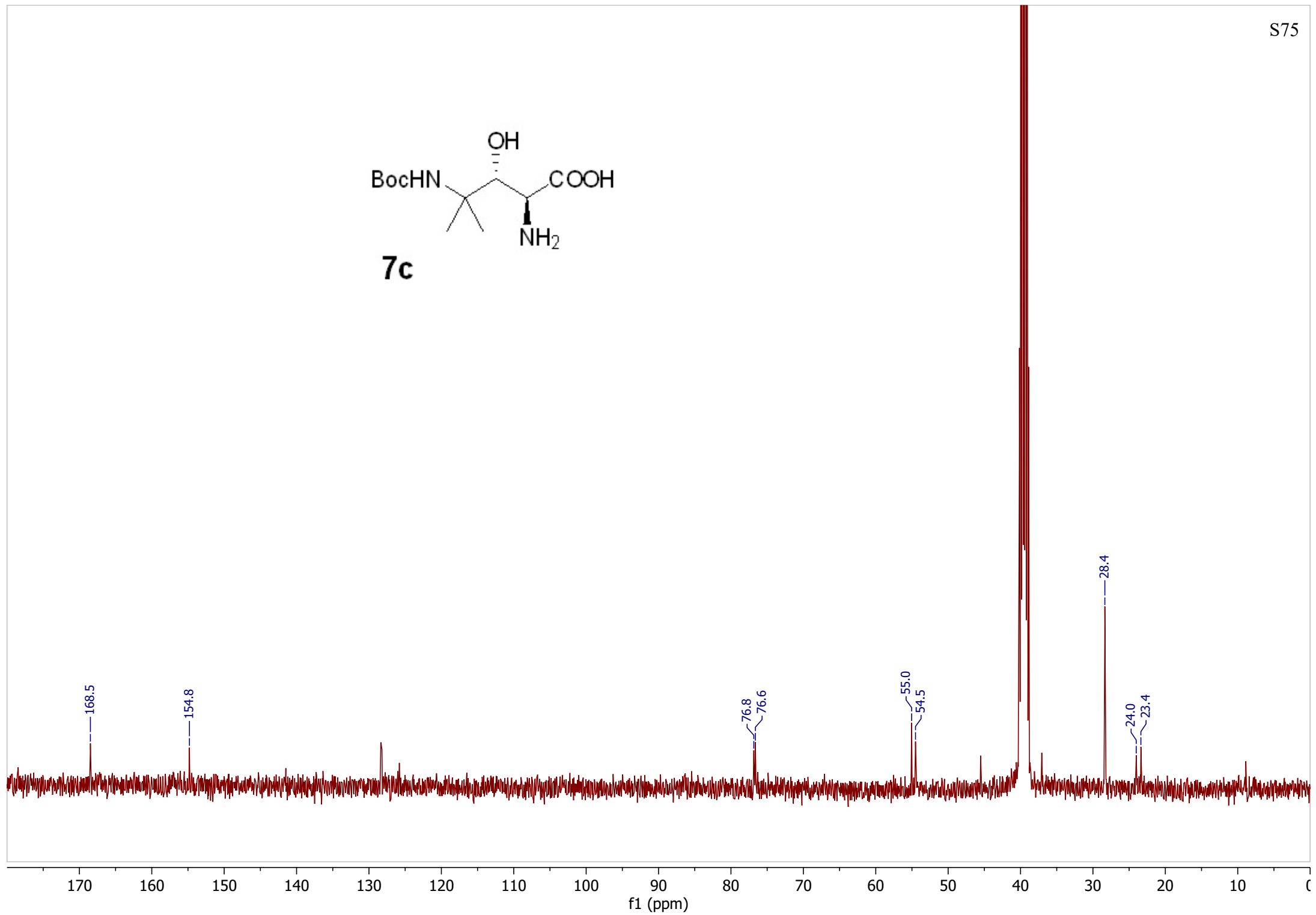
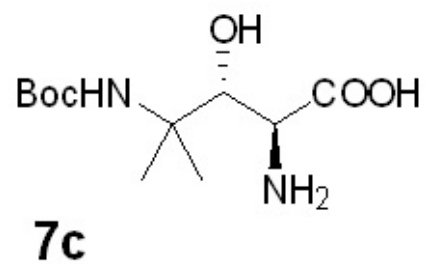


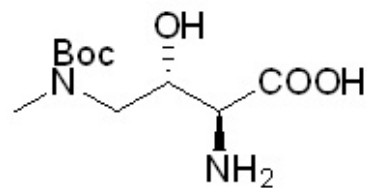




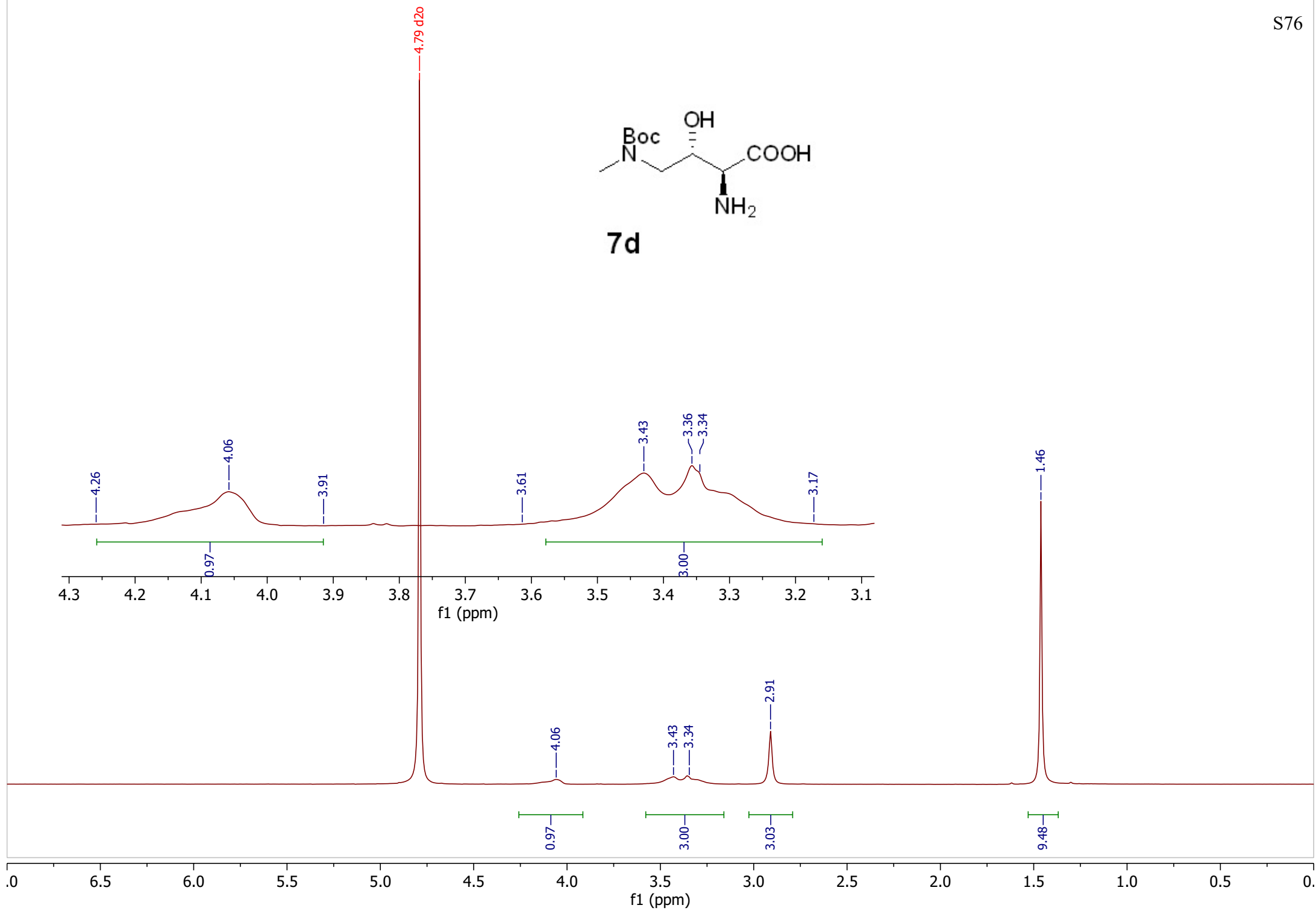
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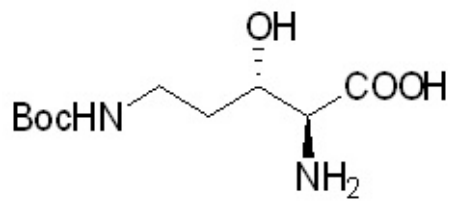




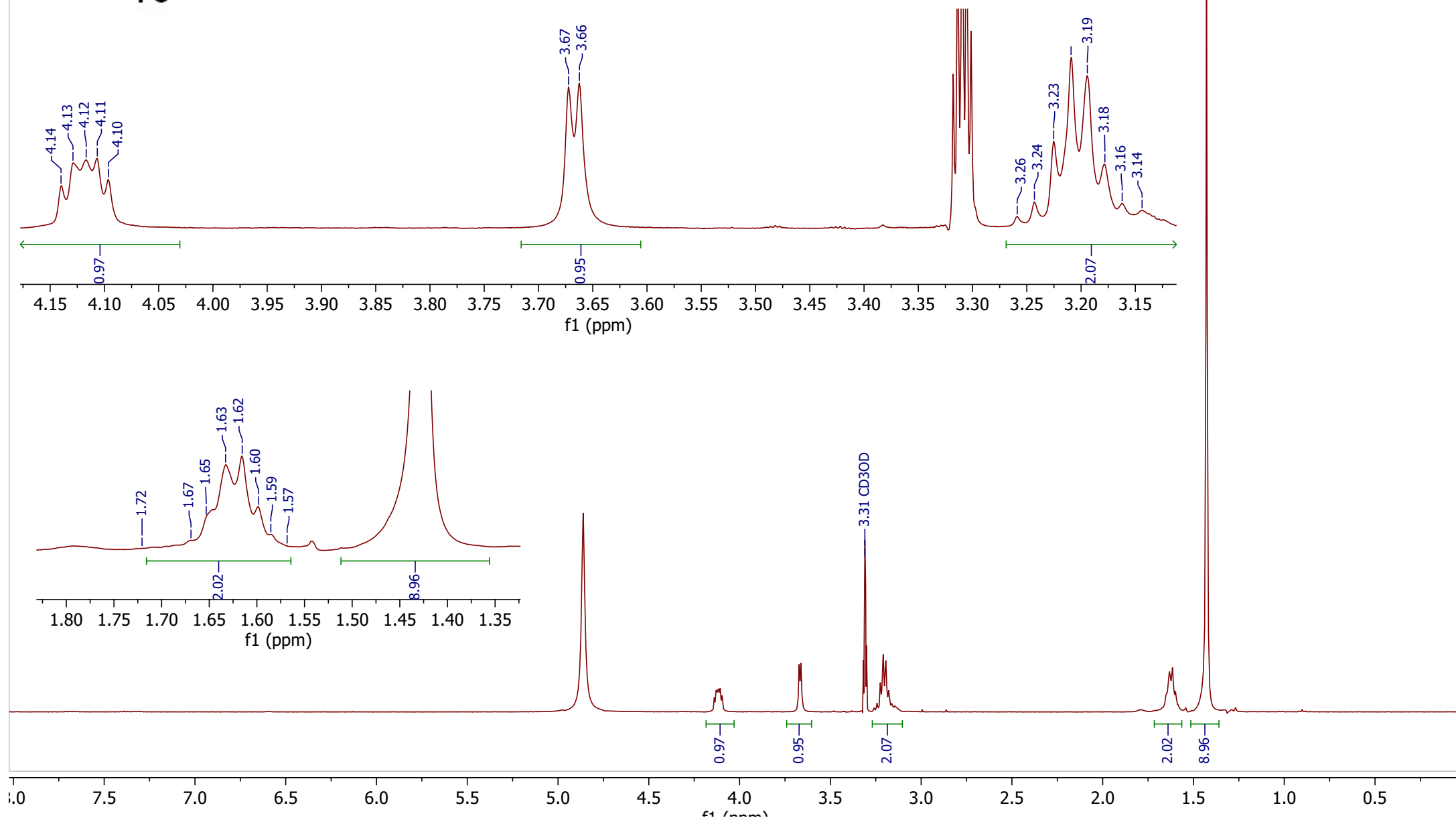


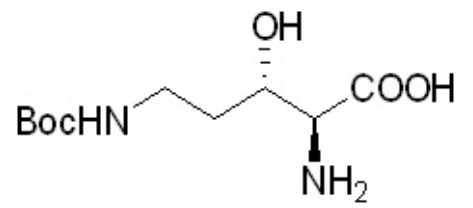
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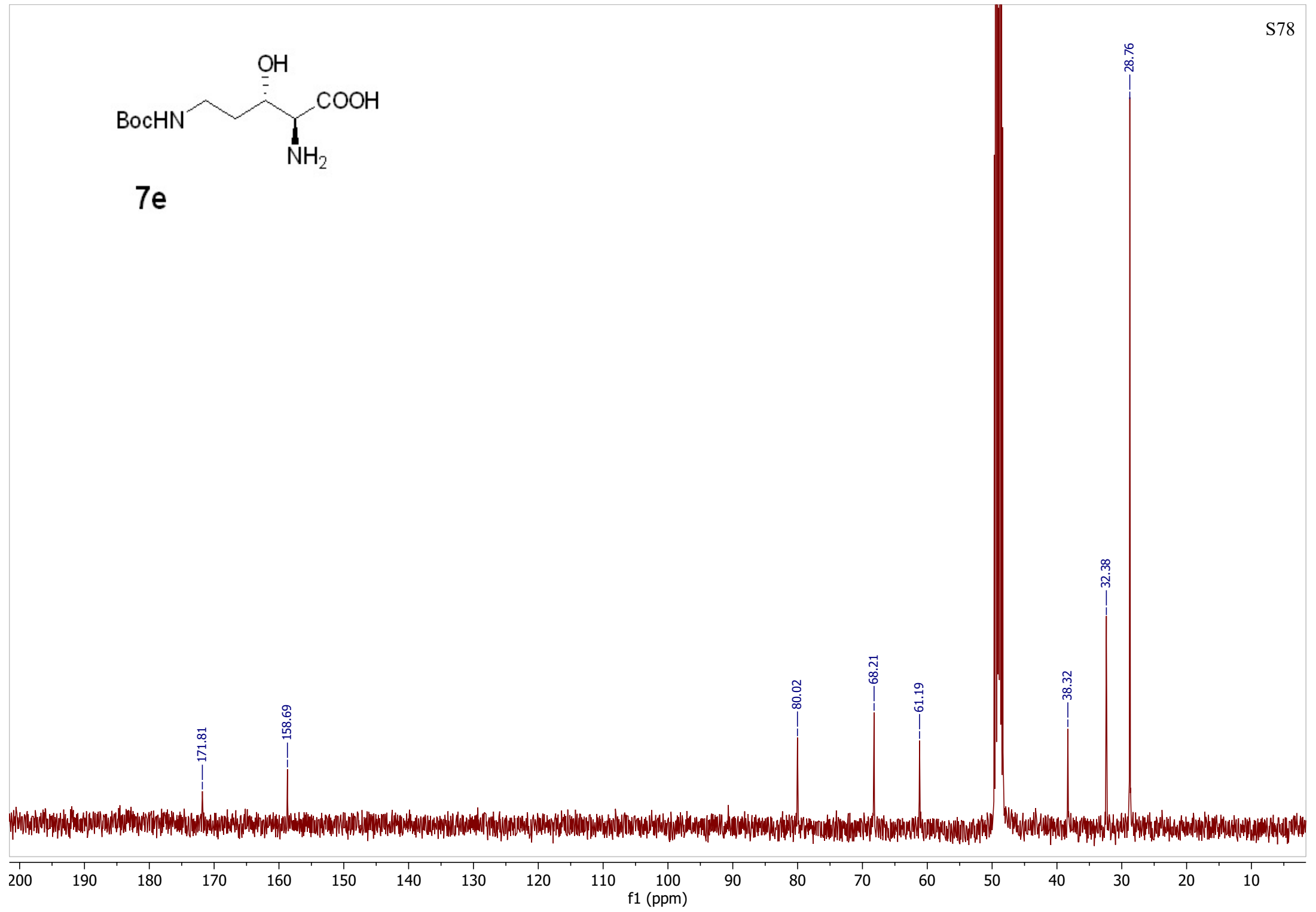


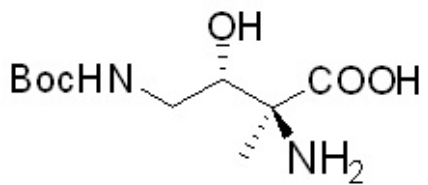
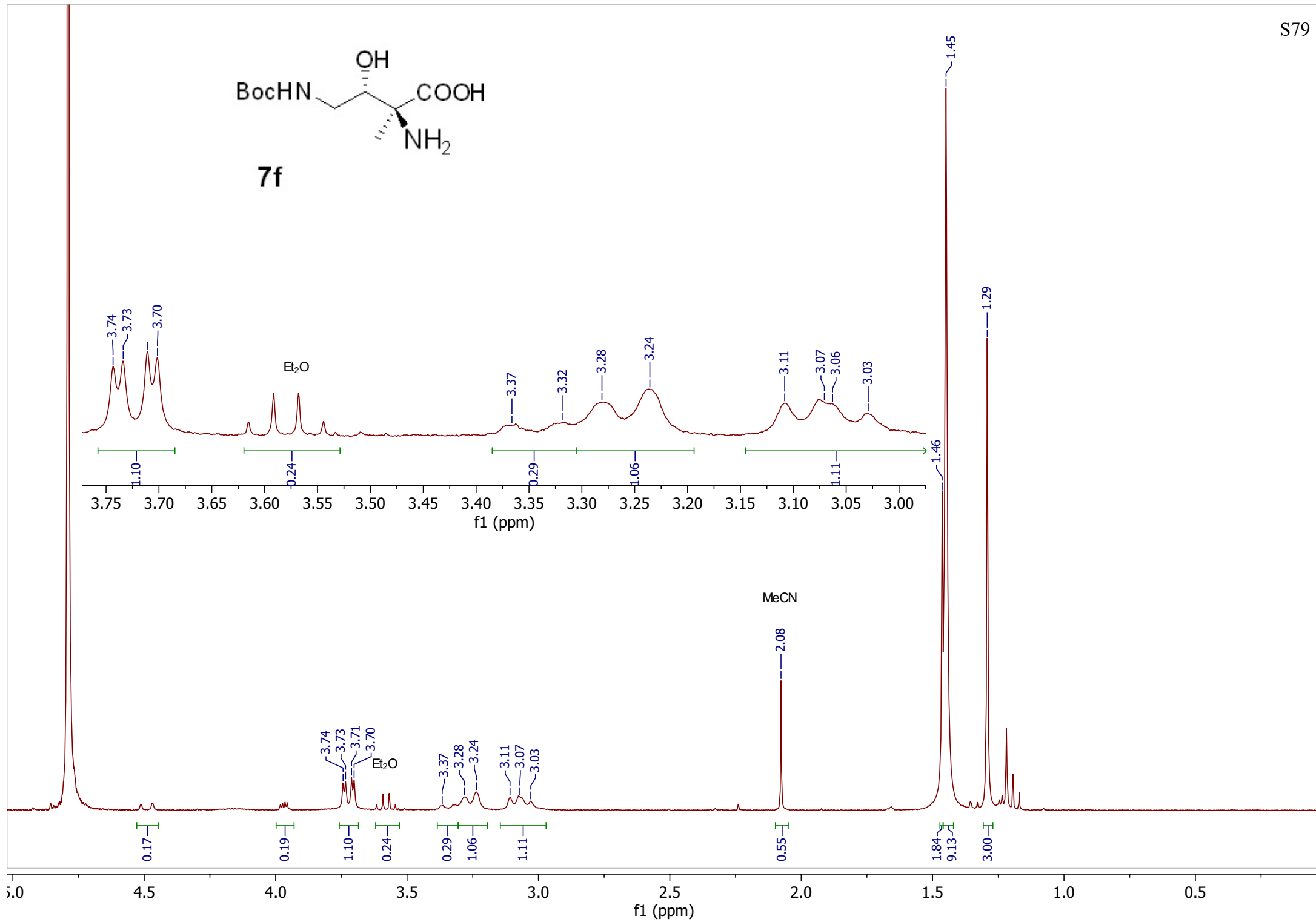
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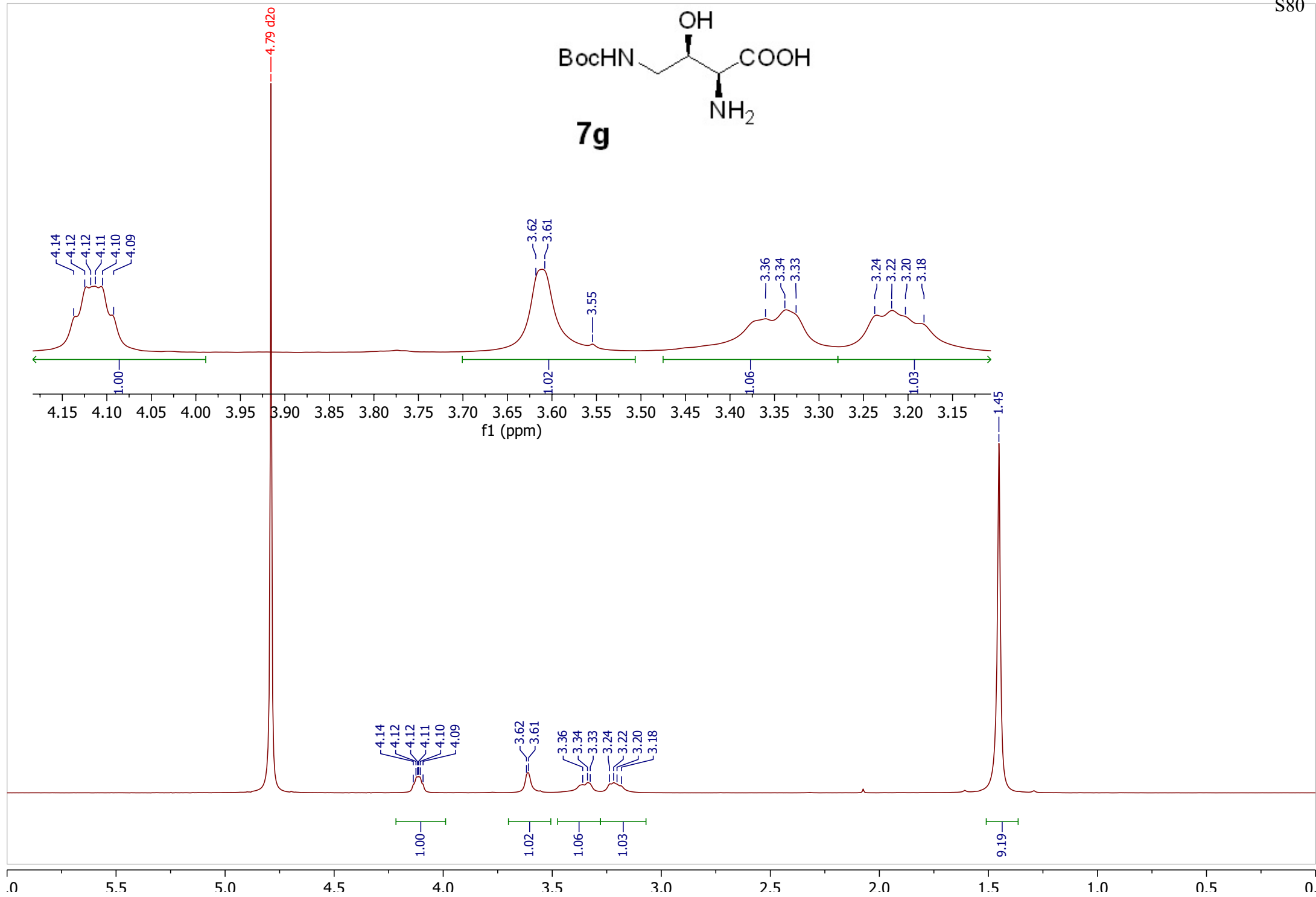
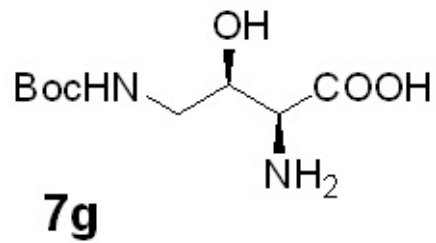


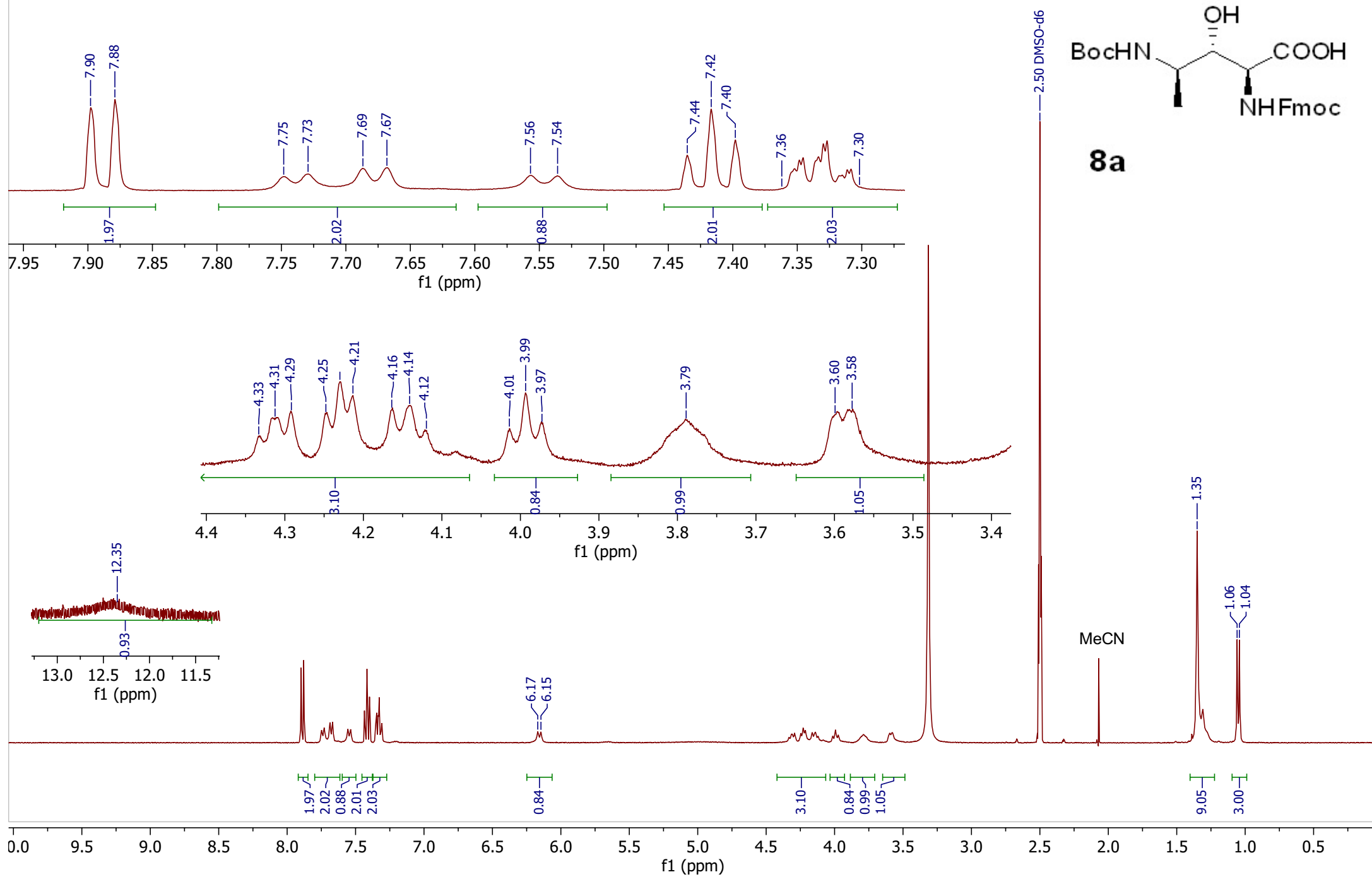


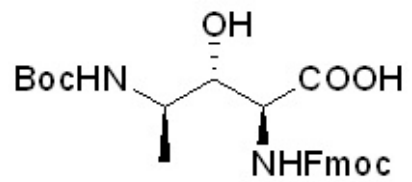
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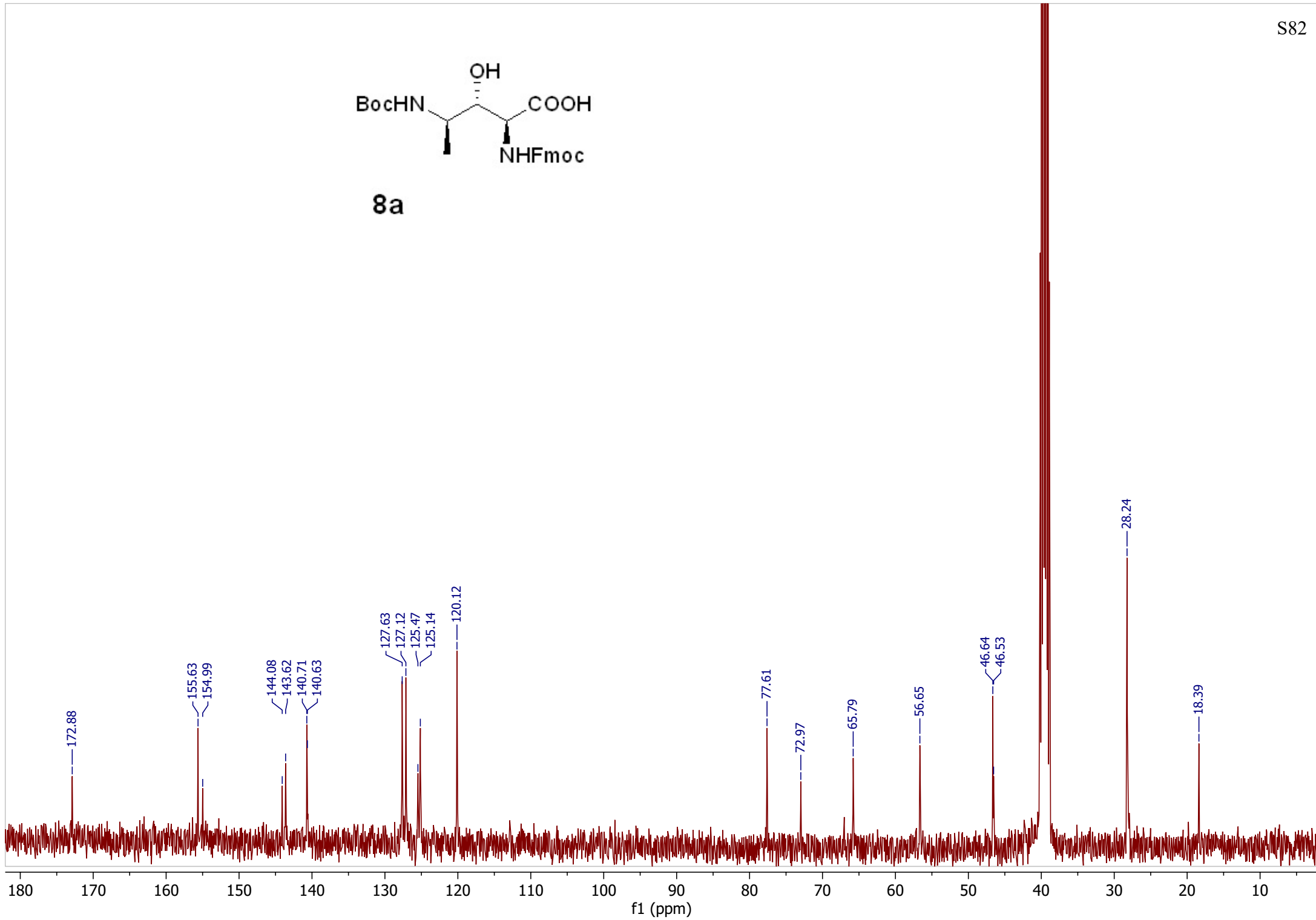
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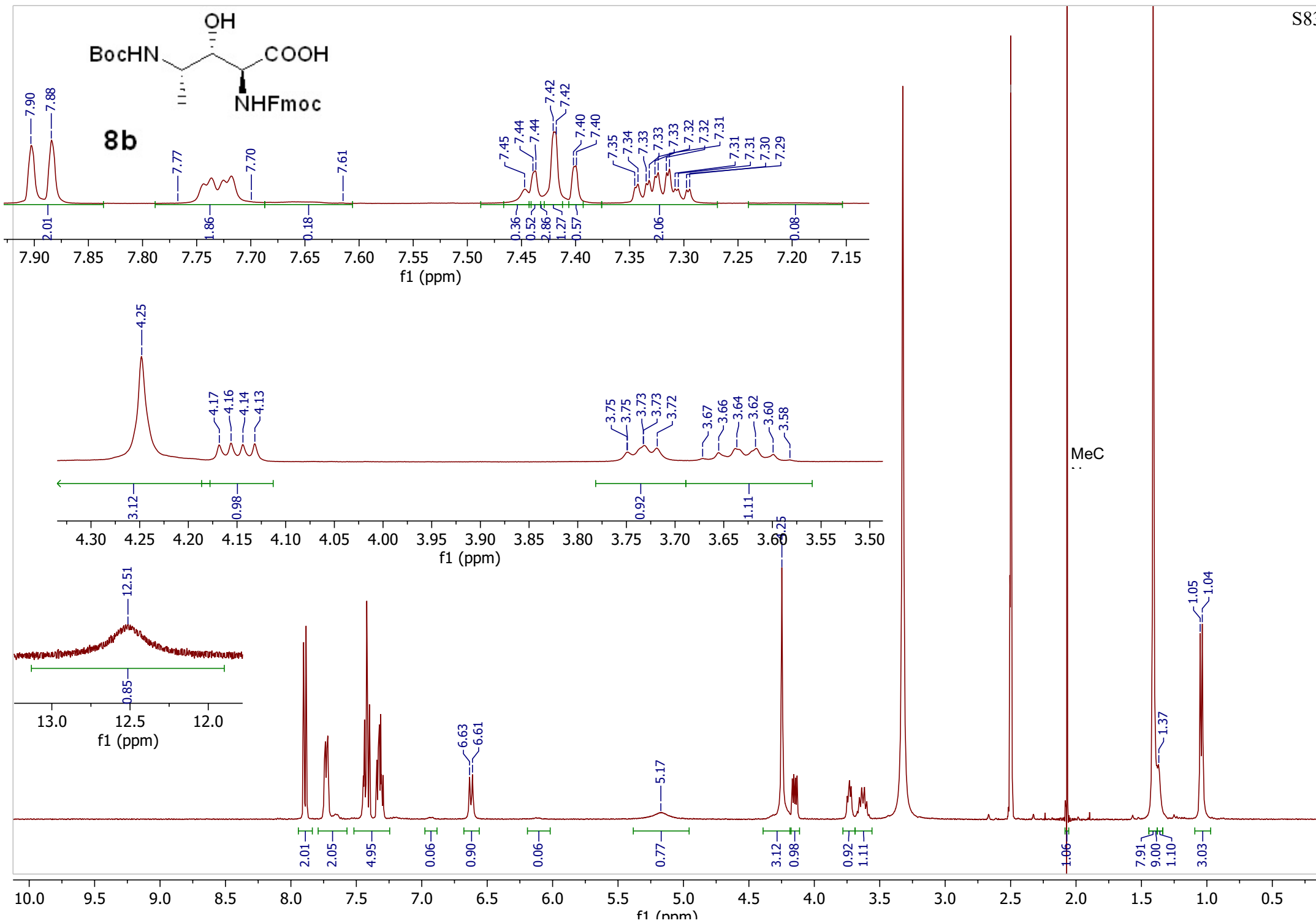


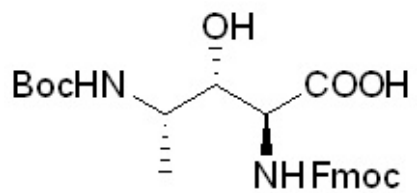
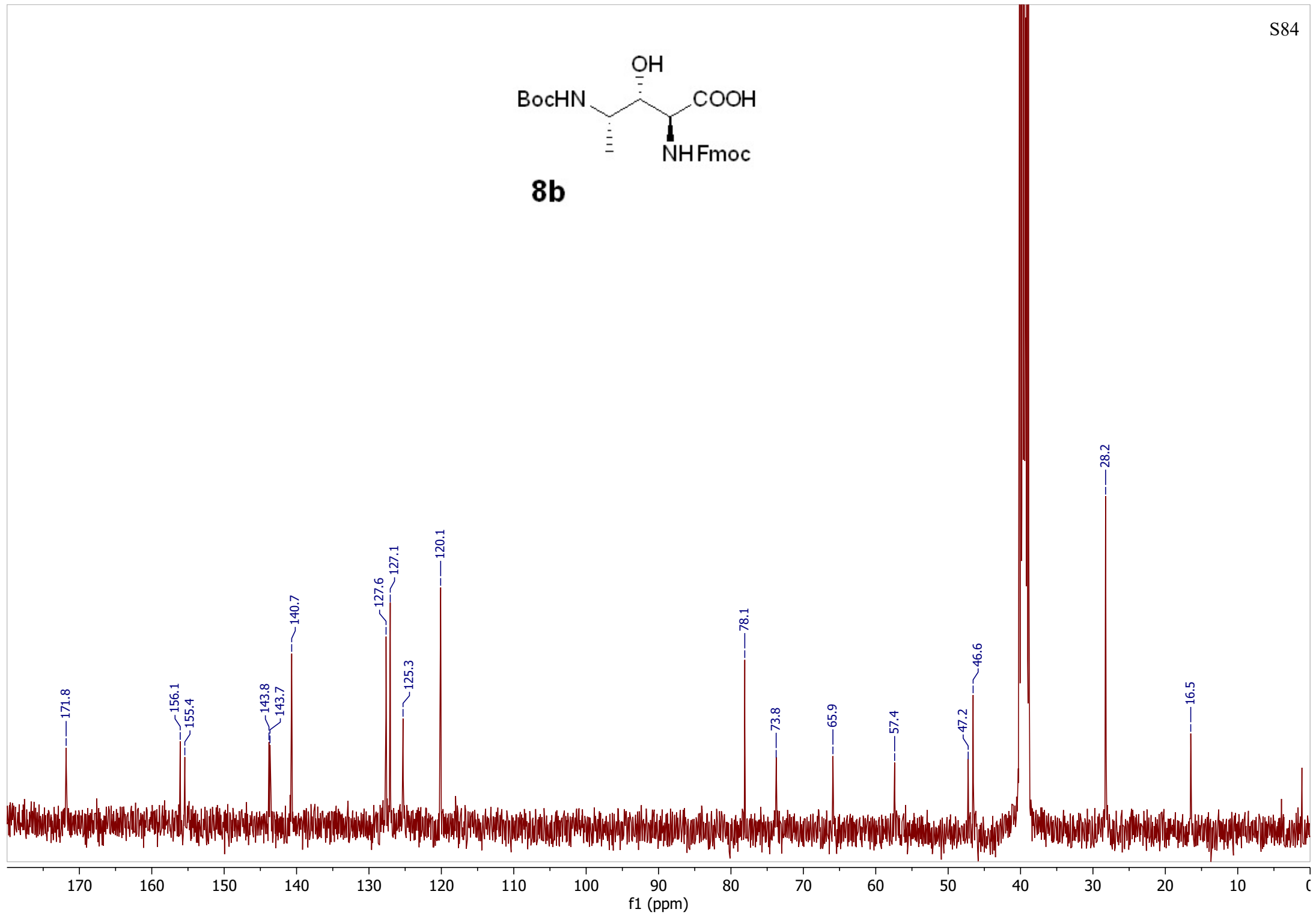


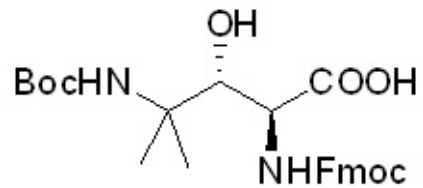


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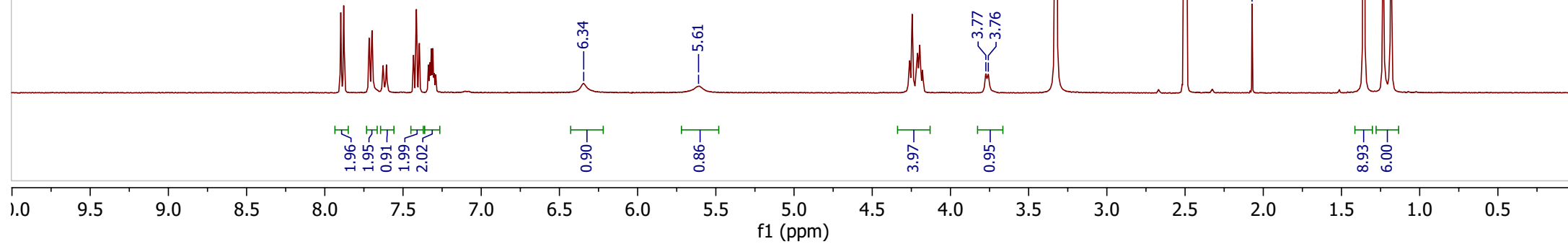
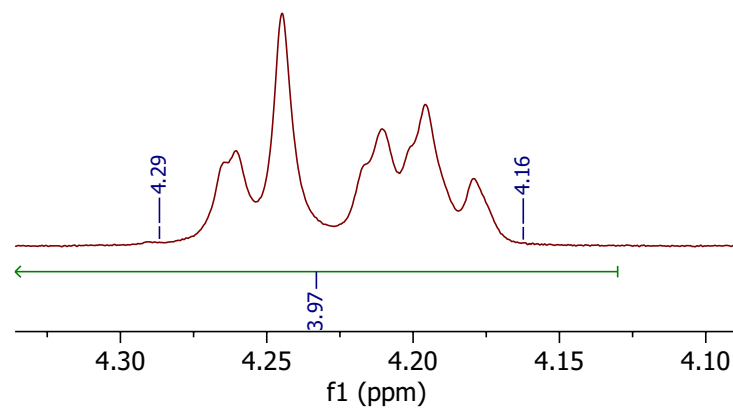
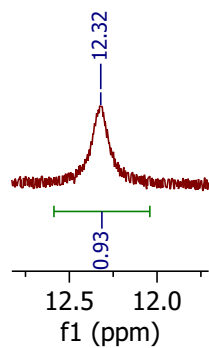
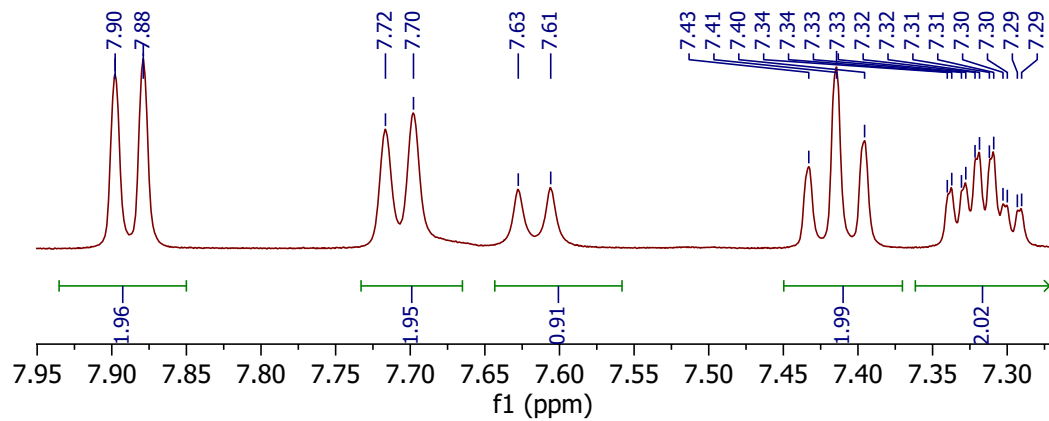


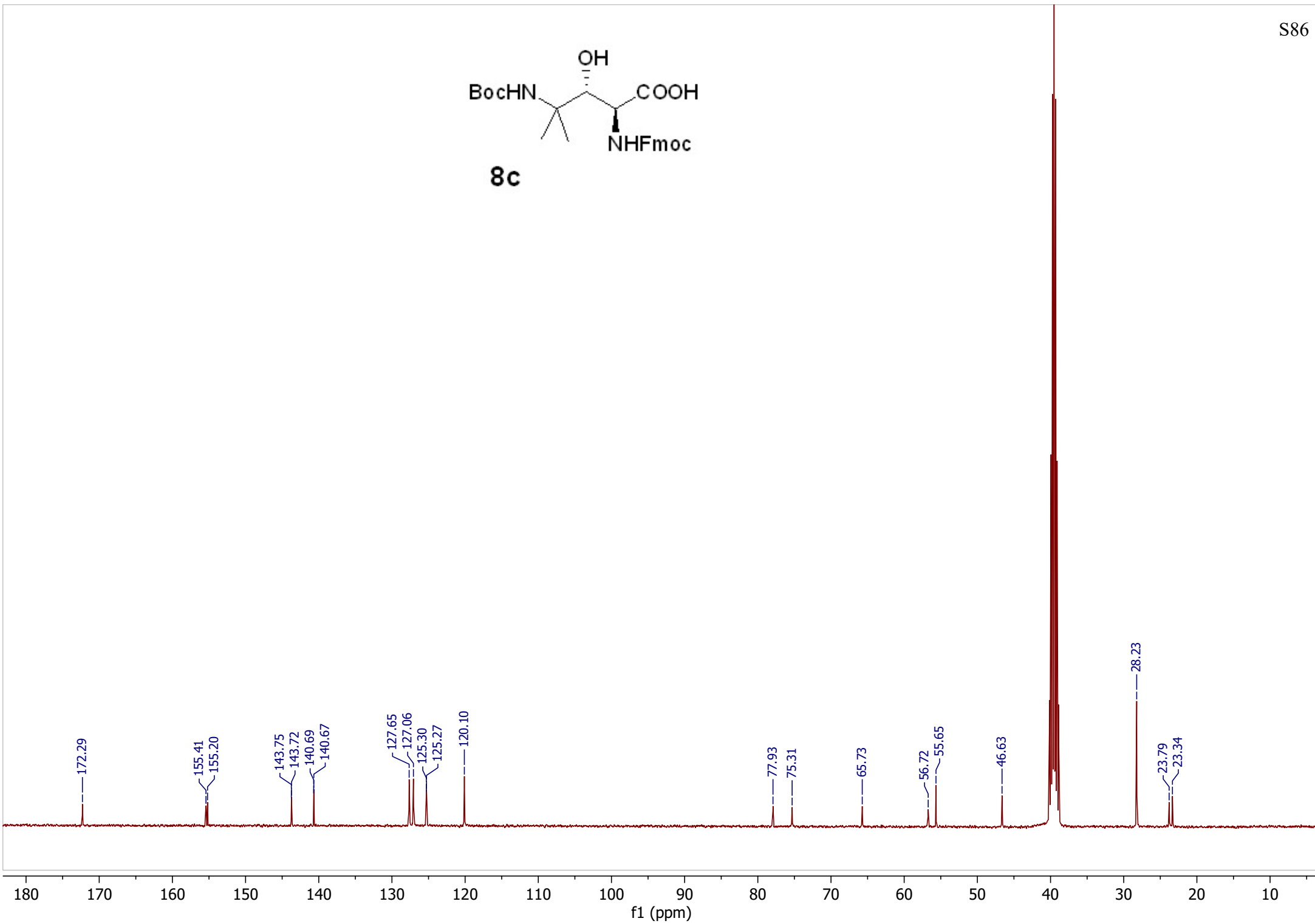
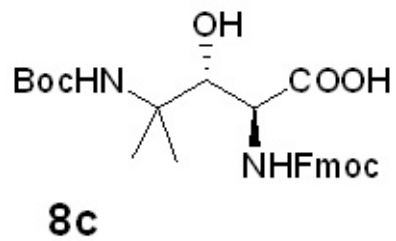


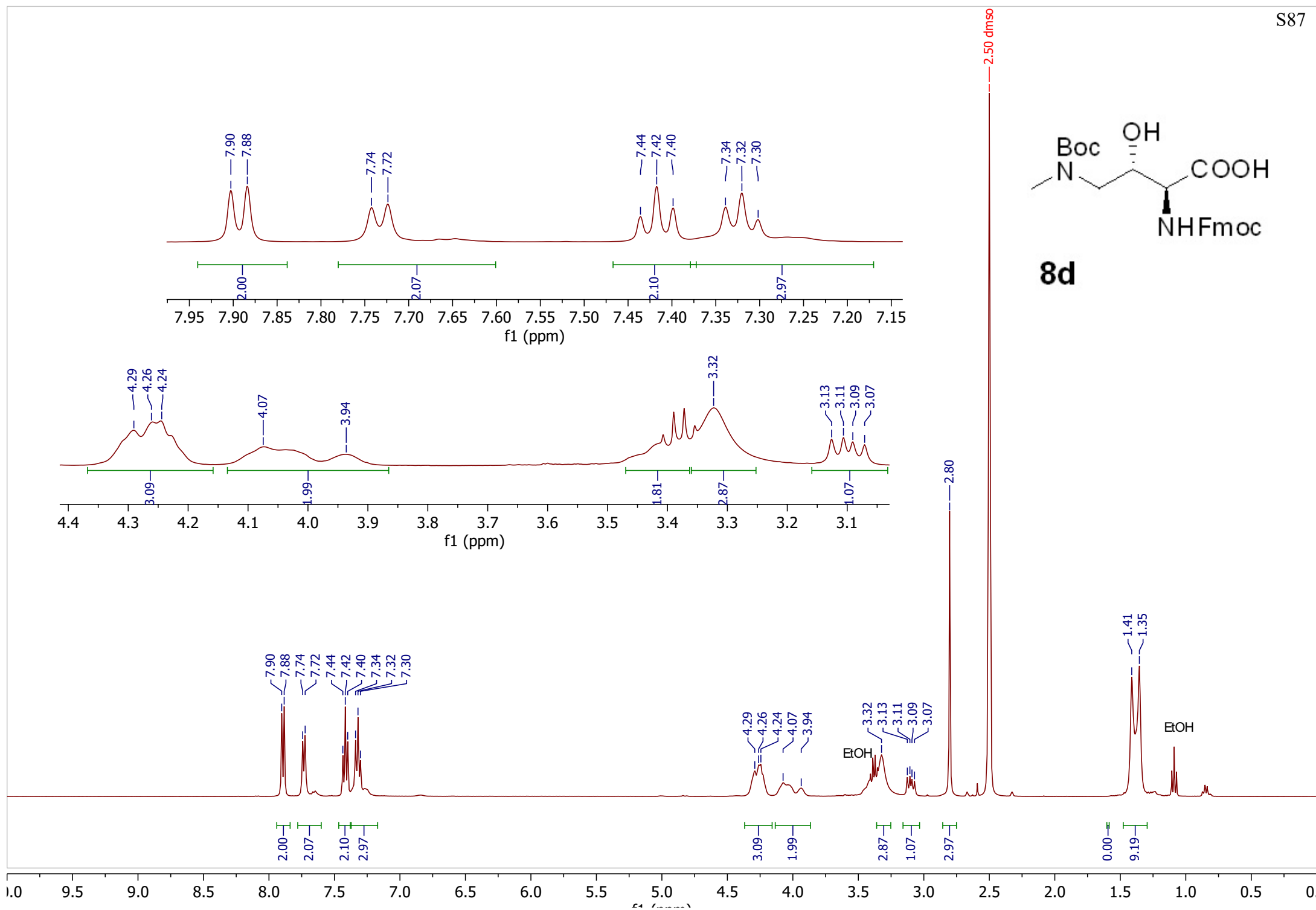
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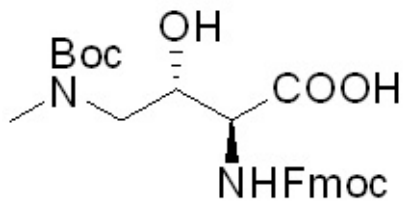
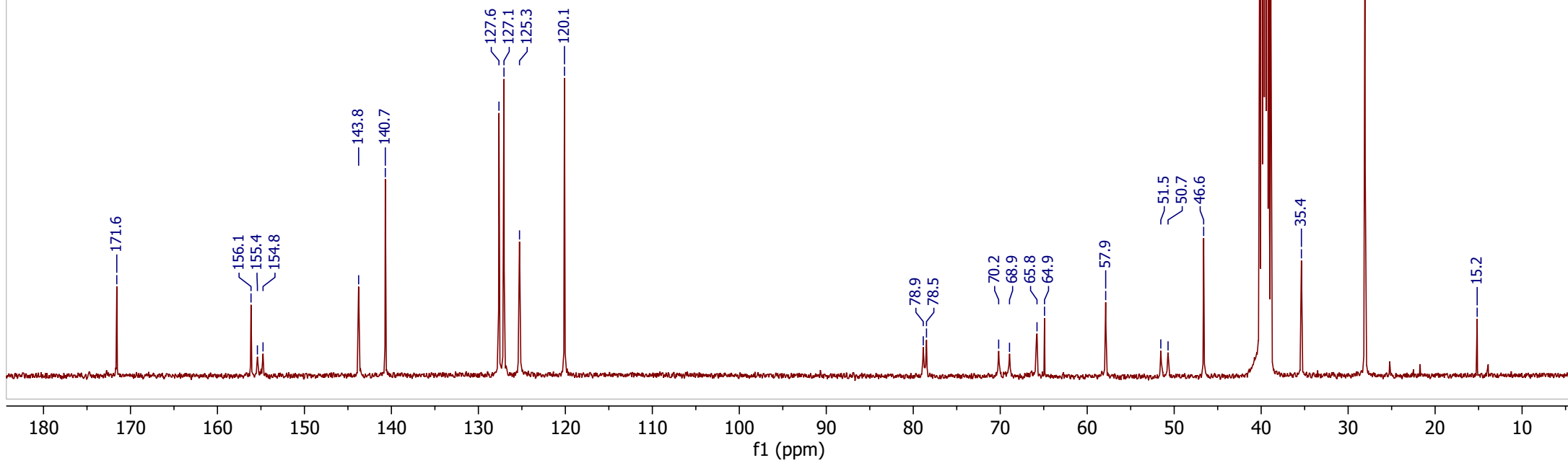


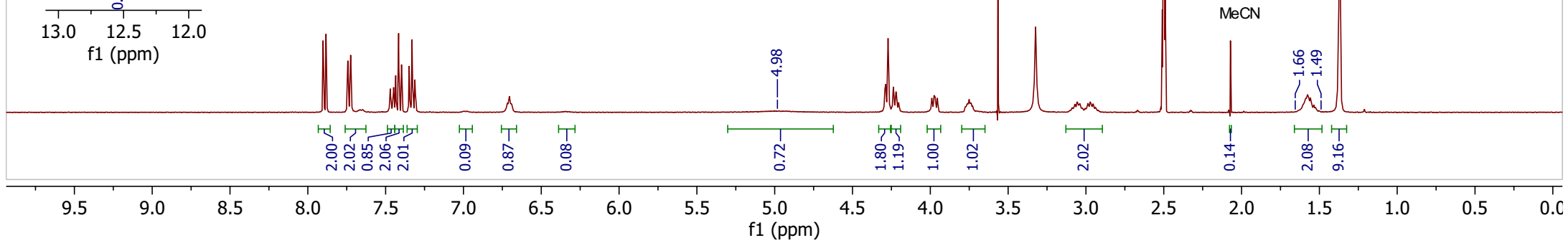
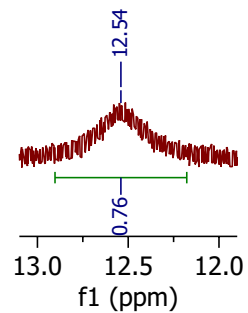
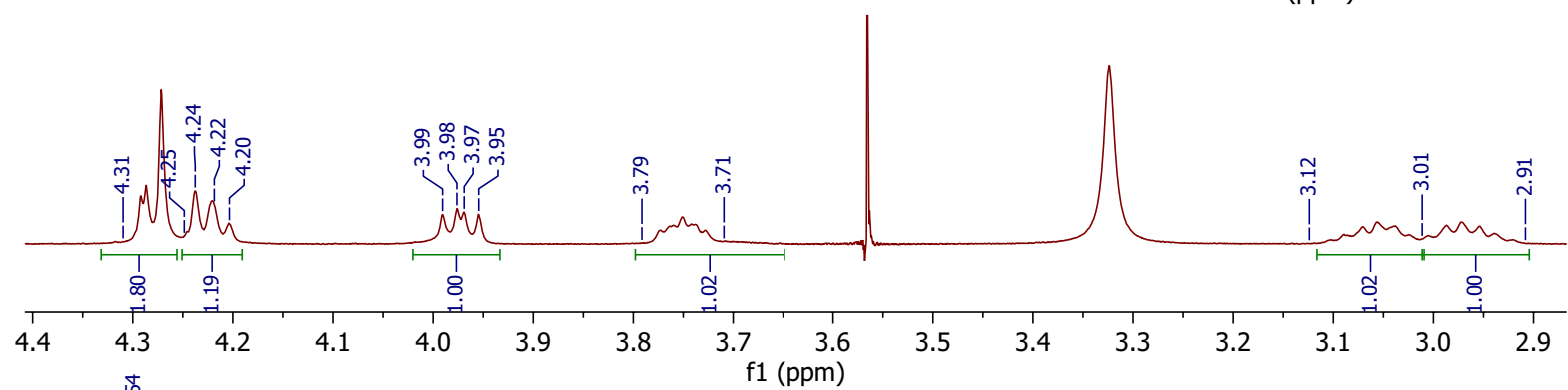
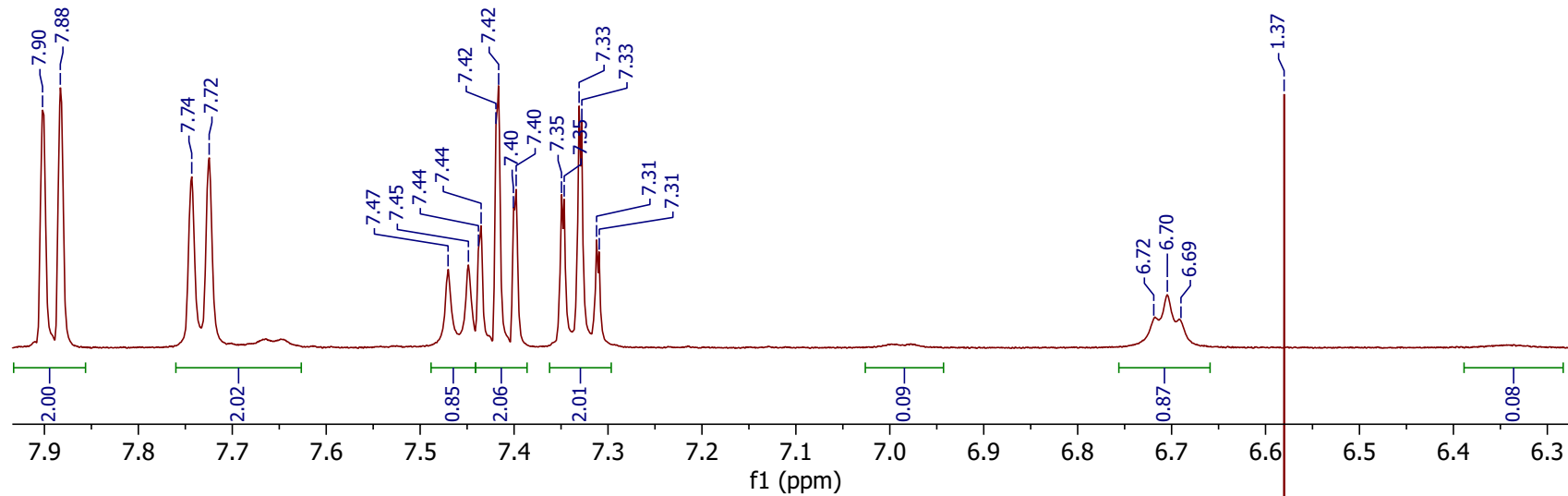
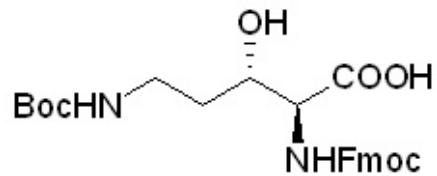
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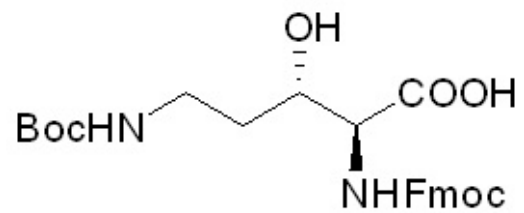
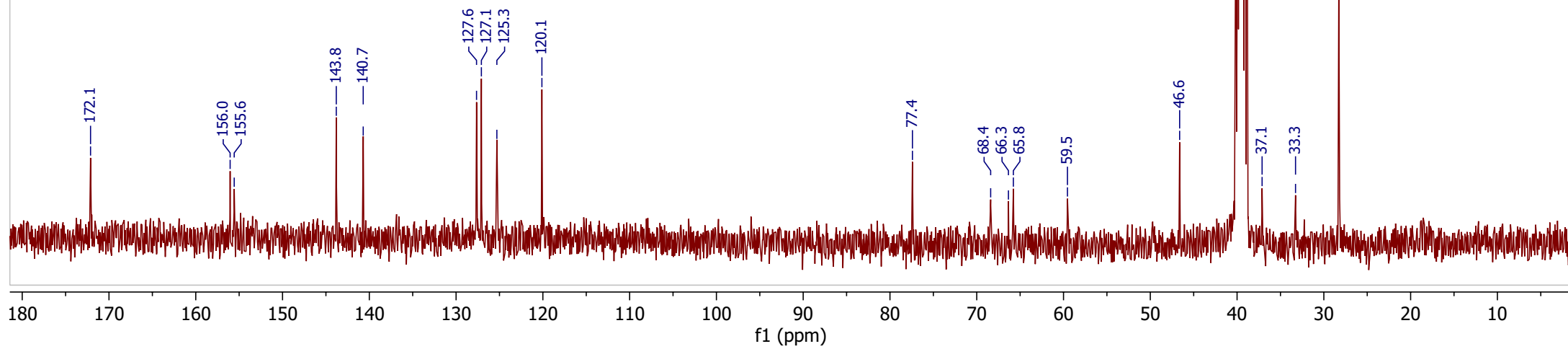


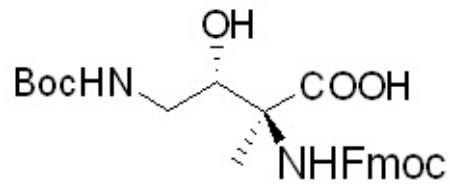




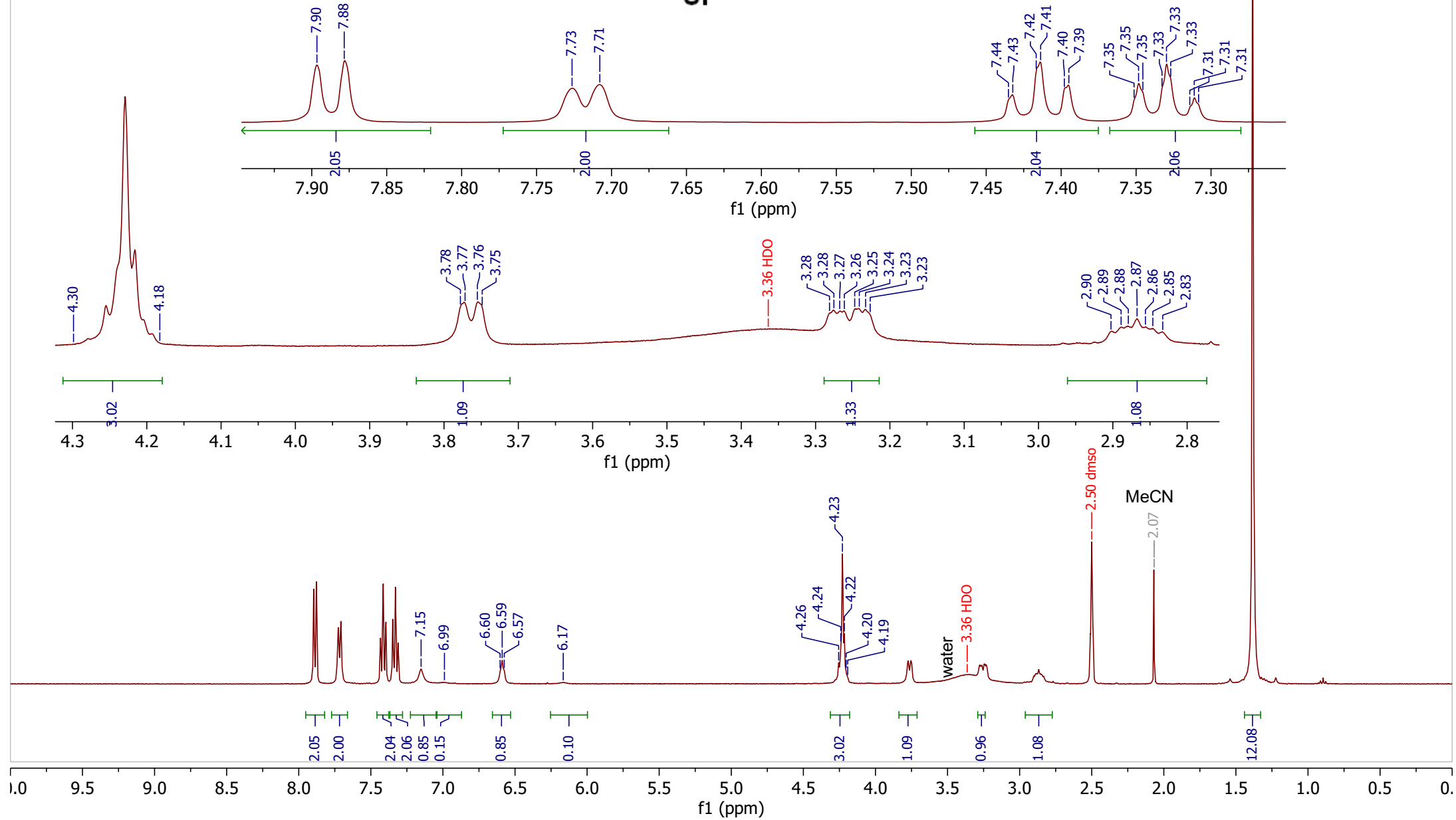
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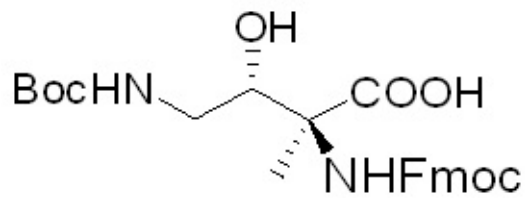
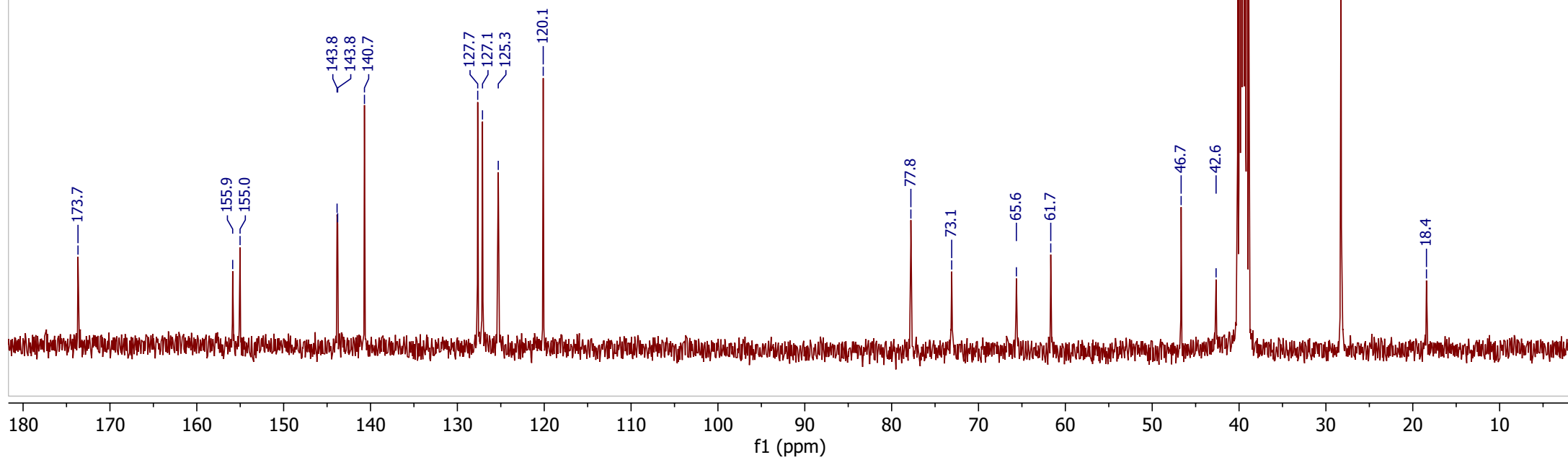


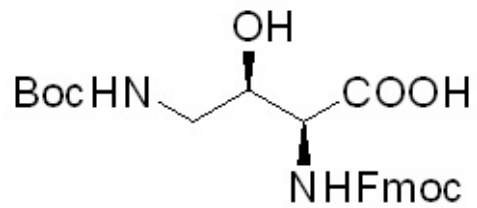
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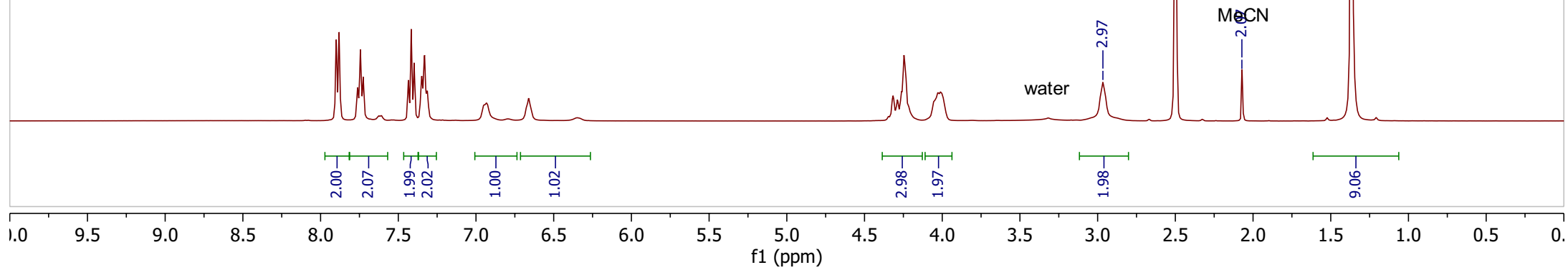
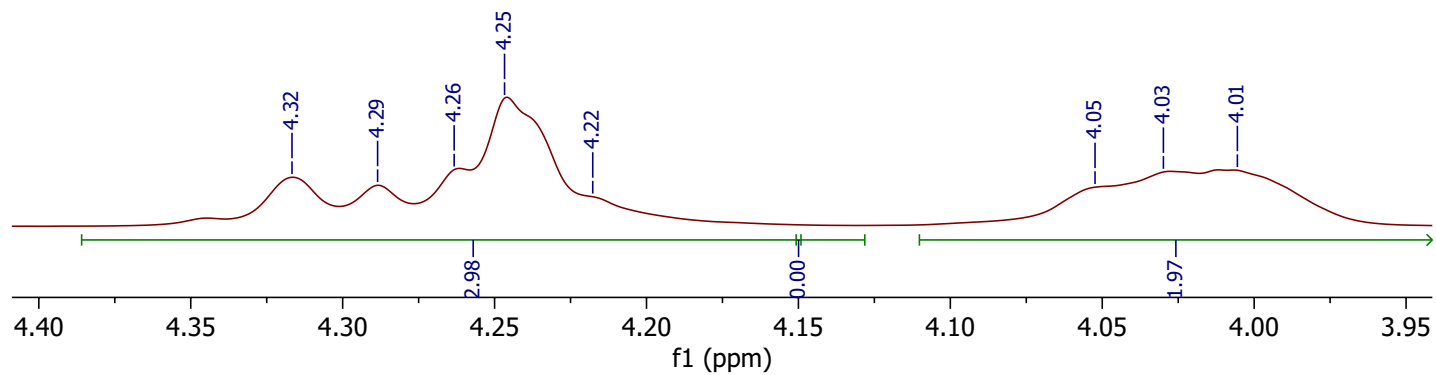
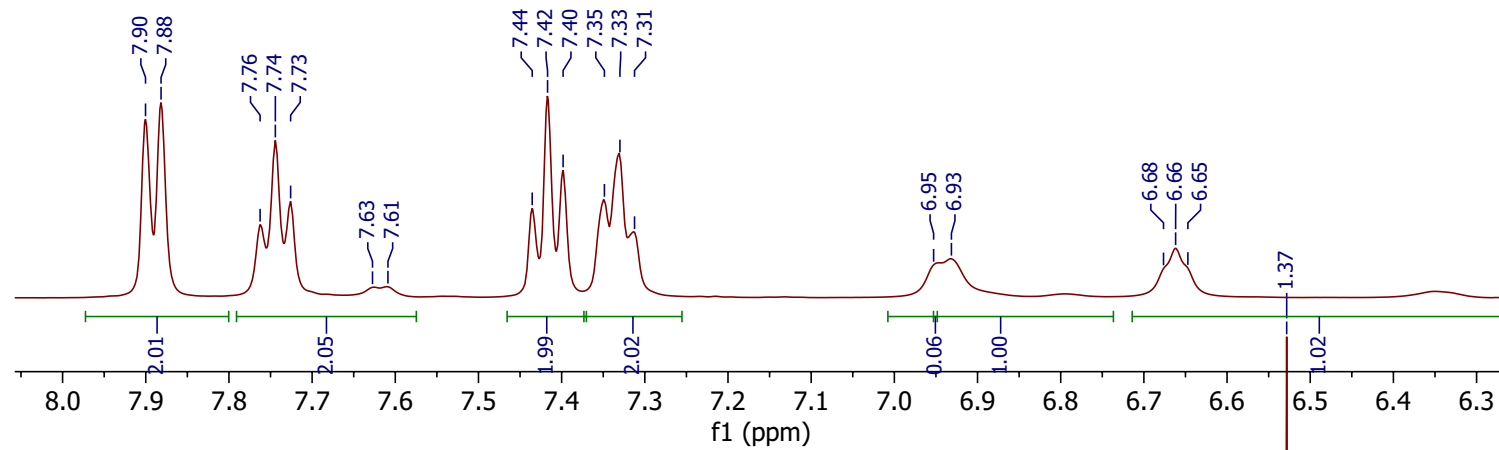
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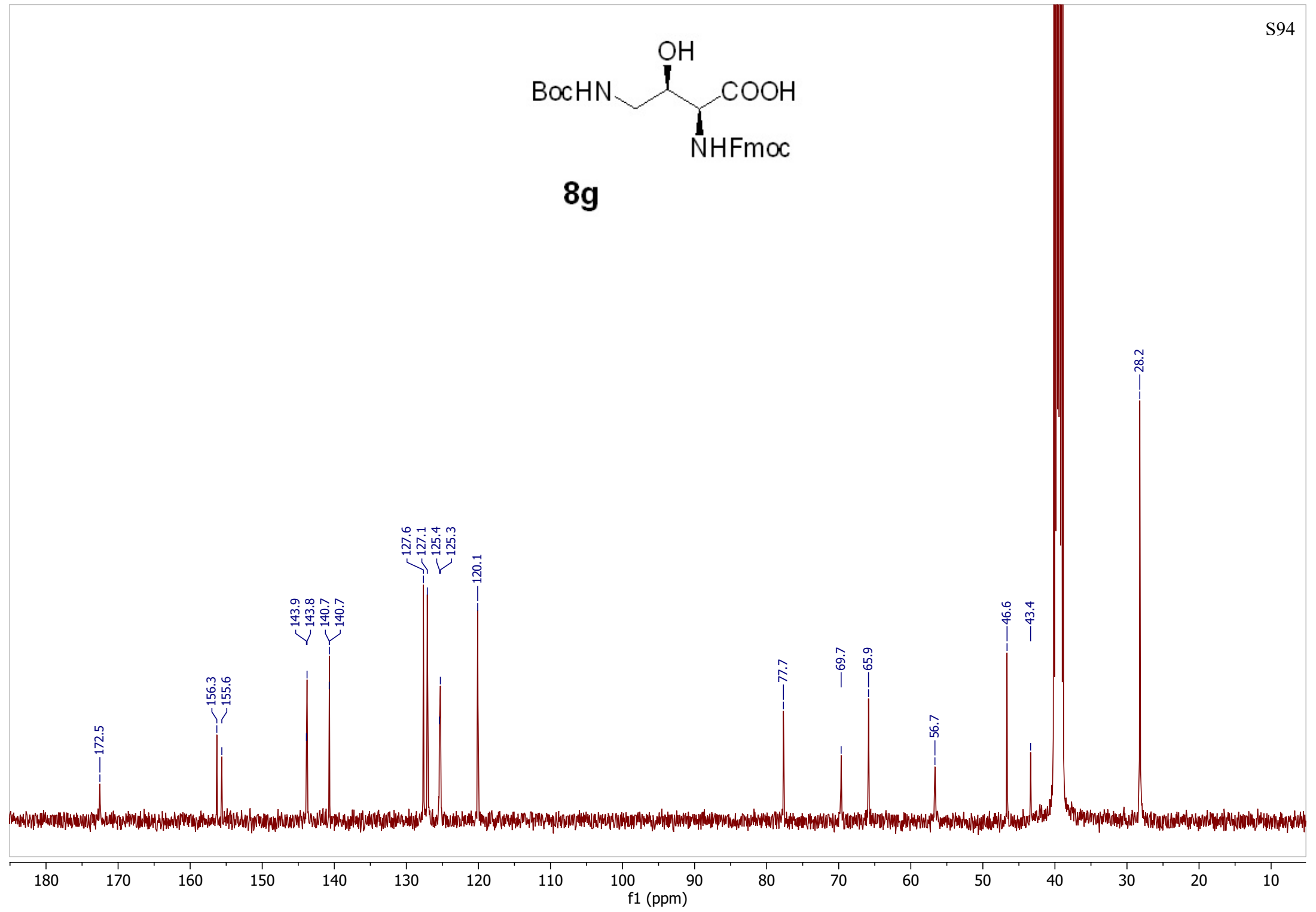
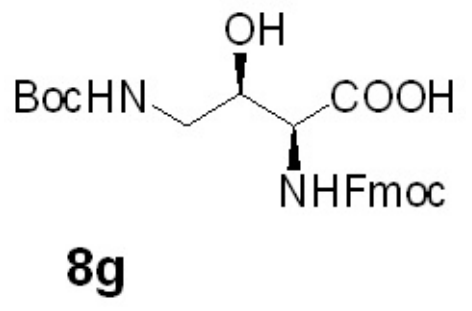


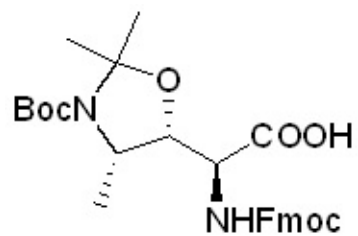
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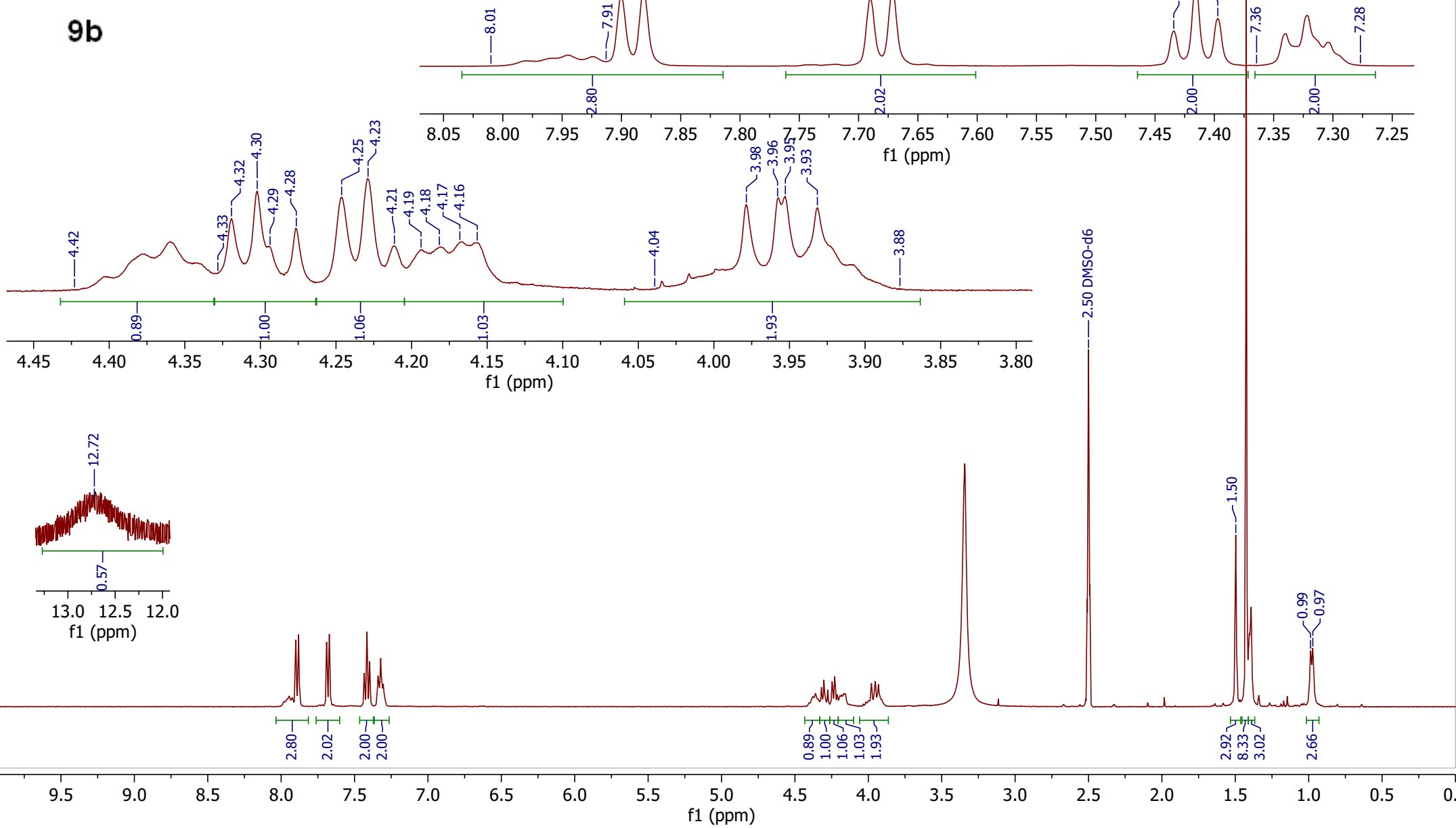
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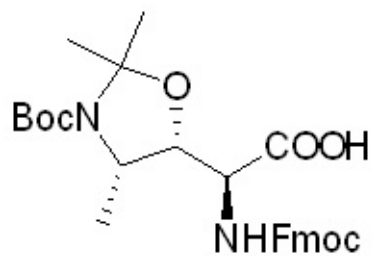
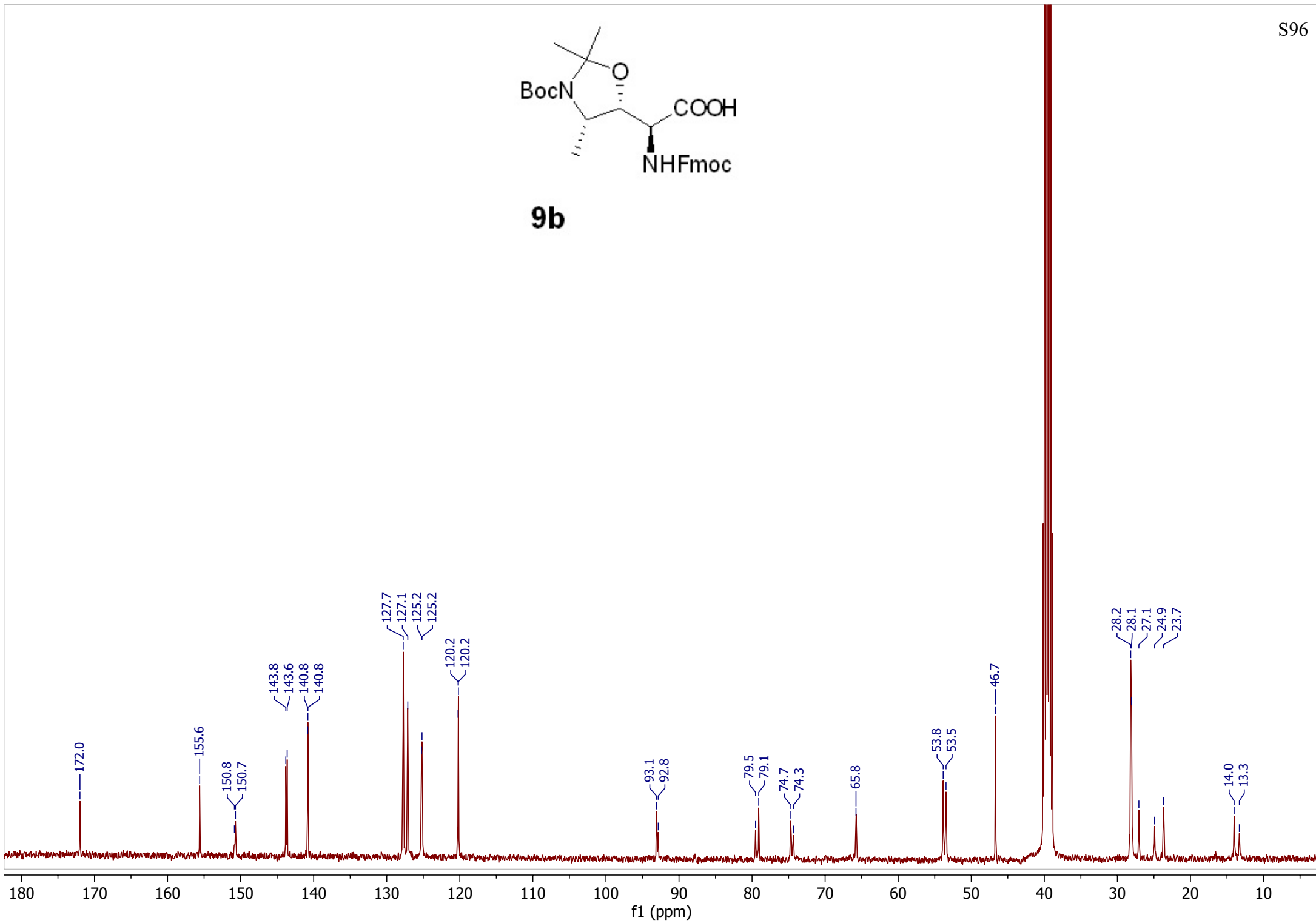


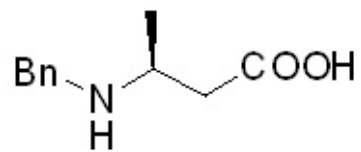




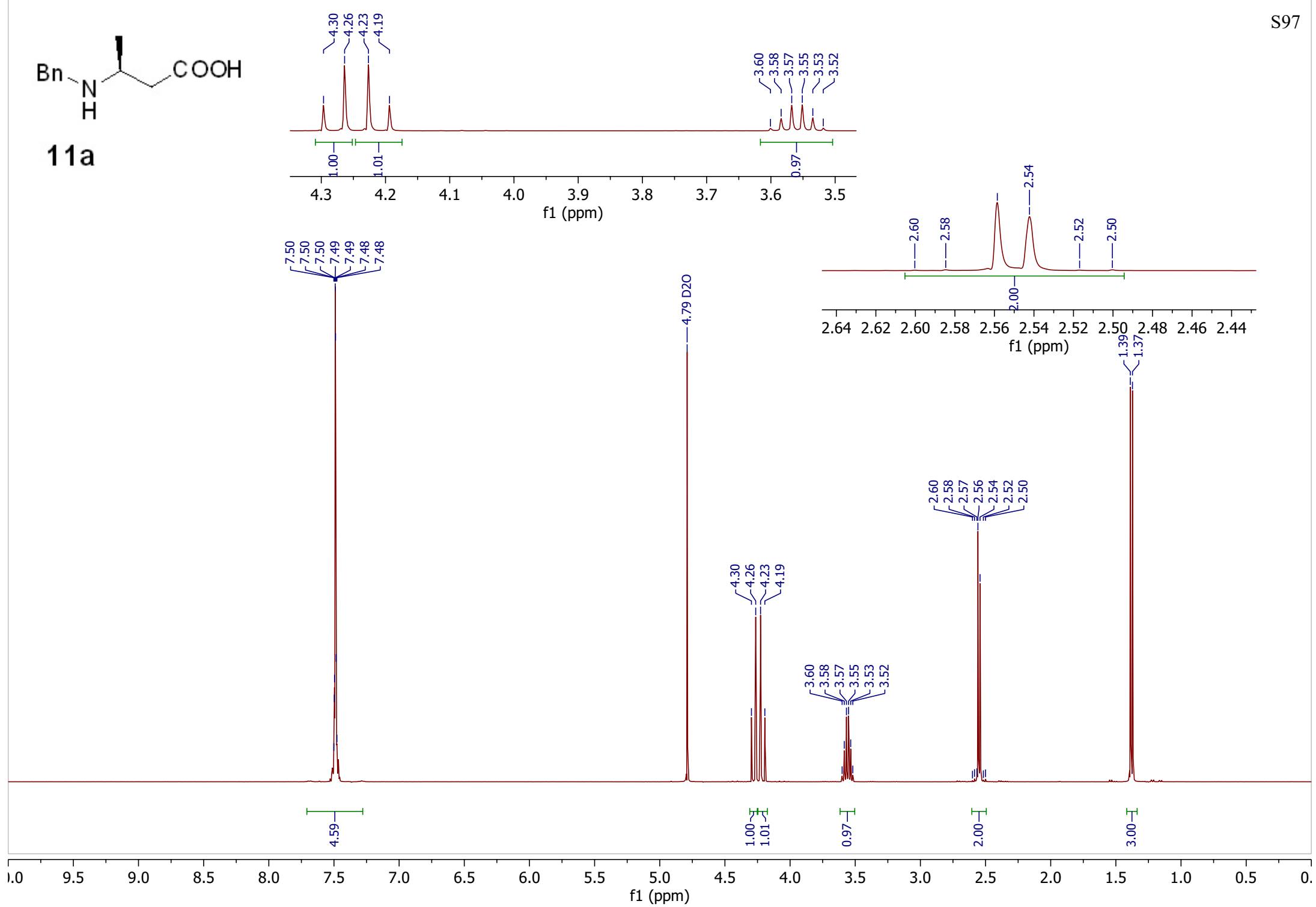
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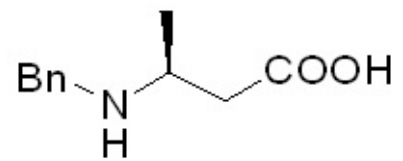
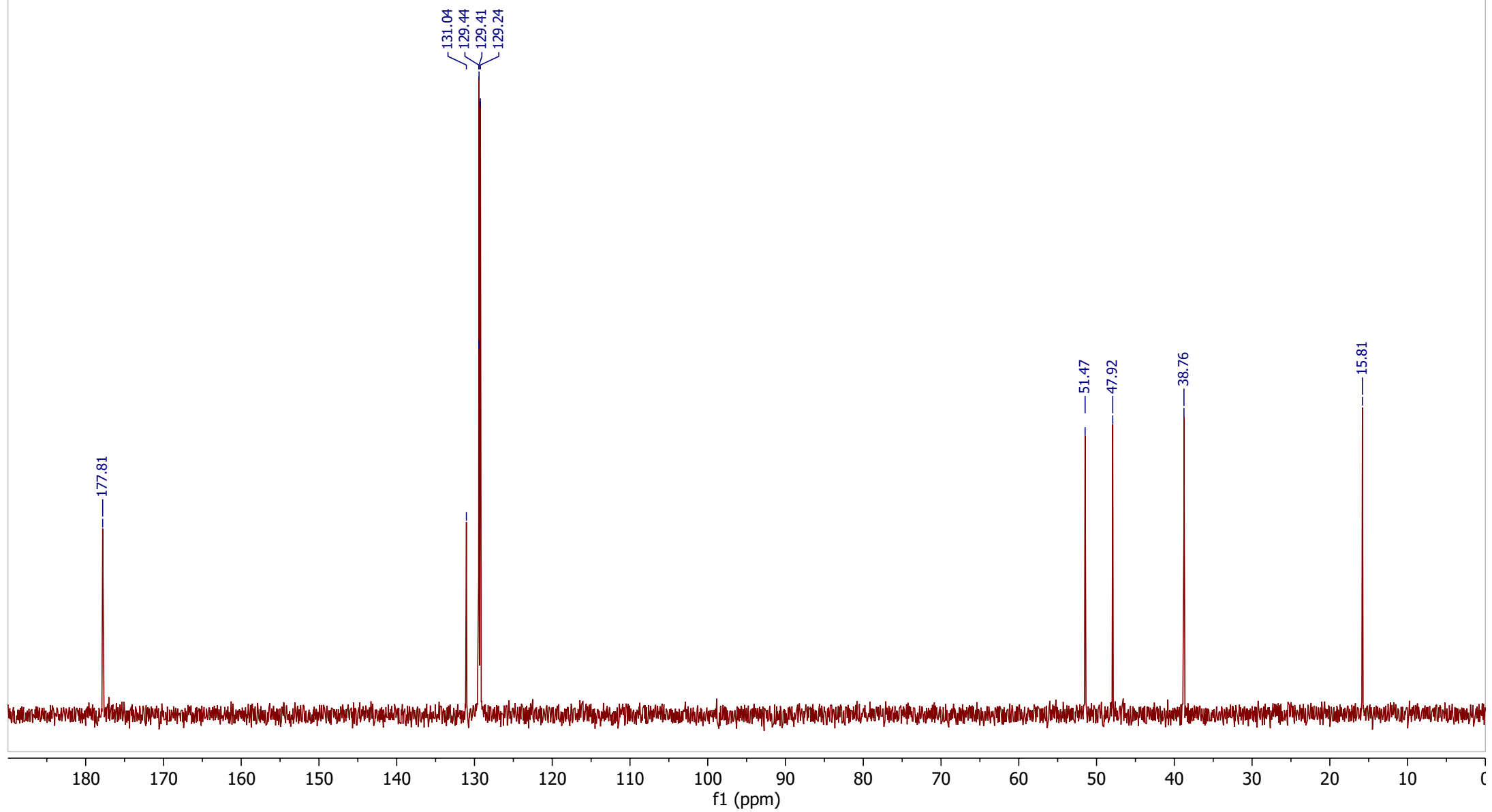


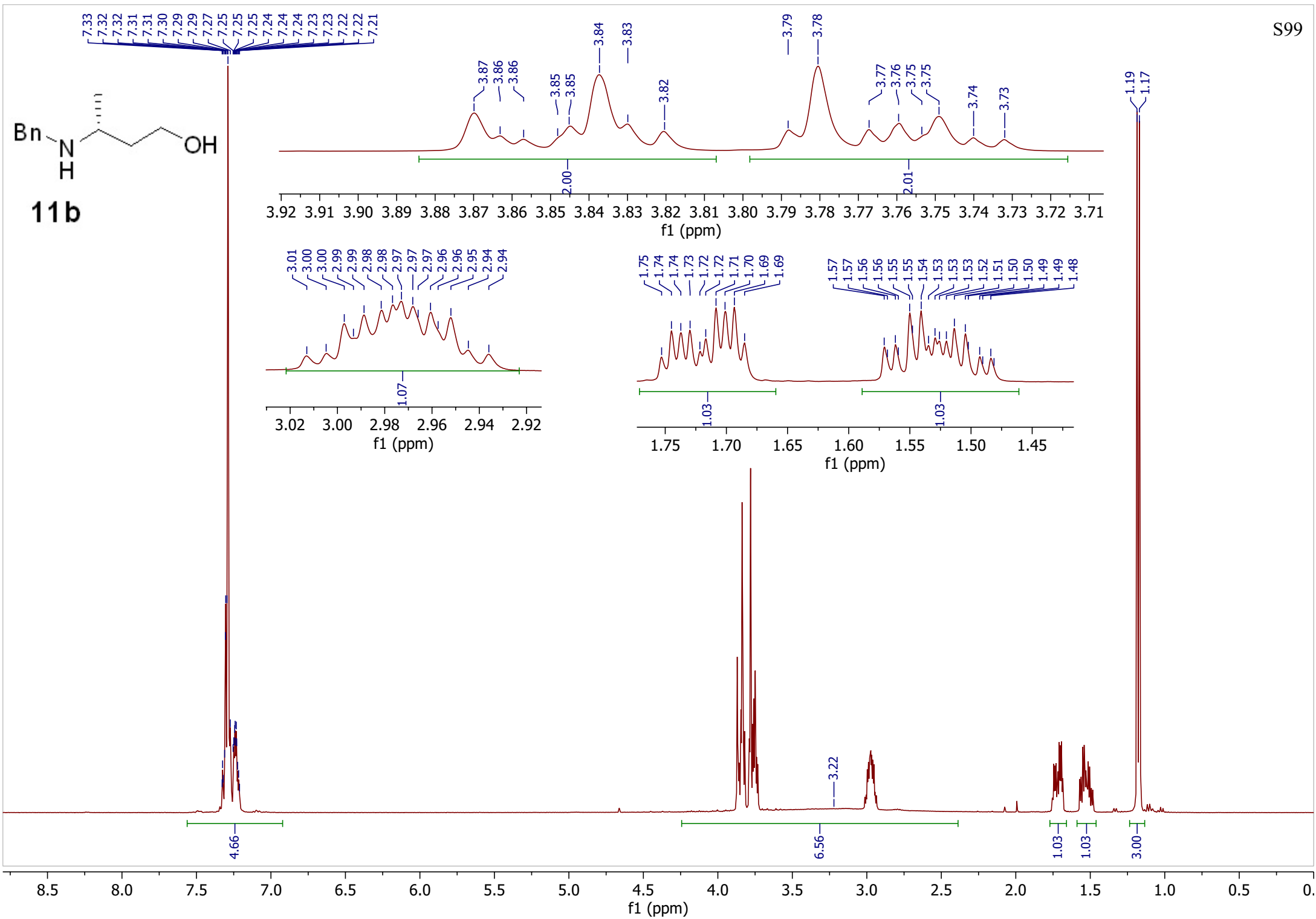
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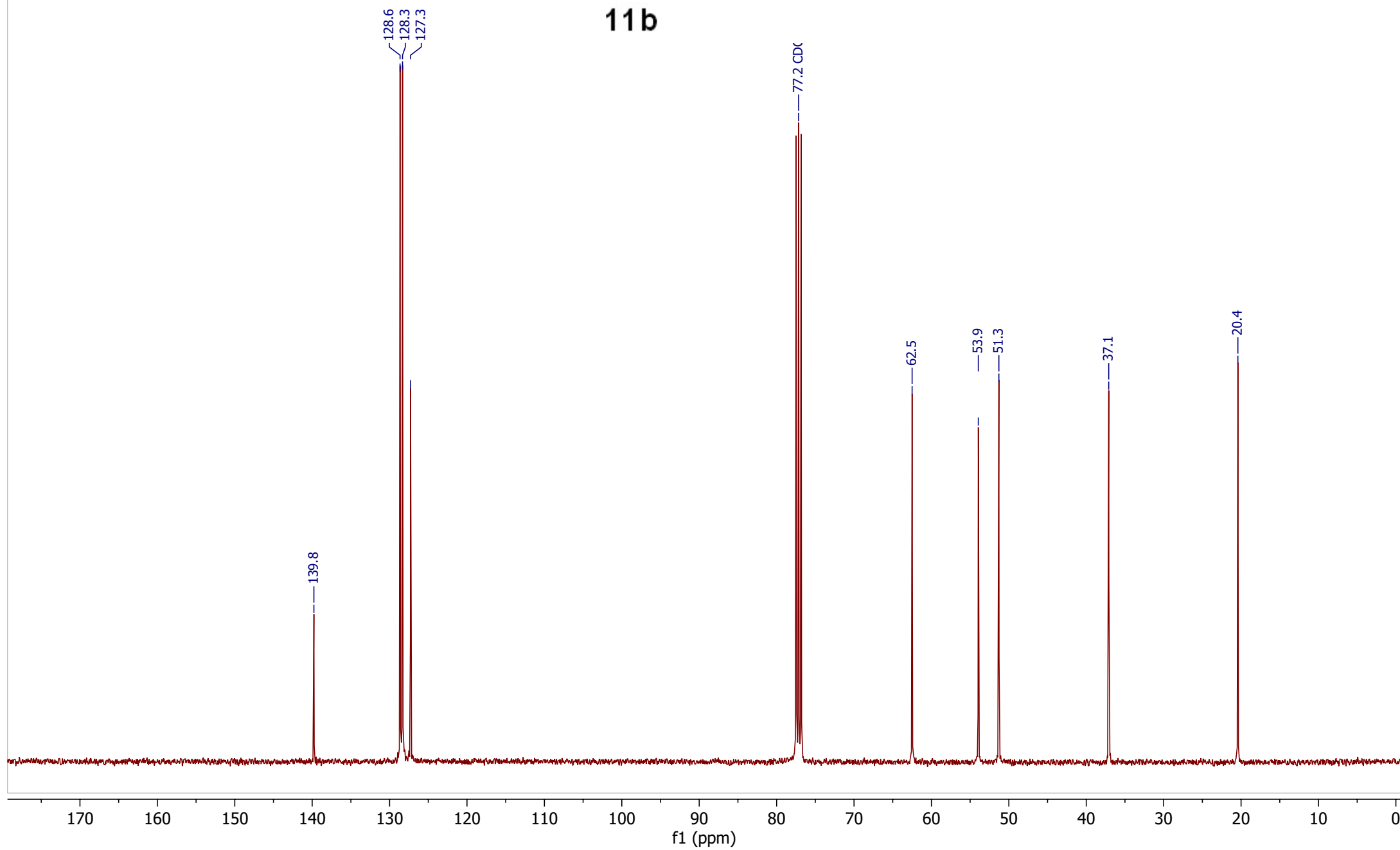
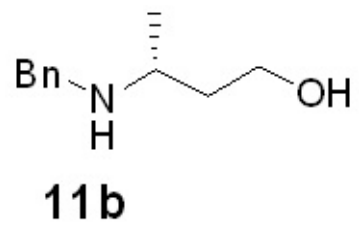


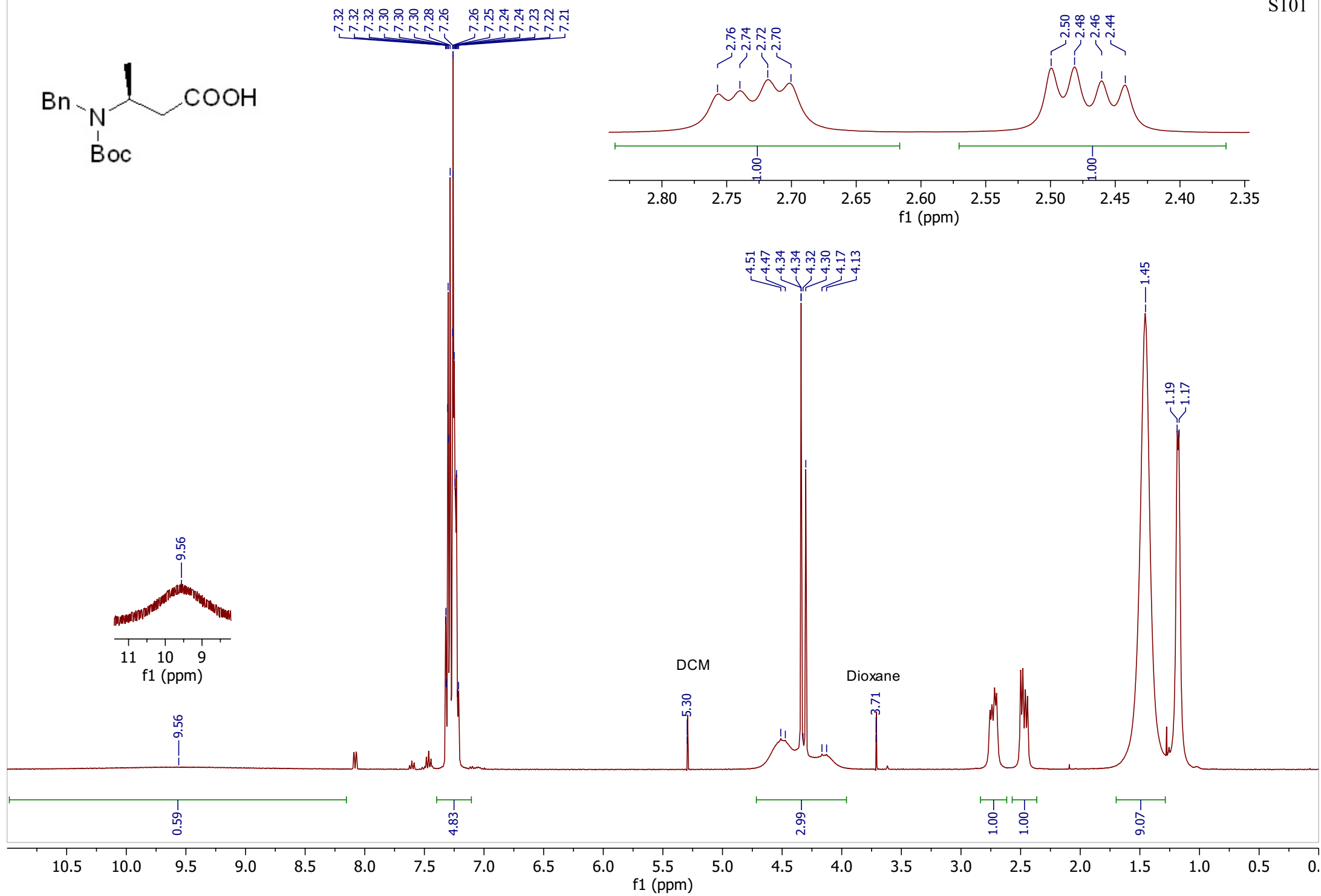
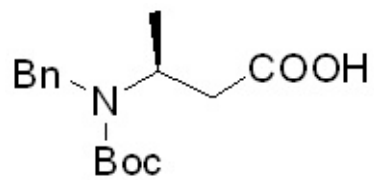
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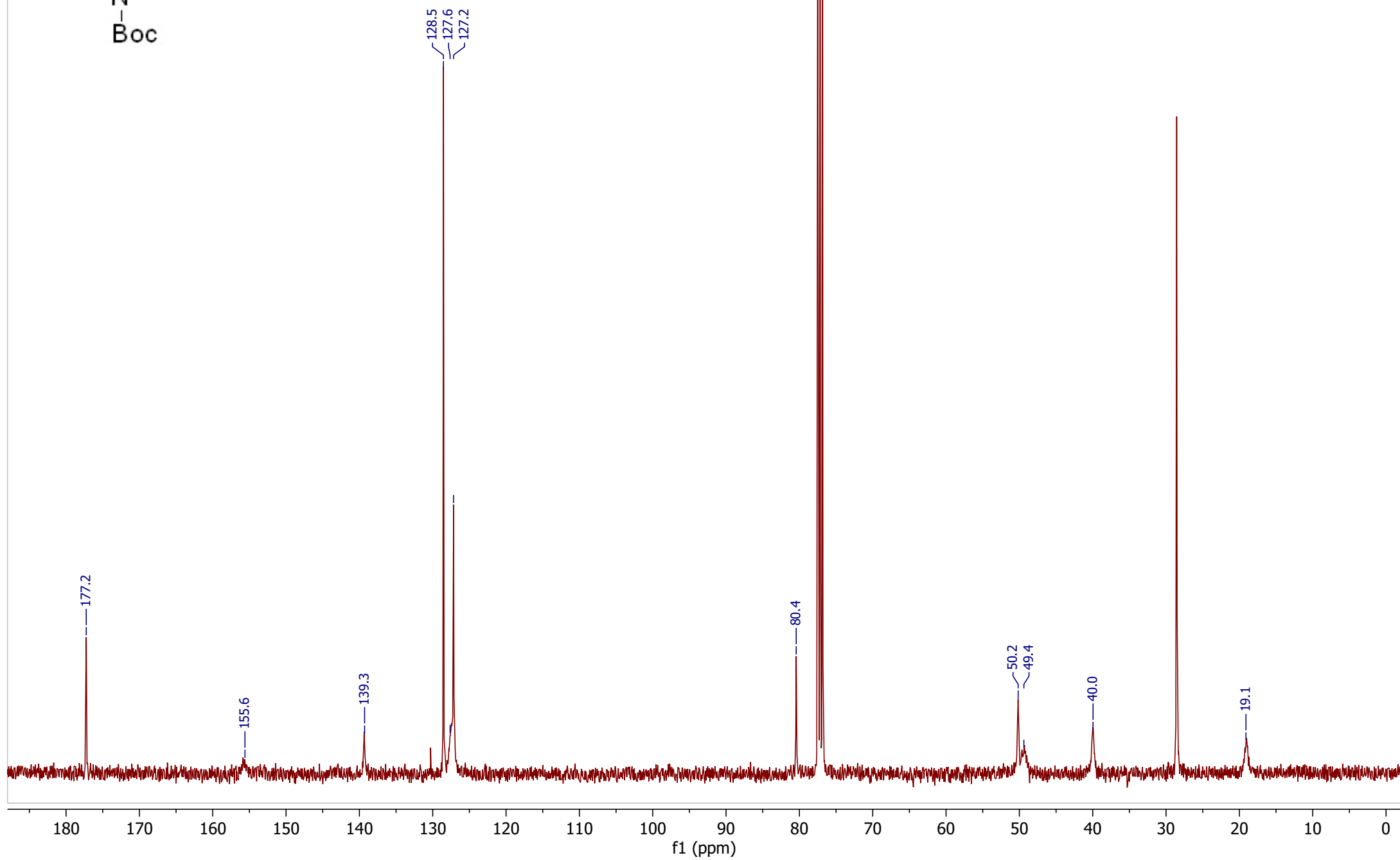
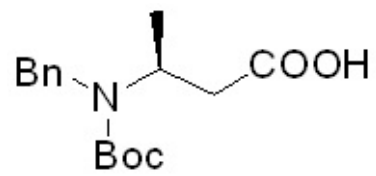


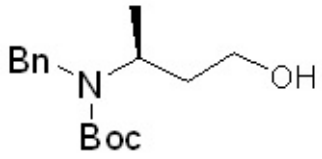
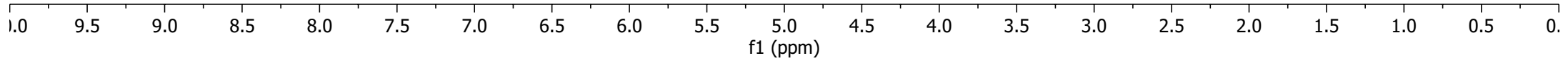
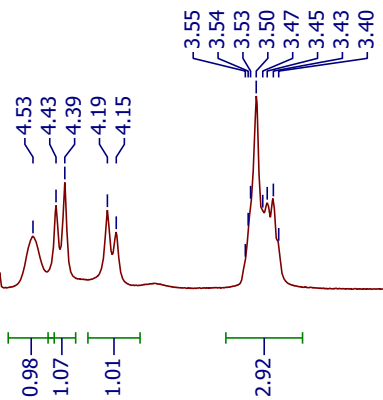
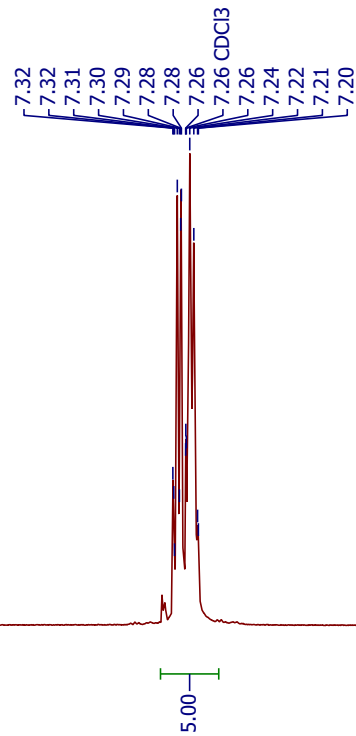
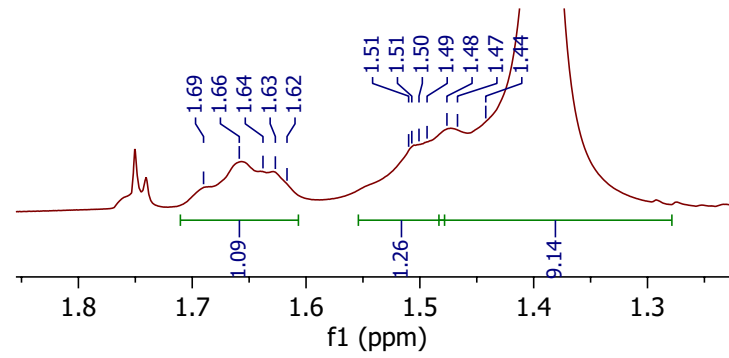
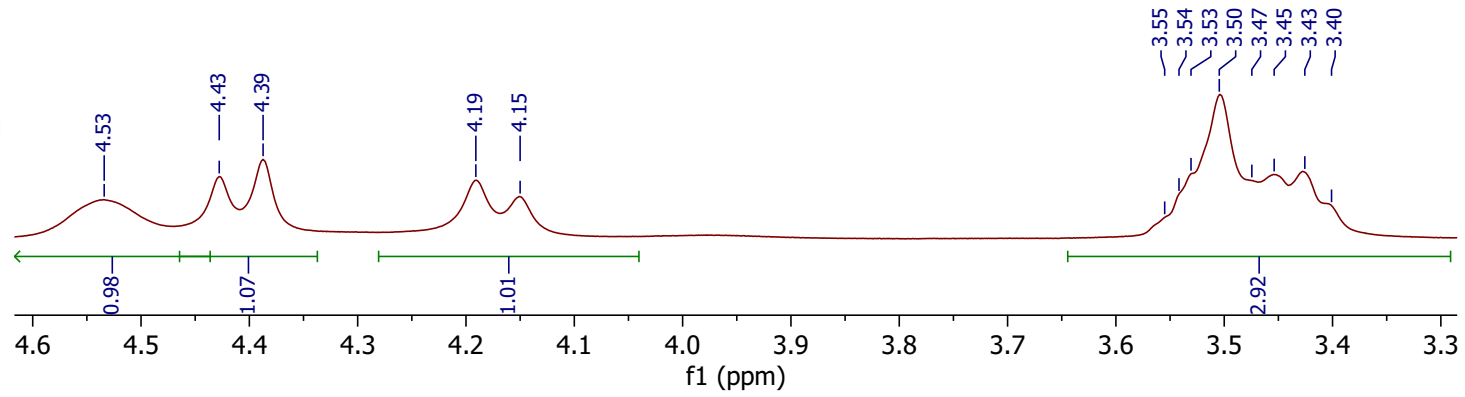
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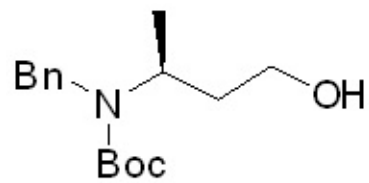
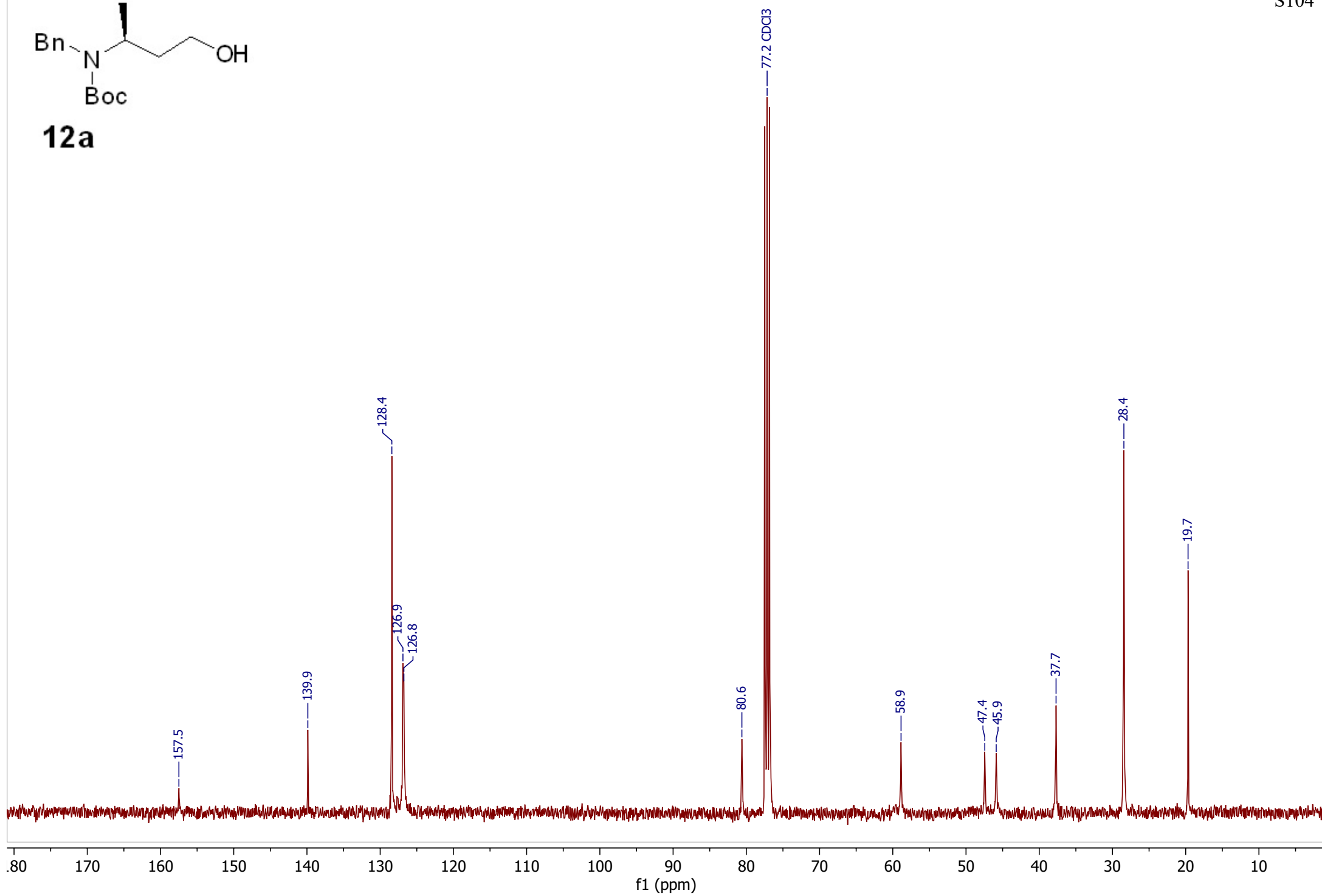


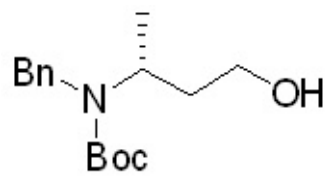
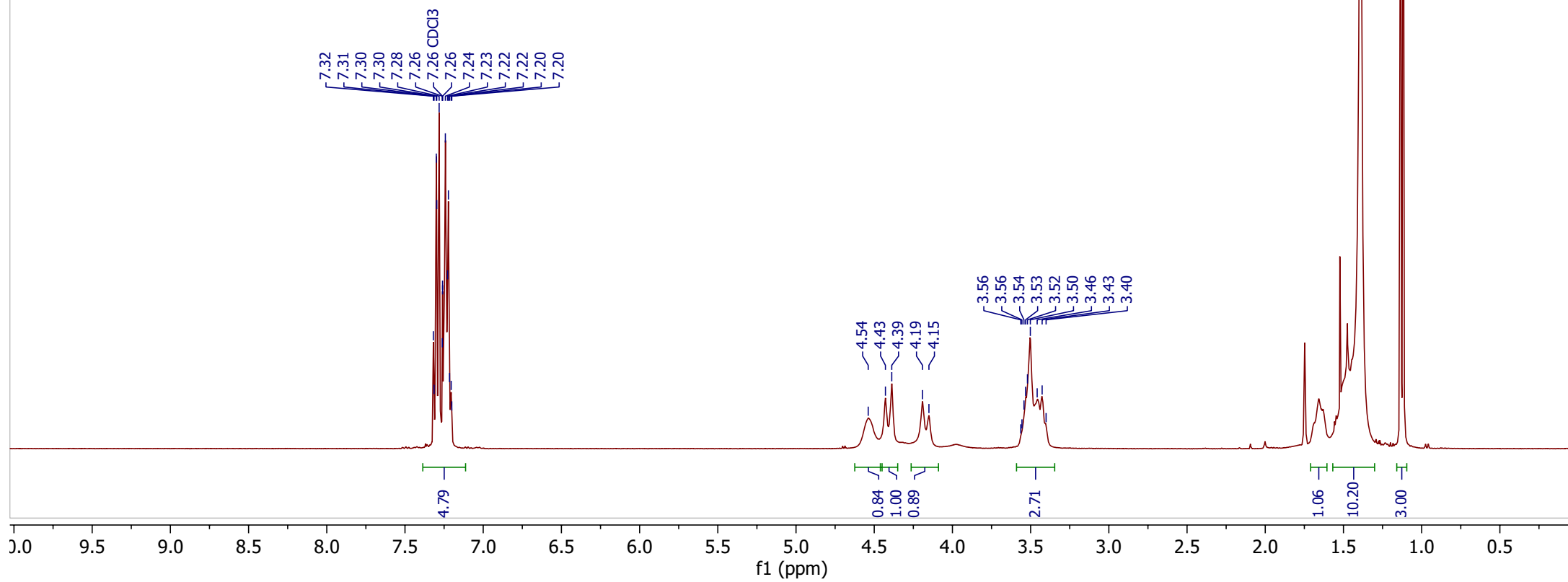


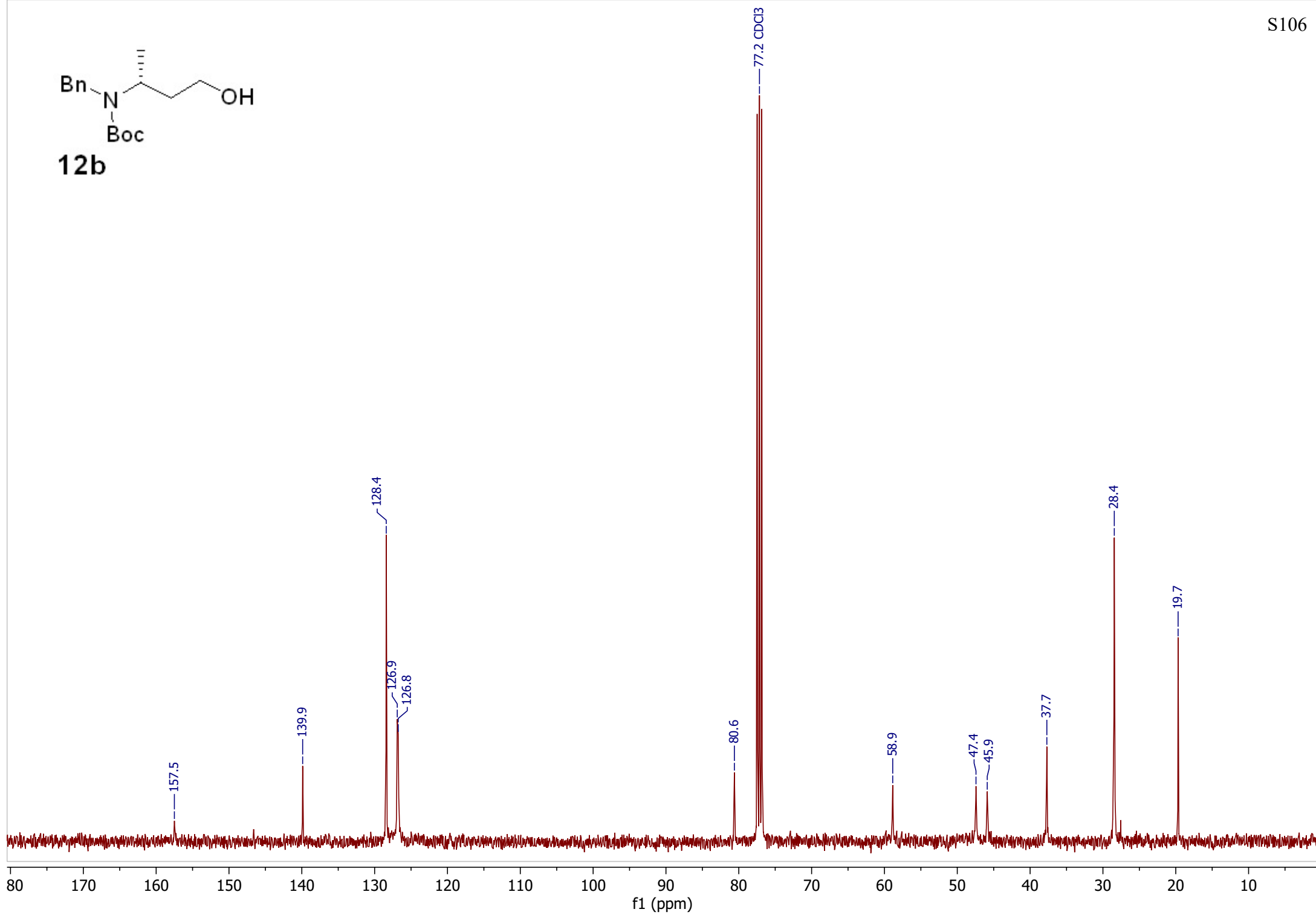
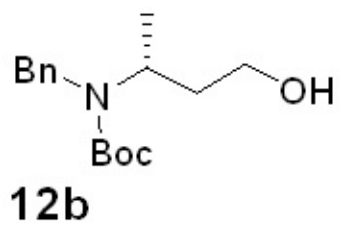


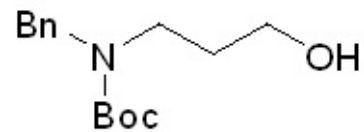
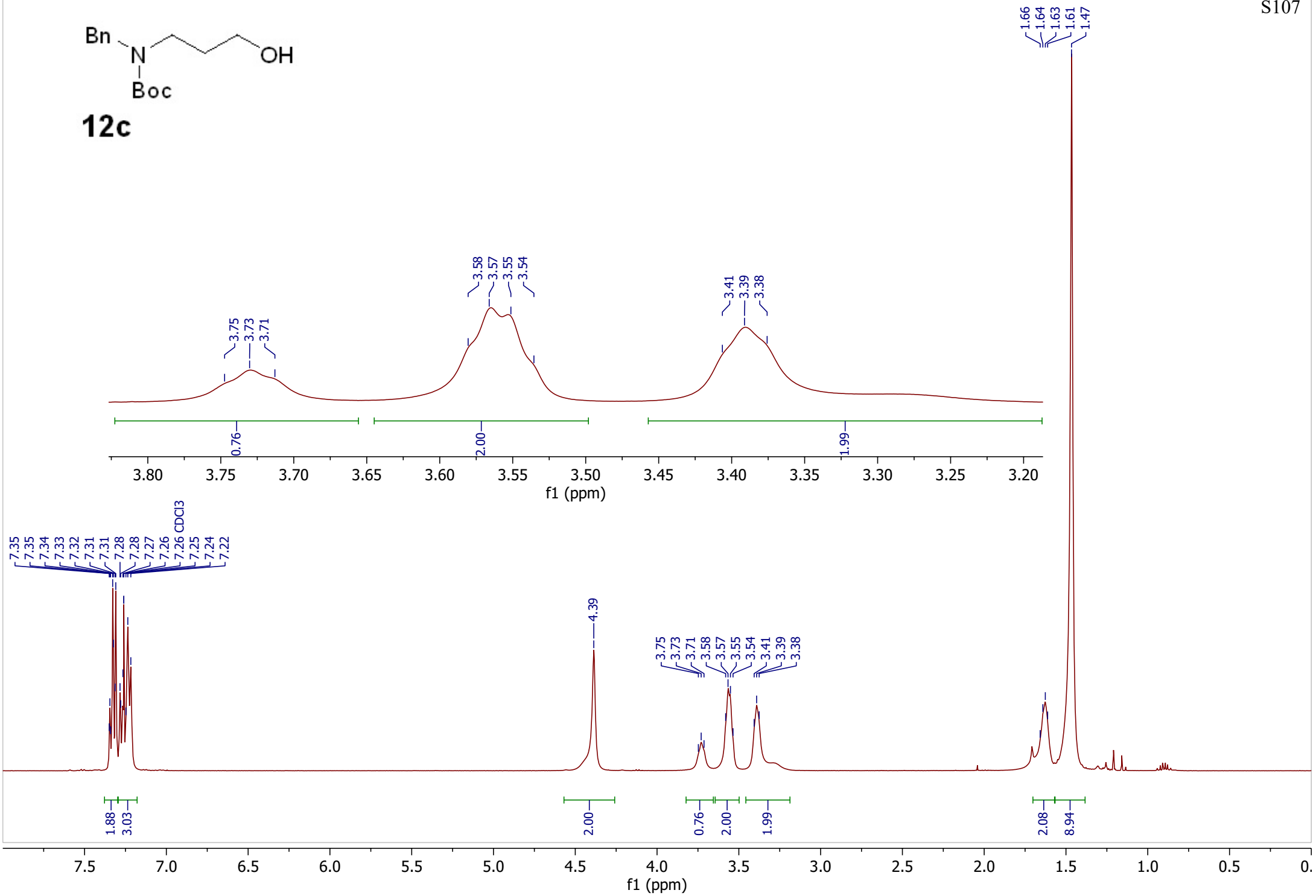


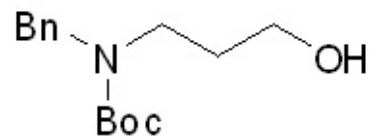
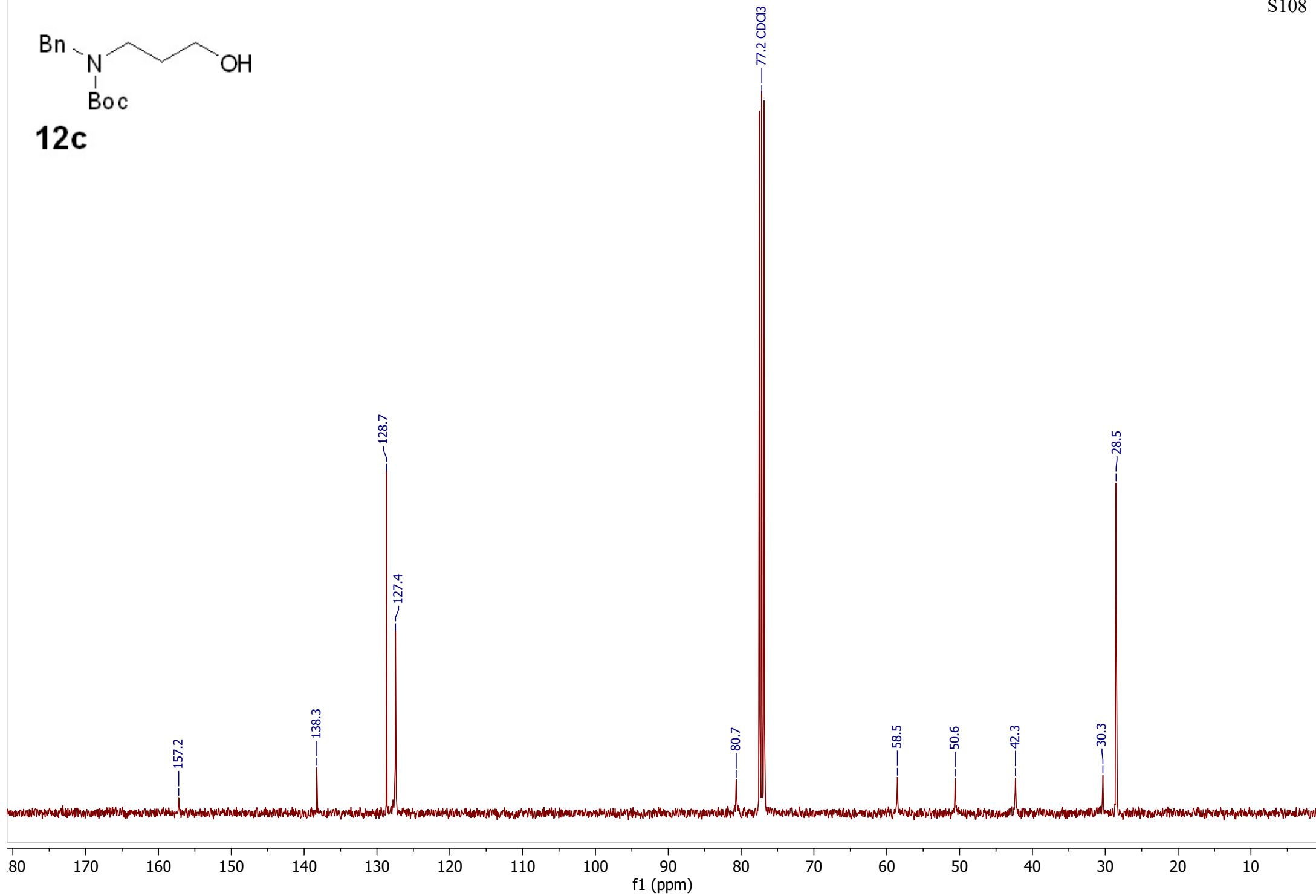
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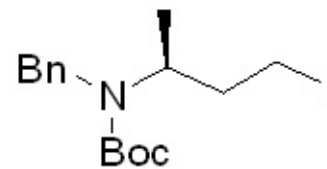
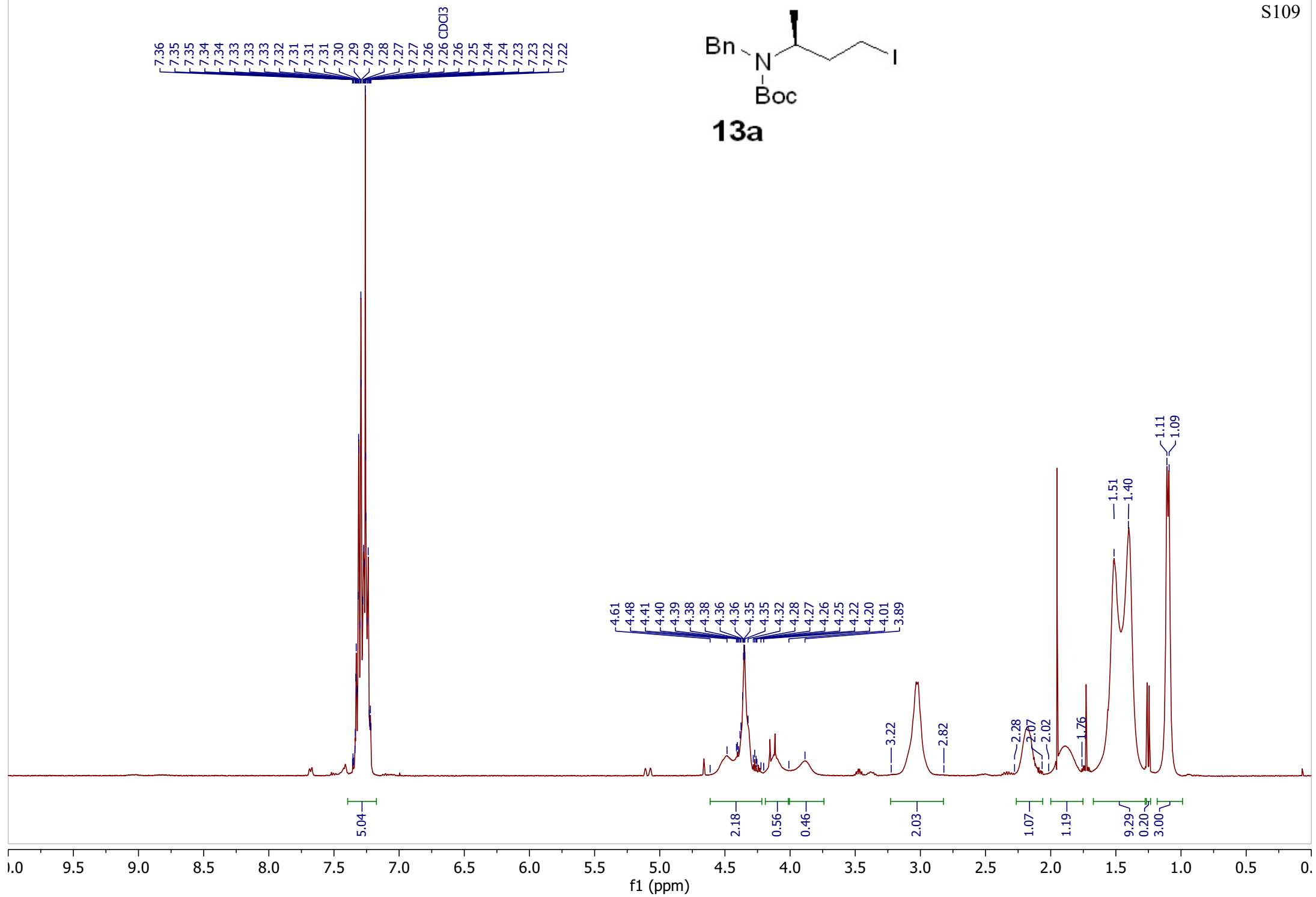
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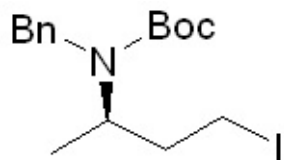
**12b**



**12c**

**12c**

**13a**

**13b**

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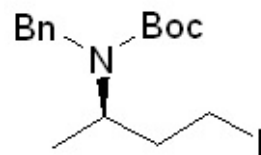
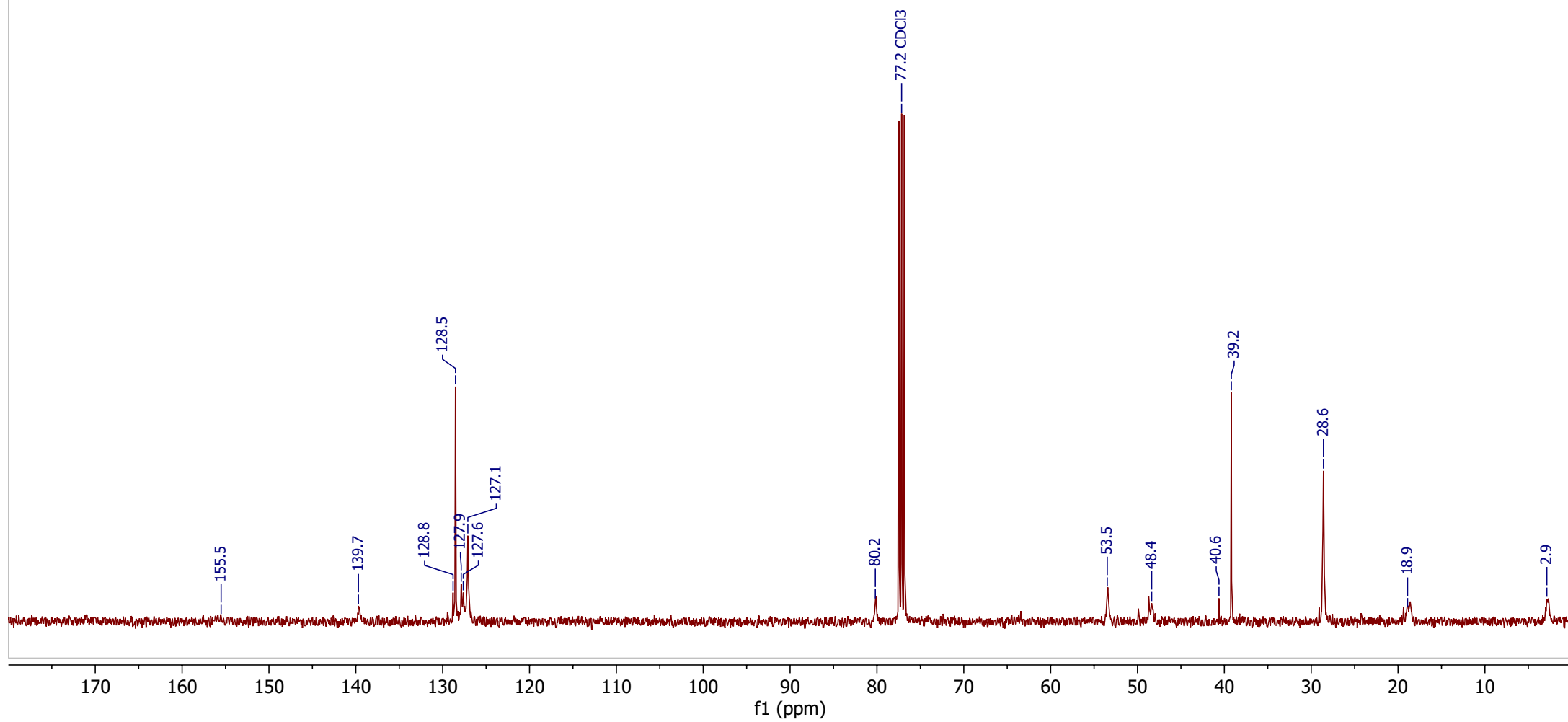
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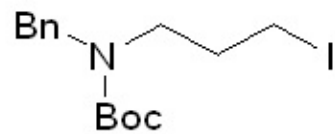
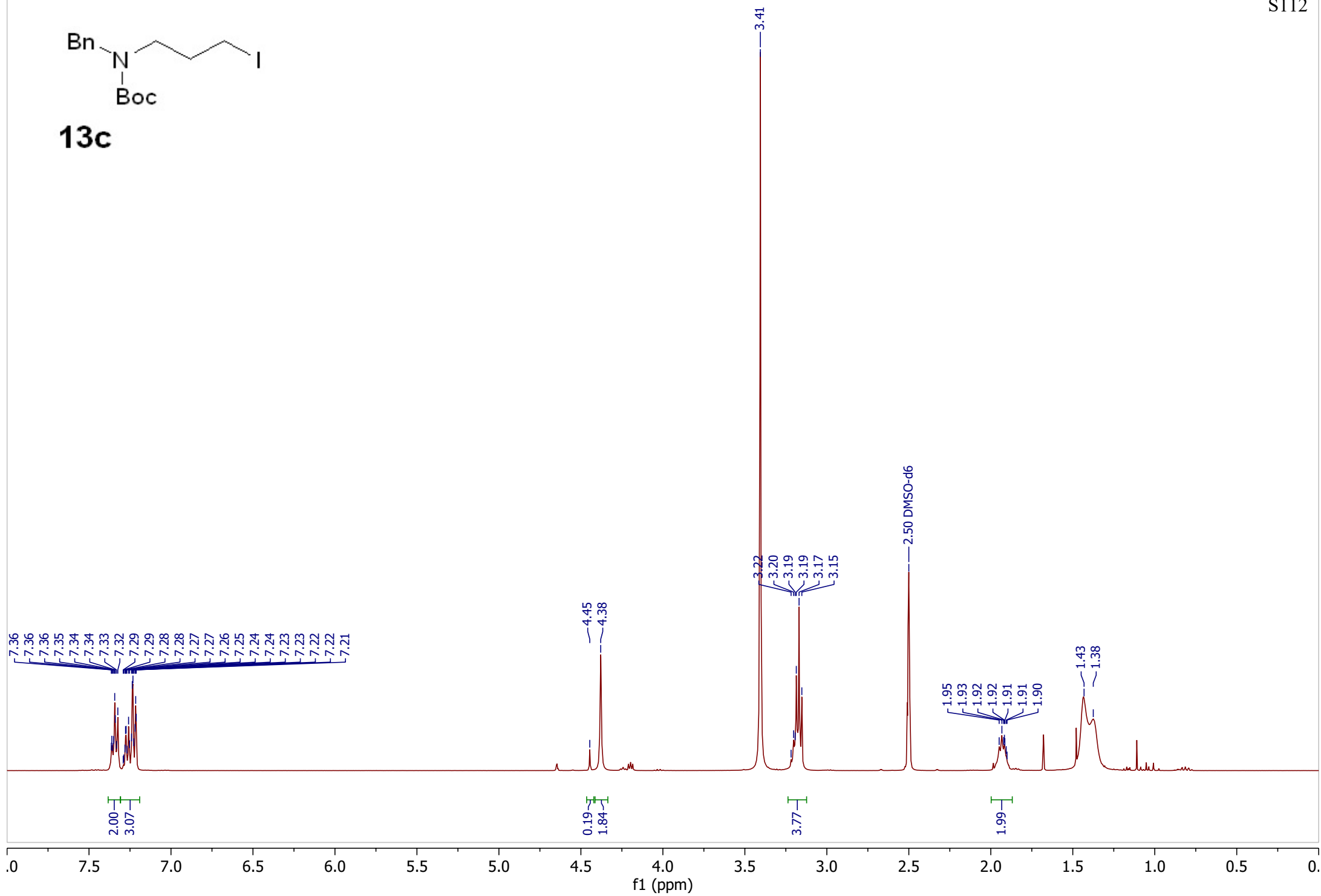
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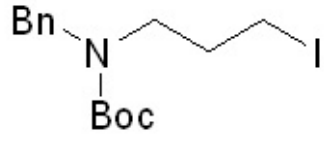
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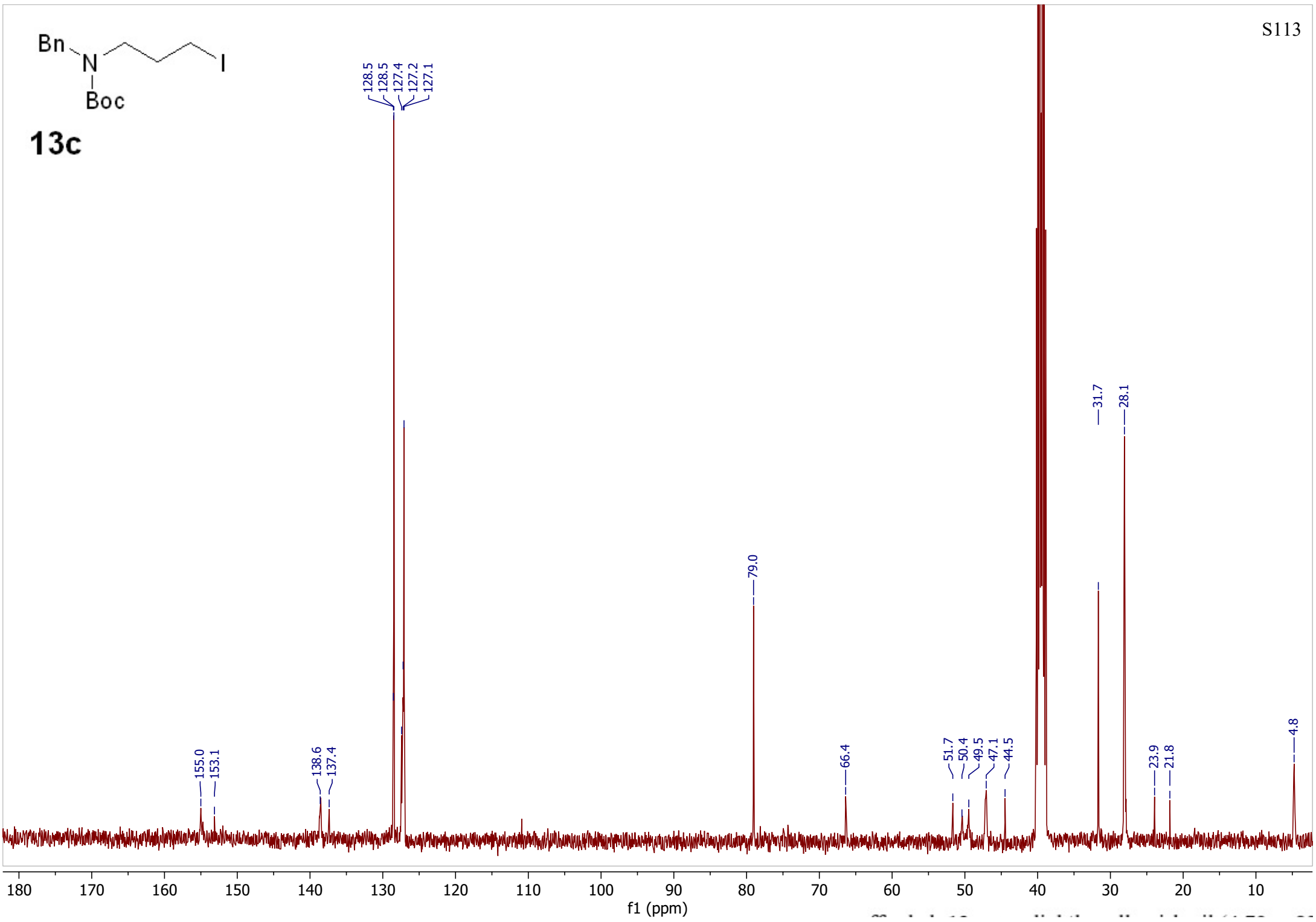
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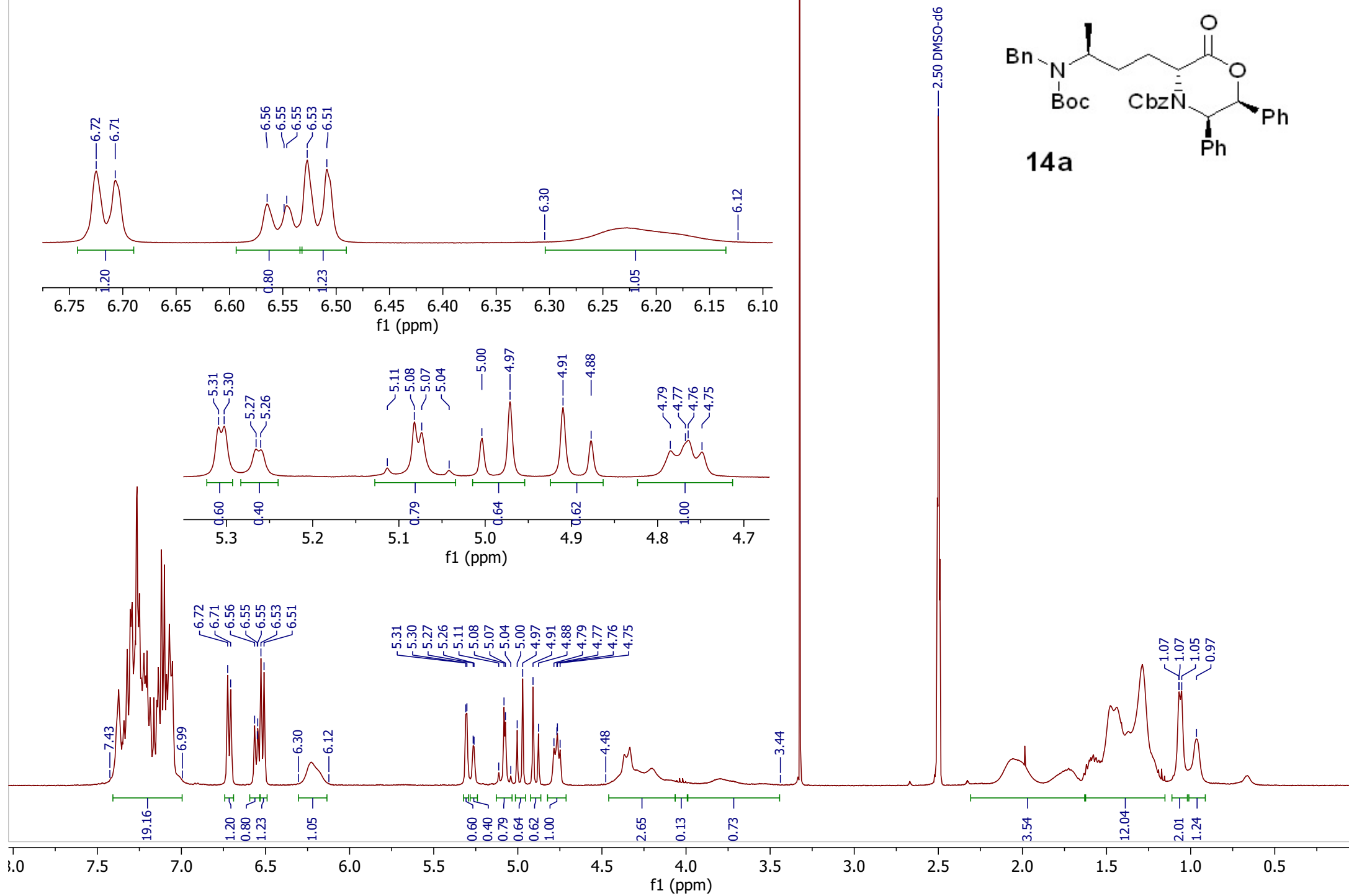
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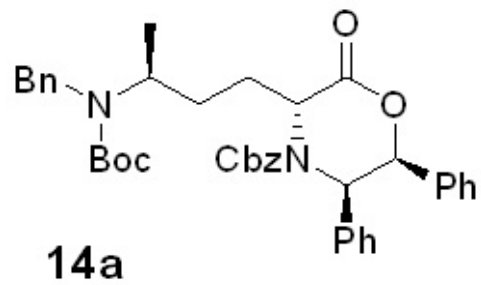
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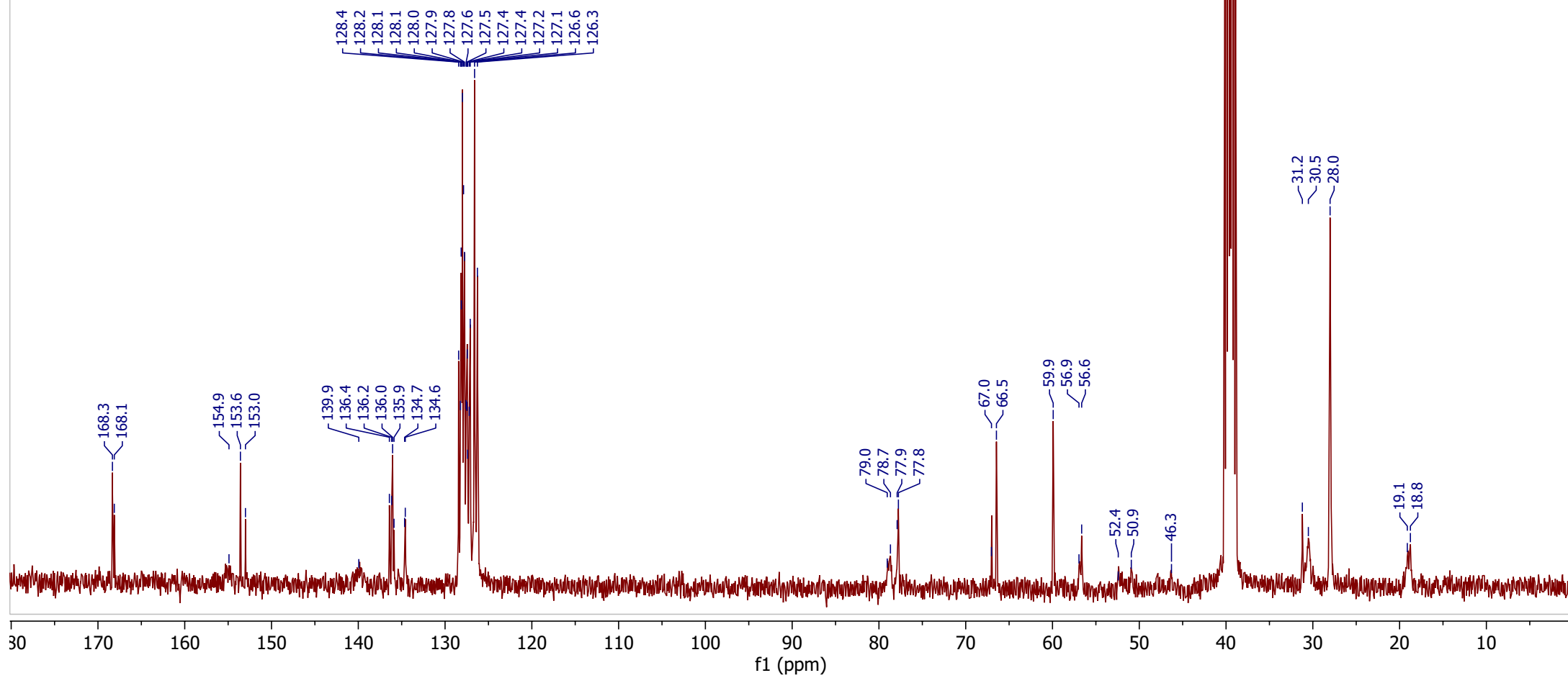
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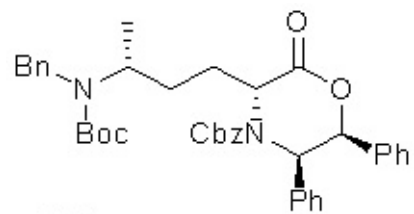
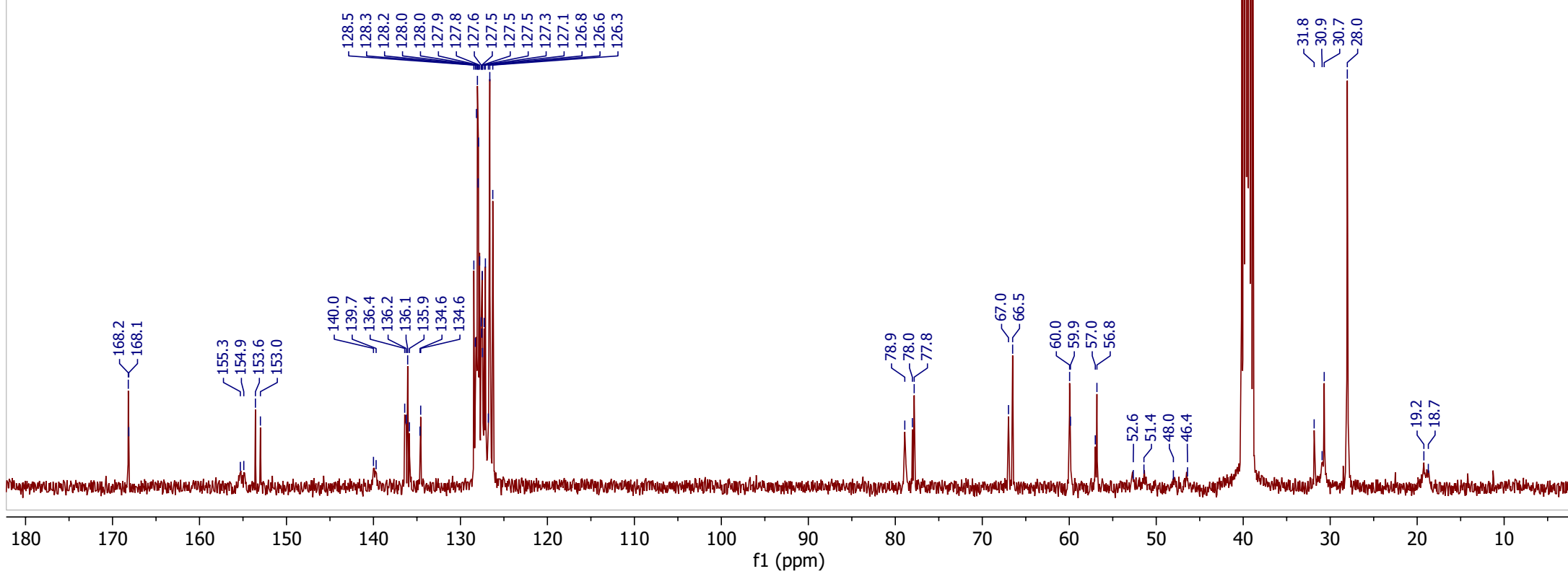


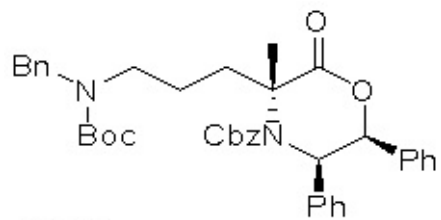
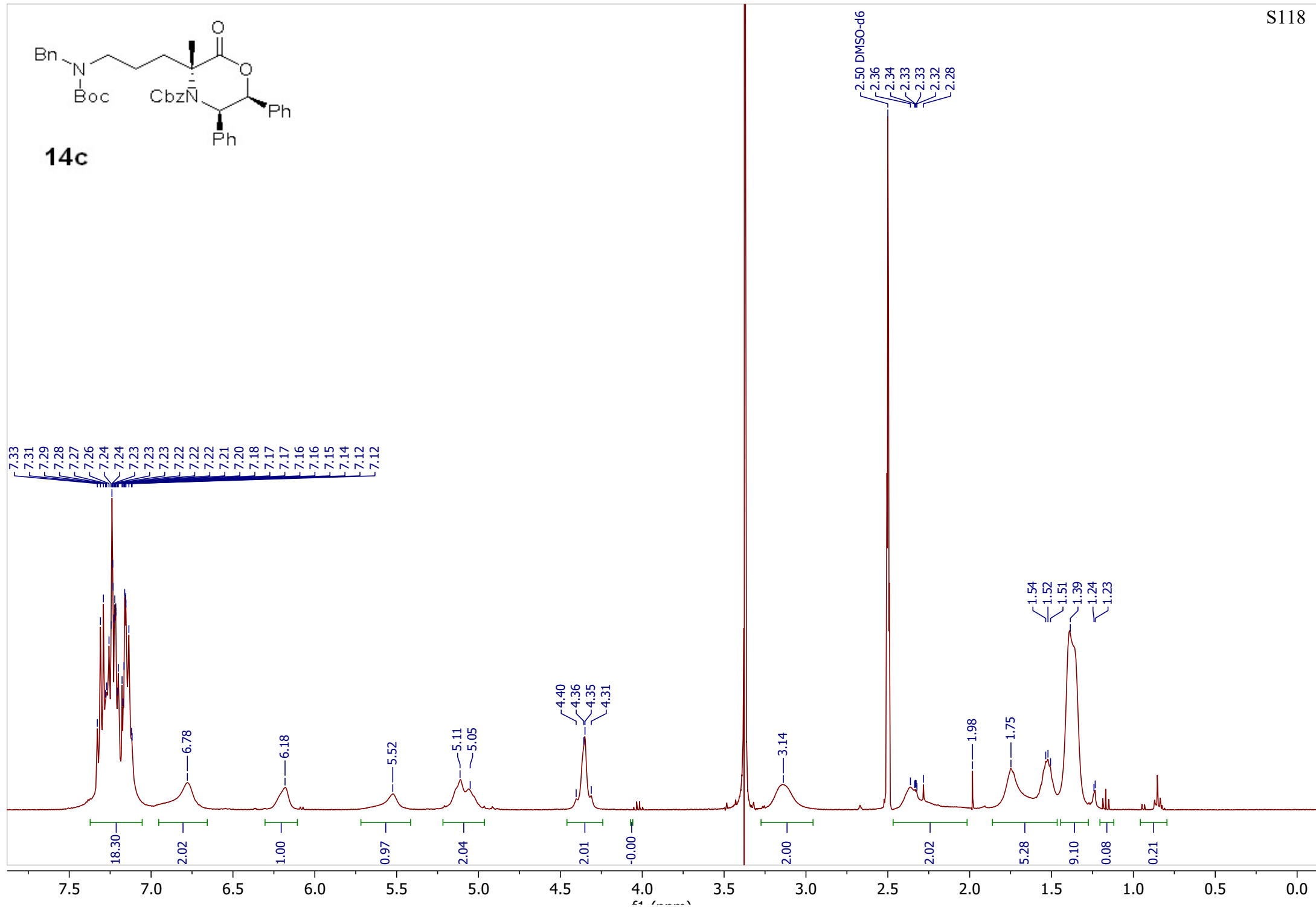


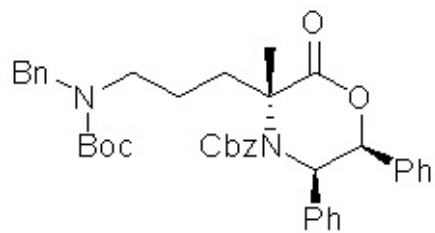
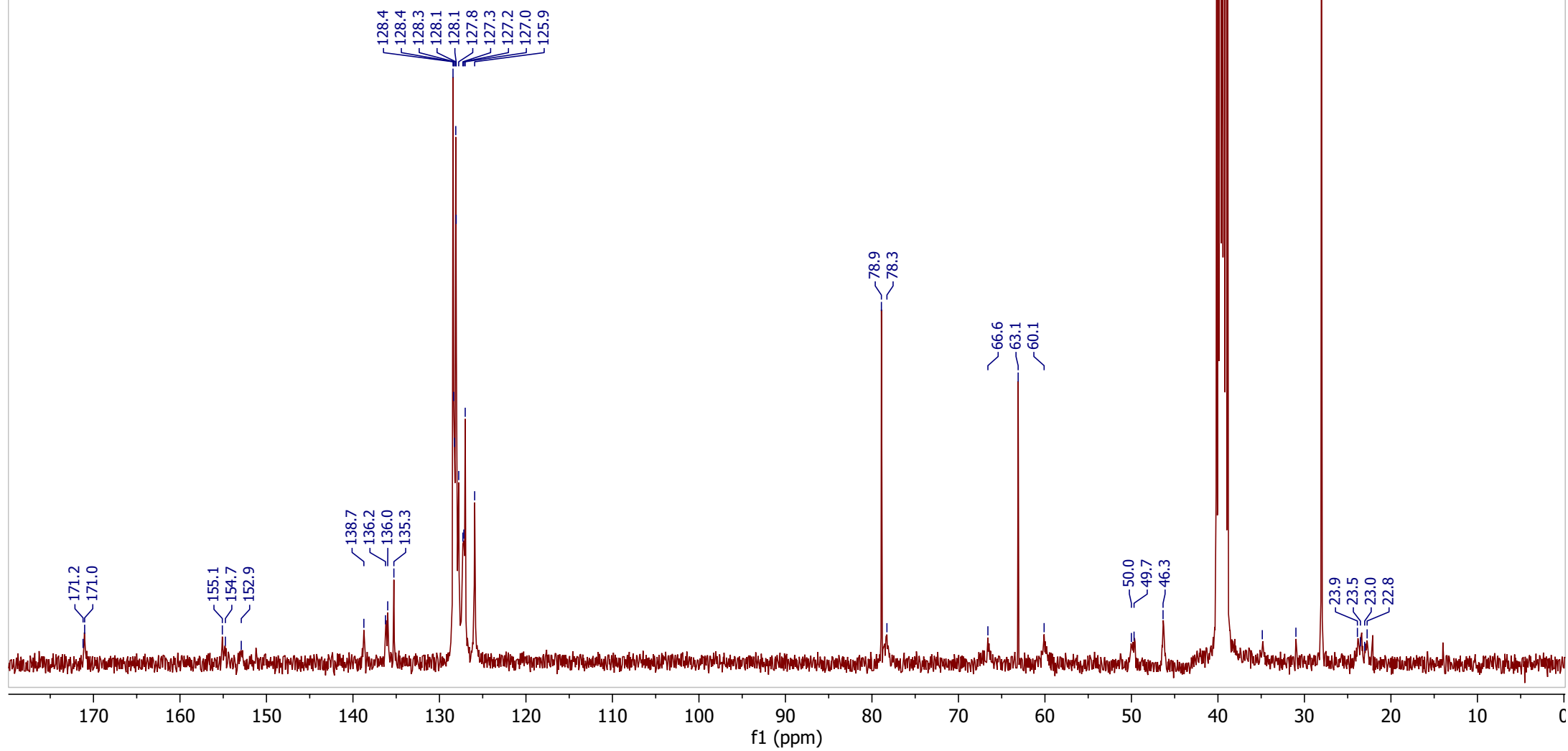


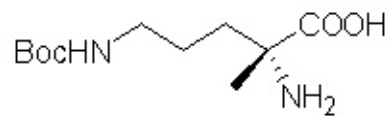
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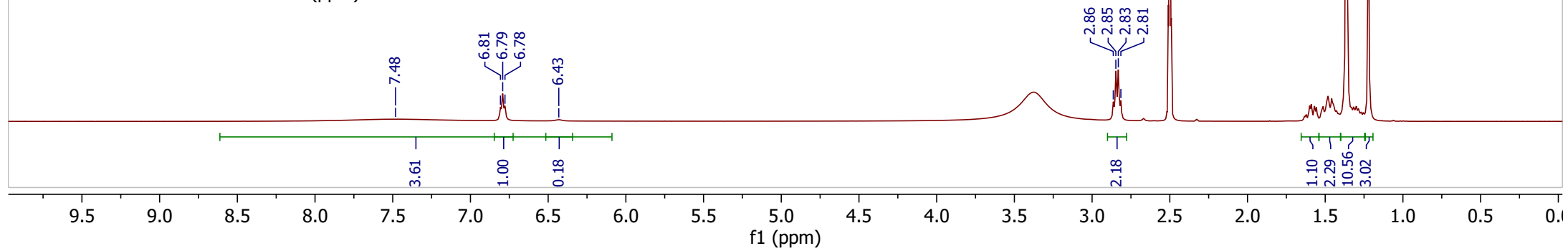
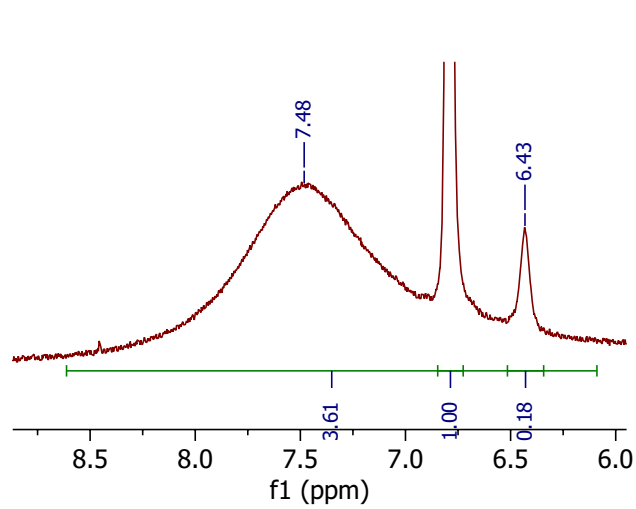
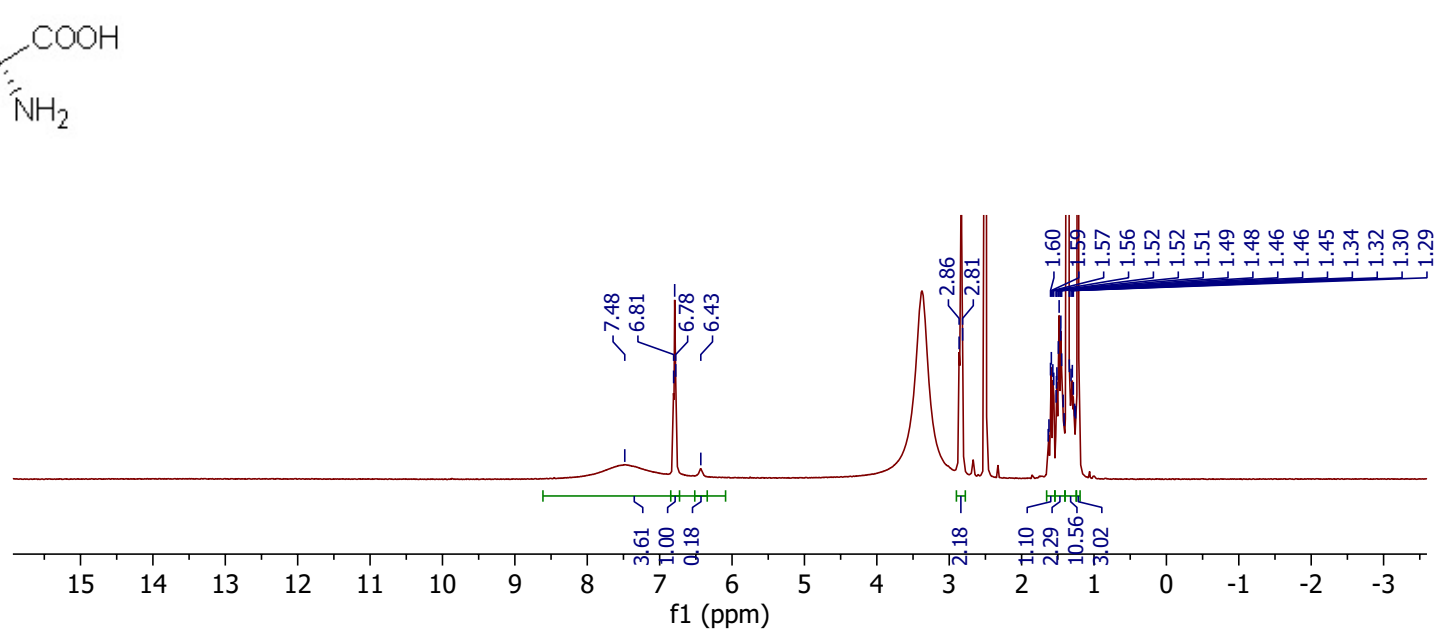
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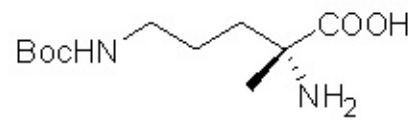
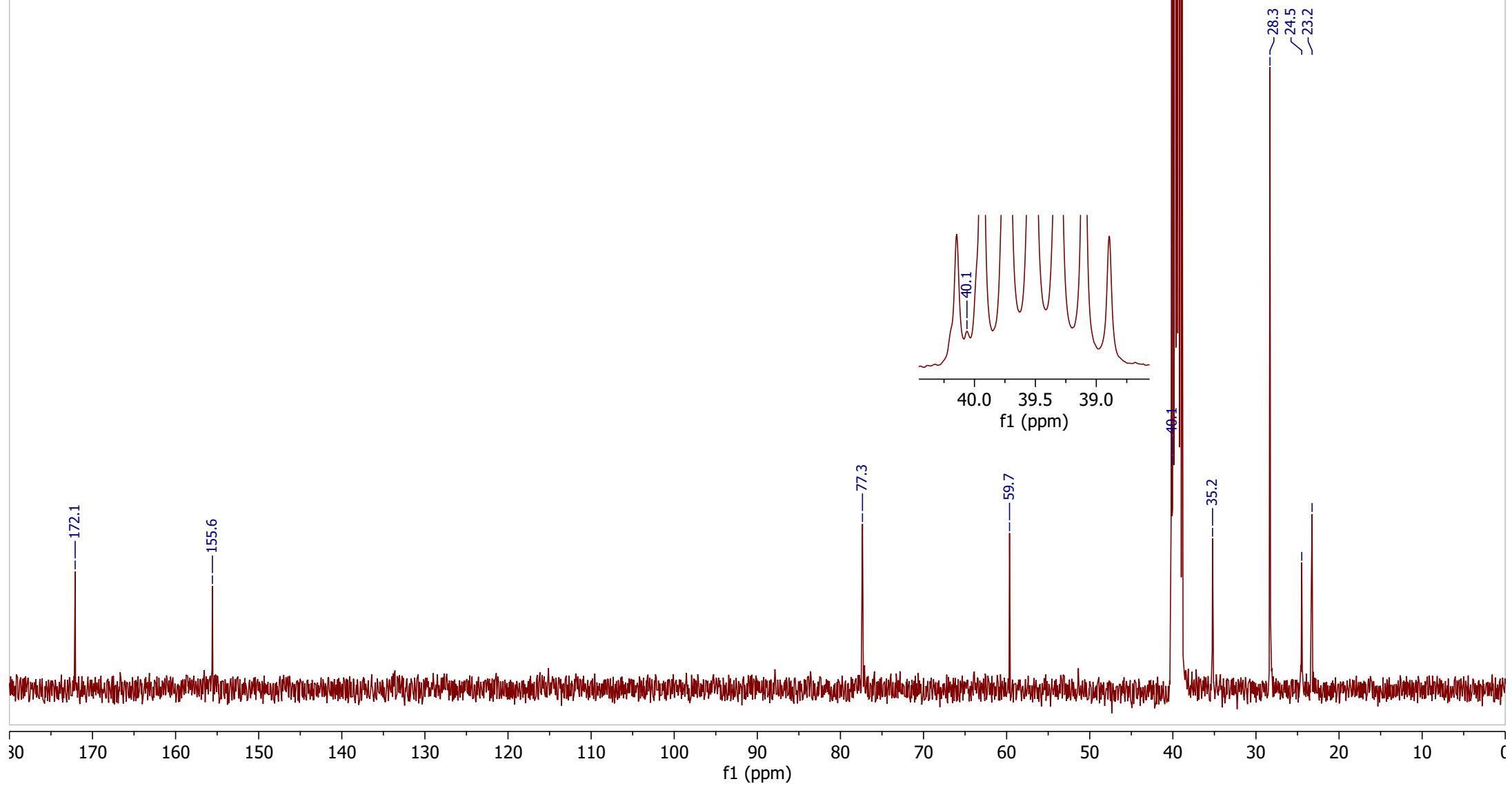
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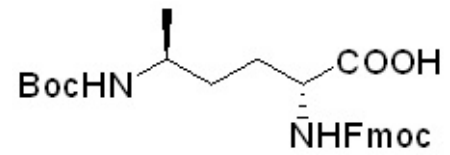
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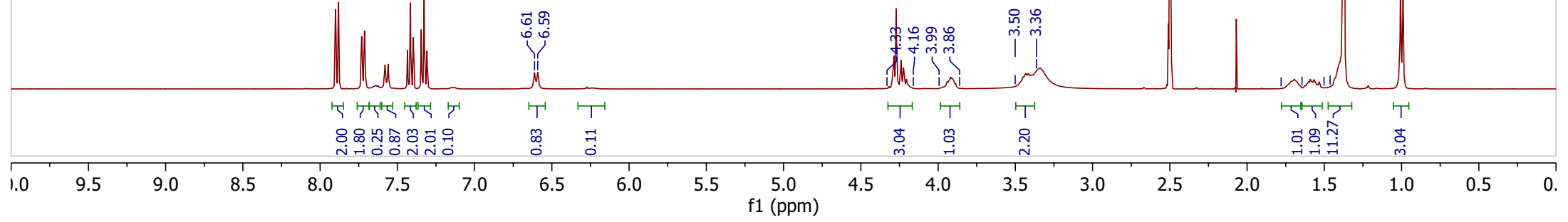
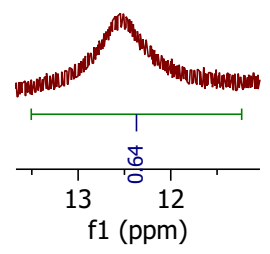
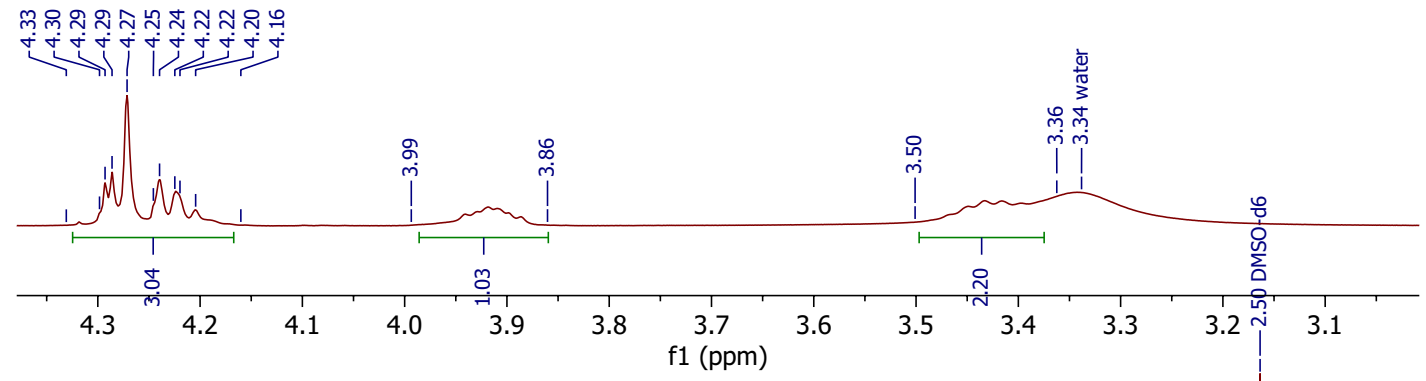
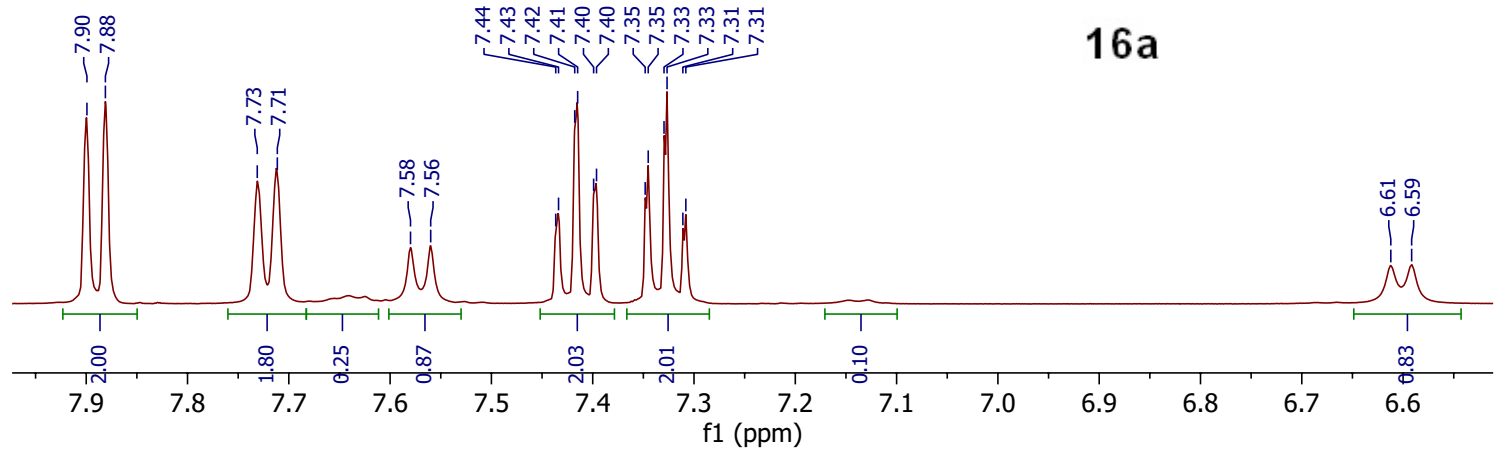
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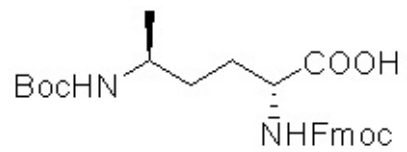
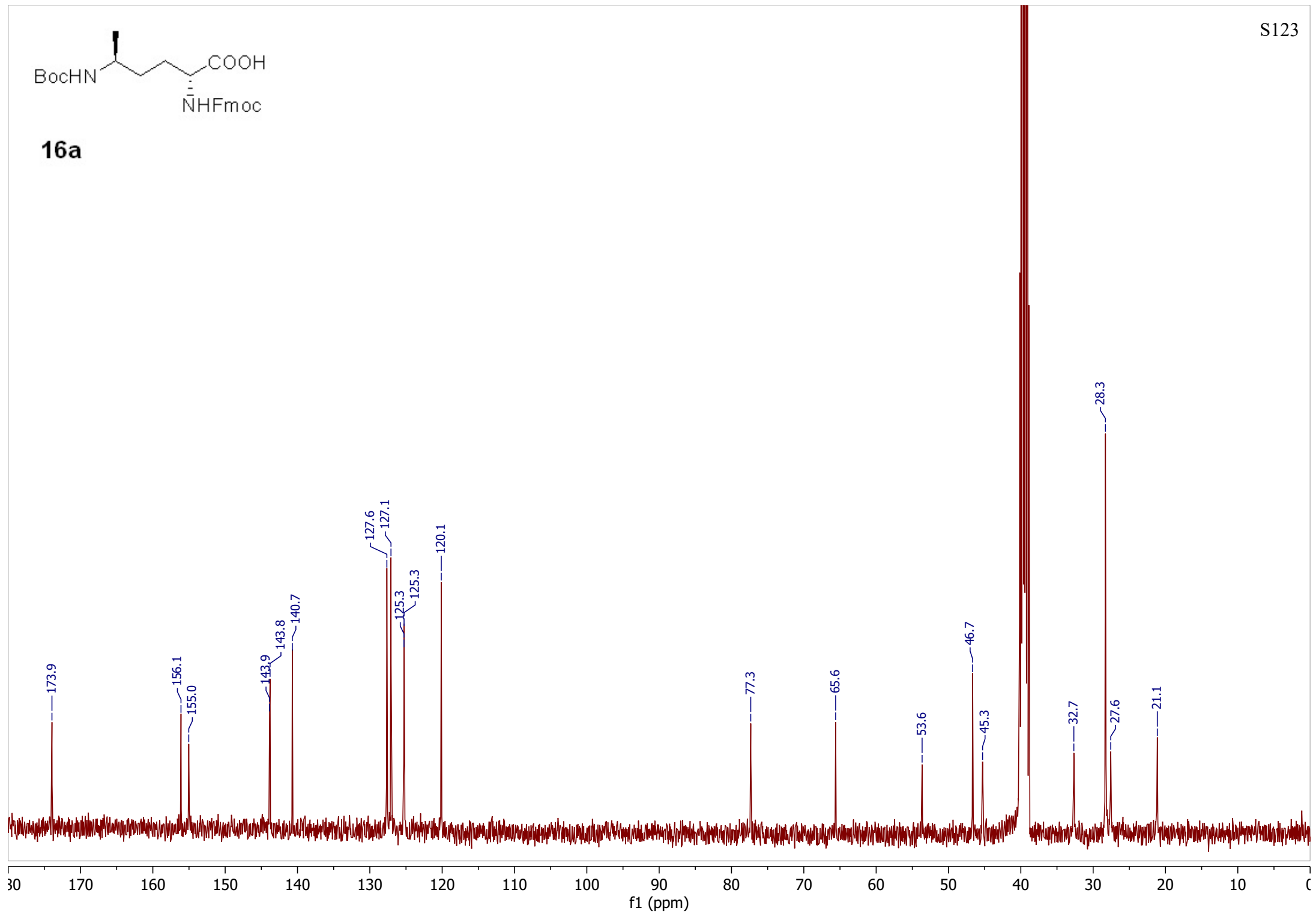


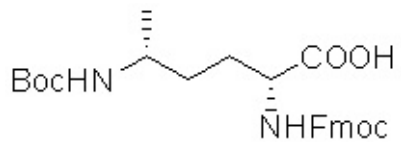
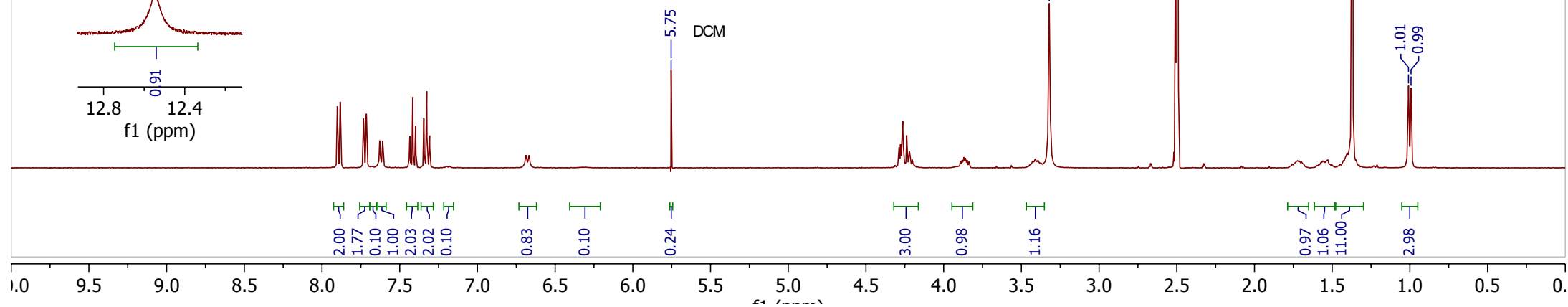
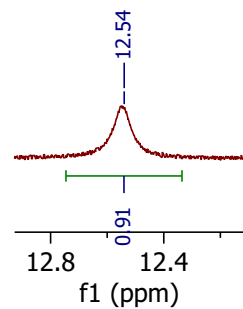
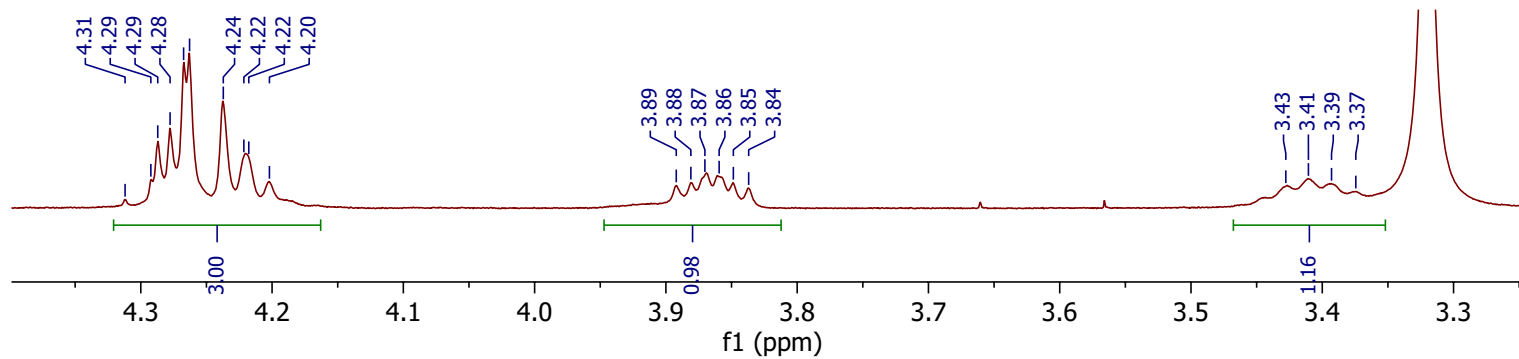
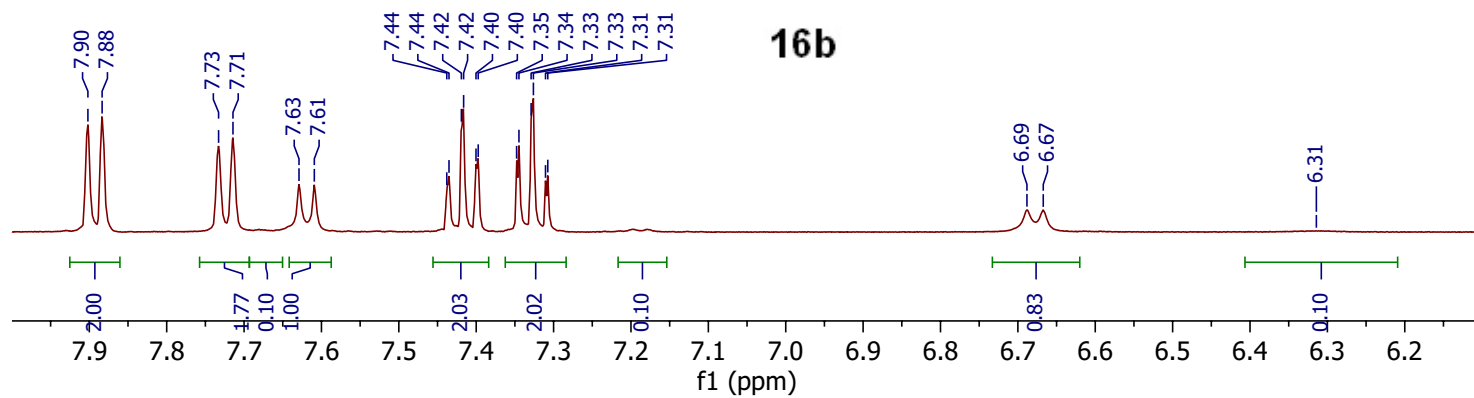
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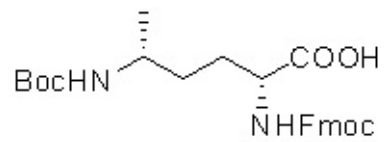
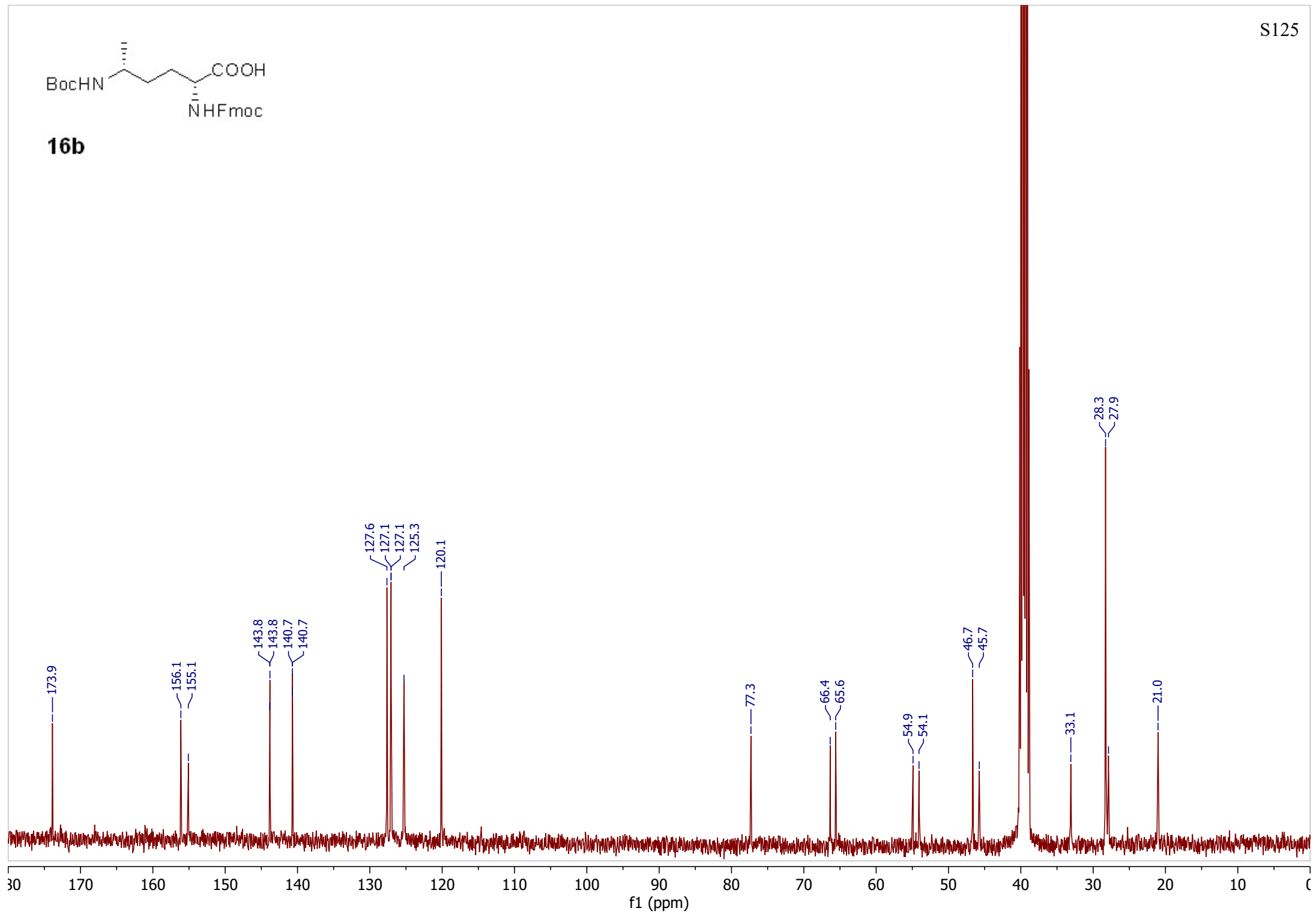


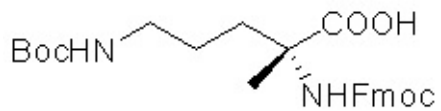
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1.46
1.38



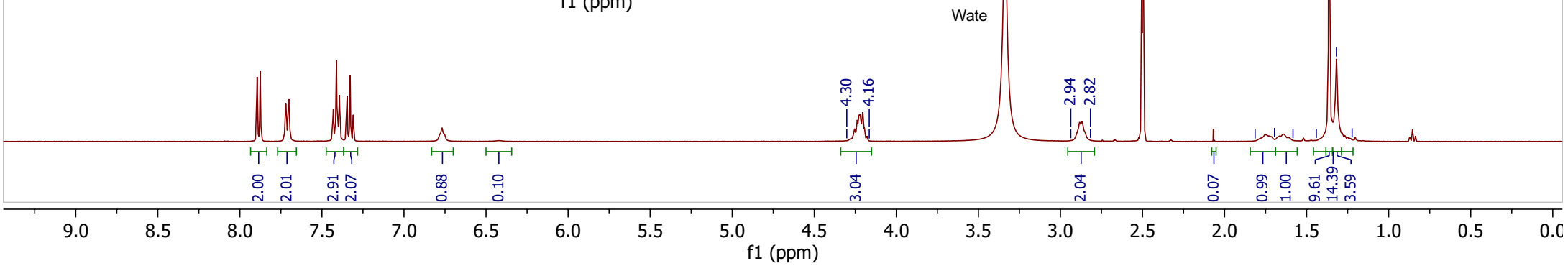
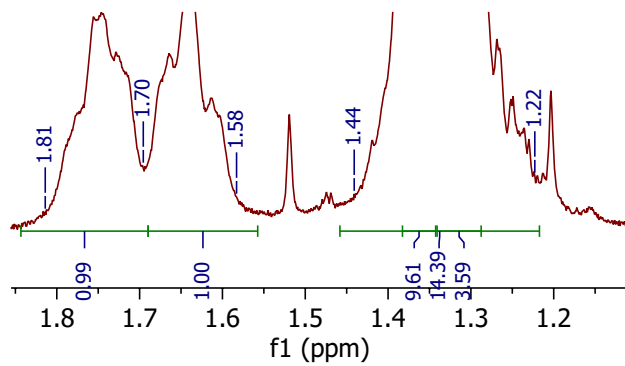
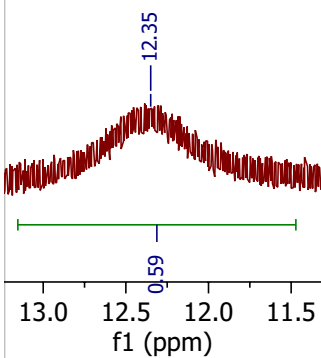
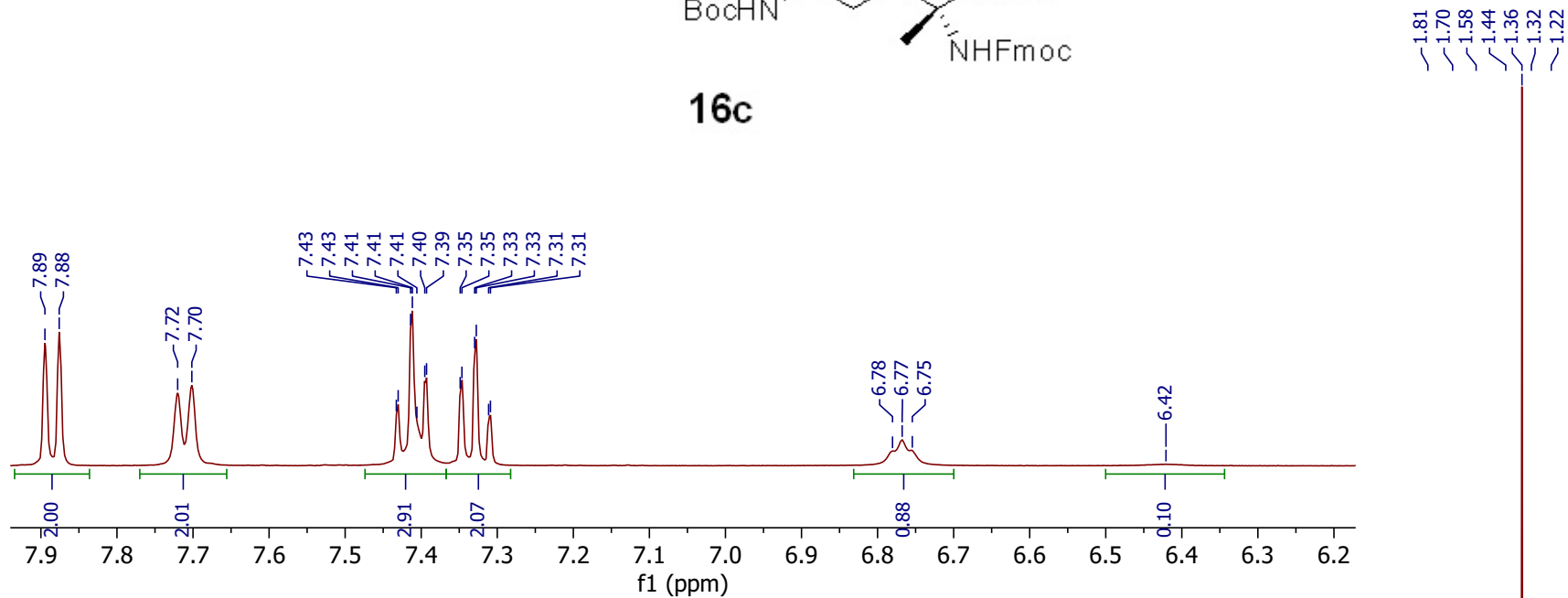
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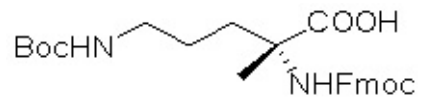
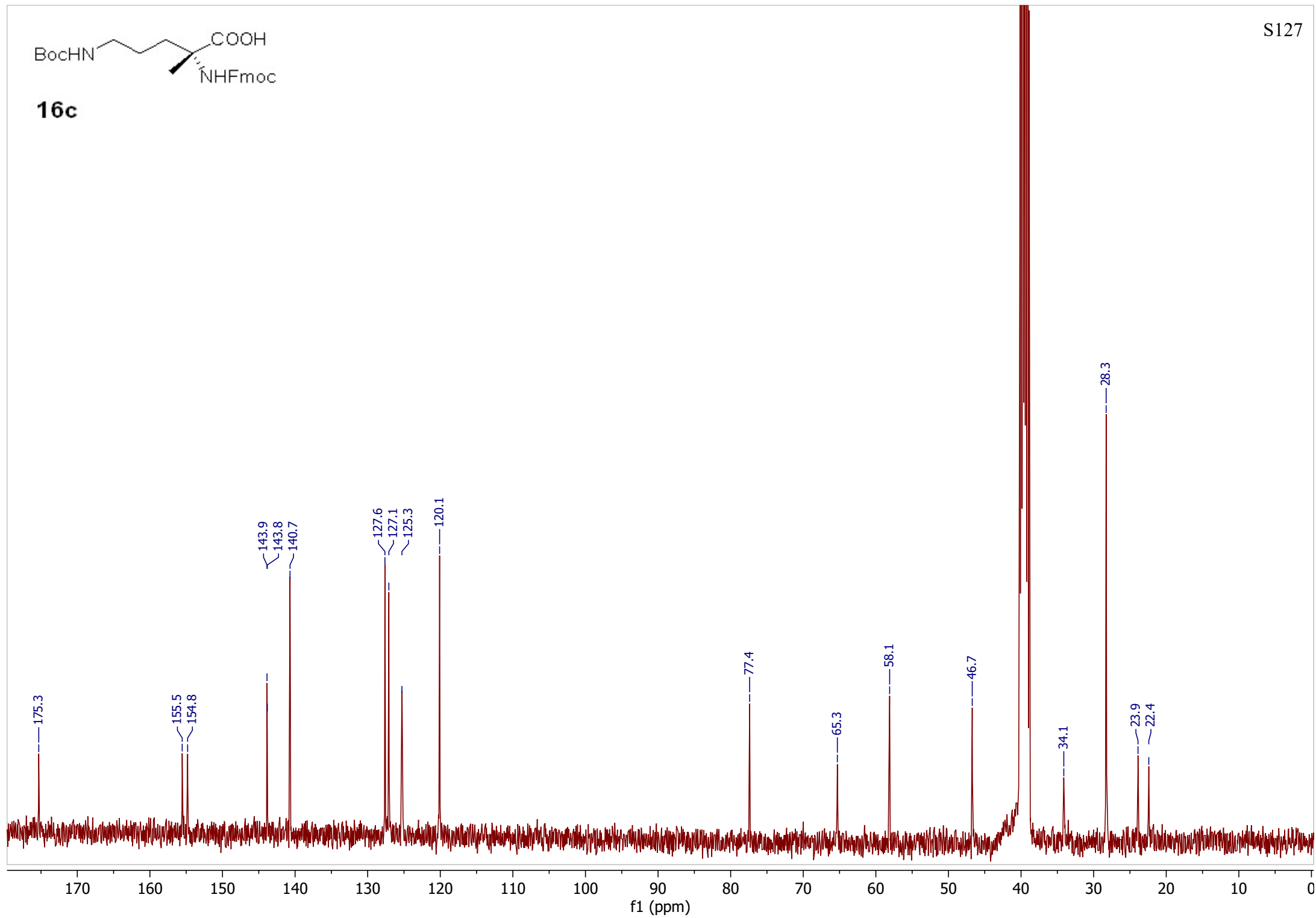
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**16b**



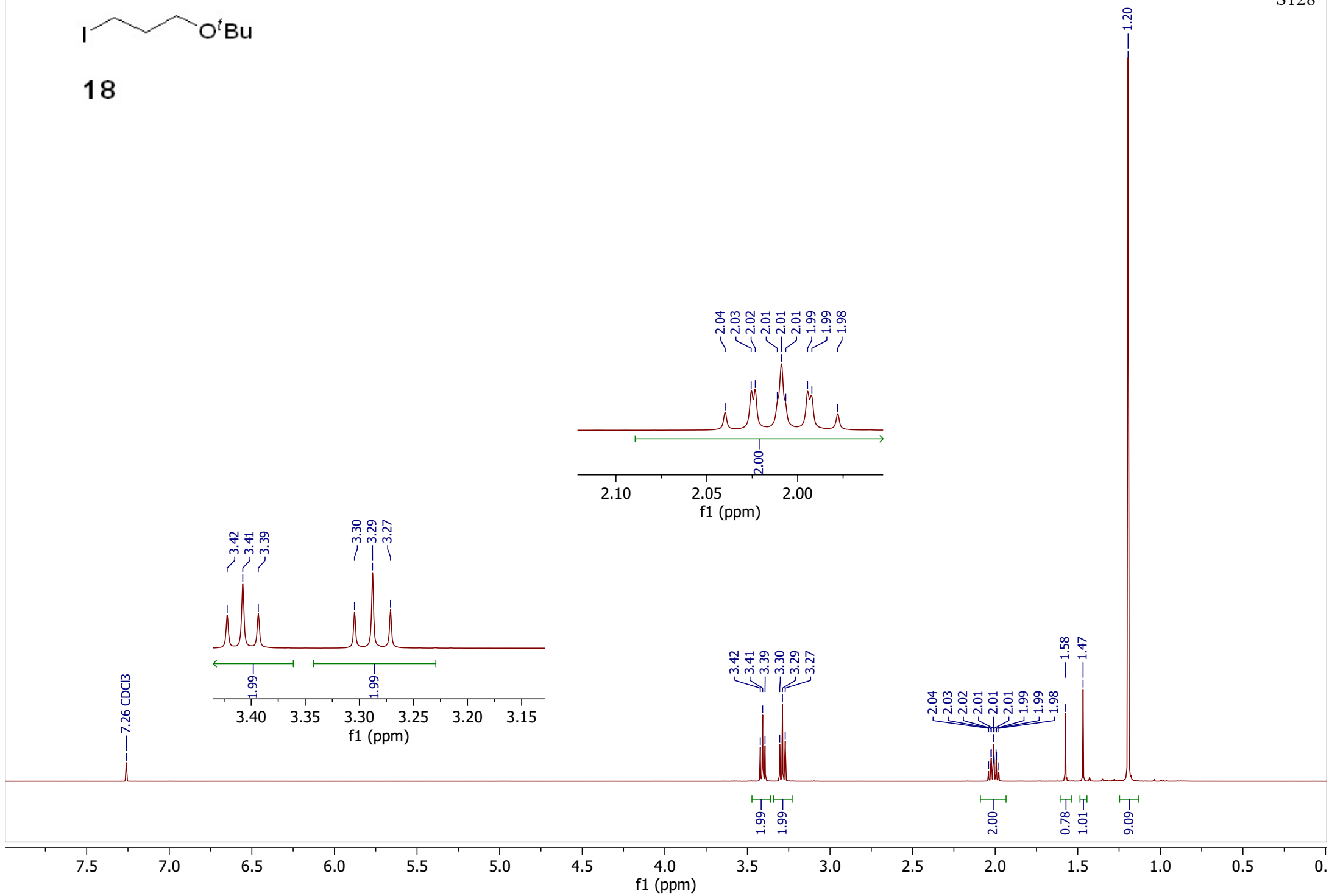
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**16c**

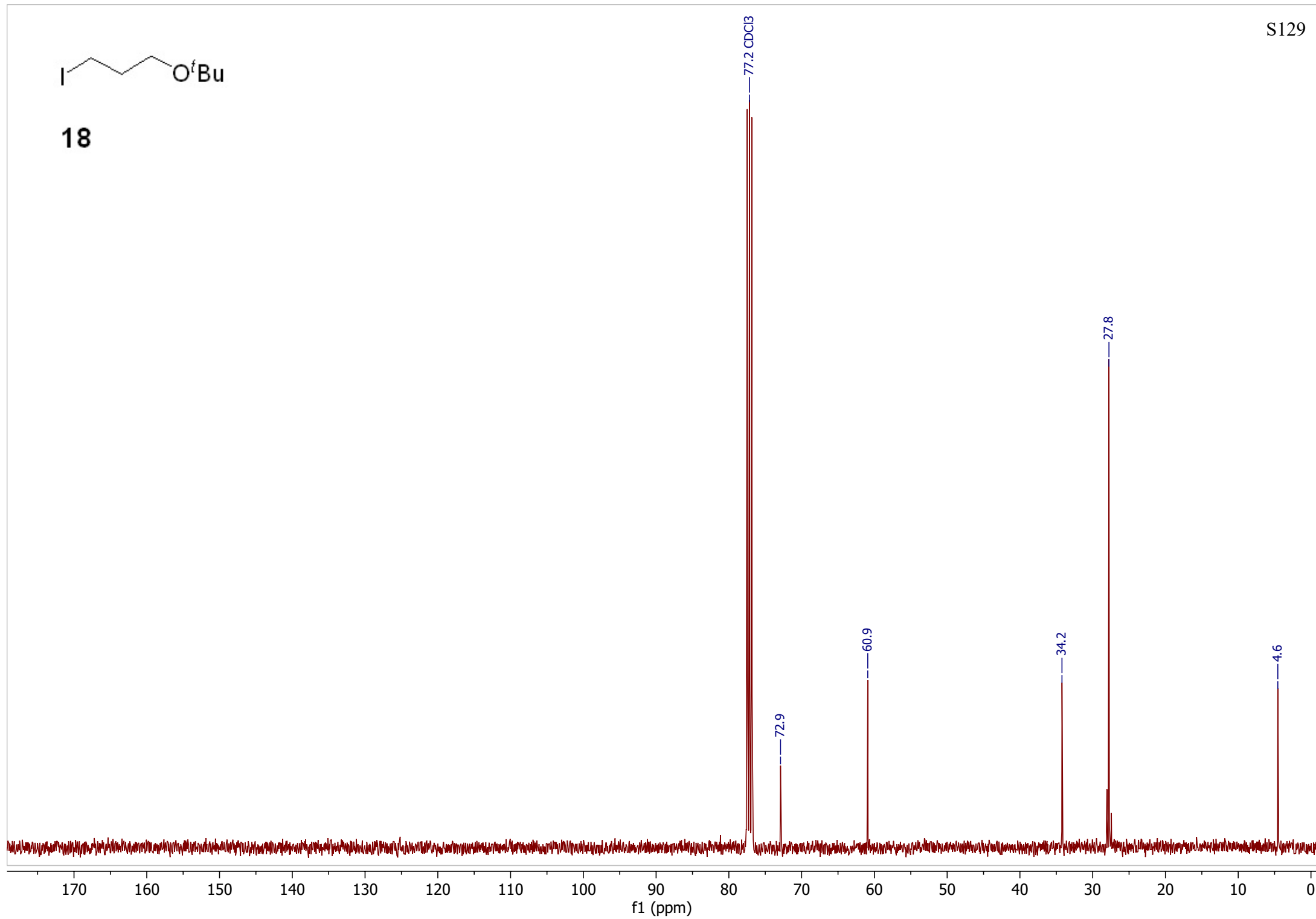


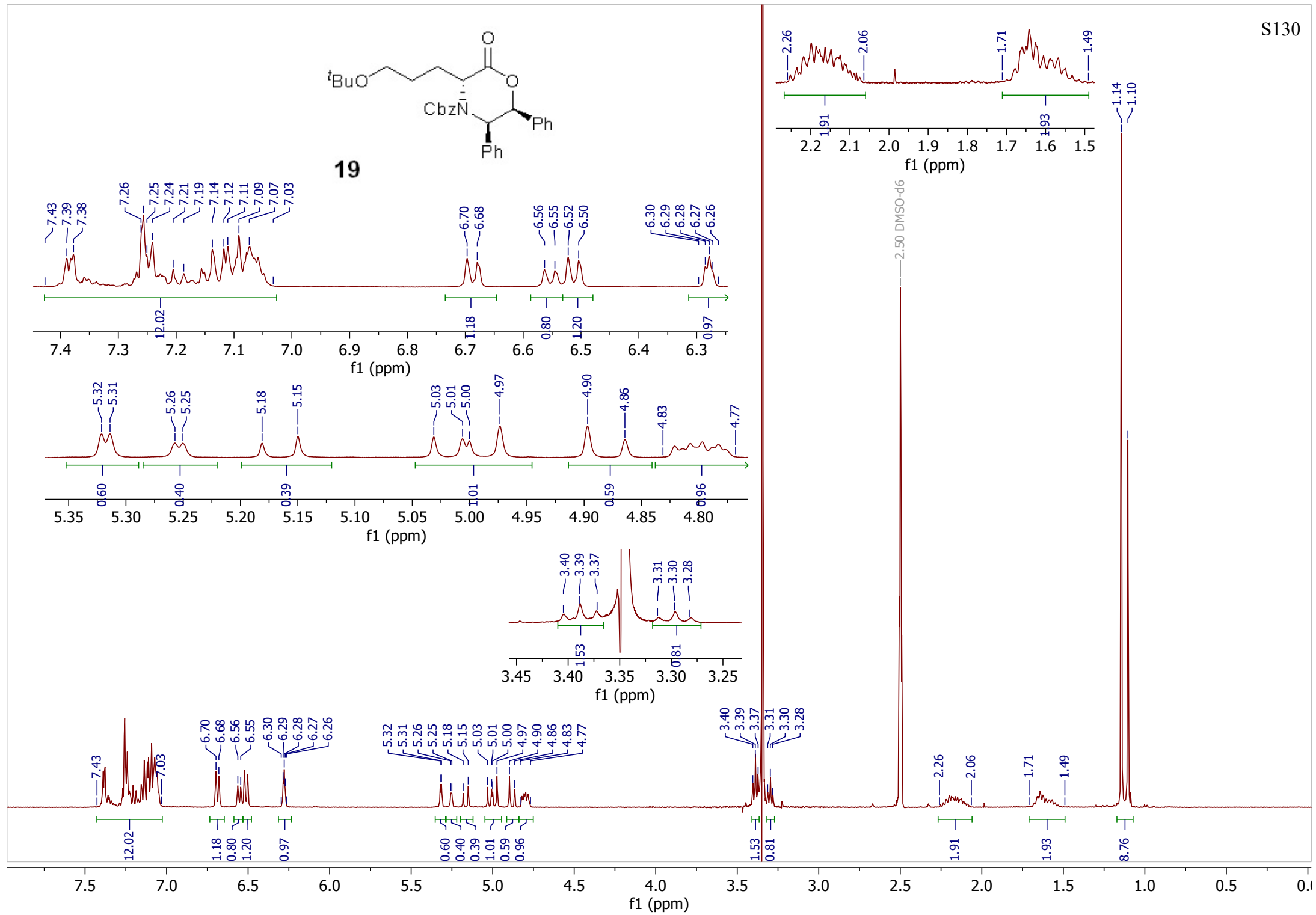
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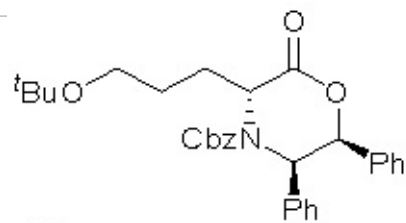
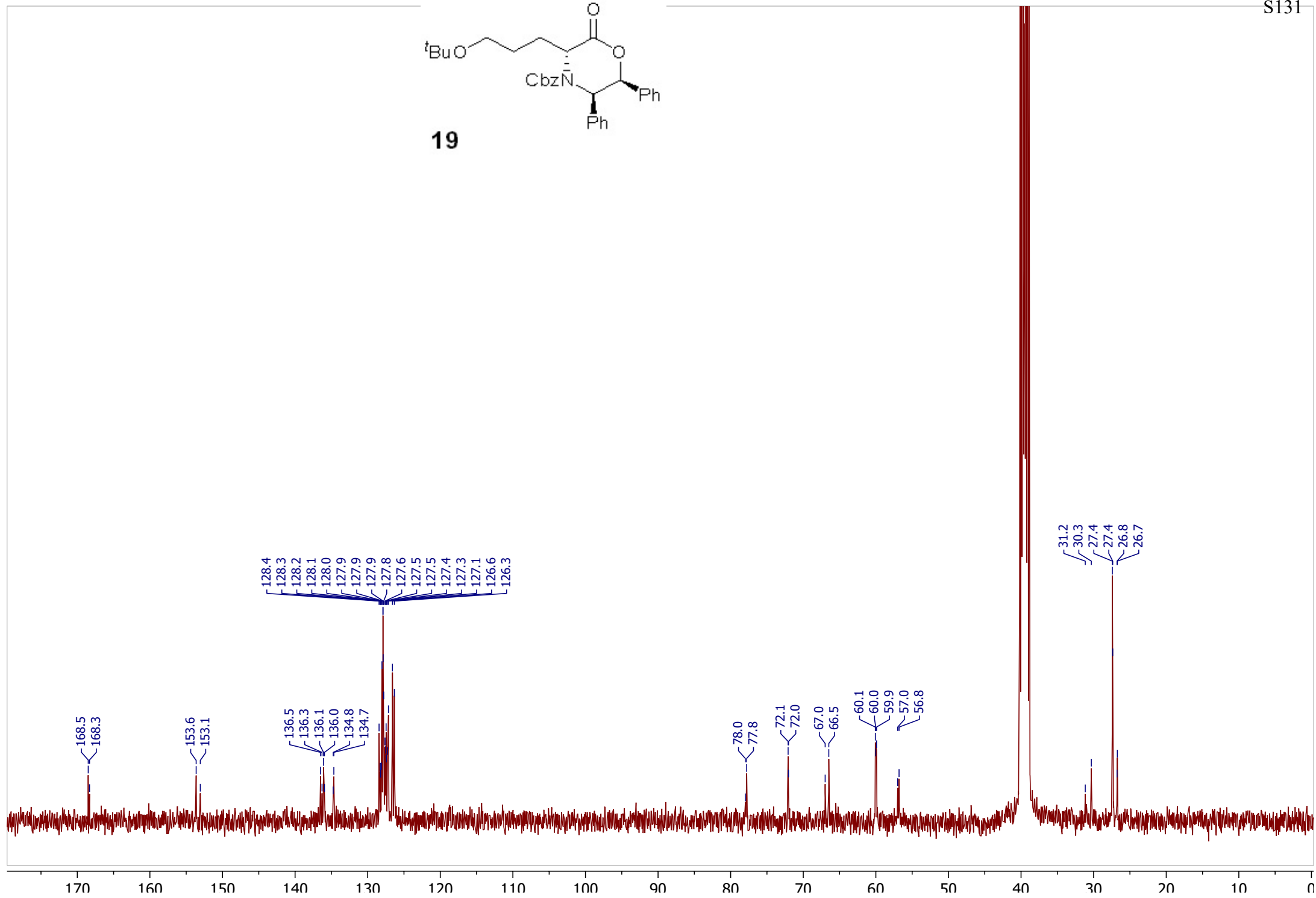


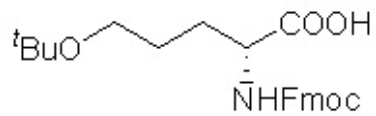


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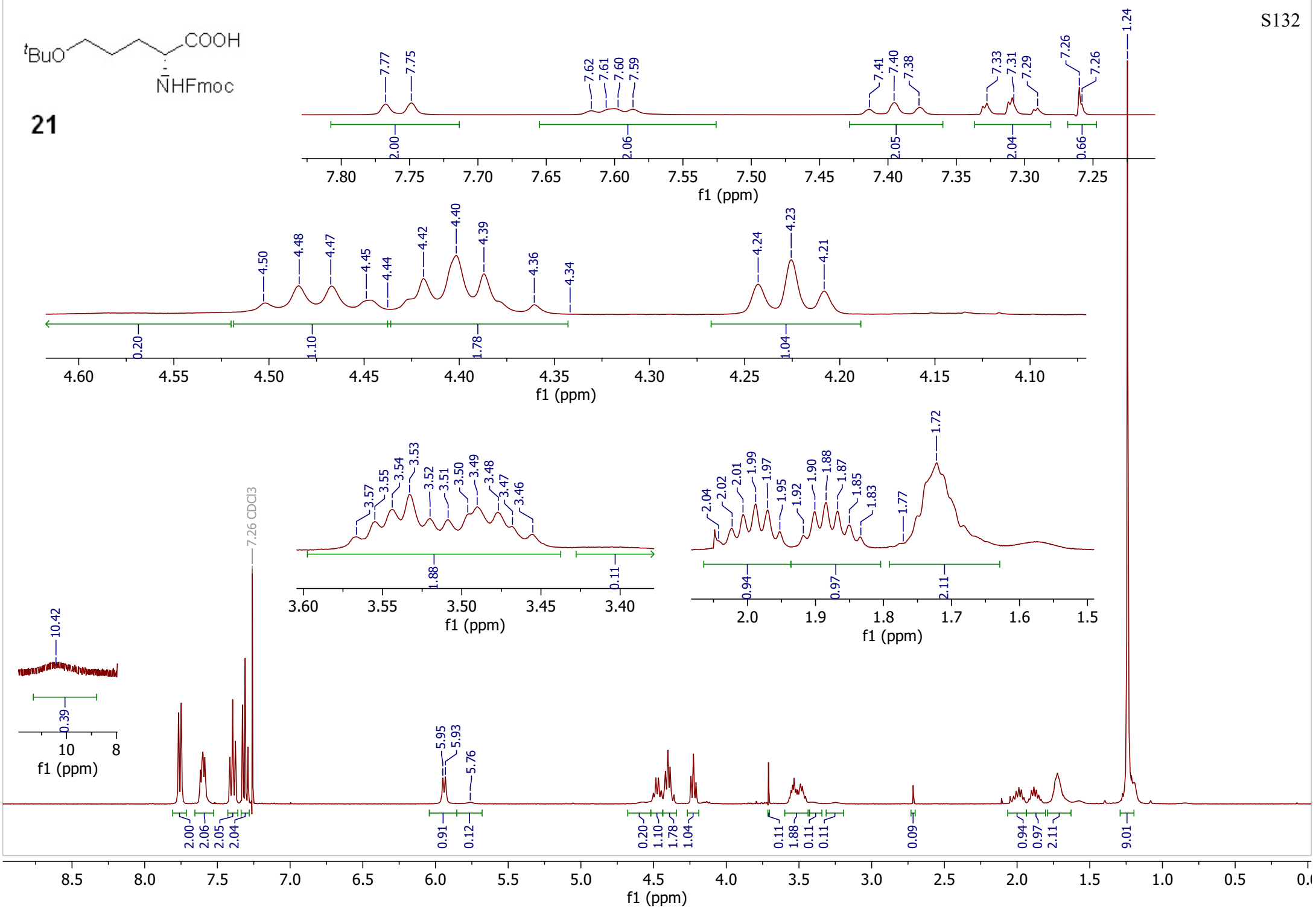


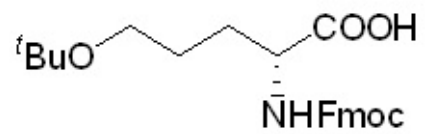


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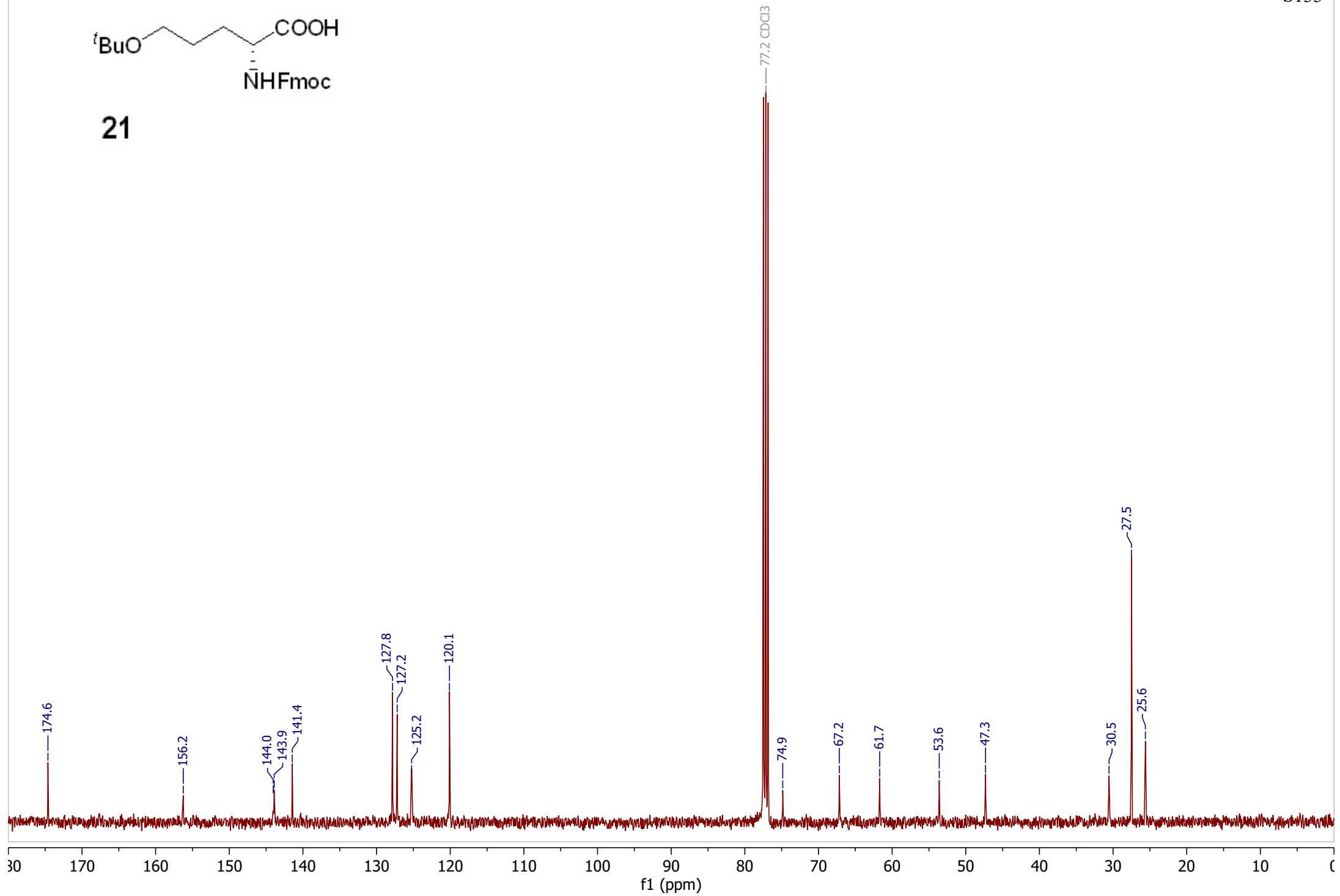


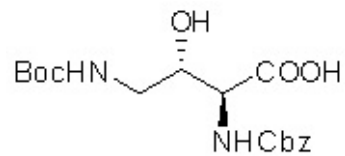
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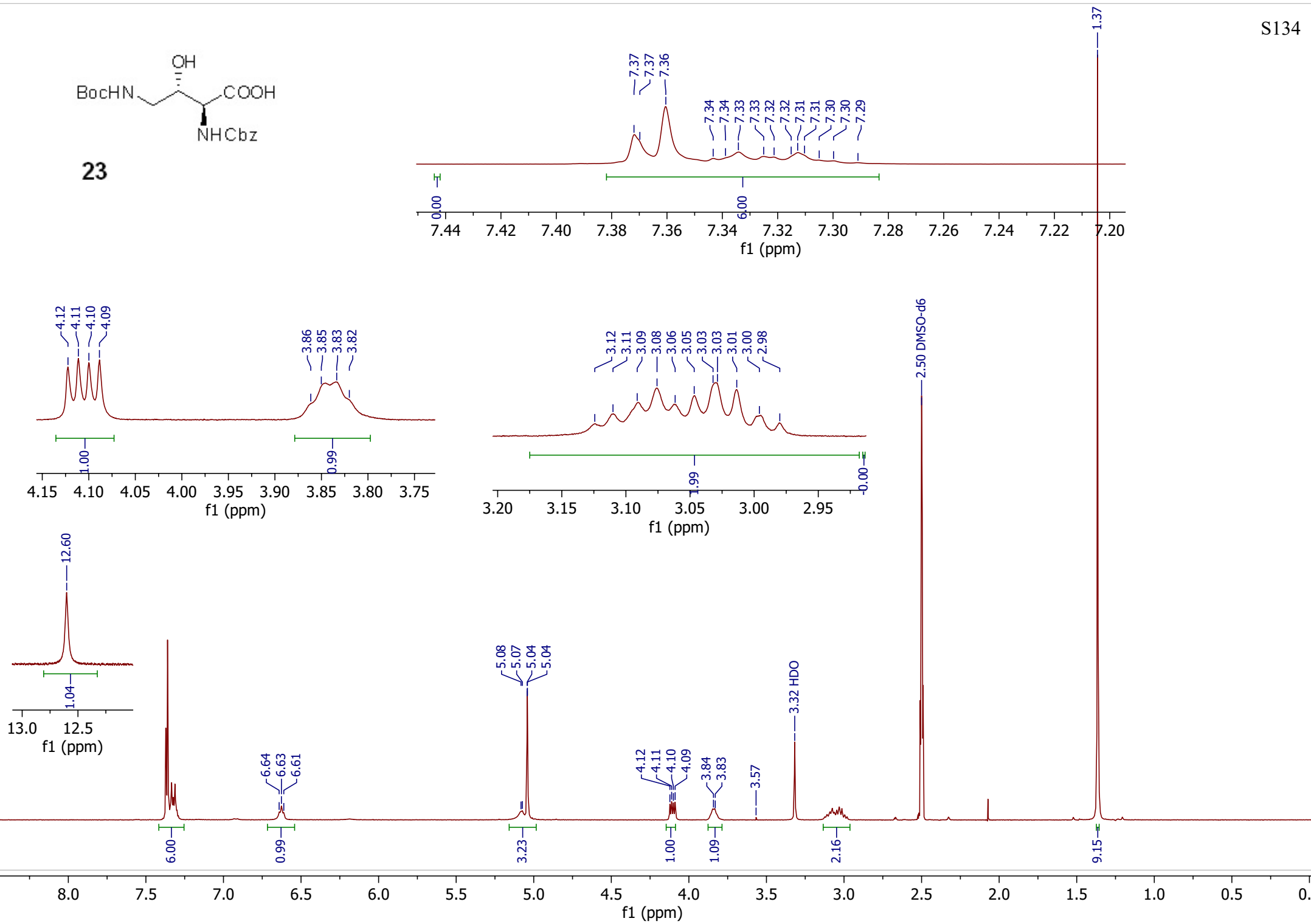


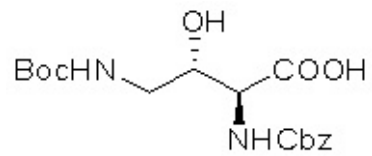
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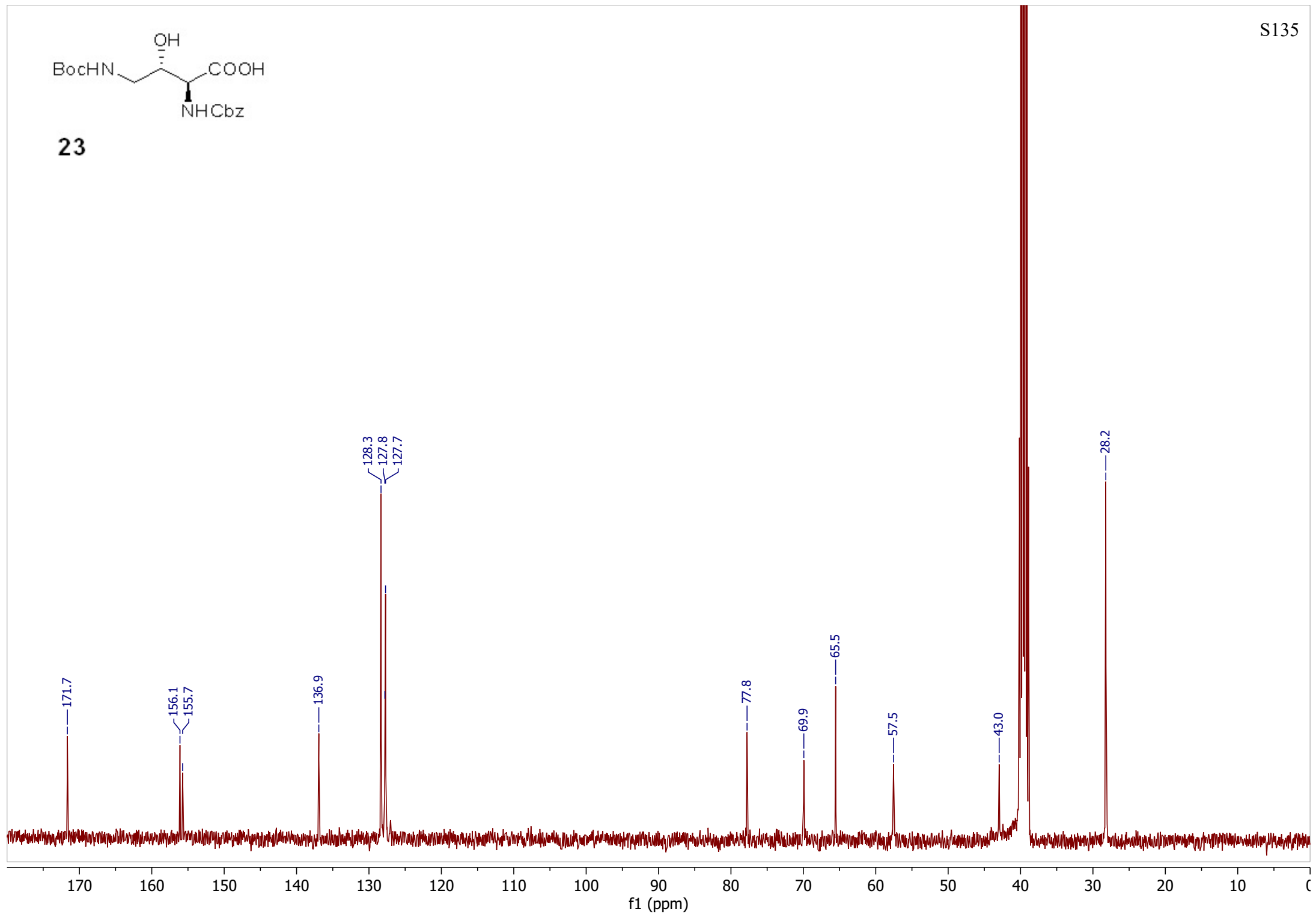


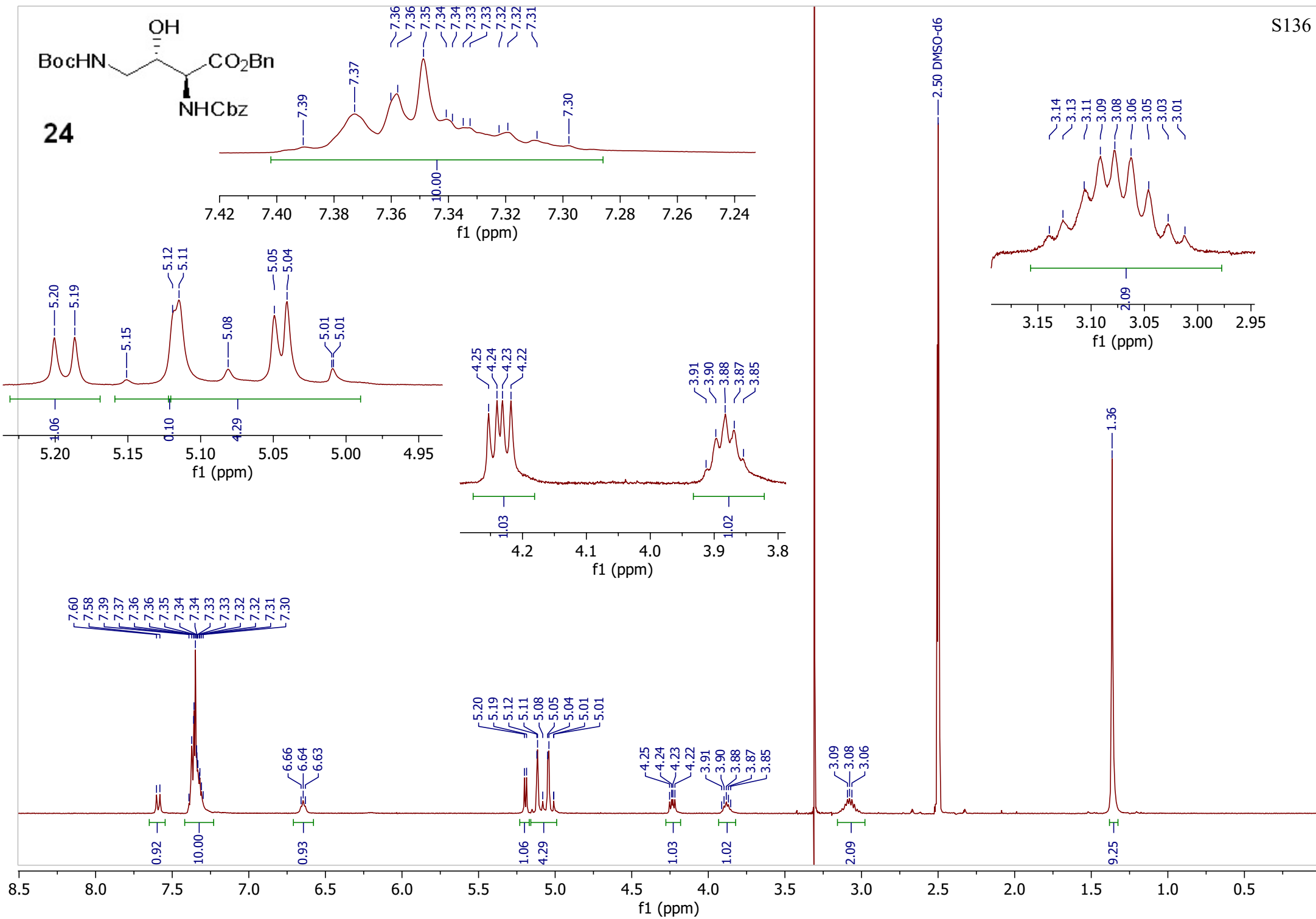
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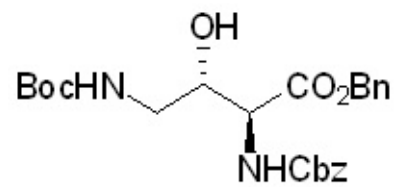




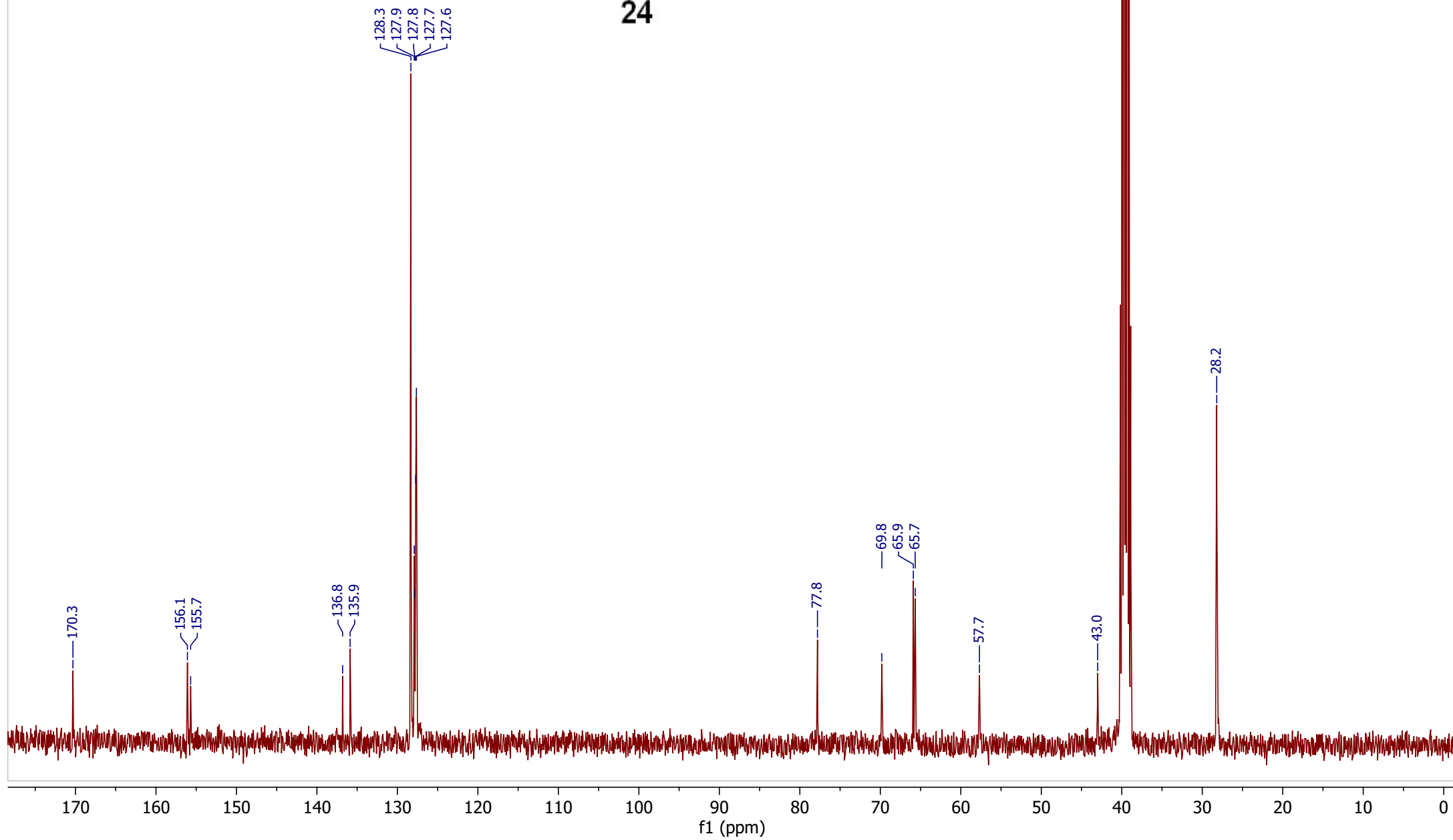
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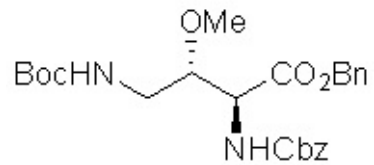




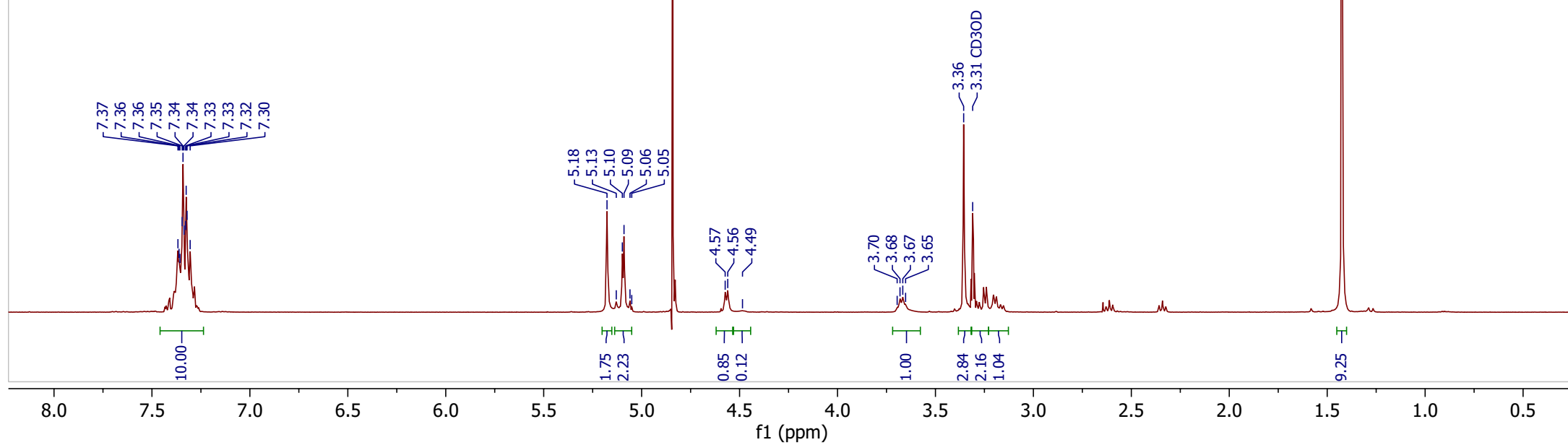
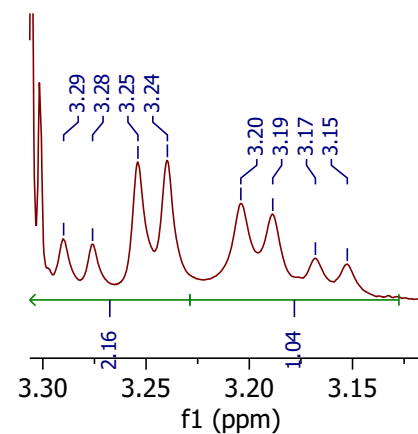
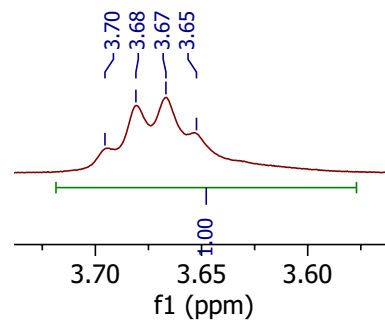
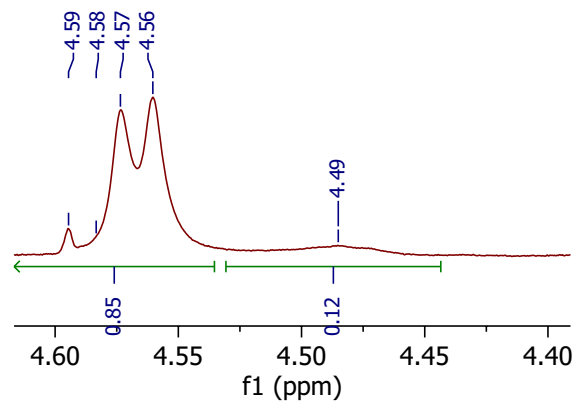
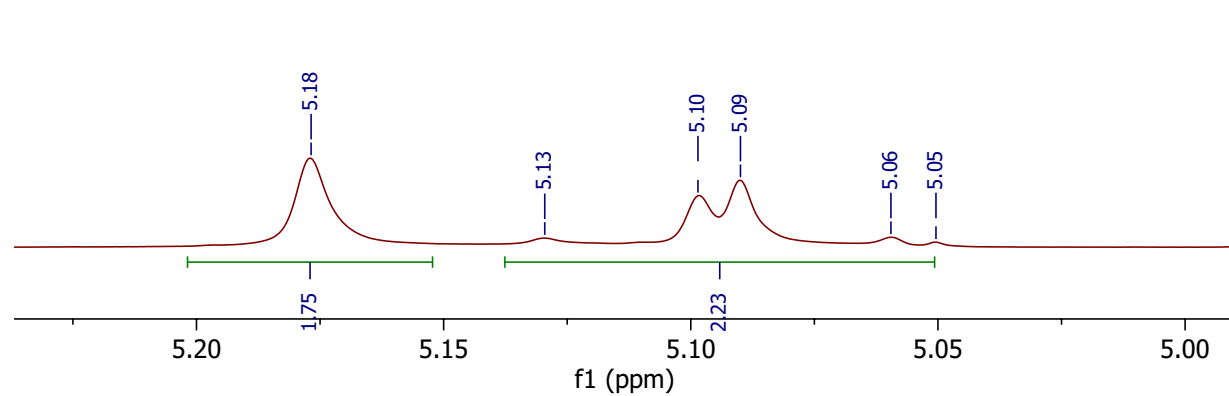


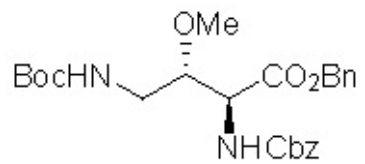
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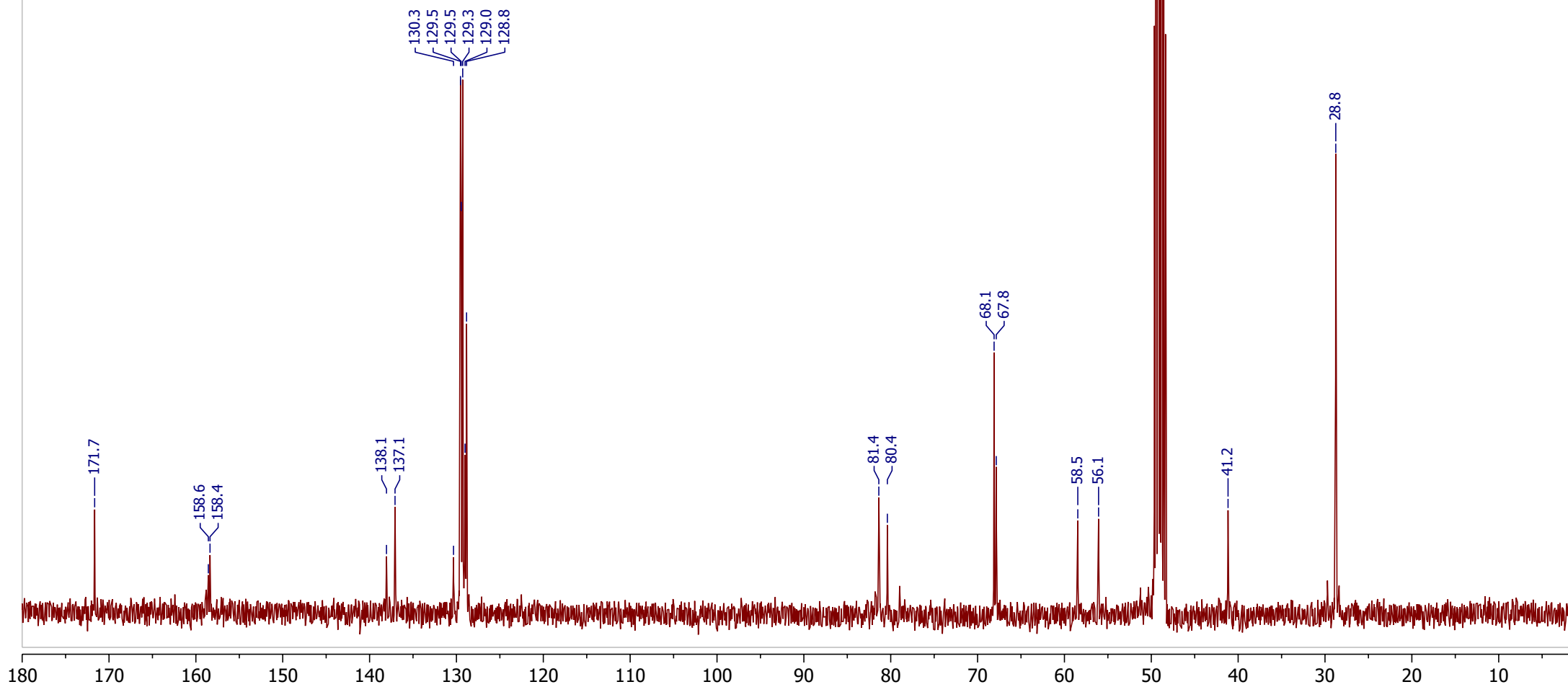


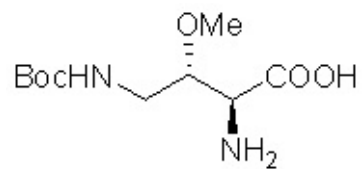
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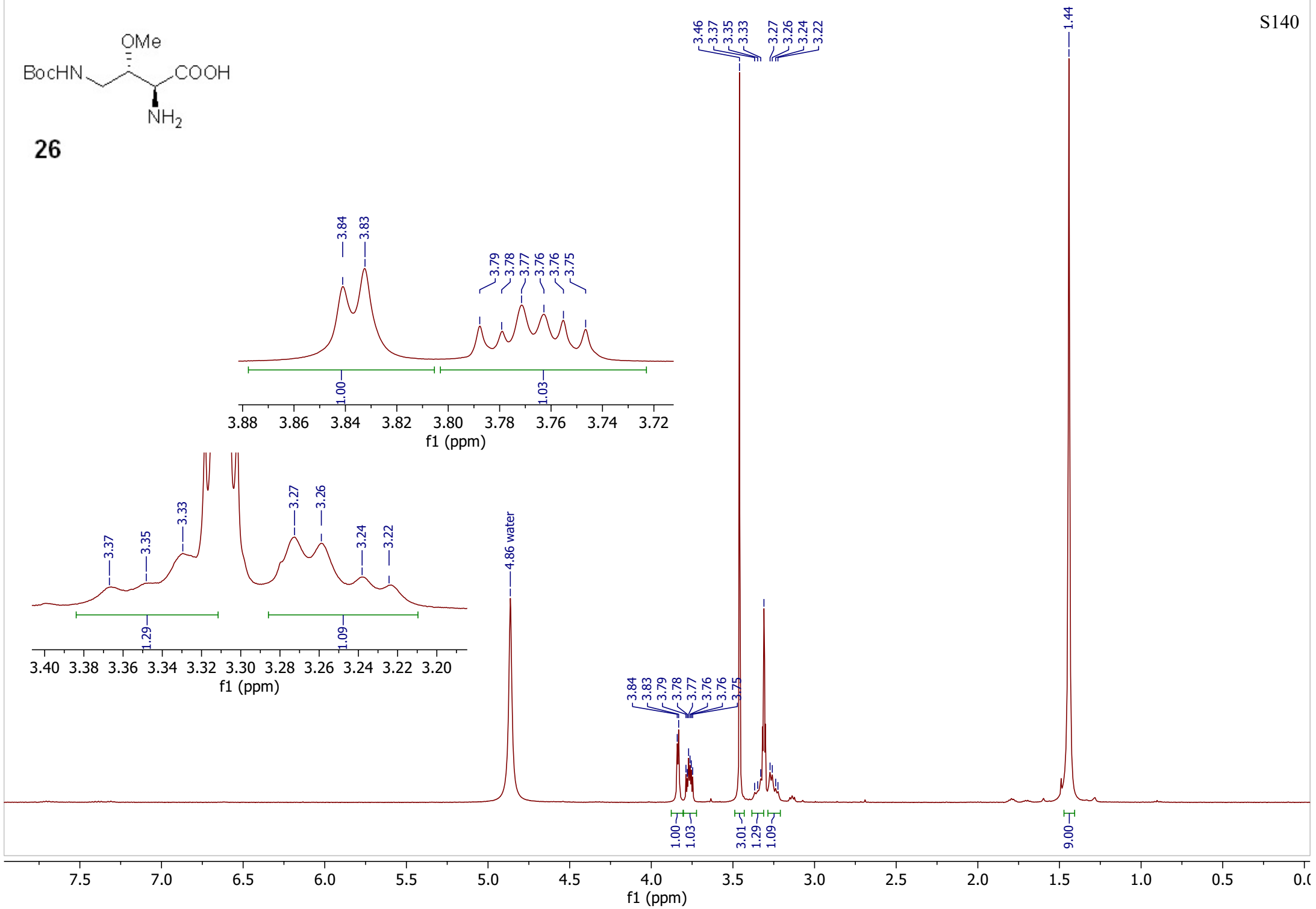
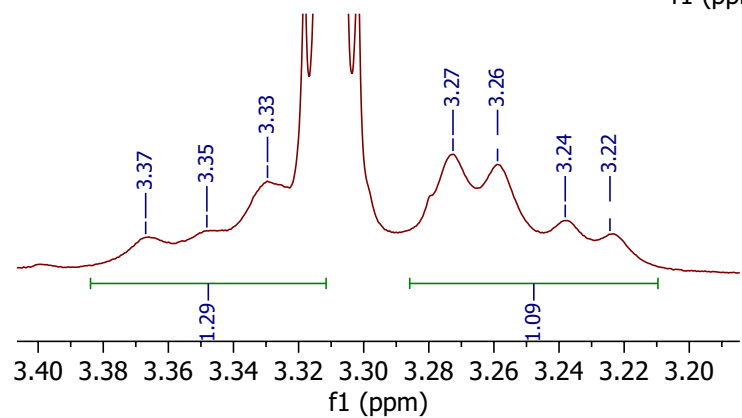
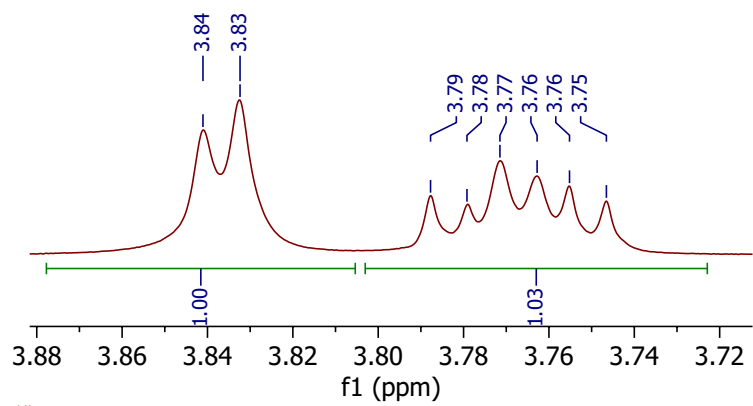


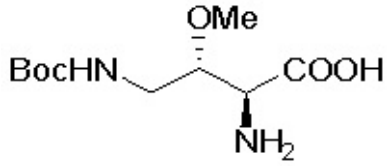
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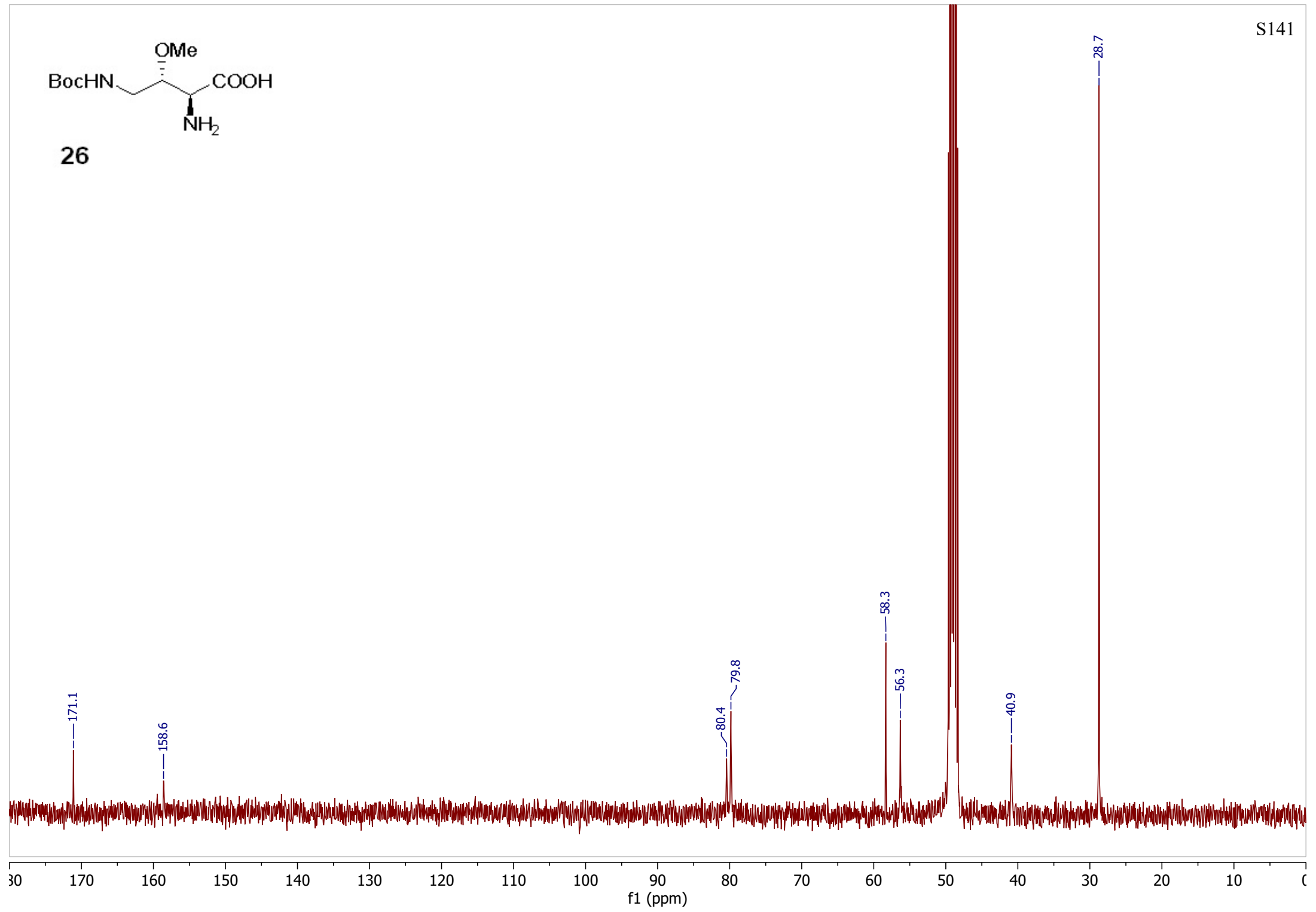


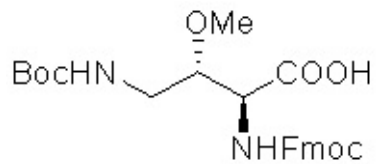
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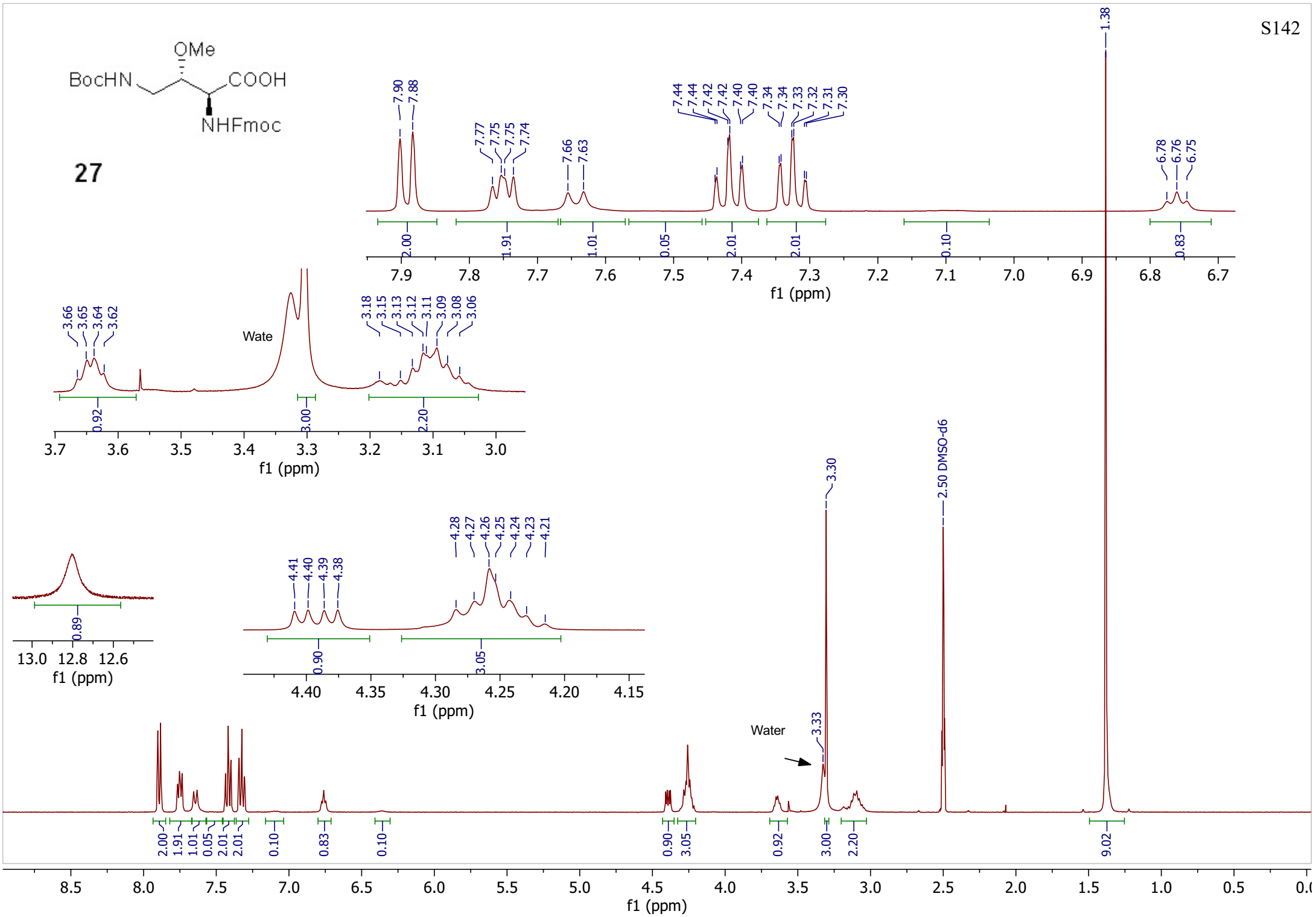


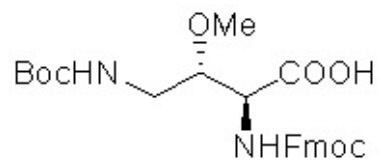
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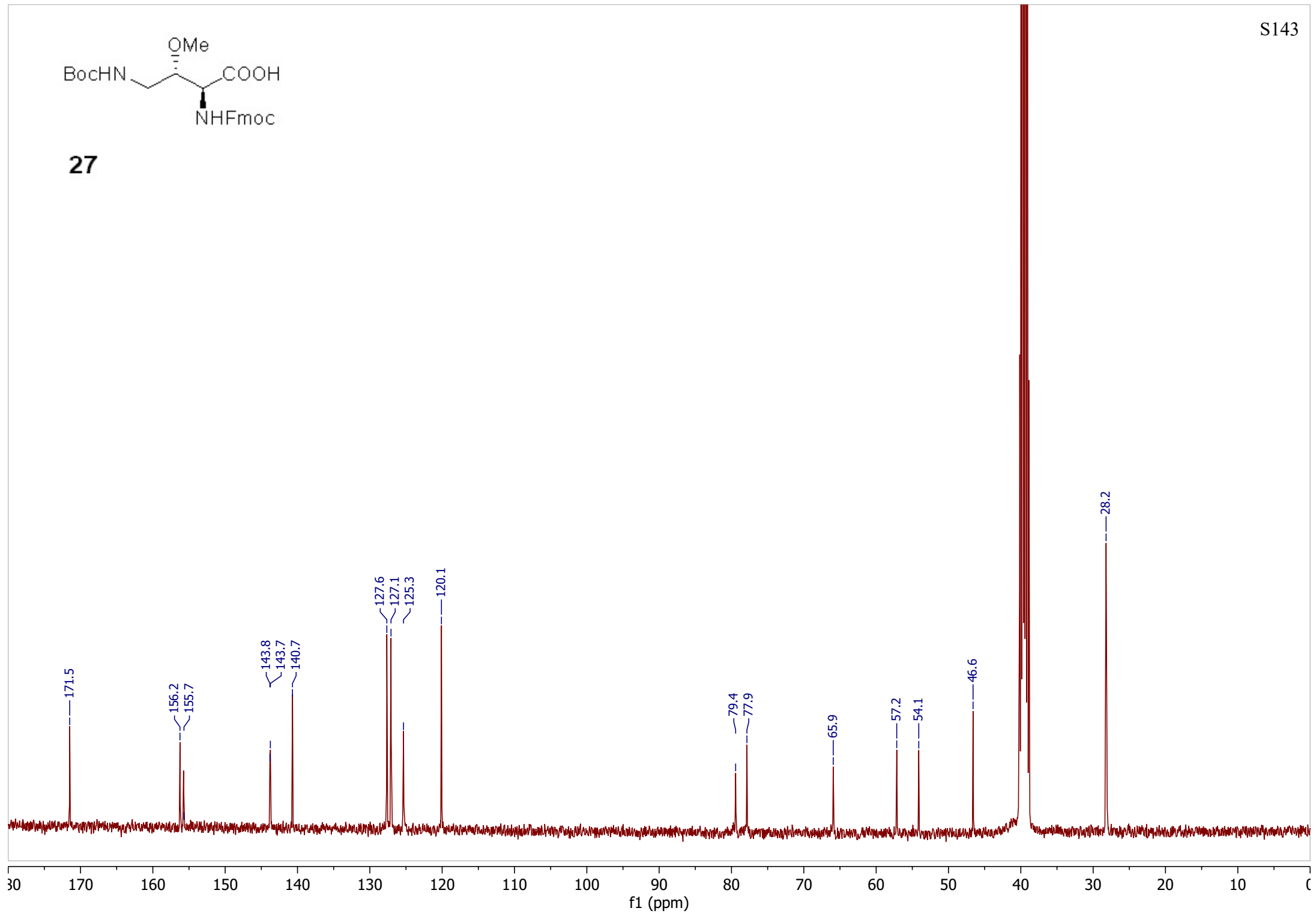


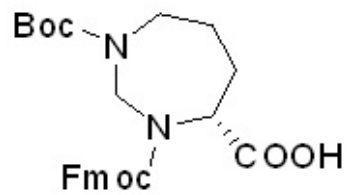
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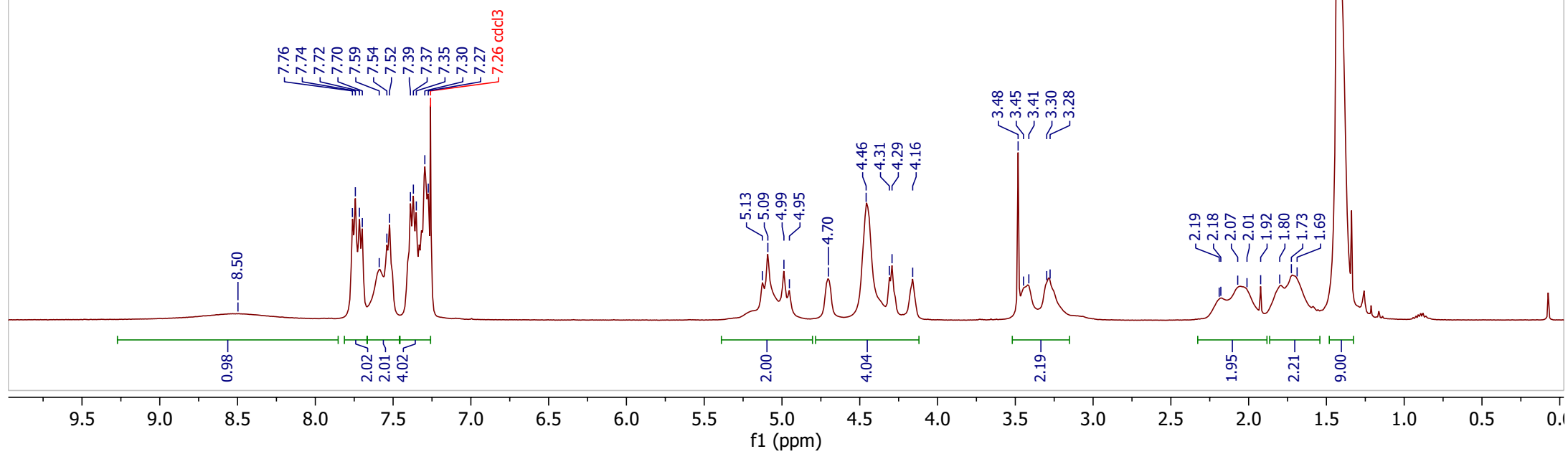


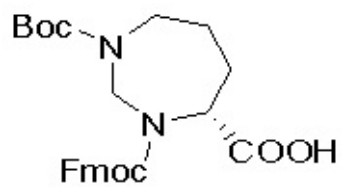
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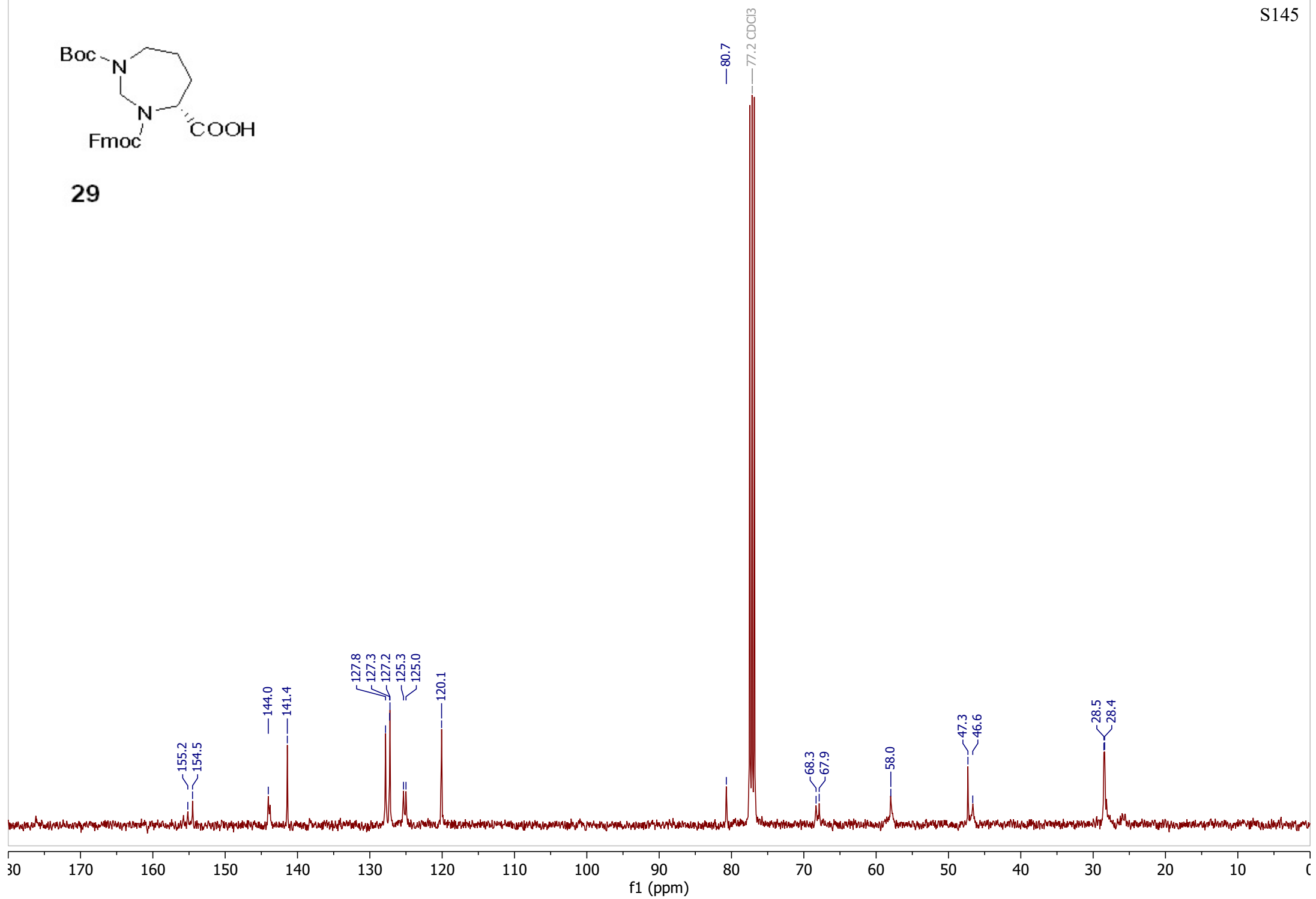


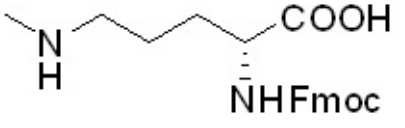
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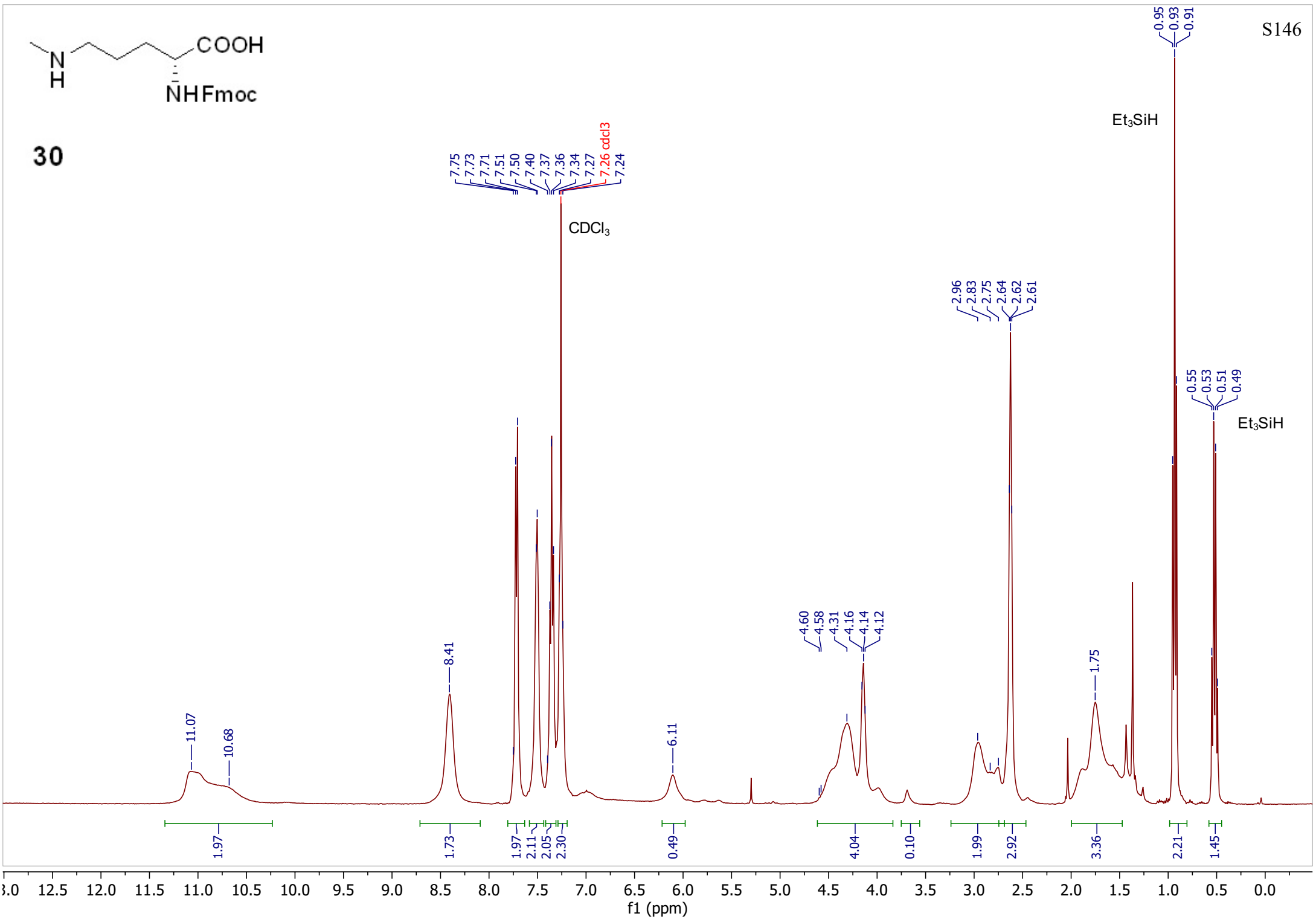


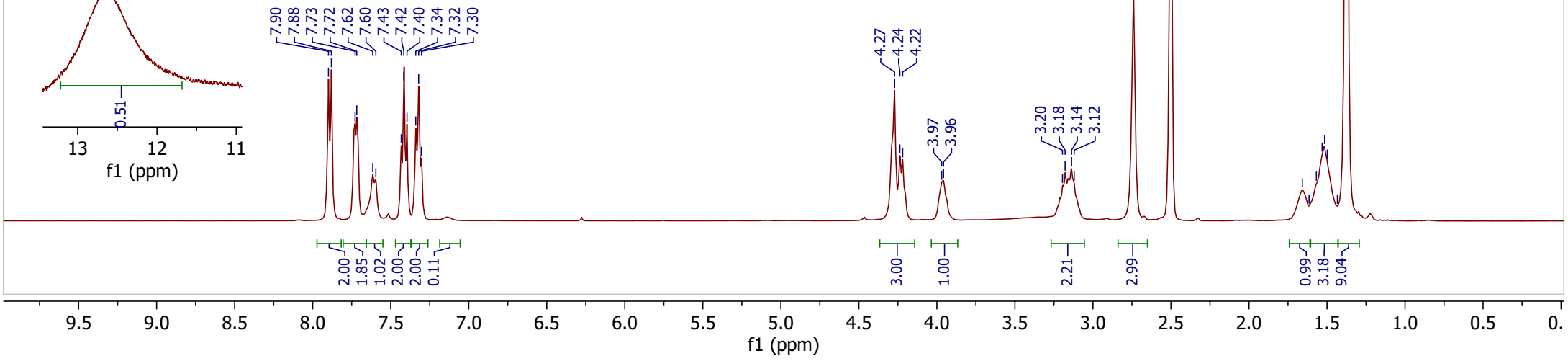
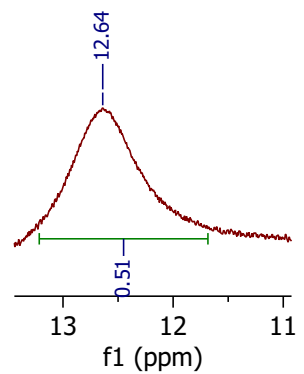
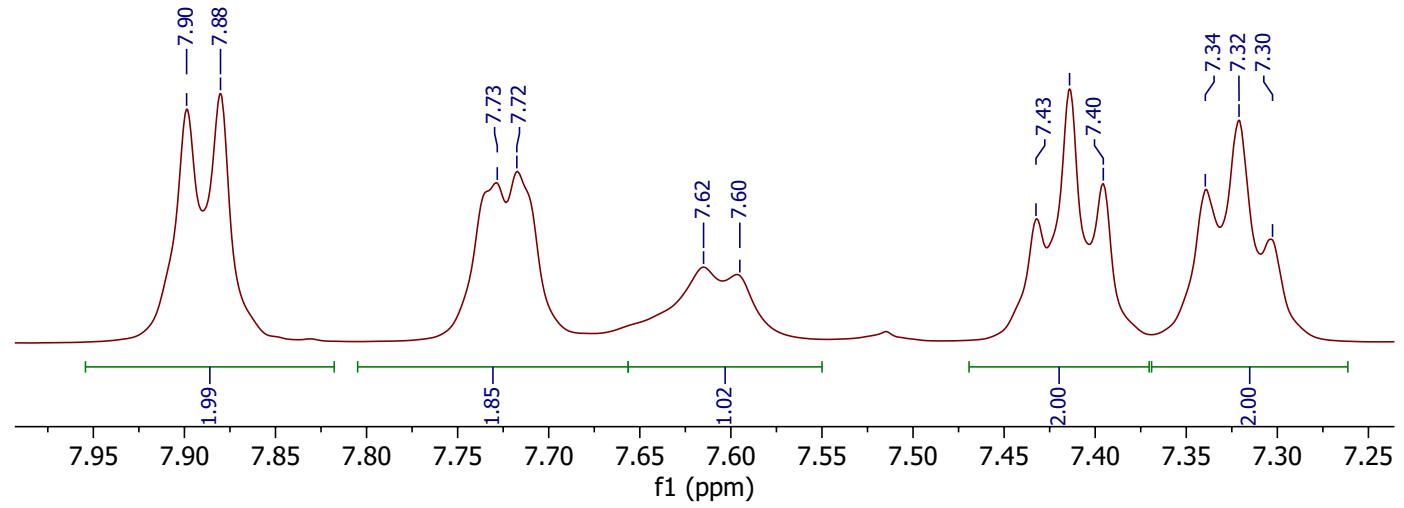
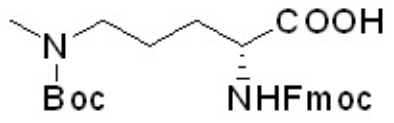
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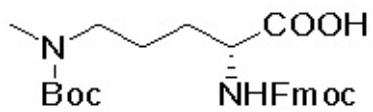
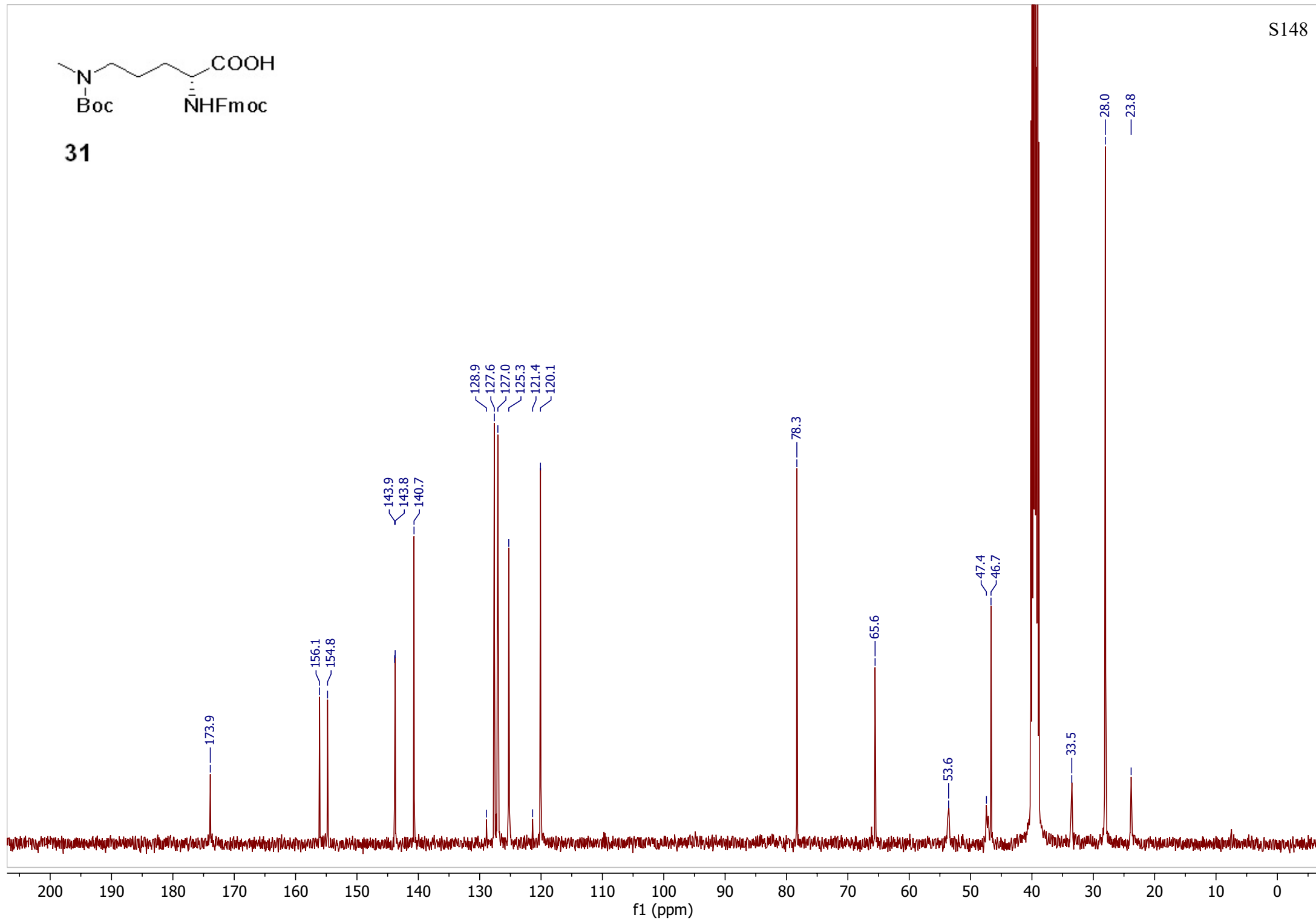


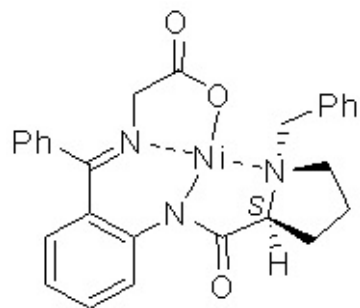
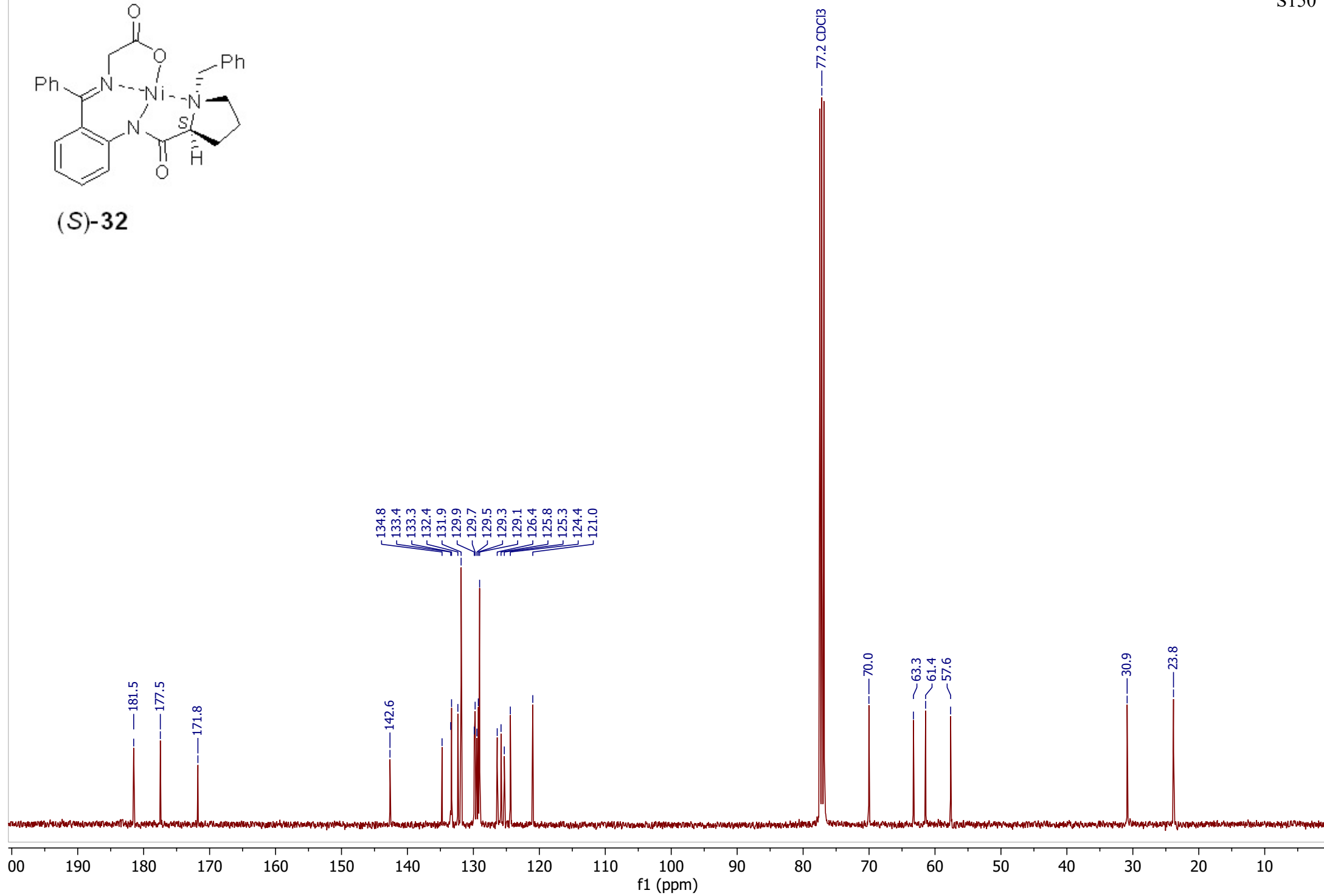


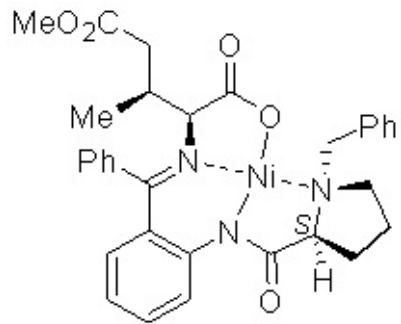
30



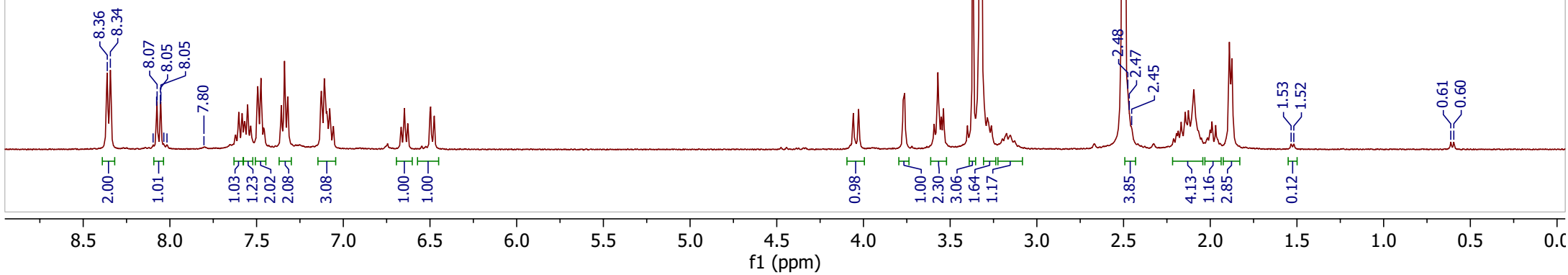
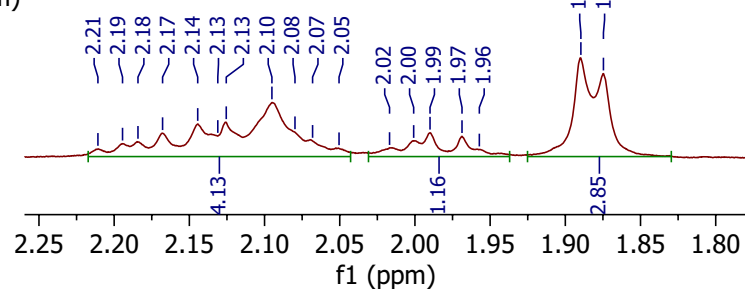
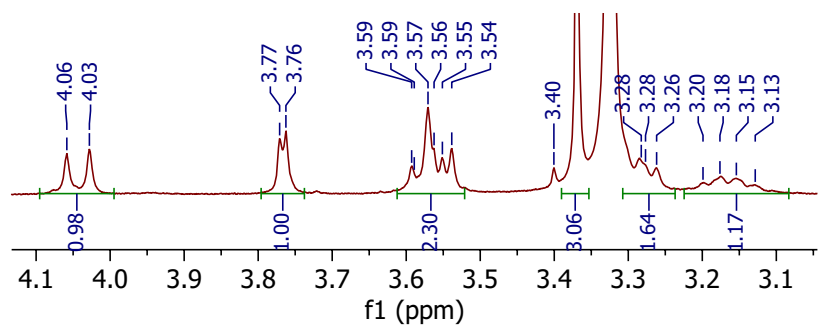
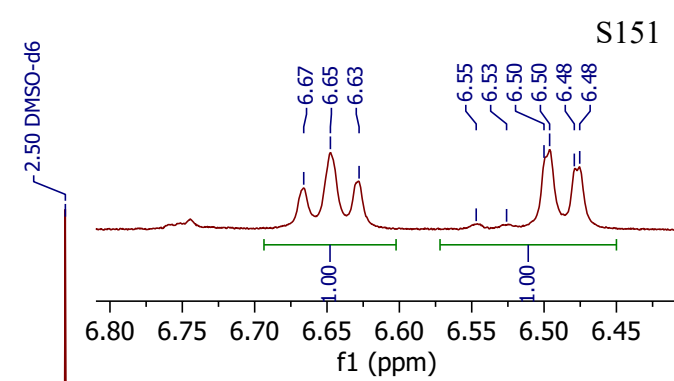
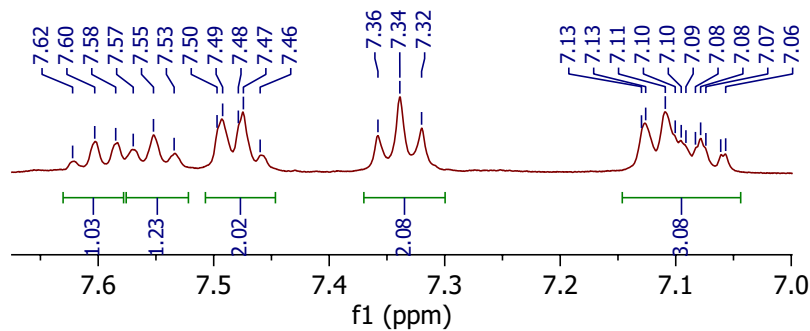


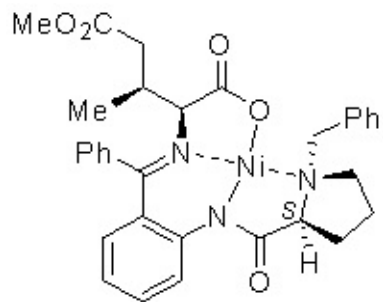
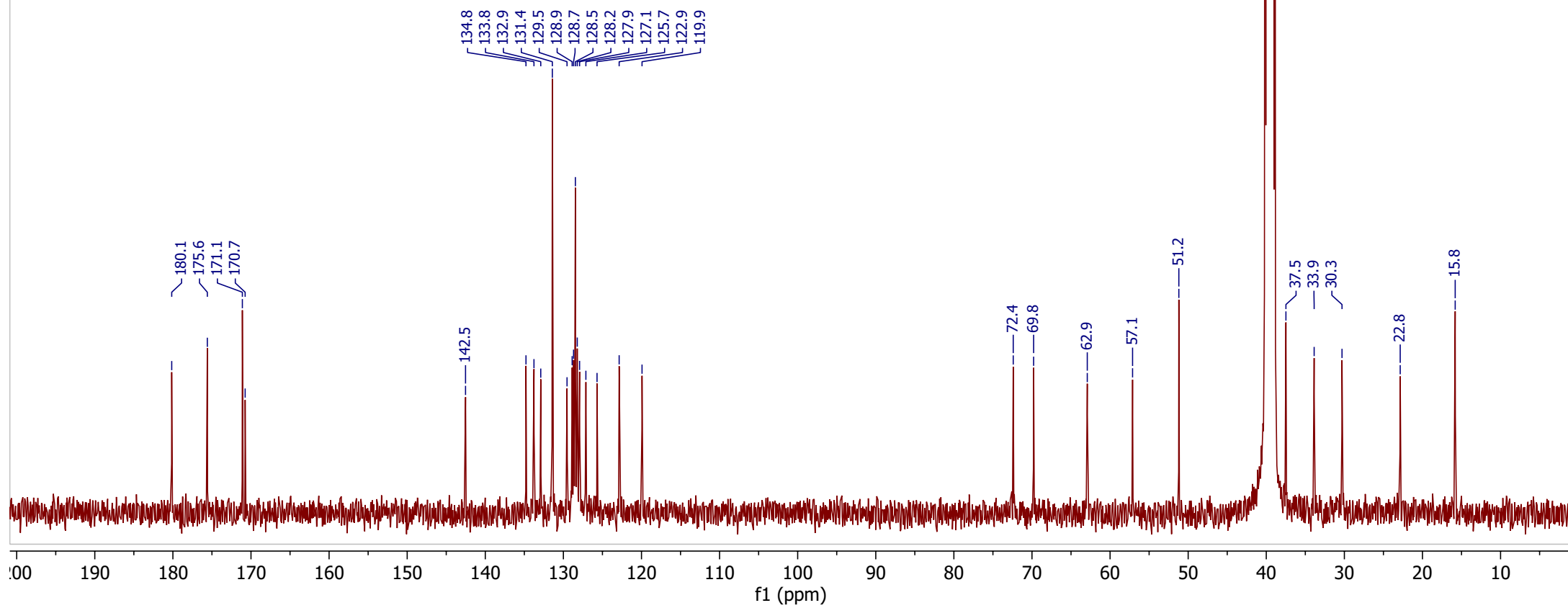
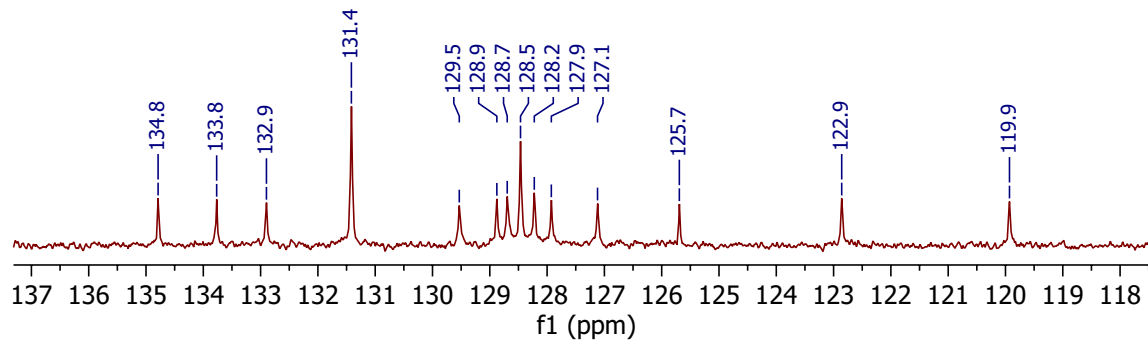
**31**

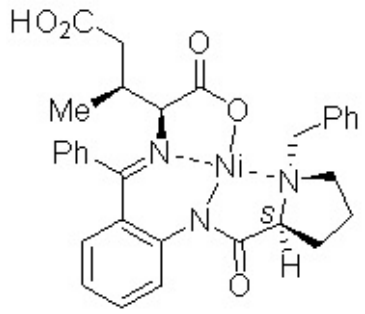
**(S)-32**



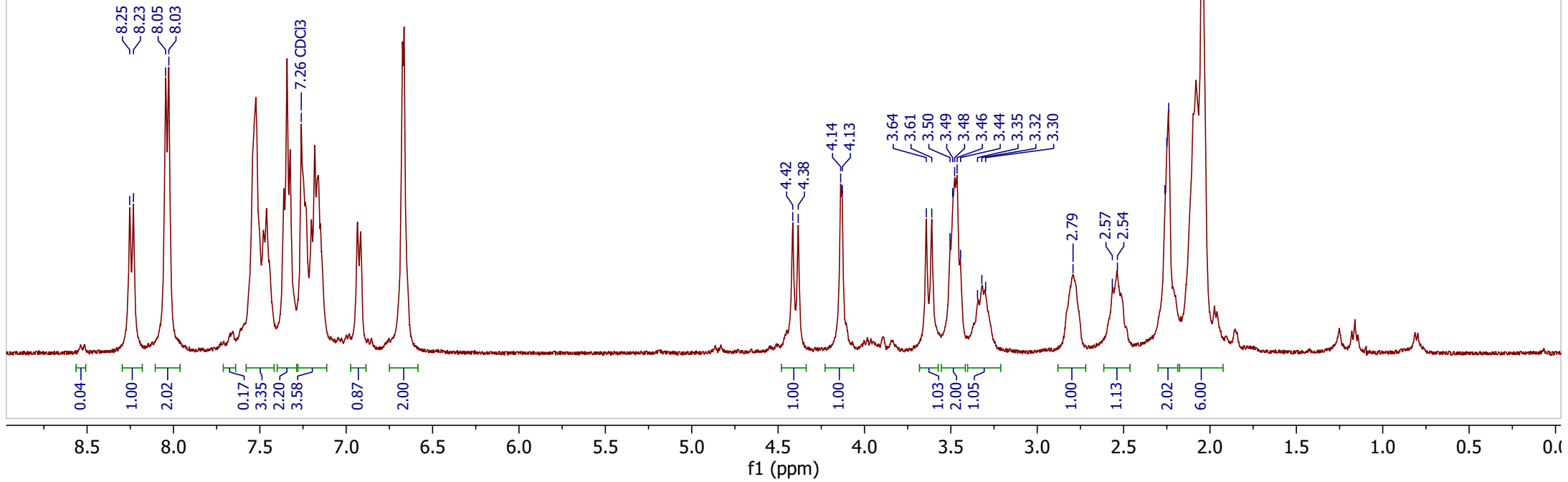
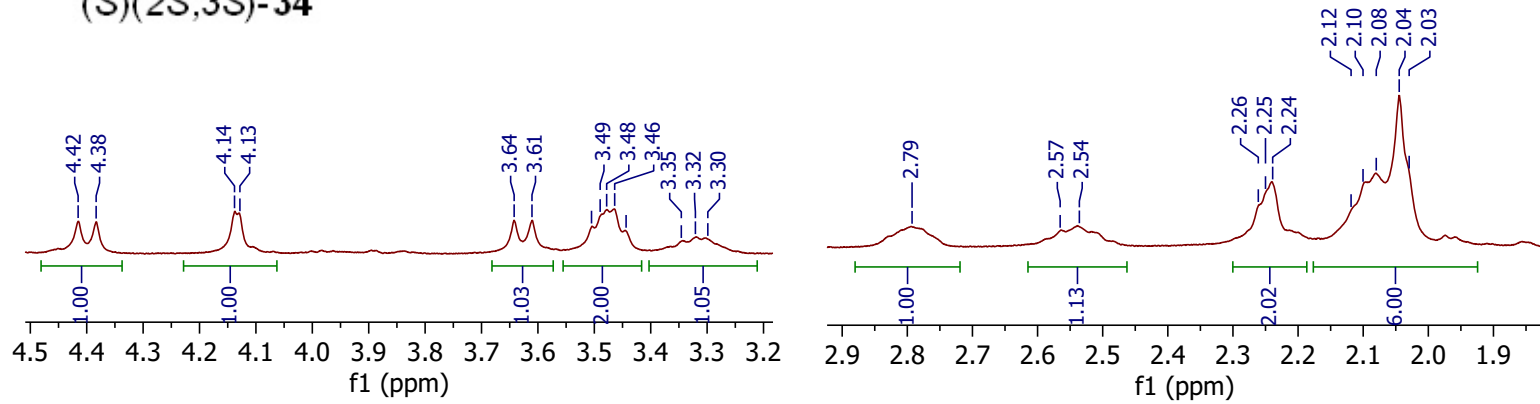
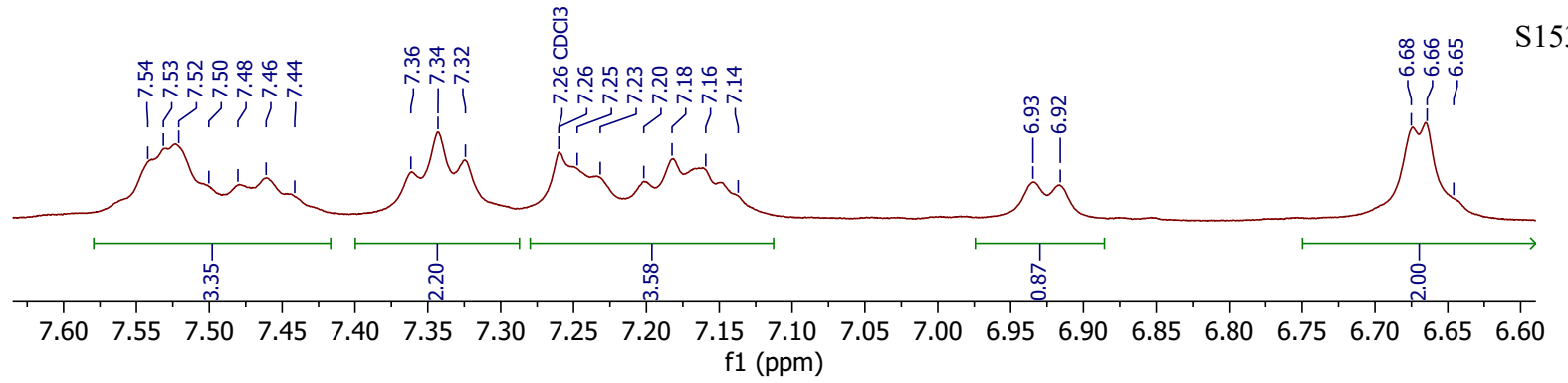
(S)(2S,3S)-33

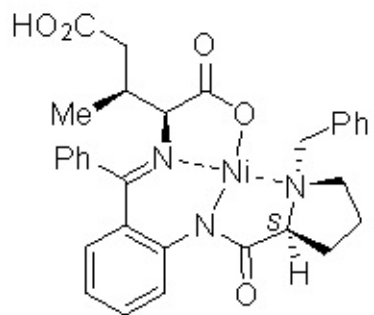
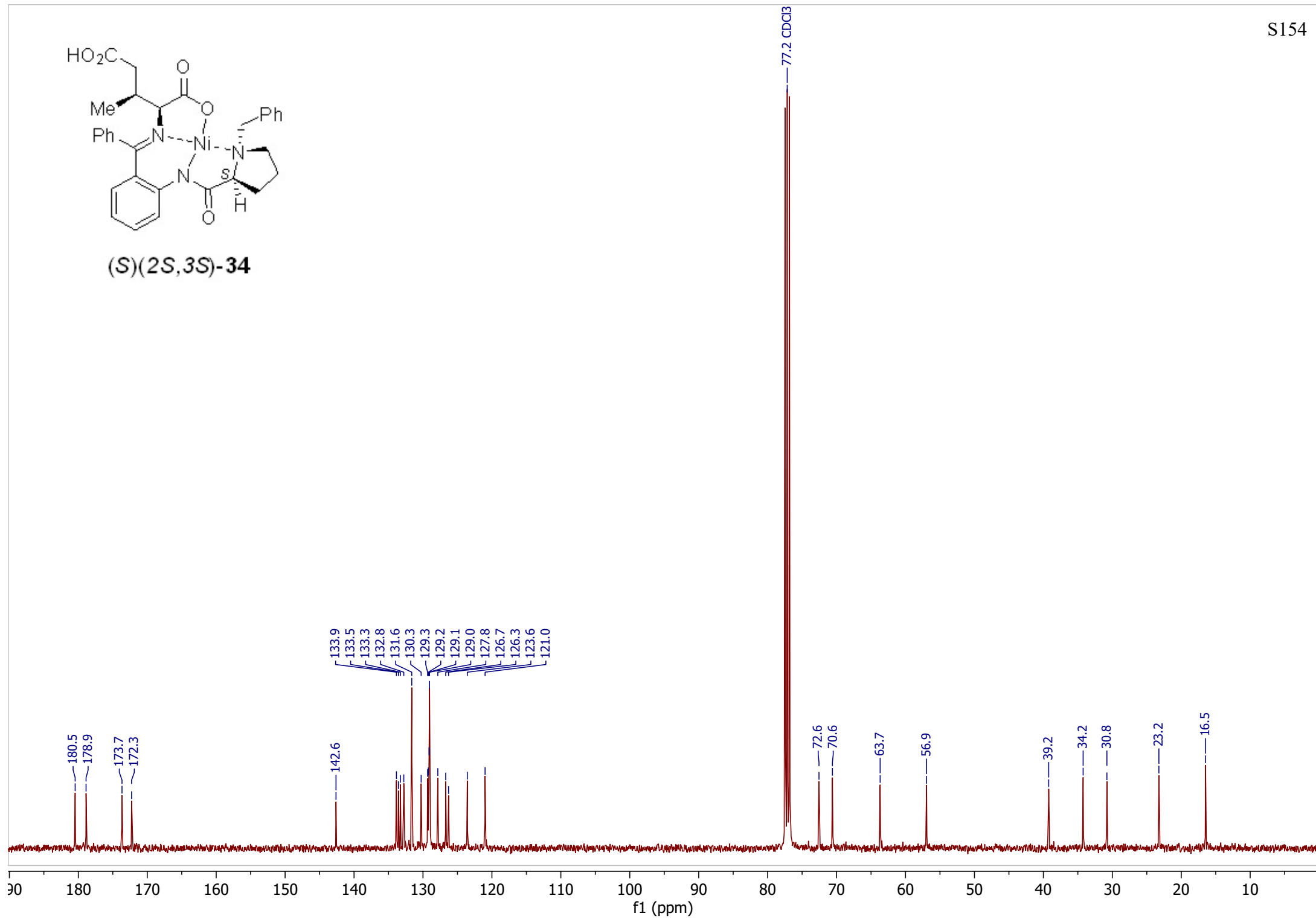


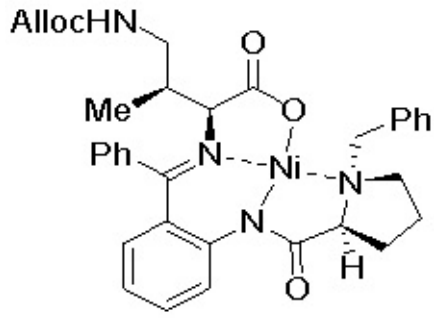
**(S)(2S,3S)-33**



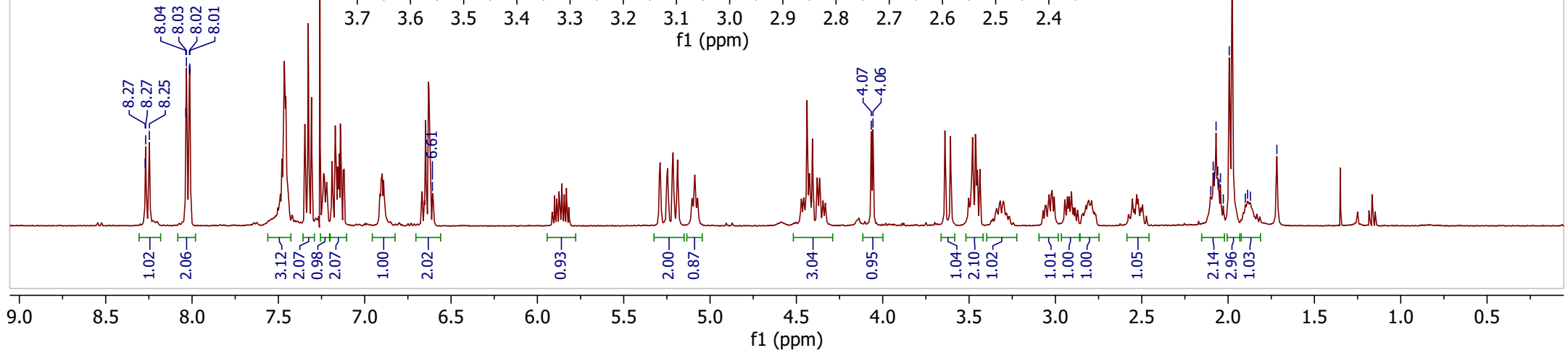
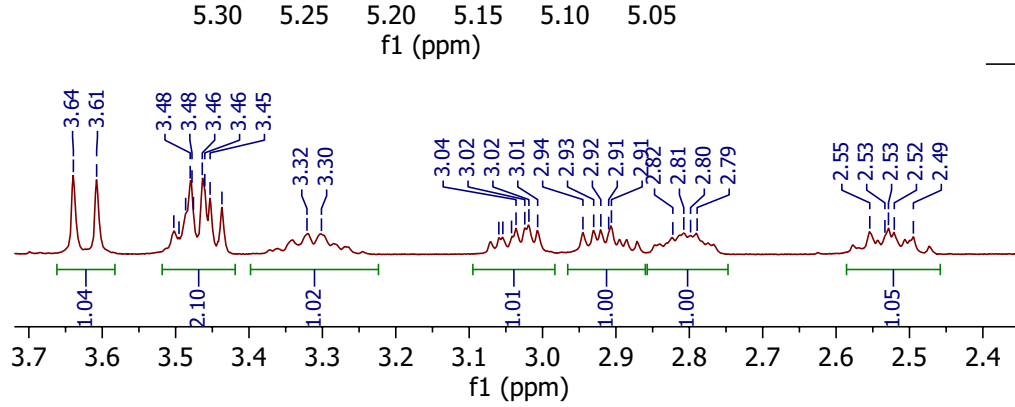
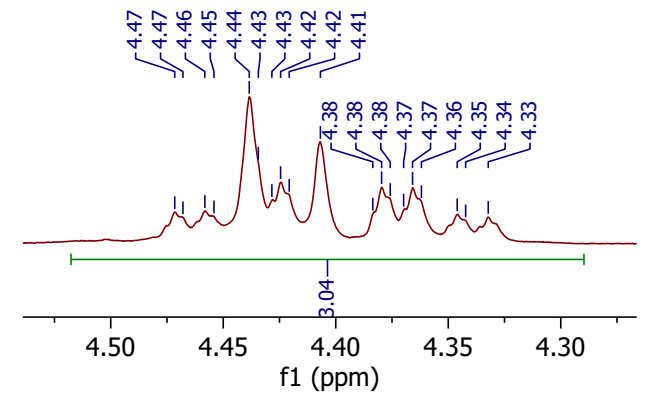
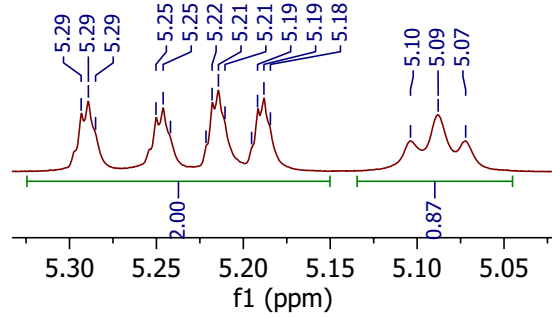
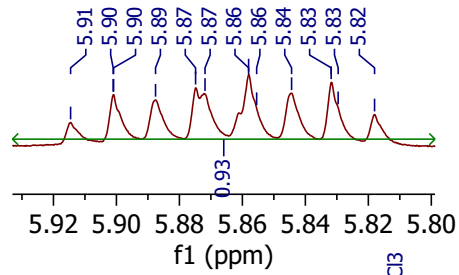
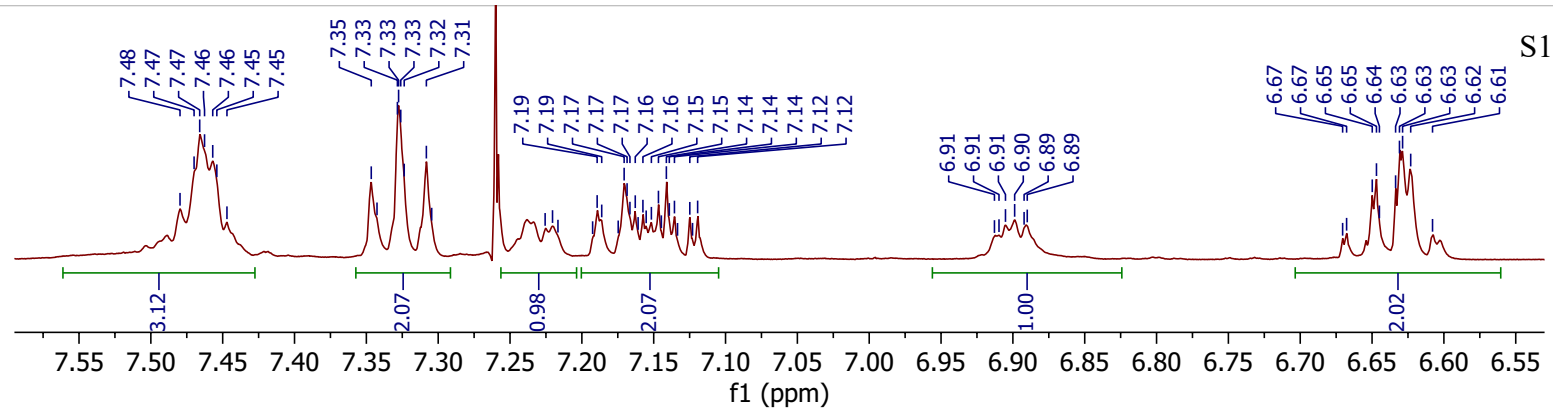
(S)(2S,3S)-34

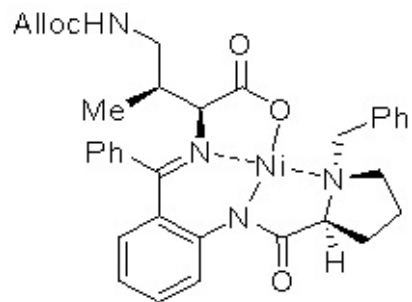
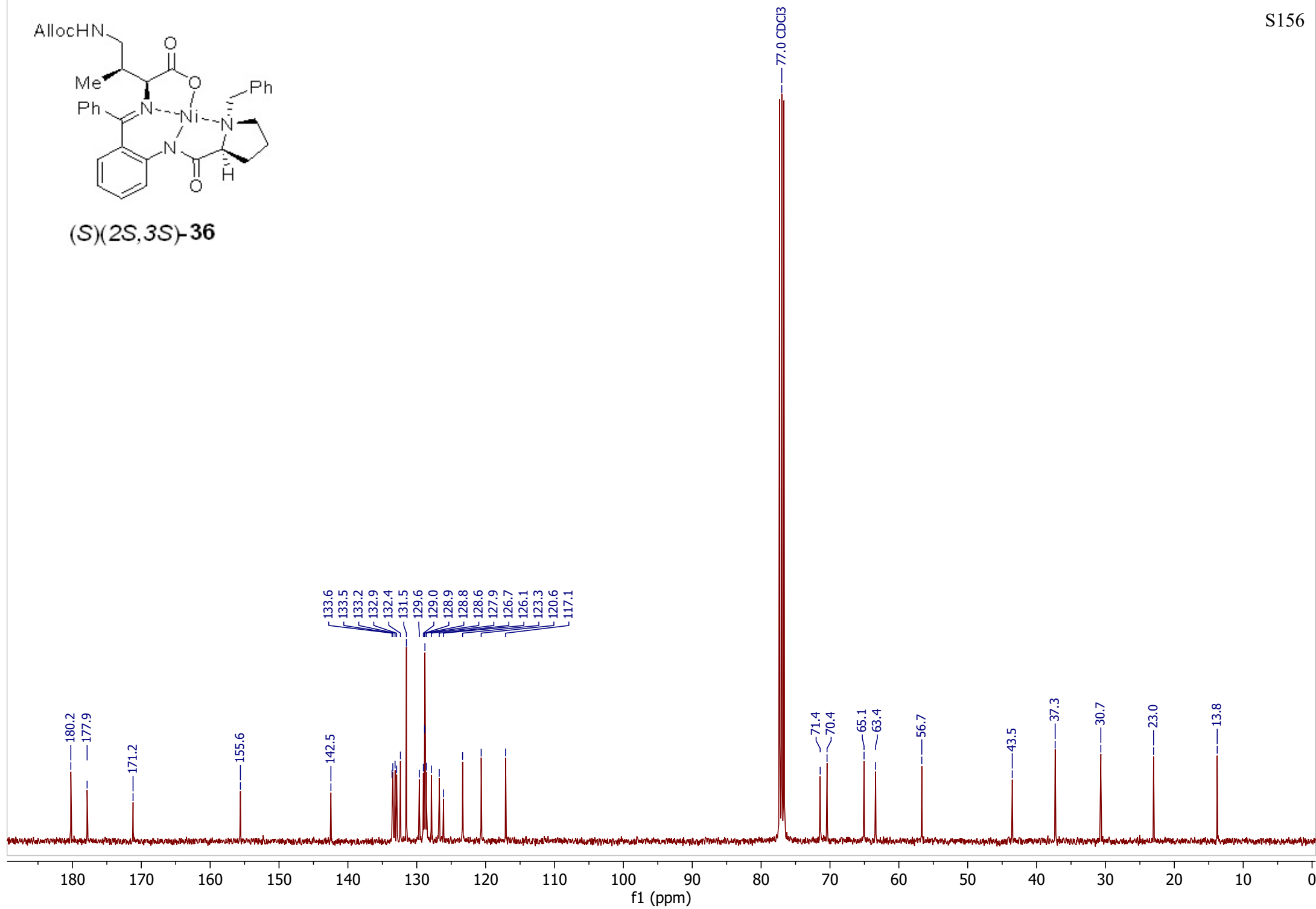


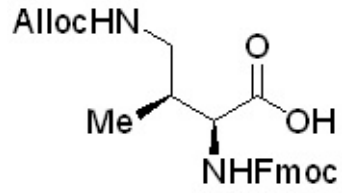
**(S)(2S,3S)-34**



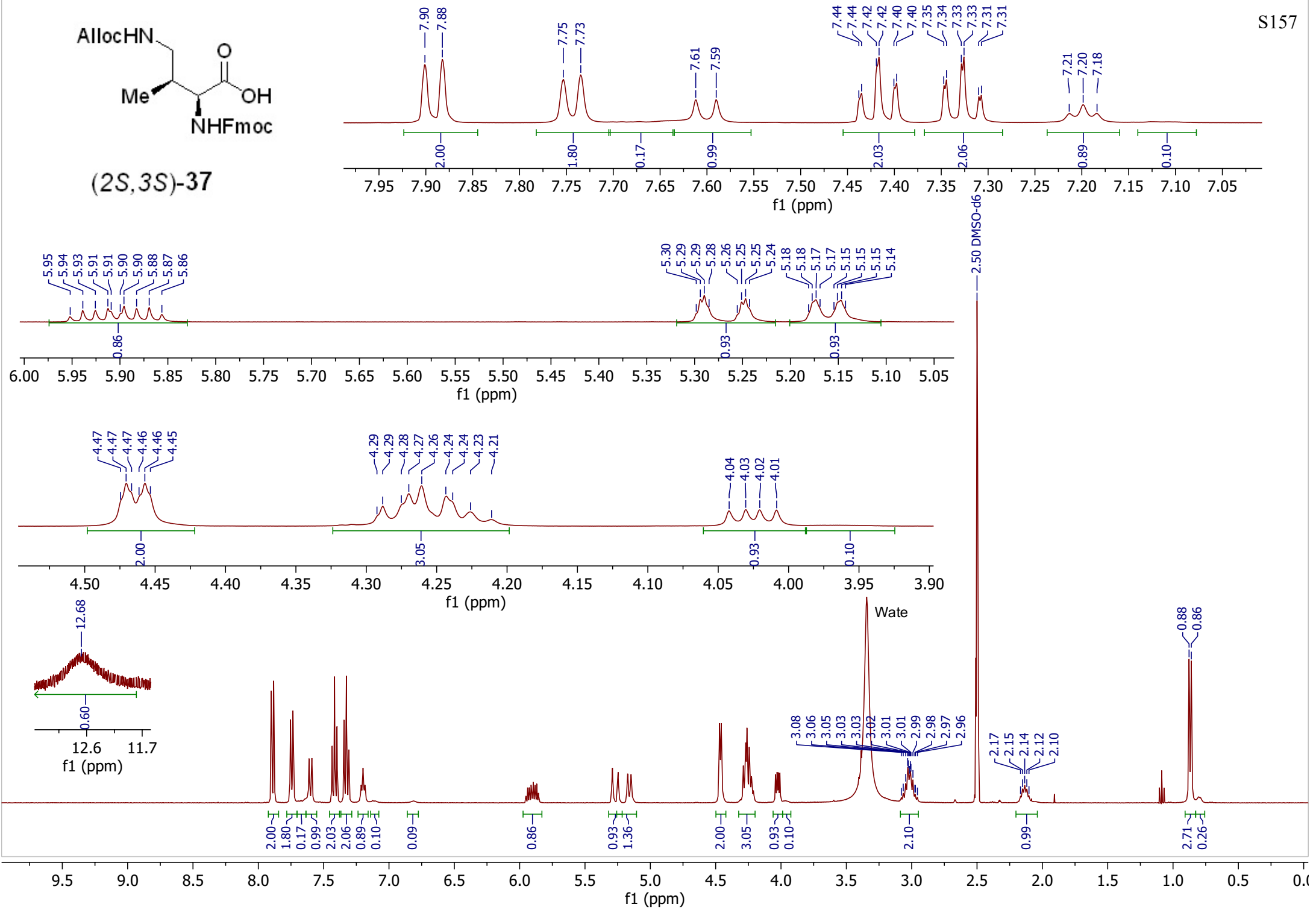
(S)(2S,3S)-36

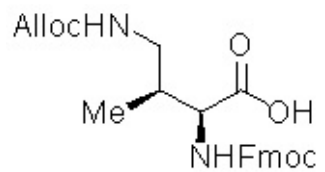
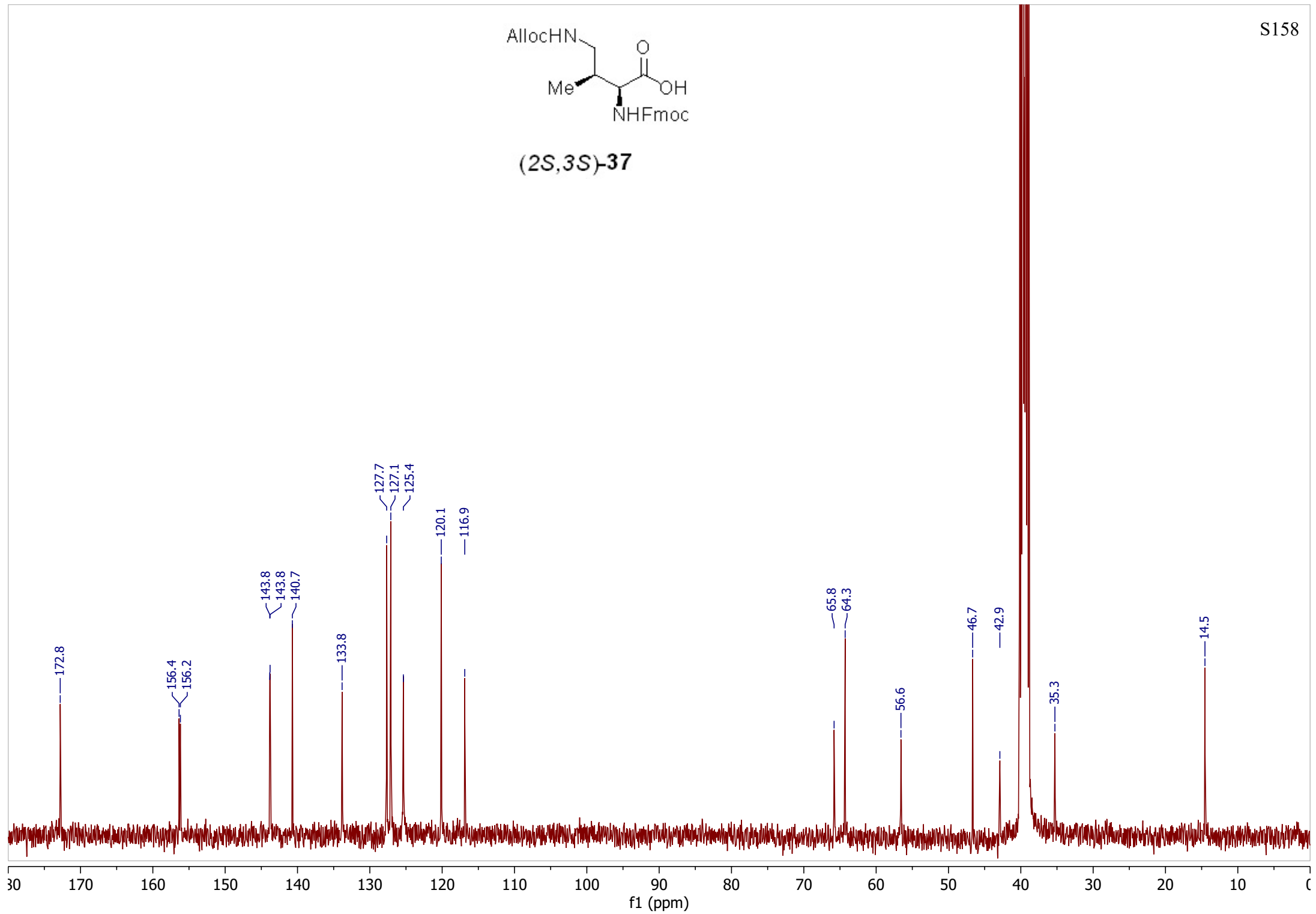


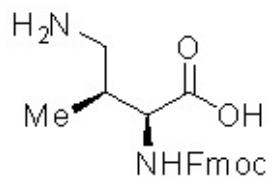
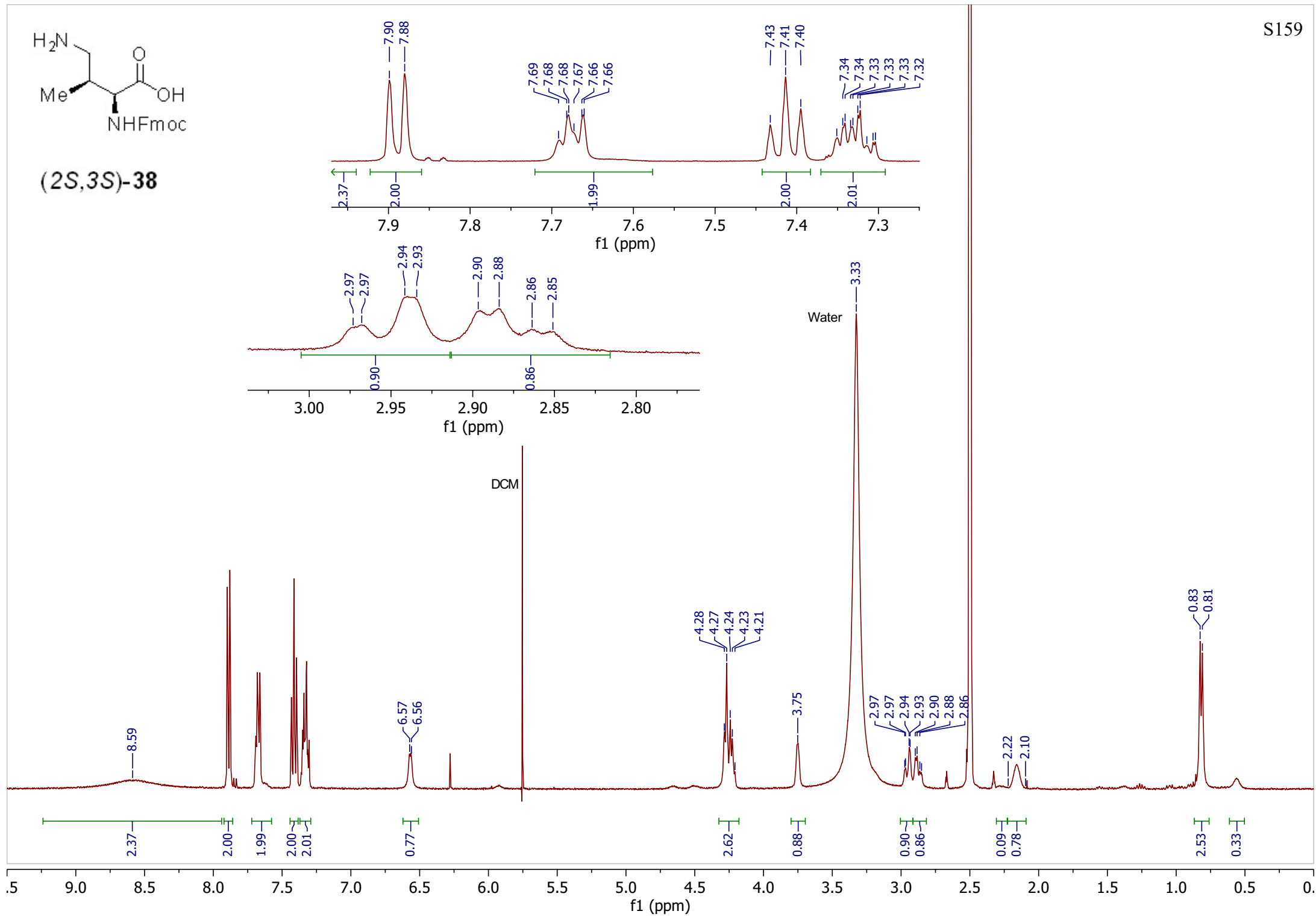
**(S)(2S,3S)-36**

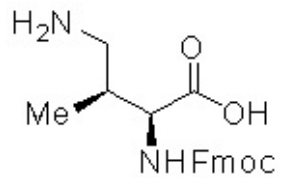
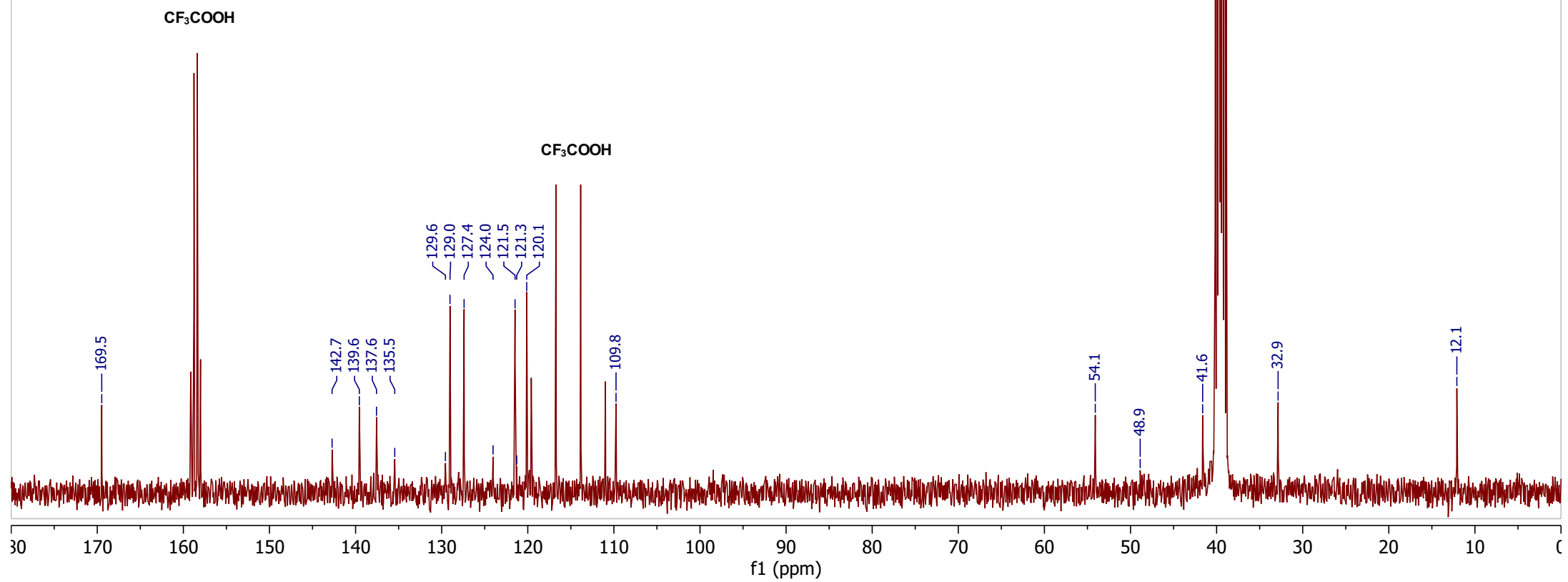


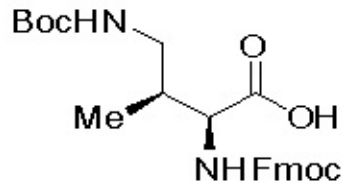
(2S,3S)-37



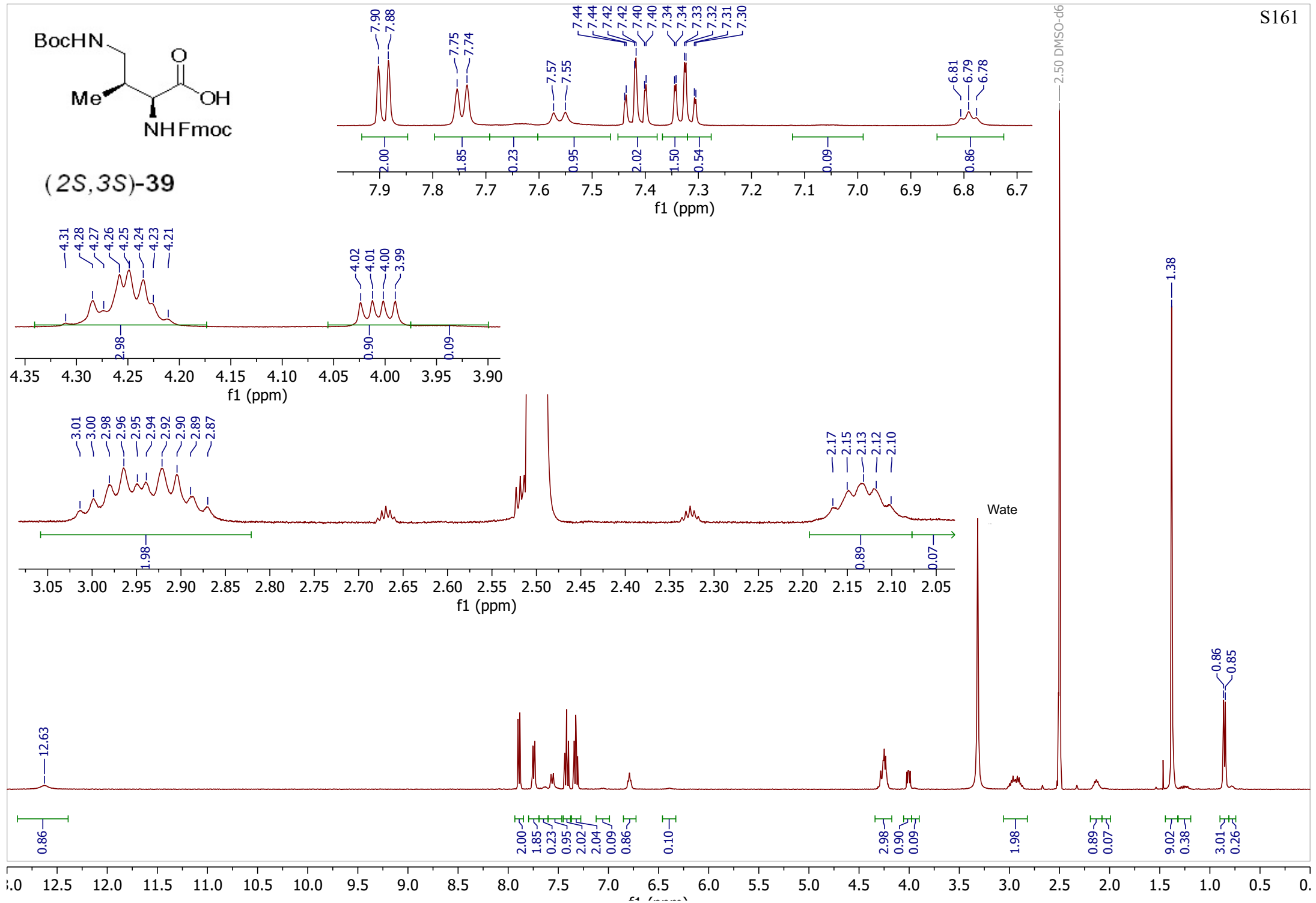
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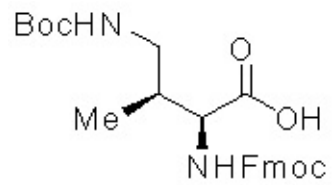
**(2S,3S)-38**

**(2S,3S)-38**



(2S,3S)-39



**(2S,3S)-39**