

## Tricyclic Diterpenoids Selectively Suppress Androgen Receptor-Positive Prostate Cancer Cells

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7.260  
7.206  
7.179  
7.034  
7.007  
6.916

2.975  
2.915  
2.850  
2.804

2.352  
2.292  
2.258

1.956

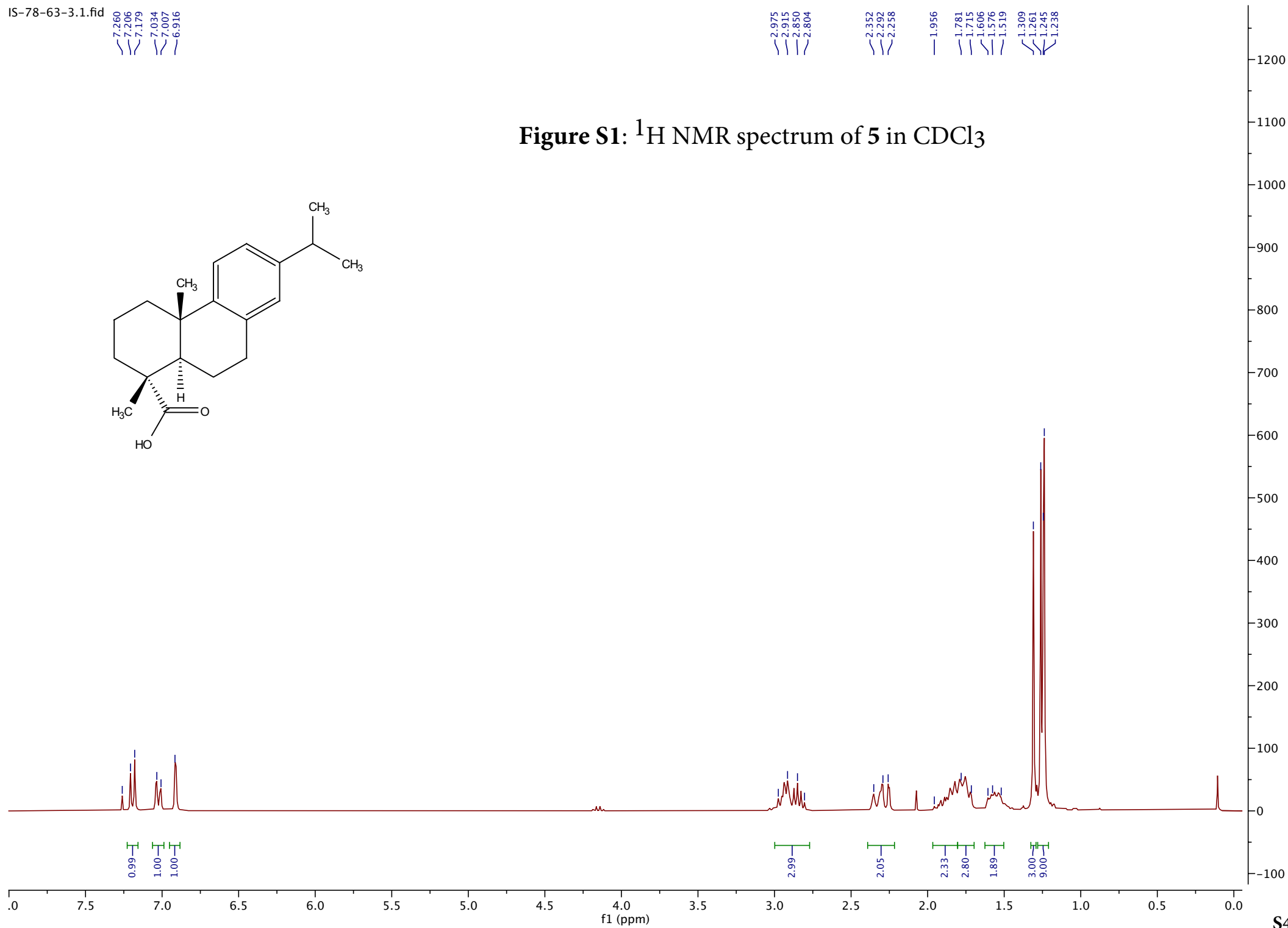
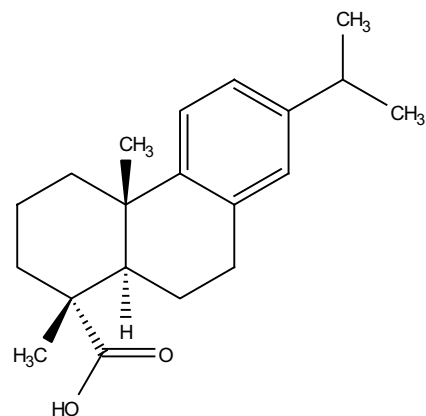
1.781  
1.715

1.606  
1.576

1.519

1.309  
1.261  
1.245  
1.238

**Figure S1:**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CDCl}_3$



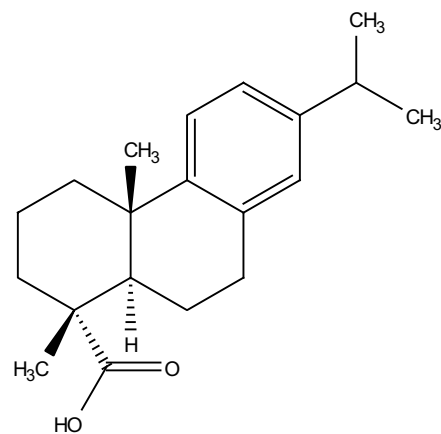
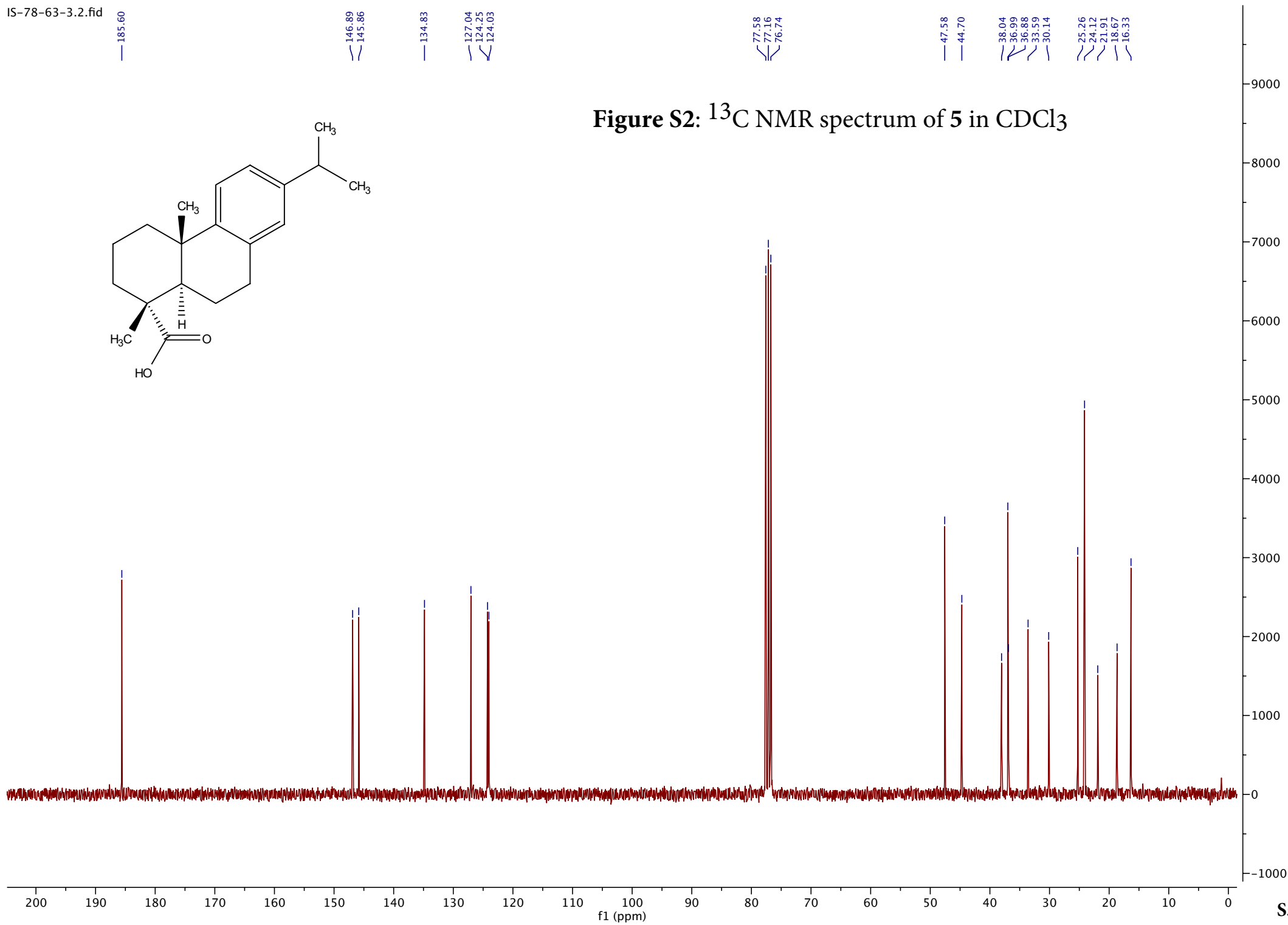


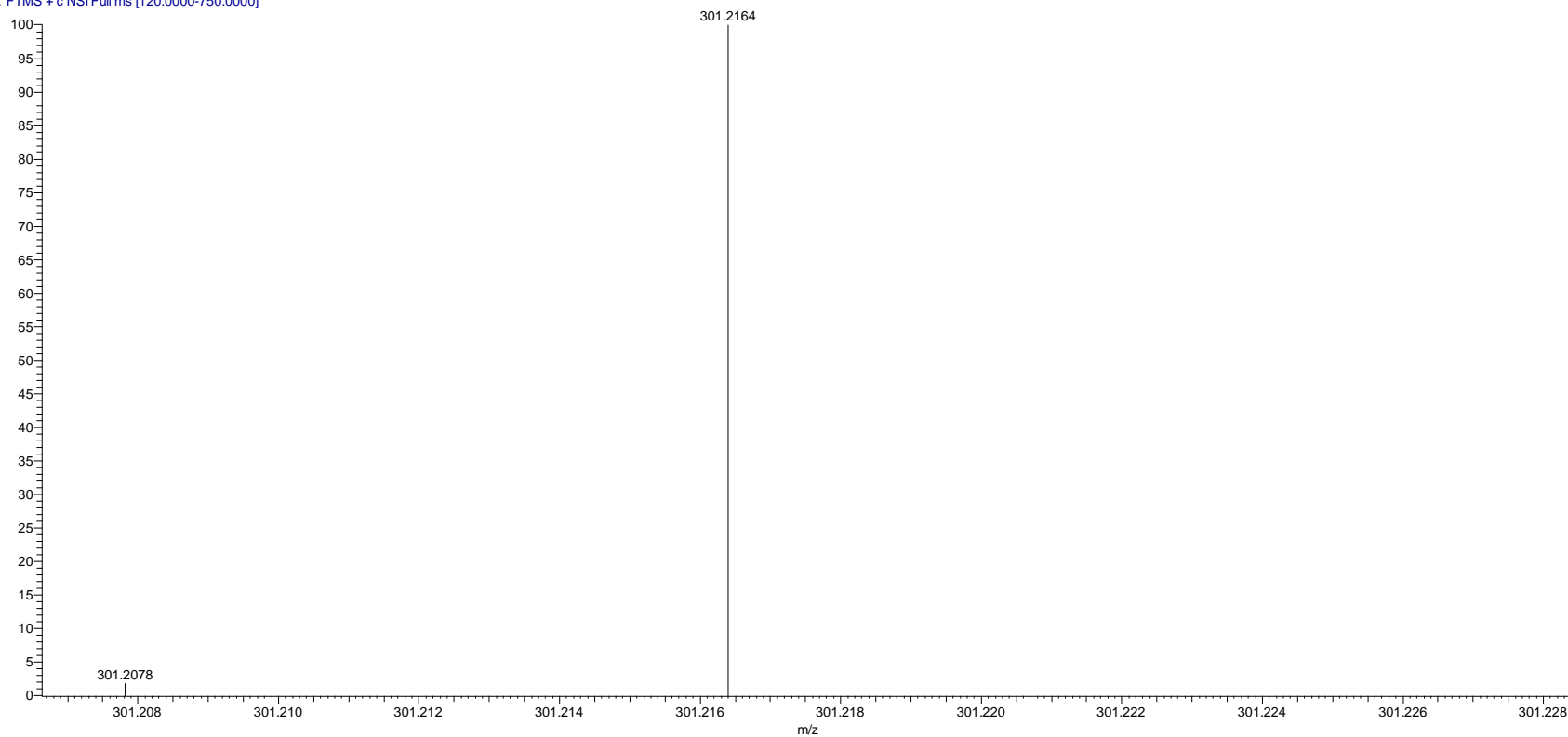
Figure S2: <sup>13</sup>C NMR spectrum of 5 in CDCl<sub>3</sub>

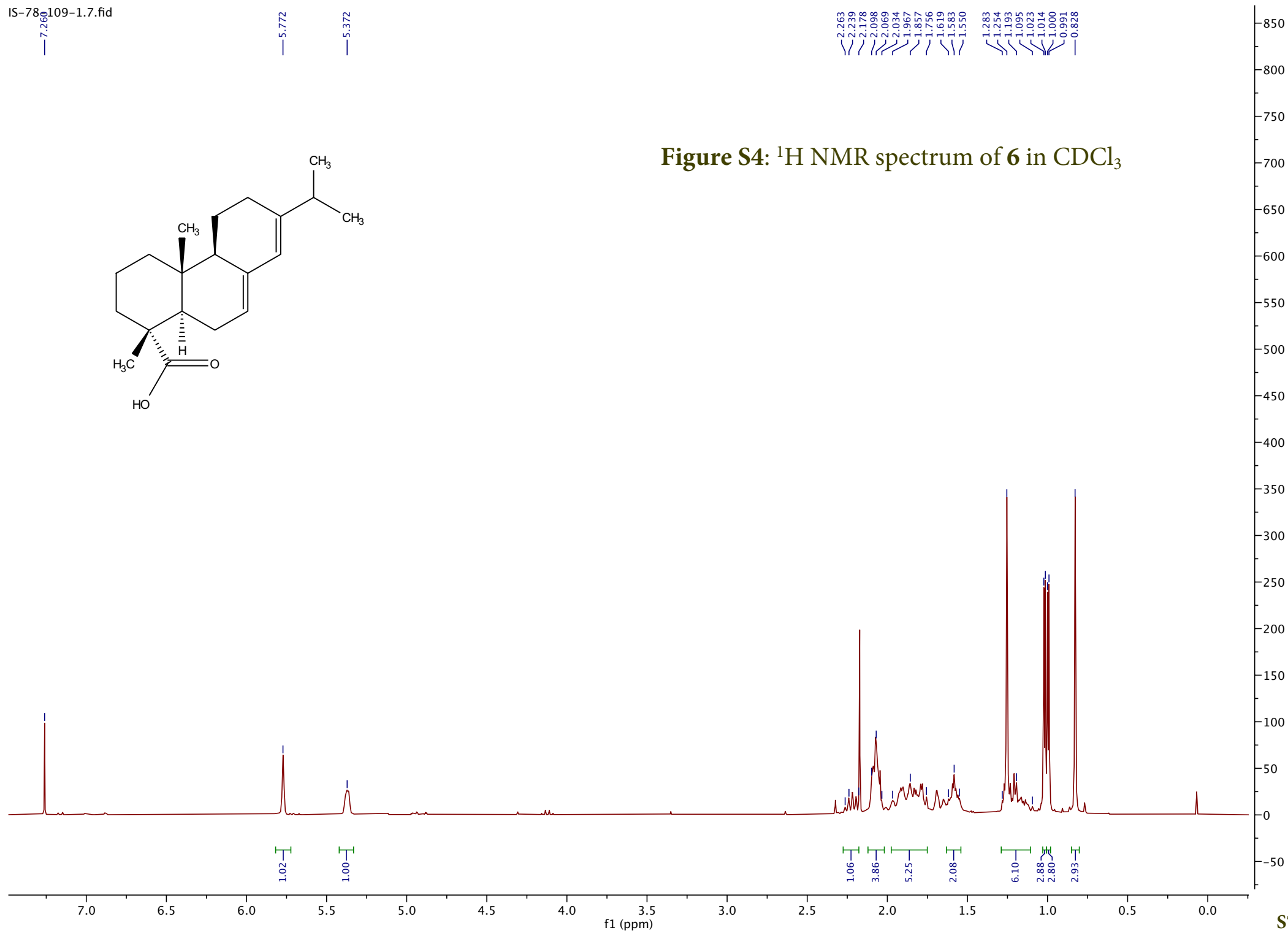


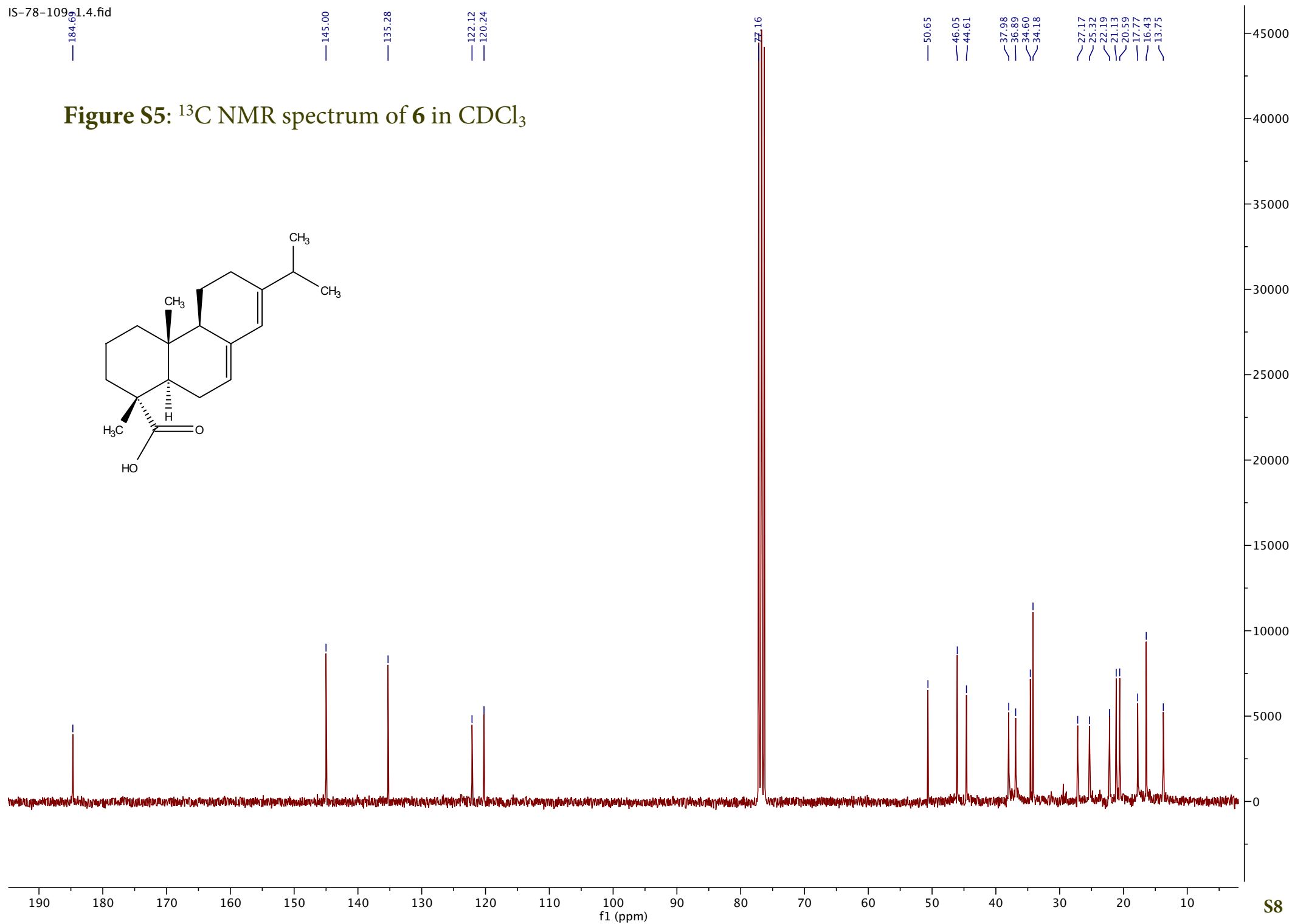
**Figure S3:** High resolution mass spectrum of **5**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-63-3	C20H28O2	300.2089	301.2167	301.2164	-0.0003	-1.13

IS-78-63-3 #2237-2505 RT: 11.95-13.39 AV: 269 NL: 2.59E6  
T: FTMS + c NSI Full ms [120.0000-750.0000]





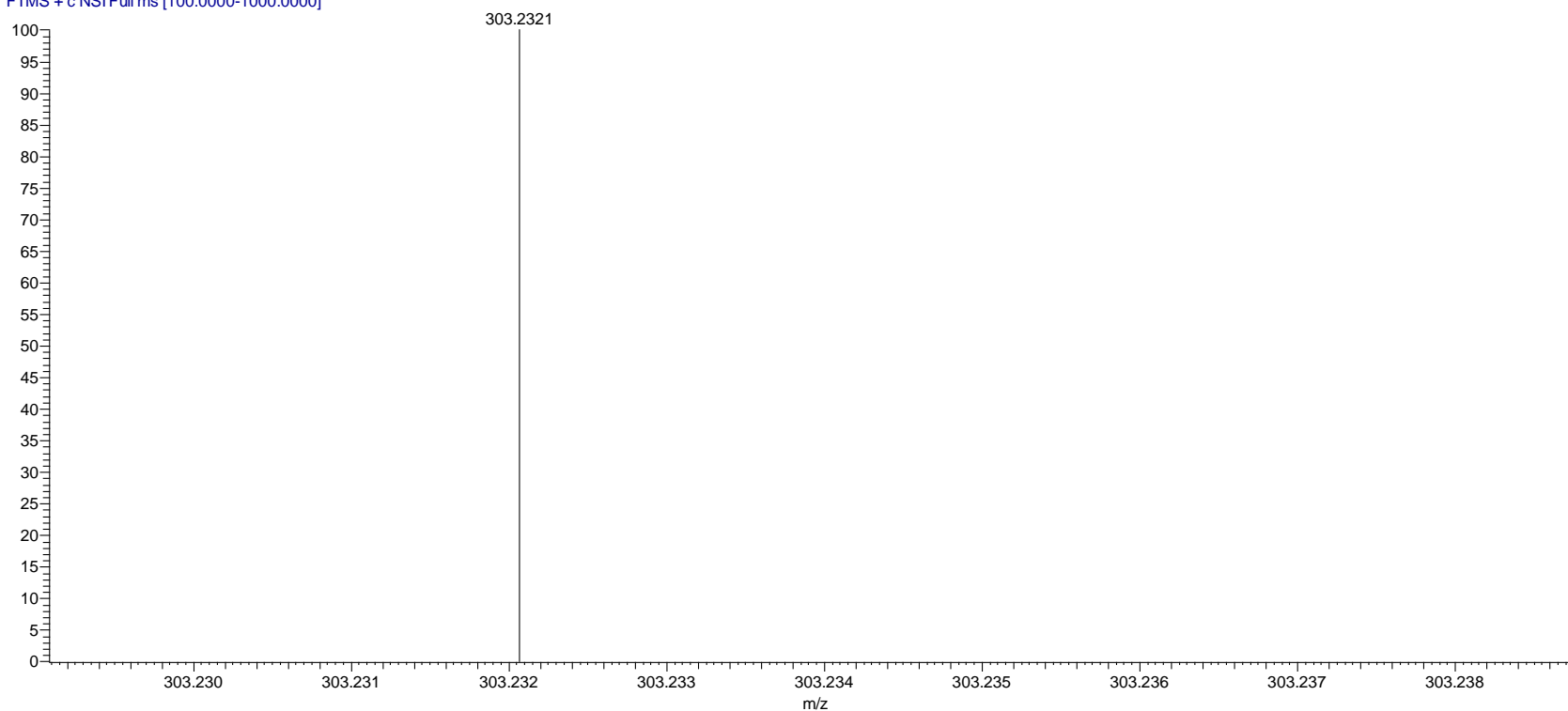




**Figure S6:** High resolution mass spectrum of **6**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-109-2	C20H30O2	302.2246	303.2324	303.2321	-0.0003	-0.96

IS-78-109-2 #2957-3058 RT: 15.49-16.02 AV: 102 NL: 2.47E5  
T: FTMS + c NSI Full ms [100.0000-1000.0000]



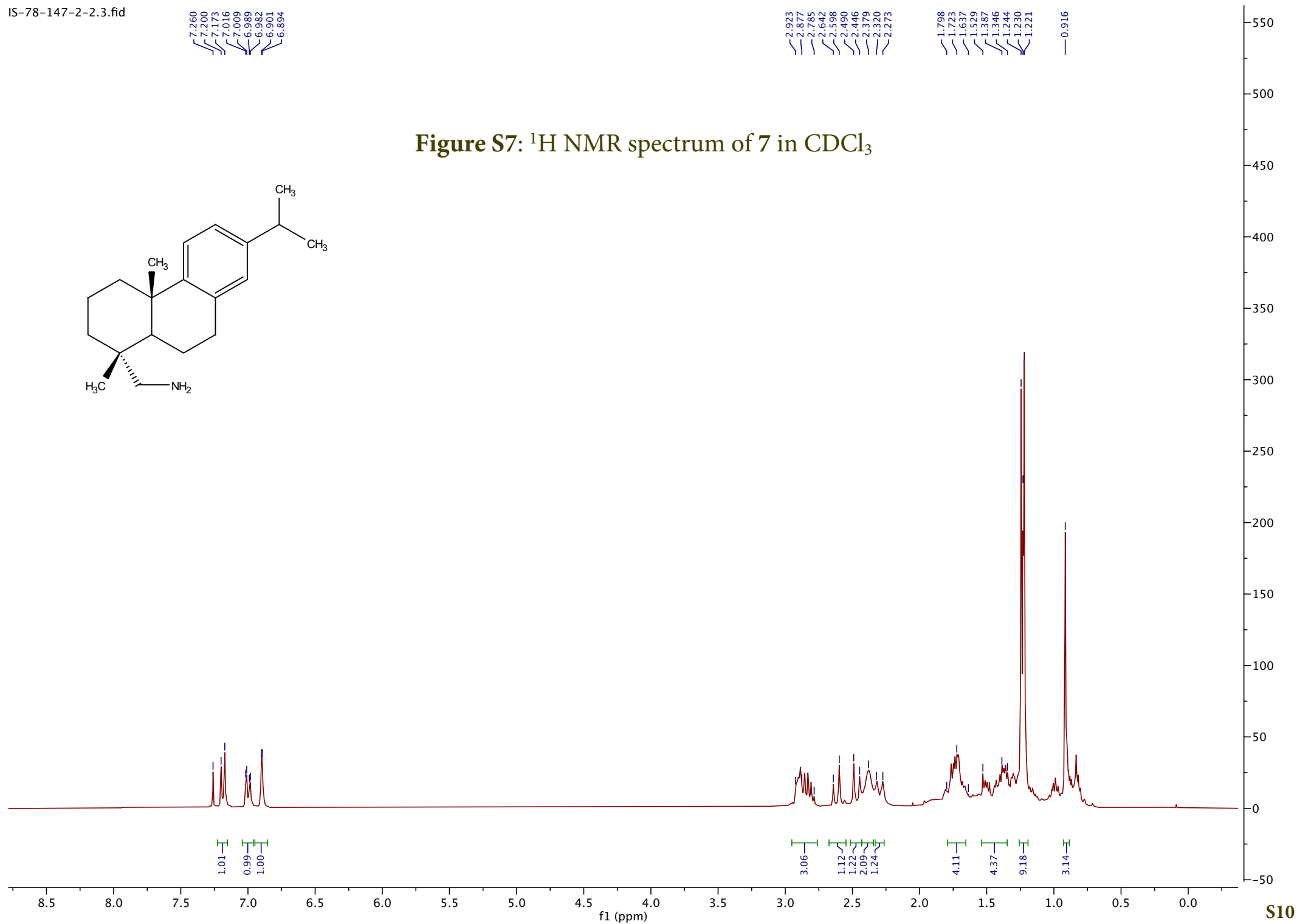
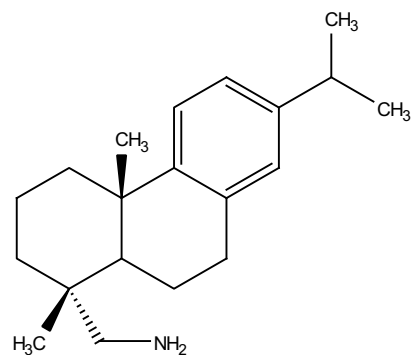
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7.009  
6.989  
6.982  
6.901  
6.894

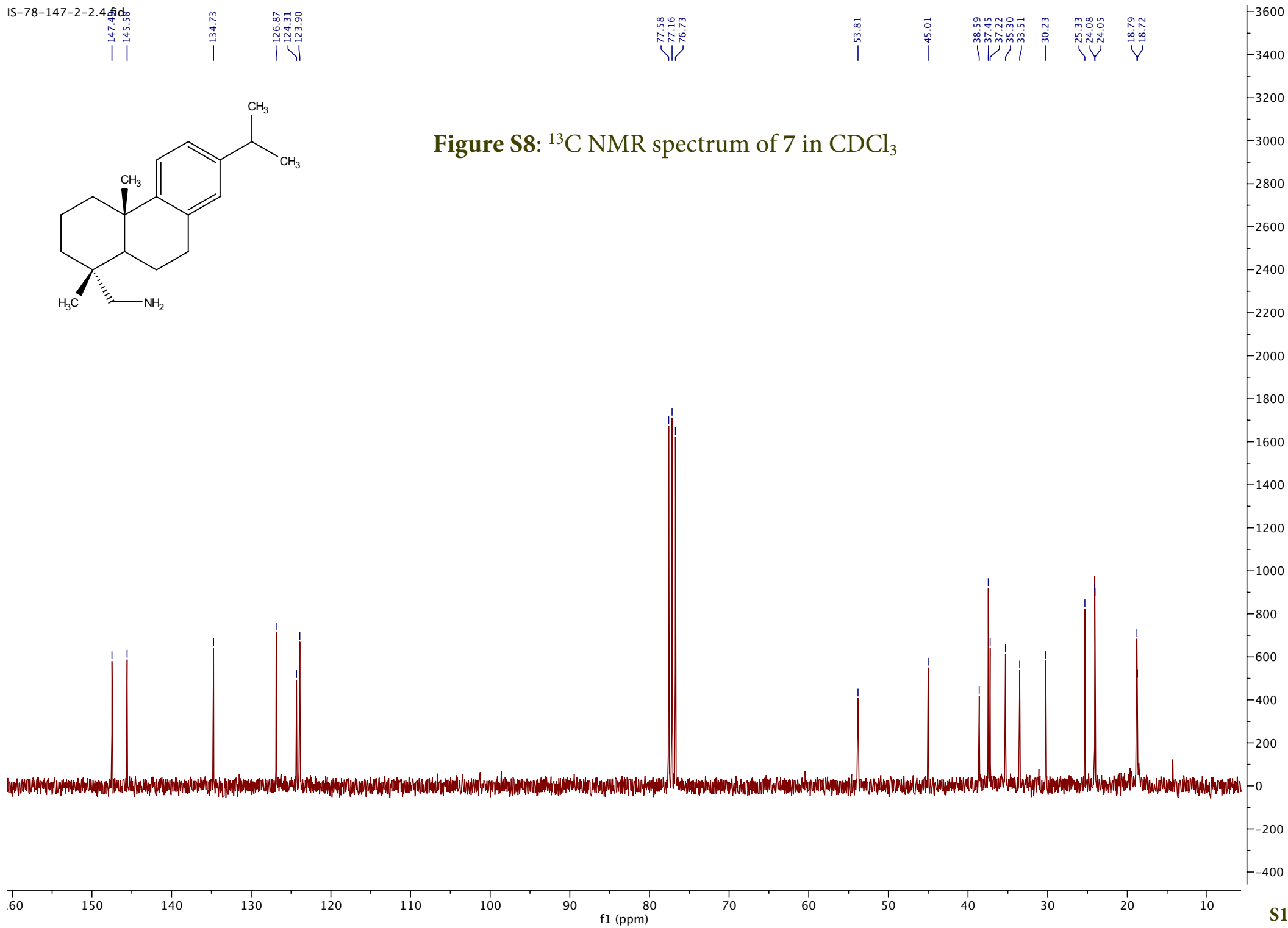
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2.877  
2.785  
2.642  
2.598  
2.490  
2.446  
2.379  
2.320  
2.273

1.798  
1.723  
1.637  
1.529  
1.387  
1.346  
1.244  
1.230  
1.221

0.916

**Figure S7:**  $^1\text{H}$  NMR spectrum of **7** in  $\text{CDCl}_3$

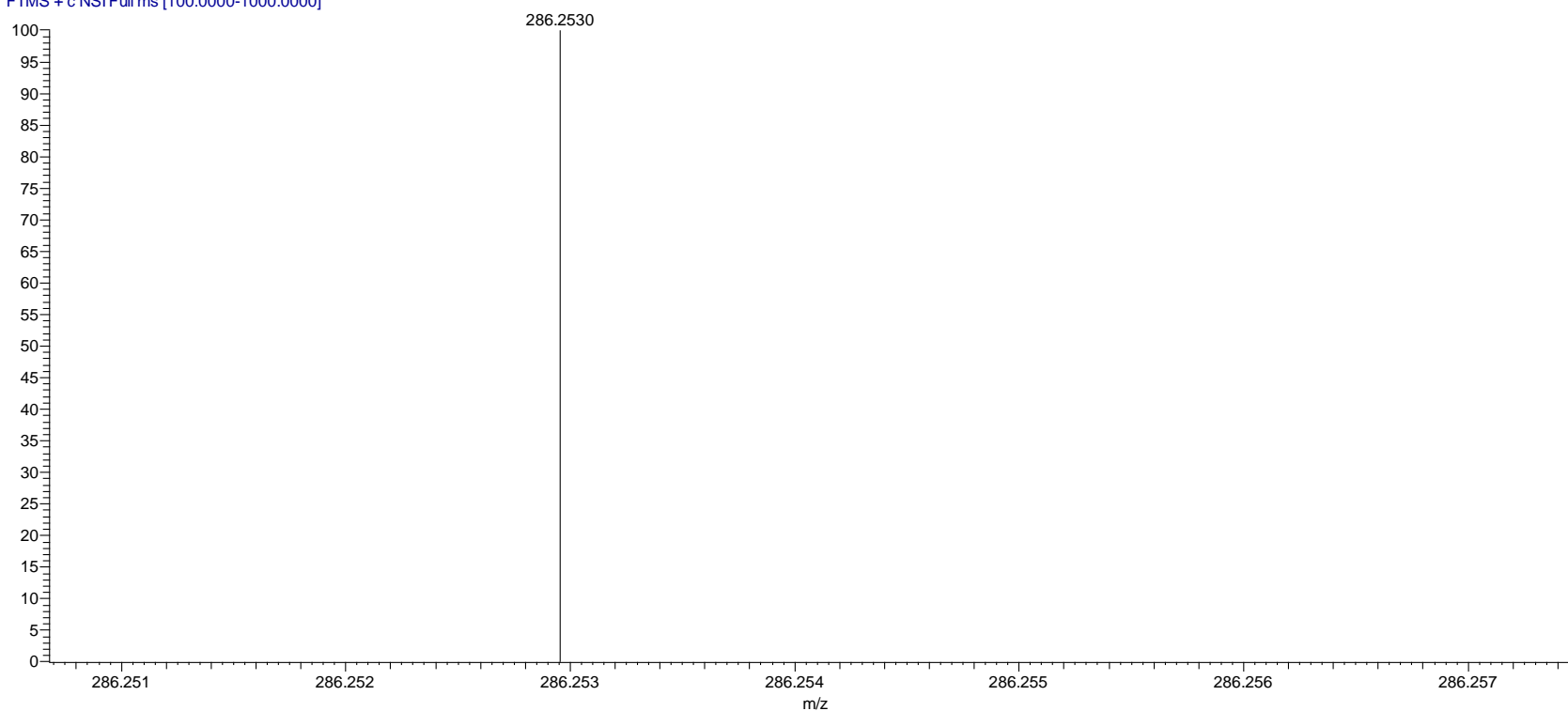


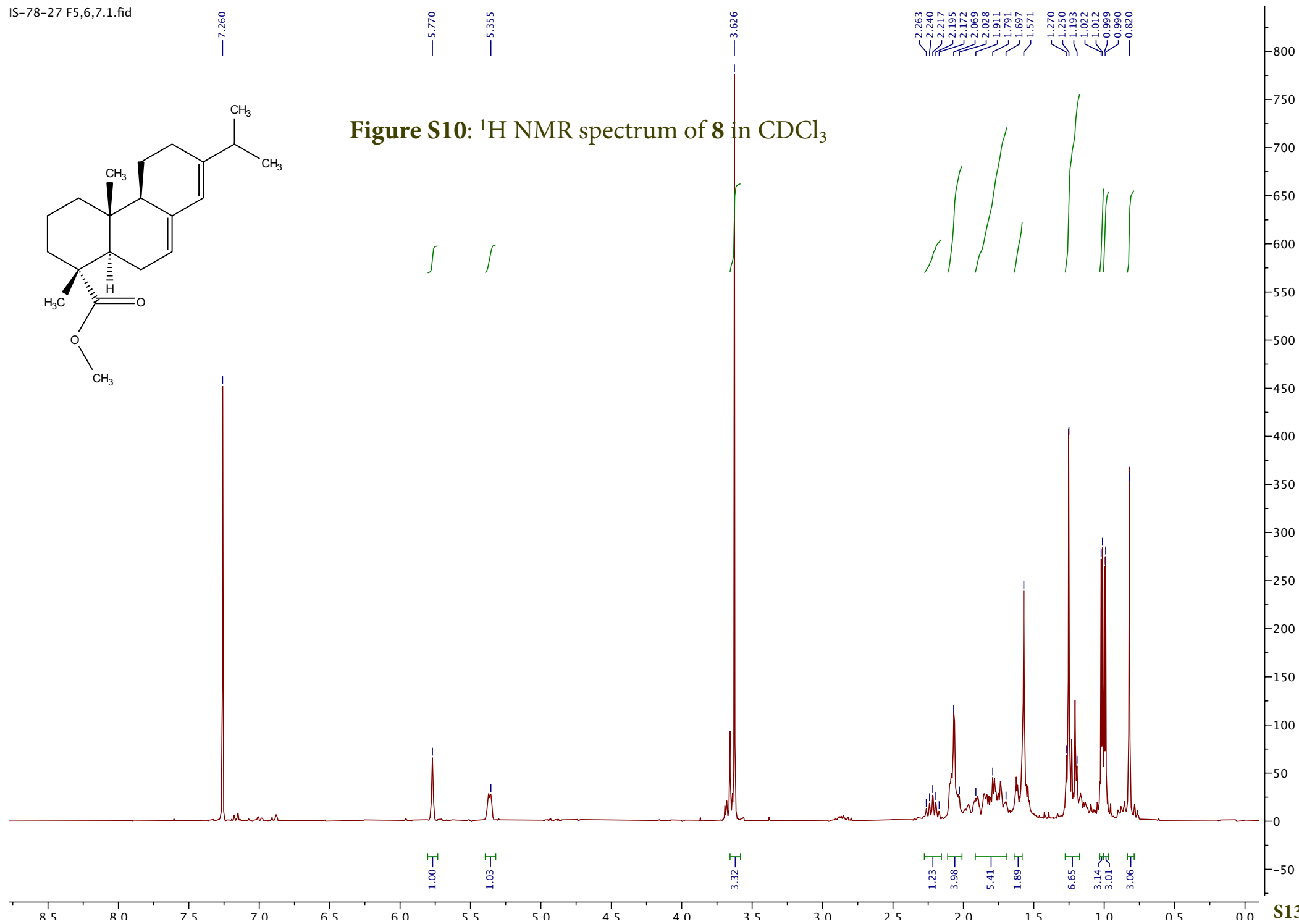


**Figure S9:** High resolution mass spectrum of **7**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-147-3	C20H31N	285.2457	286.2535	286.2530	-0.0005	-1.57

IS-78-147-3 #1900-1922 RT: 9.99-10.10 AV: 23 NL: 2.09E9  
T: FTMS + c NSI Full ms [100.0000-1000.0000]





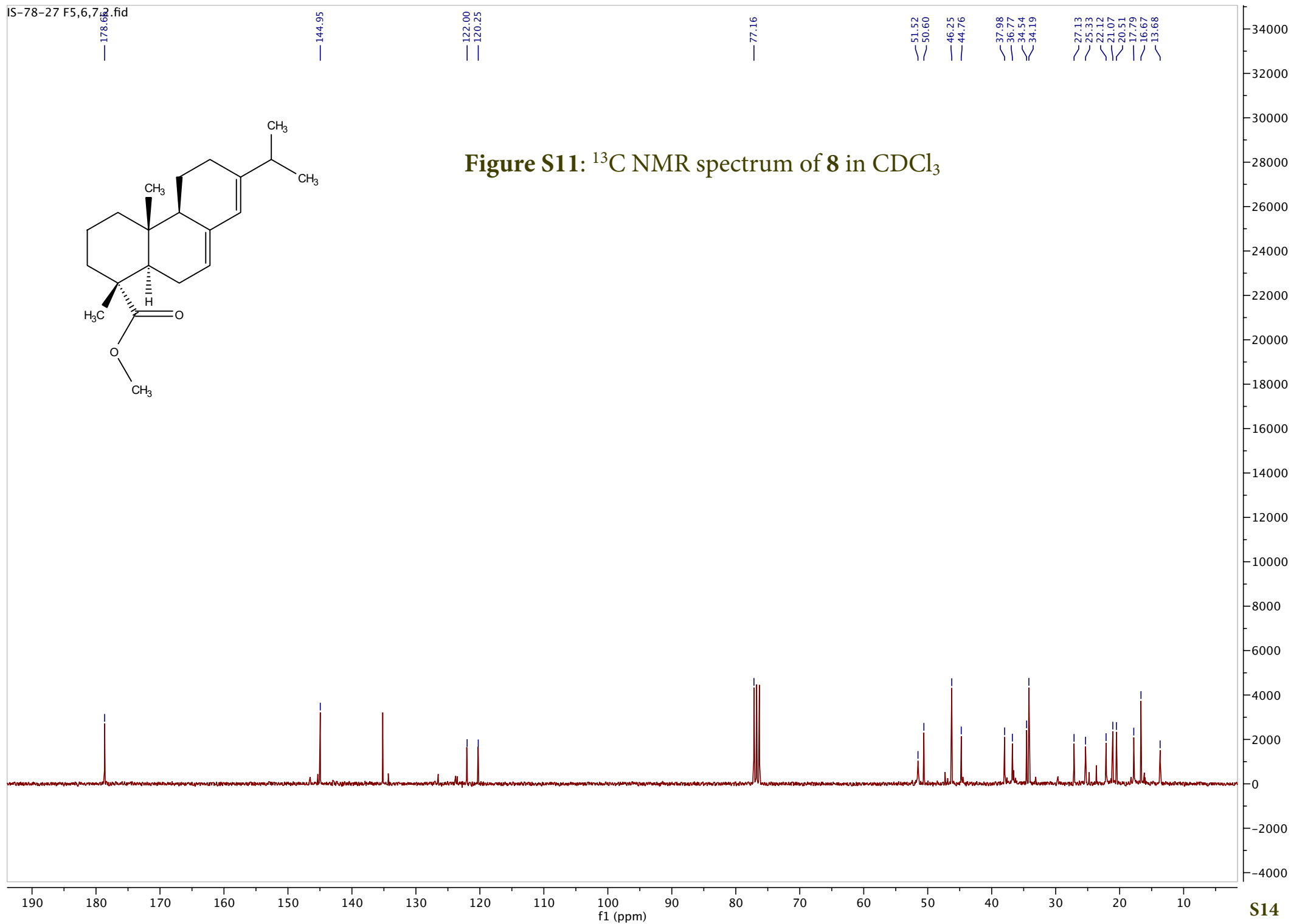
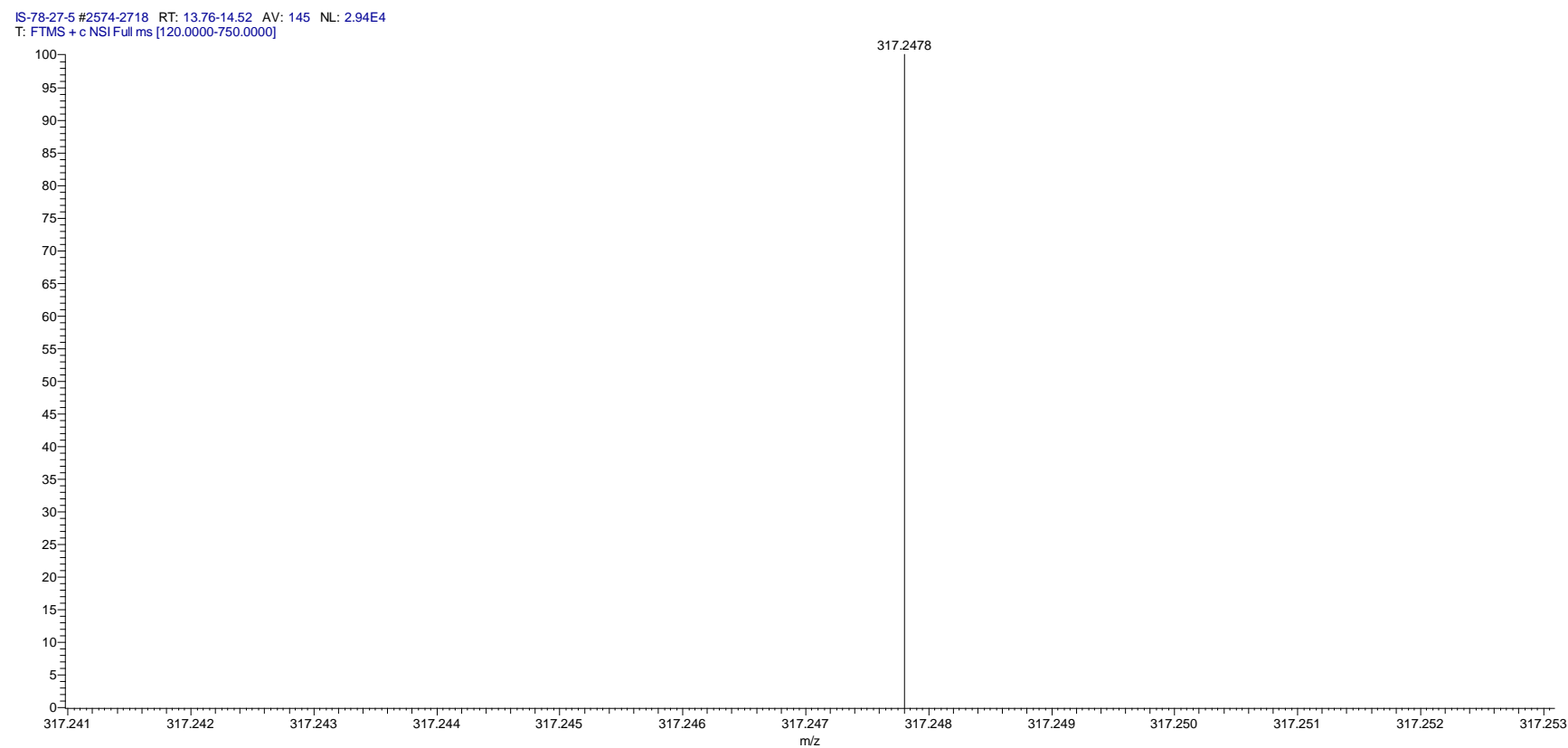


Figure S12: High resolution mass spectrum of 8

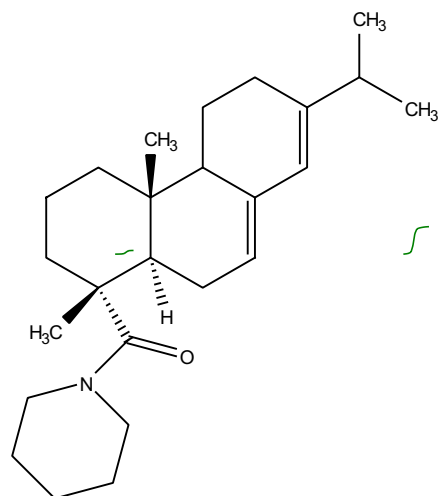
Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-27-5	C21H32O2	316.2402	317.2480	317.2478	-0.0002	-0.76



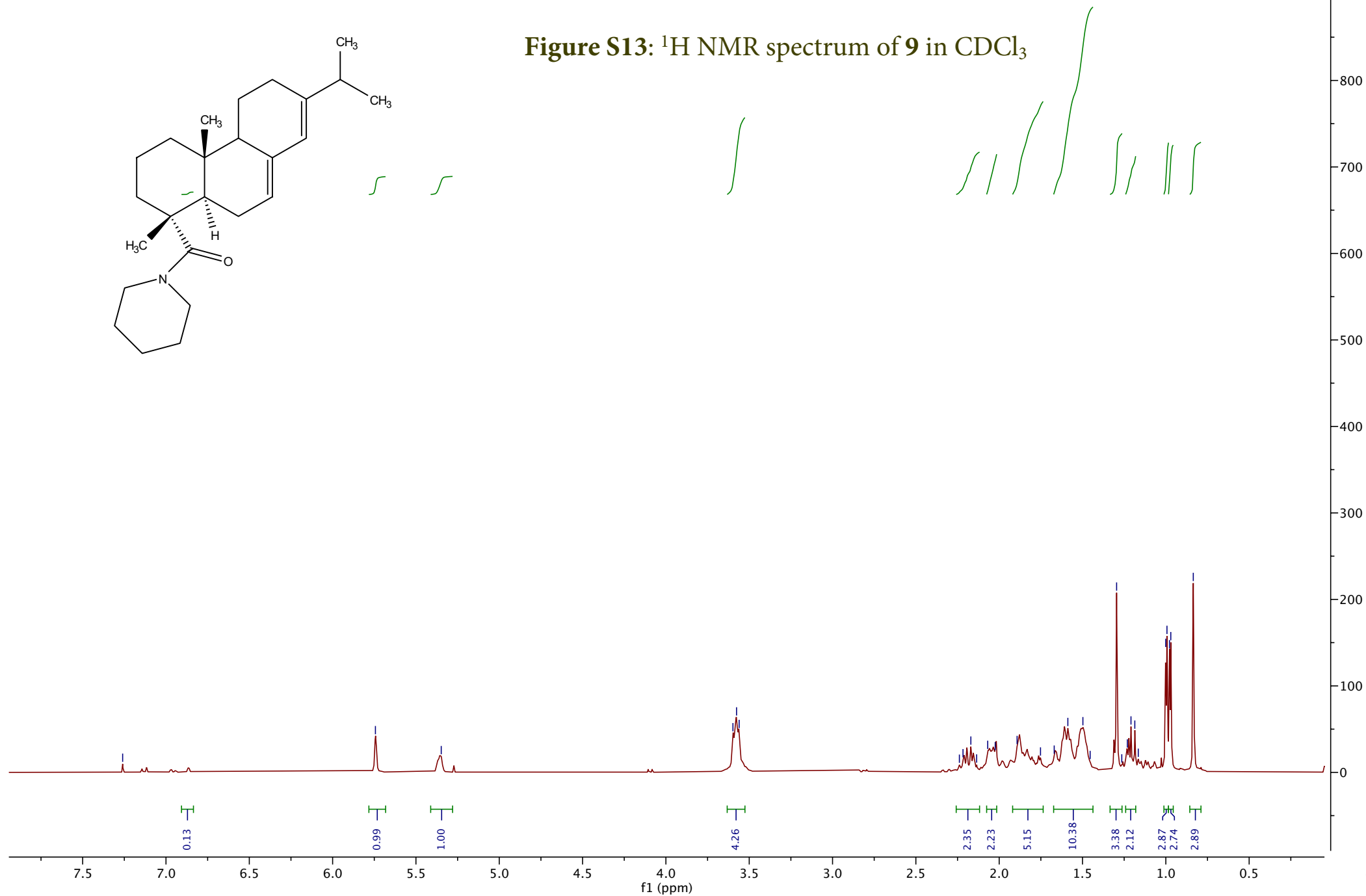
7.260

5.743

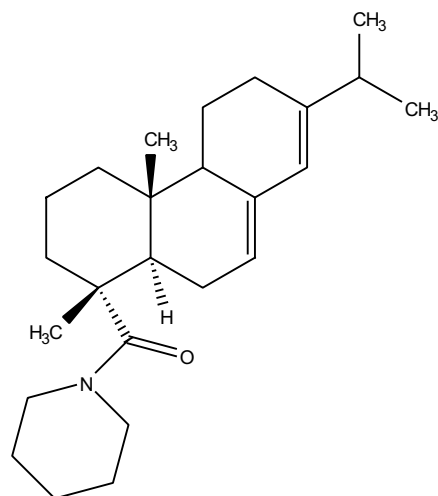
5.348

3.598  
3.576  
3.5612.239  
2.217  
2.170  
2.135  
2.069  
2.024  
1.893  
1.752  
1.670  
1.588  
1.498  
1.454  
1.295  
1.264  
1.231  
1.209  
1.186  
1.165  
1.001  
0.993  
0.978  
0.970  
0.835

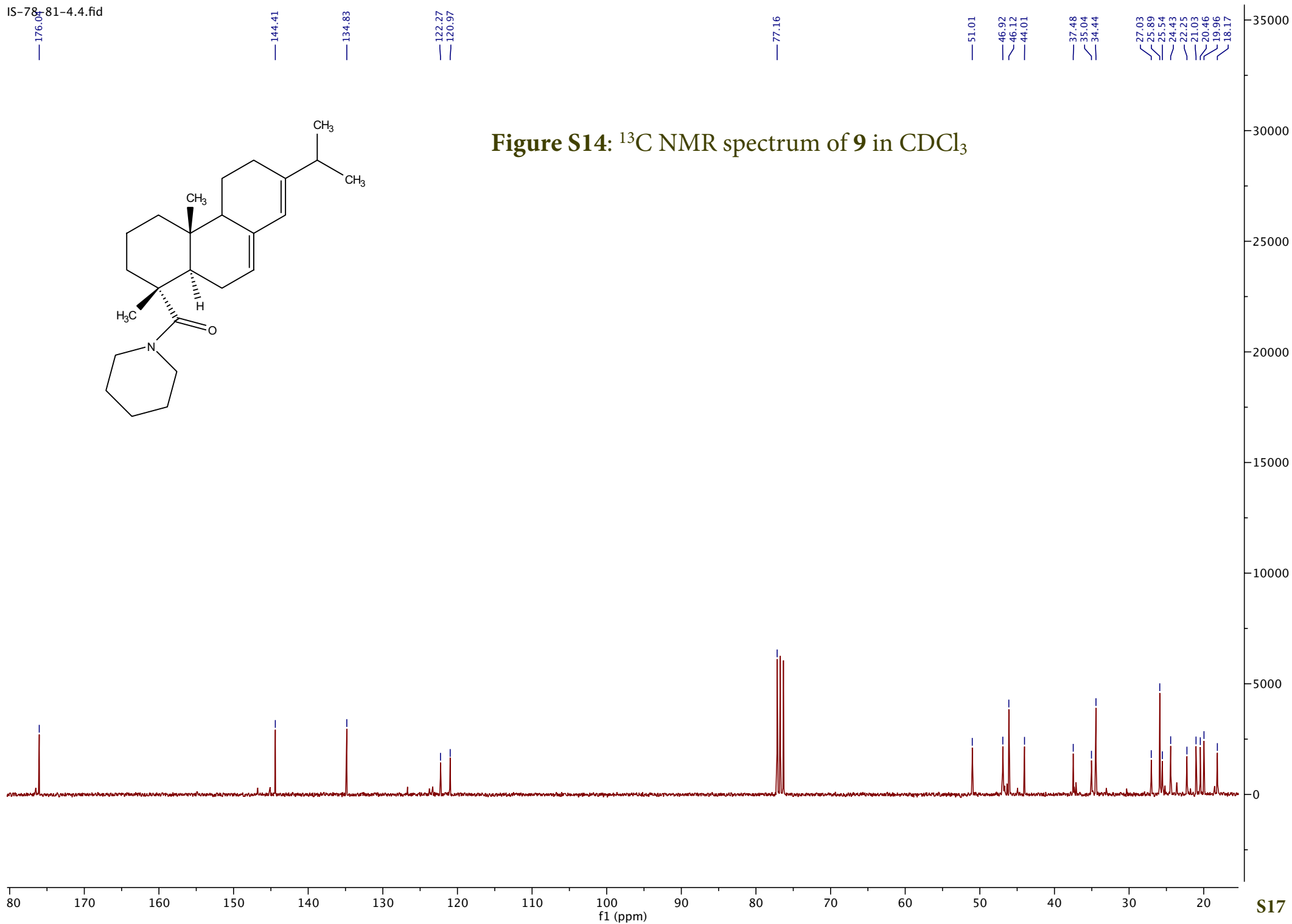
**Figure S13:**  $^1\text{H}$  NMR spectrum of **9** in  $\text{CDCl}_3$







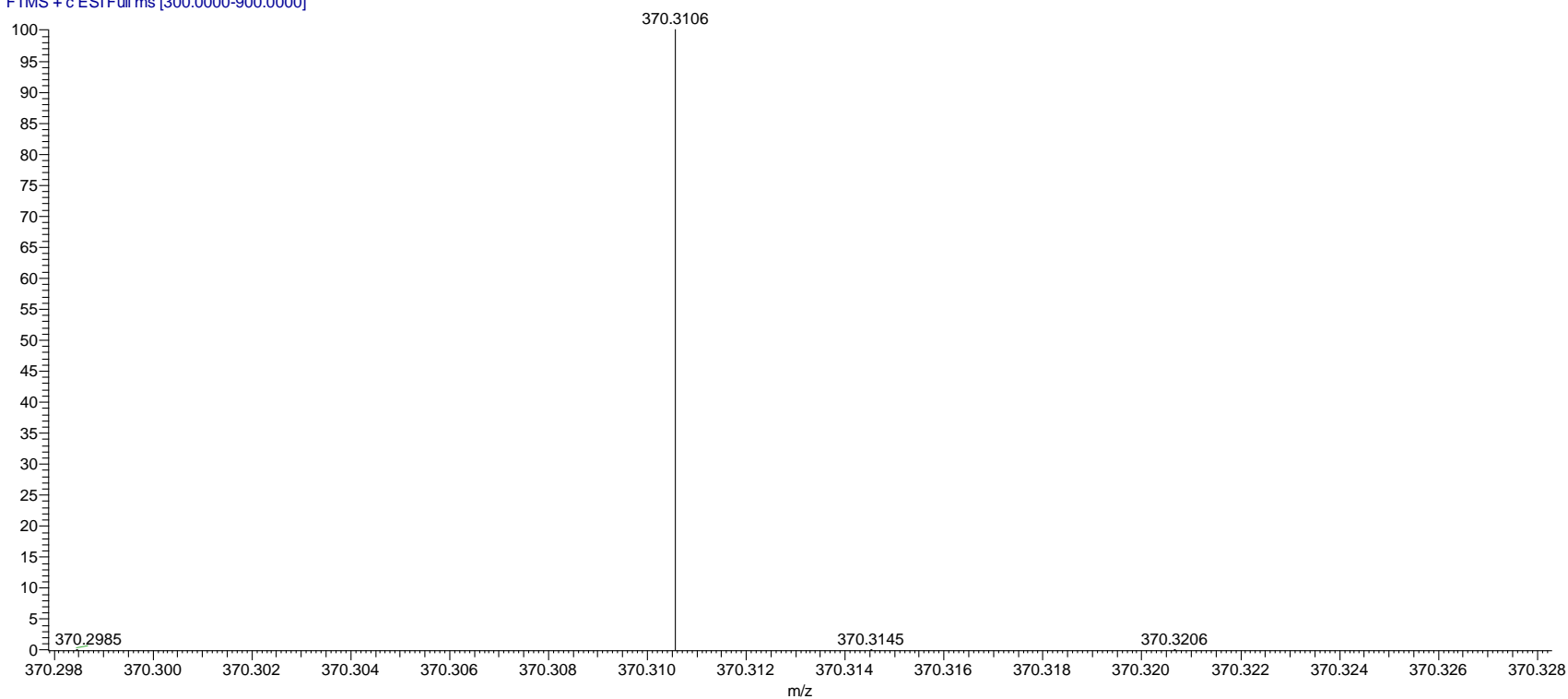
**Figure S14:** <sup>13</sup>C NMR spectrum of **9** in CDCl<sub>3</sub>

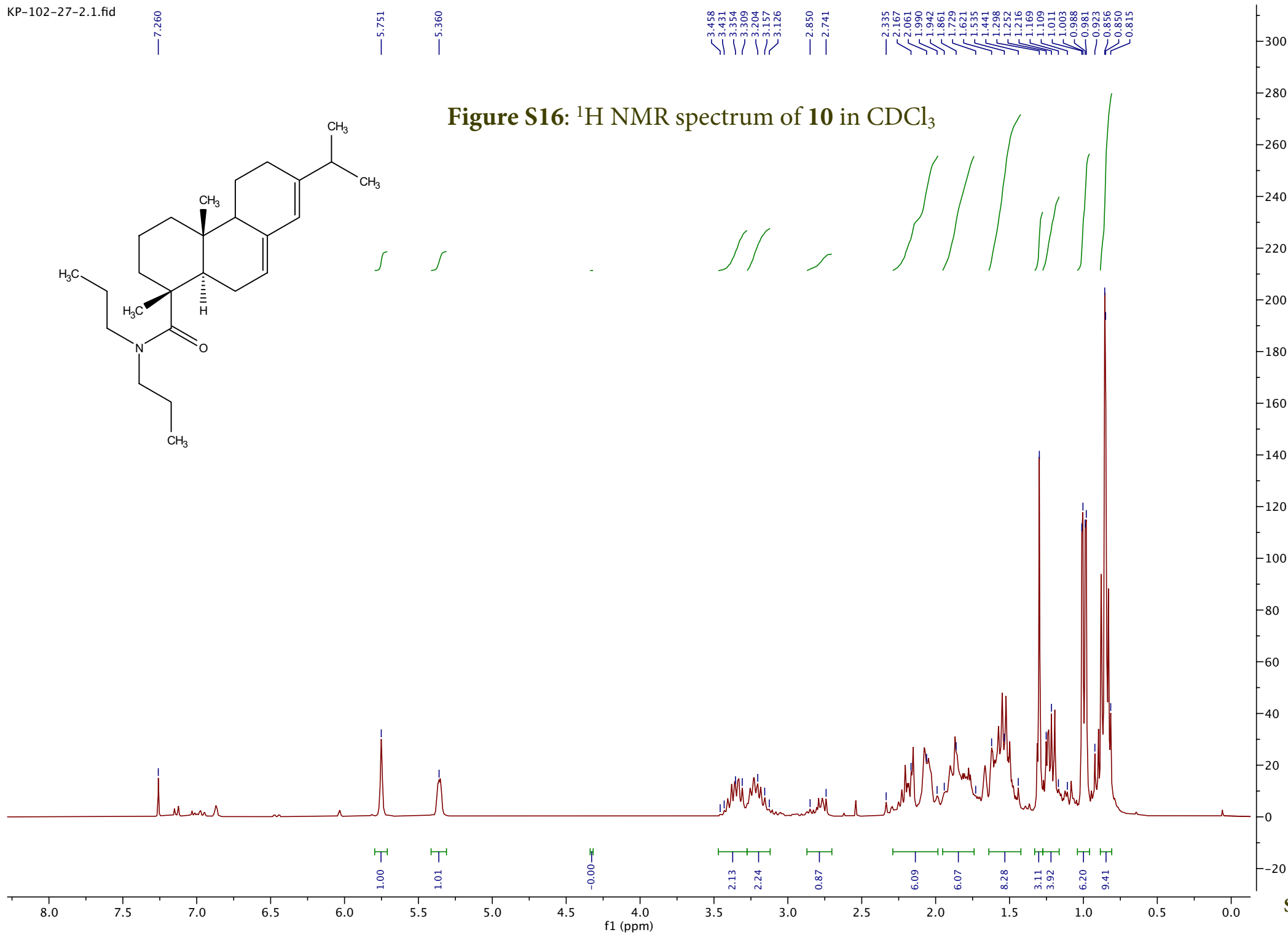


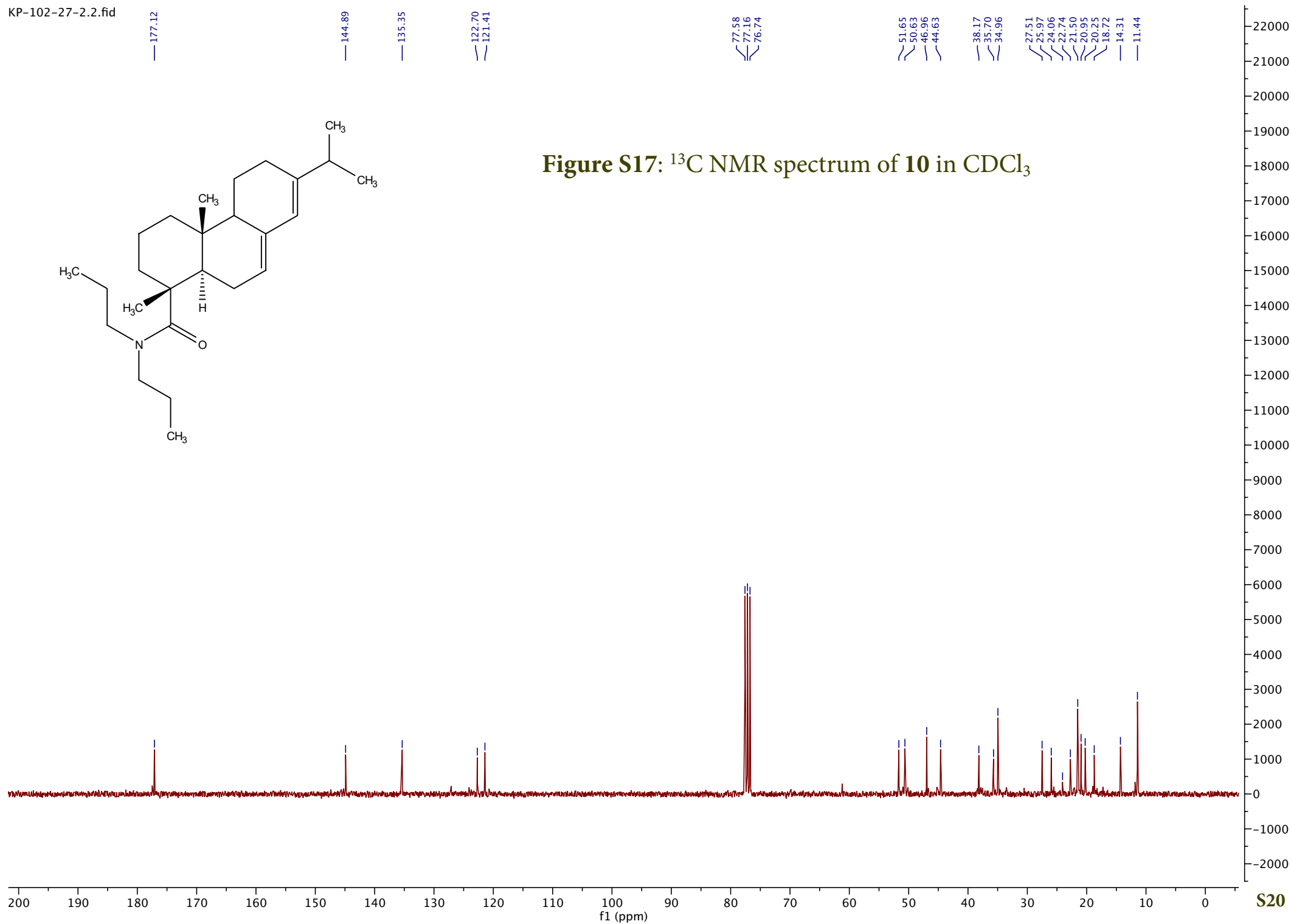
**Figure S15:** High resolution mass spectrum of **9**

Sample Name	Mol Fomula	MW(COME WITH SAMPLES)	MW(CALCULATED)	M+H	observed	delta	ppm
IS-78-81	C25H39NO	369.3032	369.30317	370.3110	<b>370.3106</b>	-0.0004	-1.00

IS-78-81 #180-692 RT: 1.29-4.46 AV: 513 NL: 7.47E6  
T: FTMS + c ESI Full ms [300.0000-900.0000]



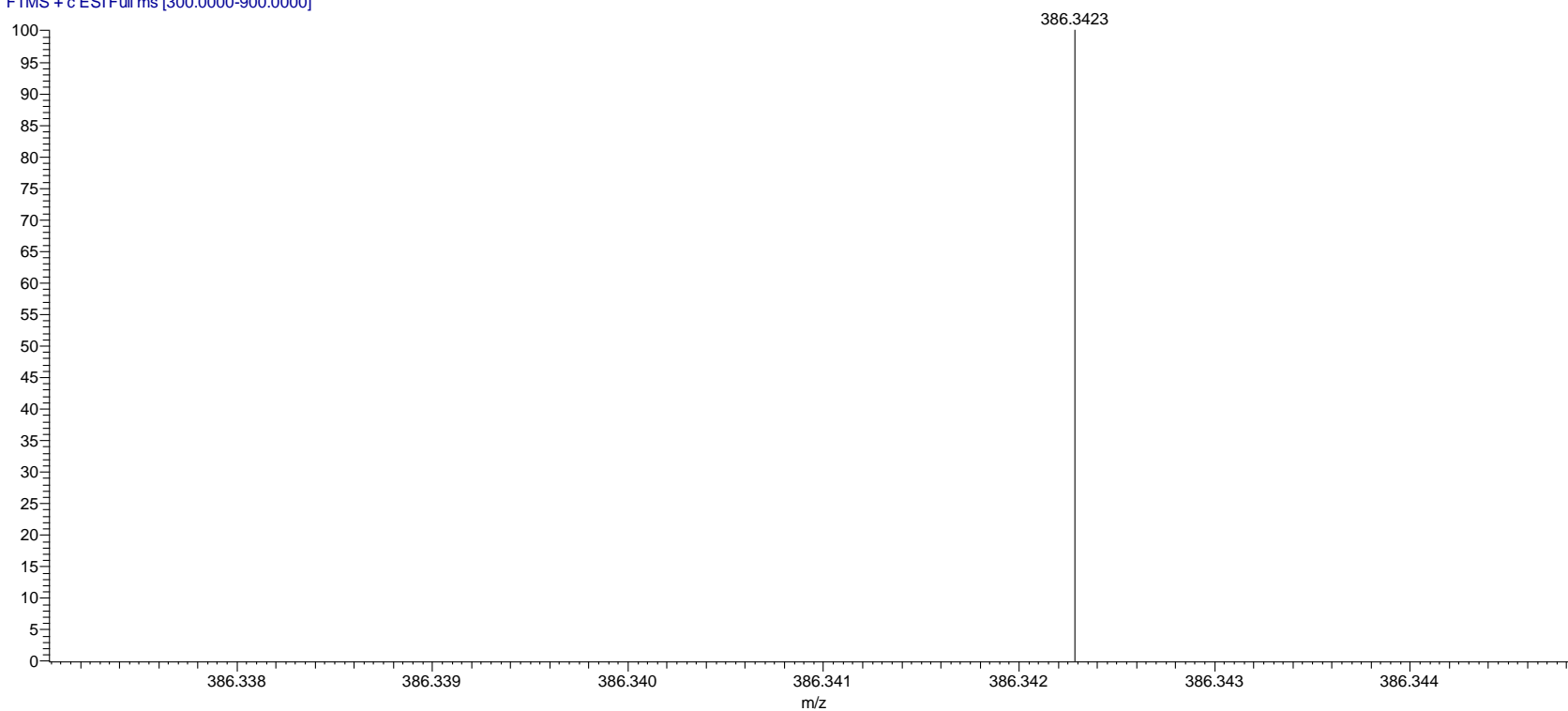


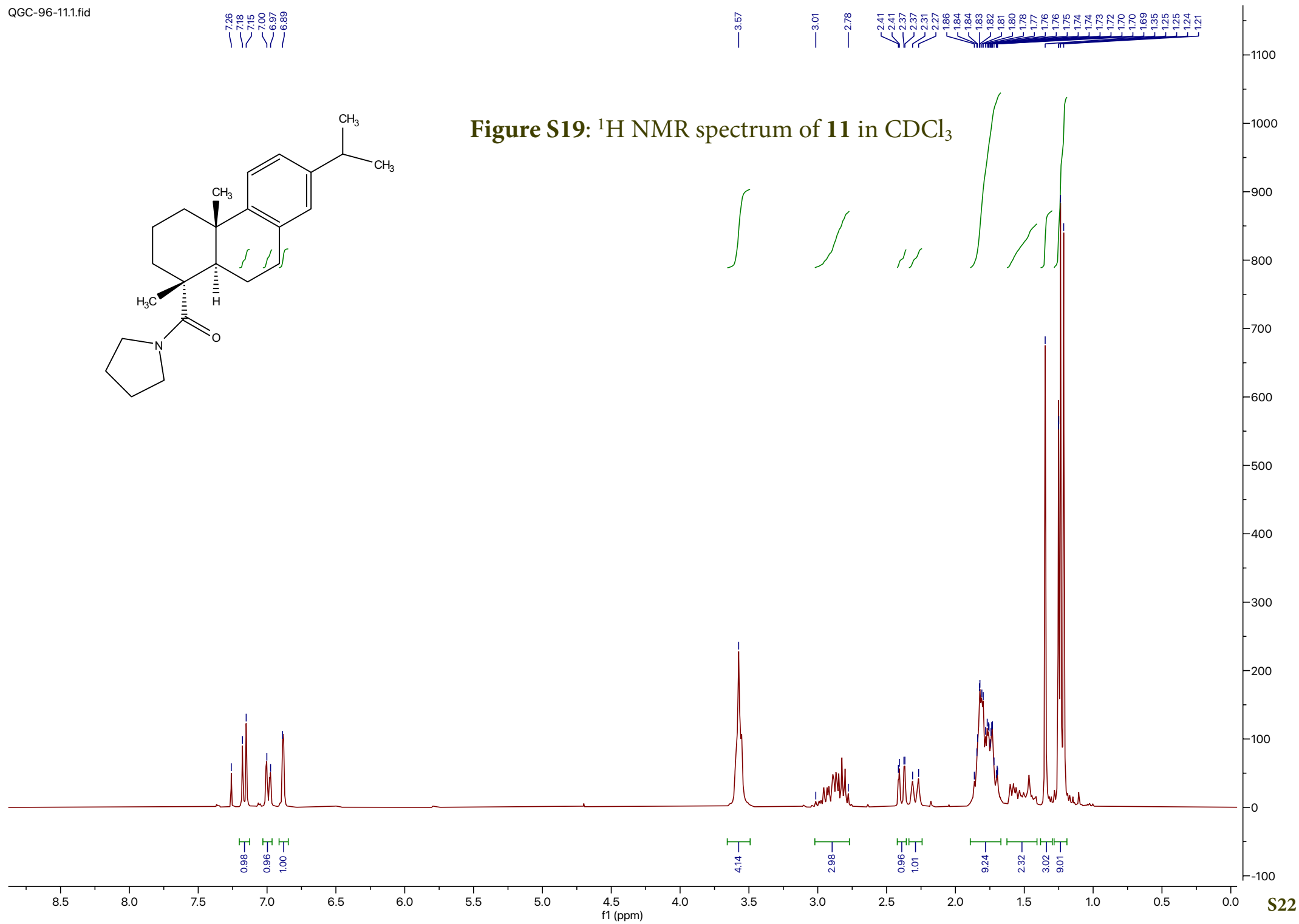


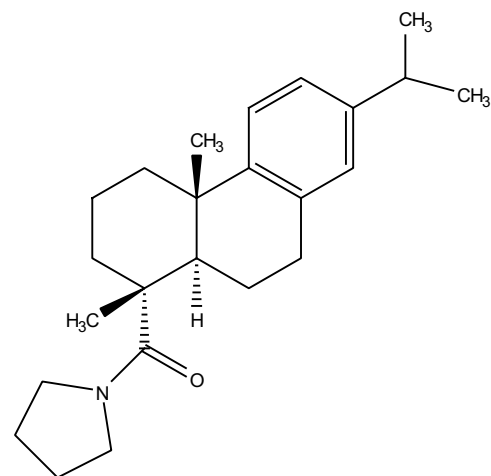
**Figure S18:** High resolution mass spectrum of **10**

Sample Name	Mol Fomula	MW(COME WITH SAMPLES)	MW(CALCULATED)	M+H	observed	delta	ppm
KP-102-27	C26H43NO	385.3345	385.33447	386.3423	<b>386.3423</b>	0.0000	0.00

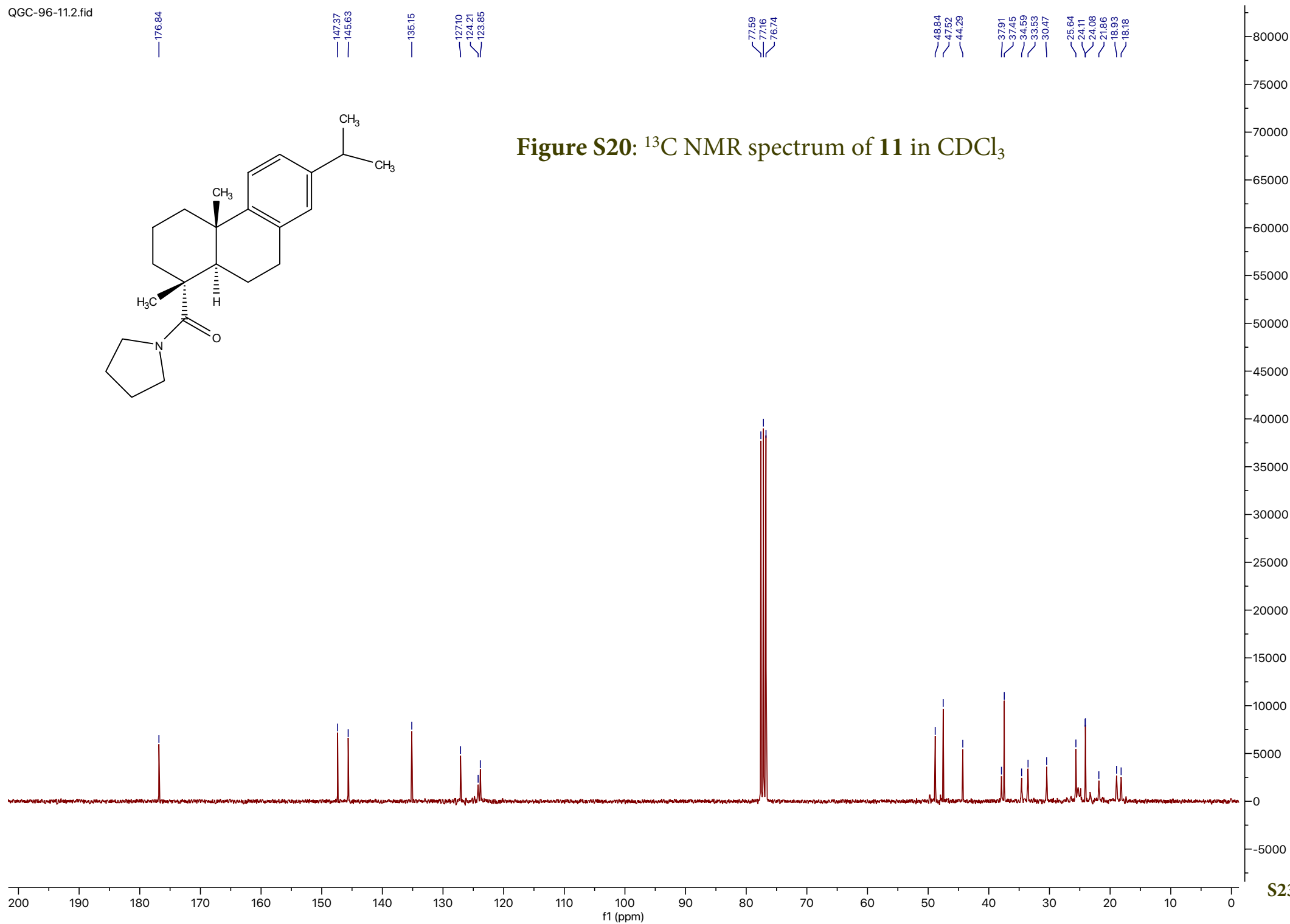
KP-102-27 #607 RT: 3.92 AV: 1 NL: 1.02E6  
T: FTMS + c ESI Full ms [300.0000-900.0000]







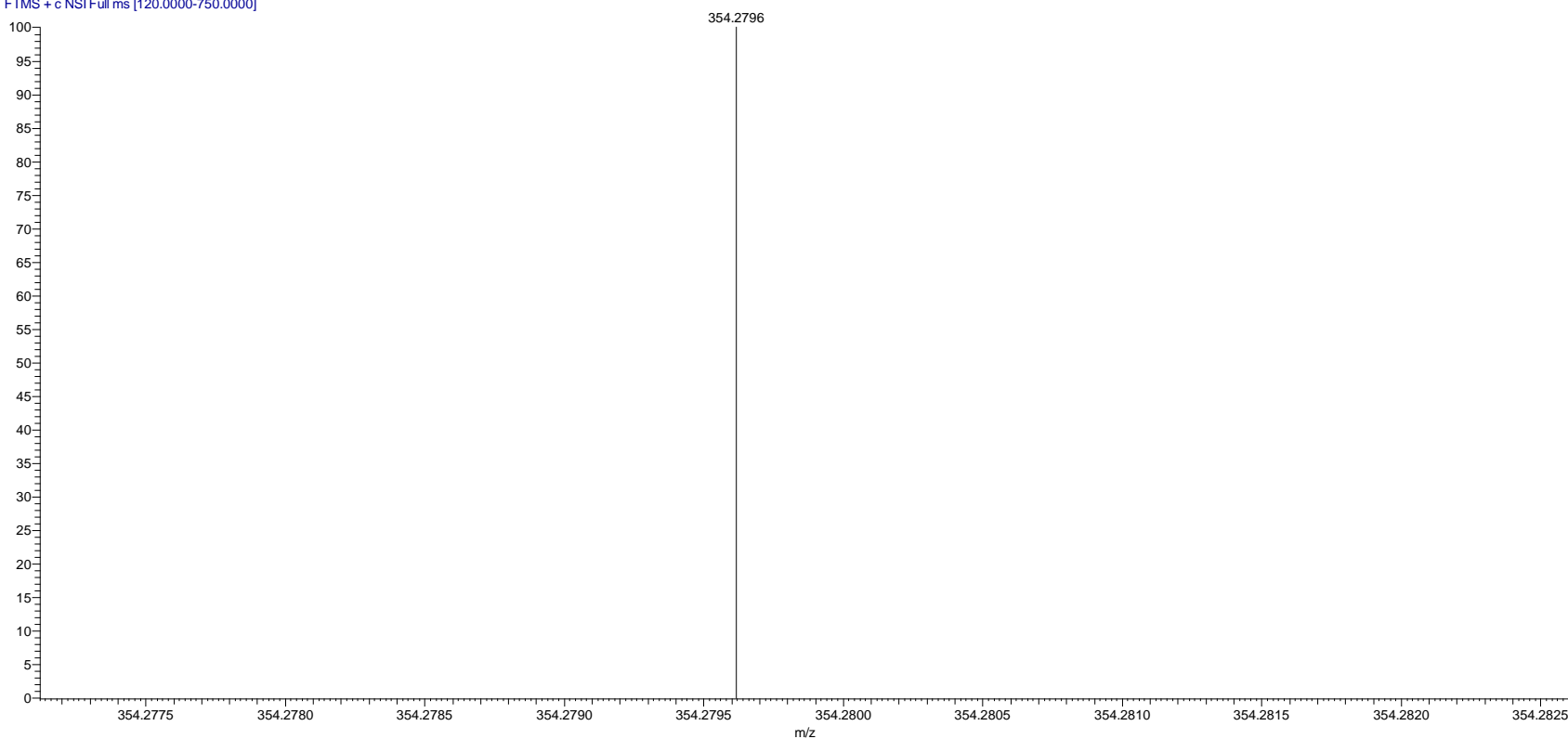
**Figure S20:**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CDCl}_3$



**Figure S21:** High resolution mass spectrum of **11**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-67	C <sub>24</sub> H <sub>35</sub> NO	353.2719	354.2797	354.2796	-0.0001	-0.17

IS-78-67- #2667-2691 RT: 14.42-14.55 AV: 25 NL: 5.73E5  
T: FTMS + c NSI Full ms [120.0000-750.0000]





7.260  
7.175  
7.147  
7.006  
6.979  
6.900

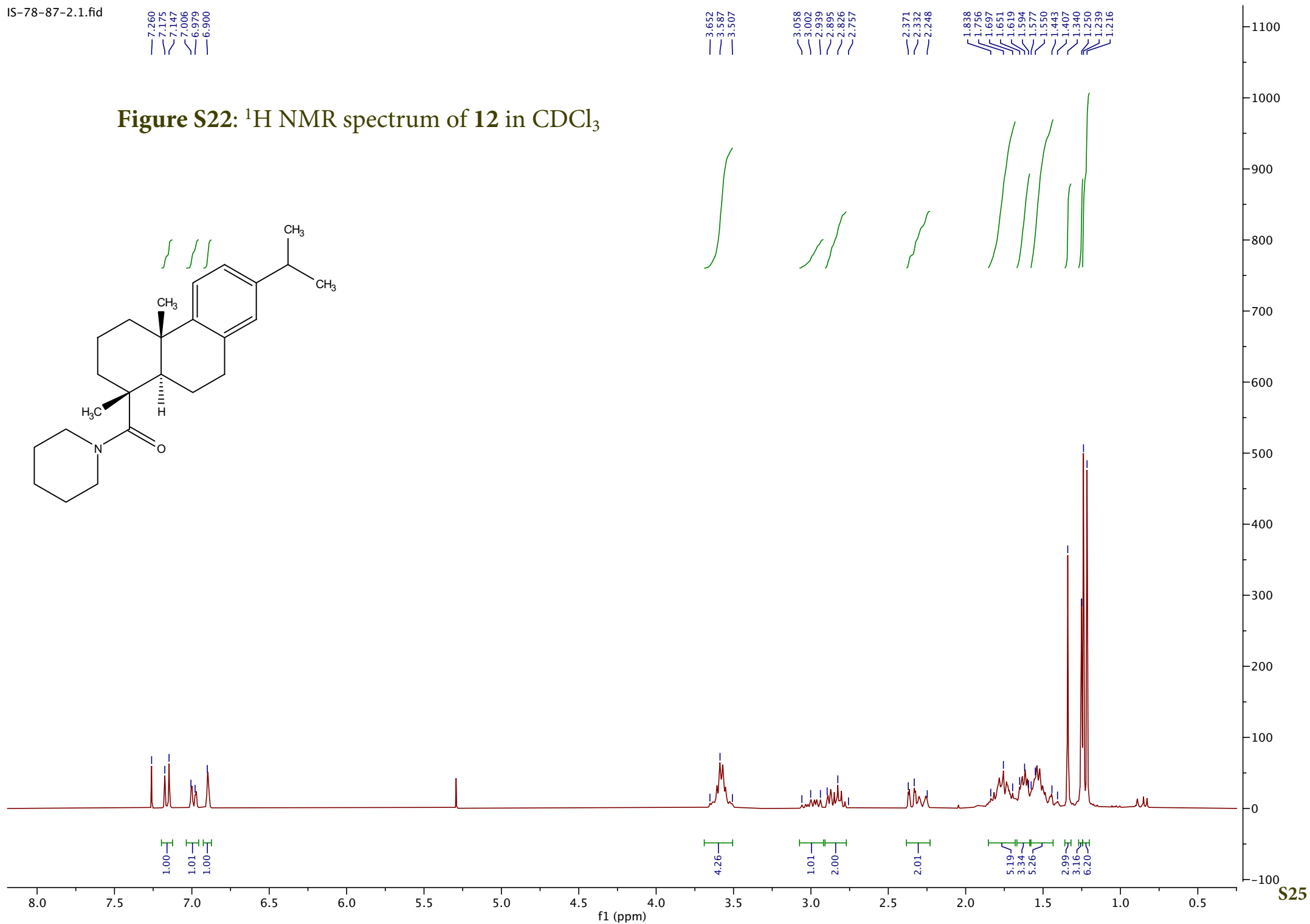
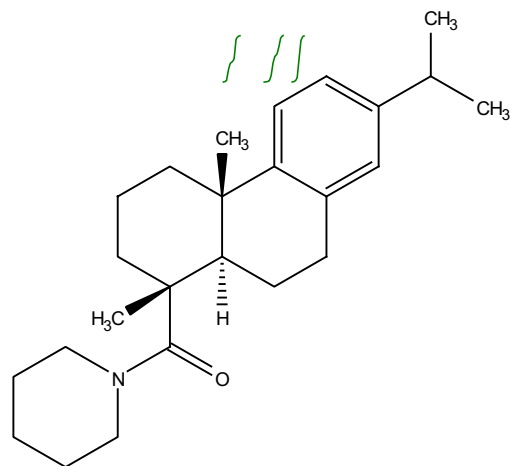
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3.587  
3.507

3.058  
3.002  
2.939  
2.895  
2.826  
2.757

2.371  
2.332  
2.248

1.838  
1.756  
1.697  
1.651  
1.619  
1.594  
1.577  
1.550  
1.443  
1.407  
1.340  
1.250  
1.239  
1.216

**Figure S22:**  $^1\text{H}$  NMR spectrum of **12** in  $\text{CDCl}_3$



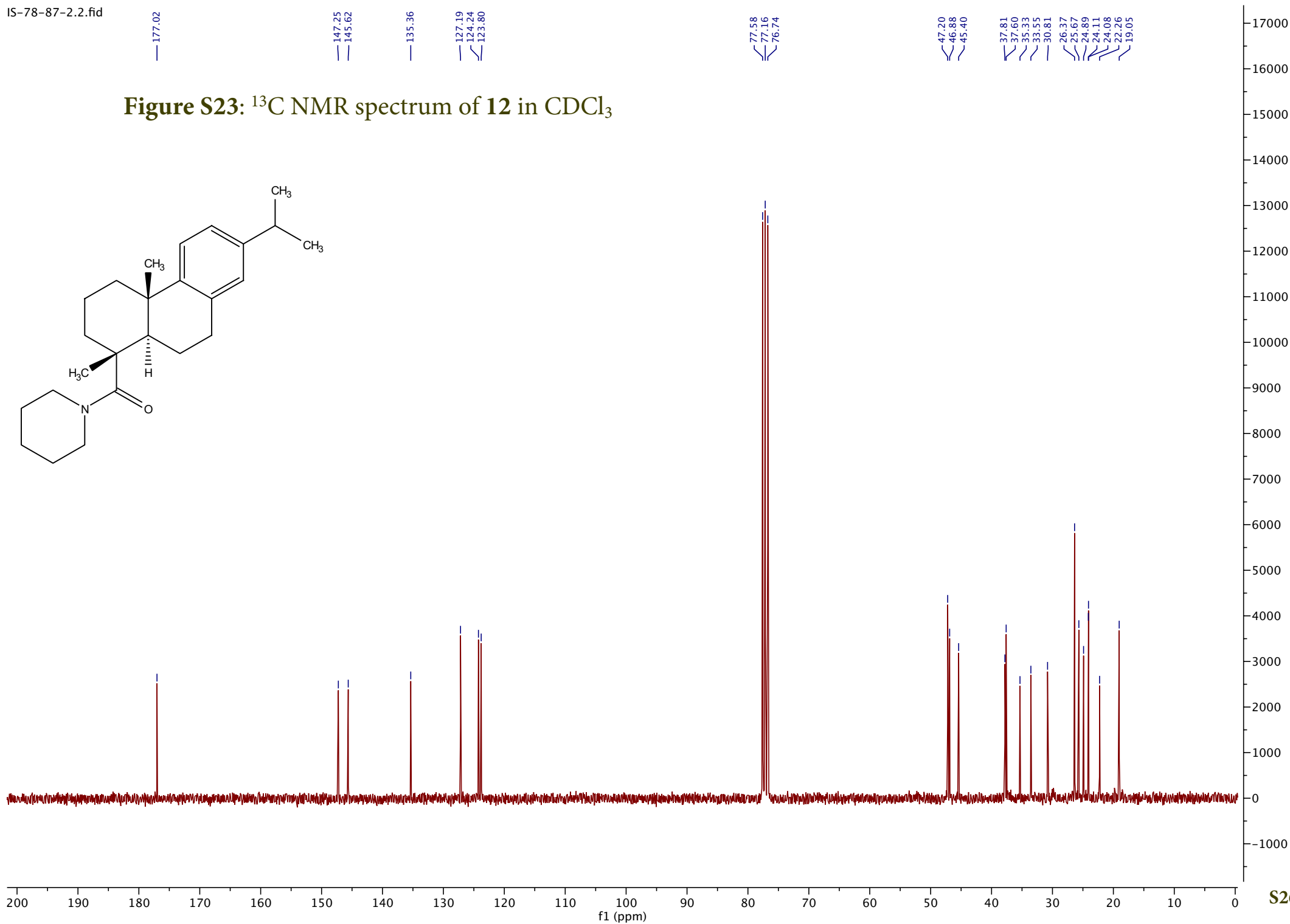
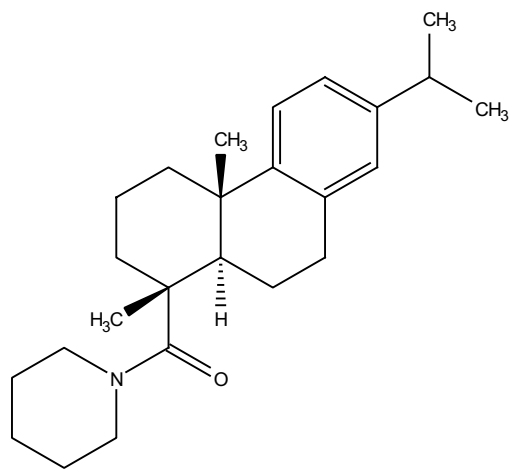
177.02

147.25  
145.62

135.36

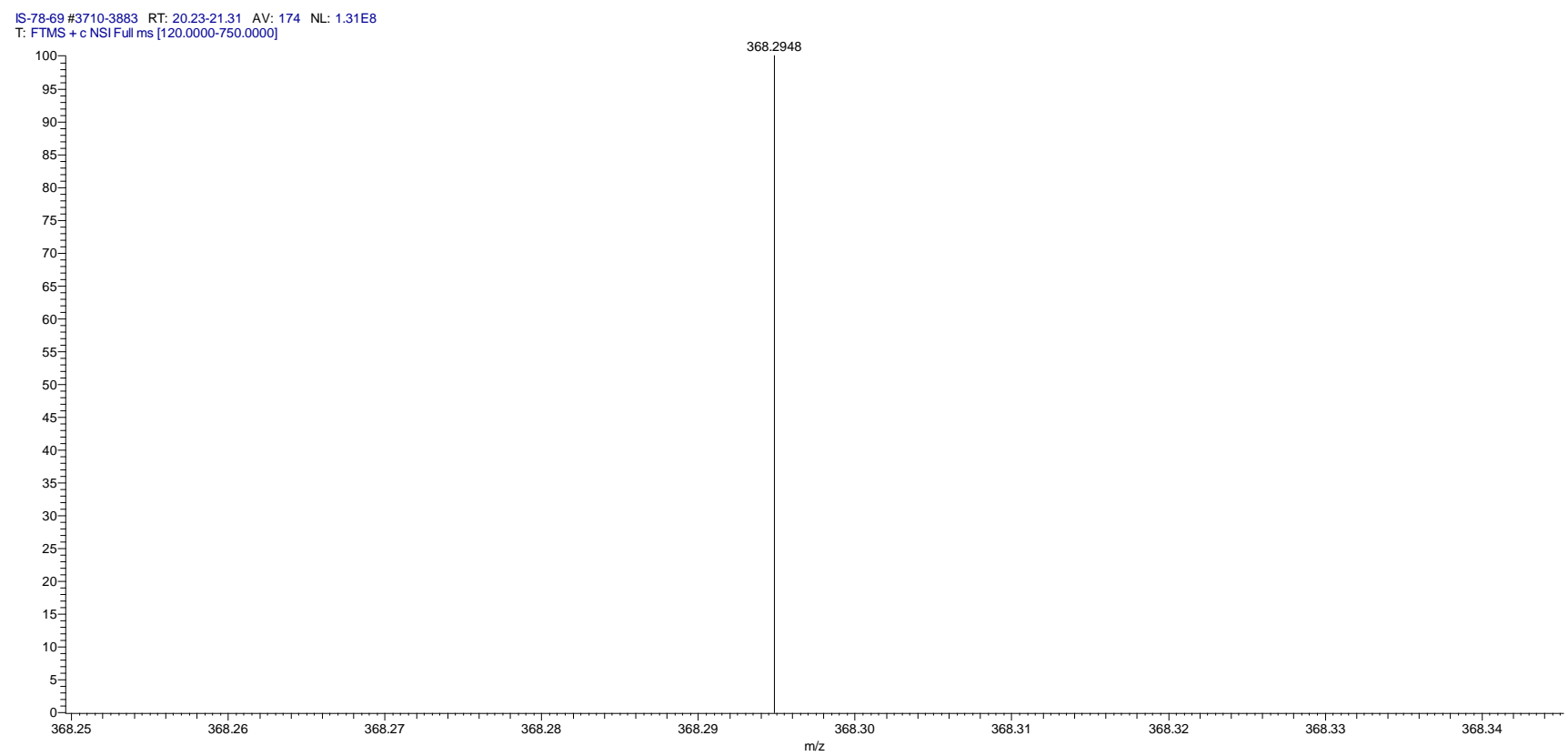
127.19  
124.24  
123.8077.58  
77.16  
76.7447.20  
46.88  
45.4037.81  
37.60  
35.33  
33.55

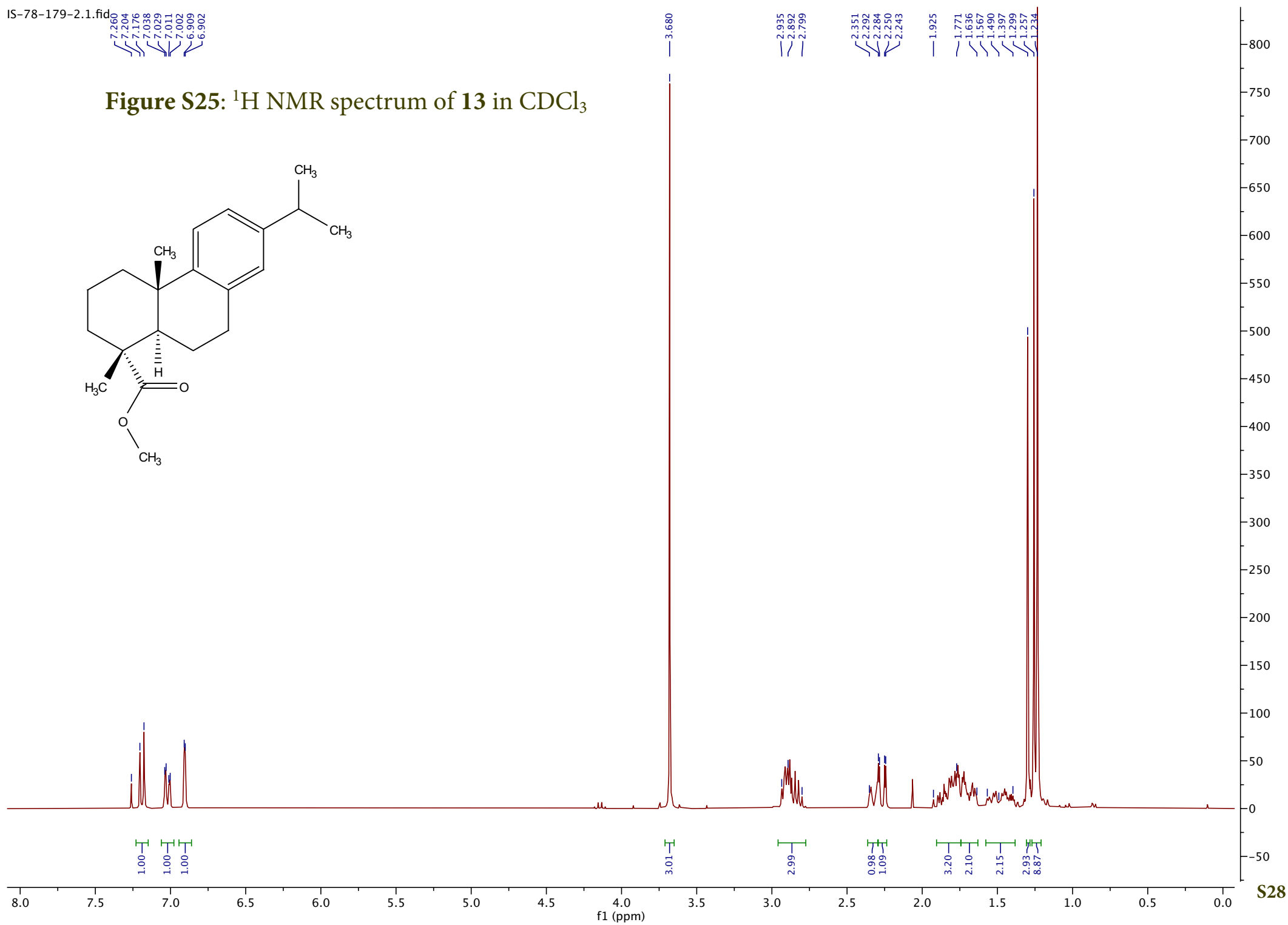
30.81

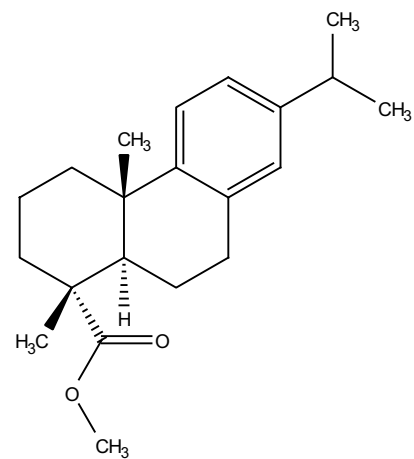
26.37  
25.67  
24.89  
24.11  
24.08  
22.26  
19.05**Figure S23:**  $^{13}\text{C}$  NMR spectrum of **12** in  $\text{CDCl}_3$ 

**Figure S24:** High resolution mass spectrum of **12**

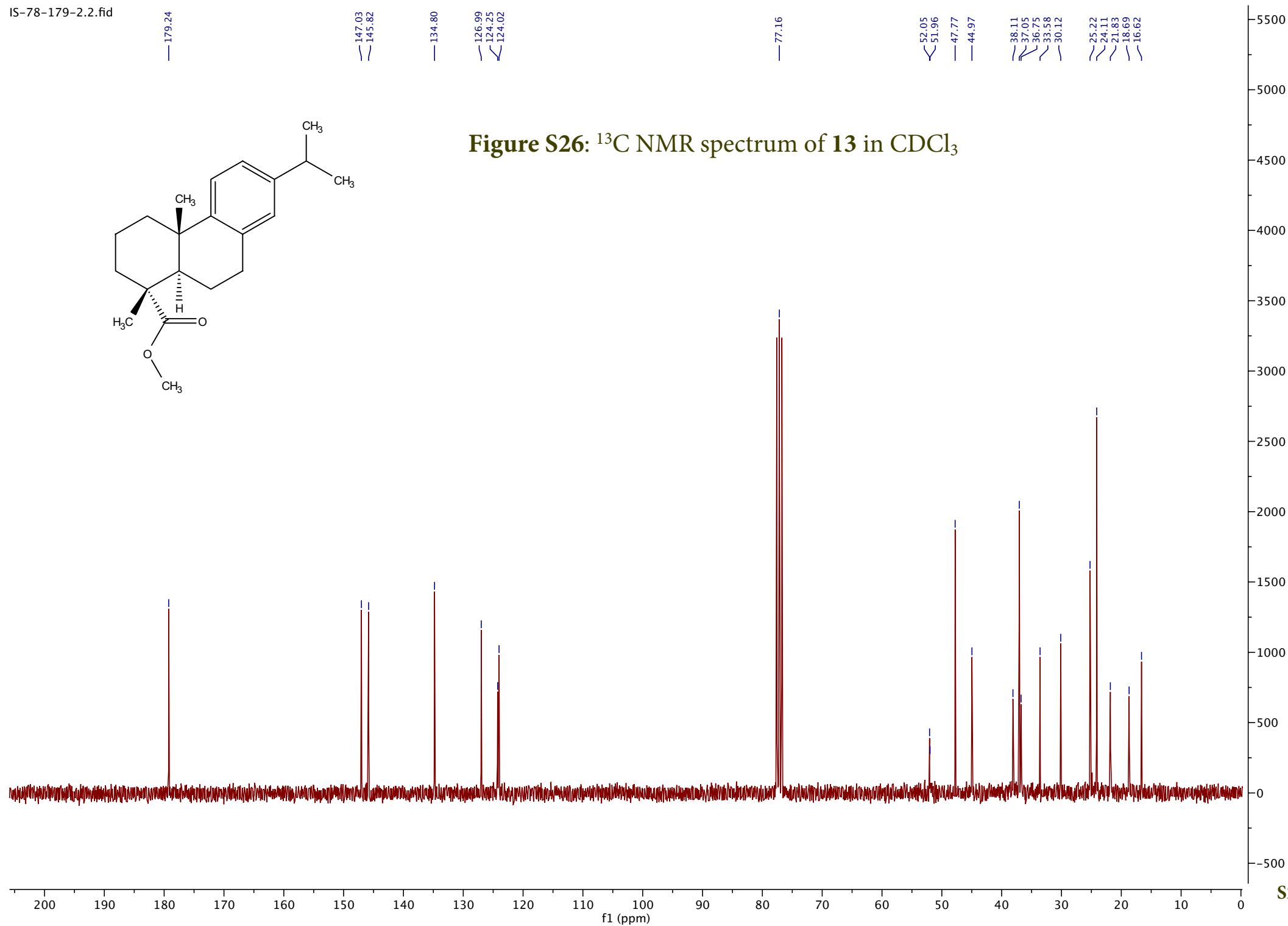
Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-69	C25H37NO	367.2875	368.2953	368.2948	-0.0005	-1.38



**Figure S25:**  $^1\text{H}$  NMR spectrum of **13** in  $\text{CDCl}_3$ 



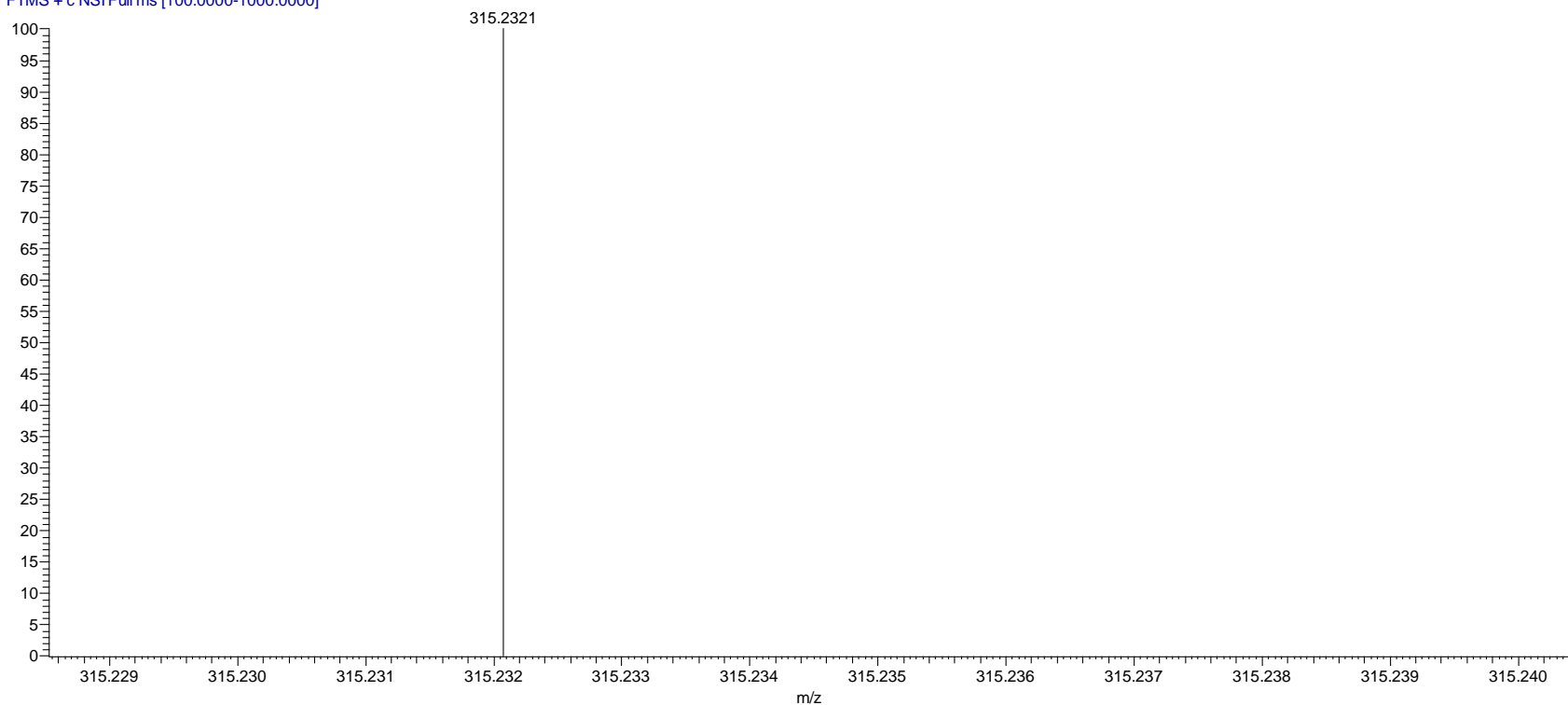
**Figure S26:** <sup>13</sup>C NMR spectrum of **13** in CDCl<sub>3</sub>

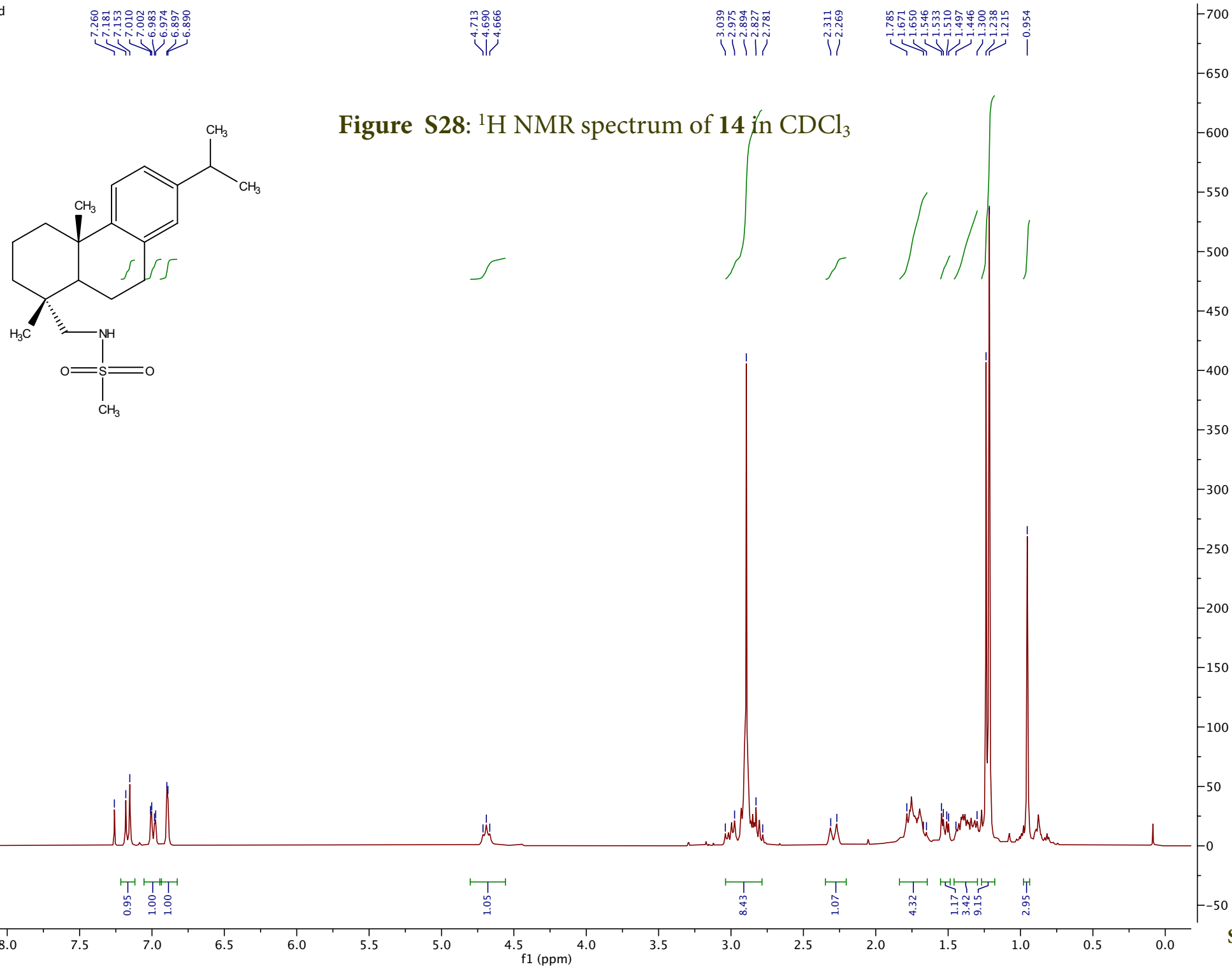


**Figure S27:** High resolution mass spectrum of **13**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-179-2	C21H31O2	314.2246	315.2324	315.2321	-0.0003	-0.92

IS-78-179-2 #2765-2885 RT: 14.49-15.12 AV: 121 NL: 1.98E7  
T: FTMS + c NSI Full ms [100.0000-1000.0000]





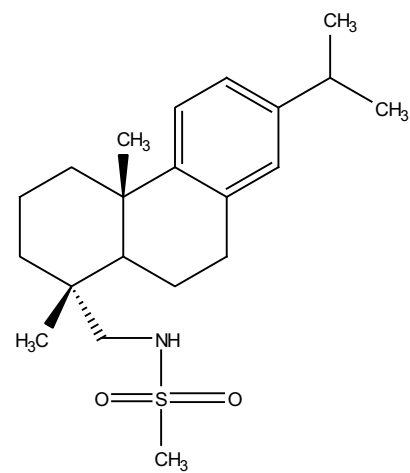


Figure S29: <sup>13</sup>C NMR spectrum of 14 in CDCl<sub>3</sub>

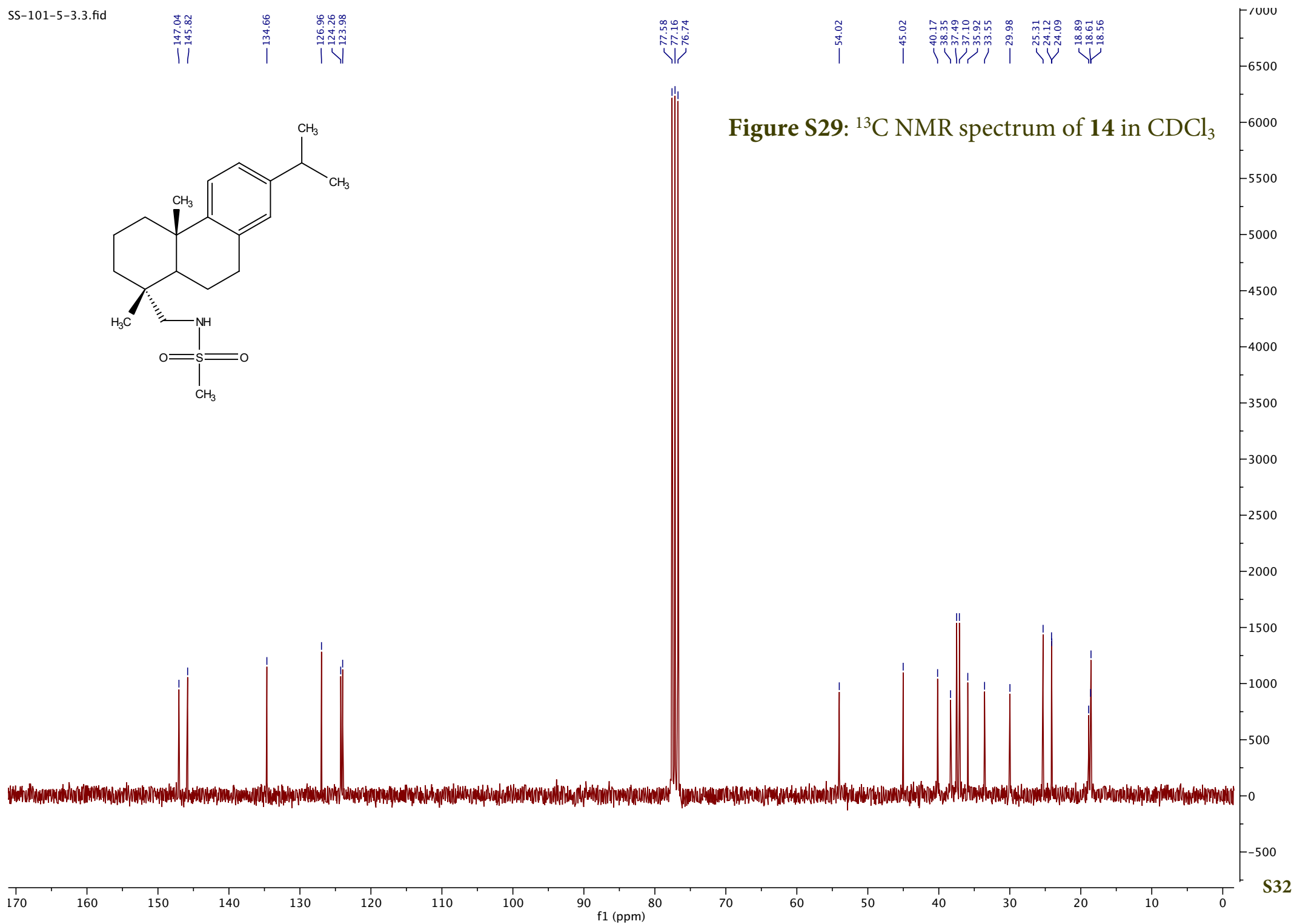
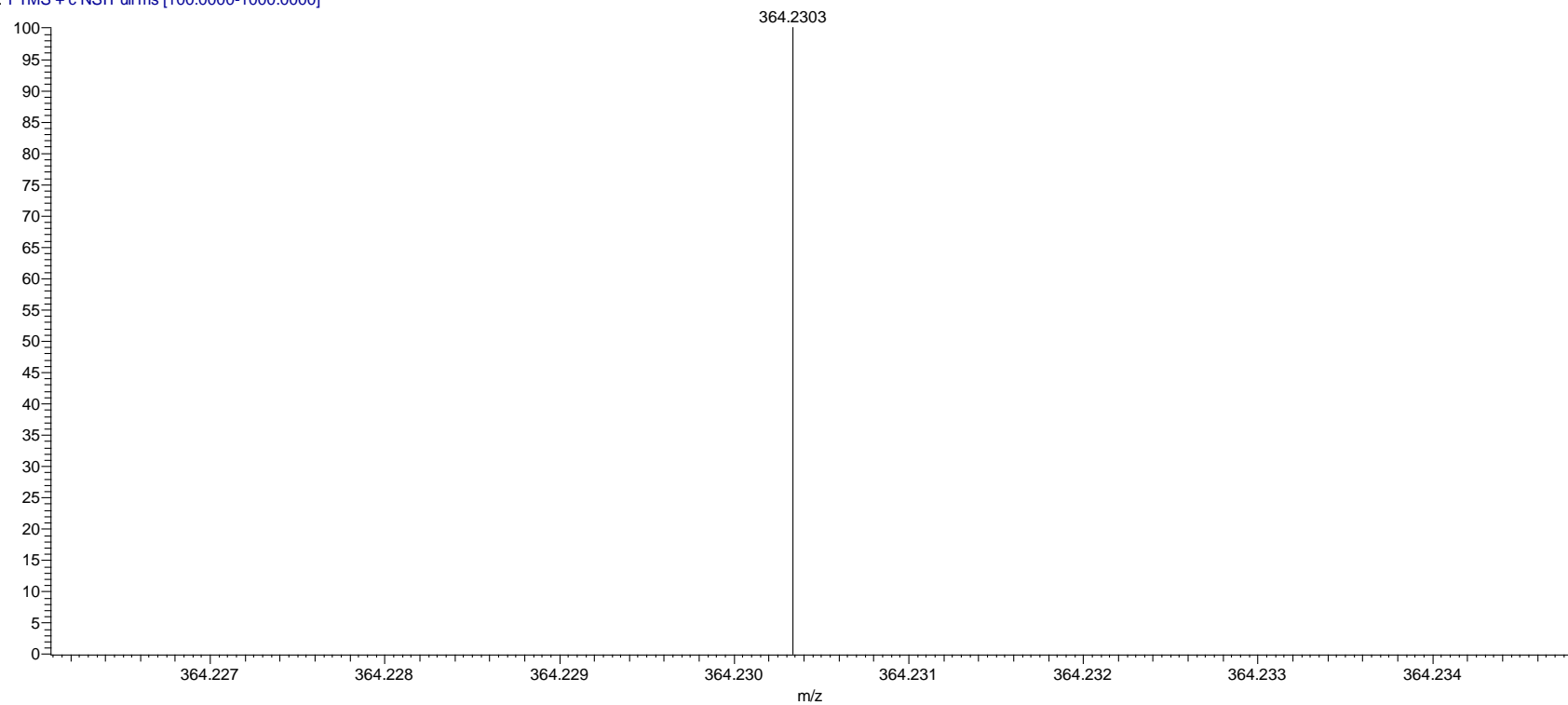


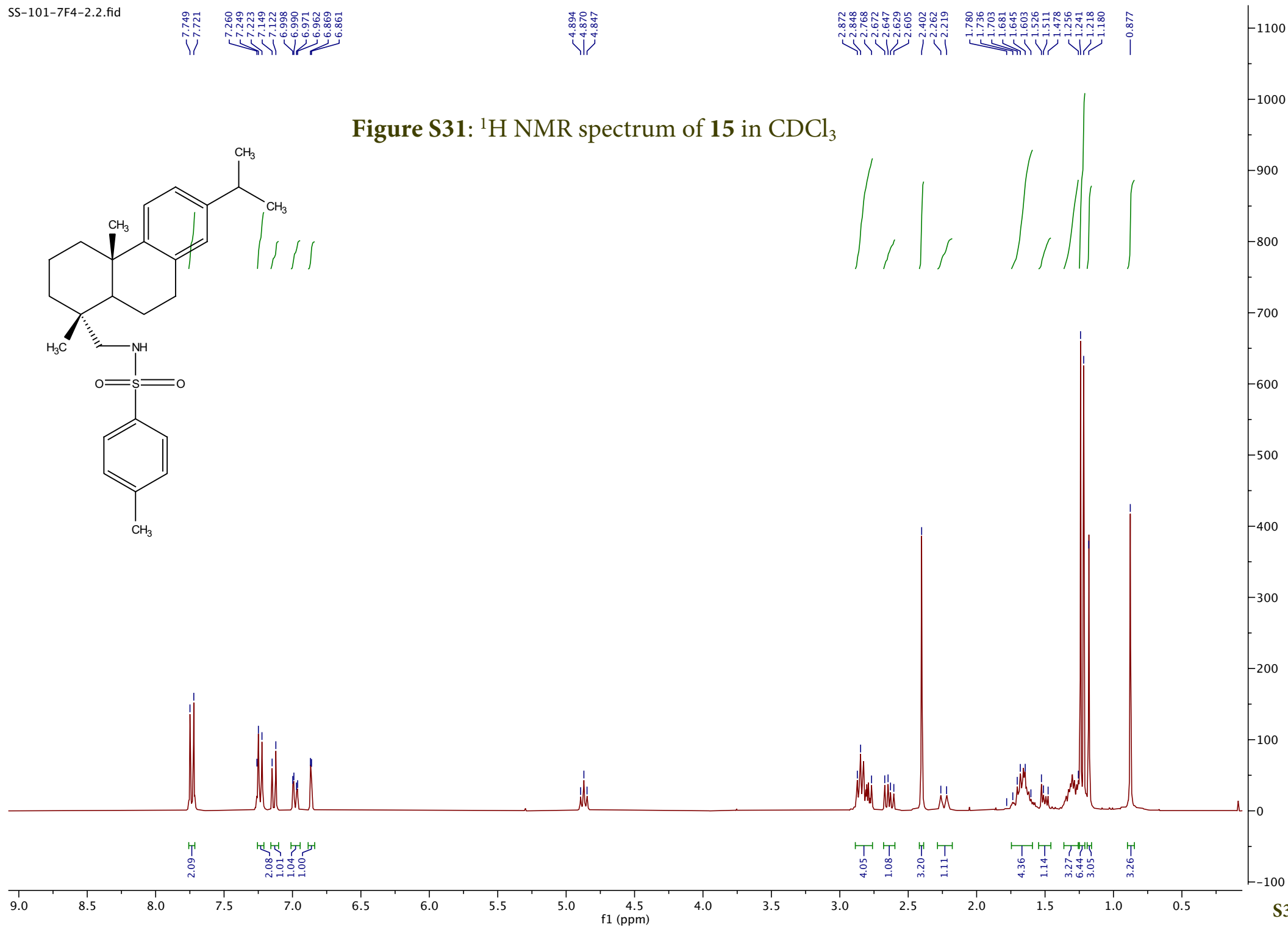


Figure S30: High resolution mass spectrum of 14

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SS-101-5-3	C21H33NO2S	363.2232	364.2310	364.2303	-0.0007	-1.92

SS-101-5-3 #2022-3892 RT: 10.74-20.54 AV: 1871 NL: 1.26E6  
T: FTMS + c NSI Full ms [100.0000-1000.0000]





147.07  
145.66  
143.33  
137.19  
134.76  
129.81  
127.08  
126.93  
124.22  
123.88

77.58  
77.16  
76.74

53.89

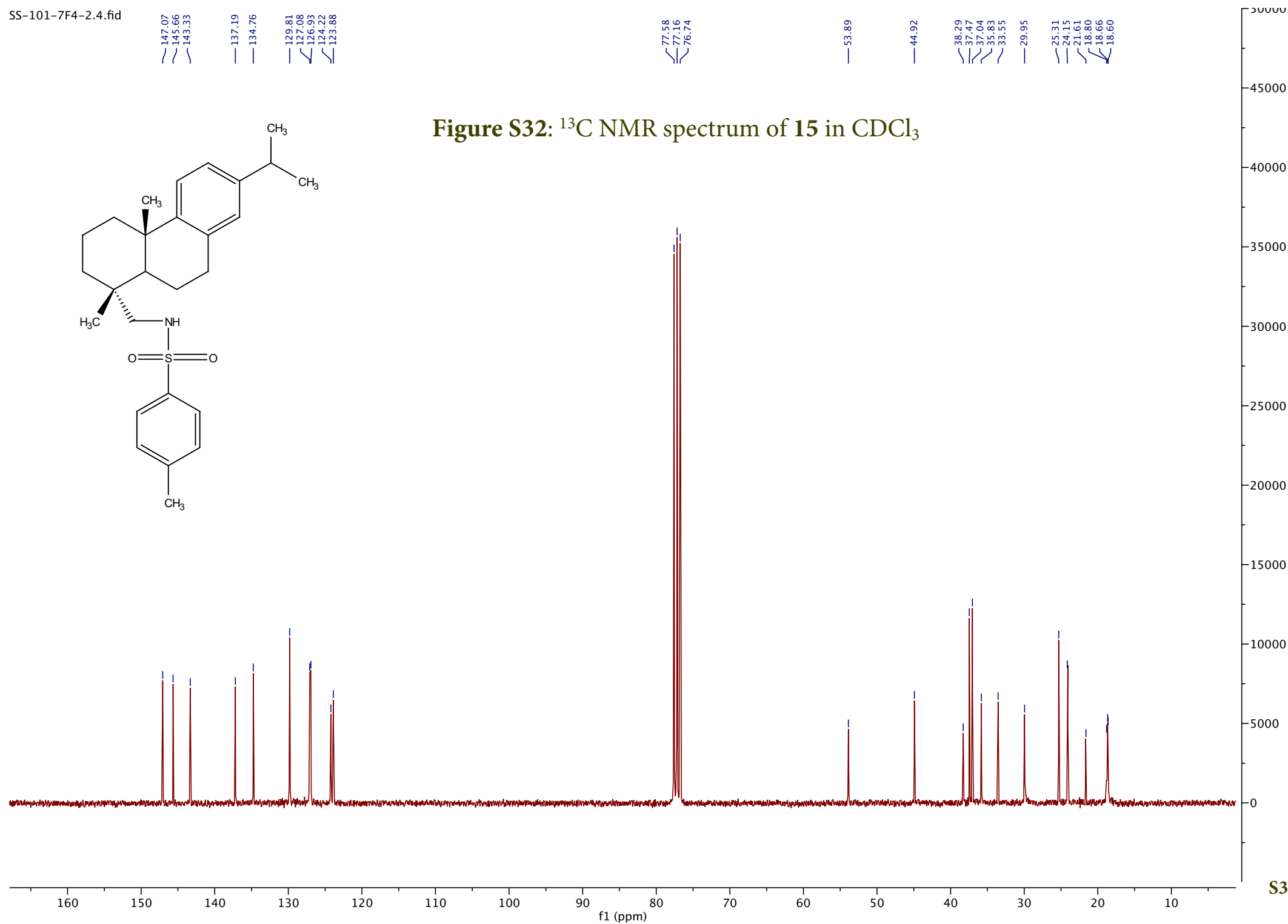
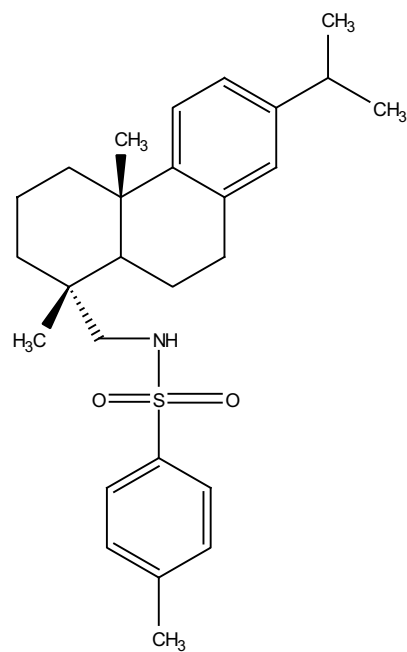
44.92

38.29  
37.47  
37.04  
35.83  
33.55

29.95

25.31  
24.15  
21.61  
18.80  
18.66  
18.60

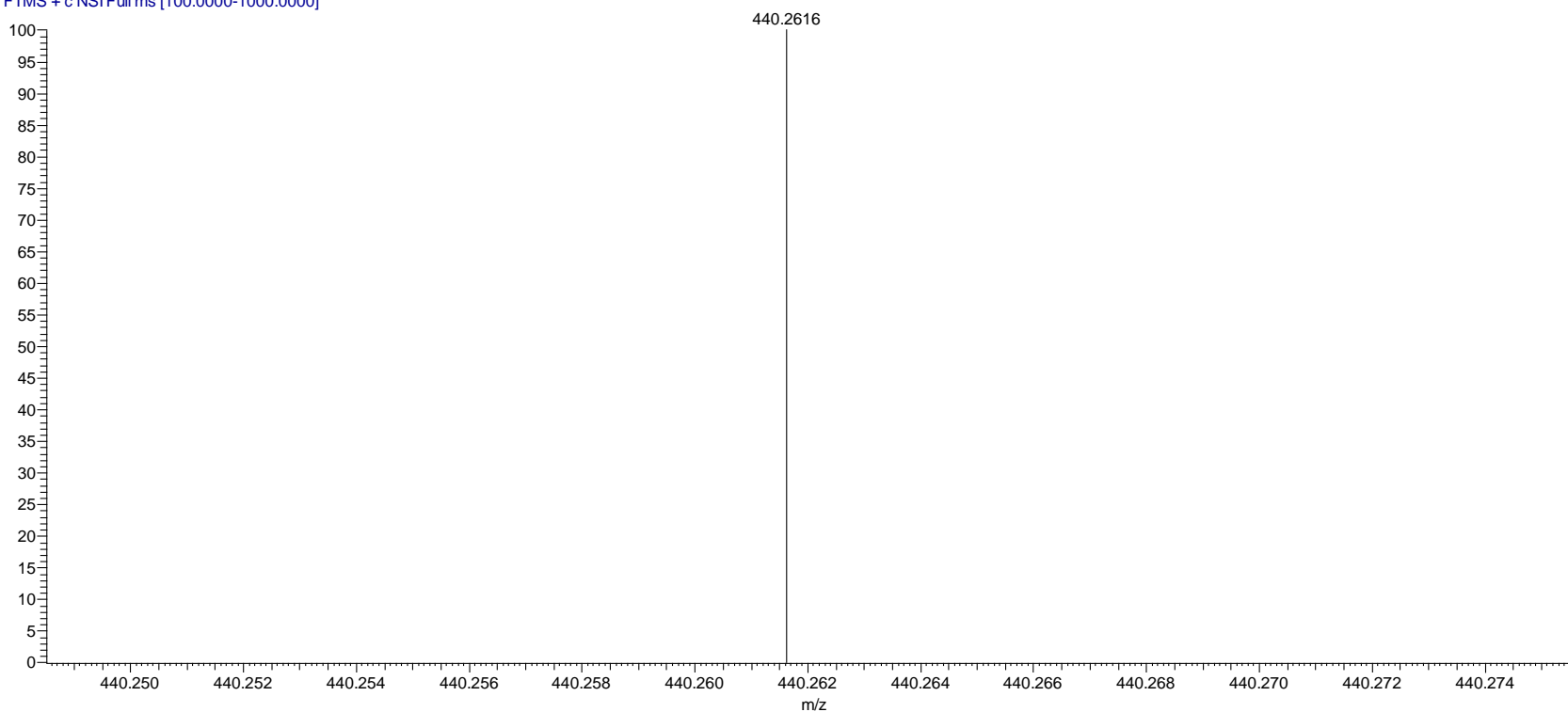
**Figure S32:**  $^{13}\text{C}$  NMR spectrum of **15** in  $\text{CDCl}_3$



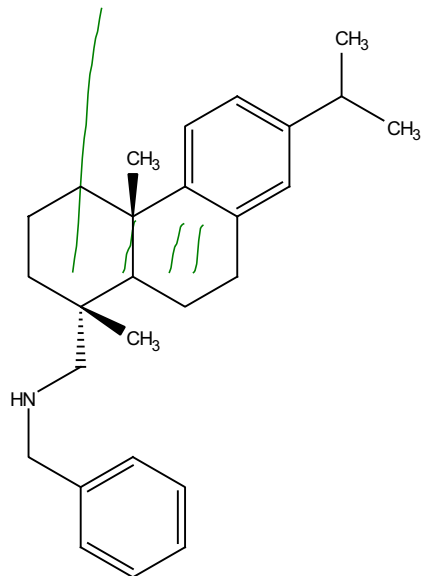
**Figure S33:** High resolution mass spectrum of **15**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SS-101-7-4	C27H37NO2S	439.2545	440.2623	440.2616	-0.0007	-1.59

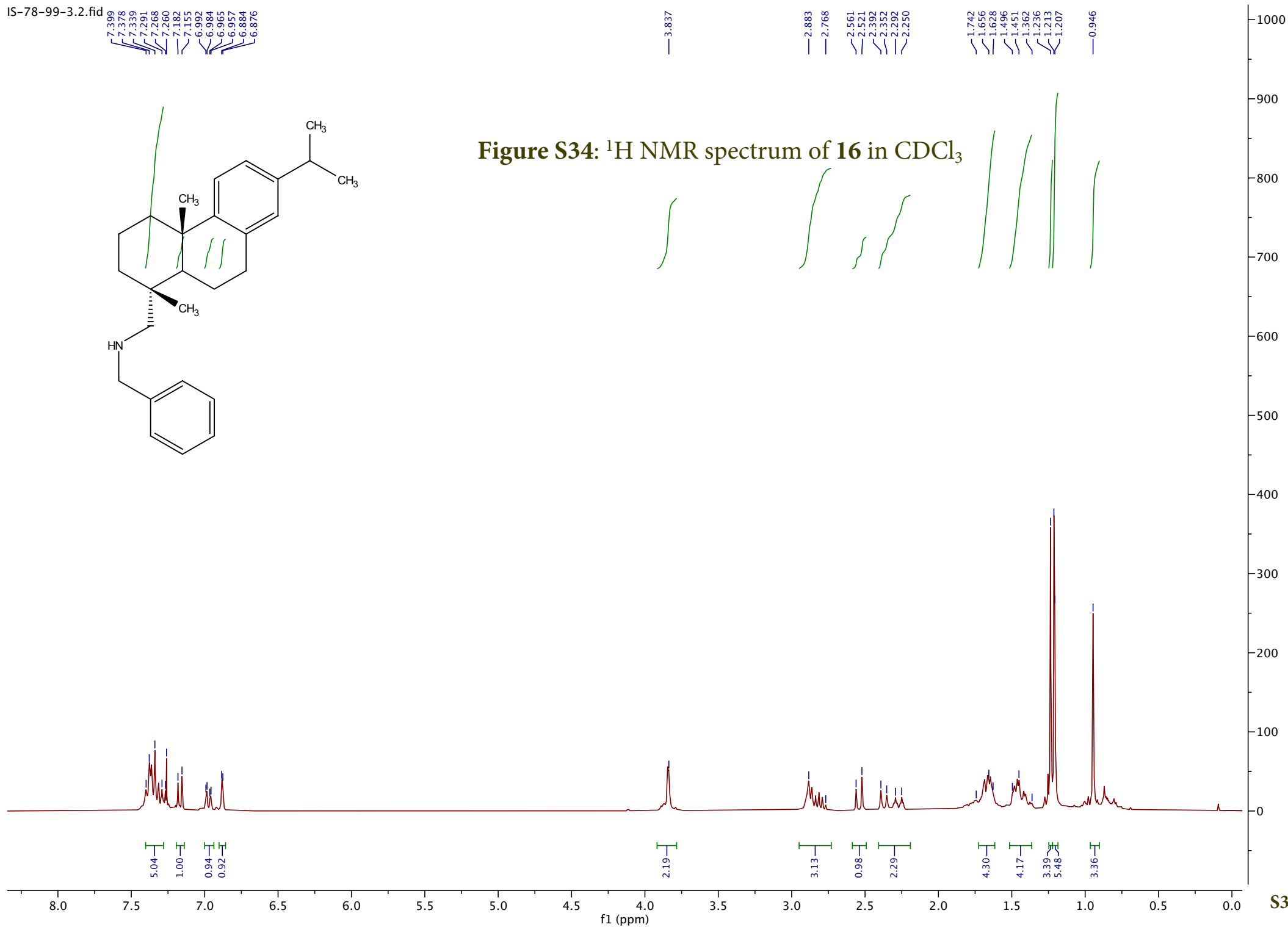
SS-101-7-4- #3988-4051 RT: 21.22-21.58 AV: 64 NL: 2.04E7  
T: FTMS + c NSI Full ms [100.0000-1000.0000]

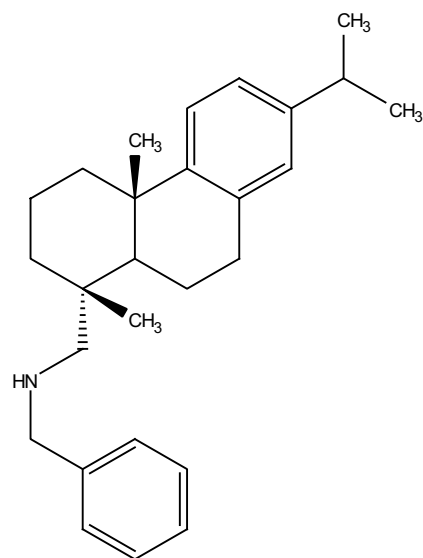


7.399  
7.378  
7.339  
7.291  
7.268  
7.260  
7.182  
7.155  
6.984  
6.982  
6.965  
6.957  
6.884  
6.876



**Figure S34:**  $^1\text{H}$  NMR spectrum of **16** in  $\text{CDCl}_3$



147.53  
145.55

134.87

128.52  
127.31  
126.89  
124.34  
123.9077.58  
77.36  
76.74

60.33

54.26

45.52

38.48  
37.55  
37.06

33.53

30.27

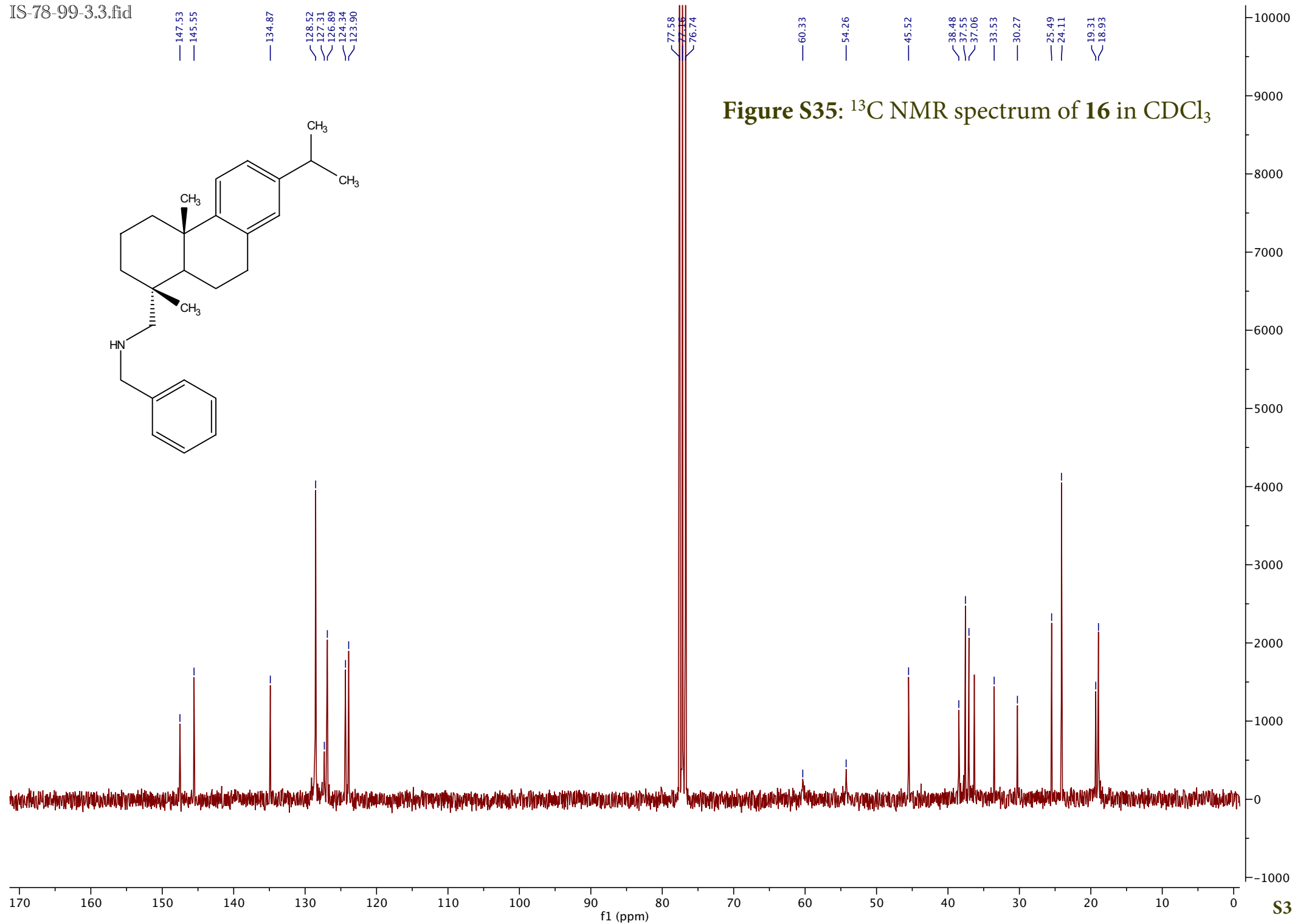
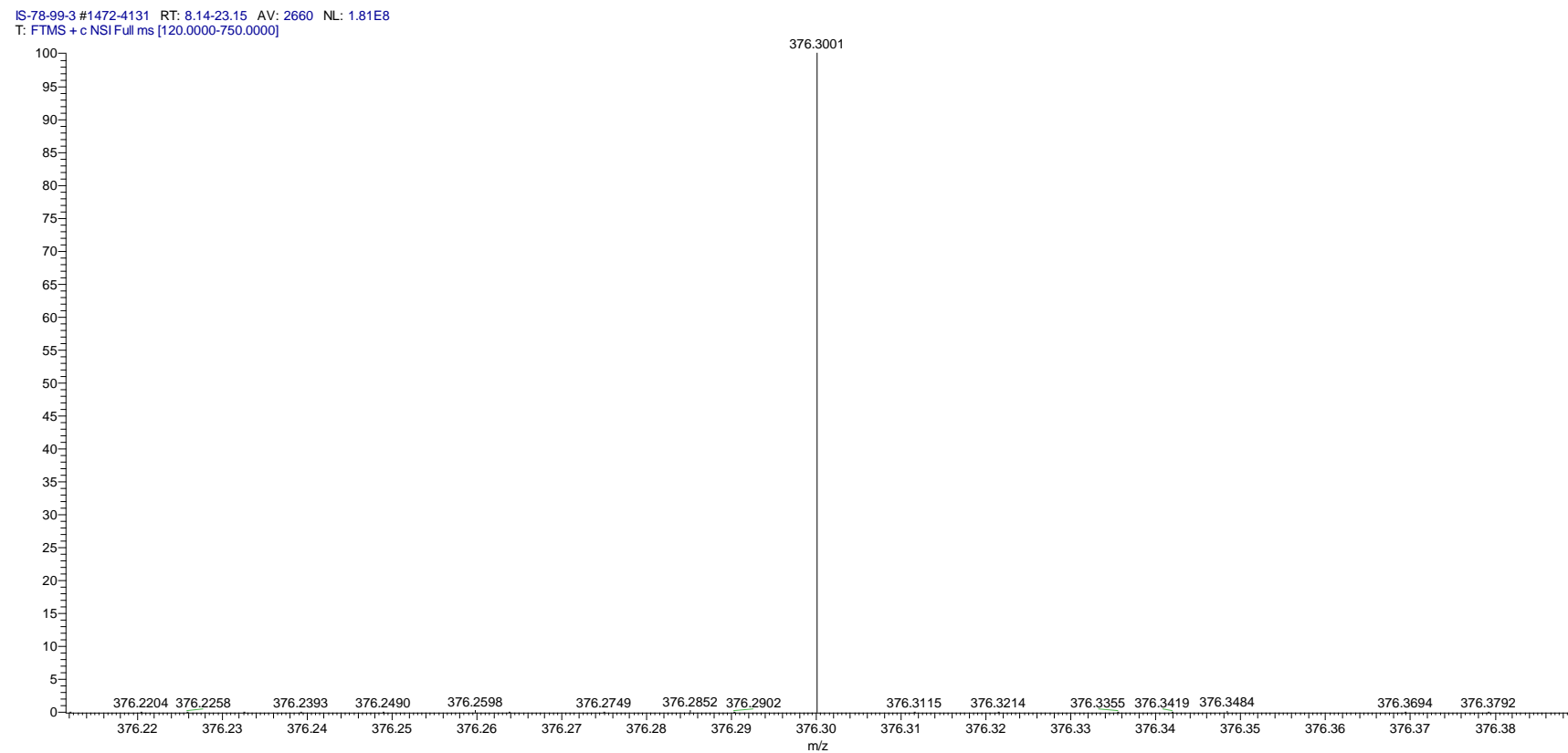
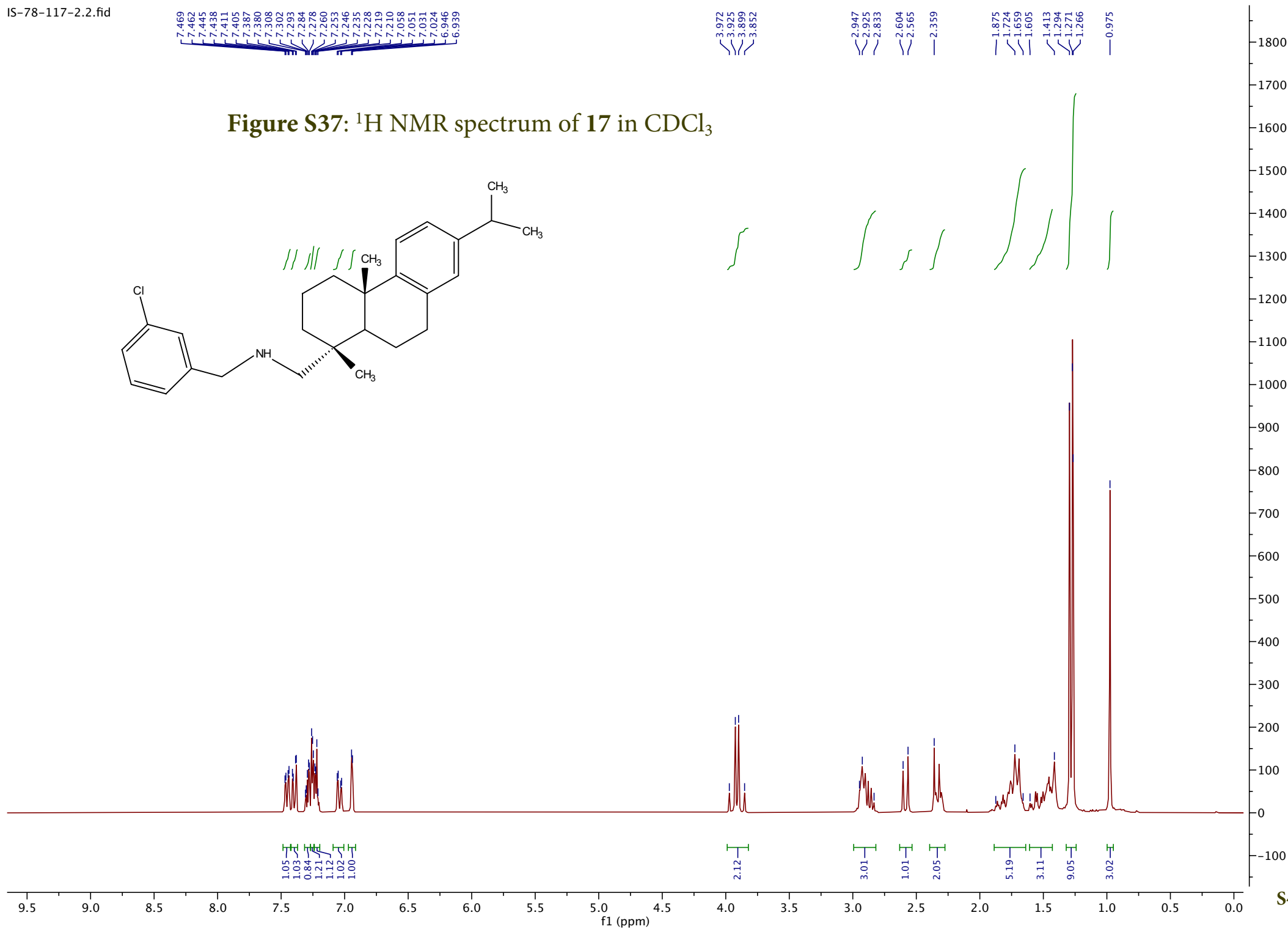
25.49  
24.1119.31  
18.93**Figure S35:**  $^{13}\text{C}$  NMR spectrum of **16** in  $\text{CDCl}_3$ 

Figure S36: High resolution mass spectrum of 16

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-99-3	C27H37N	375.2926	376.3004	376.3001	-0.0003	-0.77







147.67  
145.55138.32  
134.96  
133.76130.15  
129.51  
128.19126.92  
126.79  
124.45  
123.9277.58  
77.16  
76.73

61.02

52.30

45.34

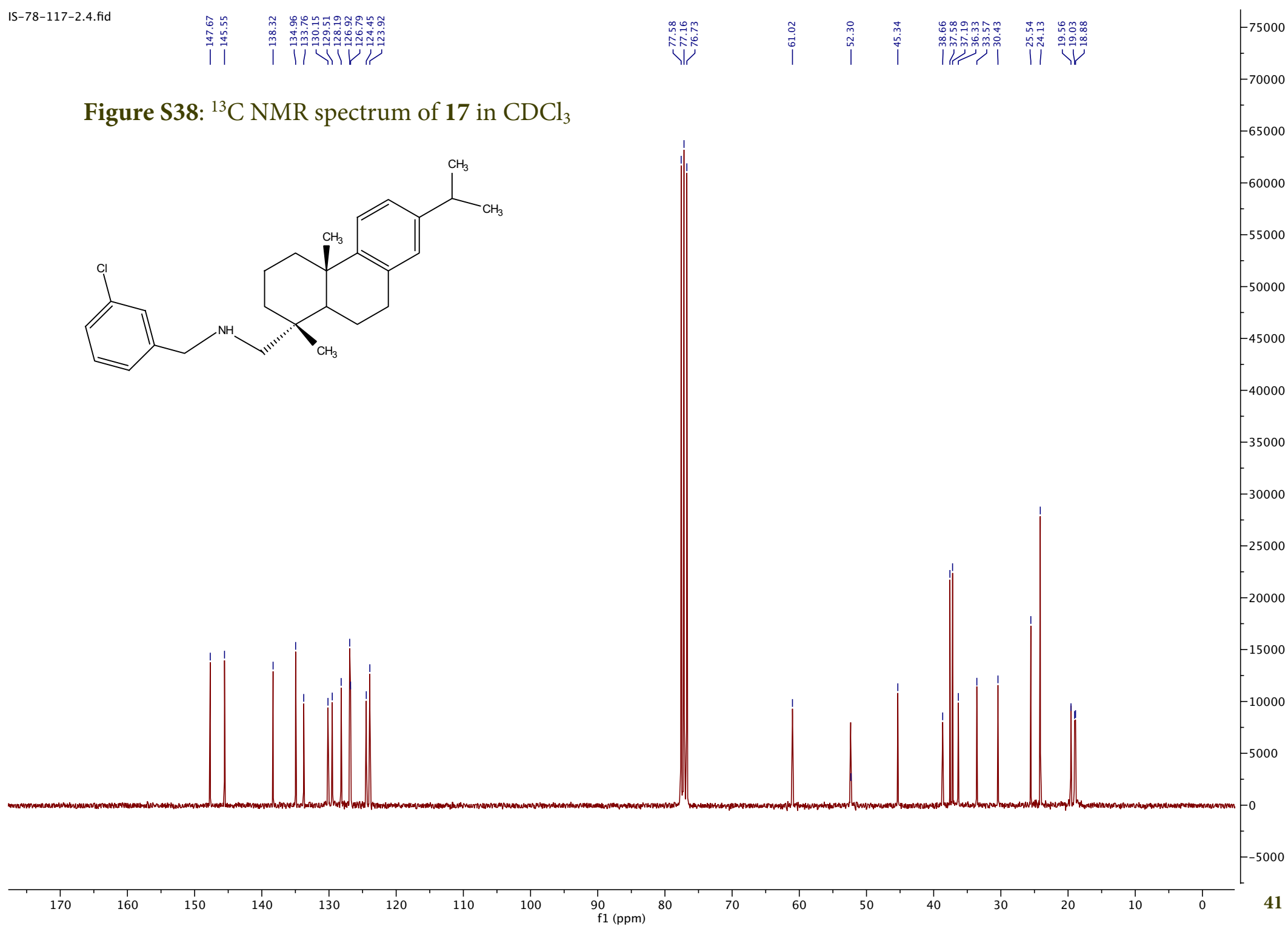
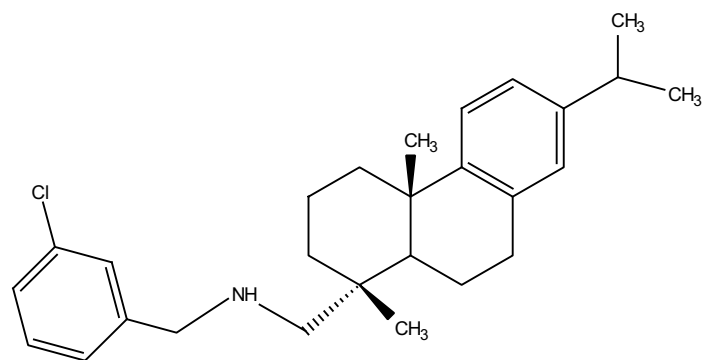
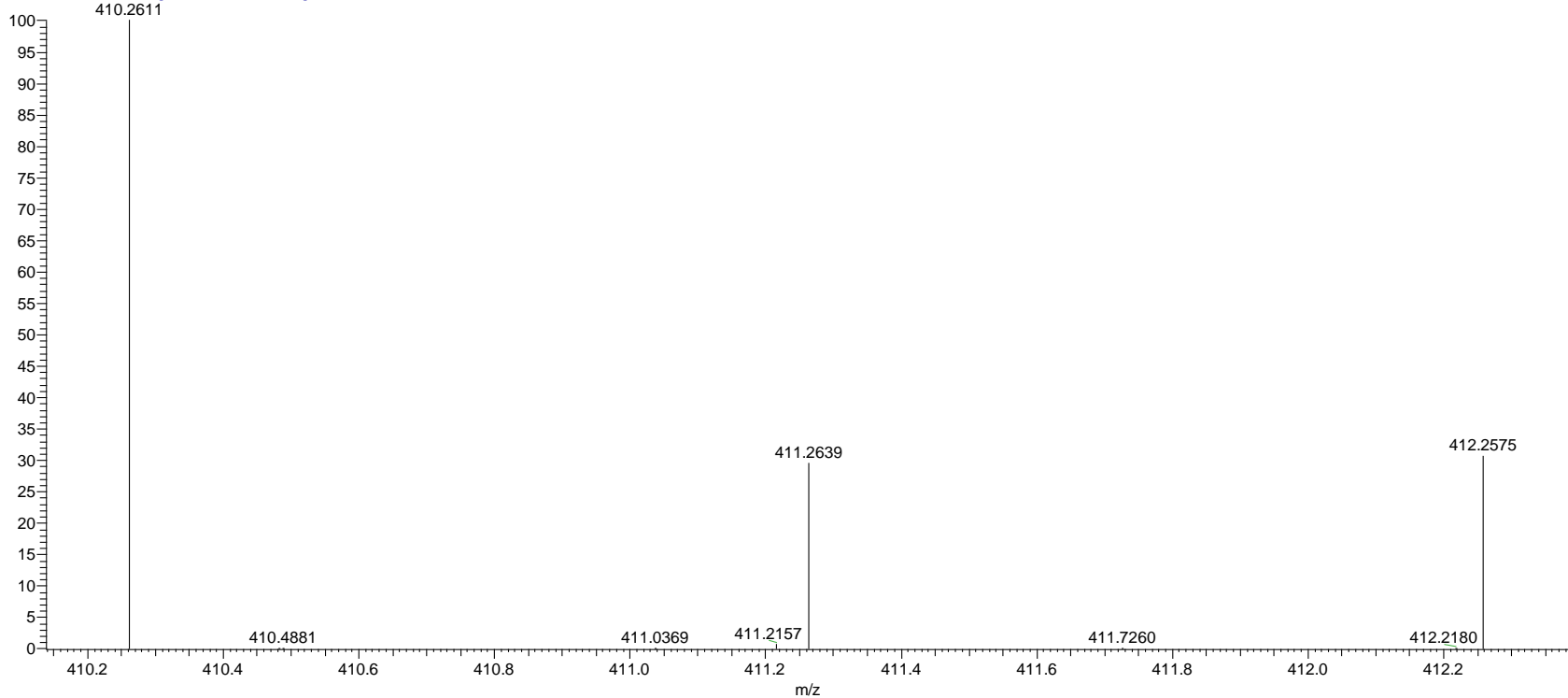
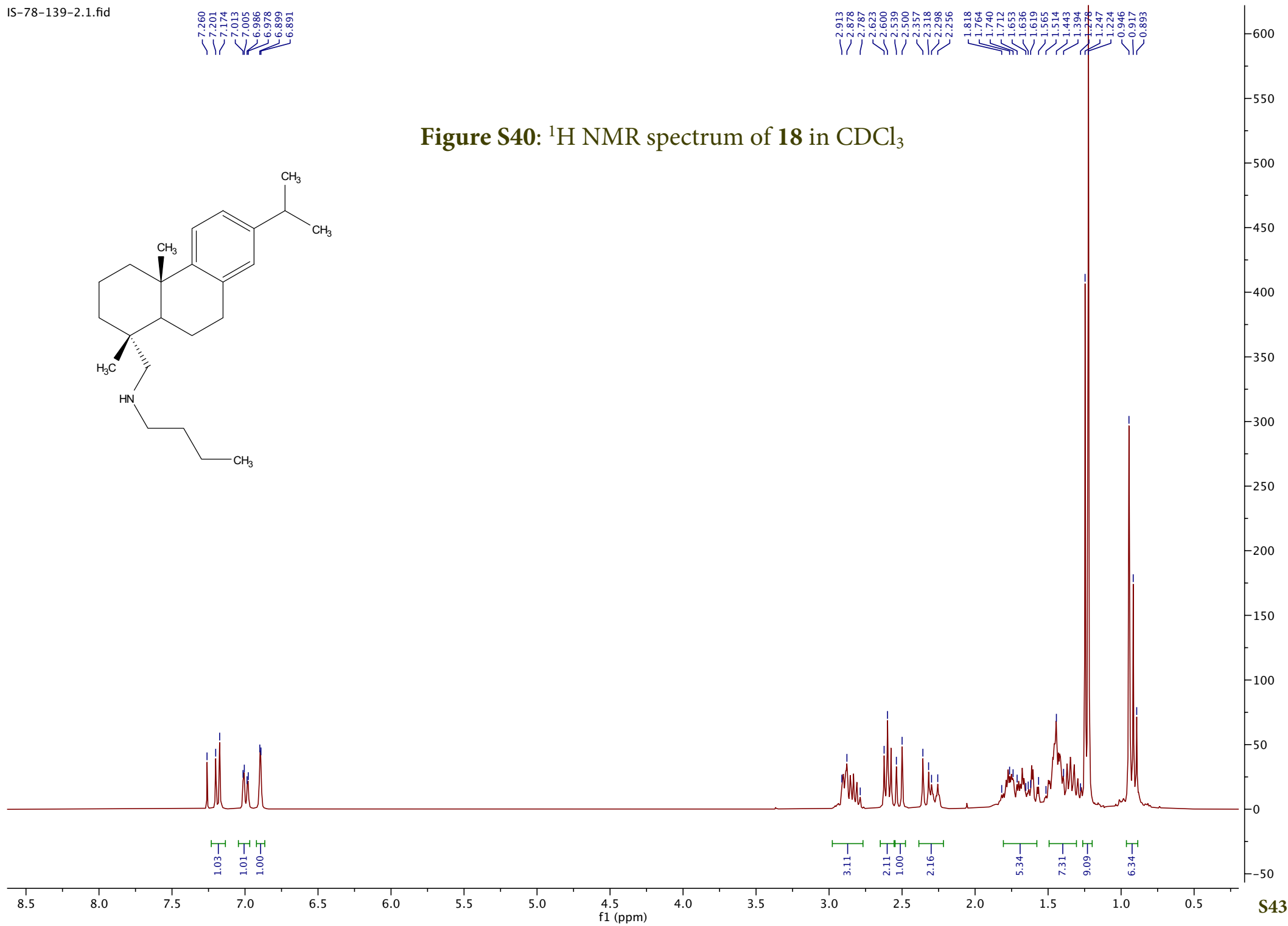
38.66  
37.58  
37.1936.33  
33.57  
30.4325.54  
24.1319.56  
19.03  
18.88**Figure S38:**  $^{13}\text{C}$  NMR spectrum of **17** in  $\text{CDCl}_3$ 

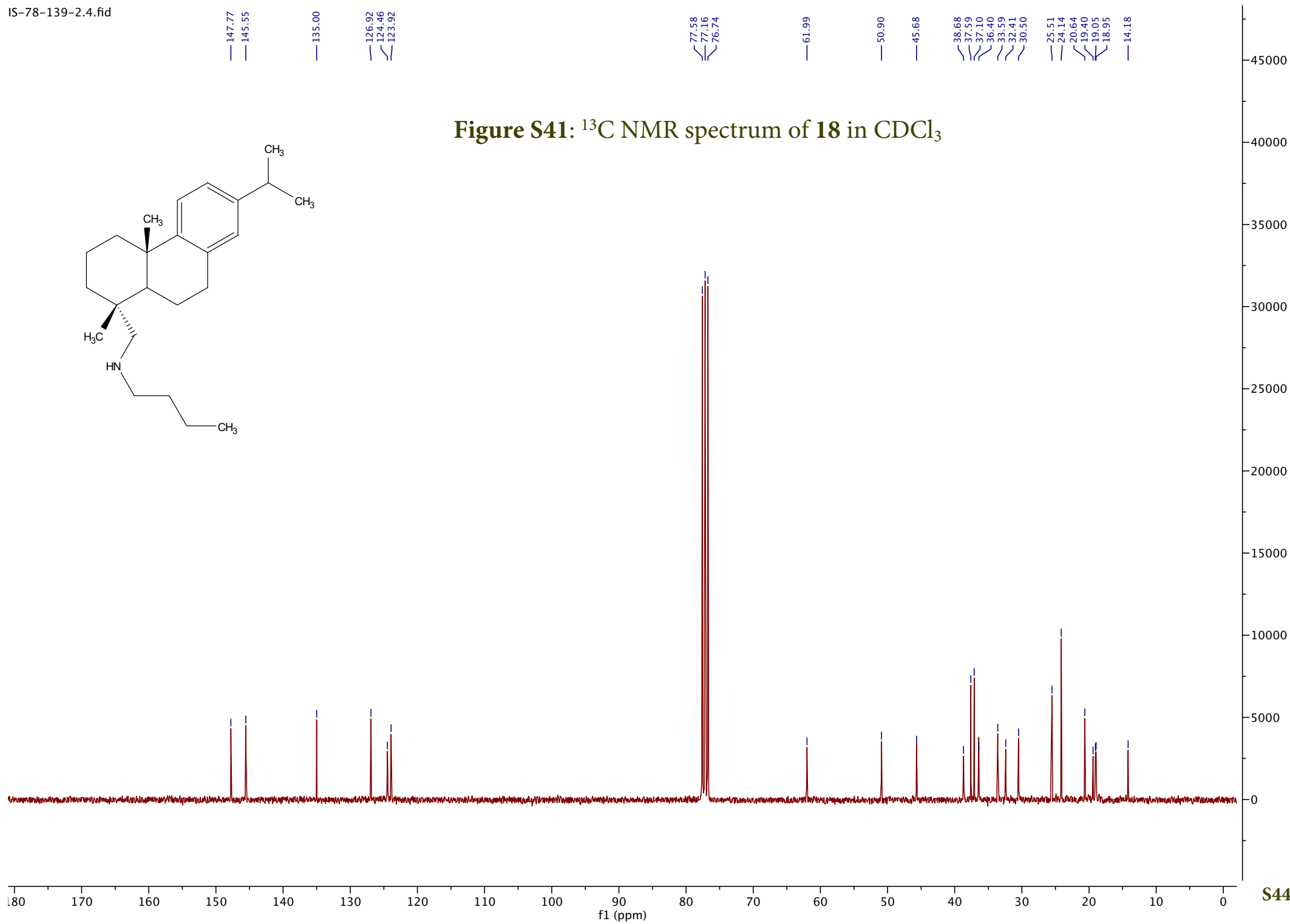
Figure S39: High resolution mass spectrum of 17

Sample Name	Mol Fomula	MW(COME WITH SAMPLES)	MW(CALCULATED)	M+H	observed	delta	ppm
IS-78-117	C27H36ClN	409.2536	409.25362	410.2614	<b>410.2611</b>	-0.0003	-0.78
			411.25067	412.2585	<b>412.2575</b>	-0.0010	-2.35

IS-78-117 #582-599 RT: 3.79-3.88 AV: 18 NL: 1.91E8  
T: FTMS + c ESI Full ms [300.0000-900.0000]



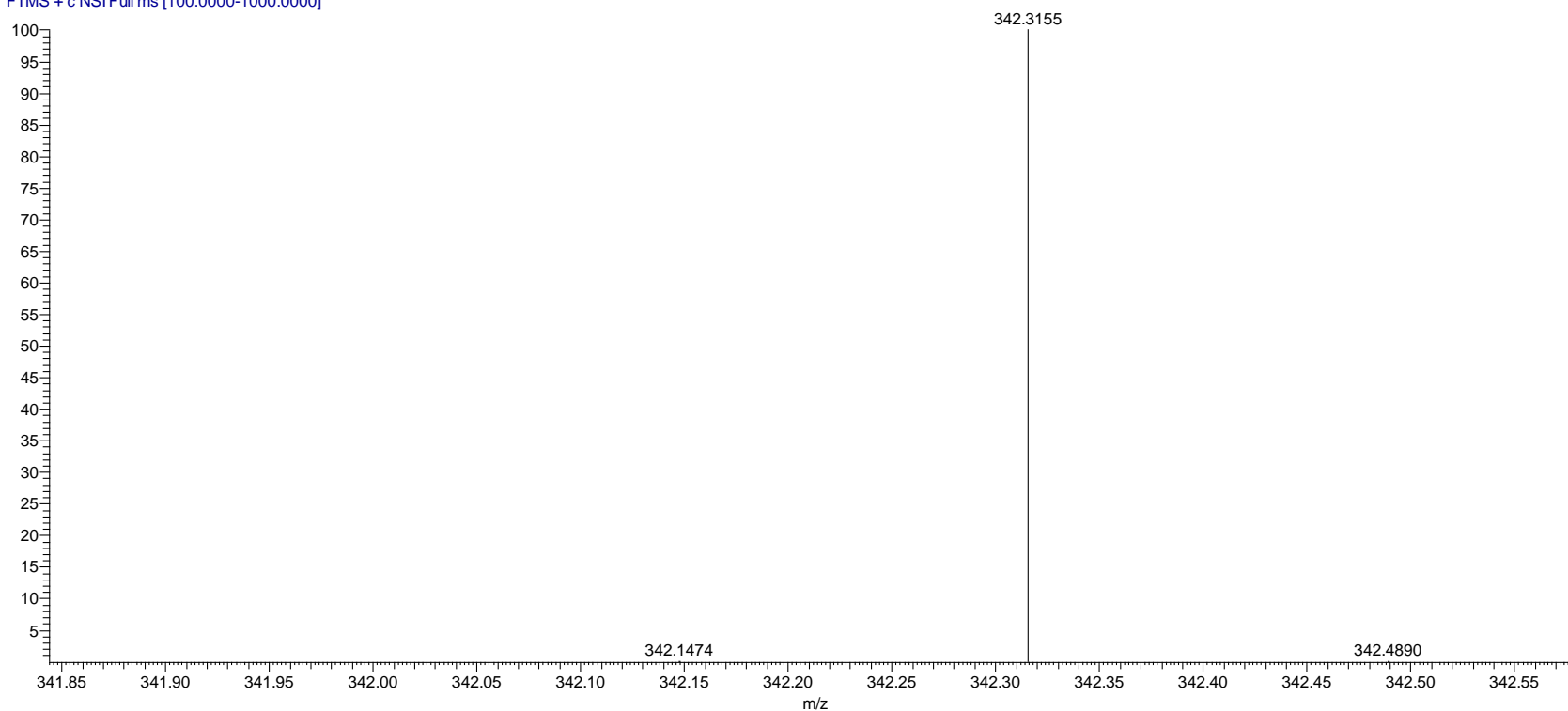




**Figure S42:** High resolution mass spectrum of **18**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-139-2	C24H39N	341.3083	342.3161	342.3155	-0.0005	-1.61

IS--78-139-2 #1991-2005 RT: 10.46-10.53 AV: 15 NL: 9.12E8  
T: FTMS + c NSI Full ms [100.0000-1000.0000]



7.260  
7.200  
7.172  
7.011  
7.003  
6.984  
6.976  
6.899  
6.891

4.230  
4.206  
4.183  
4.159

3.458  
3.400  
3.361  
3.304

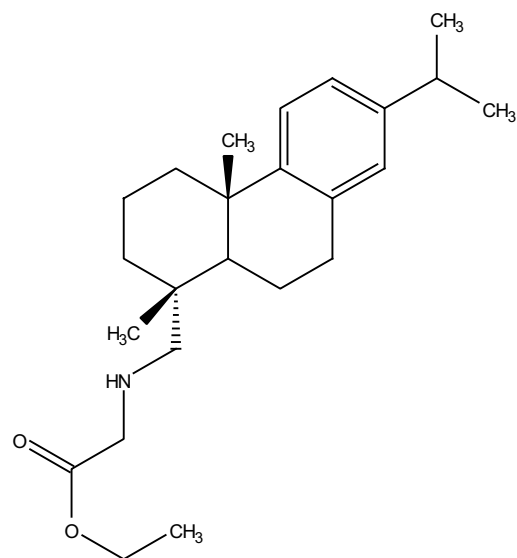
2.930  
2.917  
2.787

2.584  
2.545

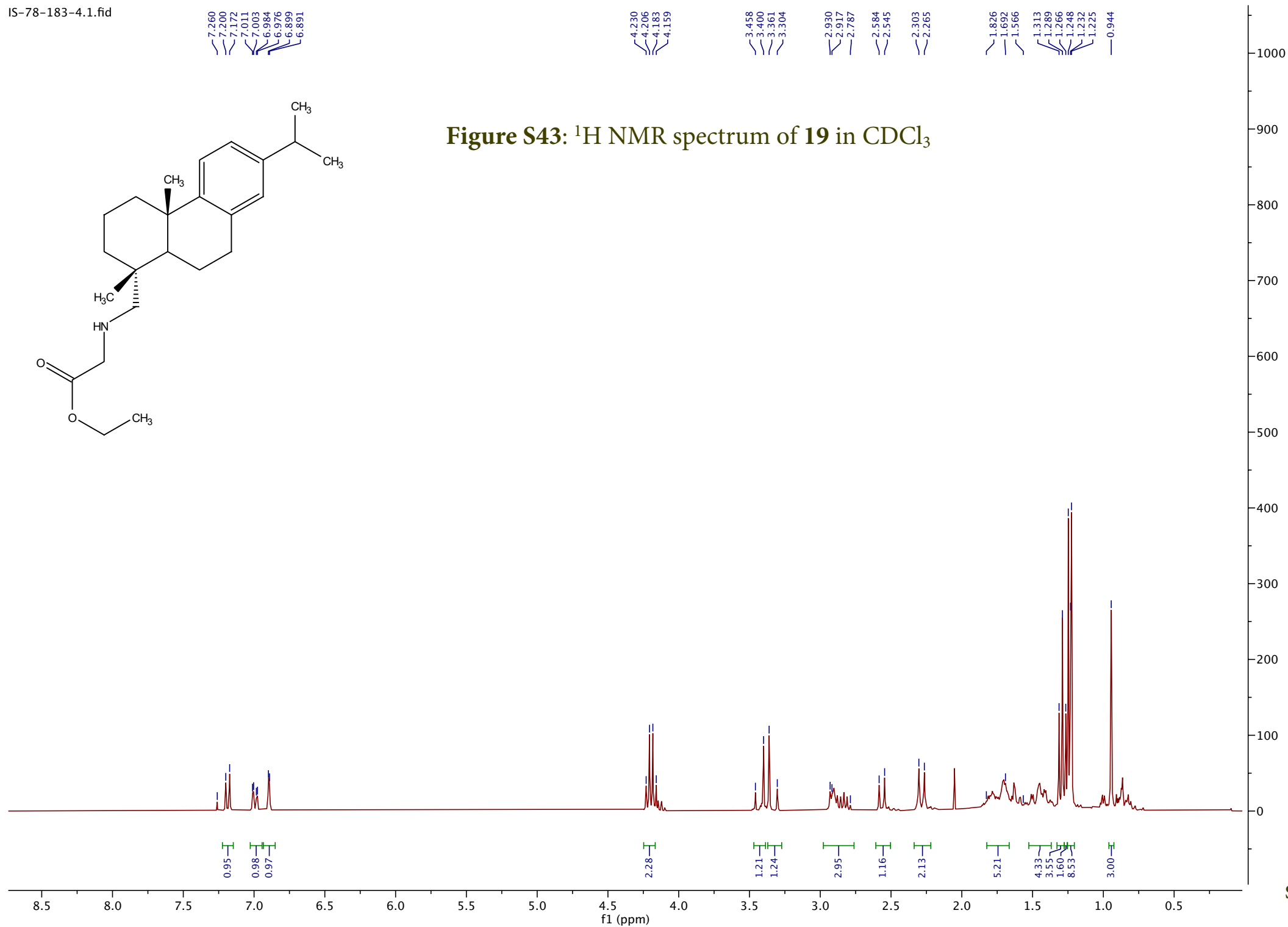
2.303  
2.265

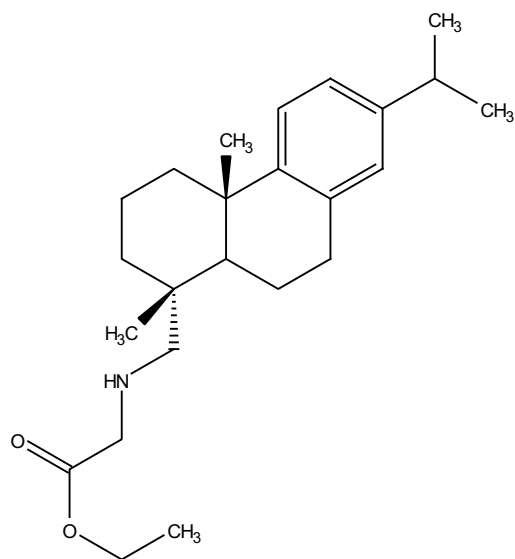
1.826  
1.692  
1.566

1.313  
1.289  
1.266  
1.248  
1.232  
1.225  
0.944

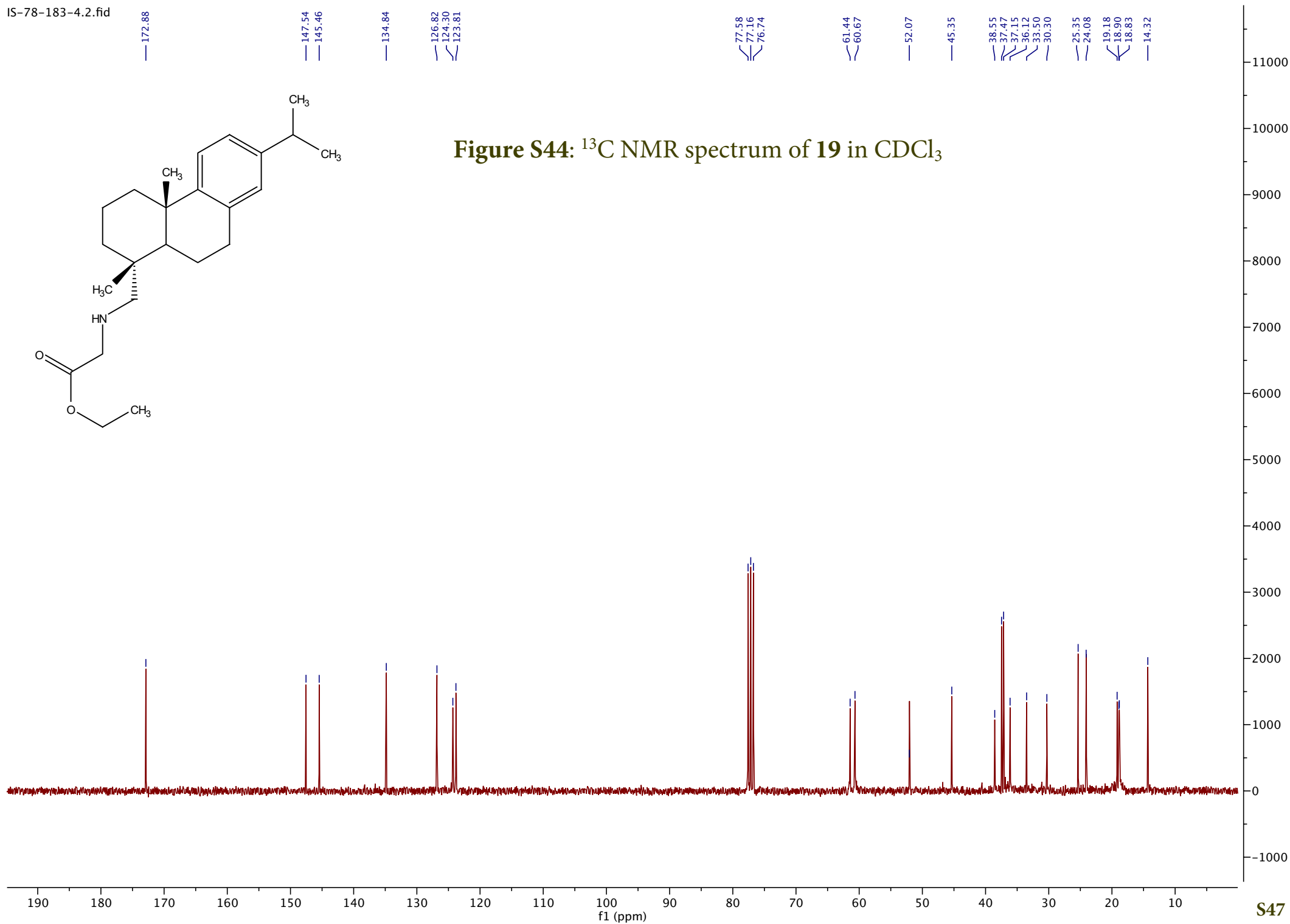


**Figure S43:** <sup>1</sup>H NMR spectrum of **19** in CDCl<sub>3</sub>





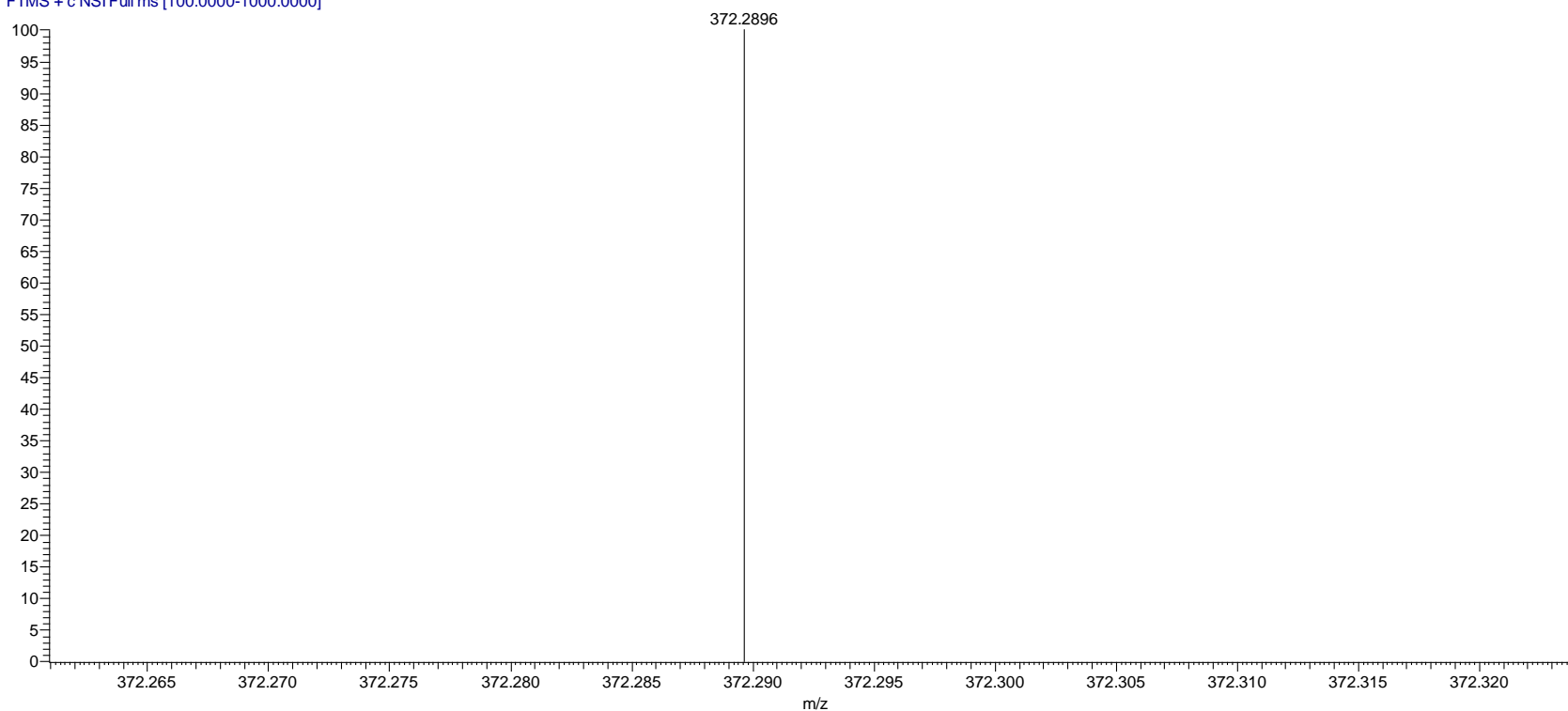
**Figure S44:** <sup>13</sup>C NMR spectrum of **19** in CDCl<sub>3</sub>



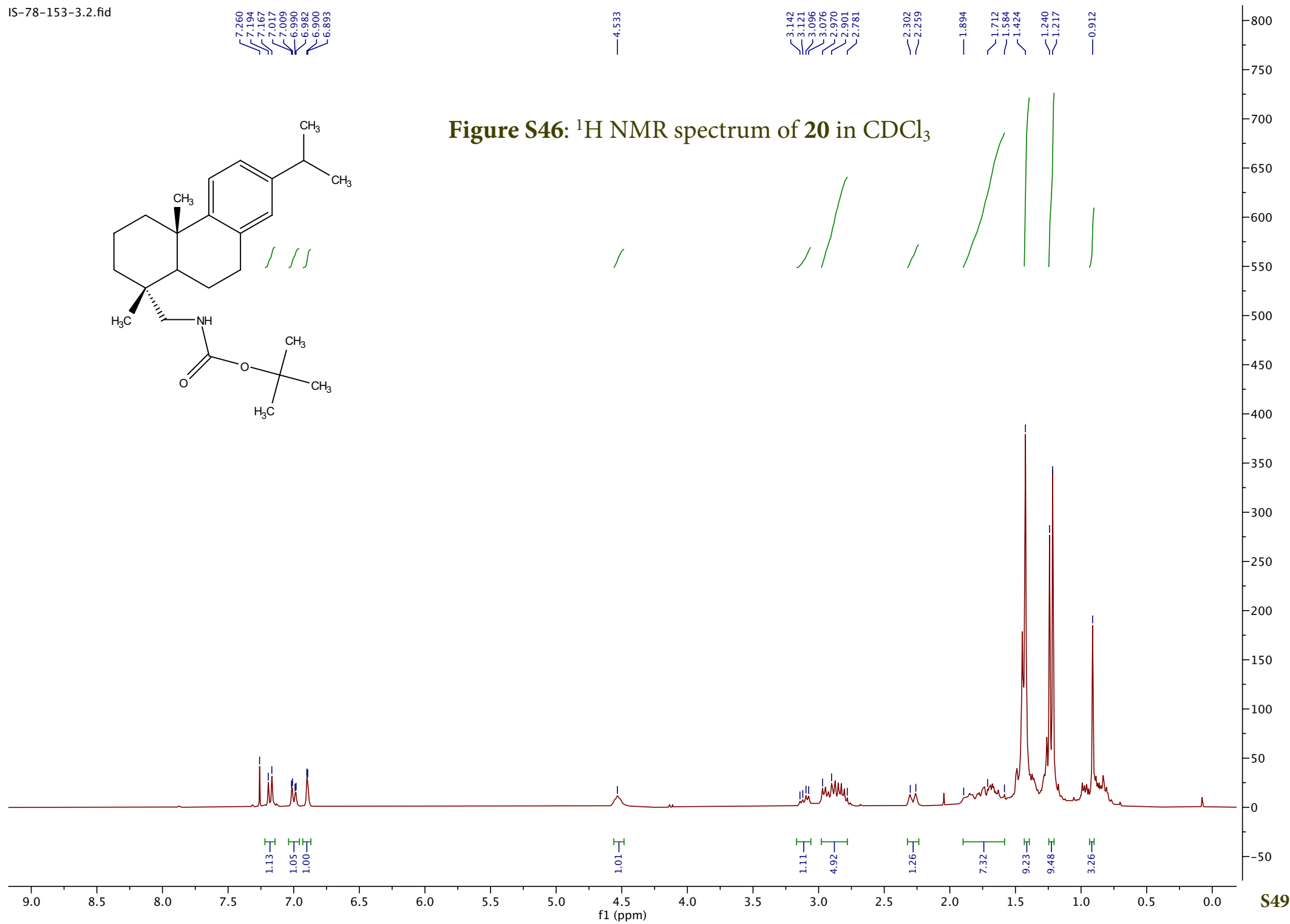
**Figure S45:** High resolution mass spectrum of **19**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-183-4	C24H37NO2	371.2824	372.2902	372.2896	-0.0006	-1.69

IS-78-183-4 #1951-1955 RT: 10.37-10.39 AV: 5 NL: 5.40E8  
T: FTMS + c NSI Full ms [100.0000-1000.0000]







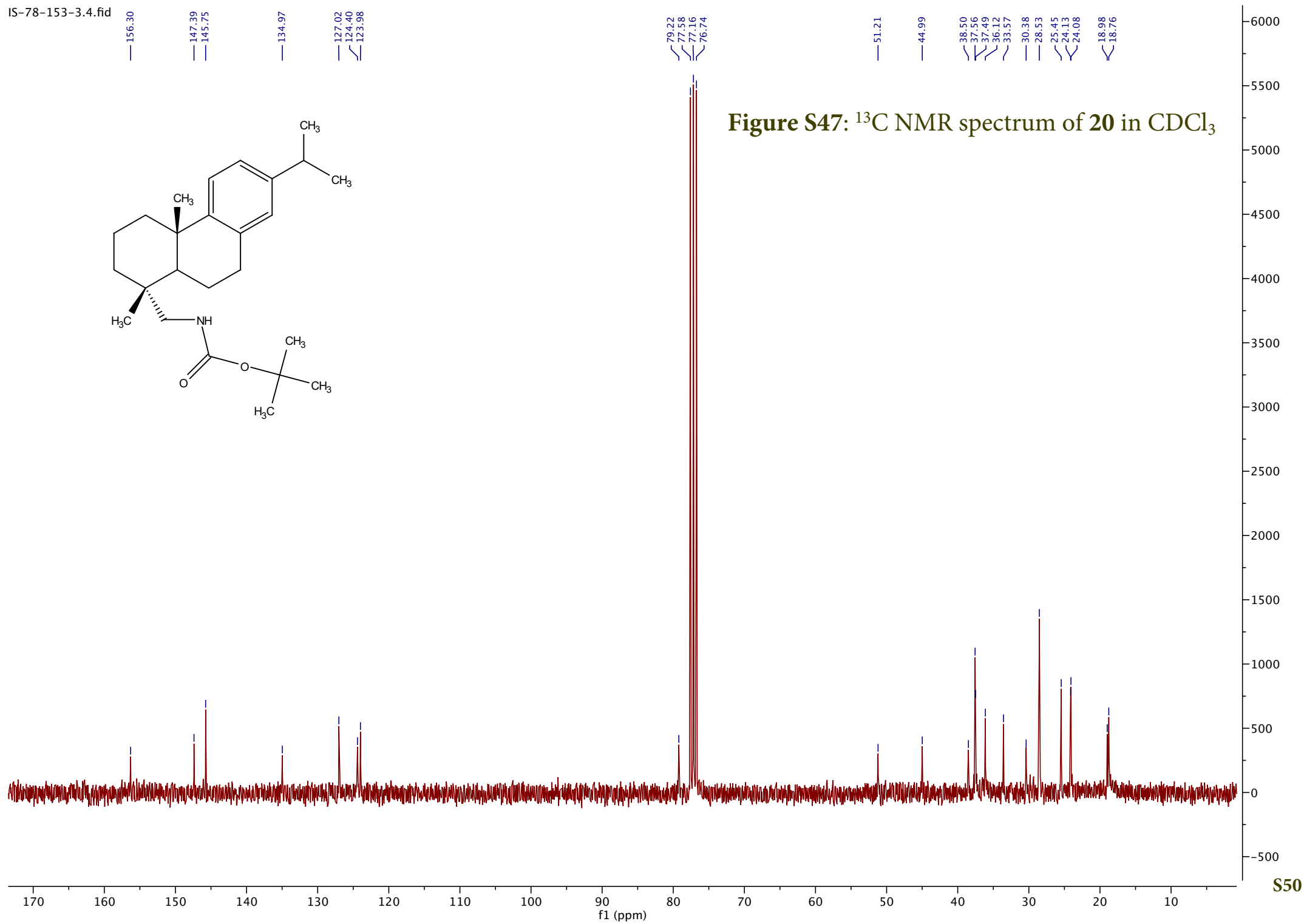
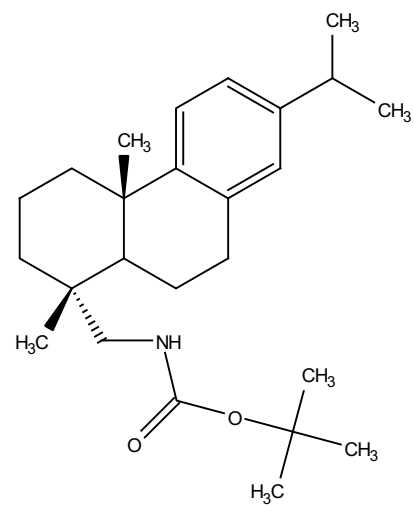
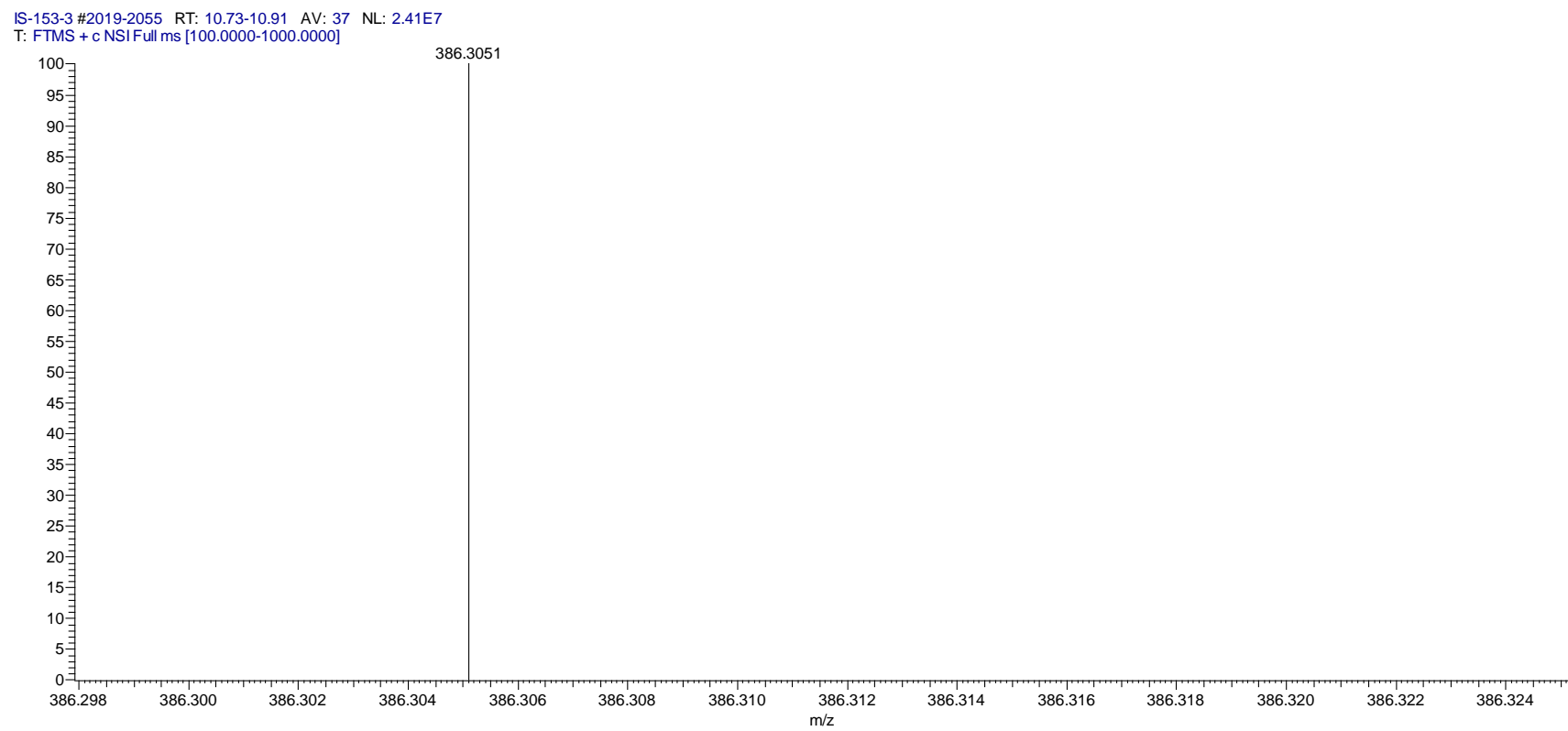


Figure S48: High resolution mass spectrum of 20

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-153(IS-78-153-3)	C25H39NO2	385.2981	386.3059	386.3051	-0.0008	-2.05

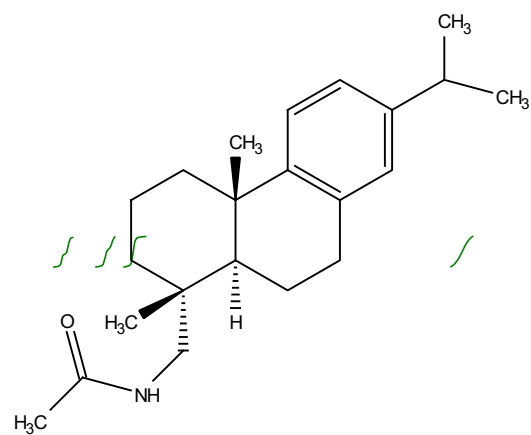


7.26  
7.19  
7.16  
7.02  
7.01  
6.98  
6.90

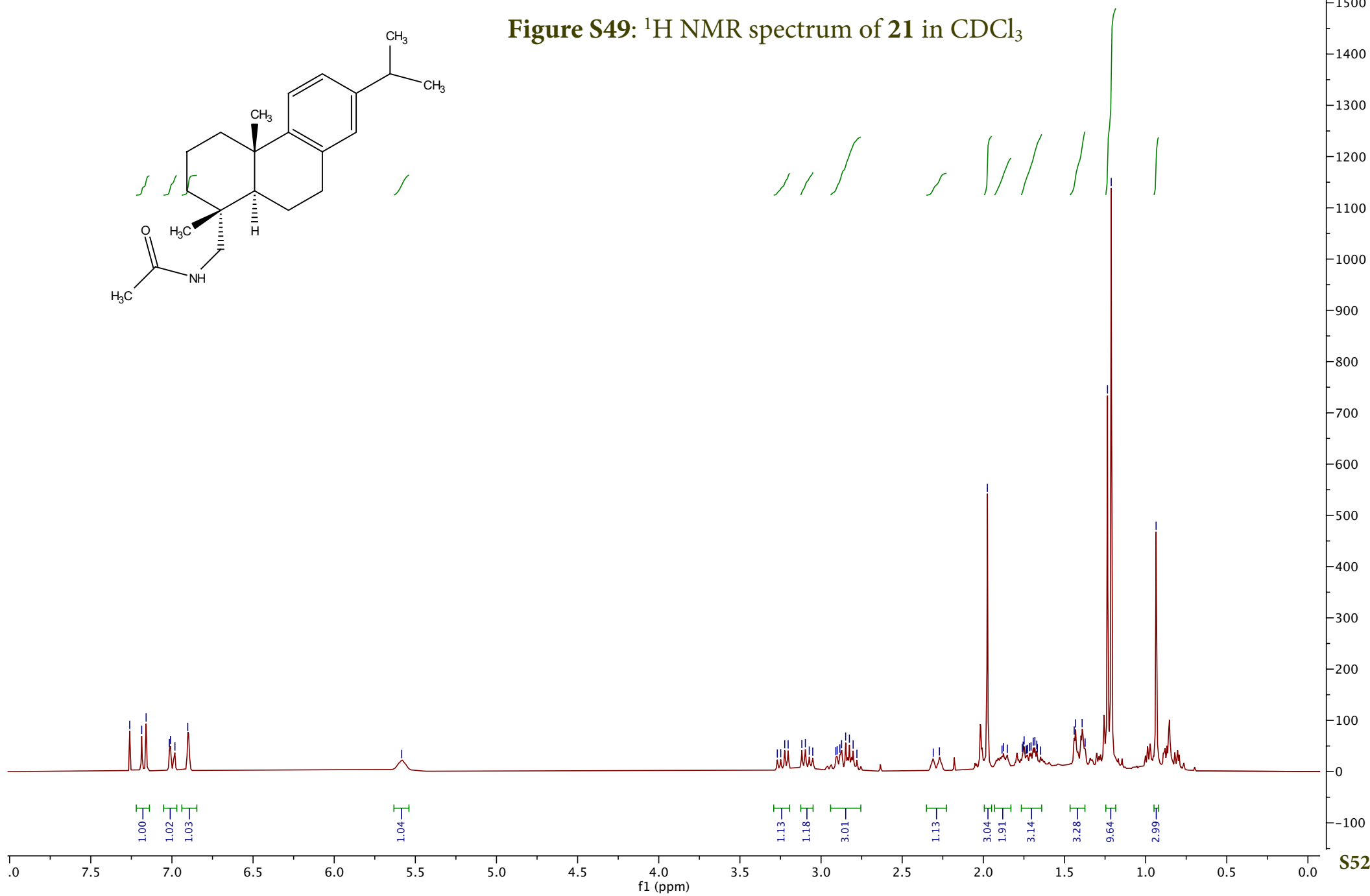
5.58

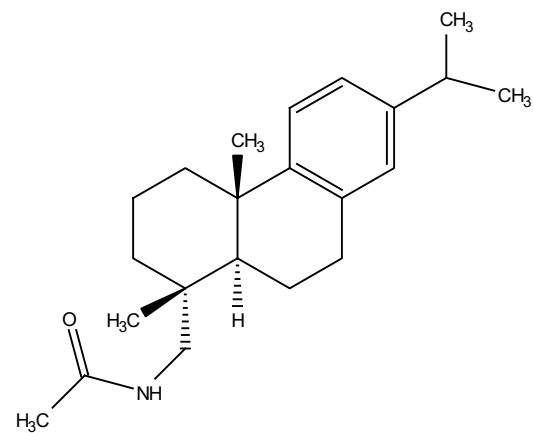
3.27  
3.25  
3.22  
3.20  
3.12  
3.10  
3.07  
3.05  
2.91  
2.90  
2.88  
2.87  
2.85  
2.83  
2.80  
2.78

2.31  
2.27  
1.98  
1.88  
1.85  
1.76  
1.75  
1.74  
1.73  
1.71  
1.69  
1.68  
1.67  
1.65  
1.44  
1.43  
1.39  
1.37  
1.23  
1.21  
0.94



**Figure S49:**  $^1\text{H}$  NMR spectrum of **21** in  $\text{CDCl}_3$





**Figure S50:** <sup>13</sup>C NMR spectrum of **21** in CDCl<sub>3</sub>

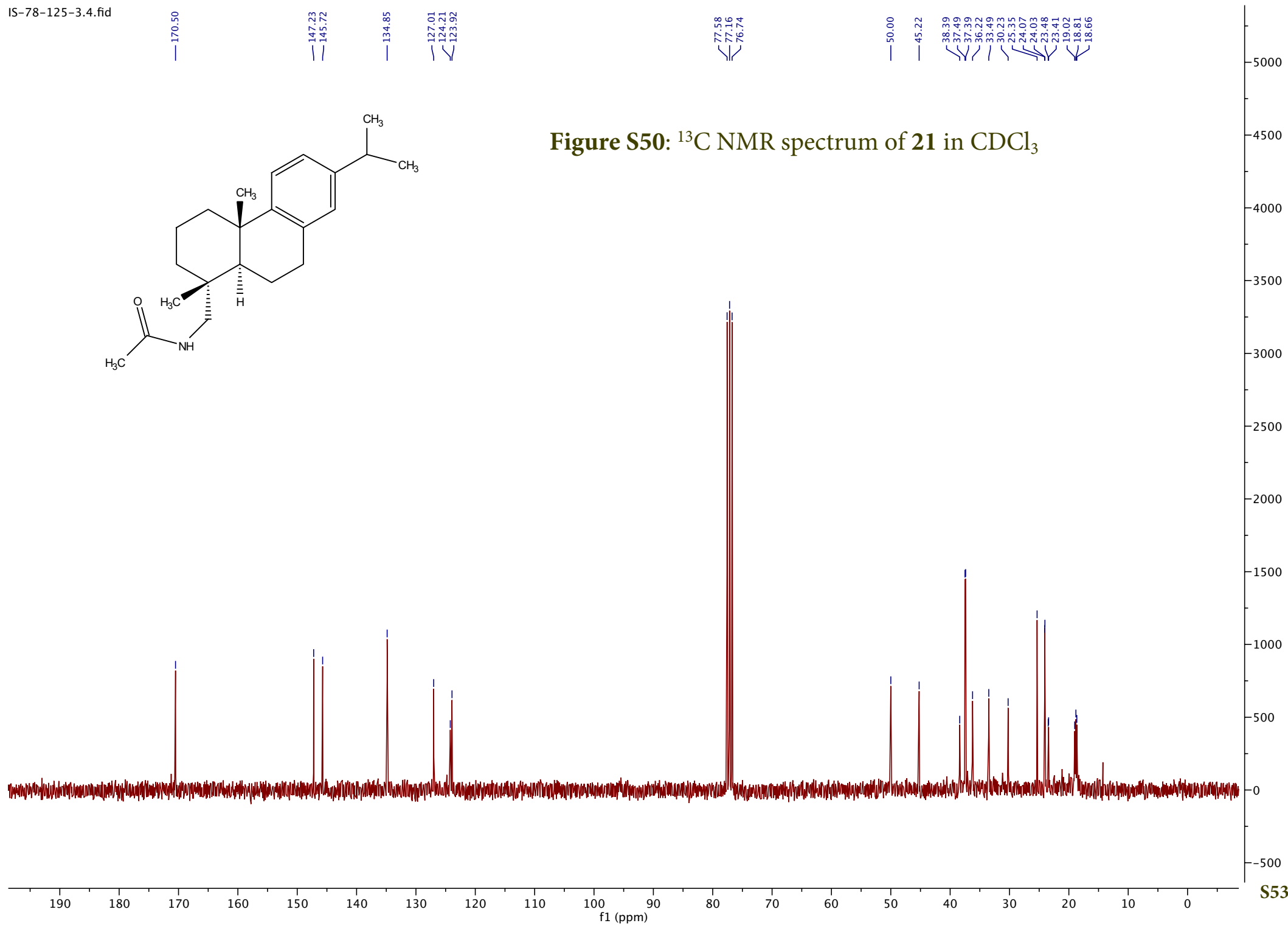
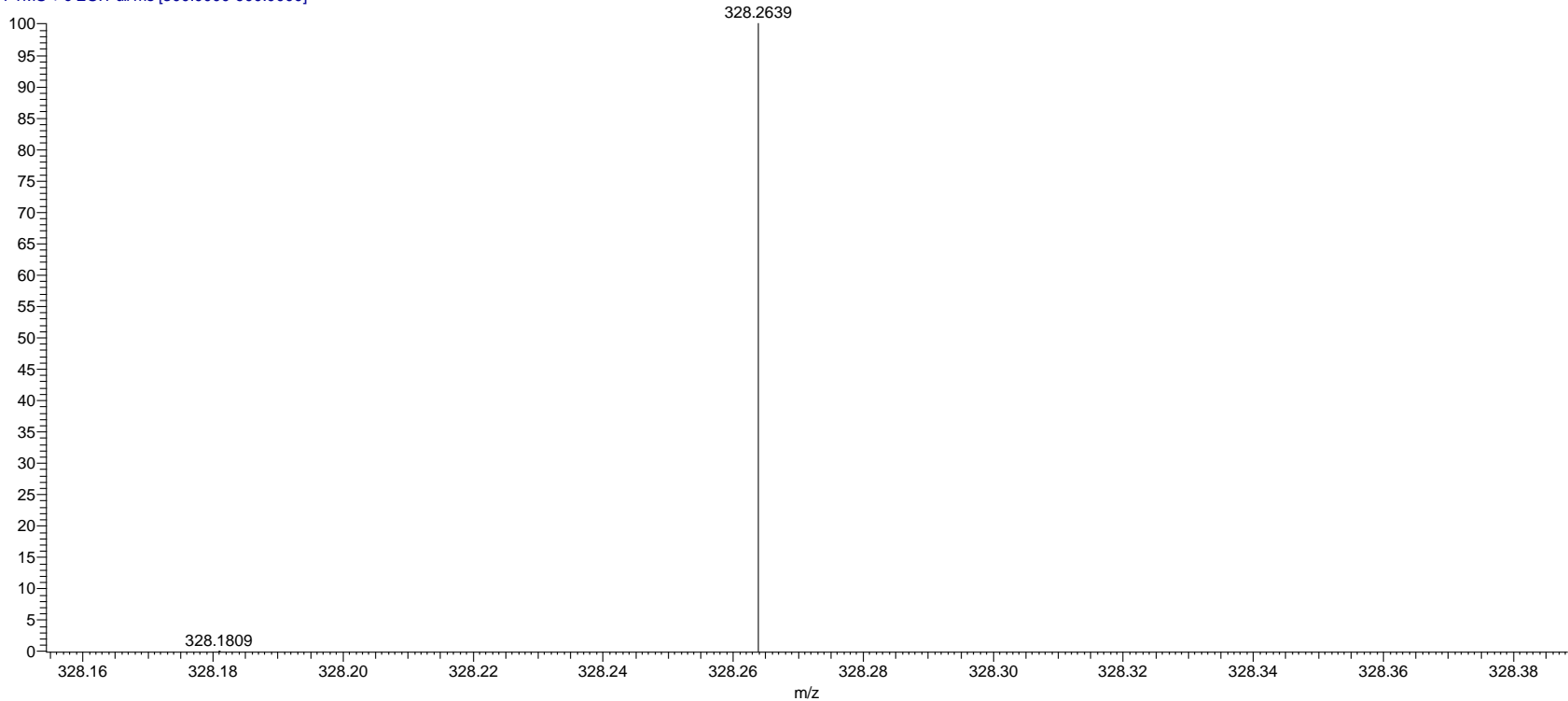
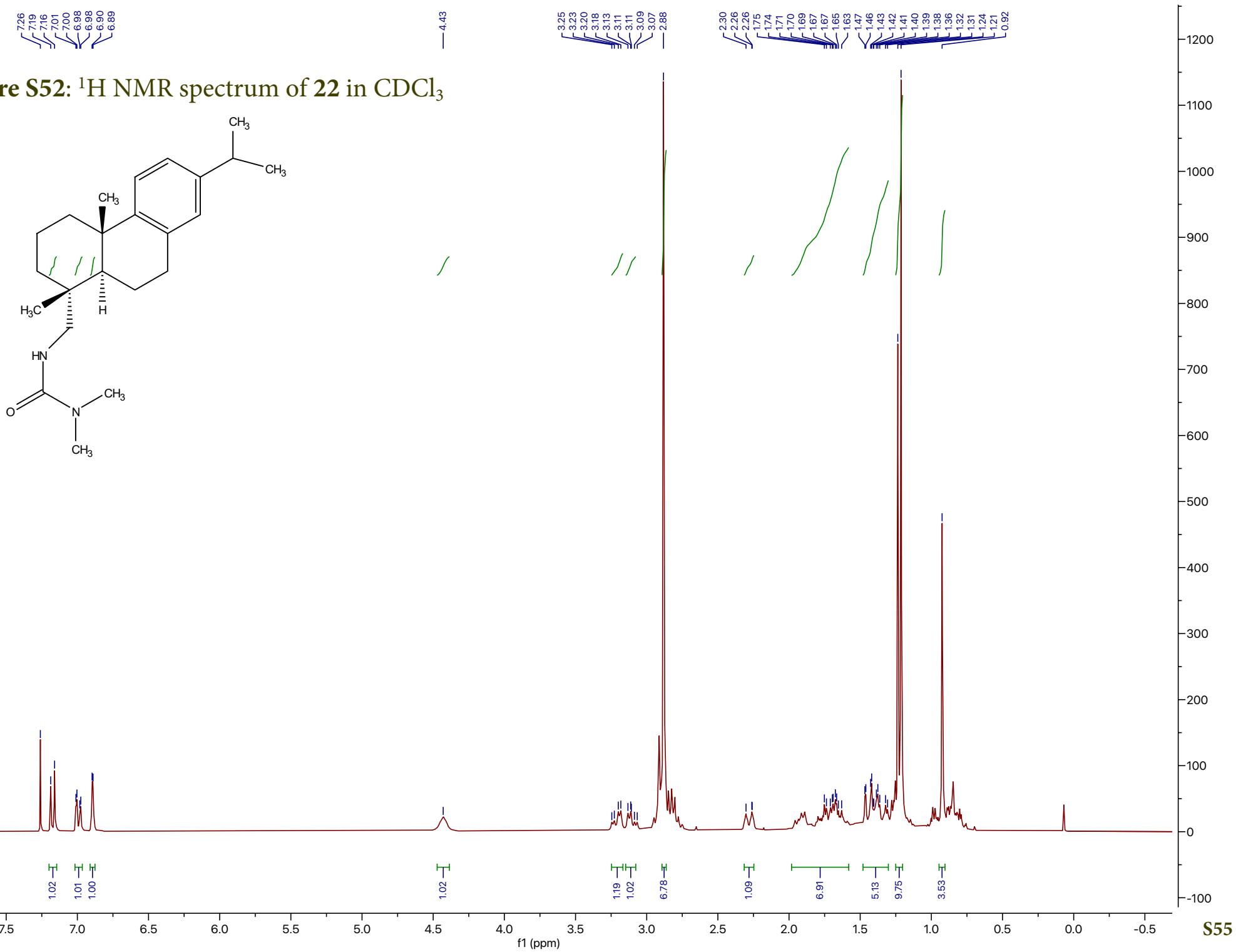


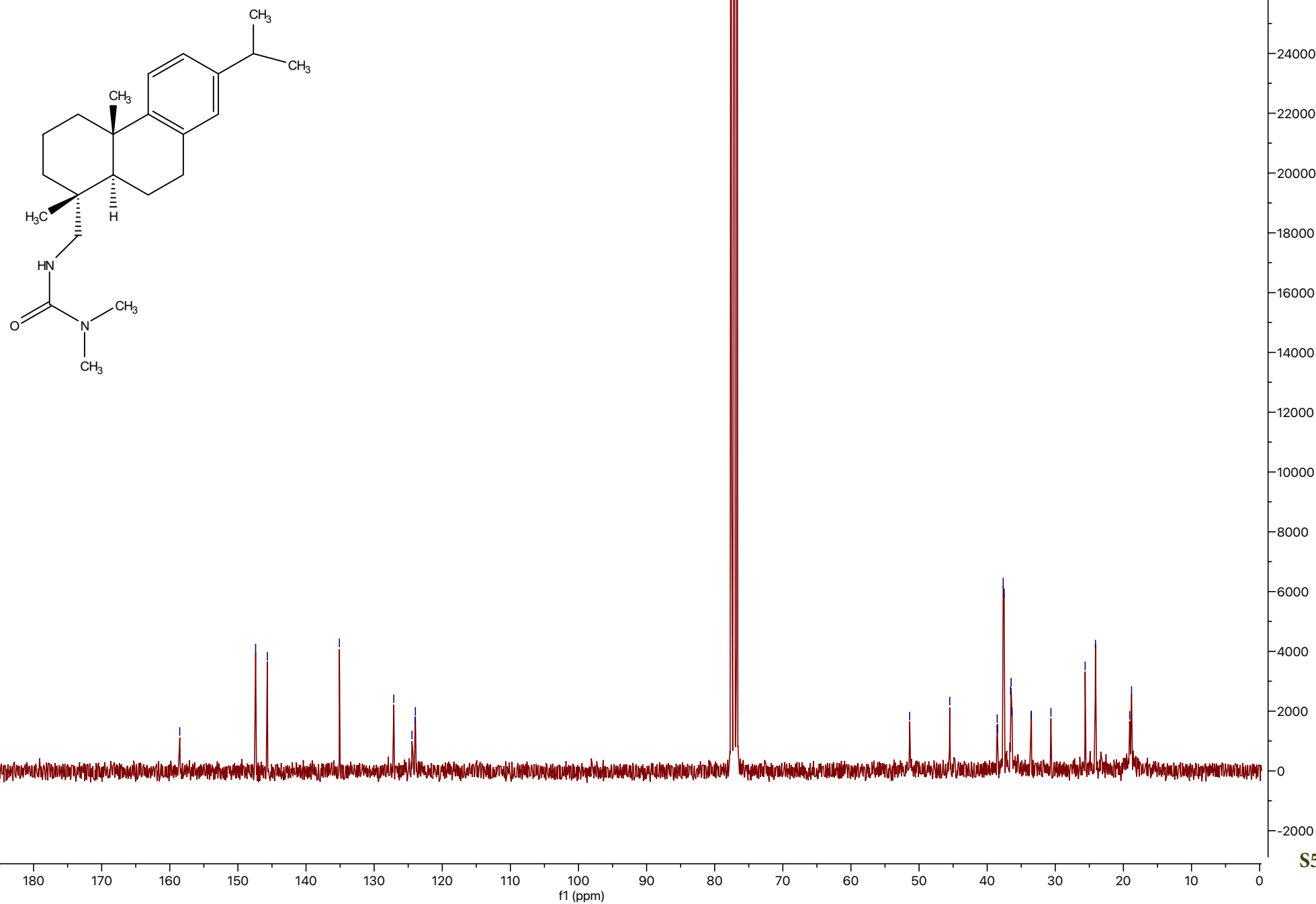
Figure S51: High resolution mass spectrum of **21**

Sample Name	Mol Fomula	MW(COME WITH SAMPLES)	MW(CALCULATED)	M+H	observed	delta	ppm
IS-78-125-3	C22H33NO	328.264	327.25621	328.2640	328.2639	-0.0001	-0.34

IS-78-125-3 #601-623 RT: 3.89-4.00 AV: 23 NL: 3.28E7  
T: FTMS + c ESI Full ms [300.0000-900.0000]





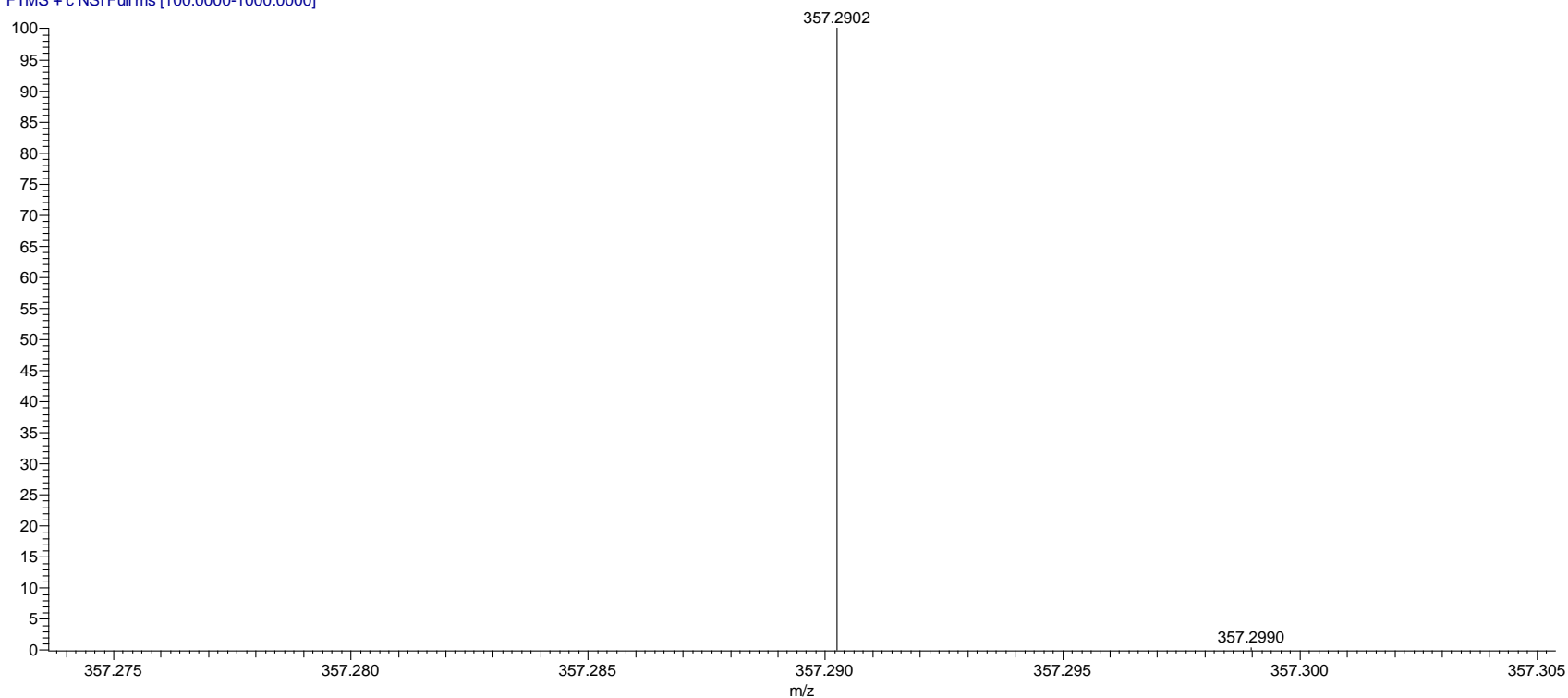
**Figure S53:**  $^{13}\text{C}$  NMR spectrum of **22** in  $\text{CDCl}_3$ 



**Figure S54:** High resolution mass spectrum of **22**

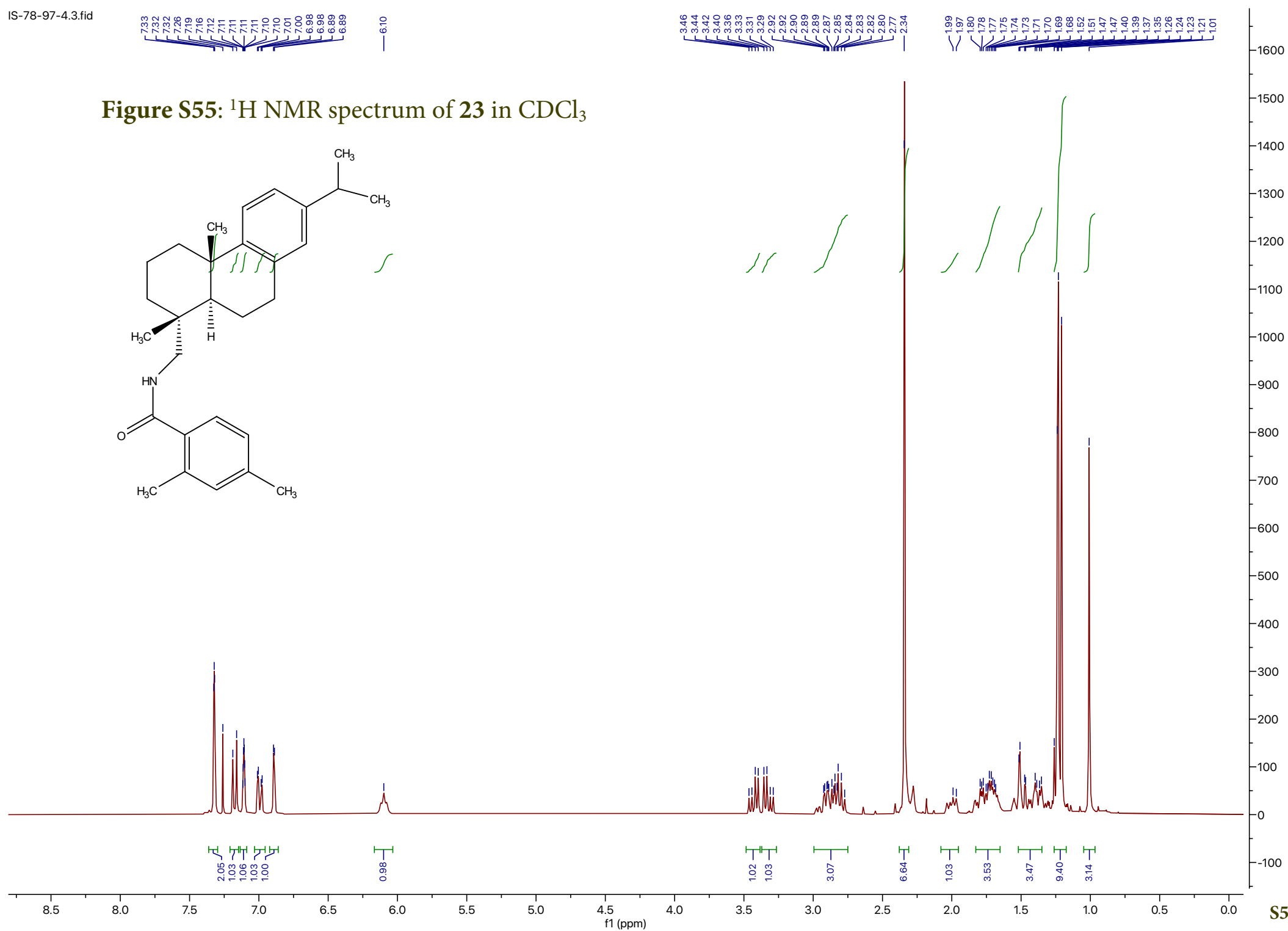
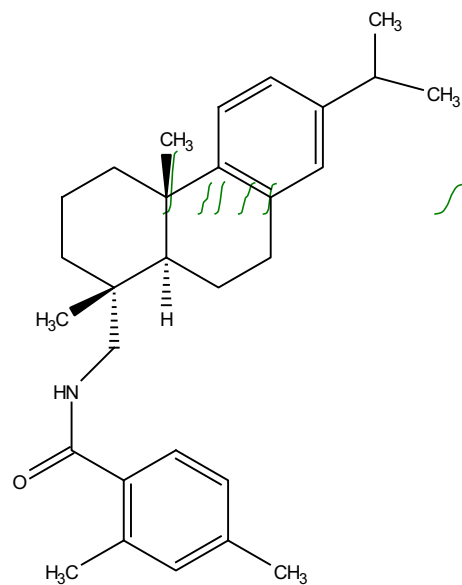
Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-163-3(IS-78-163-2)	C23H36N2O	356.2828	357.2906	357.2902	-0.0004	-1.04

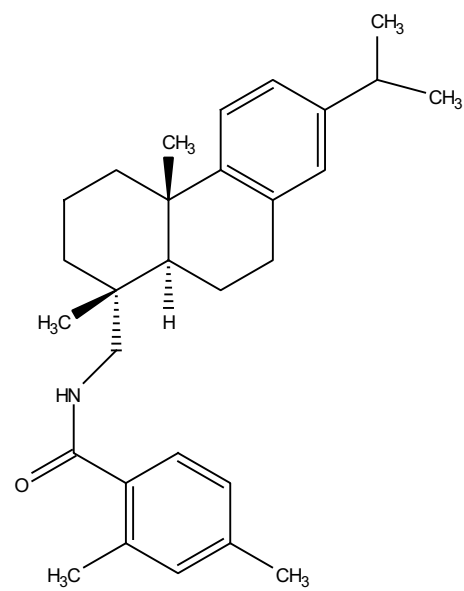
IS-78-163-2 #3608-3686 RT: 18.90-19.32 AV: 79 NL: 4.61E7  
T: FTMS + c NSI Full ms [100.0000-1000.0000]



7.33  
7.32  
7.32  
7.26  
7.19  
7.16  
7.12  
7.11  
7.11  
7.10  
7.10  
7.01  
7.00  
6.98  
6.89  
6.89

6.10

3.46  
3.44  
3.42  
3.40  
3.36  
3.33  
3.31  
3.29  
2.92  
2.90  
2.89  
2.87  
2.85  
2.84  
2.83  
2.82  
2.80  
2.77  
2.341.99  
1.97  
1.80  
1.78  
1.77  
1.75  
1.74  
1.73  
1.71  
1.70  
1.69  
1.68  
1.52  
1.51  
1.47  
1.40  
1.39  
1.37  
1.35  
1.26  
1.24  
1.23  
1.21  
1.01**Figure S55:**  $^1\text{H}$  NMR spectrum of **23** in  $\text{CDCl}_3$ 



**Figure S56:**  $^{13}\text{C}$  NMR spectrum of **23** in  $\text{CDCl}_3$

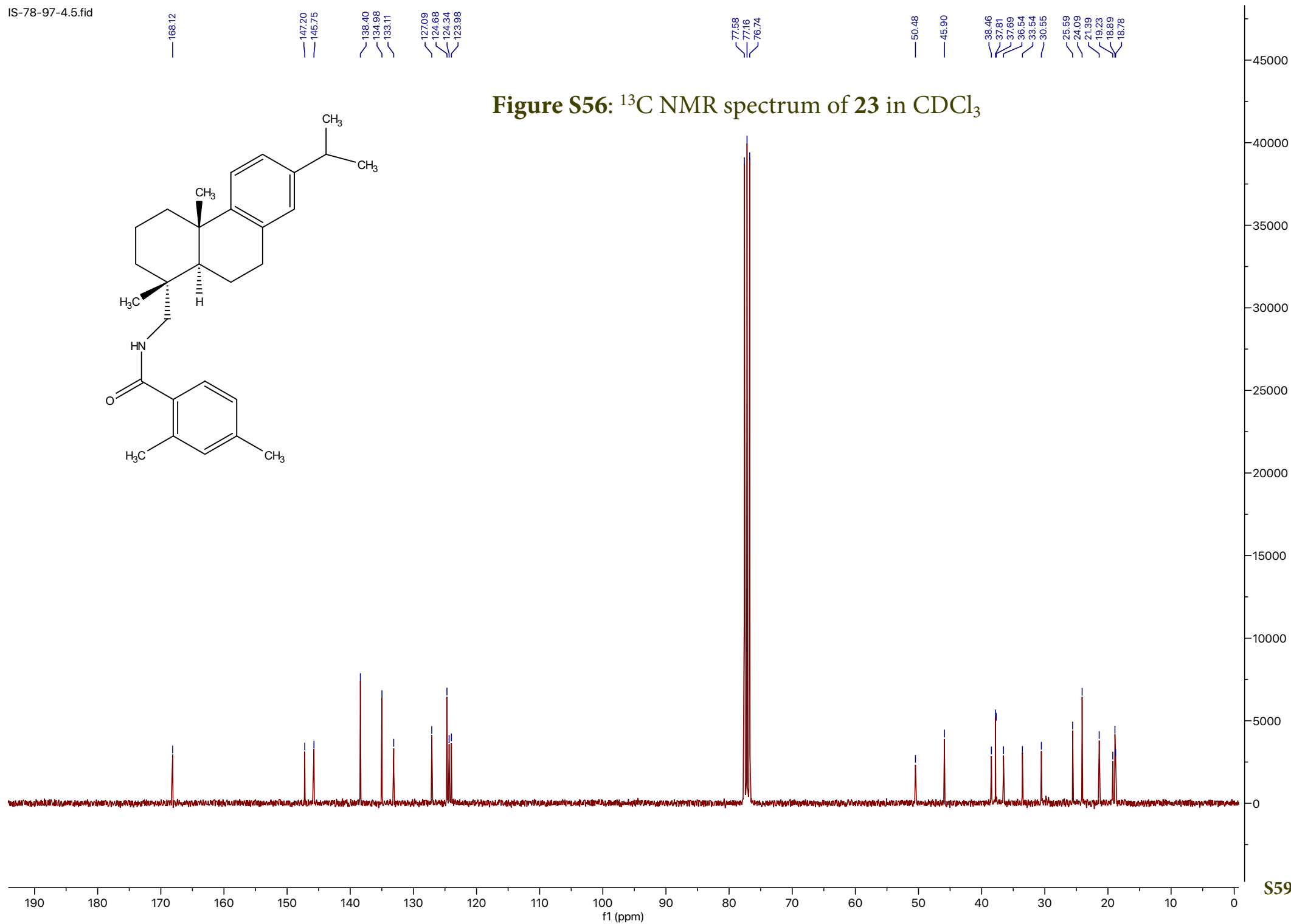
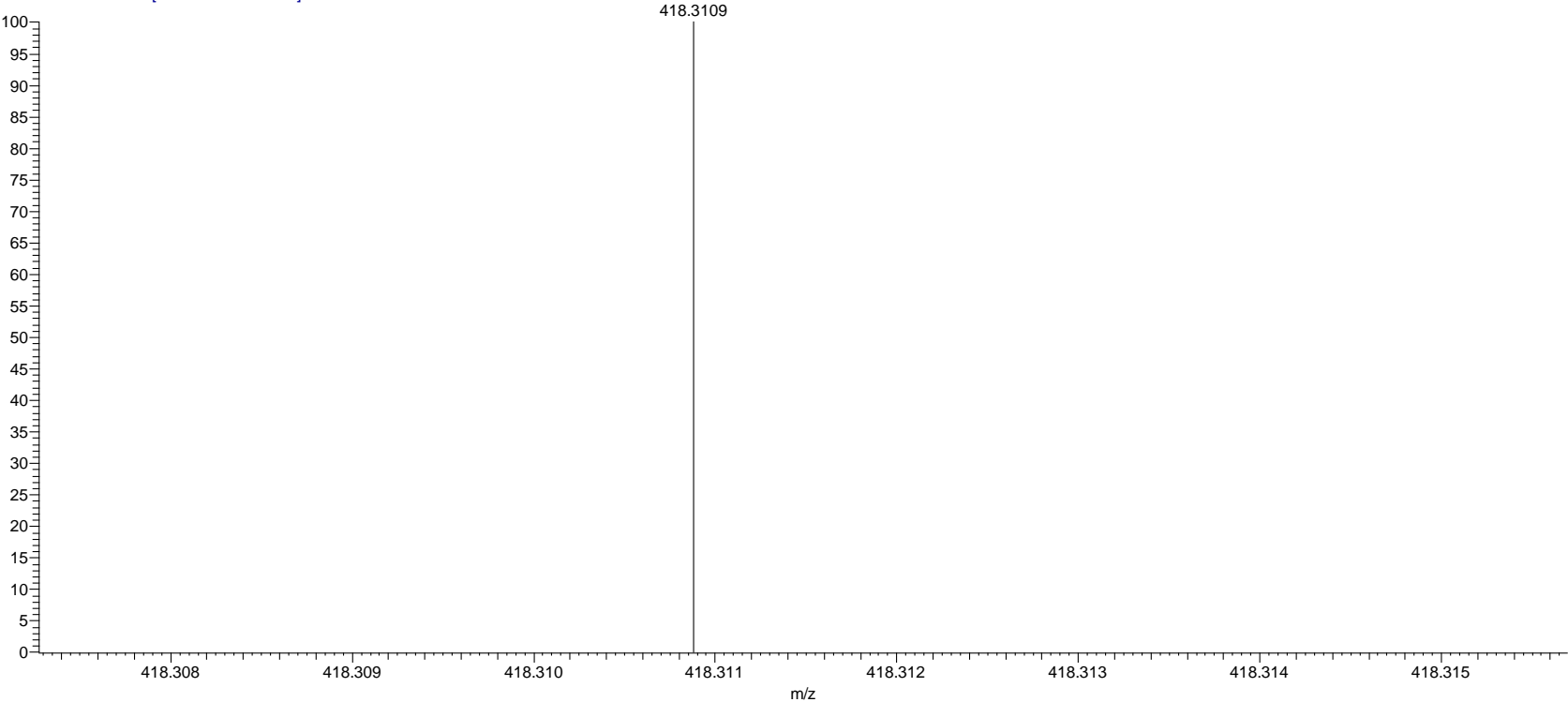
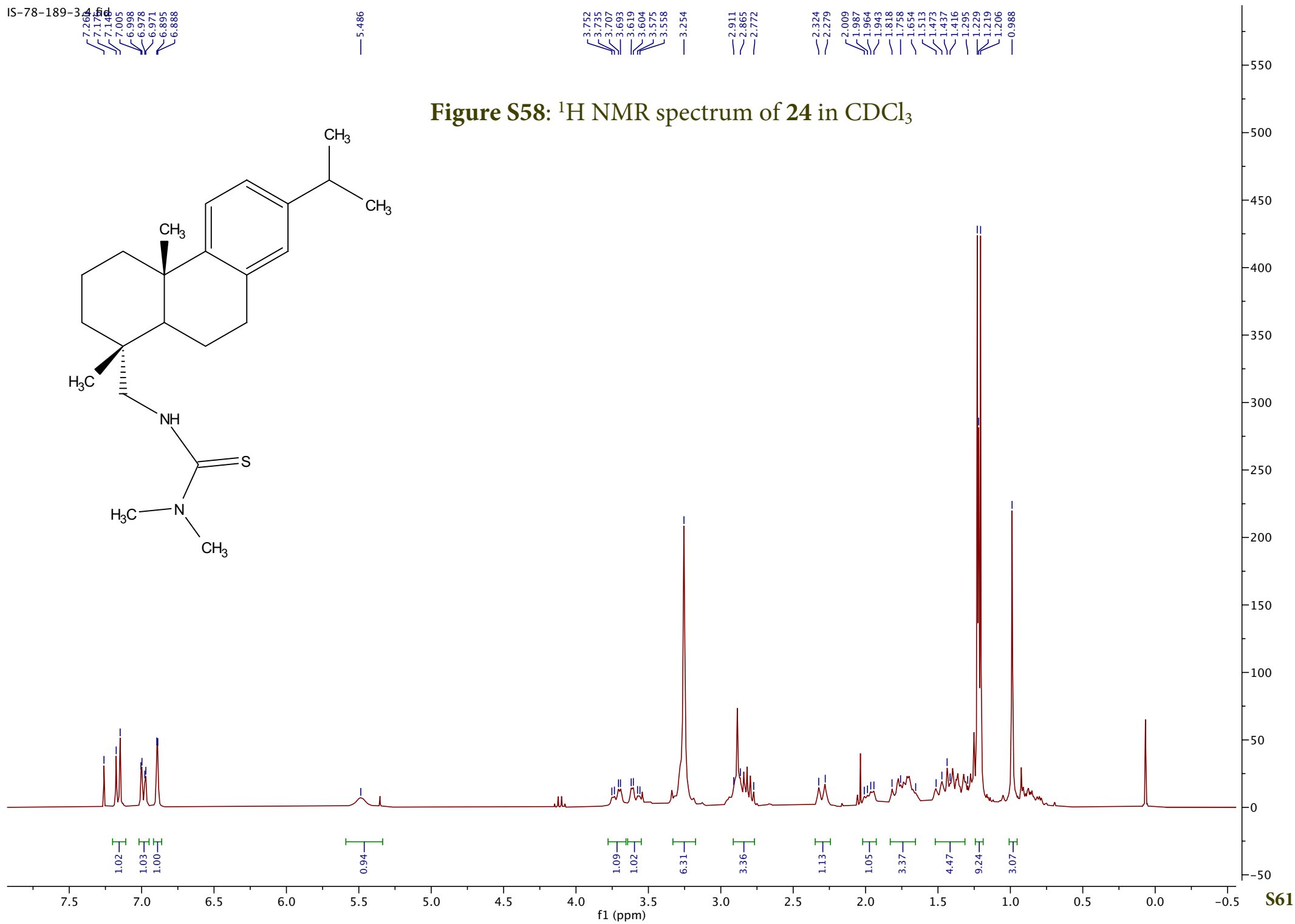


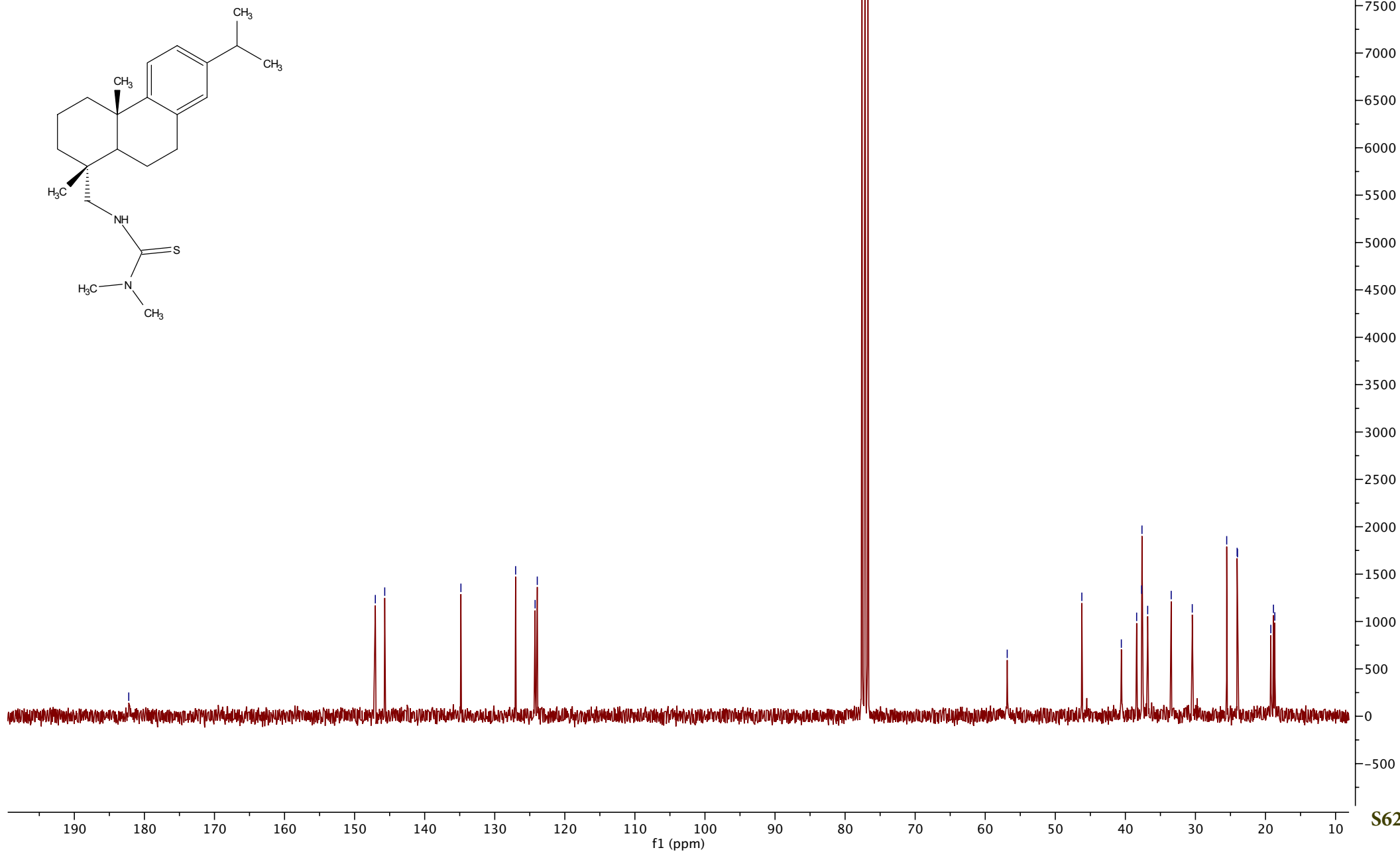
Figure S57: High resoluton mass spectrum of 23

Sample Name	Mol Fomula	MW(COME WITH SAMPLES)	MW(CALCULATED)	M+H	observed	delta	ppm
IS-78-97	C29H39NO	417.3032	417.3032	418.3110	418.3109	-0.0001	-0.17

IS-78-97 #600-612 RT: 3.88-3.94 AV: 13 NL: 7.20E5  
T: FTMS + c ESI Full ms [300.0000-900.0000]







**Figure S60:** High resolution mass spectrum of **24**

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
IS-78-189-3	C23H36N2S	372.2599	373.2677	373.2675	-0.0002	-0.59

IS-189-3 #1979-2077 RT: 10.52-11.03 AV: 99 NL: 2.13E7  
T: FTMS + c NSI Full ms [100.0000-1000.0000]

