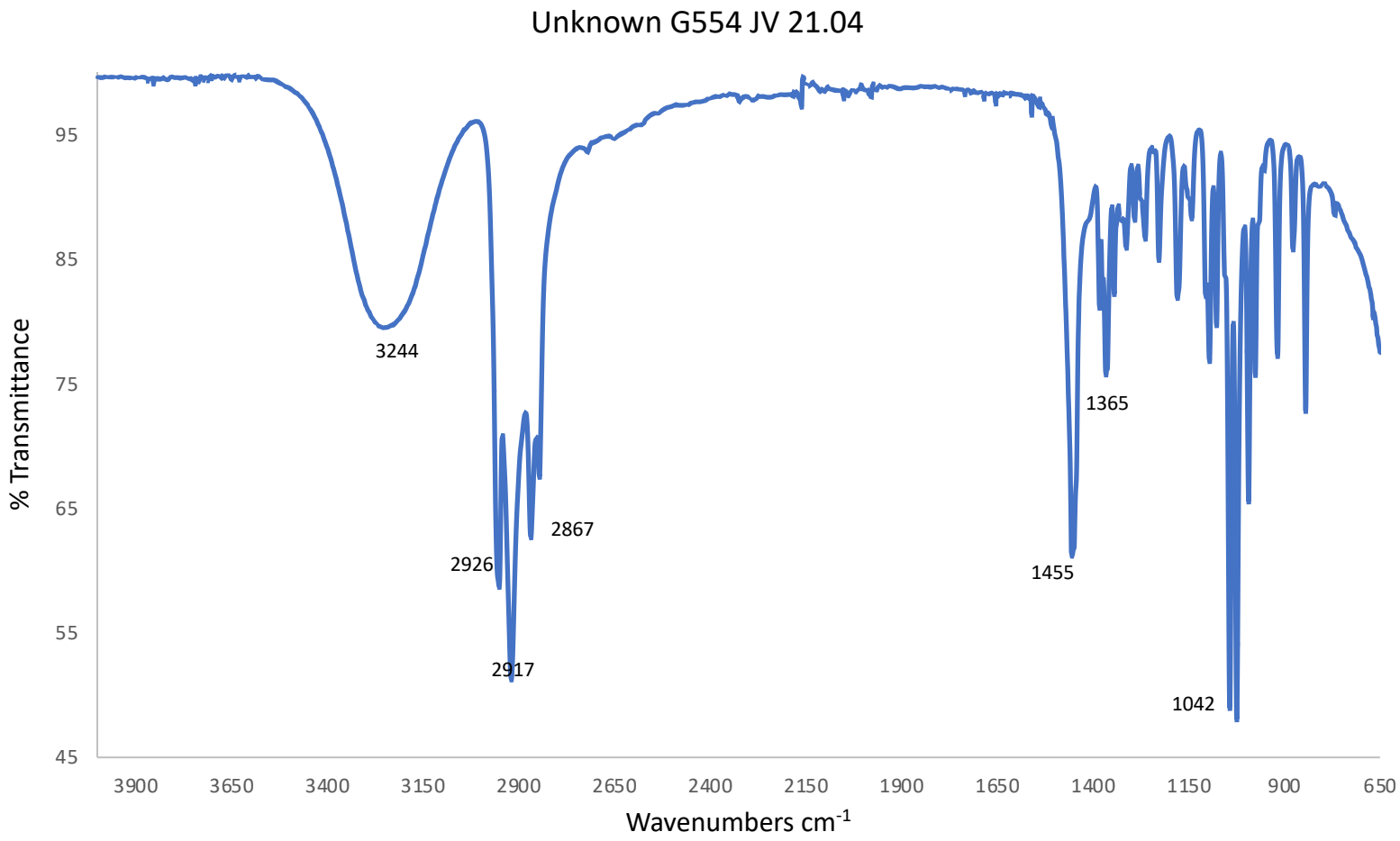
CHEM 554
Organic Spectroscopy
Unknown G554 JV21.04

By: Alexie Clover



MW: 156

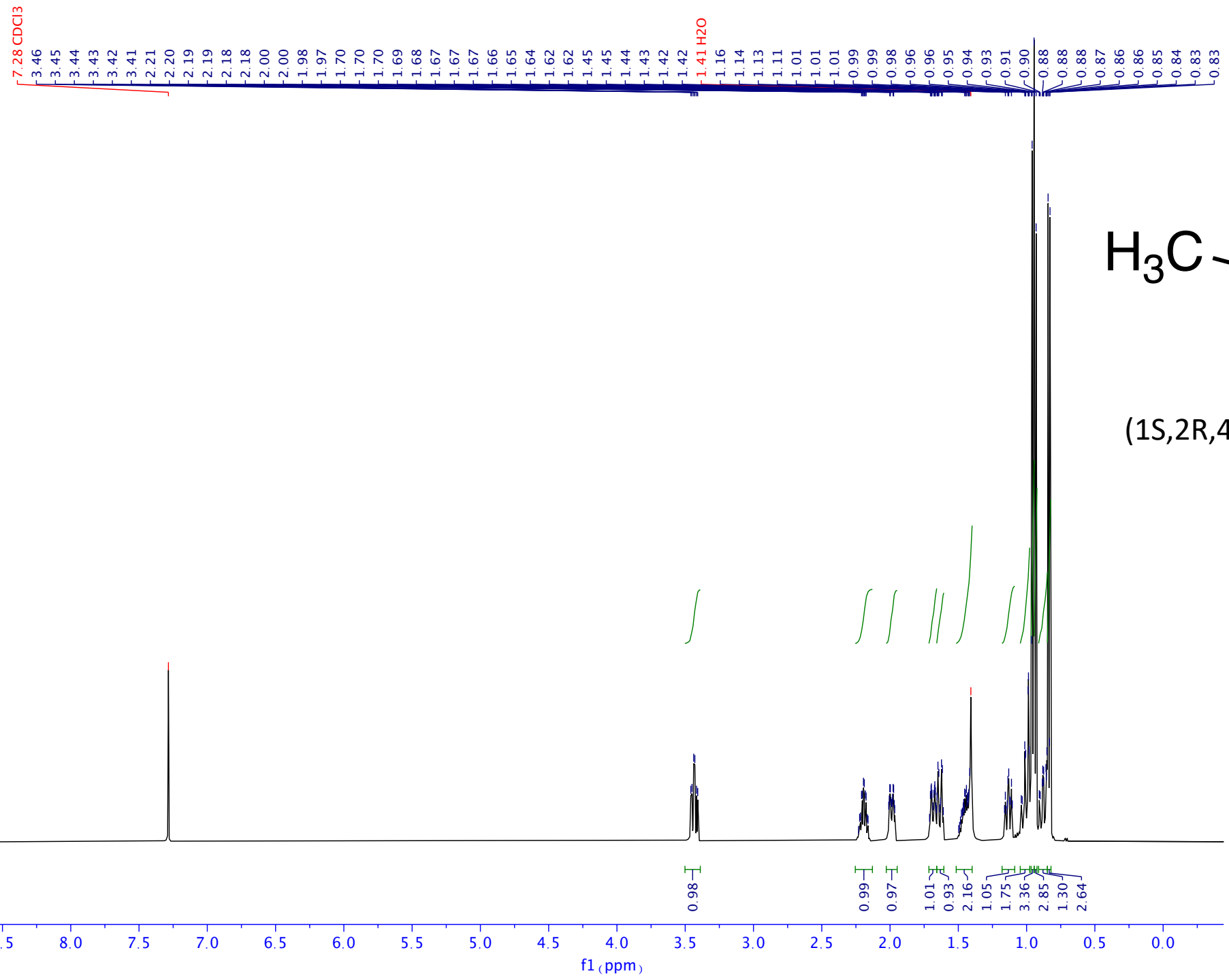
Formula: $C_{10}H_{20}O$

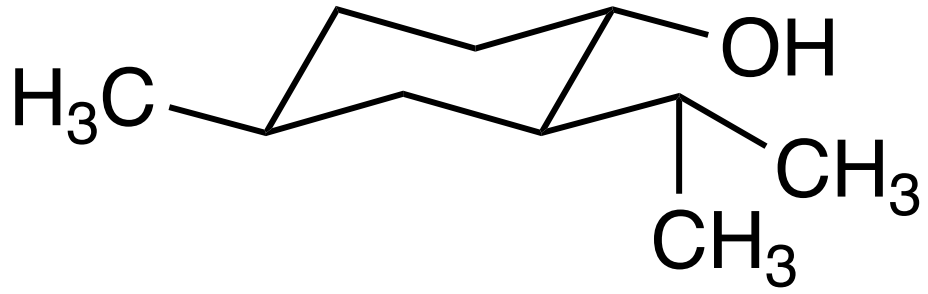
Degree of Unsaturation: 1°

cm^{-1}	Functional group and type of vibration
3227	O-H stretching
2926 and 2917	sp^3 C-H stretching
1455	Methylene bending absorbance
1365	Methyl bending absorbance
1042 and 1024	C-O stretches of alcohols

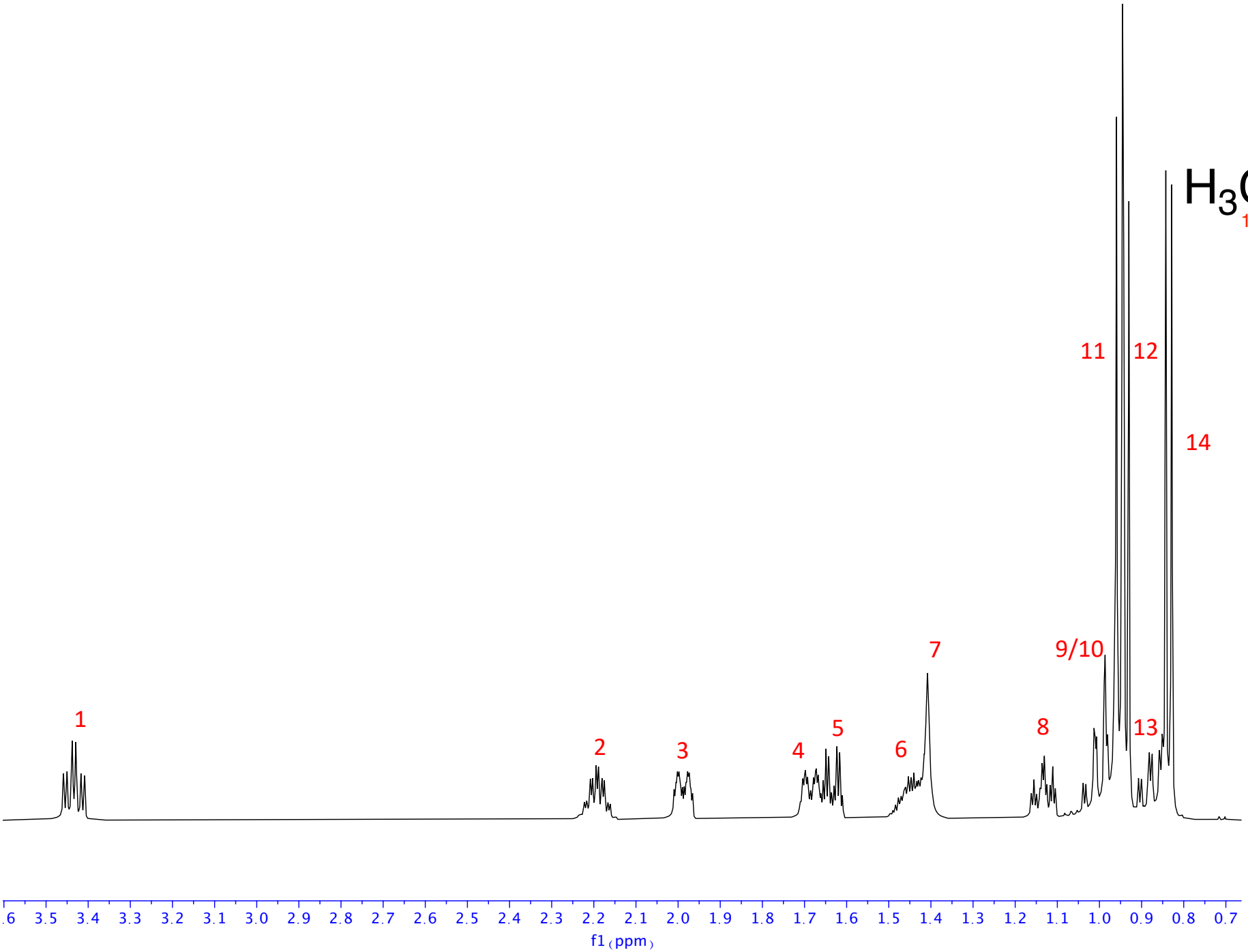
As you can see there are no absorbances from ~ 2700 – 1455 cm^{-1}

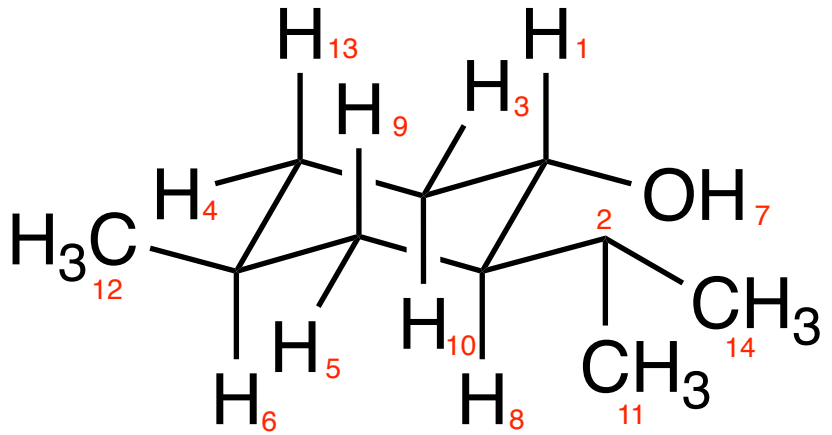
- This tells me I must have a ring to account for the 1 degree of unsaturation

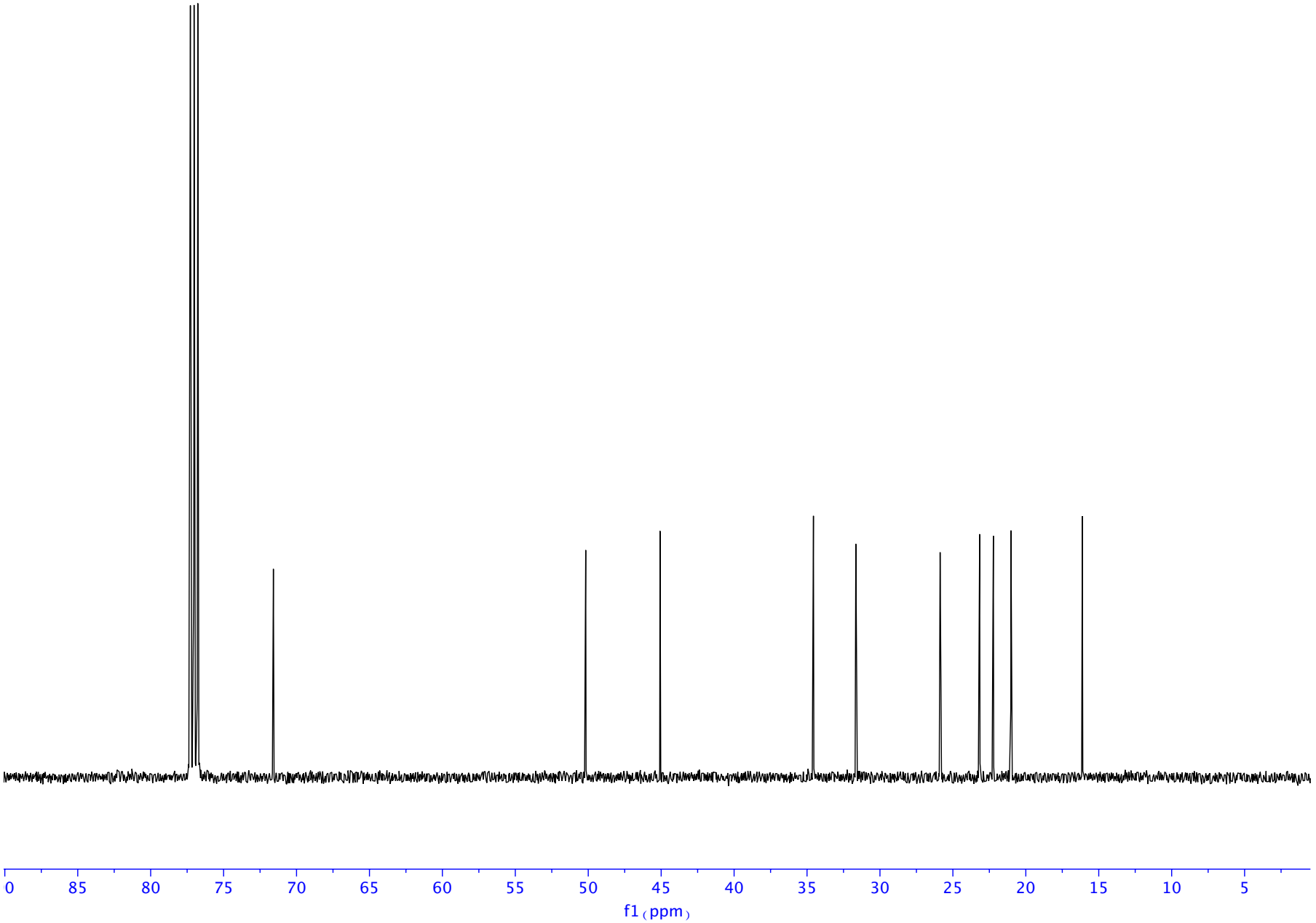


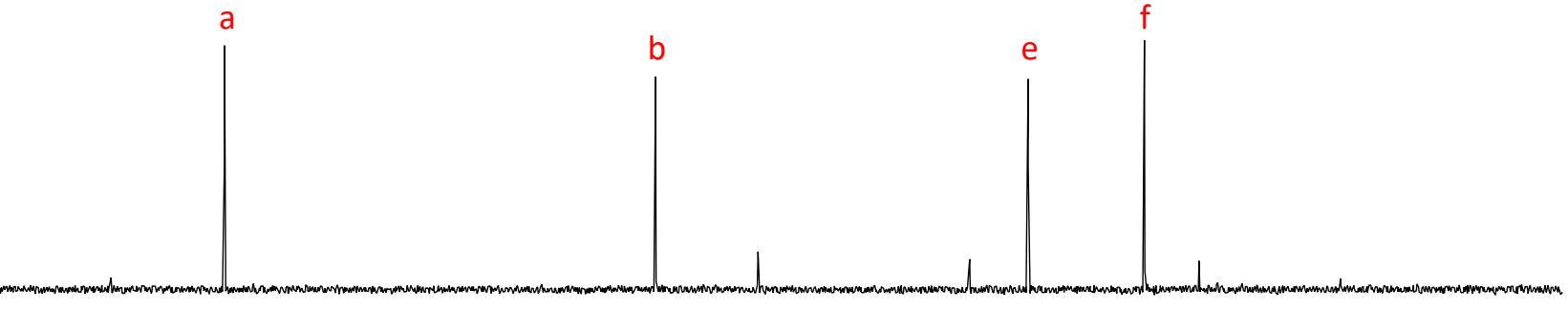


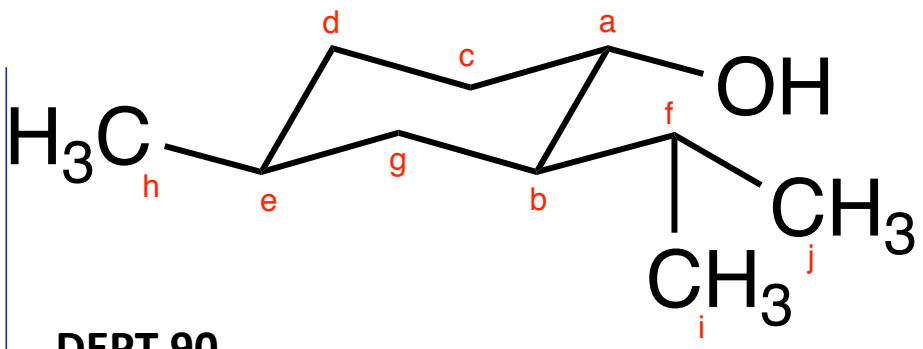
(1S,2R,4S)-2-isopropyl-4-methylcyclohexanol


1
2
3
4
5
6
7
8
9/10
11
12
13
14
.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7
f1 (ppm)

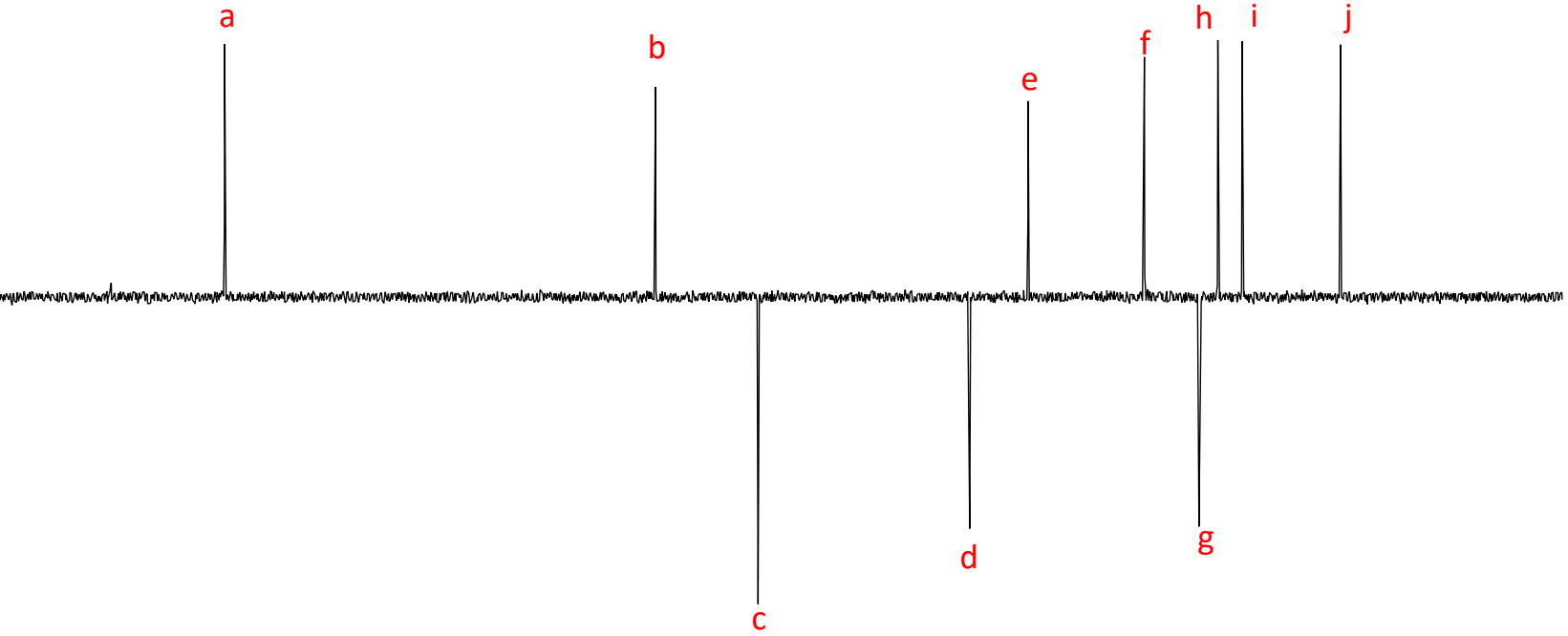

H13
H1
H3
H9
H4
OH7
2
H3C12
CH3
14
H5
H10
H6
H8
CH3
11


0
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)

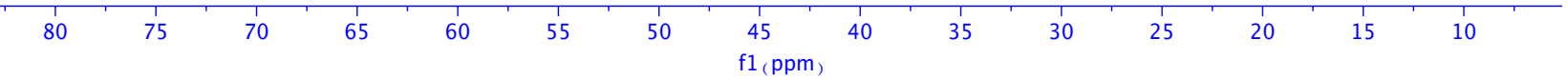




DEPT-90

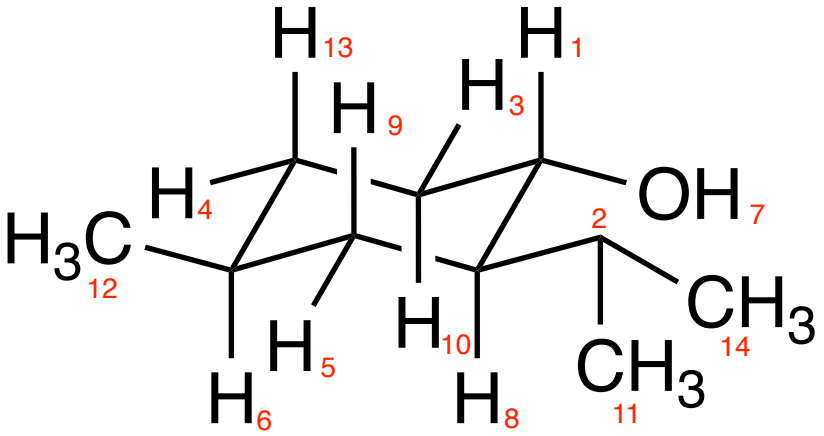


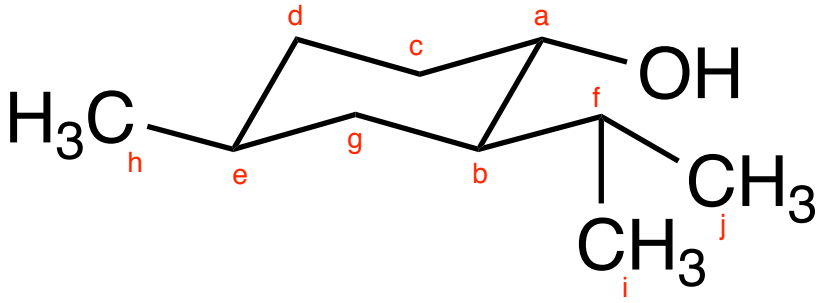
DEPT-135



We know:

- Carbons a, b, e, and f are CH's
- Carbons c, d, and g are CH_2's
- Carbons h, I, and j are CH_3's

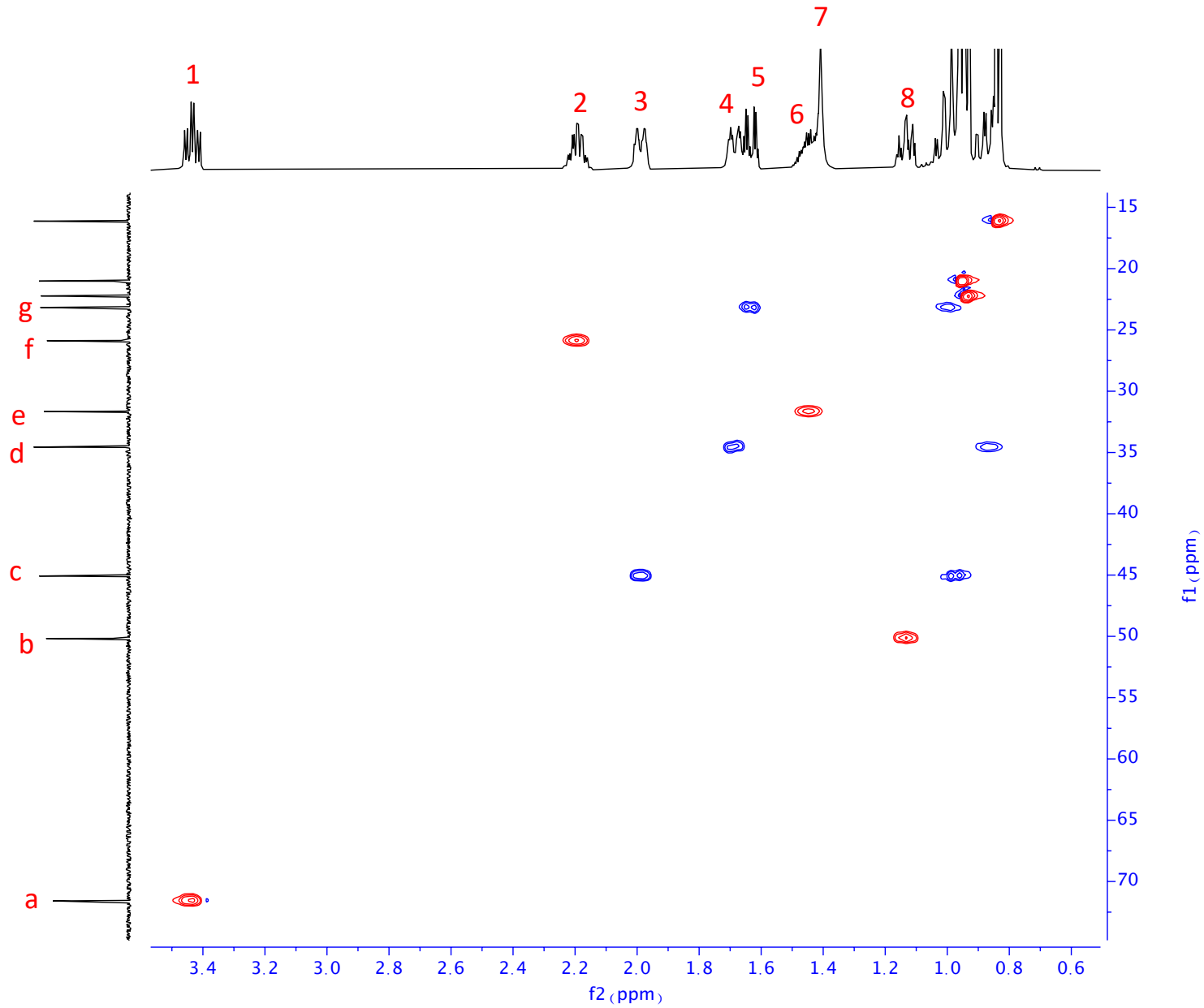


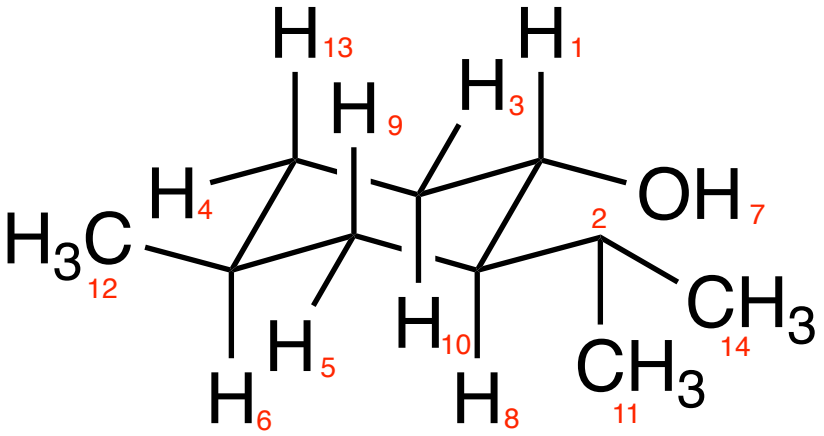


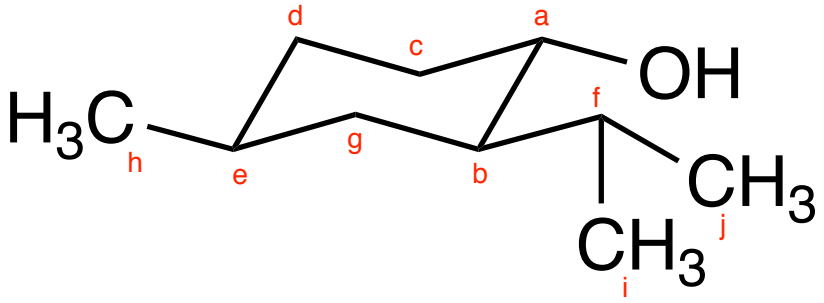
We know:

- Carbons a, b, e, and f are CH's
- Carbons c, d, and g are CH_2's
- Protons 3, 4, and 5 are CH_2's
- Carbons h, I, and j are CH_3's

HSQC

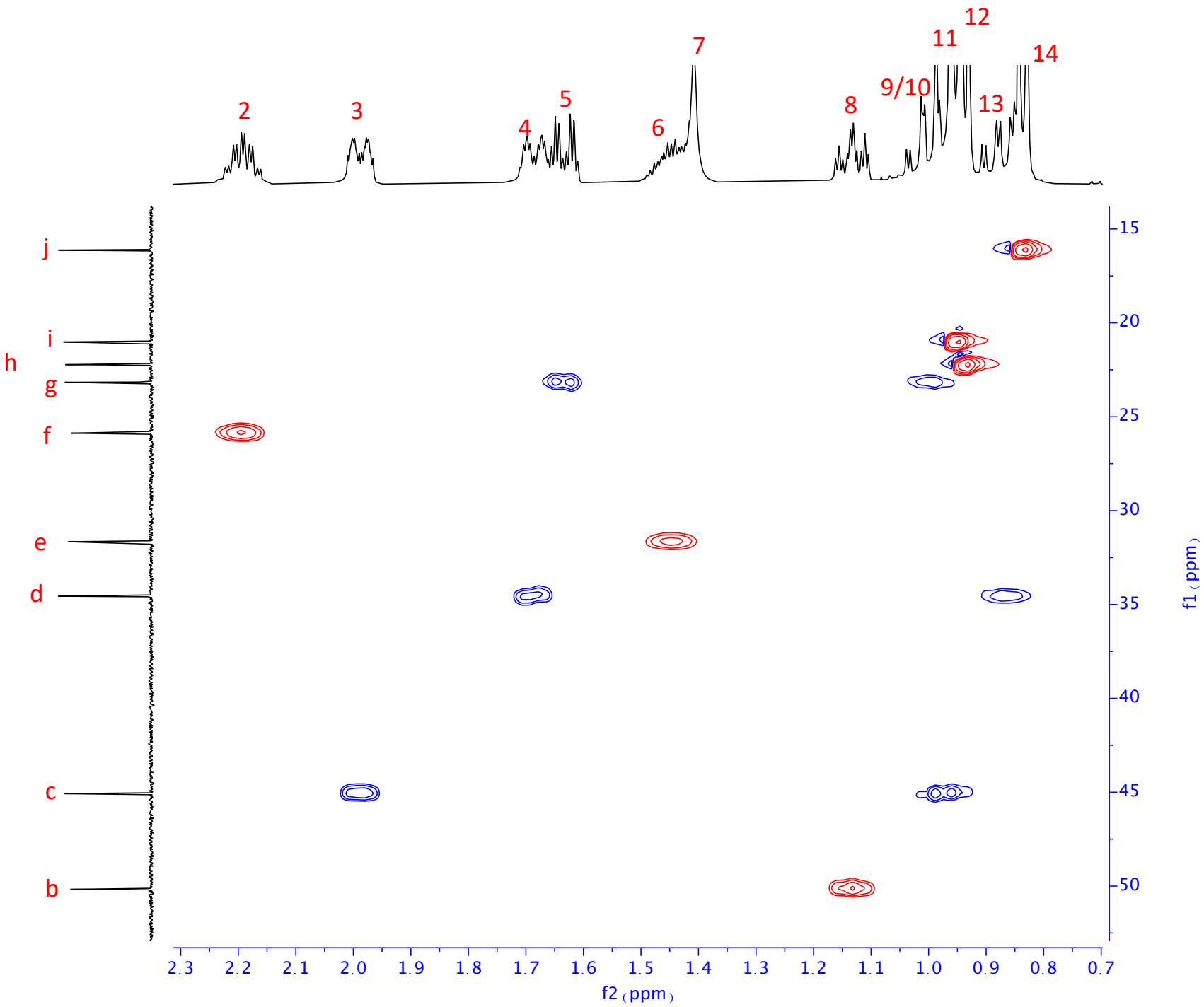




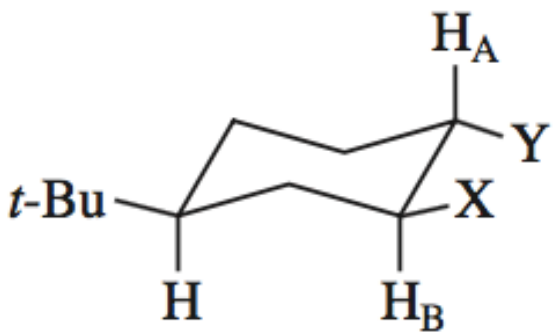


We know:

- Carbons a, b, e, and f are CH's
- Carbons c, d, and g are CH_2's
- Protons 3, 4, and 5 are CH_2's
- Carbons h, I, and j are CH_3's

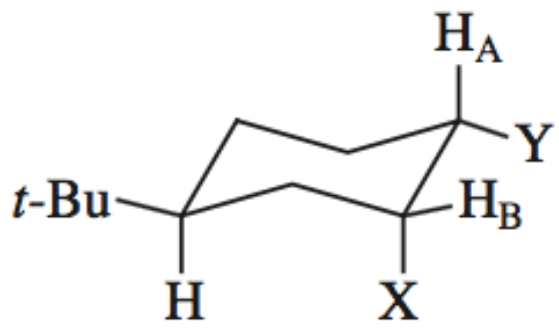


a,a



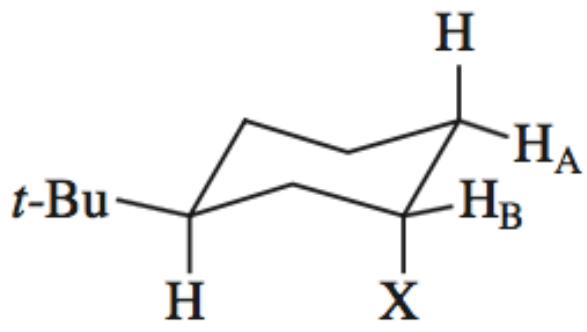
$J_{AB} = 10–14$ Hz
$\alpha = 180°$

a,e



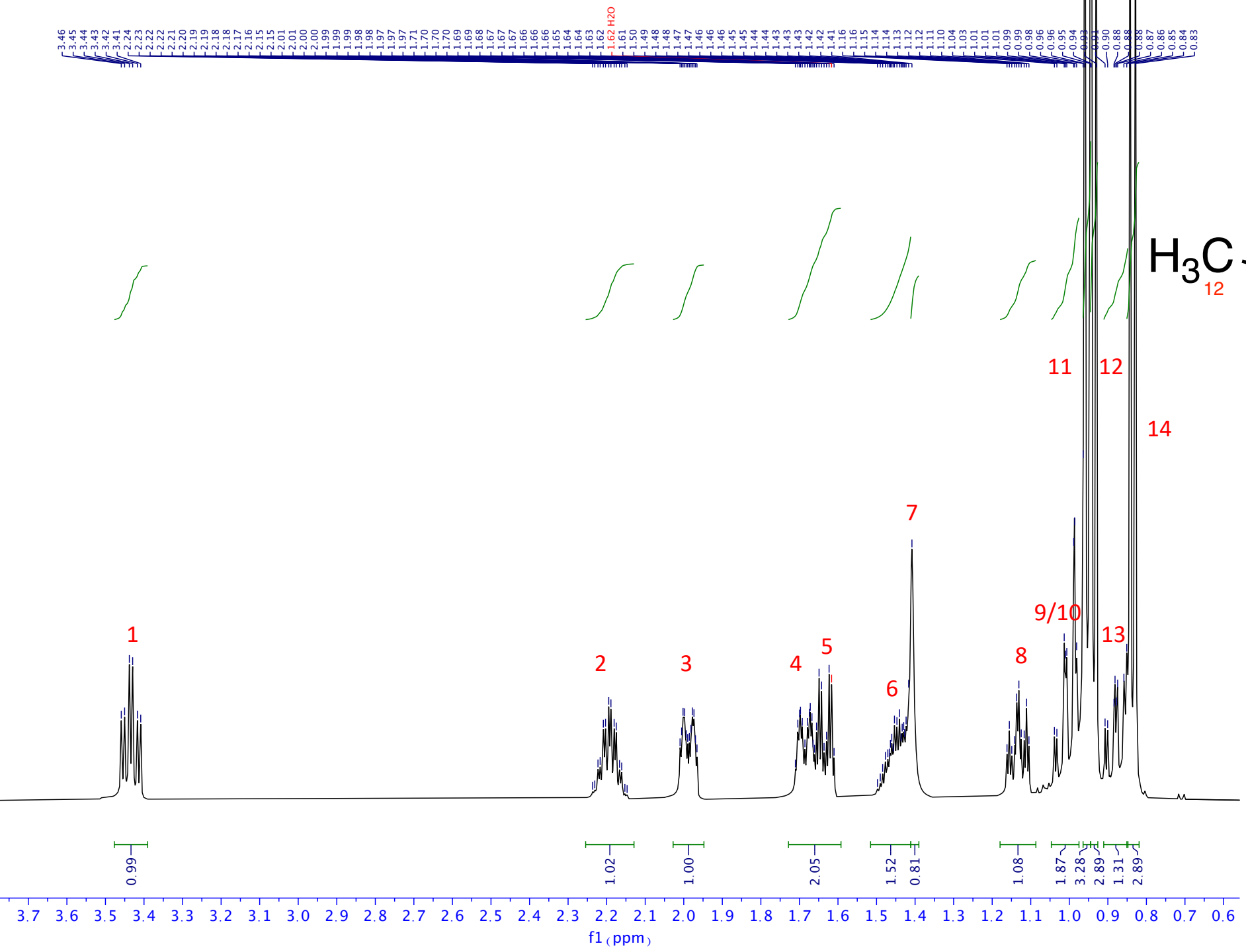
$J_{AB} = 2–6$ Hz
$\alpha = 60°$

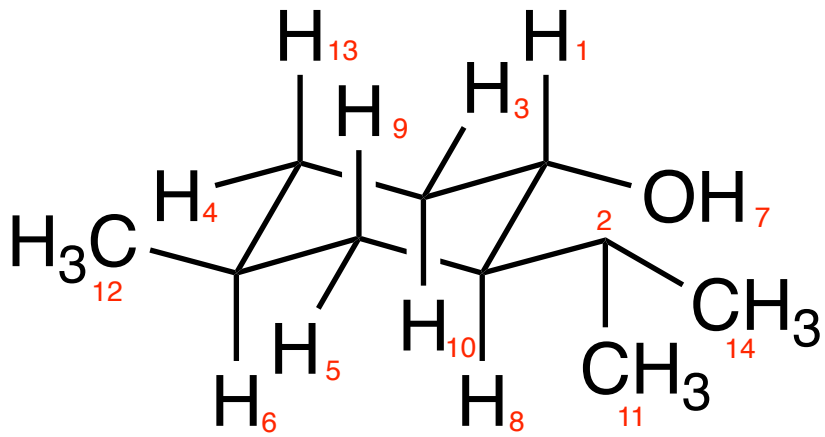
e,e

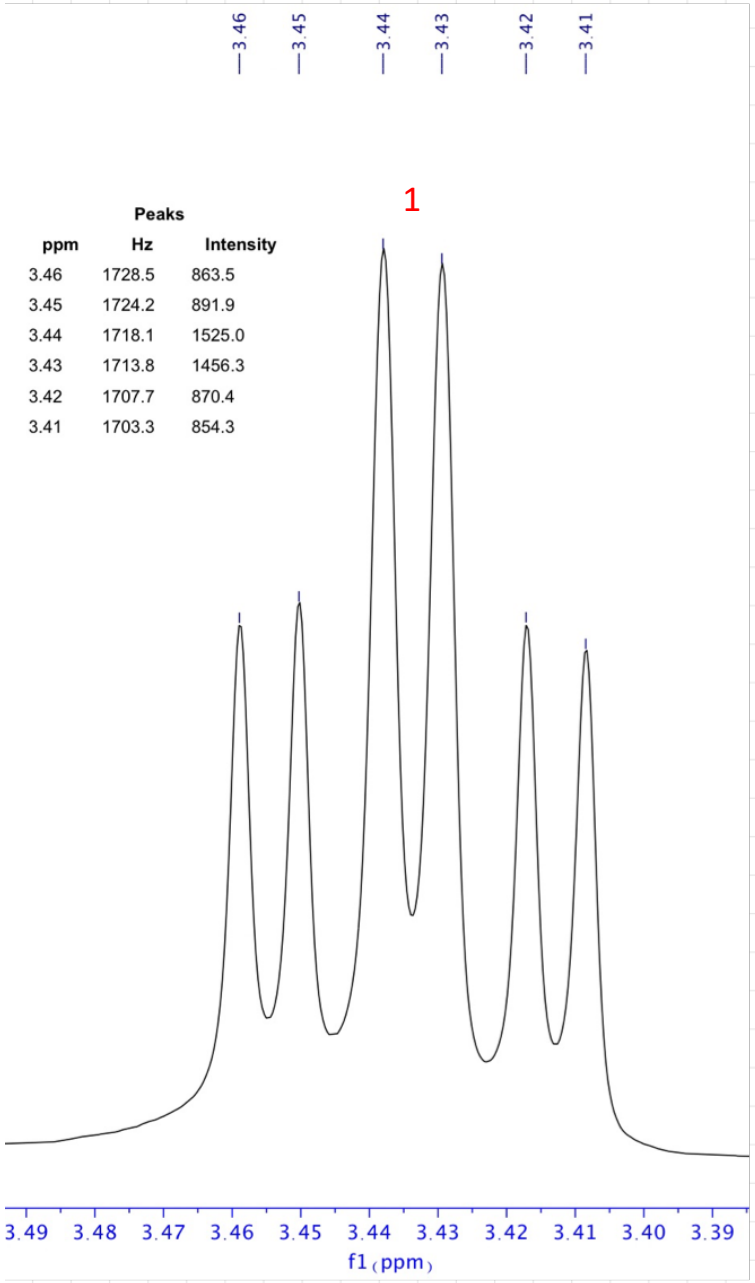


$J_{AB} = 2–5$ Hz
$\alpha = 60°$

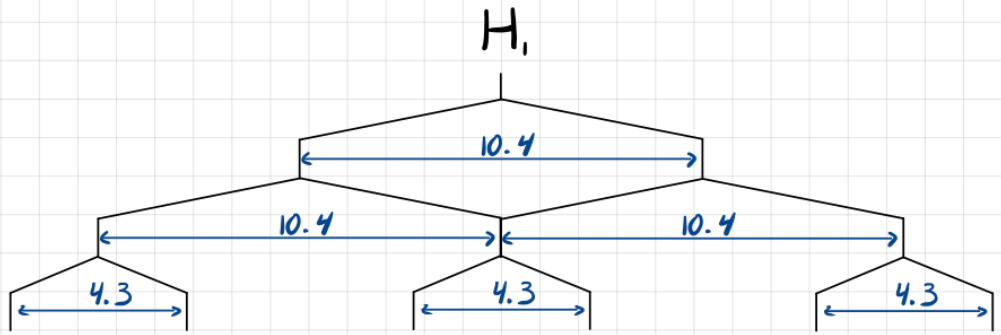
FIGURE 7.9 Vicinal couplings in cyclohexane derivatives.

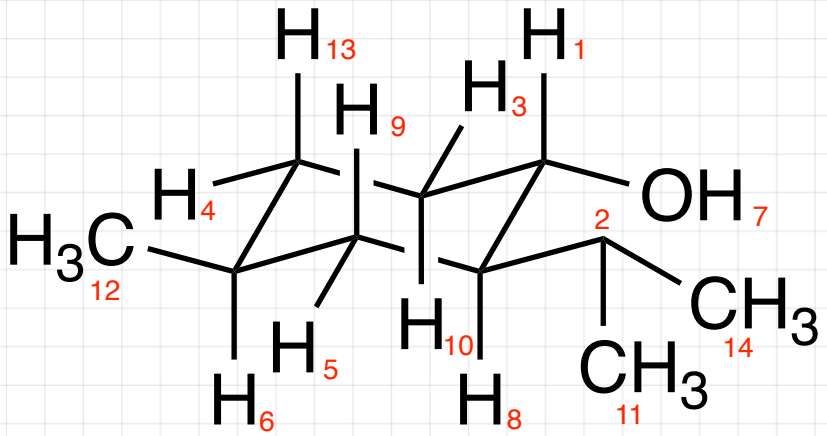

1
2
3
4
5
6
7
8
9/10
11
12
13
14
0.99
1.02
1.00
2.05
1.52
0.81
1.08
1.87
3.28
2.89
1.31
2.89
f1 (ppm)


H13
H1
H3
H9
H4
OH7
2
H3C12
CH3
14
H5
H10
H6
H8
CH3
11



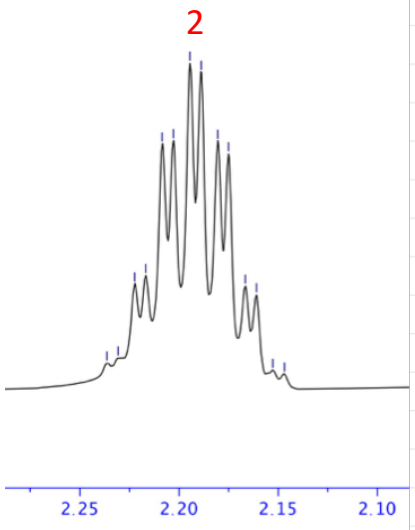
$J = 10.4, 10.4, 4.3\ Hz$

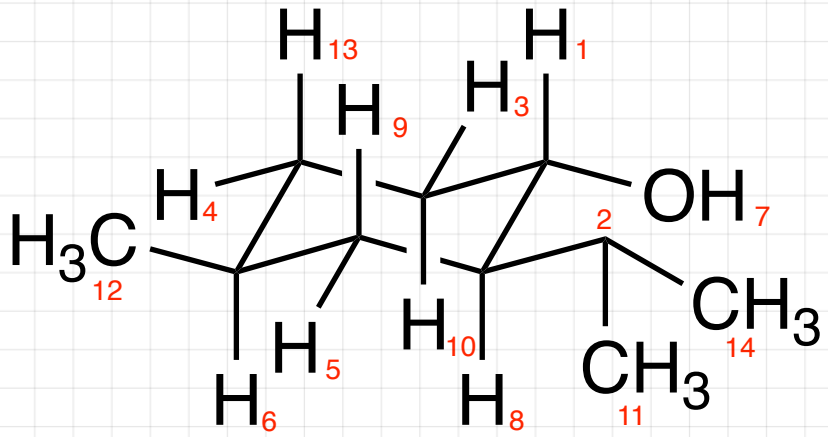




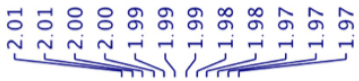
Peaks

ppm	Hz	Intensity
2.24	1117.6	45.2
2.23	1114.8	53.1
2.22	1110.6	281.3
2.22	1107.8	277.6
2.21	1103.7	692.4
2.20	1100.8	675.6
2.19	1096.7	953.0
2.19	1093.9	902.9
2.18	1089.7	722.7
2.18	1086.9	671.3
2.17	1082.7	290.5
2.16	1079.9	272.7
2.15	1075.8	41.5
2.15	1072.9	35.4





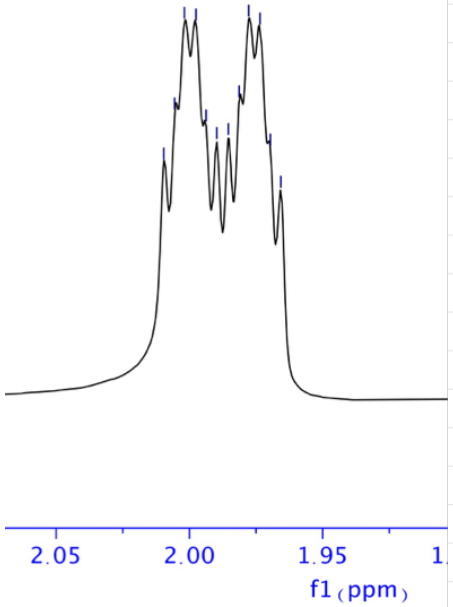
$J = 7 (X6), 2.9\ Hz$

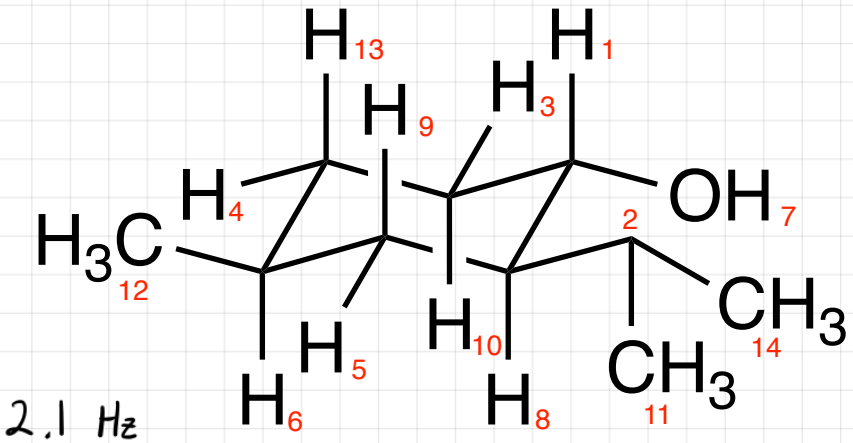


Peaks

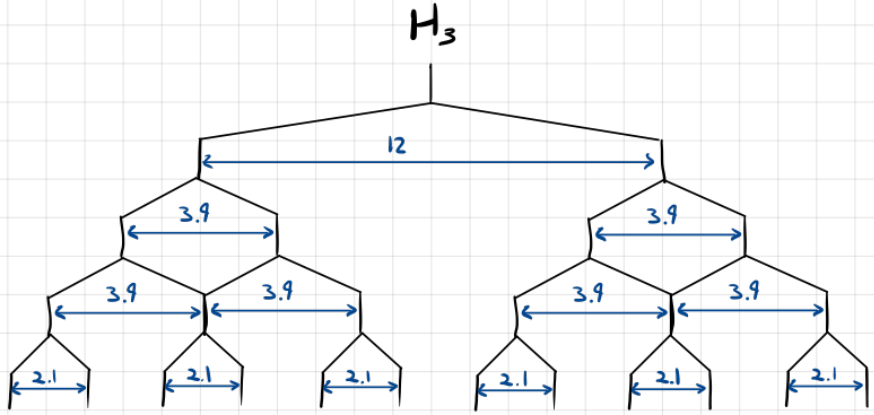
ppm	Hz	Intensity
2.01	1004.3	408.7
2.01	1002.2	357.8
2.00	1000.4	621.4
2.00	998.2	698.1
1.99	996.3	286.1
1.99	994.3	411.4
1.99	992.2	388.2
1.98	990.1	349.8
1.98	988.4	688.8
1.97	986.2	658.4
1.97	984.3	320.4
1.97	982.3	390.5

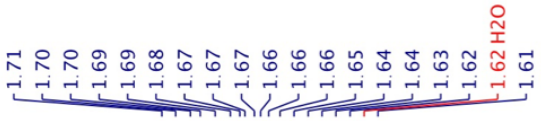
3





$J = 12.0, 3.9, 3.9, 2.1$ Hz





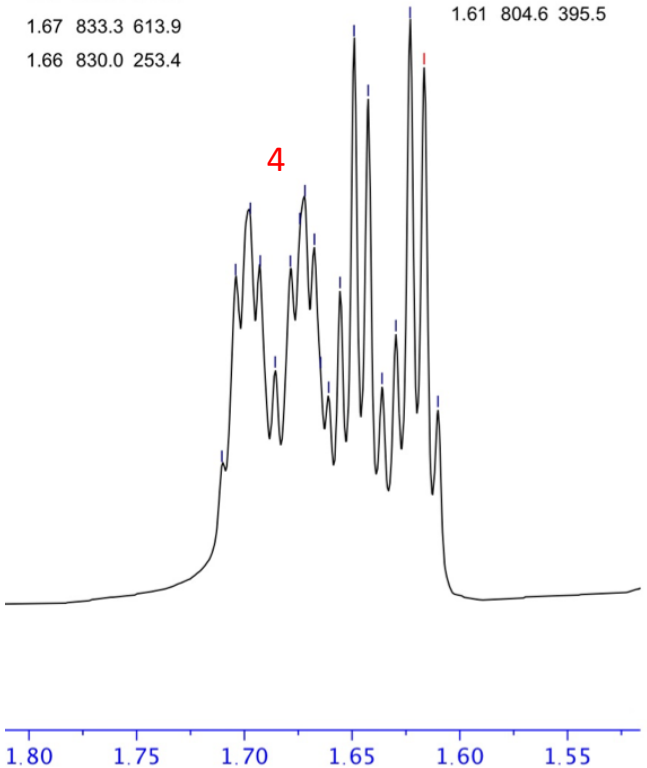
$J = 12.4, 5.6, 5.6, 3.4\ Hz$

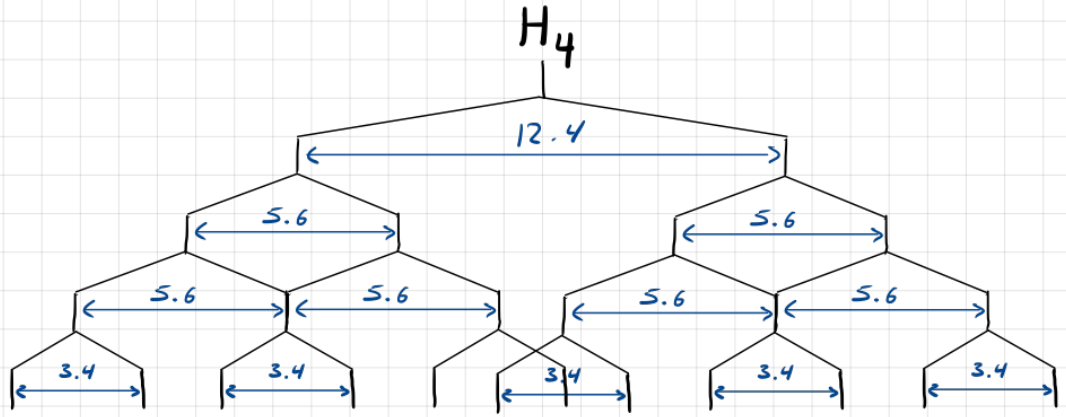
Peaks

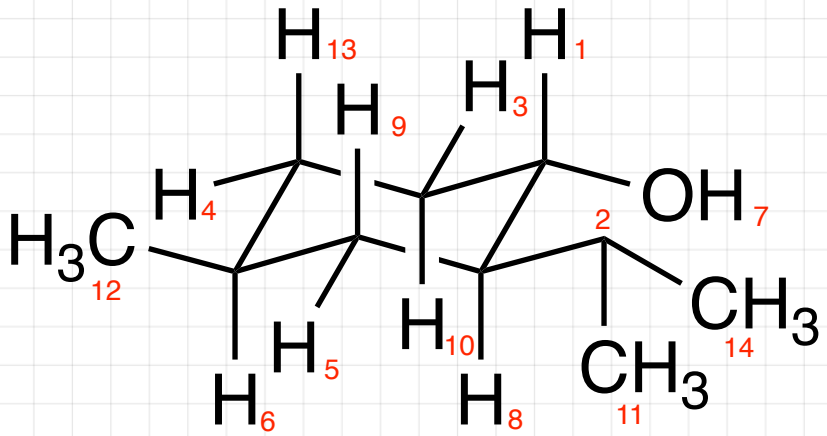
ppm	Hz	Intensity
1.71	854.8	148.2
1.70	851.6	638.6
1.70	848.1	717.4
1.69	845.9	573.9
1.69	842.4	323.9
1.68	838.8	469.2
1.67	835.5	639.6
1.67	833.3	613.9
1.66	830.0	253.4

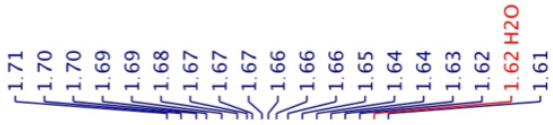
Peaks

ppm	Hz	Intensity
1.66	827.3	602.9
1.65	824.1	1259.3
1.64	820.8	1114.8
1.64	817.6	388.1
1.63	814.4	537.6
1.62	811.1	1342.9
1.62	807.8	1223.5
1.61	804.6	395.5







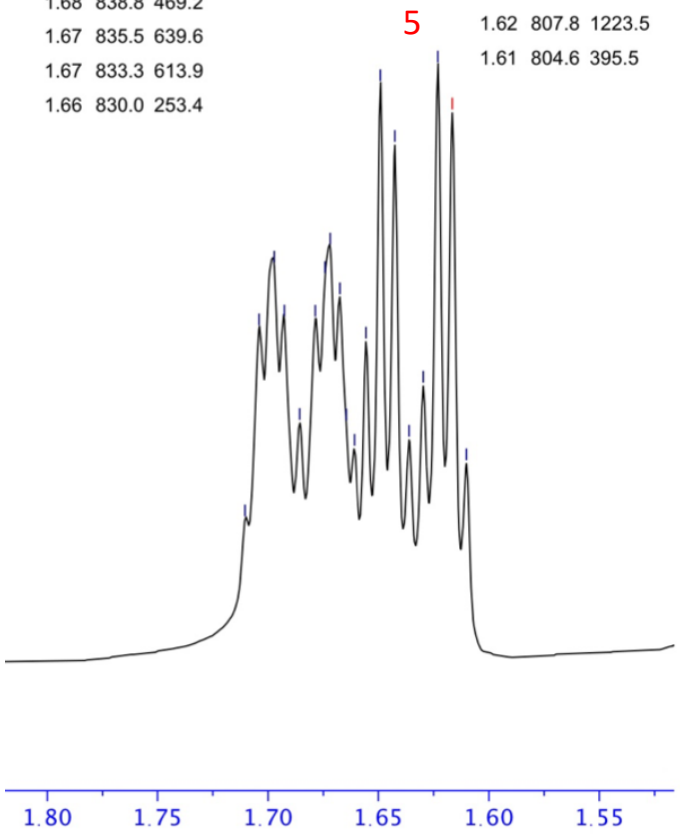


Peaks

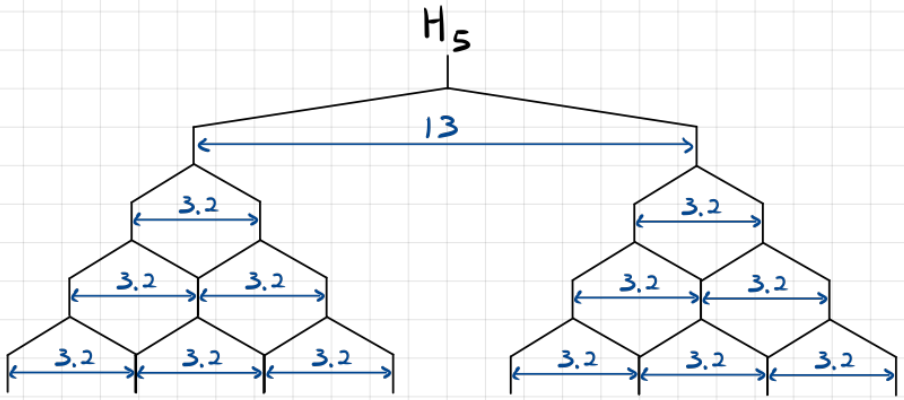
ppm	Hz	Intensity
1.71	854.8	148.2
1.70	851.6	638.6
1.70	848.1	717.4
1.69	845.9	573.9
1.69	842.4	323.9
1.68	838.8	469.2
1.67	835.5	639.6
1.67	833.3	613.9
1.66	830.0	253.4

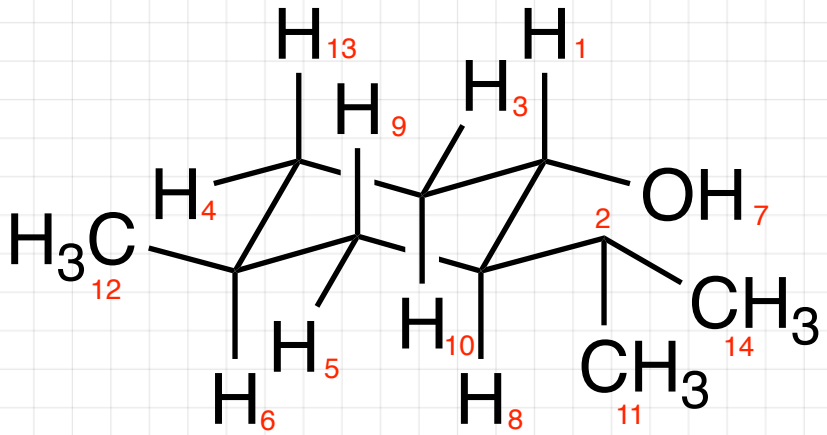
Peaks

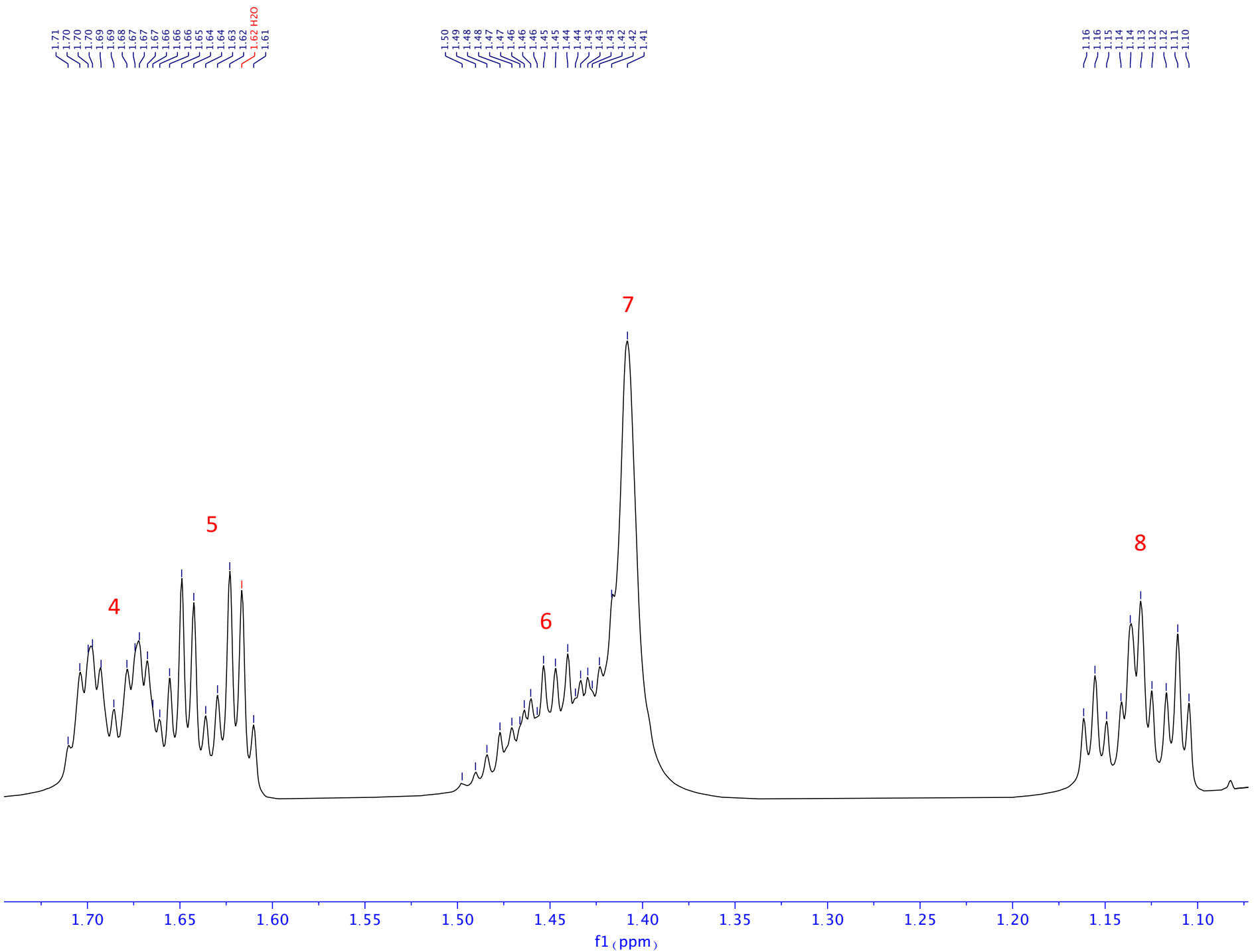
ppm	Hz	Intensity
1.66	827.3	602.9
1.65	824.1	1259.3
1.64	820.8	1114.8
1.64	817.6	388.1
1.63	814.4	537.6
1.62	811.1	1342.9
1.62	807.8	1223.5
1.61	804.6	395.5



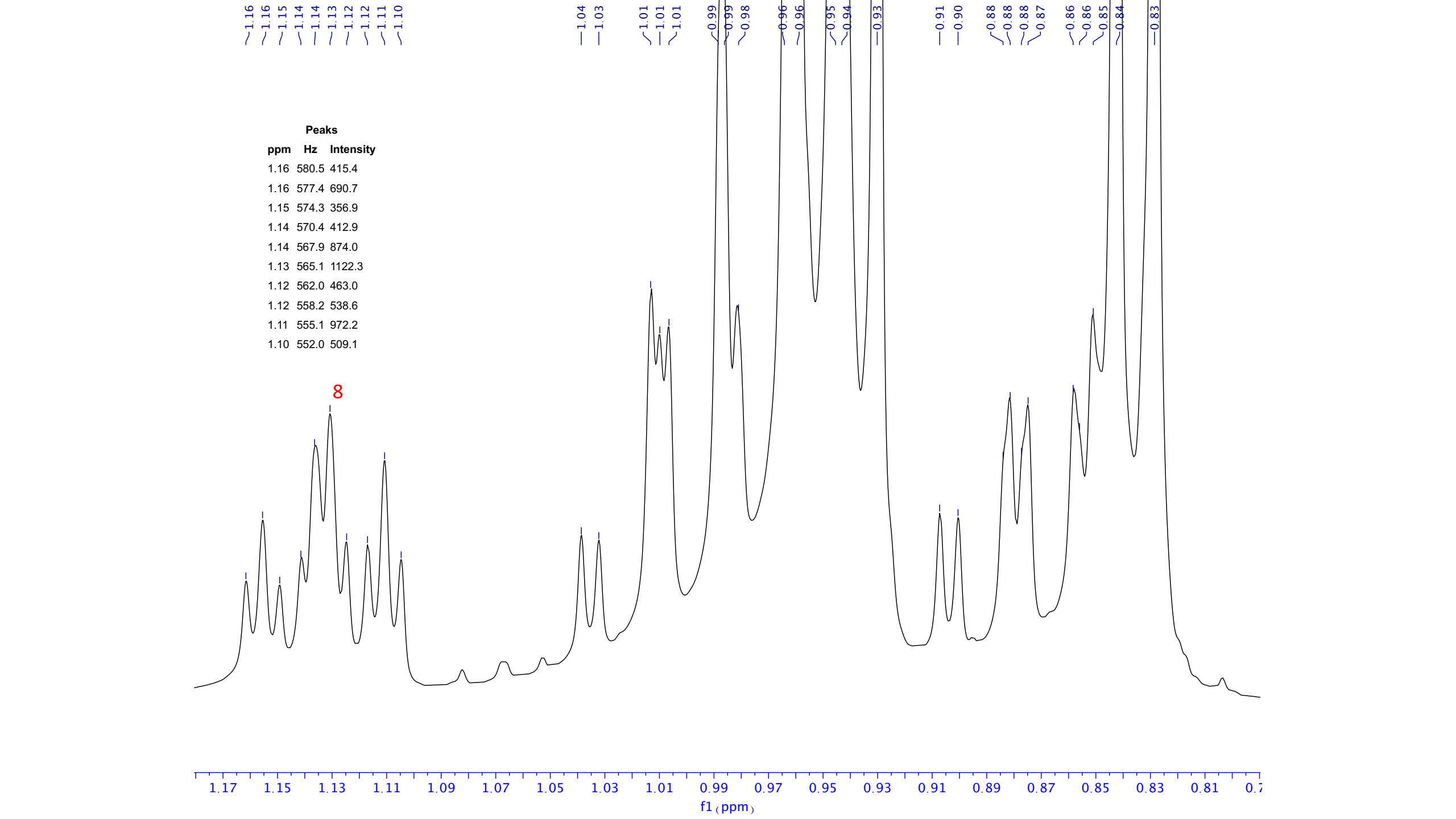
$J = 13.0, 3.2, 3.2, 3.2$ Hz

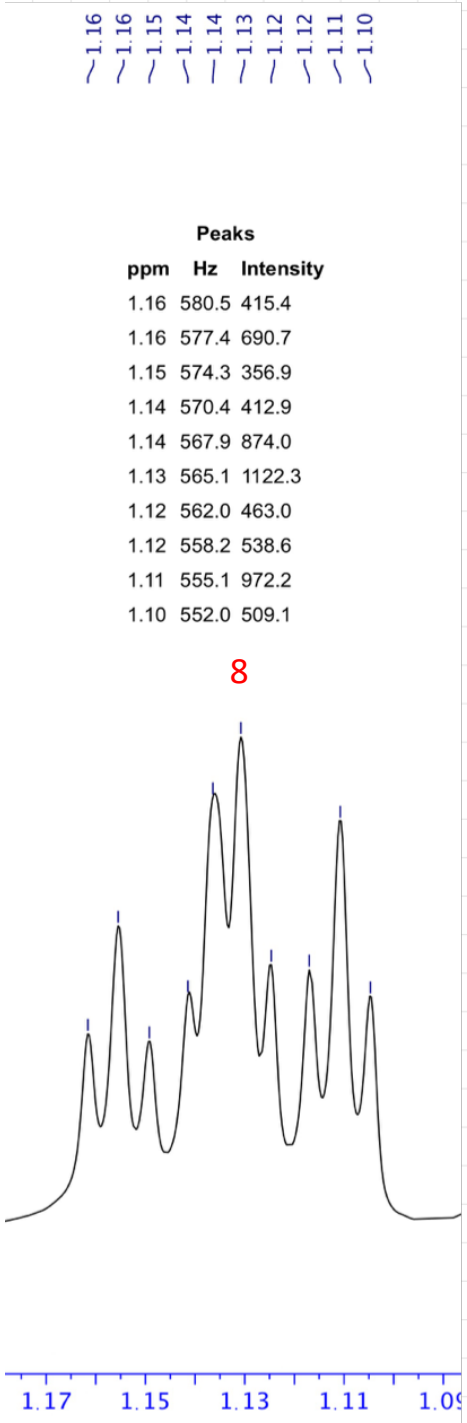




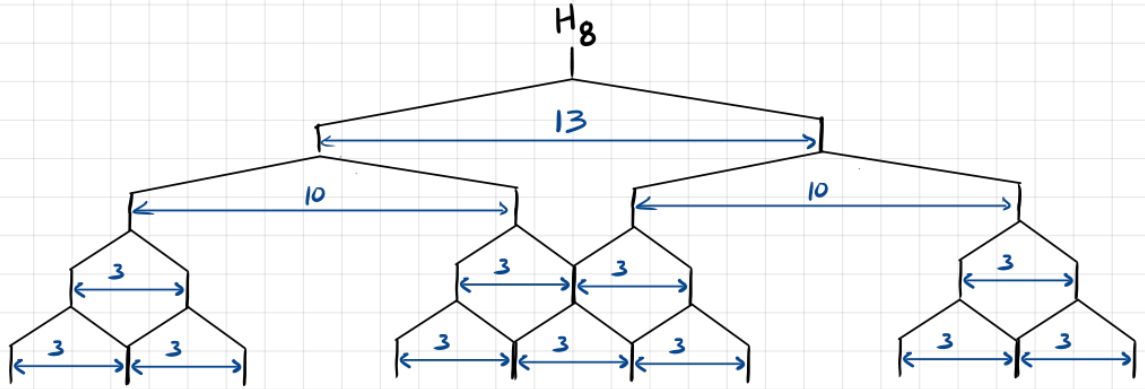


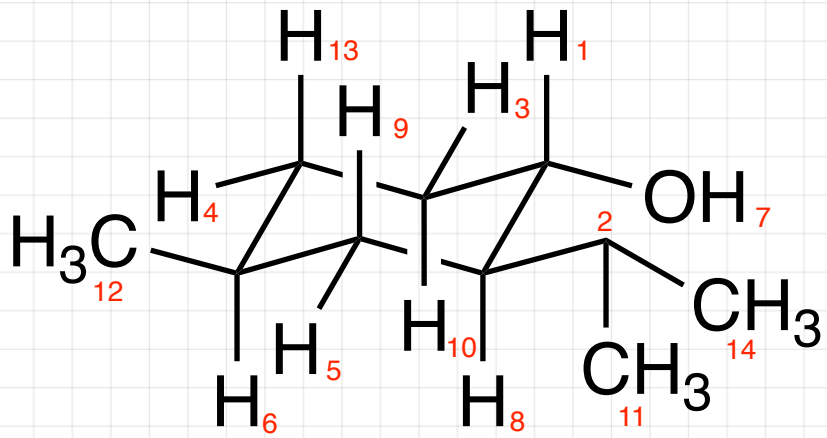
I'm going to skip signals 6 & 7 to the proton signal of 8.

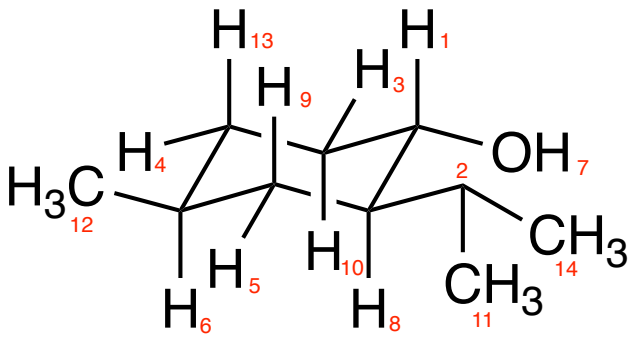

Peaks
ppm Hz Intensity
1.16 580.5 415.4
1.16 577.4 690.7
1.15 574.3 356.9
1.14 570.4 412.9
1.14 567.9 874.0
1.13 565.1 1122.3
1.12 562.0 463.0
1.12 558.2 538.6
1.11 555.1 972.2
1.10 552.0 509.1
8
f1 (ppm)

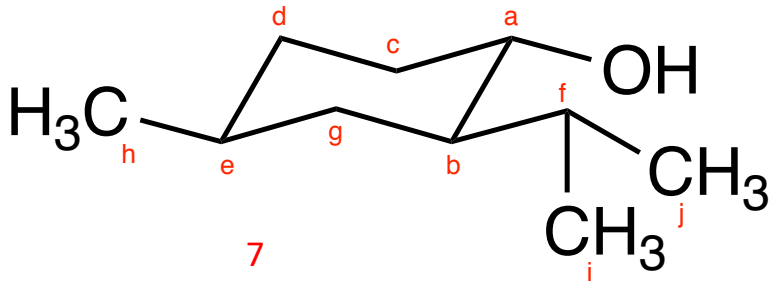

~1.16
~1.16
~1.15
~1.14
~1.14
~1.13
~1.12
~1.12
~1.11
~1.10
Peaks
ppm Hz Intensity
1.16 580.5 415.4
1.16 577.4 690.7
1.15 574.3 356.9
1.14 570.4 412.9
1.14 567.9 874.0
1.13 565.1 1122.3
1.12 562.0 463.0
1.12 558.2 538.6
1.11 555.1 972.2
1.10 552.0 509.1
8
1.17
1.15
1.13
1.11
1.09

J = 13, 10, 3, 3 Hz


H8
13
10
10
3
3
3
3
3
3
3
3
3
3
3
3

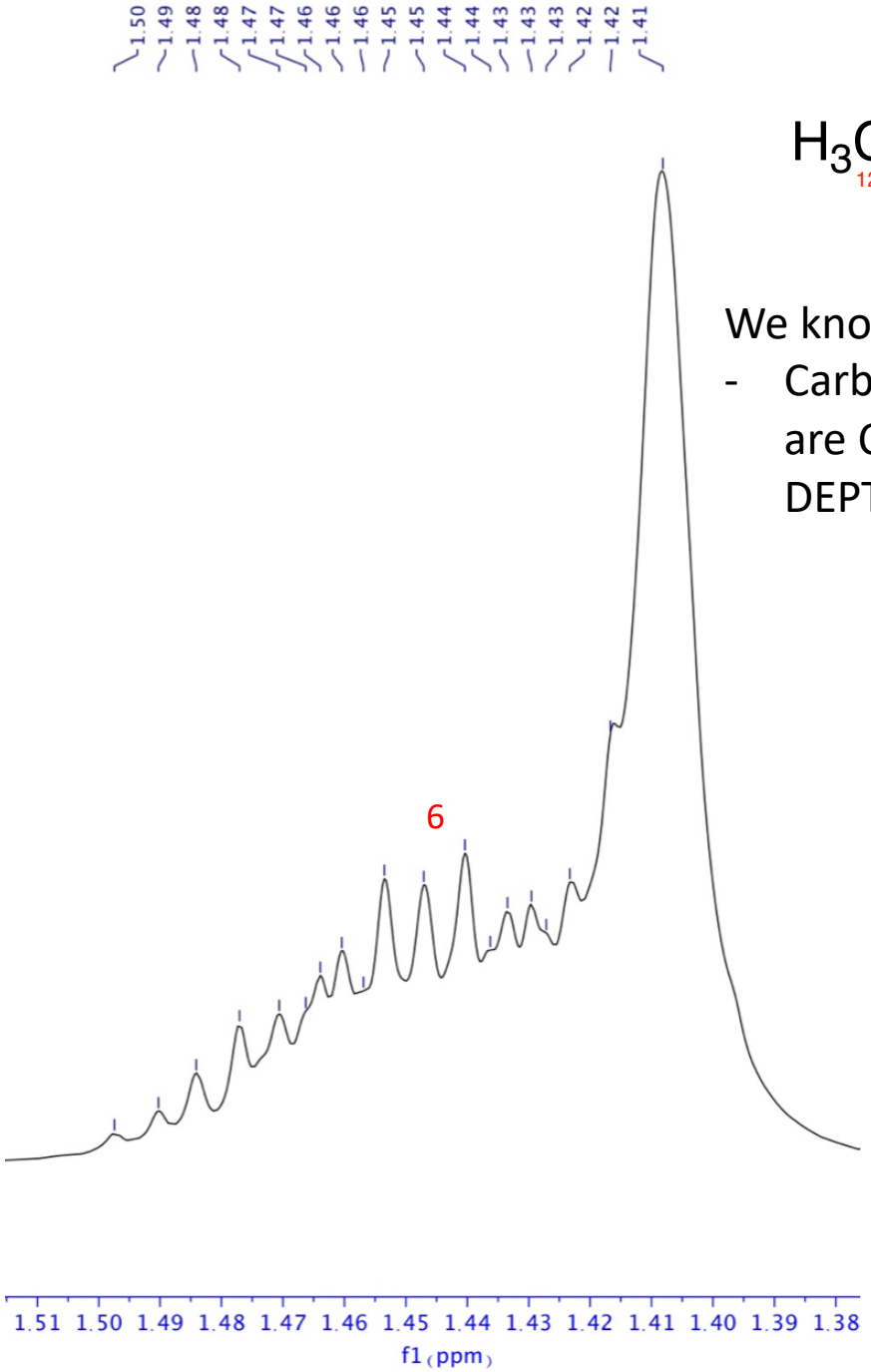

H13
H1
H9
H3
H4
OH7
2
H3C12
CH3
14
H10
H5
H6
H8
CH3
11

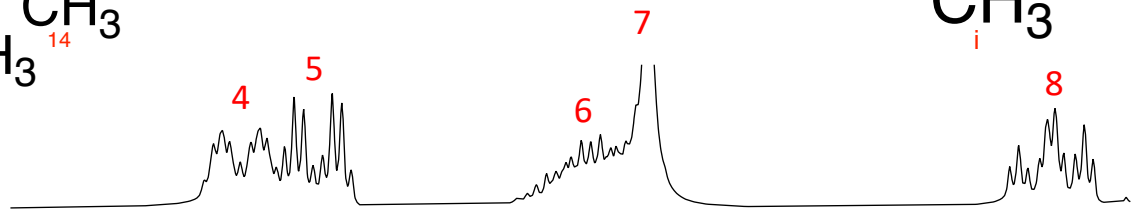


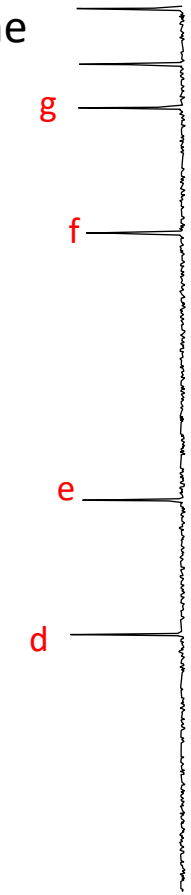


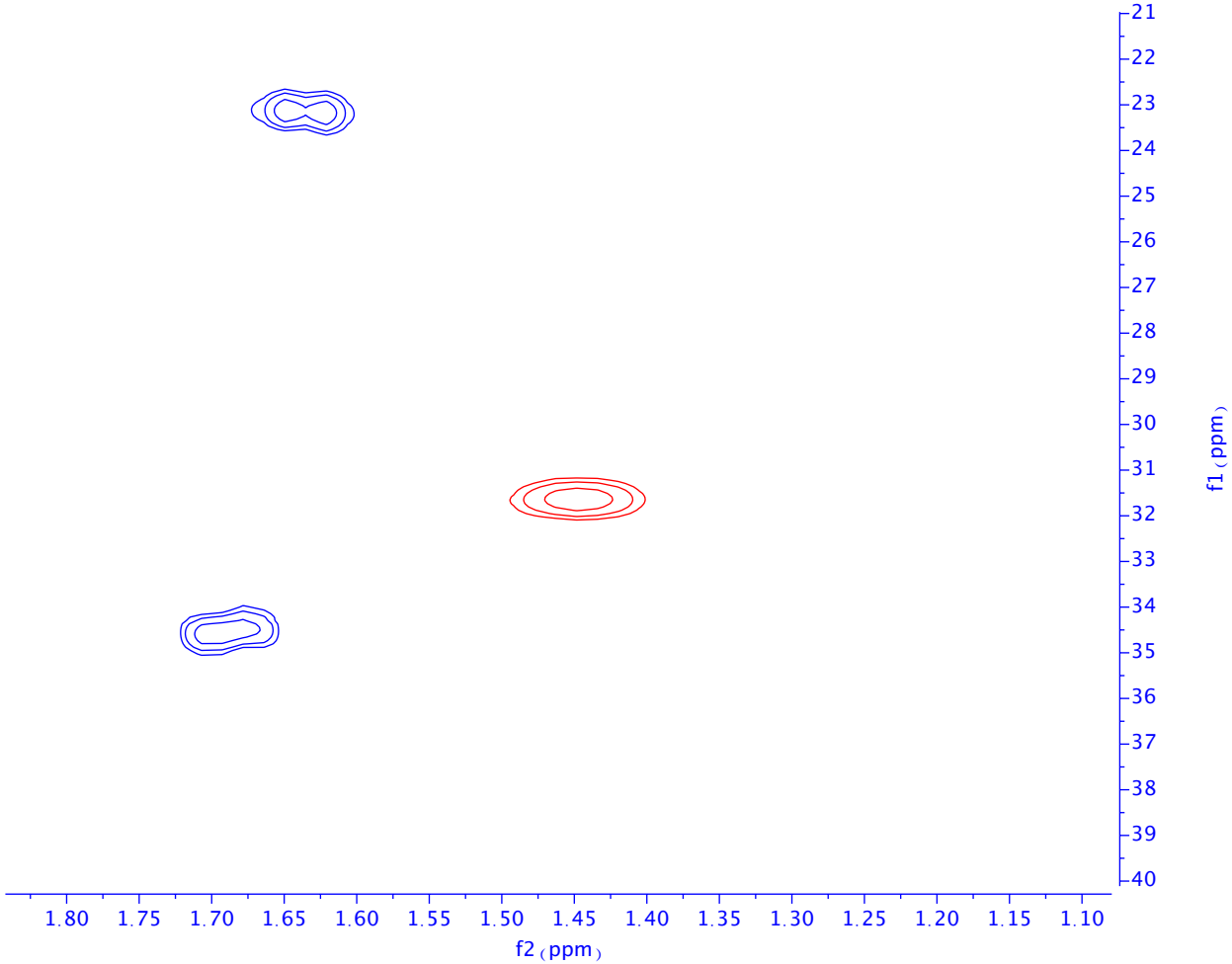
We know:

- Carbons a, b, e, and f are CH's from the DEPT-90

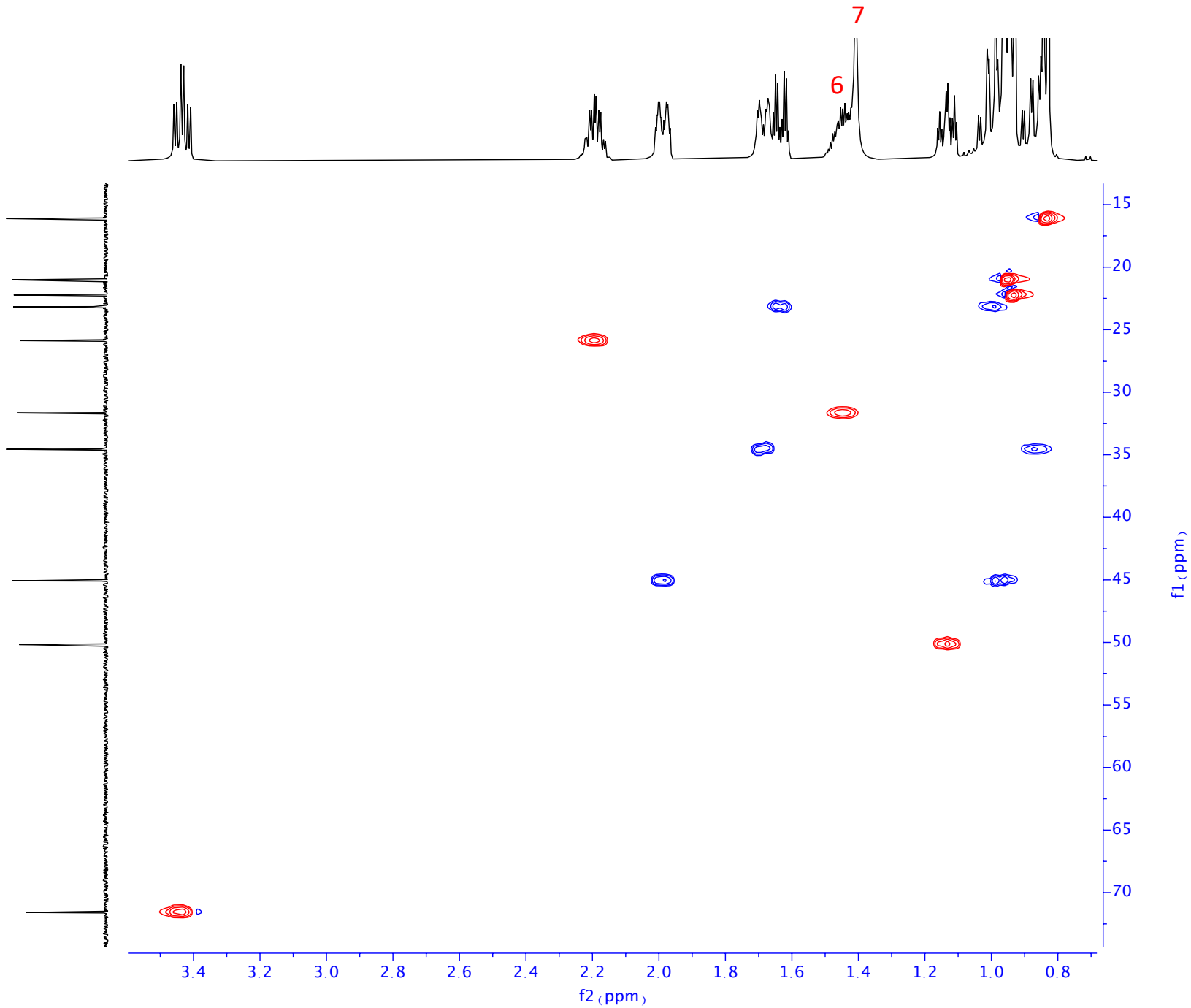


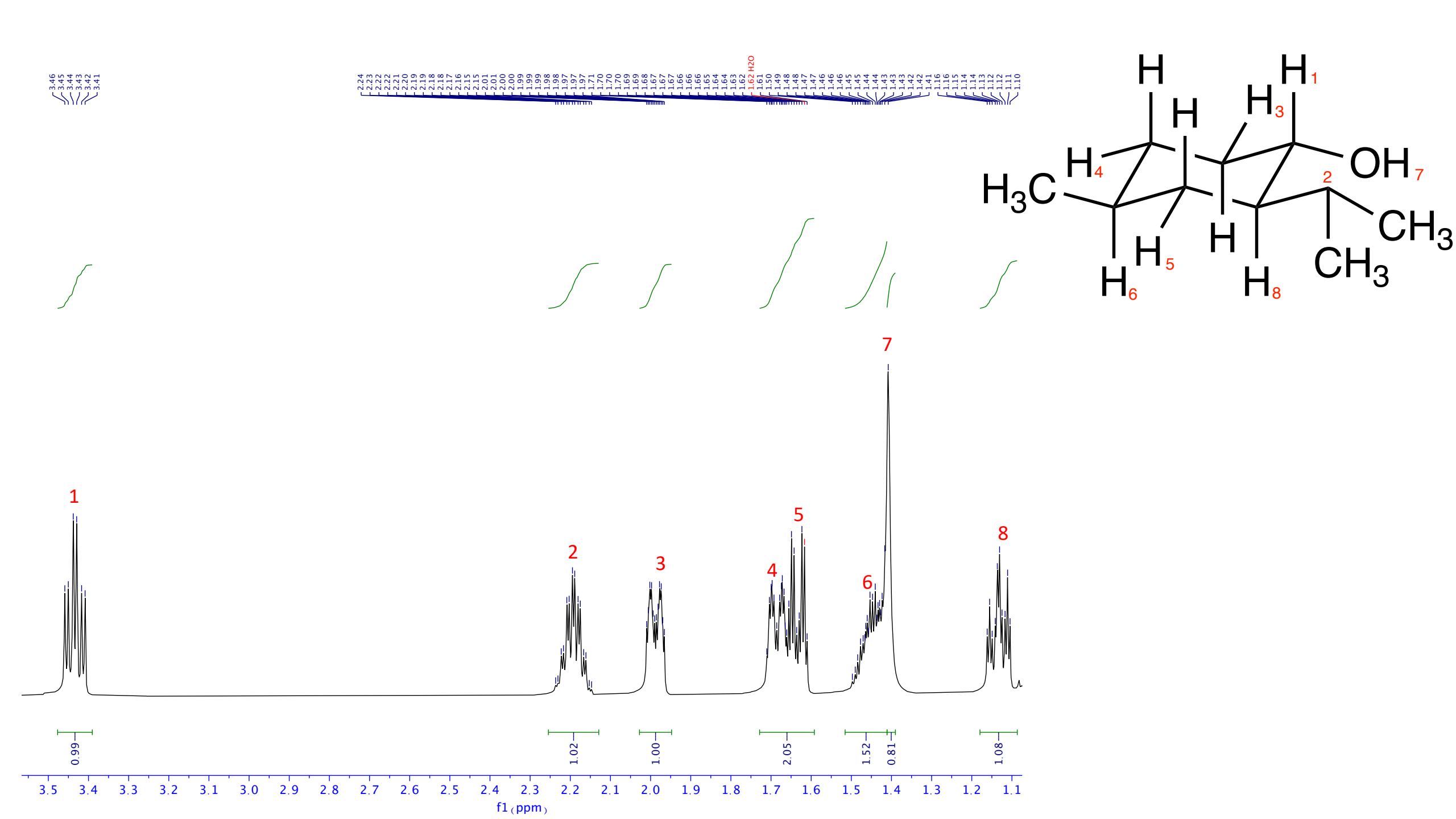


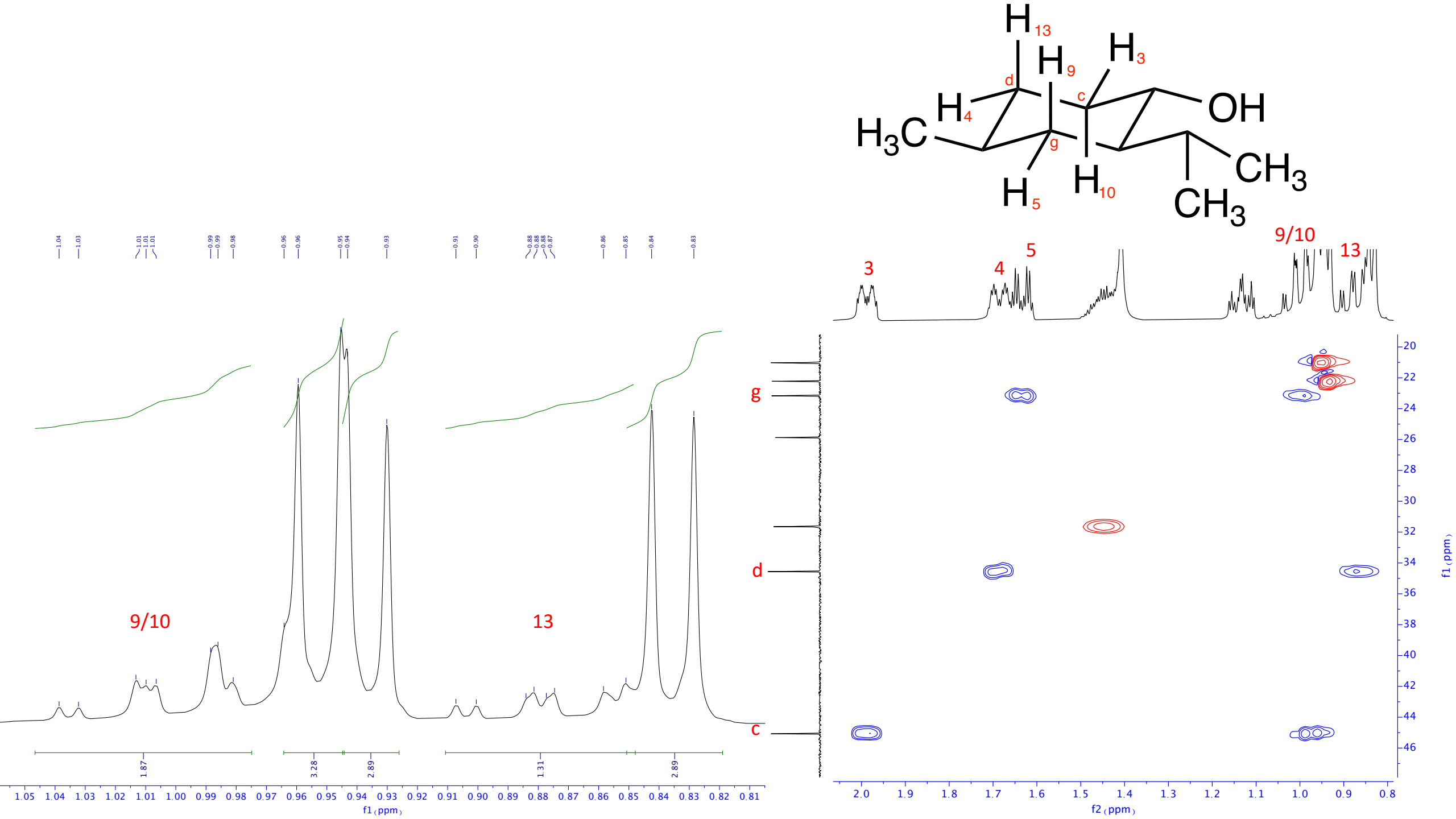




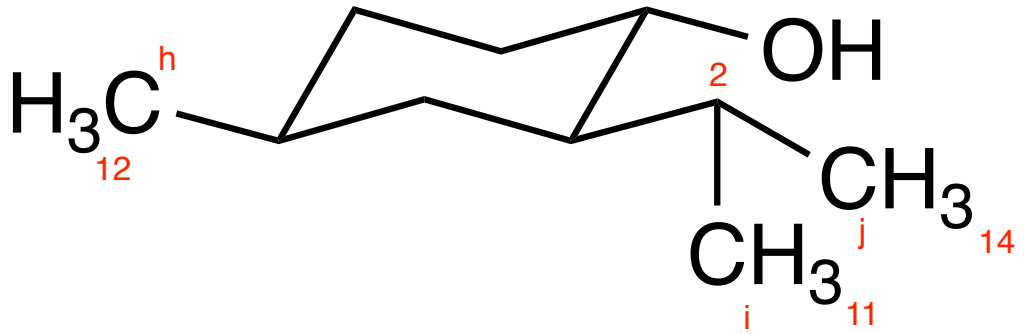
Finding the O-H proton.

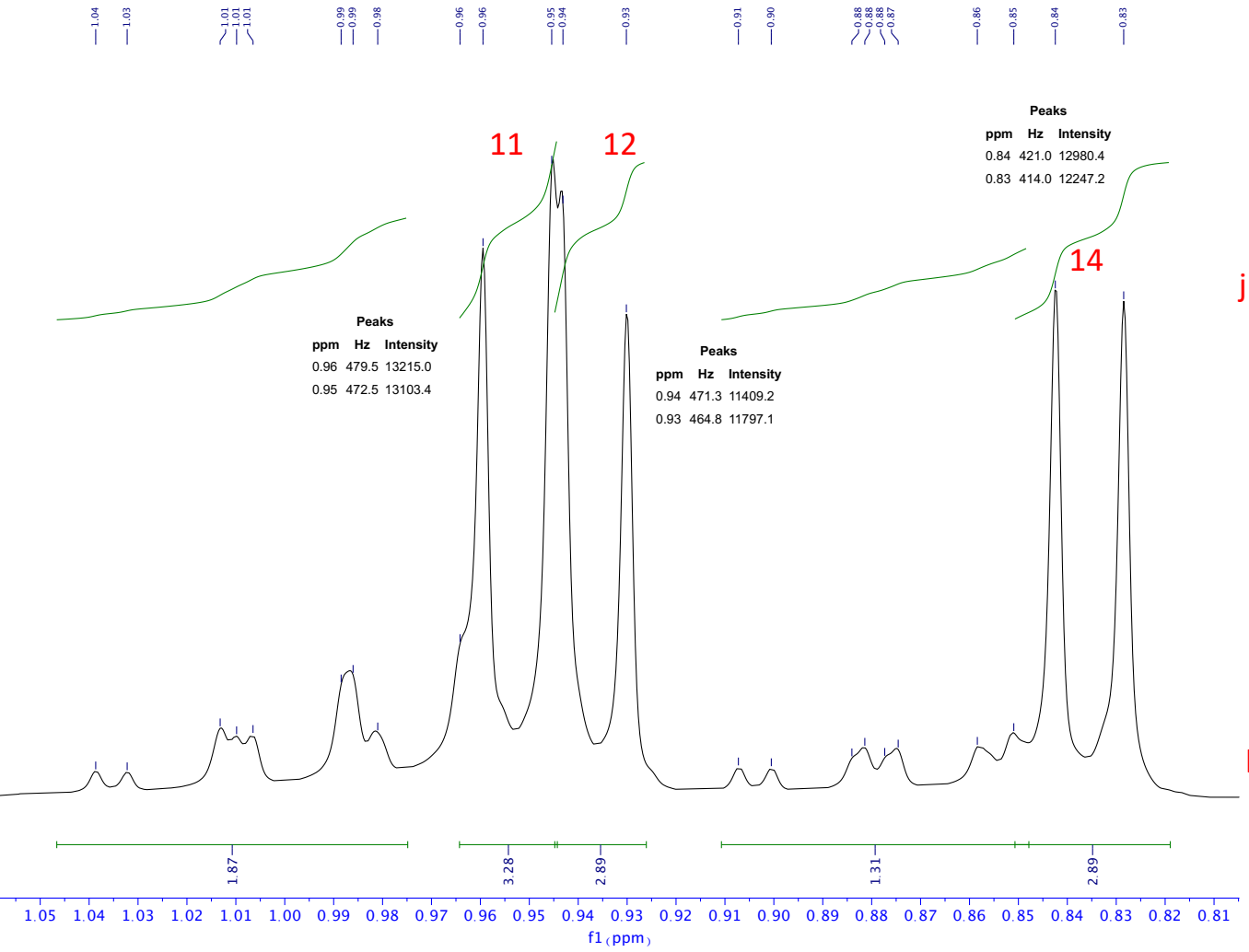


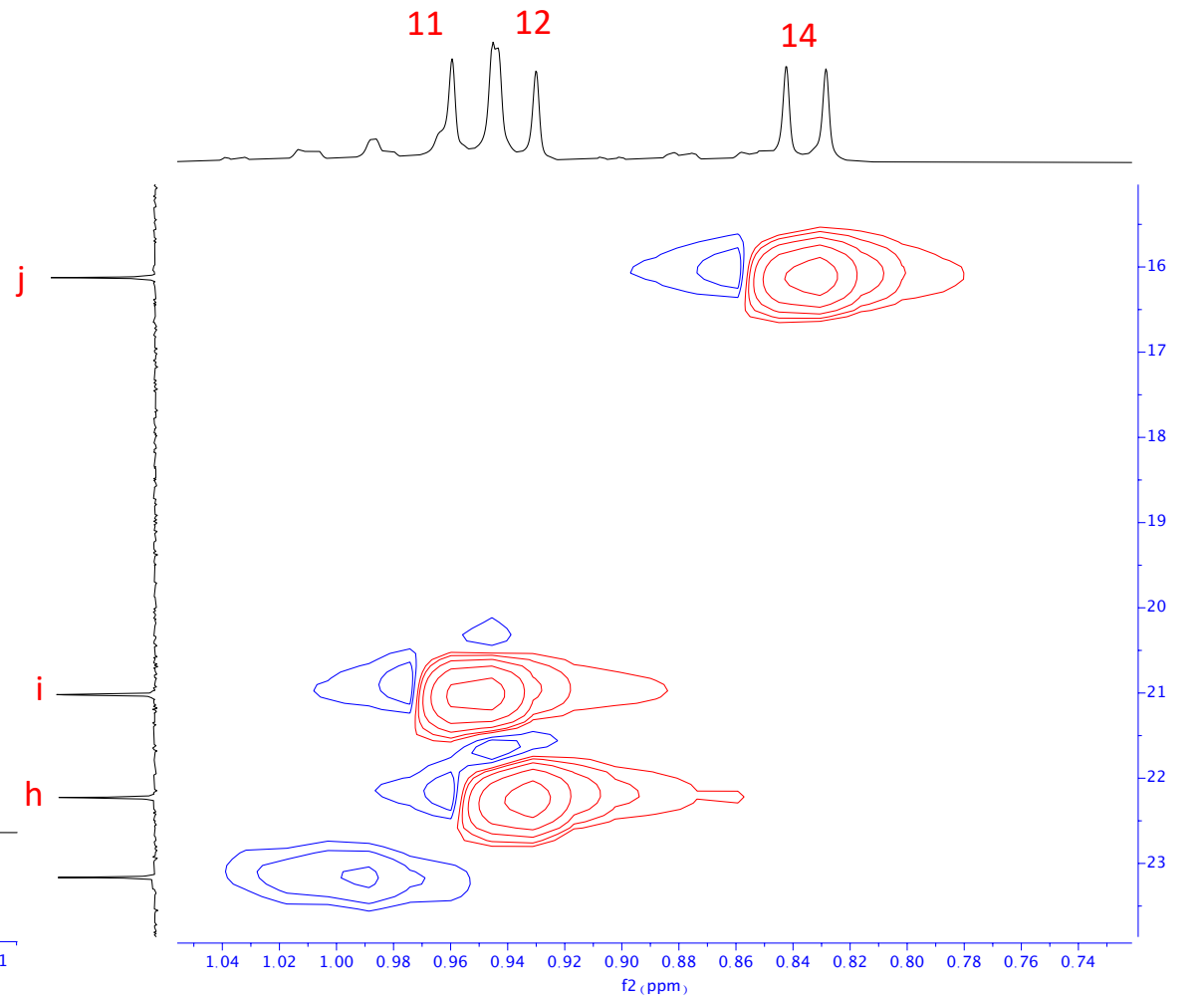

H
H
H1
H3
H4
H3C
OH7
2
CH3
H5
H
CH3
H6
H8
1
2
3
4
5
6
7
8
0.99
1.02
1.00
2.05
1.52
0.81
1.08
f1 (ppm)

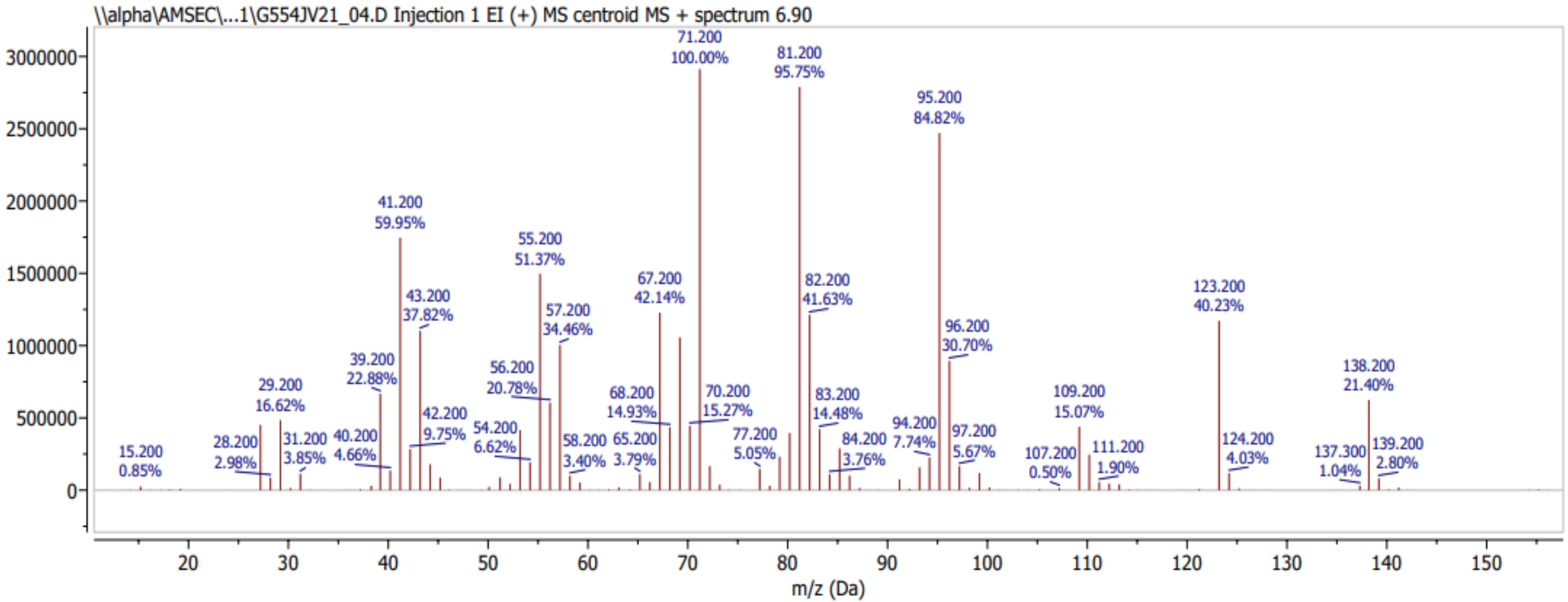

H13
H9
H3
d
c
H4
OH
H3C
g
CH3
H5
H10
CH3
9/10
13
3
4
5
9/10
13
g
d
c
1.87
3.28
2.89
1.31
2.89
f1 (ppm)
f2 (ppm)
f1 (ppm)

Signal	δ (ppm)	Multiplicity	Integration	Coupling constant (Hz)	Conclusion
2	2.20	Heptet of doublets	1	J = 7 and 2.9	CH-CH-isopropyl
11	0.95	d	3	J = 7	CH_3-CH
12	0.93	d	3	J = 6.5	CH_3-CH
14	0.83	d	3	J = 7	CH_3-CH



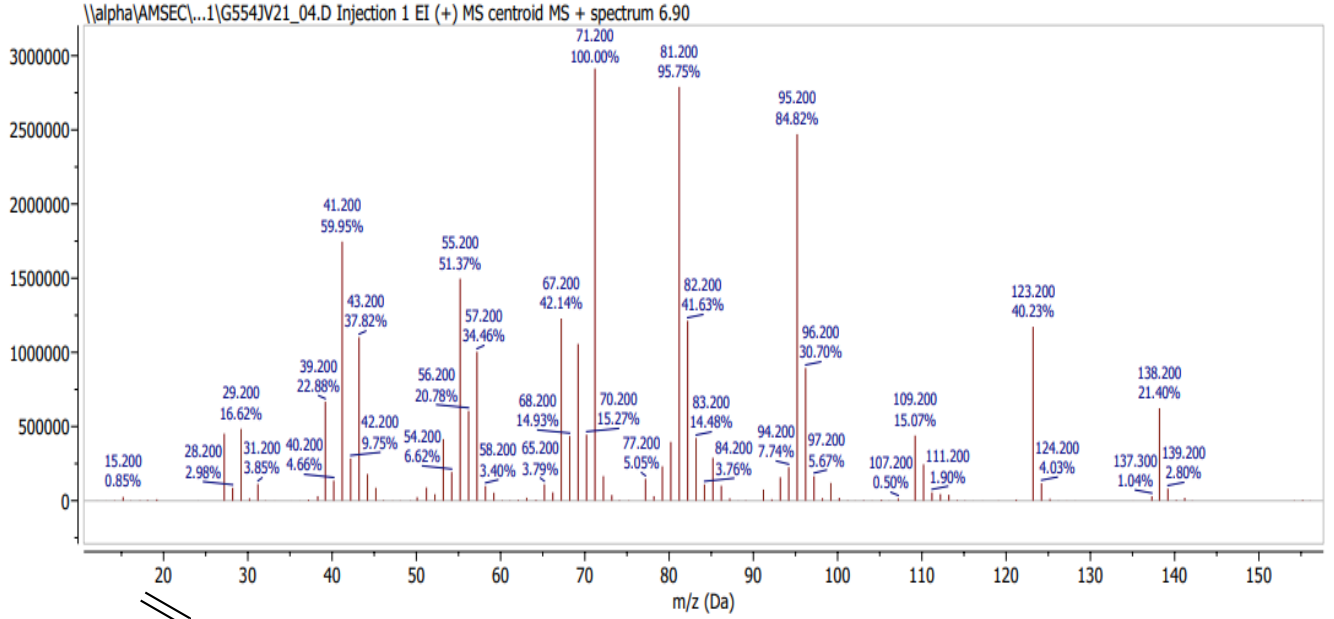


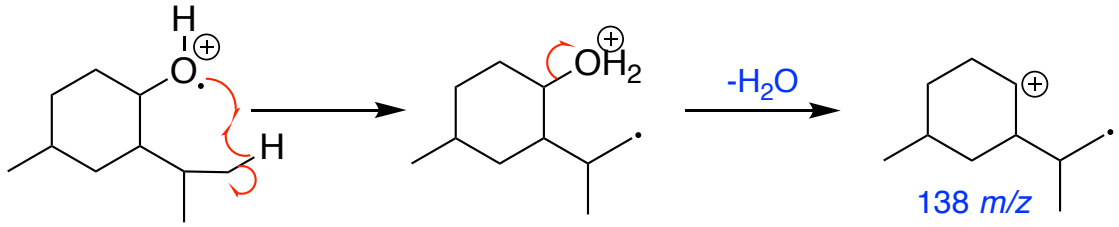


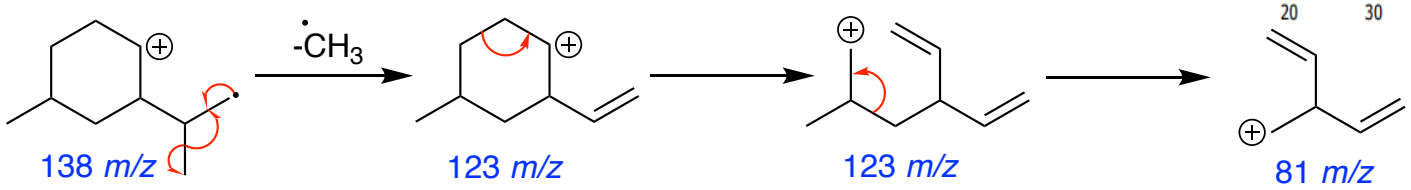

\\alpha\AMSEC\...1\G554JV21_04.D Injection 1 EI (+) MS centroid MS + spectrum 6.90
3000000
2500000
2000000
1500000
1000000
500000
0
71.200
100.00%
81.200
95.75%
95.200
84.82%
41.200
59.95%
55.200
51.37%
67.200
42.14%
82.200
41.63%
123.200
40.23%
43.200
37.82%
57.200
34.46%
96.200
30.70%
39.200
22.88%
56.200
20.78%
138.200
21.40%
29.200
16.62%
68.200
14.93%
70.200
15.27%
109.200
15.07%
83.200
14.48%
42.200
9.75%
54.200
6.62%
94.200
7.74%
124.200
4.03%
40.200
4.66%
77.200
5.05%
97.200
5.67%
28.200
2.98%
31.200
3.85%
58.200
3.40%
65.200
3.79%
84.200
3.76%
111.200
1.90%
139.200
2.80%
15.200
0.85%
107.200
0.50%
137.300
1.04%
20
30
40
50
60
70
80
90
100
110
120
130
140
150
m/z (Da)

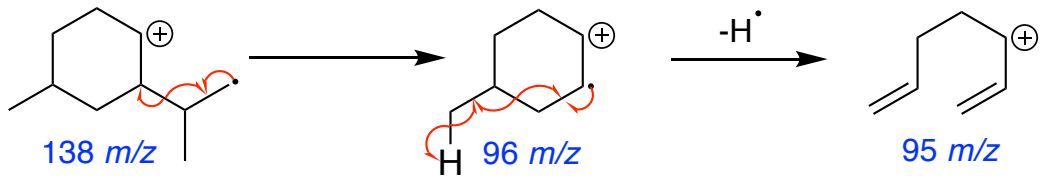
Fragmentations

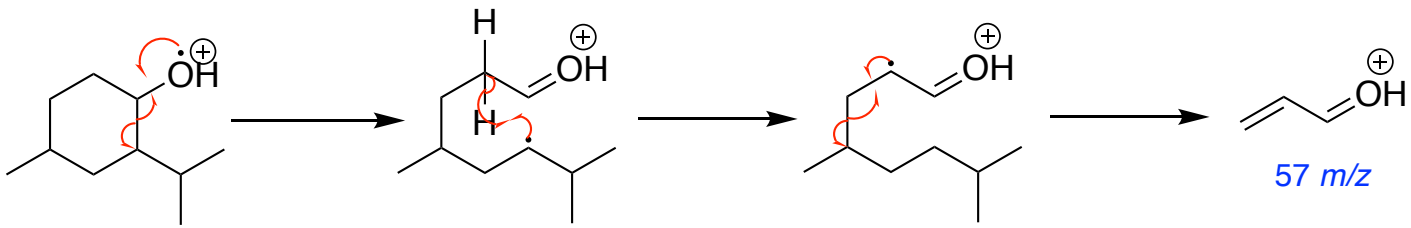
Base peak at 156 *m/z*











Thank you for listening!
Any questions?

References

Pavia, D.; Lampman, G.; Kriz, G.; Vyvyan, J. Introduction to Spectroscopy, Fifth Edition.; Cengage learning, 2015. http://dl.iranchembook.ir/ebook/organic-chemistry-2753.pdf