Tetrabutylammonium fluoride (TBAF)-catalyzed addition of substituted trialkylsilylalkynes to aldehydes, ketones and trifluoromethyl ketones

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Supporting Information

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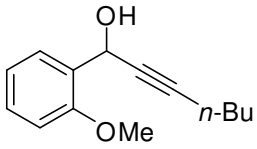
General Information. All reactions were carried out under inert atmosphere using oven dried glassware and a magnetic stirrer. THF was distilled and dried over sodium. Trialkylsilylalkynes, tetrabutylammonium fluoride and all aldehydes/ketones were purchased from commercial sources and used without further purification. Products were purified via column chromatography using hexane/ethyl acetate. ^{1}H and ^{13}C NMR spectra were obtained on a 300 and 400 MHz NMR spectrometer. All NMR spectra were taken in $CDCl_3$ otherwise reported. Thin layer chromatography was used to monitor reaction progress.

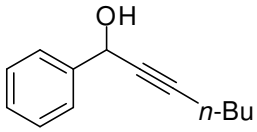
References for known compounds:

1-(2'-methoxyphenyl)hept-2-yn-1-ol (Table 1, entry 1)[1]:



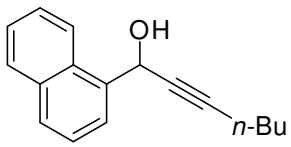
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 75 % of a yellow oil.

1-Phenylhept-2-yn-1-ol (Table 2, entry 2)[1]:



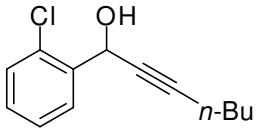
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 78 % of a yellow oil.

1-(napthalen-1-yl)hept-2-yn-1-ol (Table 2, entry 3)[1]:



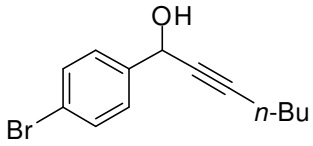
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 72 % of a yellow oil.

1-(4′-Bromophenyl)hept-2-yn-1-ol (Table 2, entry 4)[2]:



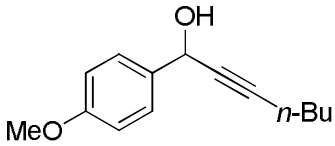
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 99 % of a yellow oil.

1-(4′-Bromophenyl)hept-2-yn-1-ol (Table 2, entry 5)[1]:



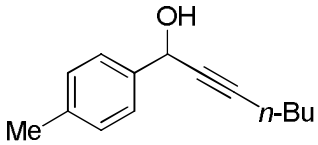
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 83 % of a yellow oil.

1-(4′-methoxyphenyl)hept-2-yn-1-ol (Table 2, entry 6)[1]:



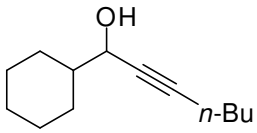
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 79 % of a yellow oil.

1-*p*-Tolylhept-2-yn-1-ol (Table 2, entry 7)[1]:



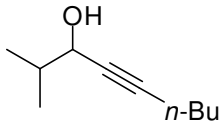
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 75 % of a yellow oil.

1-cyclohexylhept-2-yn-1-ol (Table 2, entry 8)[1]:



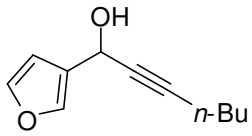
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 91 % of a colorless oil.

2-methylnon-4-yn-3-ol (Table 2, entry 9)[1]:



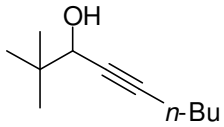
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 91% of a colorless oil.

1-(furan-3-yl)hept-2-yn-1-ol (Table 2, entry 10)[1]:



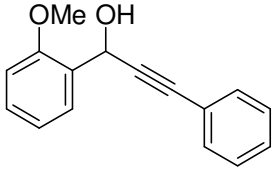
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 72 % of a red oil.

2,2-Dimethylnon-4-yn-3-ol (Table 2, entry 11)[1]:



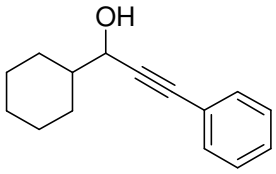
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 84 % of a yellow oil.

1-(2-Methoxy-phenyl)-3-phenyl-prop-2-yn-1-ol (Table 3, entry 1)[3]:



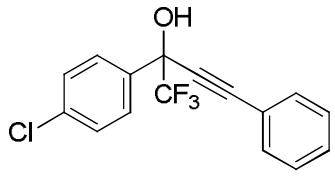
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 76 % of a yellow oil.

1-Cyclohexyl-3-phenyl-prop-2-yn-1-ol (Table 3, entry 2)[4]:



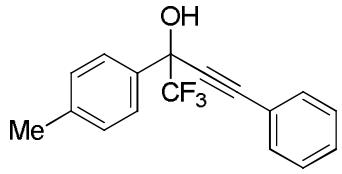
Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 75 % of a yellow oil.

2-(4-Chlorophenyl)-1,1,1-trifluoro-4-phenylbut-3-yn-2-ol (Table 4, entry 2): [5]



Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 98% as colorless oil.

1,1,1-Trifluoro-4-phenyl-2-(p-tolyl)but-3-yn-2-ol (Table 4, entry 3): [5]



Purified via flash column chromatography with 10 % ethyl acetate/hexane, yielding 90% as colorless oil.

References:

1. Scheidt,K. A.; Lettan, R. B. *Org. Lett*. **2005**, *7*, 3227-3230.
2. Braga, A. L.; Appelt, H. R.; Silveira, C. C.; Wessjohann, L. A.; Schneider, P. H. *Tetrahedron* **2002**, *58*, 10413-10416.
3. Xu, M.; Pu, L. *Org. Lett*. **2002**, *4*, 4555-4557.

4. Ishikawa, T.; Mizuta, T.; Hagiwara, K.; Aikawa, T.; Kudo, T.; Saito, S. *J. Org. Chem*. **2003**, *68*, 3702-3705.

5. (a) Motoki, R.; Kanai, M.; Shibasaki, M. *Org. Lett.* **2007**, *9*, 2997-3000. (b) Linderman, R. J.; Lonikar, M. *J. Org. Chem*. **1988**, *53*, 6013-6022.

KW273, CDCL3
300MHz
12/06/06

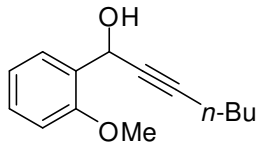
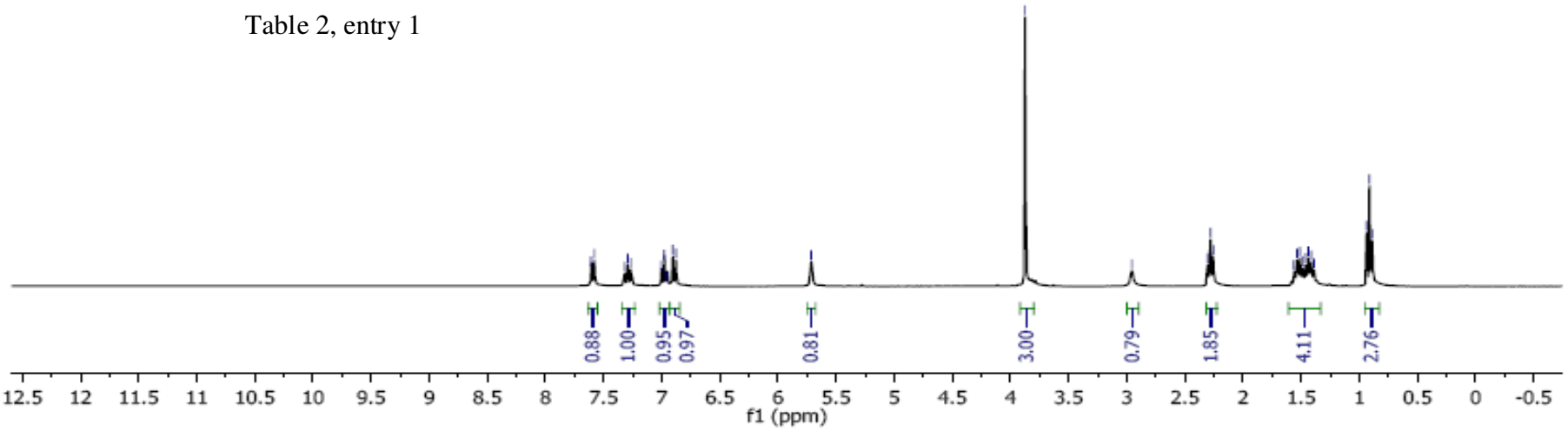


Table 2, entry 1



KW273,CDCL3
75MHz
12/06/06

156.992
129.714
129.538
128.140
120.997
110.903
87.418
79.334
77.730
77.306
76.882
61.455
55.719
30.930
22.204
18.810
13.853

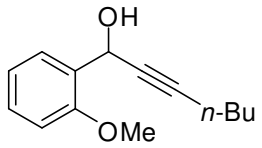
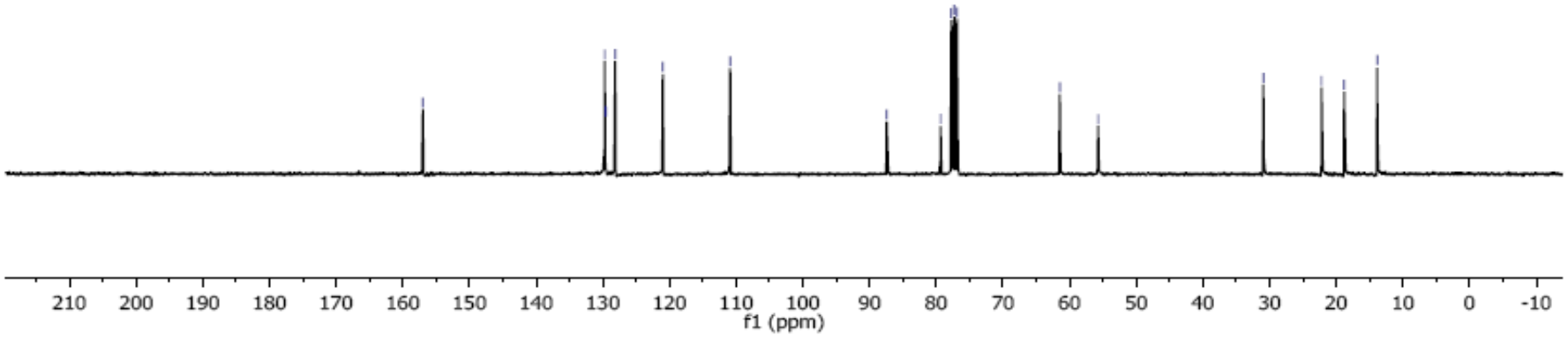


Table 2, entry 1



KW268,CDCl3
300MHz

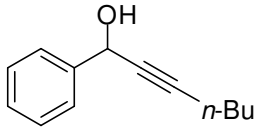
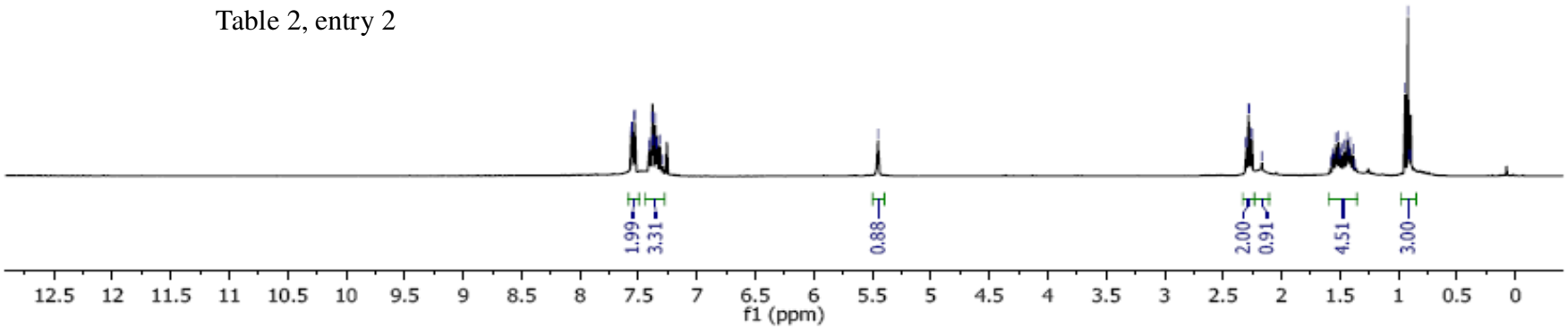
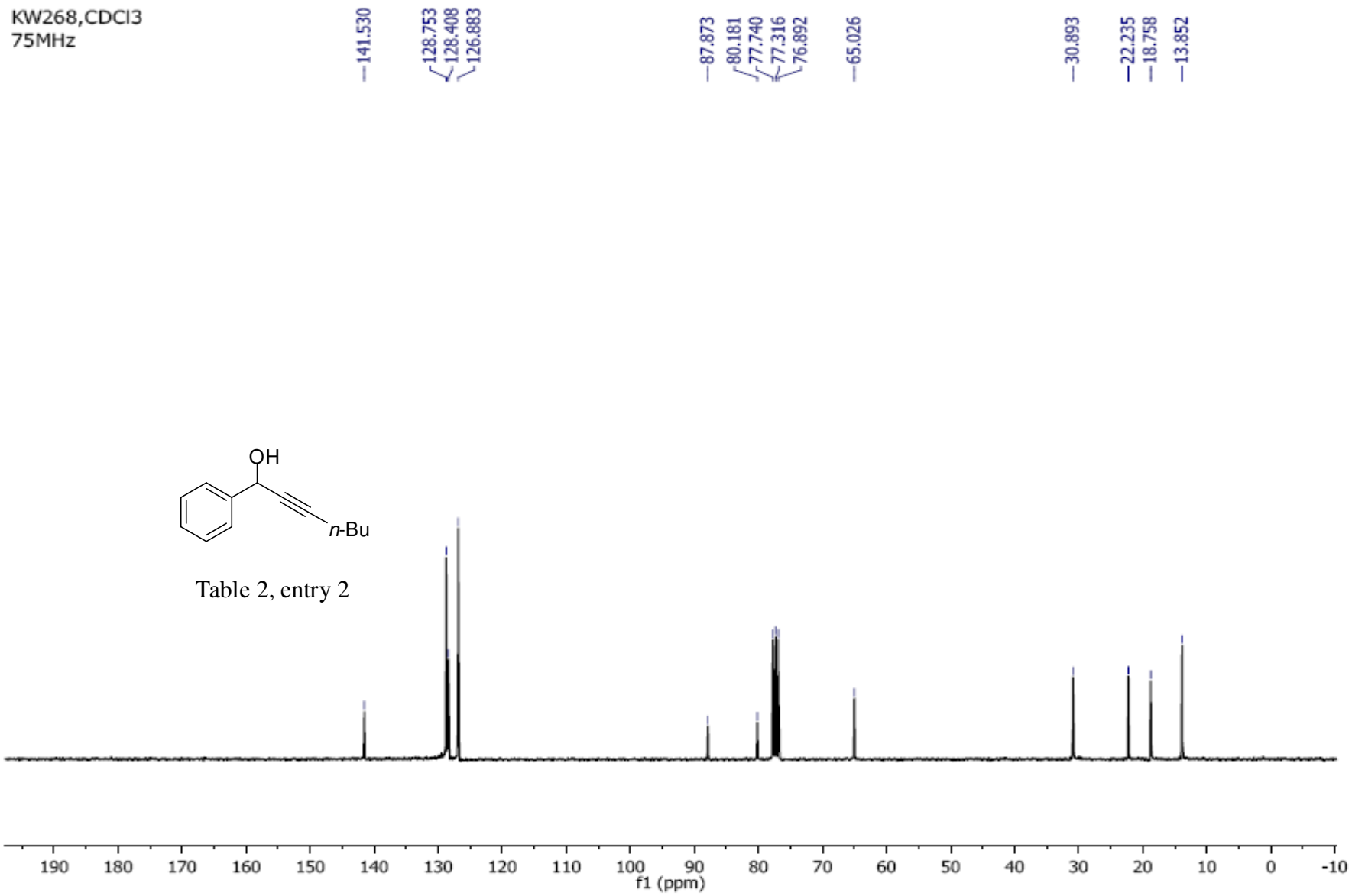


Table 2, entry 2

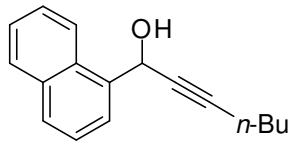



KW268,CDCl3
75MHz
141.530
128.753
128.408
126.883
87.873
80.181
77.740
77.316
76.892
65.026
30.893
22.235
18.758
13.852
OH
n-Bu
Table 2, entry 2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

KW298,CDCL3
300MHz
01/24/07

8.337 8.310 7.824 7.541 7.509 7.480 7.452 7.258 6.116

2.466 2.330 2.300 2.277 1.528 1.450 1.400 0.953 0.929 0.905



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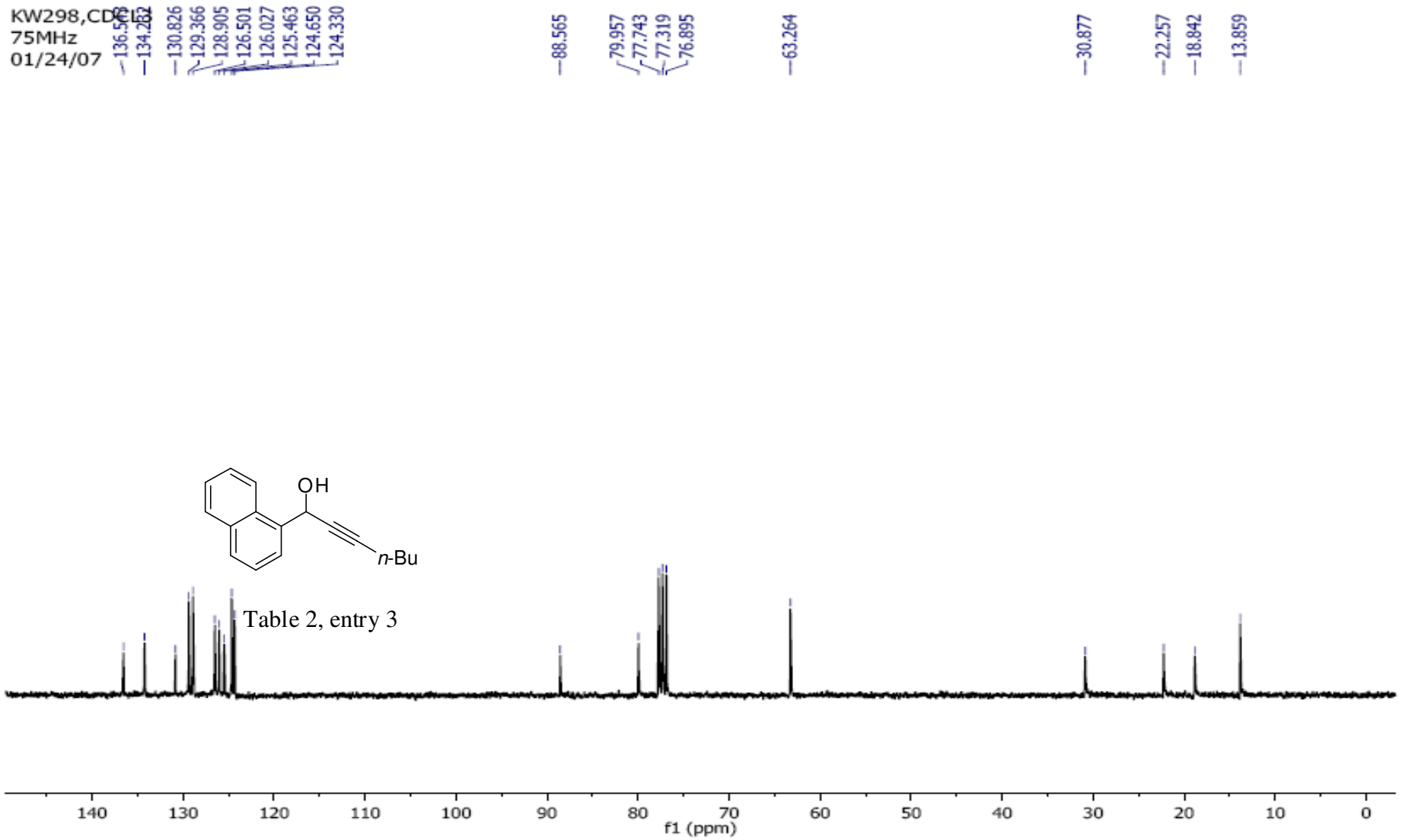

KW298,CDCl3
75MHz
01/24/07
136.565
134.252
130.826
129.366
128.905
126.501
126.027
125.463
124.650
124.330
88.565
79.957
77.743
77.319
76.895
63.264
30.877
22.257
18.842
13.859
OH
n-Bu
Table 2, entry 3
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

KW277. CDCl3
400MHz

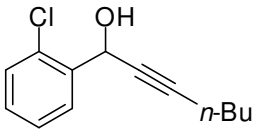
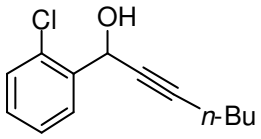


Table 2, entry 4

KW277, CDCl3
100MHz

138.696
132.943
129.843
129.662
128.526
127.359
88.018
78.996
77.637
77.320
77.002
62.286
30.818
22.227
18.768
13.857



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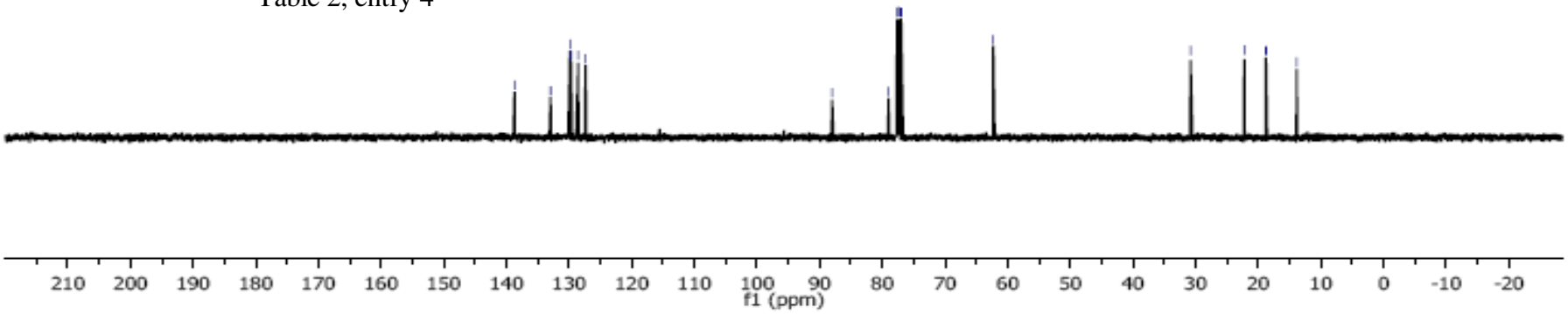
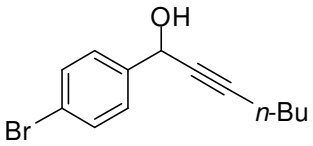


KW278,CDCl3
400MHz



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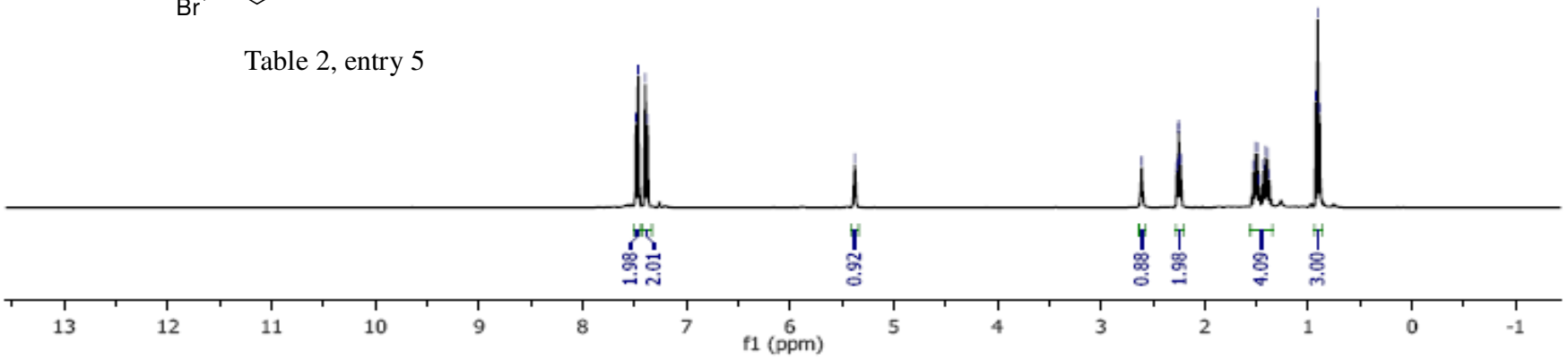


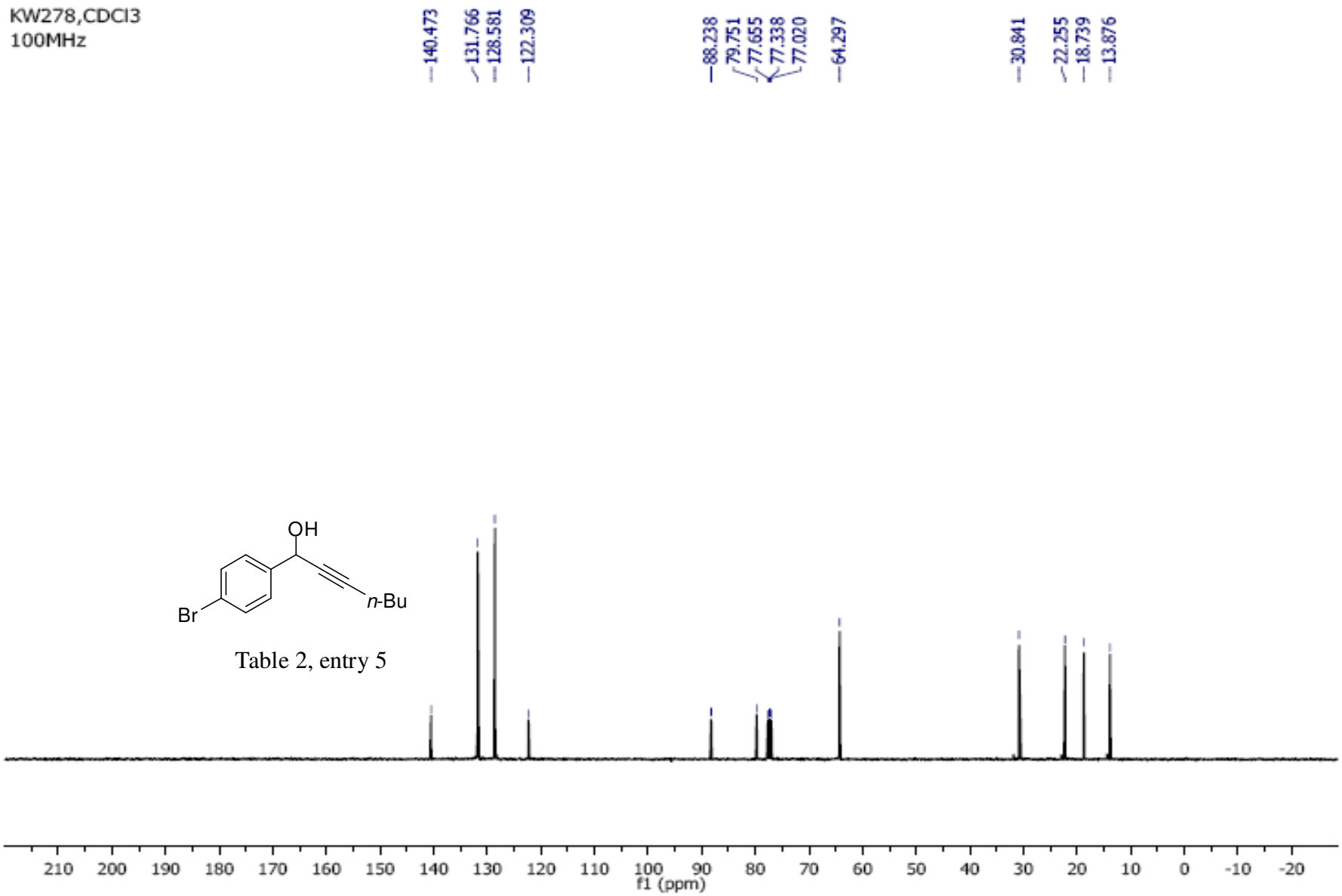
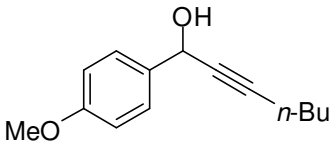


Table 2, entry 5

KW274,CDCl3
400MHz



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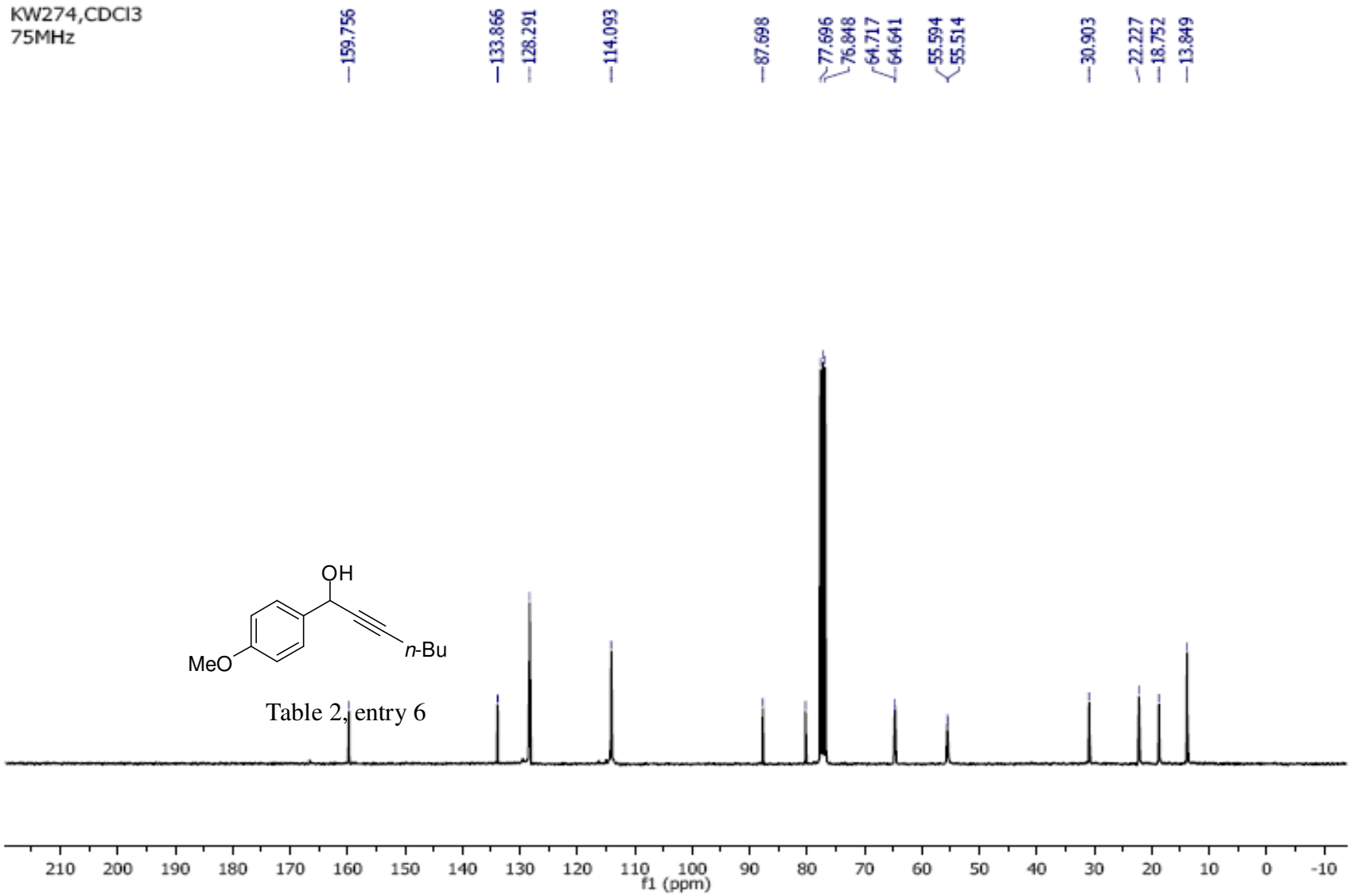

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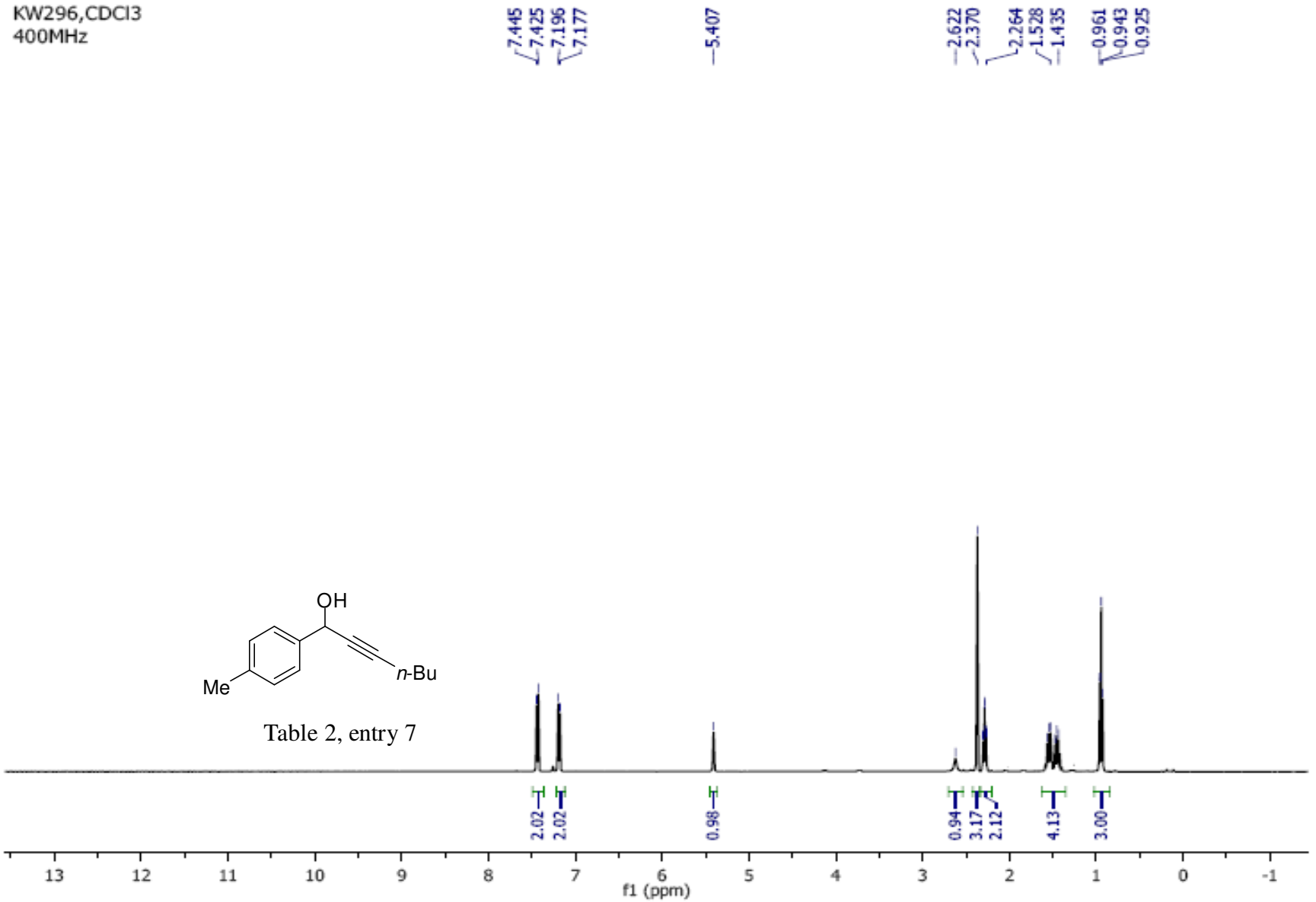


Table 2, entry 7

KW296,CDCl3
100MHz

138.763
138.073
129.385
126.865
87.510
80.441
77.408
77.090
64.798
30.961
22.281
18.804
13.901

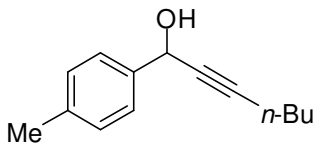


Table 2, entry 7

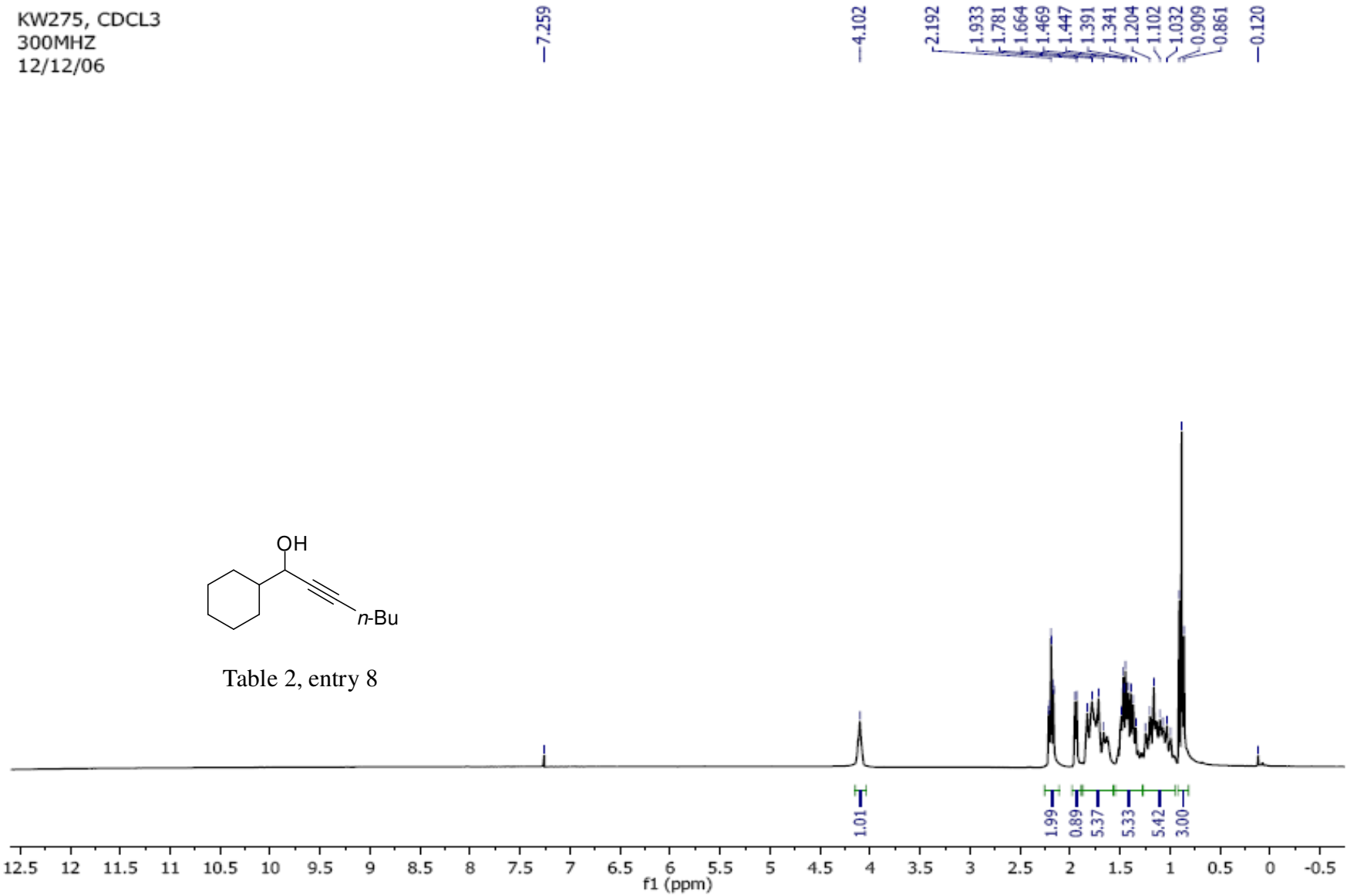


Table 2, entry 8

KW275C1, CDCL3
75MHz
12/12/06

86.369
80.359
77.708
77.284
76.860
67.618
67.557
44.547
31.023
28.832
28.281
26.657
26.136
22.152
18.595
13.783

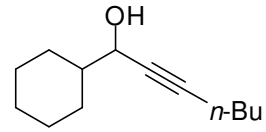


Table 2, entry 8

KW285, CDCL3
300MHz
12/20/06

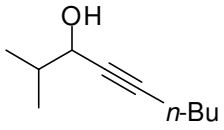
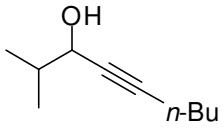


Table 2, entry 9

KW285,CDCL3
75MHz
12/20/06

86.264
80.021
77.702
77.279
76.854
68.216
34.827
30.990
22.101
18.347
13.754



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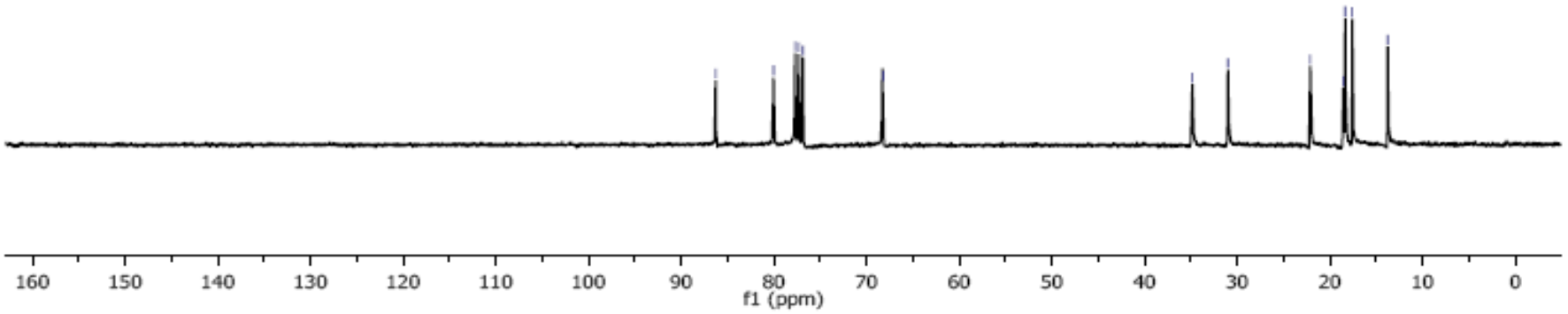
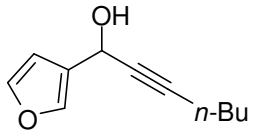


KW322,CDCL3
300MHz
02/28/07



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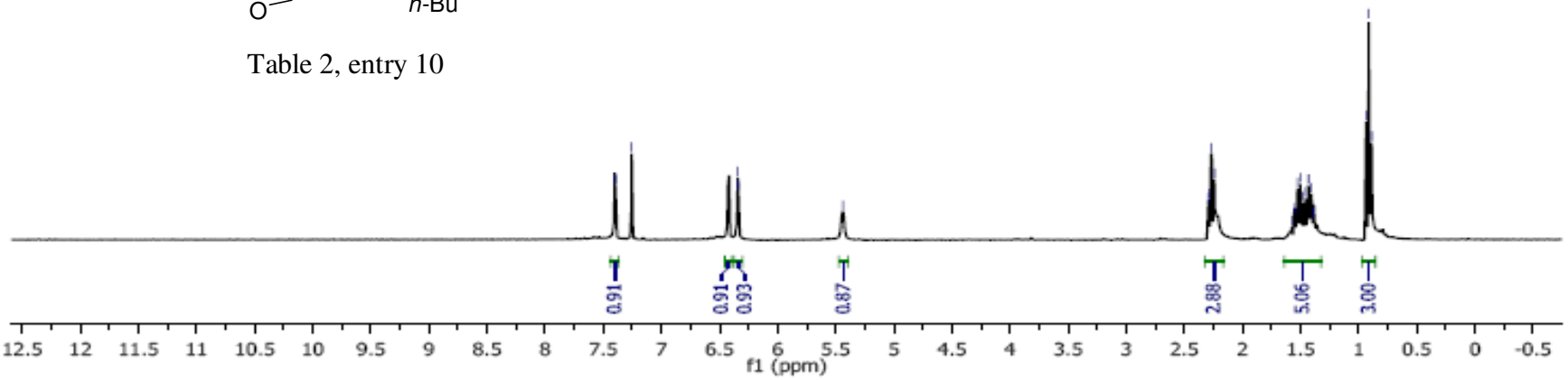

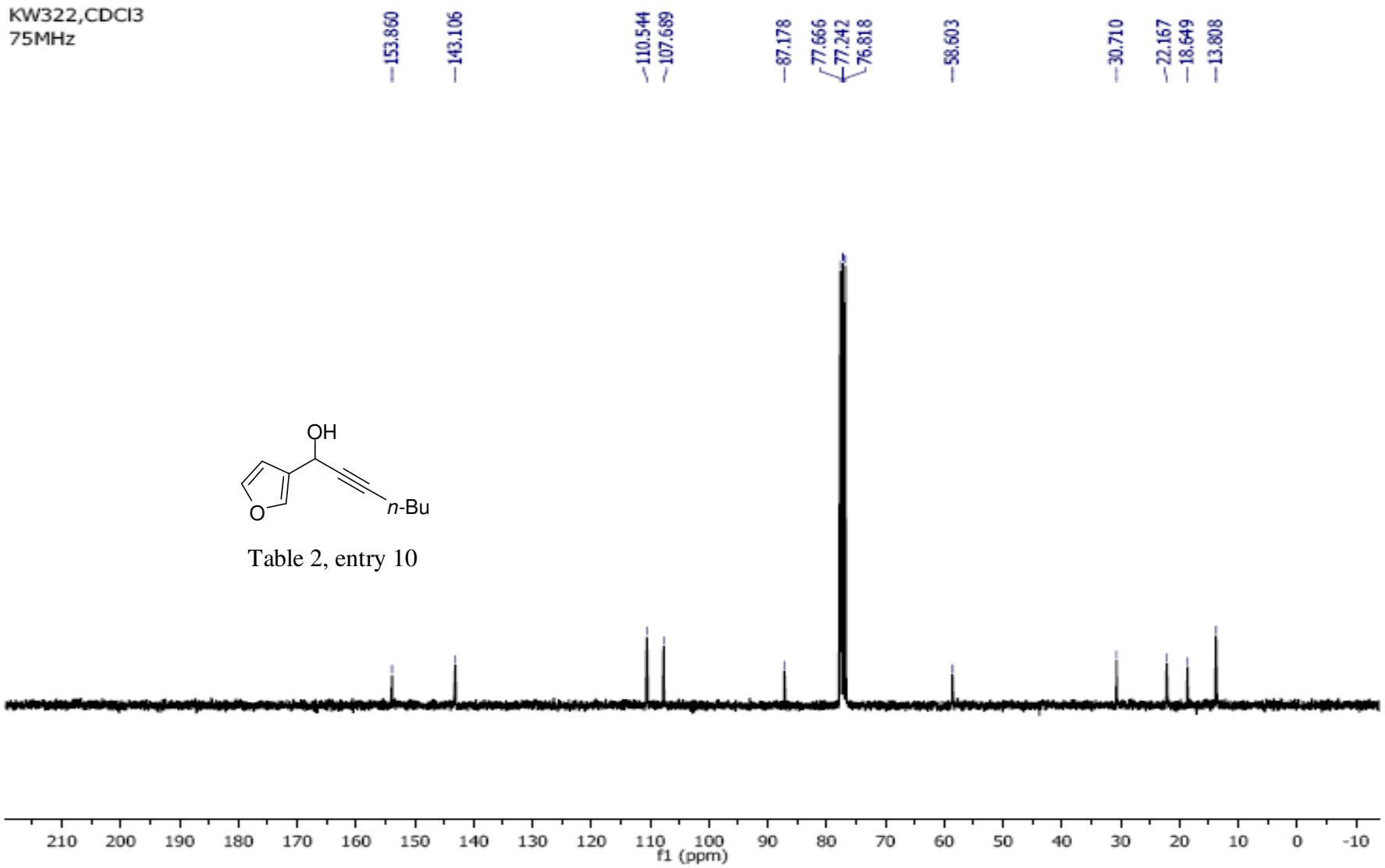

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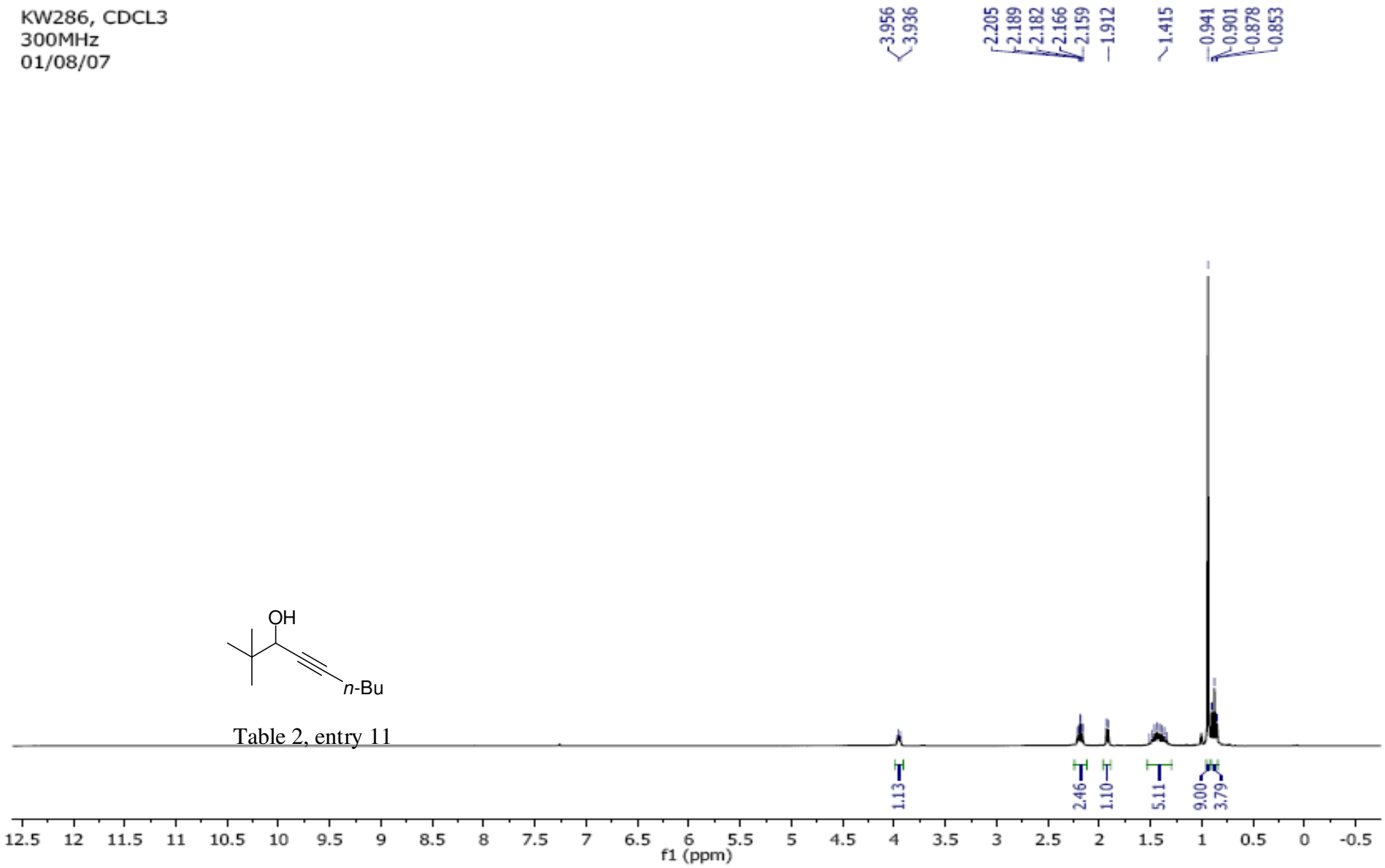


Table 2, entry 11

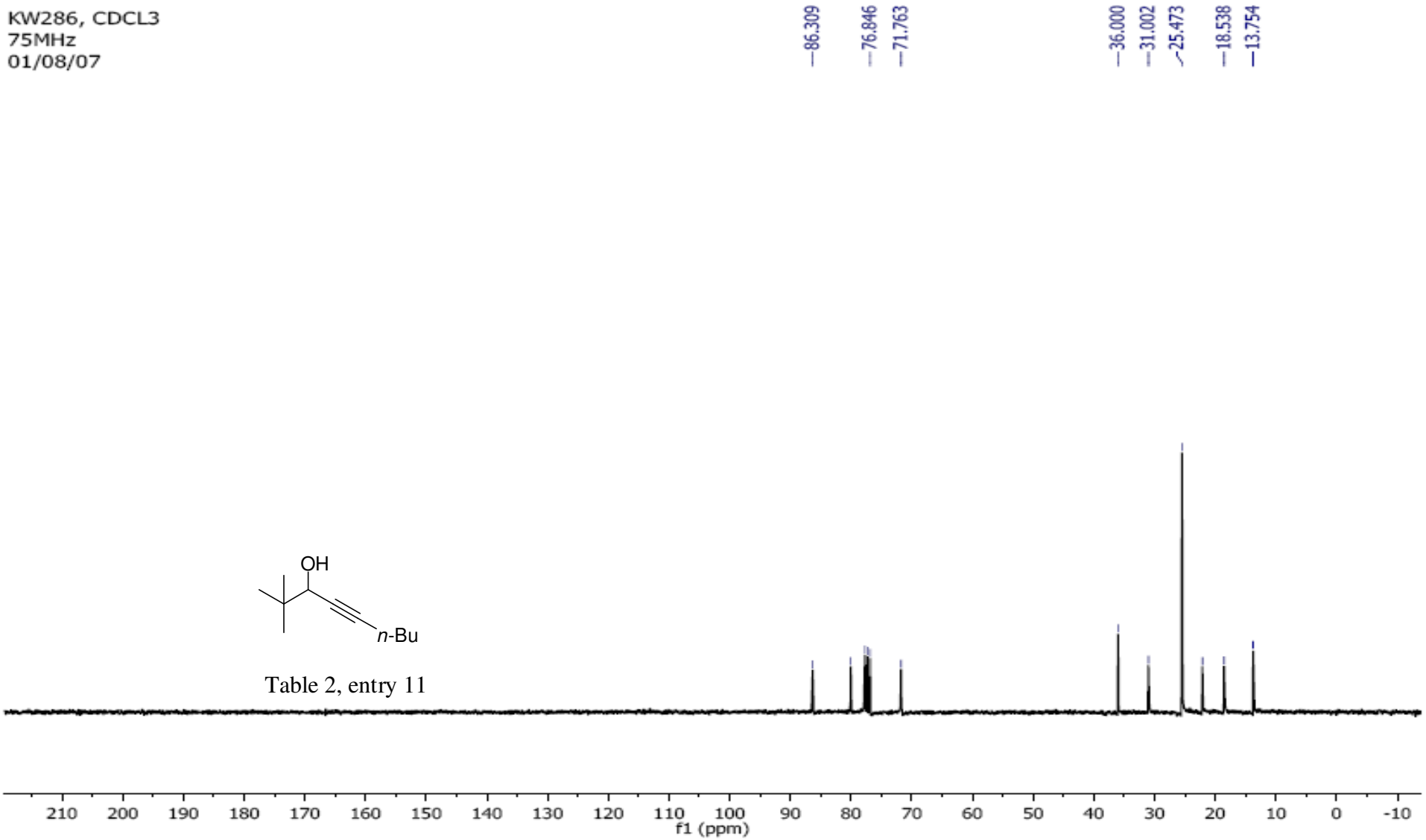


Table 2, entry 11

KW313,CDCl3
300MHz

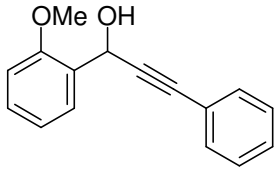
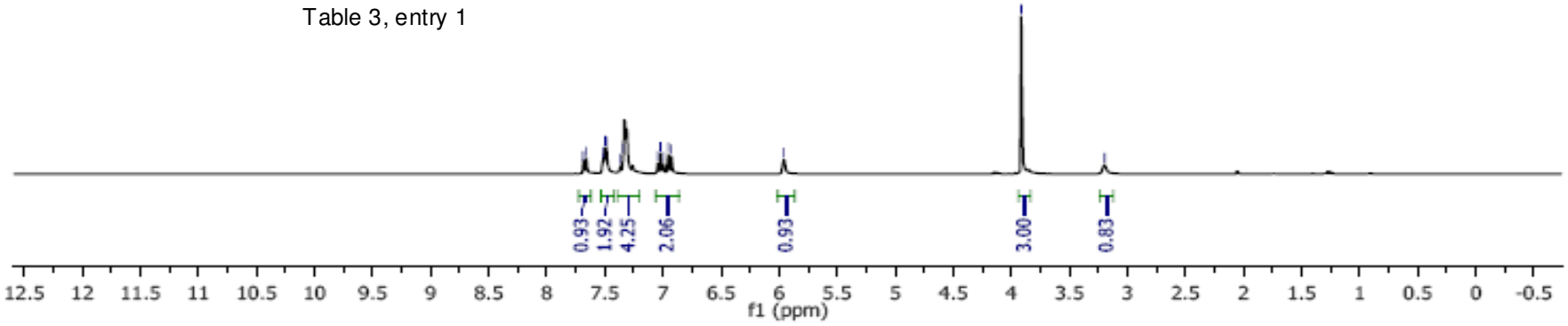
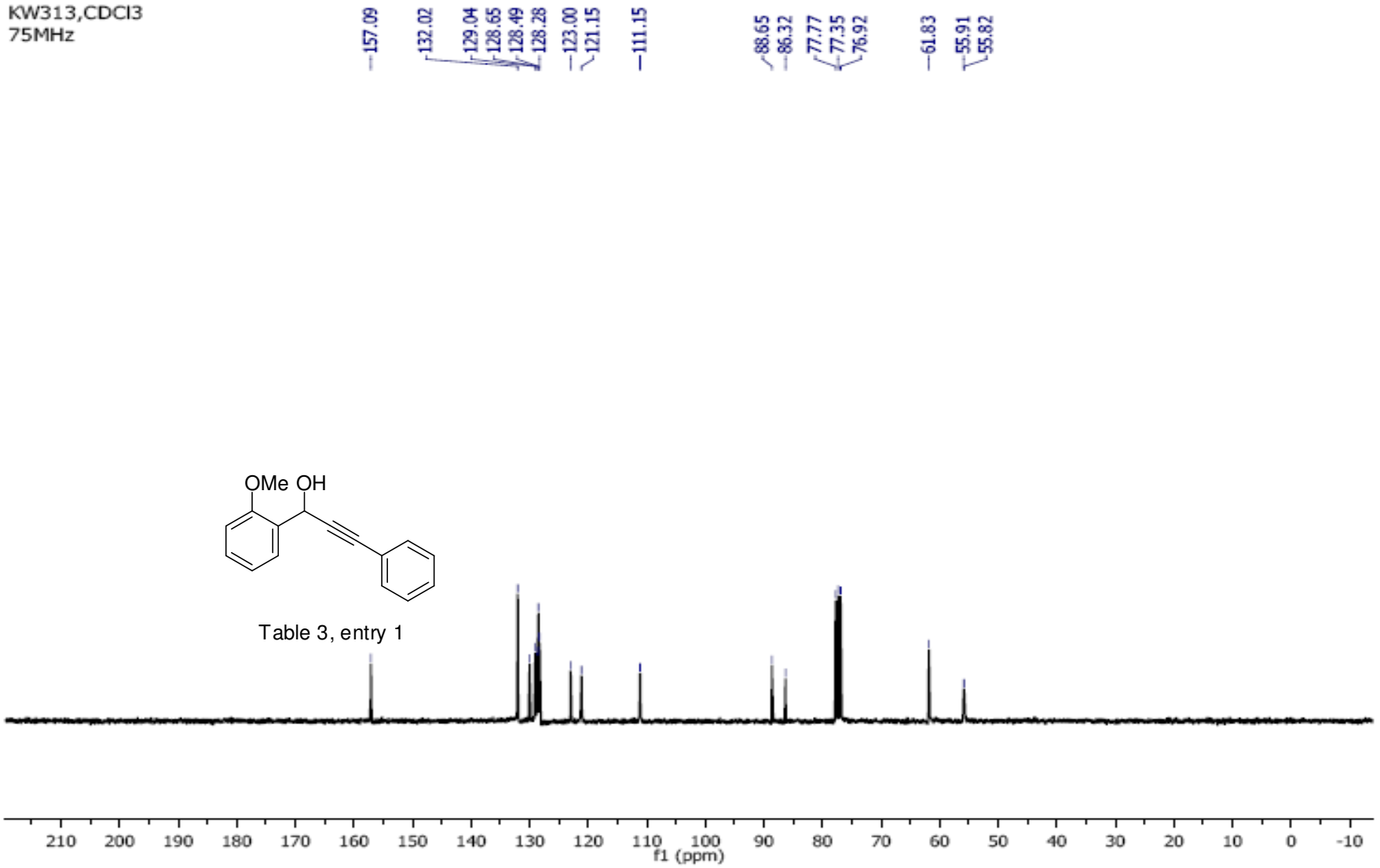


Table 3, entry 1




KW313,CDCl3
75MHz
157.09
132.02
129.04
128.65
128.49
128.28
123.00
121.15
111.15
88.65
86.32
77.77
77.35
76.92
61.83
55.91
55.82
OMe OH
Table 3, entry 1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

KW312,CDCl3
300MHz

7.453
7.444
7.436
7.424
7.306
7.297
7.290
7.283
7.251
4.394
4.374
2.520
1.945
1.708
1.672
1.222
1.187
1.147
1.116

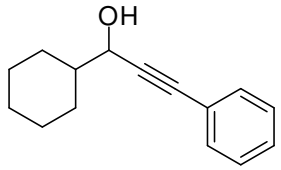


Table 3, entry 2

KW312,CDCl3
75MHz

131.93
128.50
123.01
89.54
85.87
77.74
77.32
76.90
67.89
44.54
28.93
28.45
26.65
26.16

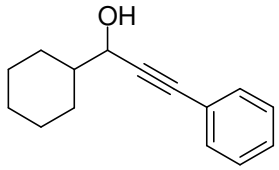


Table 3, entry 2

KW464, CDCl3
400MHz
YELLOW OIL

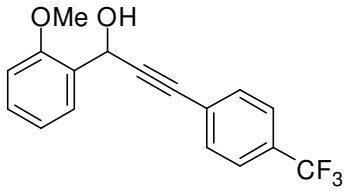


Table 3, entry 3

KW464C,CDCl3
100MHz

157.038
132.220
125.456
125.420
125.382
125.344
121.186
111.179
91.116
84.839
77.261
76.943
61.959
55.861

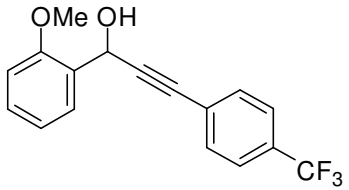
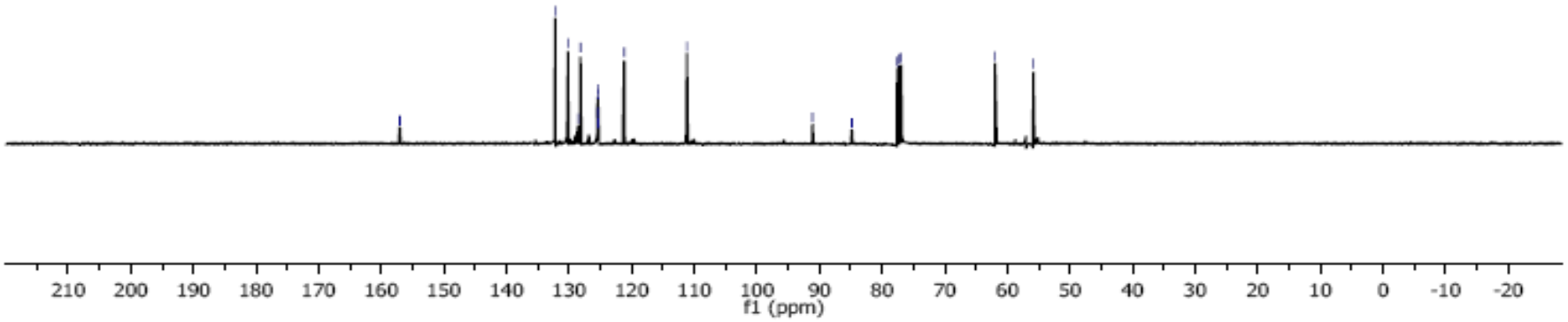


Table 3, entry 3



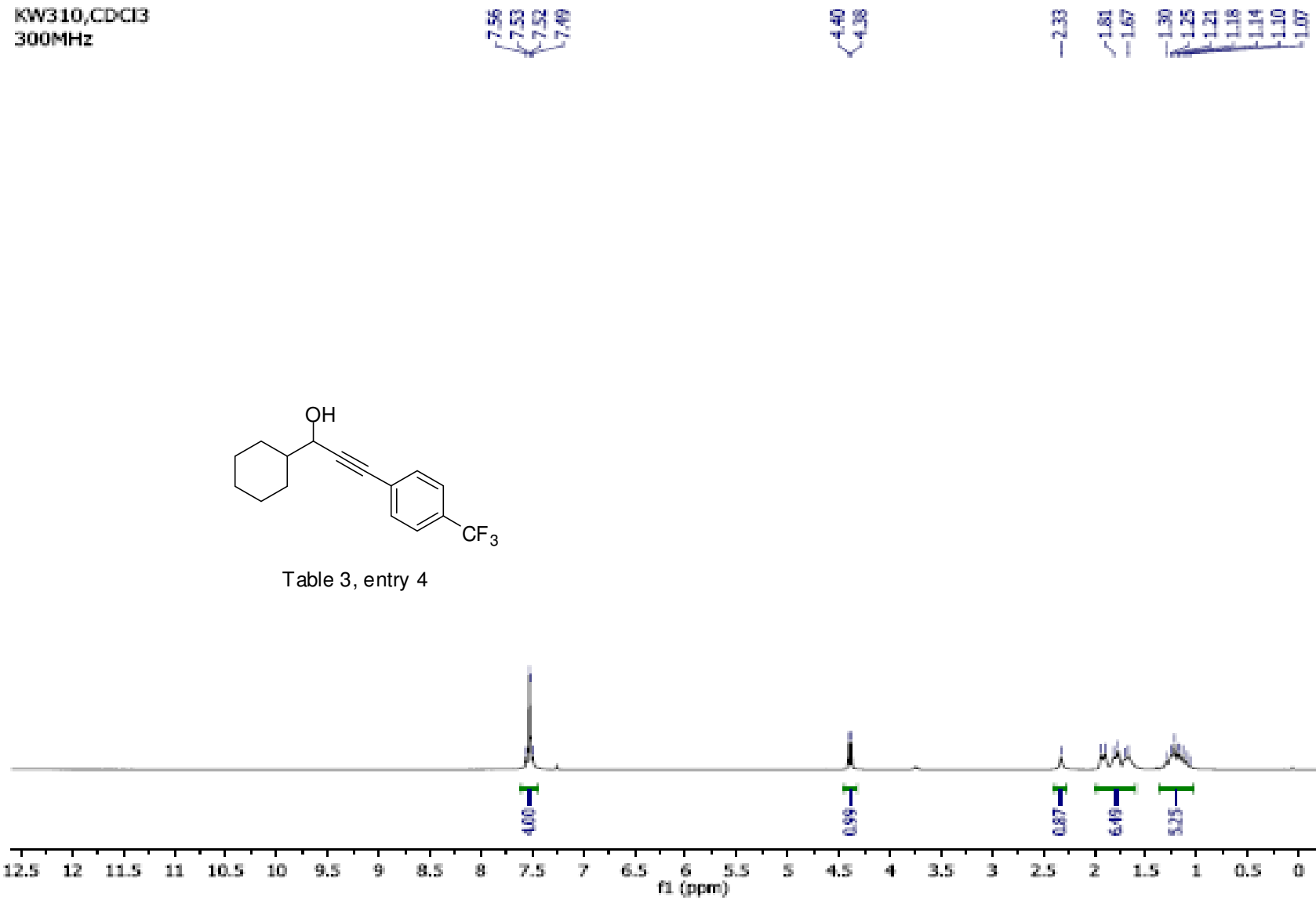


Table 3, entry 4

KW310,CDCl3
75MHz

132.12
130.90
130.47
130.04
129.60
126.80
125.89
125.42
125.37
122.28
92.06
84.52
77.27
76.84
67.80
44.44
28.89
28.46
26.56
26.08

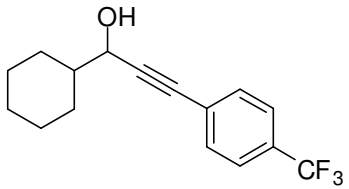
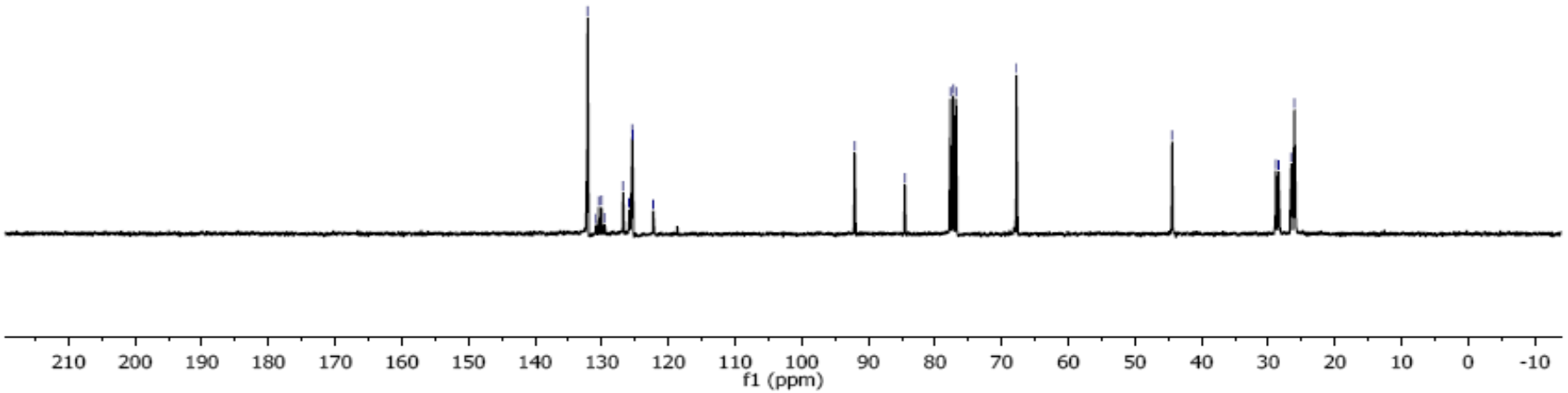
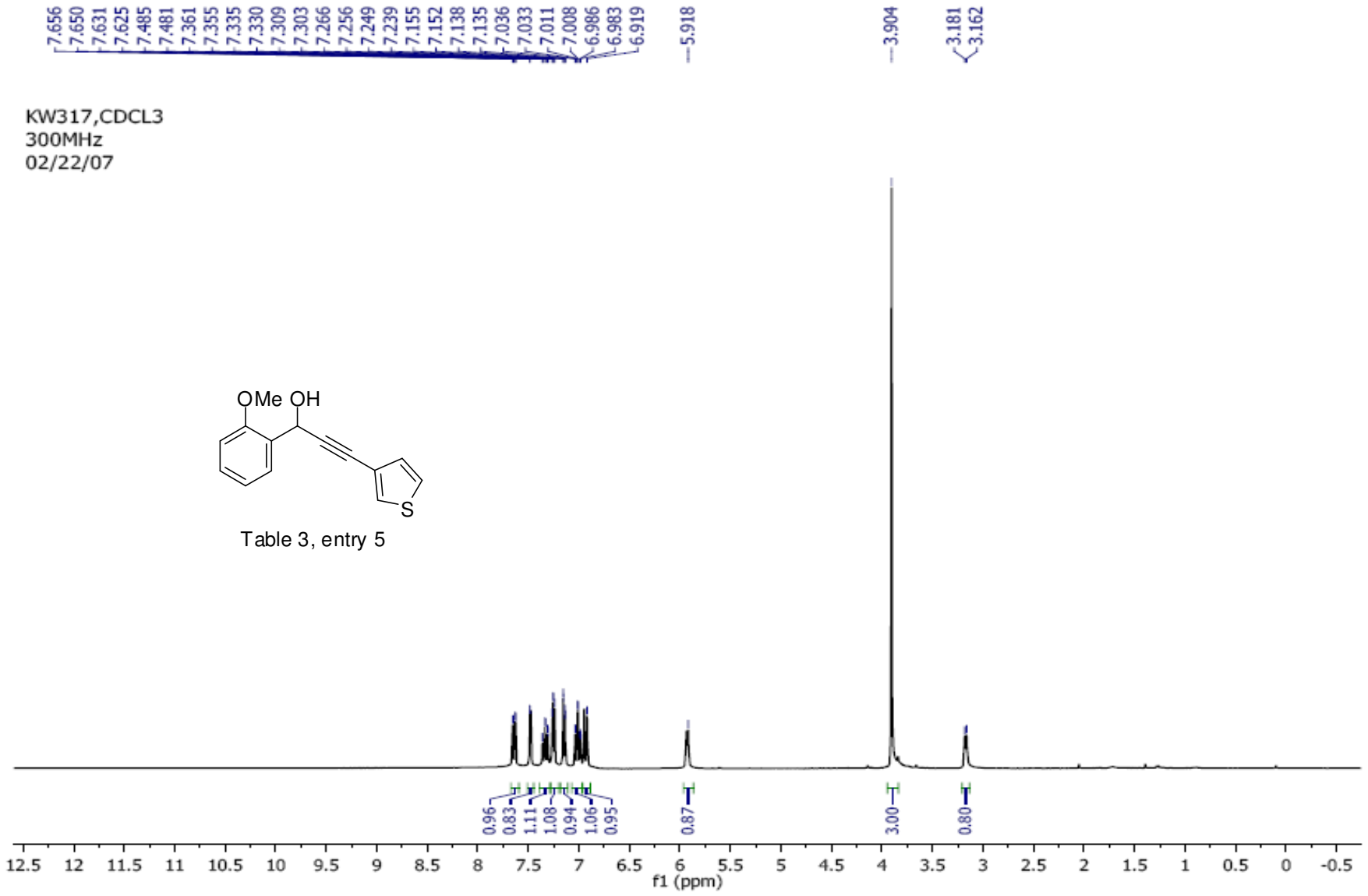


Table 3, entry 4




7.656
7.650
7.631
7.625
7.485
7.481
7.361
7.355
7.335
7.330
7.309
7.303
7.266
7.256
7.249
7.239
7.155
7.152
7.138
7.135
7.036
7.033
7.011
7.008
6.986
6.983
6.919
5.918
3.904
3.181
3.162
KW317,CDCL3
300MHz
02/22/07
OMe OH
S
Table 3, entry 5
0.96
0.83
1.11
1.08
0.94
1.06
0.95
0.87
3.00
0.80
12.5 12 11.5 11 10.5 10 9.5 9 8.5 8 7.5 7 6.5 6 5.5 5 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0 -0.5
f1 (ppm)

KW317,CDCL3
75MHz
02/22/07

157.045
130.201
129.989
129.315
128.962
128.258
125.486
121.998
121.139
111.134
88.218
81.499
77.764
77.340
76.916
61.848
55.892
55.815

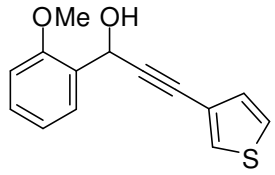
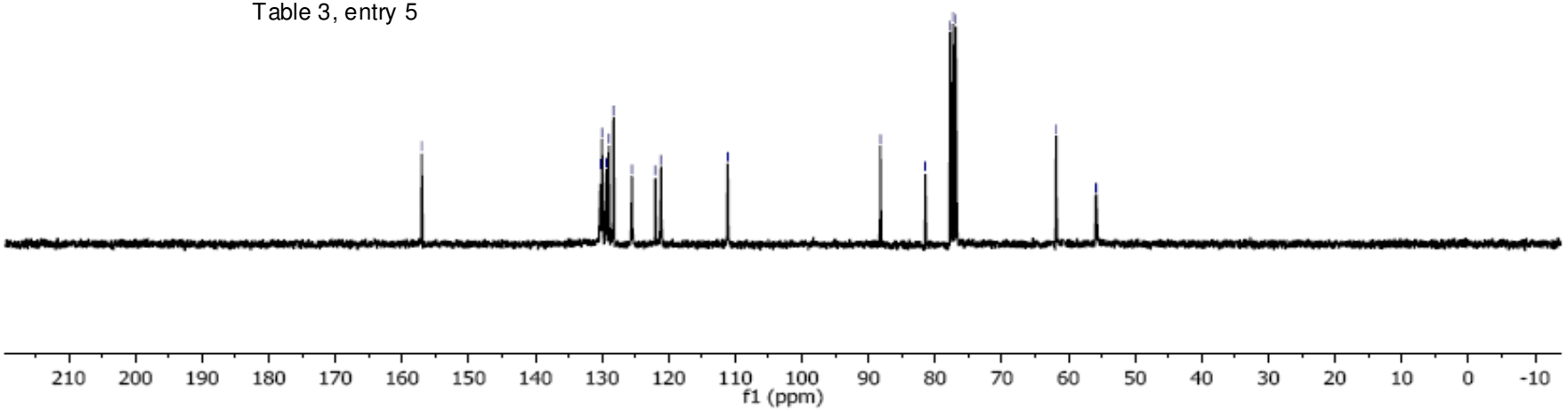


Table 3, entry 5



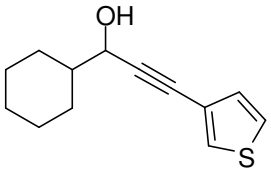
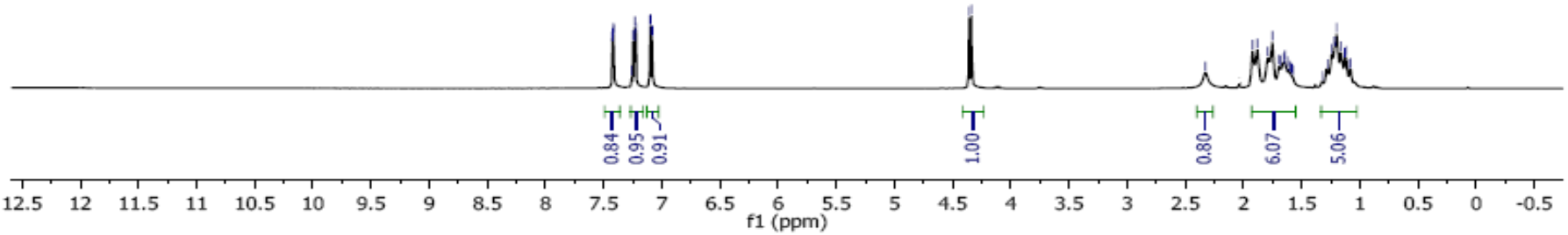


Table 3, entry 6



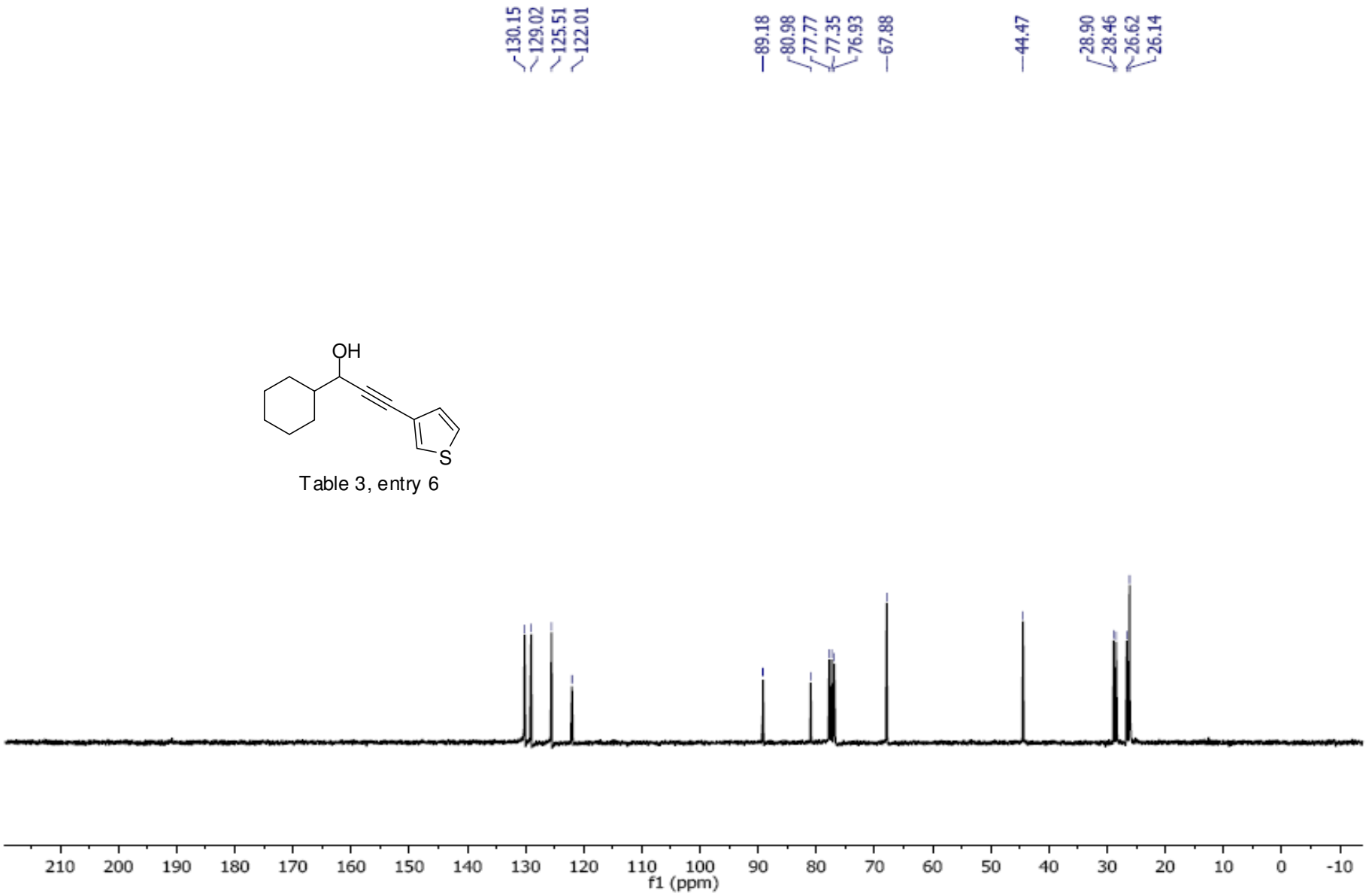


Table 3, entry 6

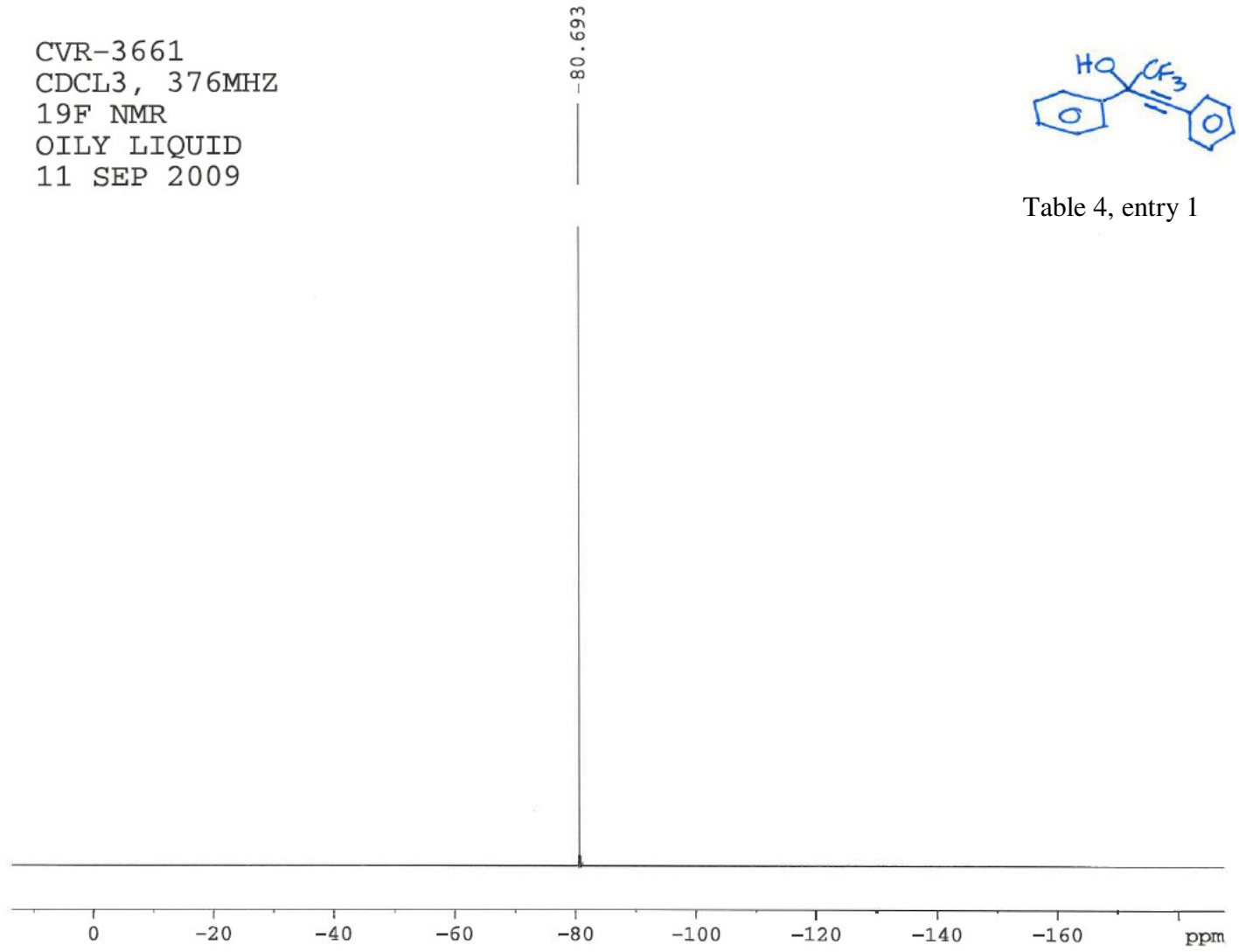


Table 4, entry 1

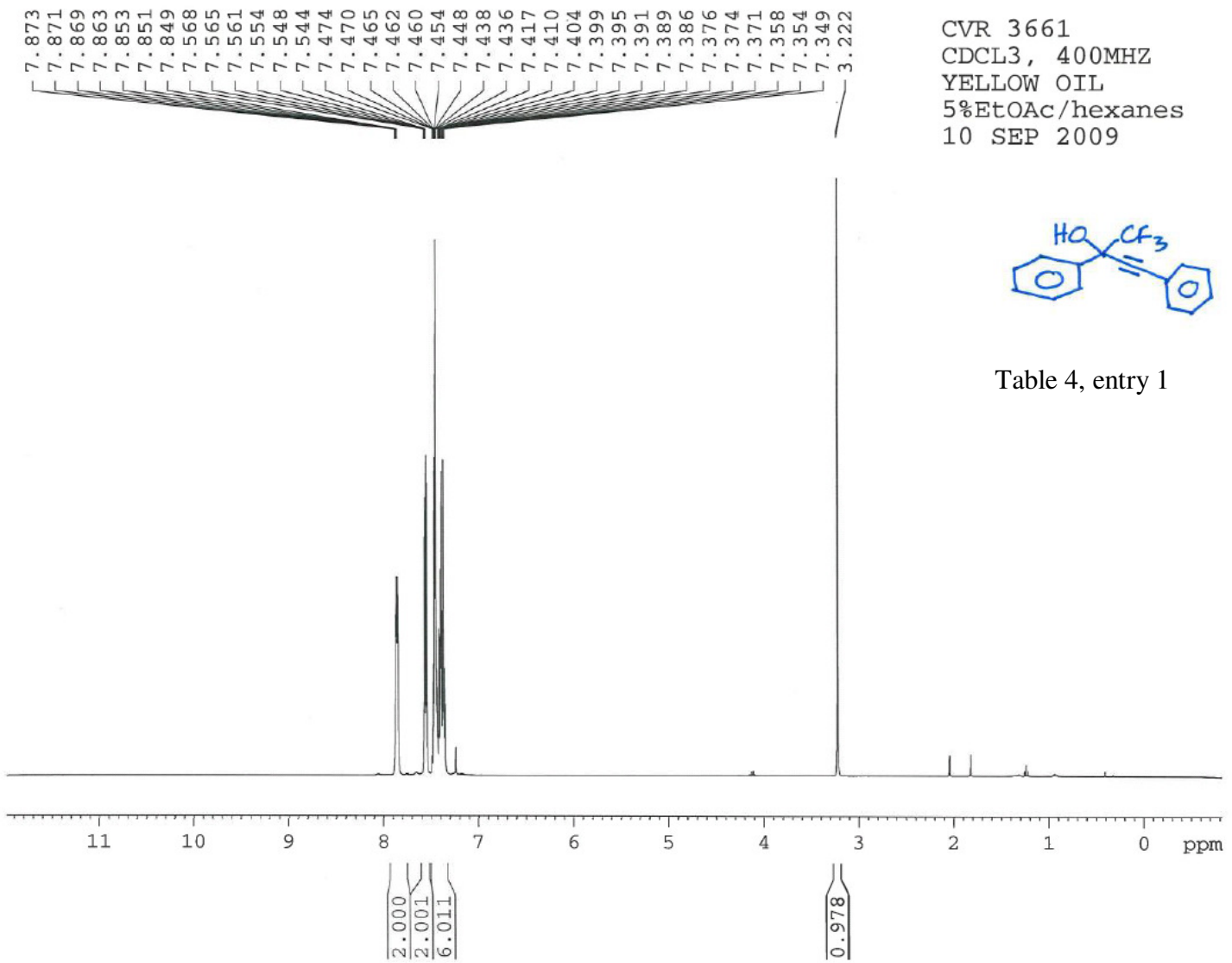


Table 4, entry 1

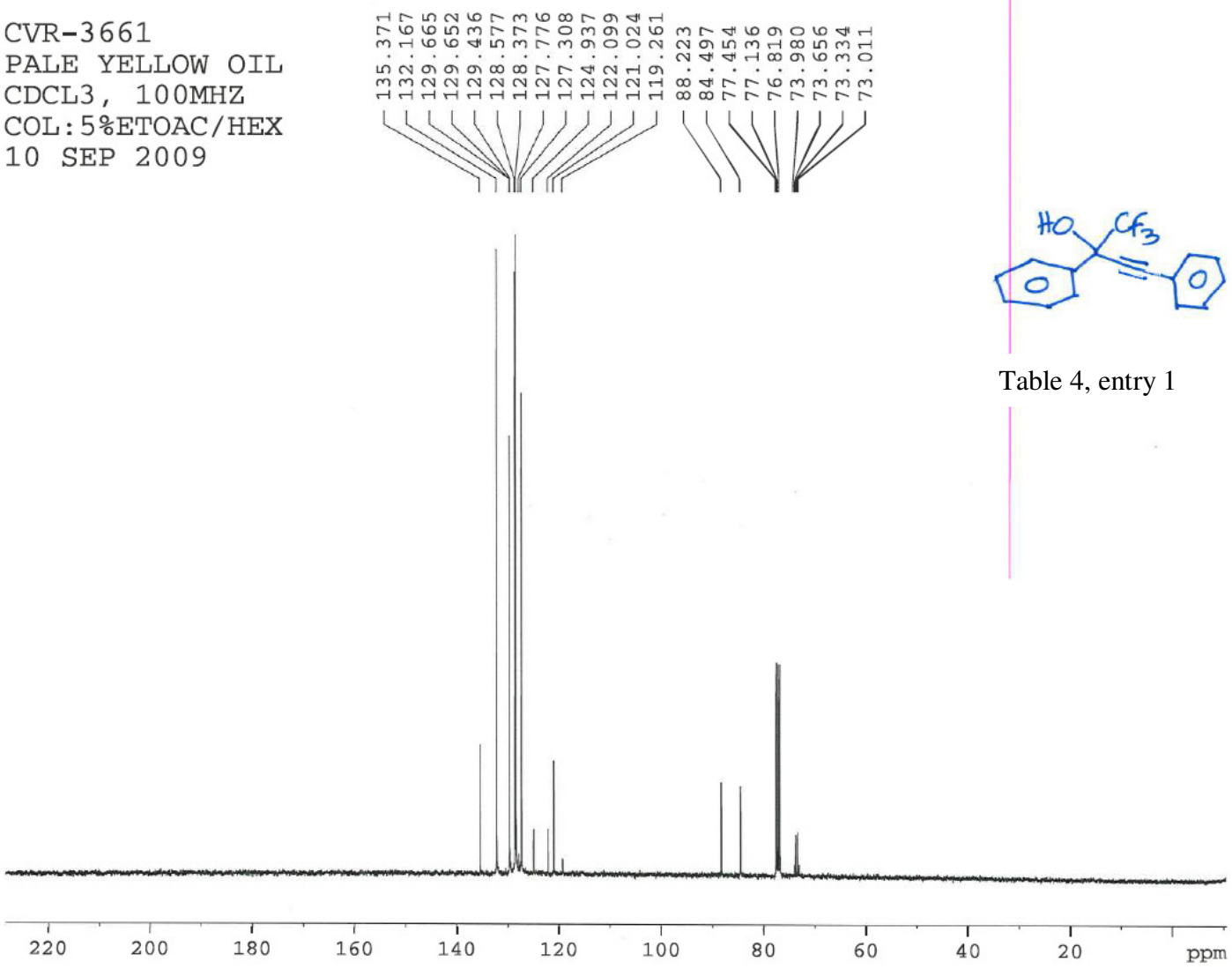


Table 4, entry 1

Manual Peak Matching Report
For Accurate Mass Determination

Theoretical mass	Experimental mass	PFK matching mass	Deviation*
276.07620	276.07667	230.98582	1.7 ppm

* The deviation is obtained from the following equation:

$$\text{deviation} = \frac{\text{experimental mass - theoretical mass}}{\text{nominal mass}}$$

Where nominal mass takes in account only ^{12}C, ^{1}H, ^{16}O, ^{14}N etc...

Theoretical mass correspond to the mass of the most abundant isotope peak

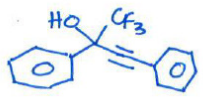


Table 4, entry 1

```
LIST:  fin084755                          14-SEP-09   REG   :  00:20.7      #9
Samp:  CVR-3661                                       Start :  16:52:39      22
Comm:  70 eV EI
Mode:  EI +Q1MS LMR UP LR
Oper:                 Client:  Venkat                 Inlet :
Base:  207.2                  Inten :   47335472      Masses:  35 > 650
Norm:  207.2                  RIC   :   259532488     #peaks:  620
Peak:  1000.00  mmu
Data:  + #9= 9>21
```

No.	Mass	Intensity (11360513)	%RA	%RIC	Flags
1	205.	18760960	39.63	7.23	F#
2	207.	42938368	90.71	16.54	FM#
3	207.	47335424	100.00	18.24	FM#
4	208.	13645312	28.83	5.26	FM#
5	276.	16788992	35.47	6.47	F#

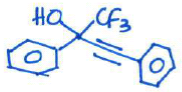


Table 4, entry 1

```
Date: Mon Sep 14 16:54:18 2009   ICIS: 8.3.0 SP2 for OSF1 (V4.0) build 98-238 from 26-Aug-98
```

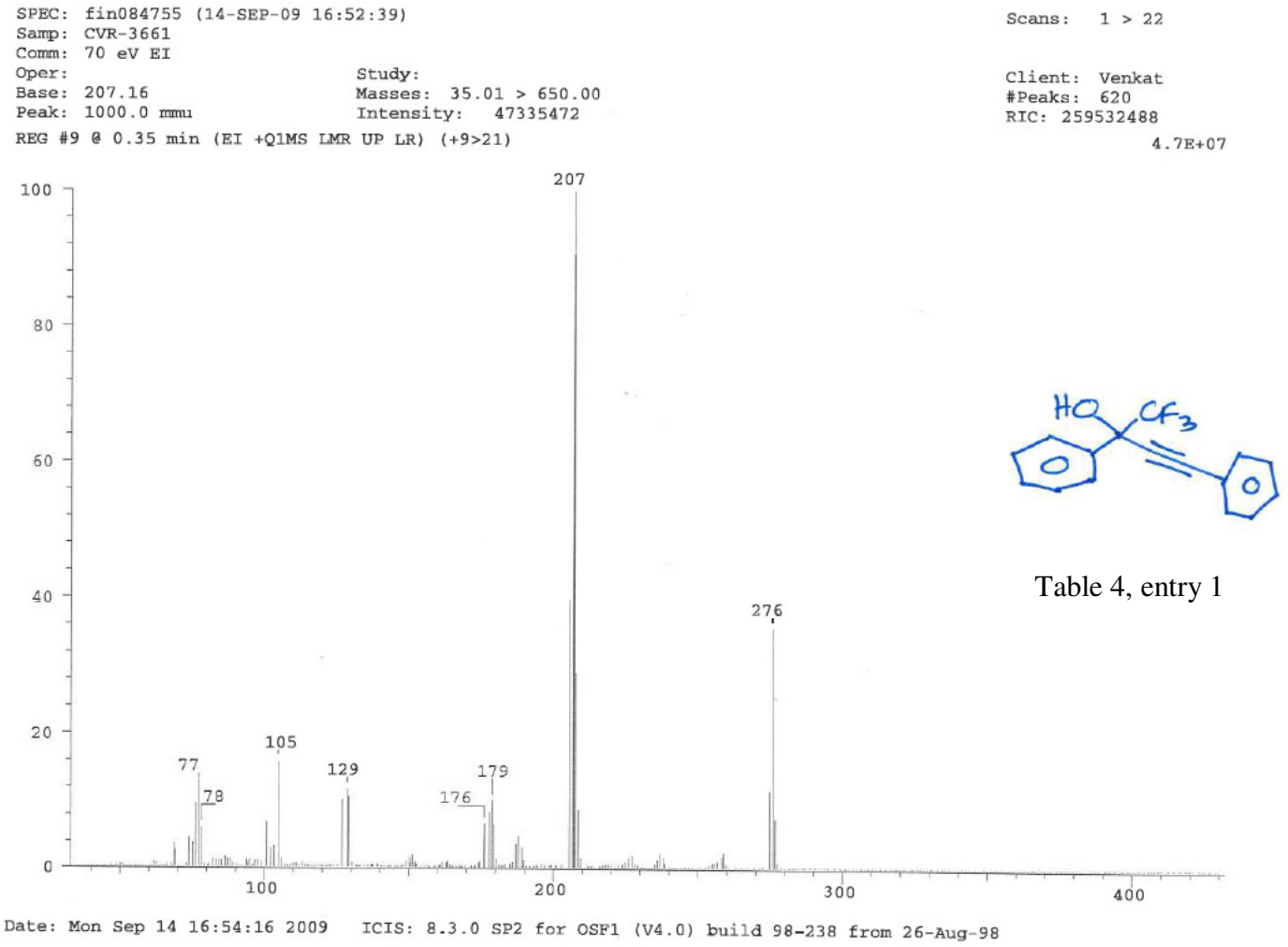


Table 4, entry 1

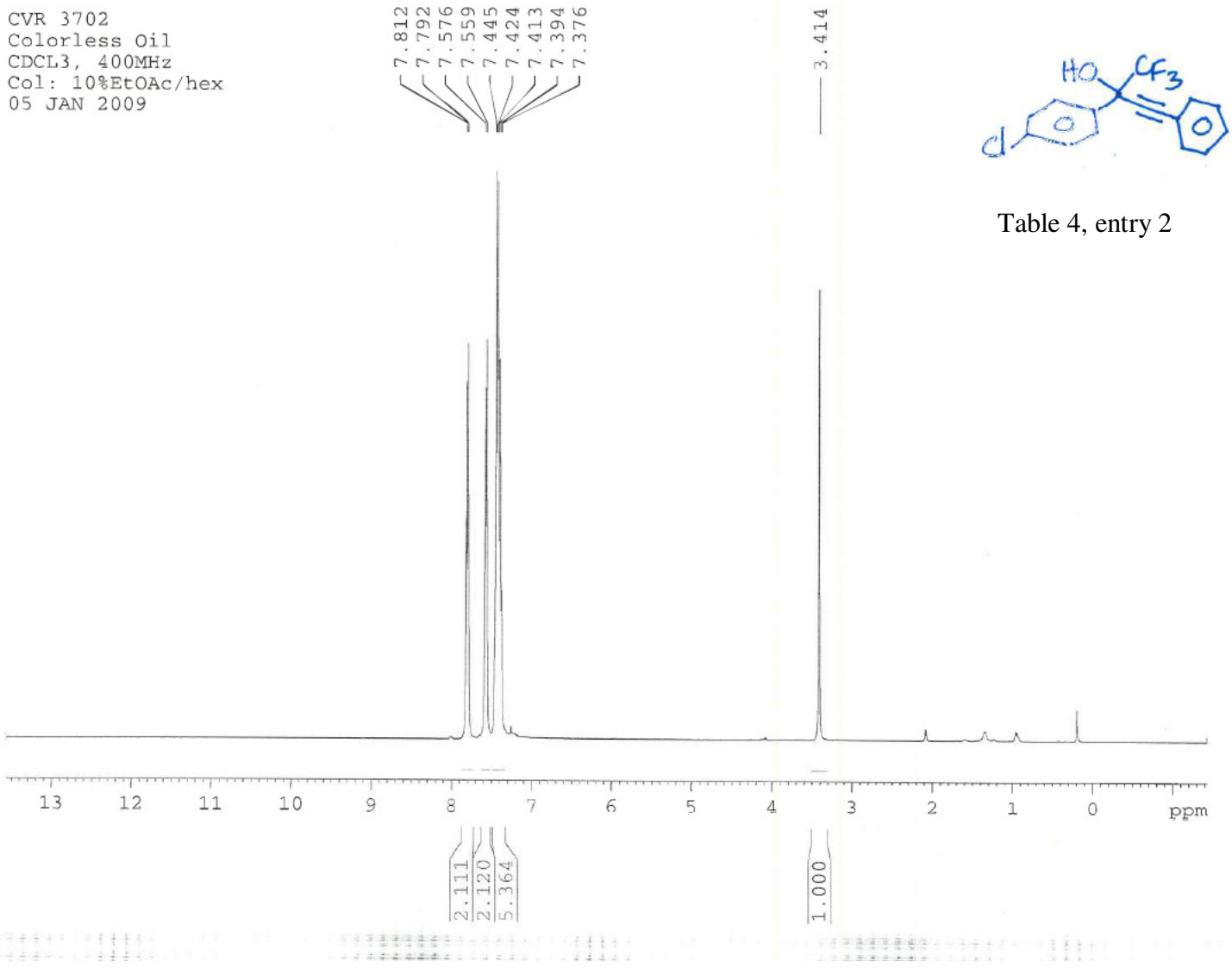


Table 4, entry 2

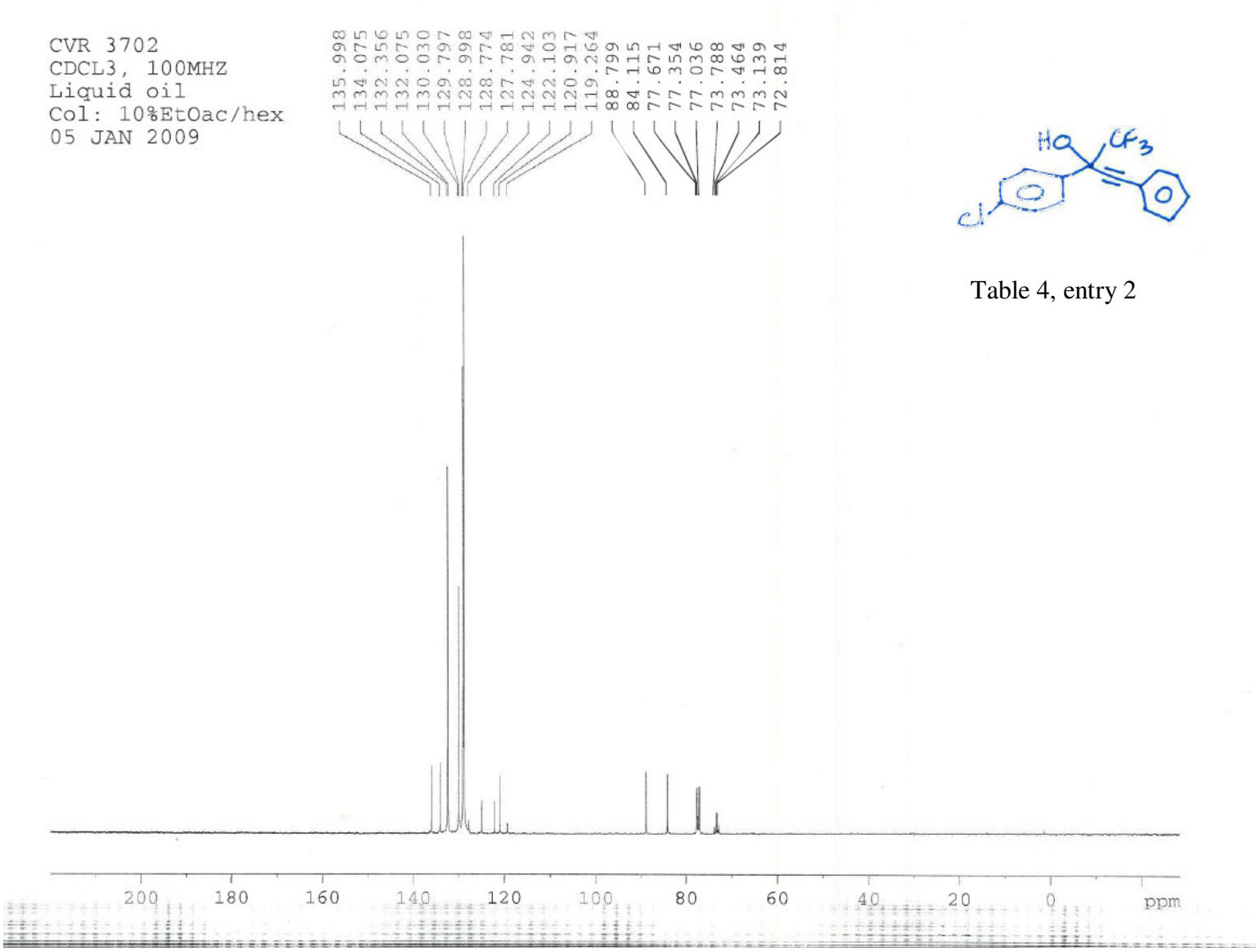


Table 4, entry 2

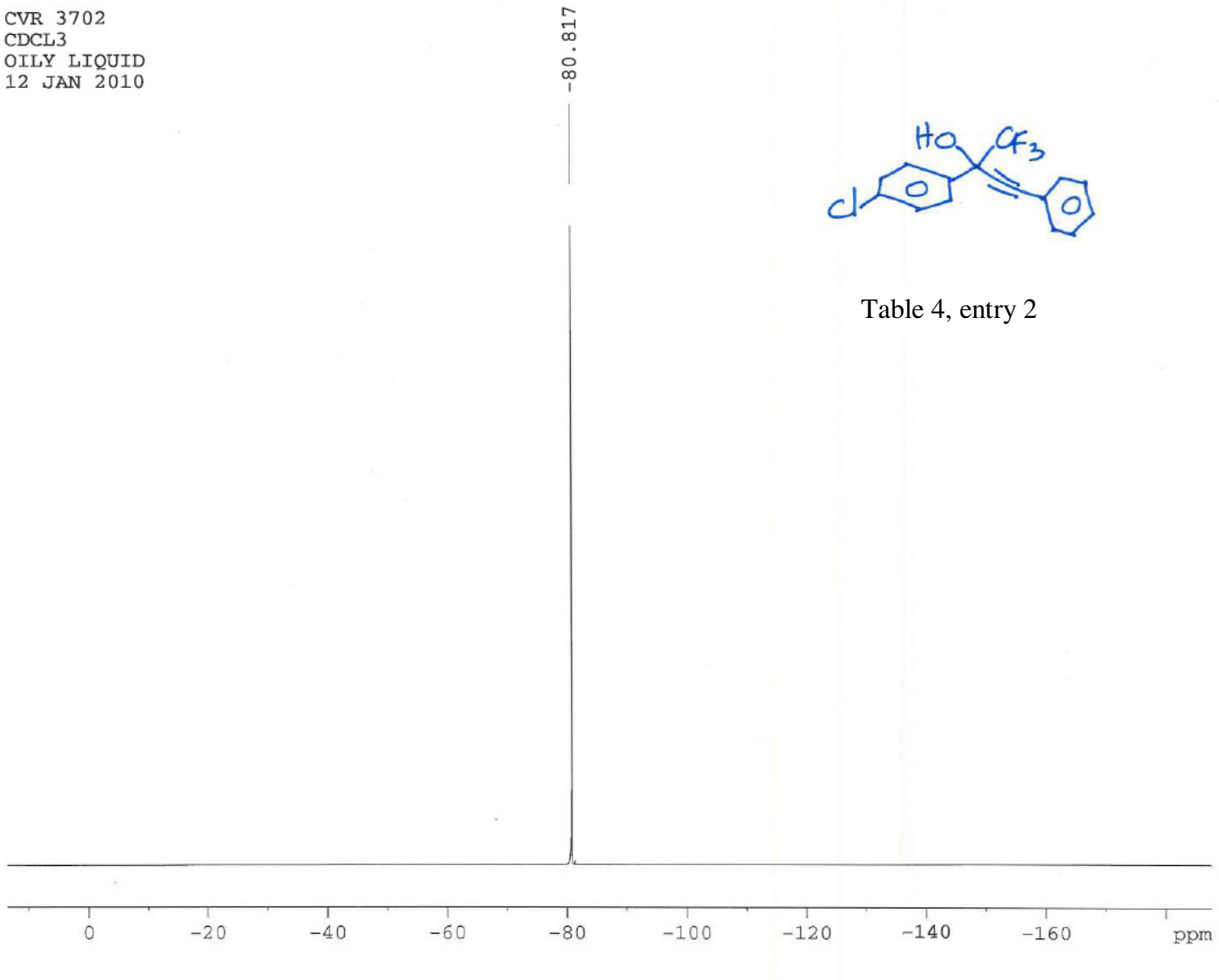


Table 4, entry 2

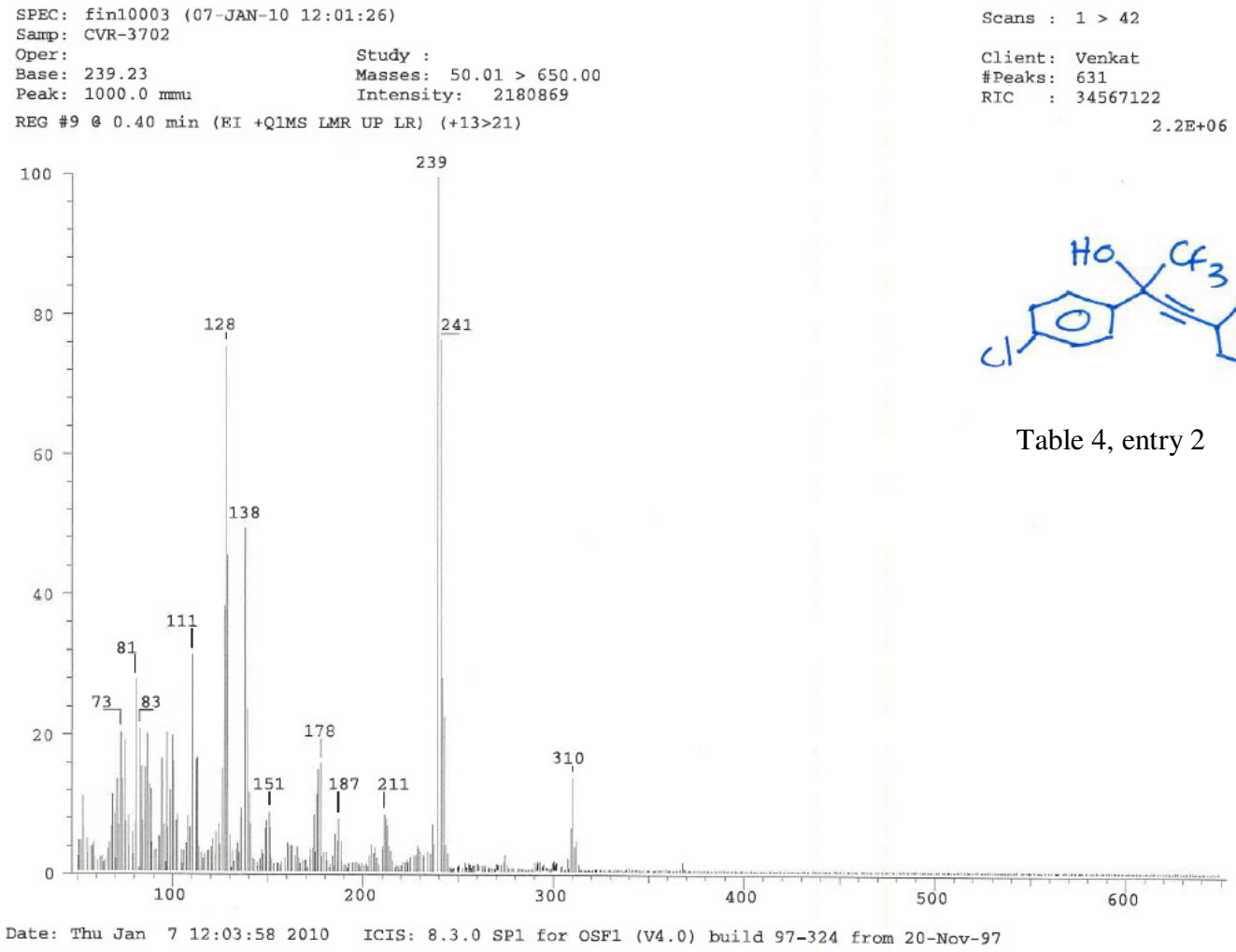


Table 4, entry 2

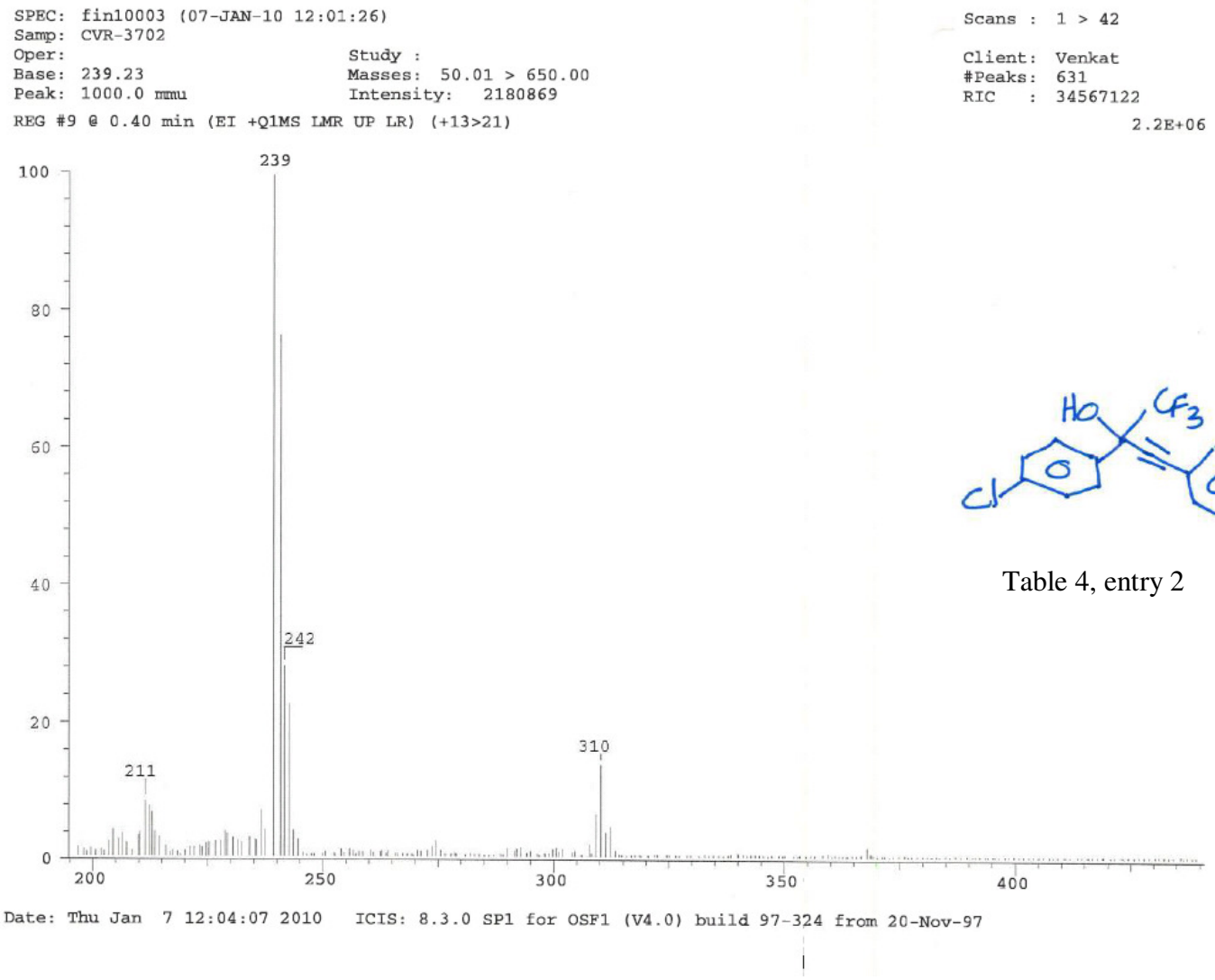


Table 4, entry 2

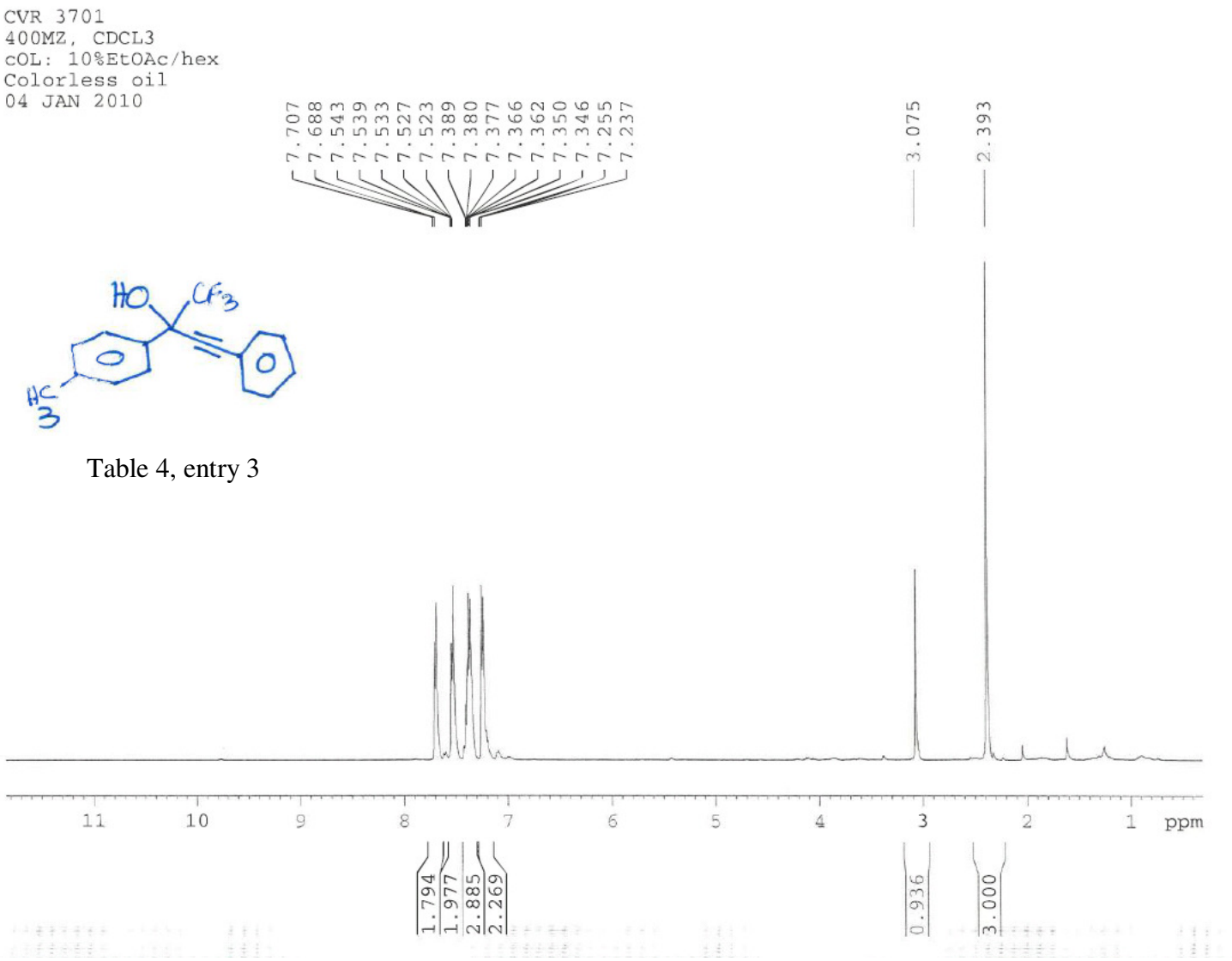


Table 4, entry 3

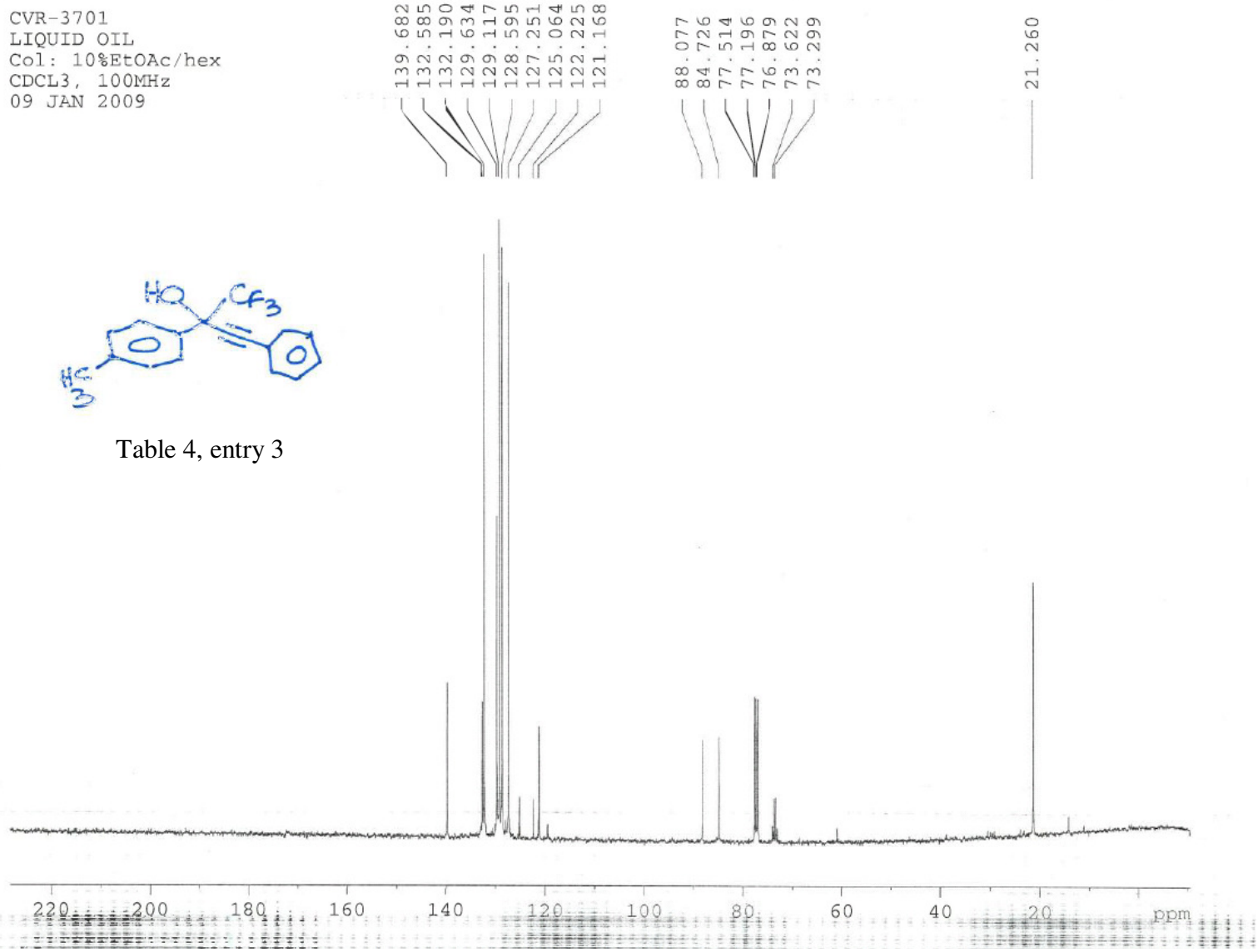


Table 4, entry 3

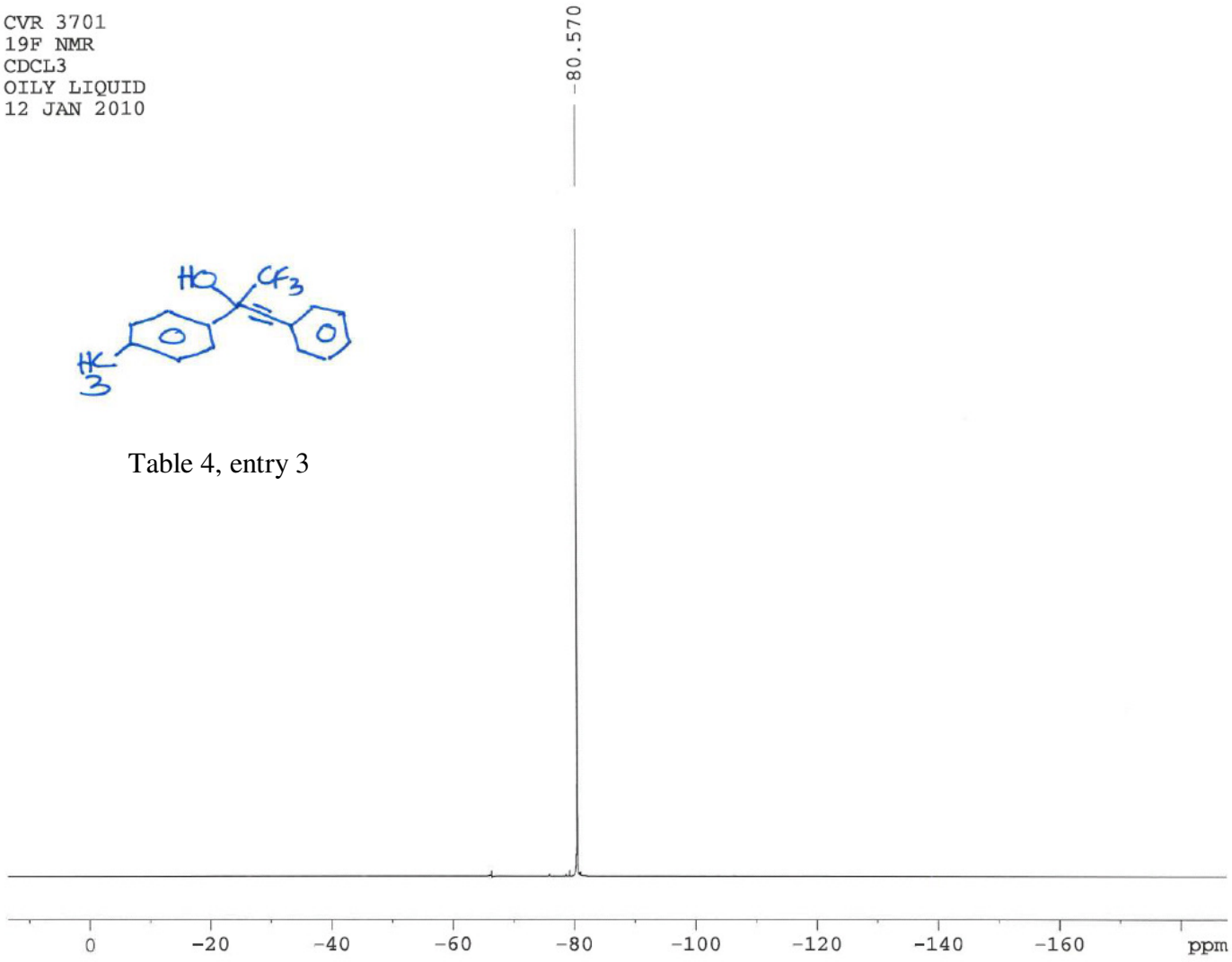


Table 4, entry 3

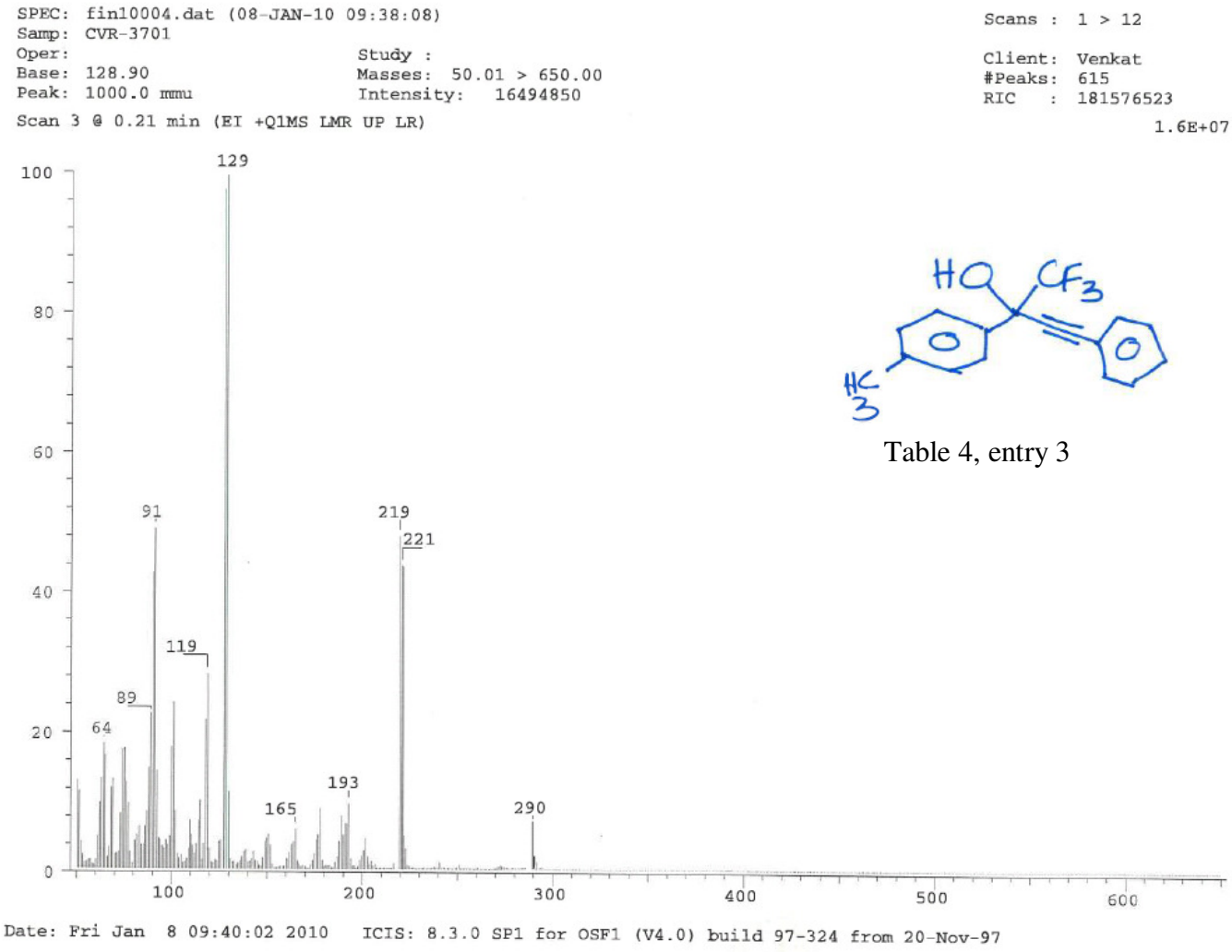


Table 4, entry 3

LIST: fin10004 08-JAN-10 Elapse: 00:12.9 3
Samp: CVR-3701 Start : 09:38:08 12
Mode: EI +Q1MS LMR UP LR
Oper: Client: Venkat Inlet :
Base: 128.9 Inten : 16494850 Masses: 50 > 650
Norm: 128.9 RIC : 181576523 #peaks: 615
Peak: 1000.00 mmu

659794

No.	Mass		Intensity	%RA	%RIC	Flags
1	50.		2105104	12.76	1.16	FM
2	51.		1856859	11.26	1.02	F
3	61.		770019	4.67	0.42	F
4	62.		1574076	9.54	0.87	F
5	63.		2162760	13.11	1.19	F
6	64.		2983203	18.09	1.64	F
7	65.		2702122	16.38	1.49	F
8	68.		1932277	11.71	1.06	F
9	69.		2138042	12.96	1.18	F
10	73.		1309887	7.94	0.72	F
11	74.		2833079	17.18	1.56	F
12	75.		2864436	17.37	1.58	F
13	76.		2065642	12.52	1.14	F
14	77.		1566815	9.50	0.86	F
15	82.		804434	4.88	0.44	FM
16	83.		1007563	6.11	0.55	FM
17	86.		1004412	6.09	0.55	F
18	87.		1369969	8.31	0.75	F
19	88.		2411677	14.62	1.33	F
20	89.		3705893	22.47	2.04	F
21	90.		7033073	42.64	3.87	F
22	91.		8079235	48.98	4.45	F
23	92.		2338223	14.18	1.29	F
24	93.		736684	4.47	0.41	FM
25	94.		690355	4.19	0.38	F
26	97.		682300	4.14	0.38	F
27	99.		777398	4.71	0.43	F
28	100.		2900467	17.58	1.60	F
29	101.		3955192	23.98	2.18	F
30	102.		1368895	8.30	0.75	F
31	110.		1164337	7.06	0.64	FM
32	110.		810583	4.91	0.45	F
33	114.		1158855	7.03	0.64	F
34	115.		1628733	9.87	0.90	F
35	118.		3555300	21.55	1.96	F
36	119.		4636006	28.11	2.55	FM
37	126.		687916	4.17	0.38	F
38	128.	S	16159944	97.97	8.90	F
39	129.	S	16494850	100.00	9.08	F
40	130.		1844466	11.18	1.02	F
41	150.		742827	4.50	0.41	F
42	151.		828491	5.02	0.46	F
43	165.		947398	5.74	0.52	F
44	176.		695228	4.21	0.38	F
45	177.		815183	4.94	0.45	F
46	178.		1442261	8.74	0.79	F
47	189.		1273792	7.72	0.70	F
48	190.		820220	4.97	0.45	F
49	191.		1083400	6.57	0.60	F
50	192.		1083838	6.57	0.60	F
51	193.		1556378	9.44	0.86	FM
52	202.		734804	4.45	0.40	FM
53	219.		7915911	47.99	4.36	F
54	221.		7218822	43.76	3.98	F
55	221.		7191125	43.60	3.96	F
56	222.		804339	4.88	0.44	F
57	290.		1135846	6.89	0.63	F

Date: Fri Jan 8 09:46:51 2010 ICIS: 8.3.0 SP1 for OSF1 (V4.0) build 97-324 from 20-Nov-97

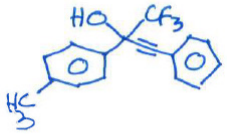


Table 4, entry 3

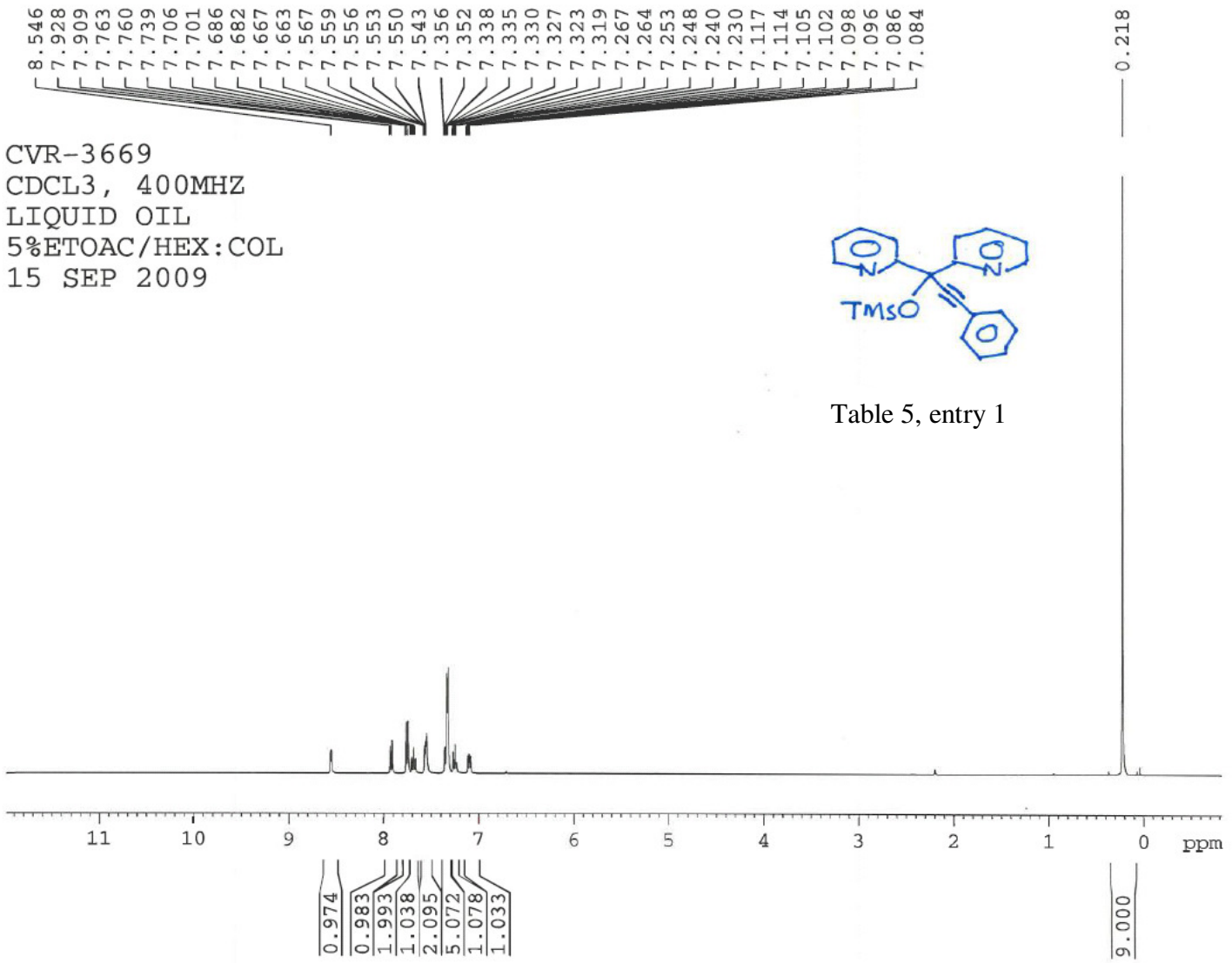


Table 5, entry 1

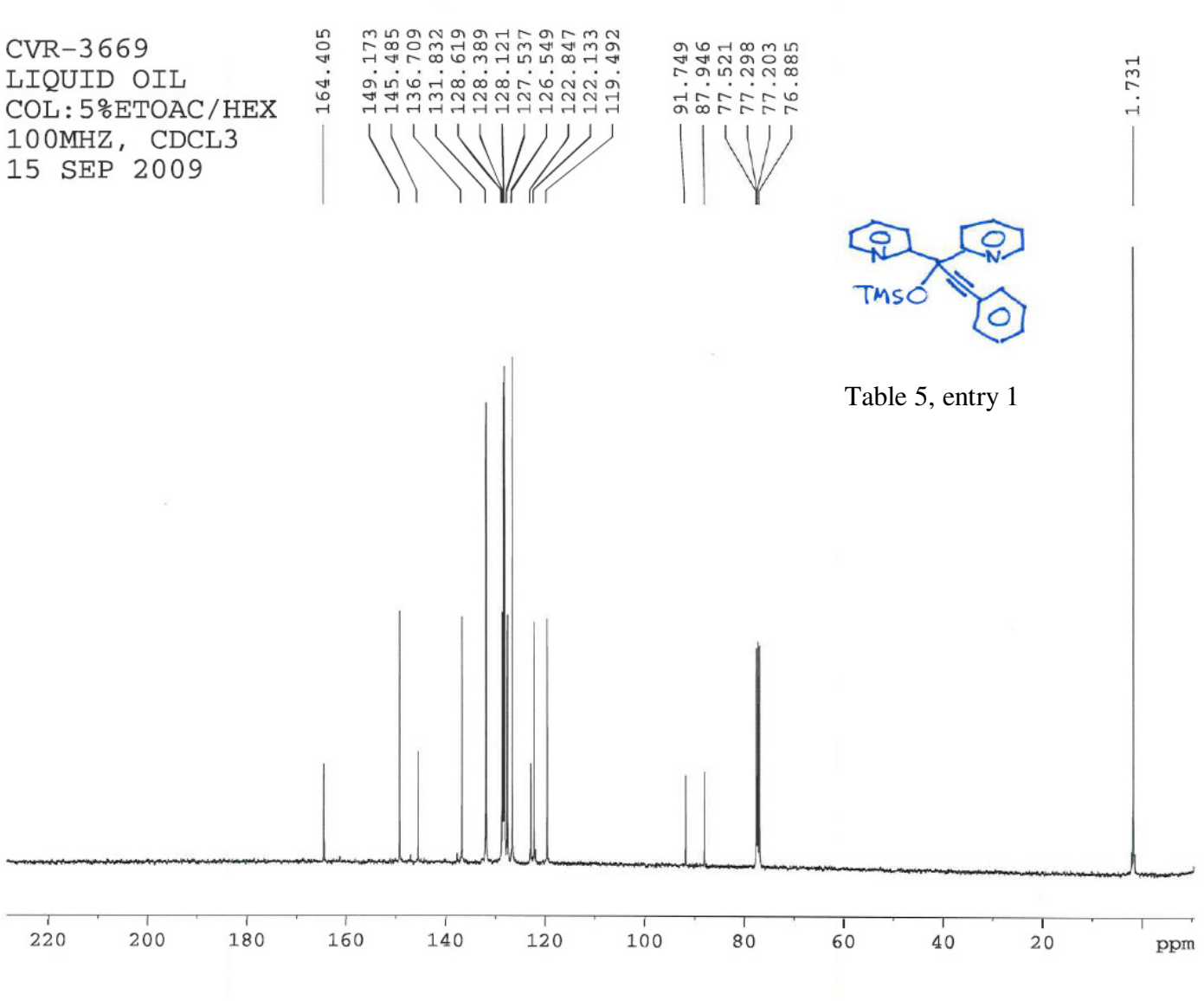


Table 5, entry 1

Manual Peak Matching Report
For Accurate Mass Determination

Theoretical mass	Experimental mass	PFK matching mass	Deviation*
358.15013	358.15108	330.99923	2.6 ppm

* The deviation is obtained from the following equation:

$$\text{deviation} = \frac{\text{experimental mass - theoretical mass}}{\text{nominal mass}}$$

Where nominal mass takes in account only ^{12}C, ^{1}H, ^{16}O, ^{14}N etc...

Theoretical mass correspond to the mass of the most abundant isotope peak

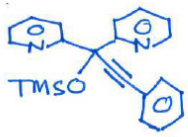


Table 5, entry 1

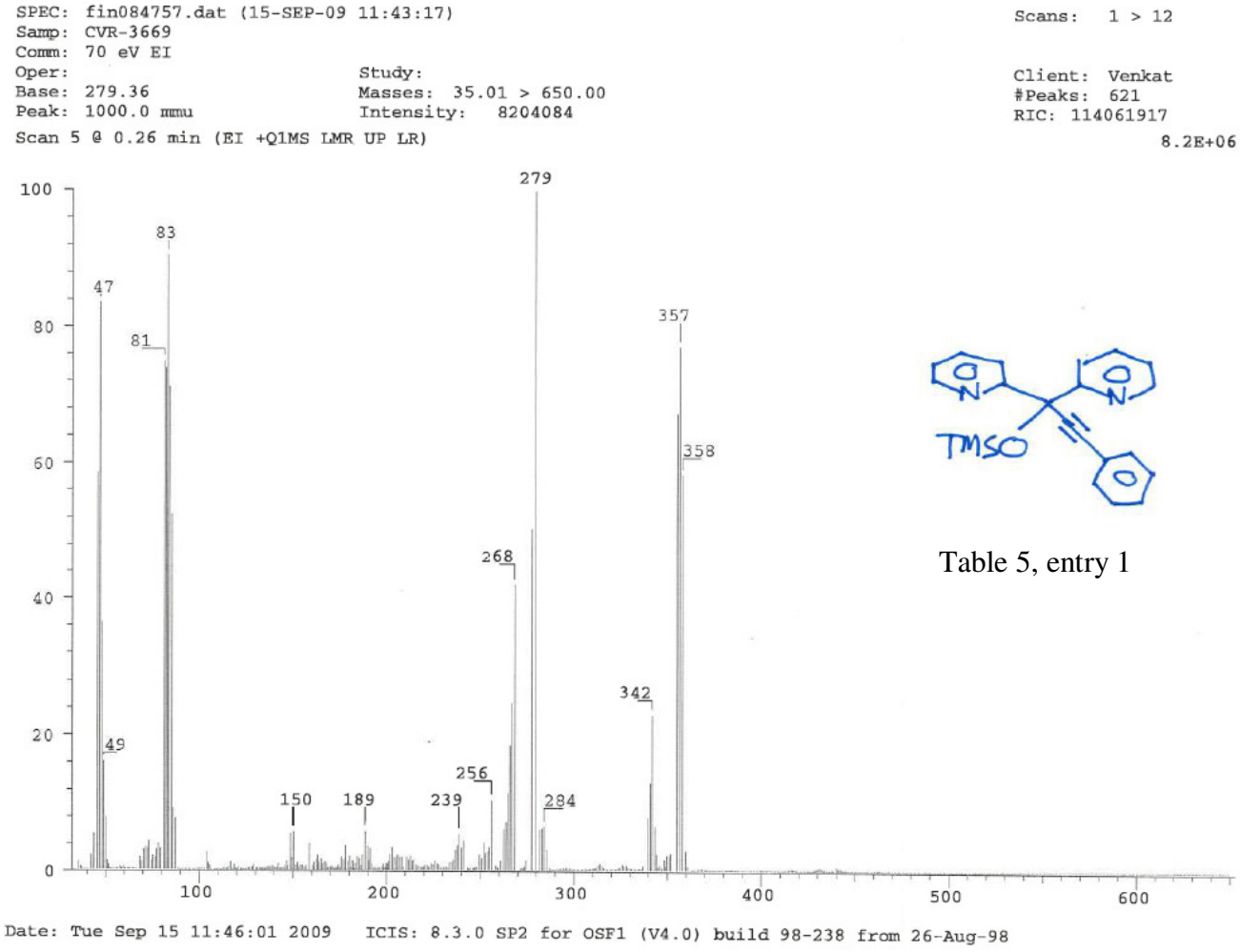


Table 5, entry 1

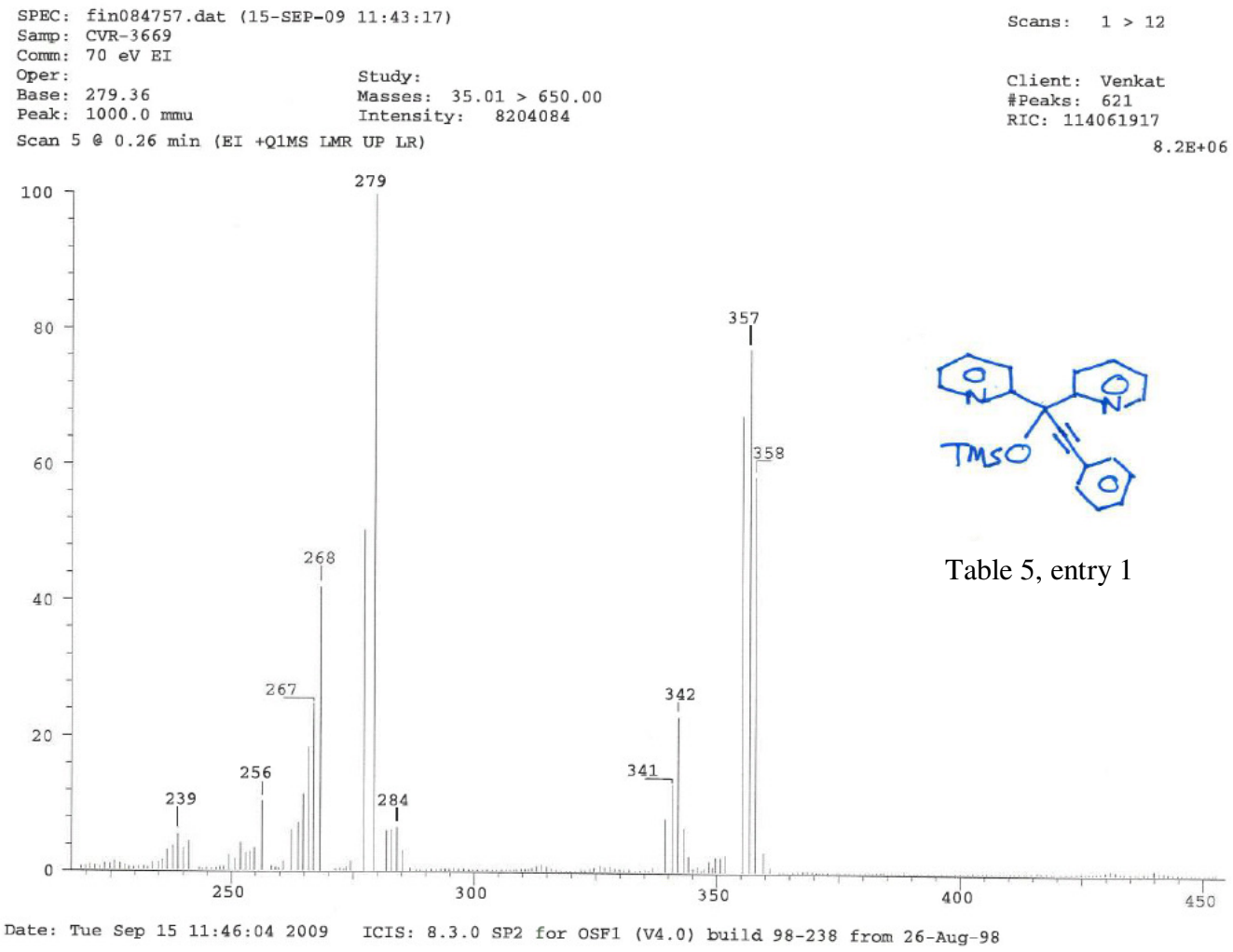


Table 5, entry 1

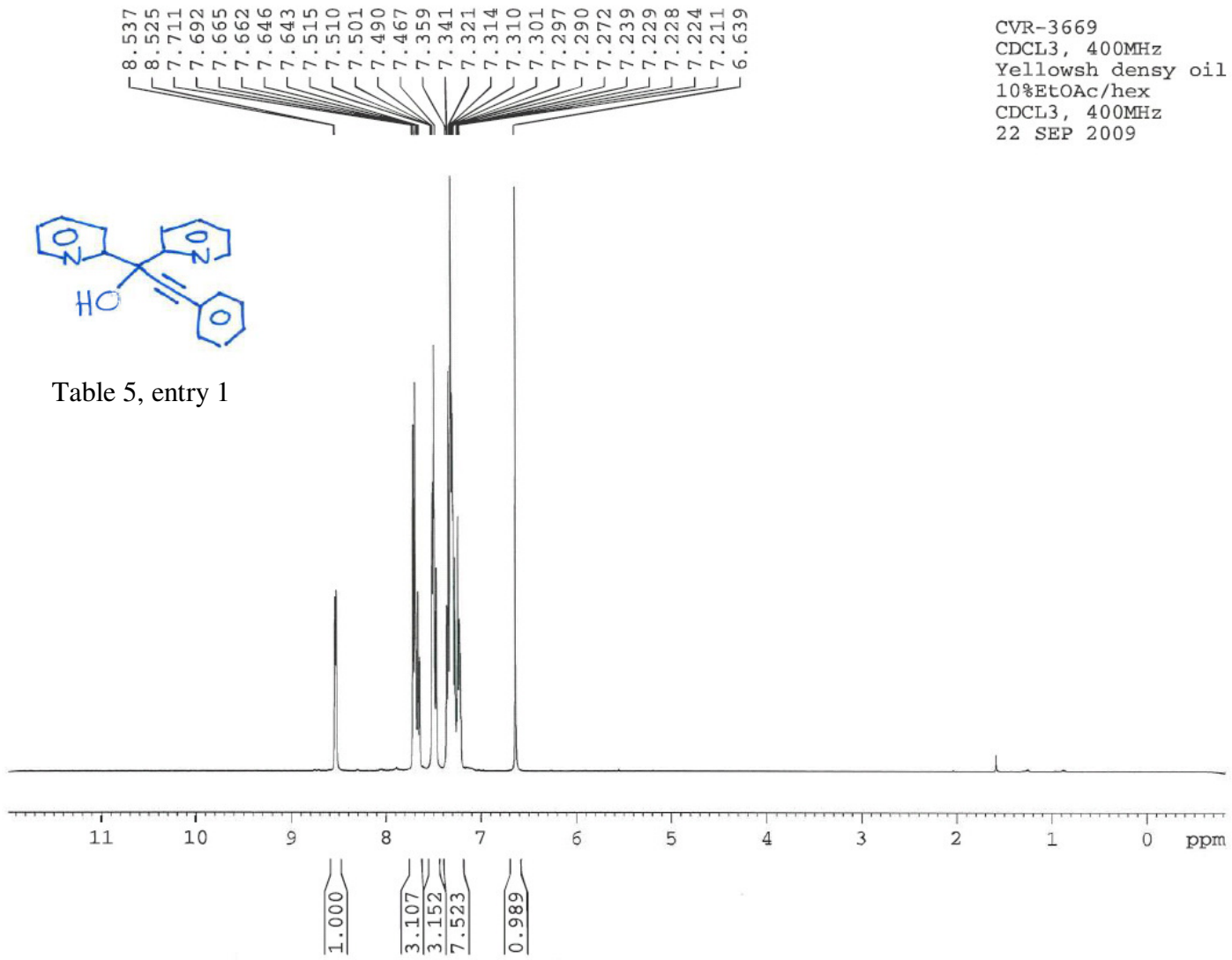


Table 5, entry 1

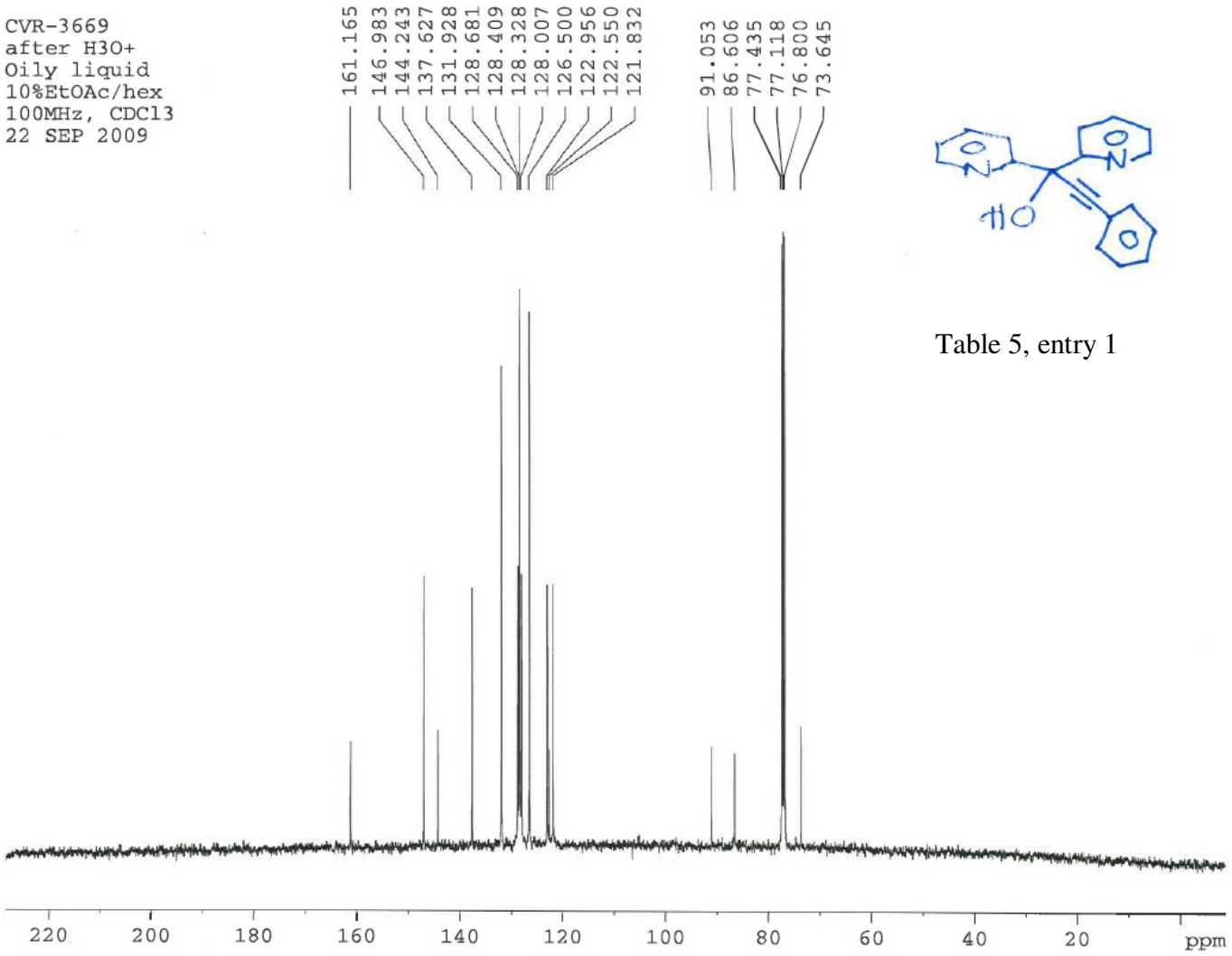


Table 5, entry 1

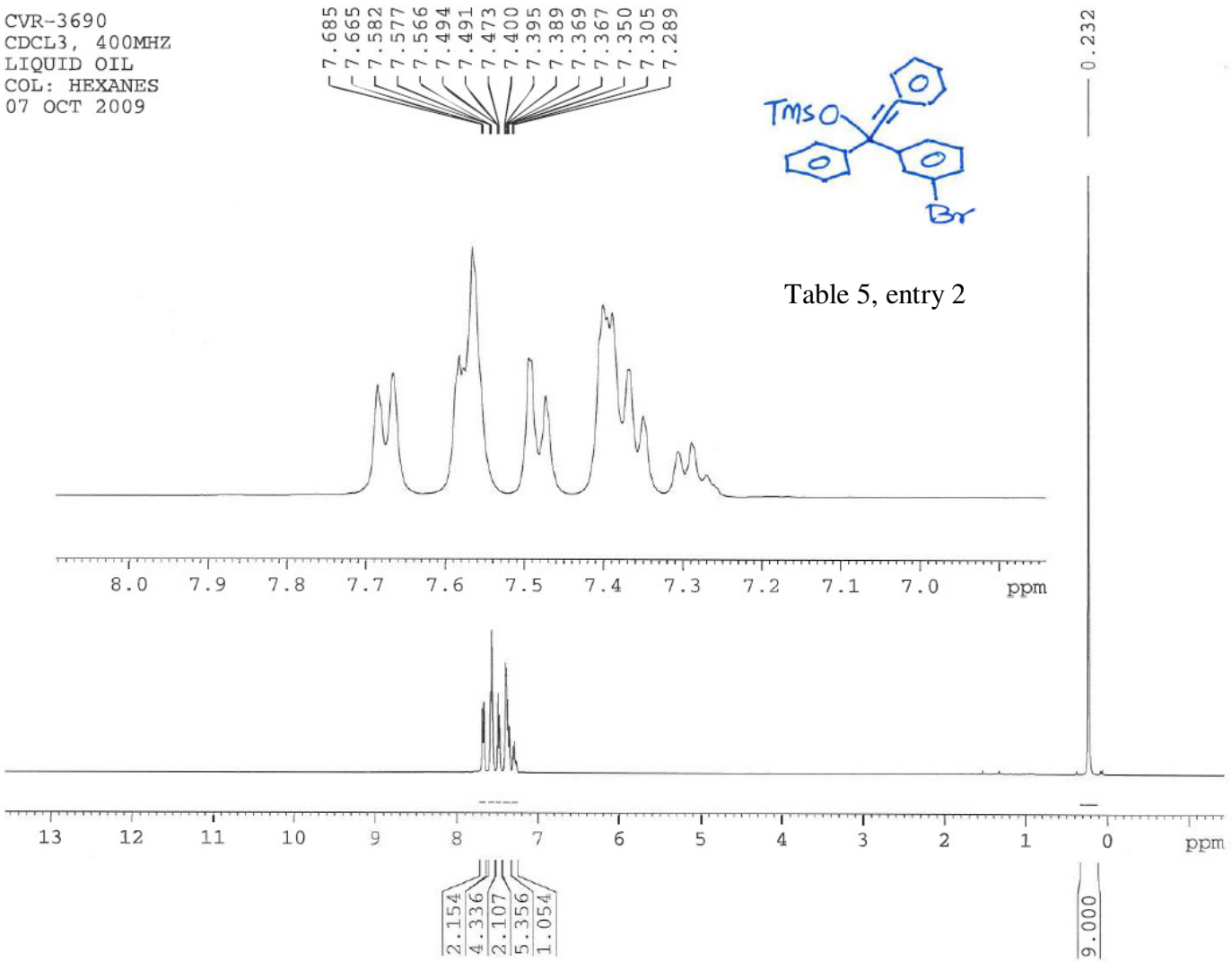


Table 5, entry 2

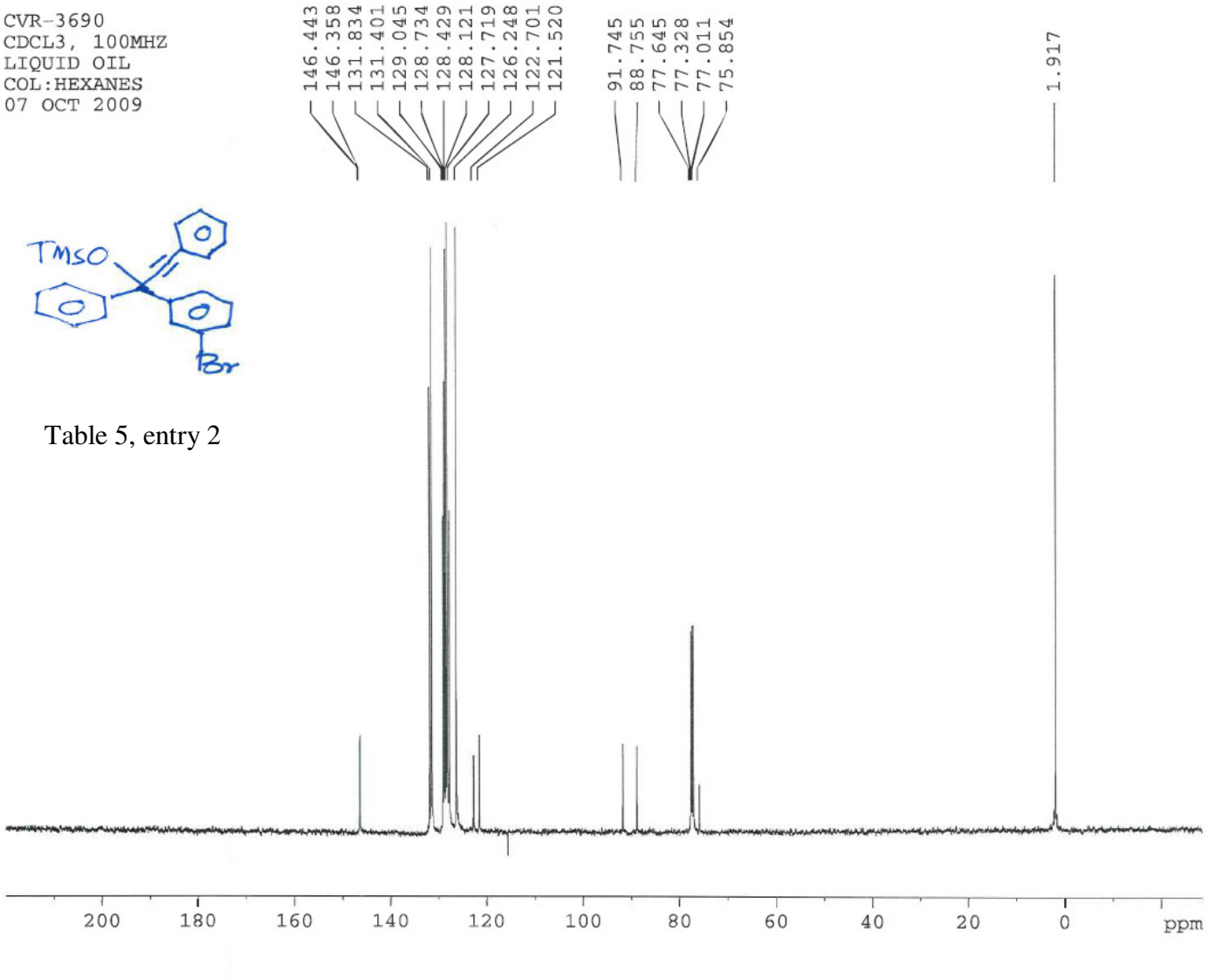


Table 5, entry 2

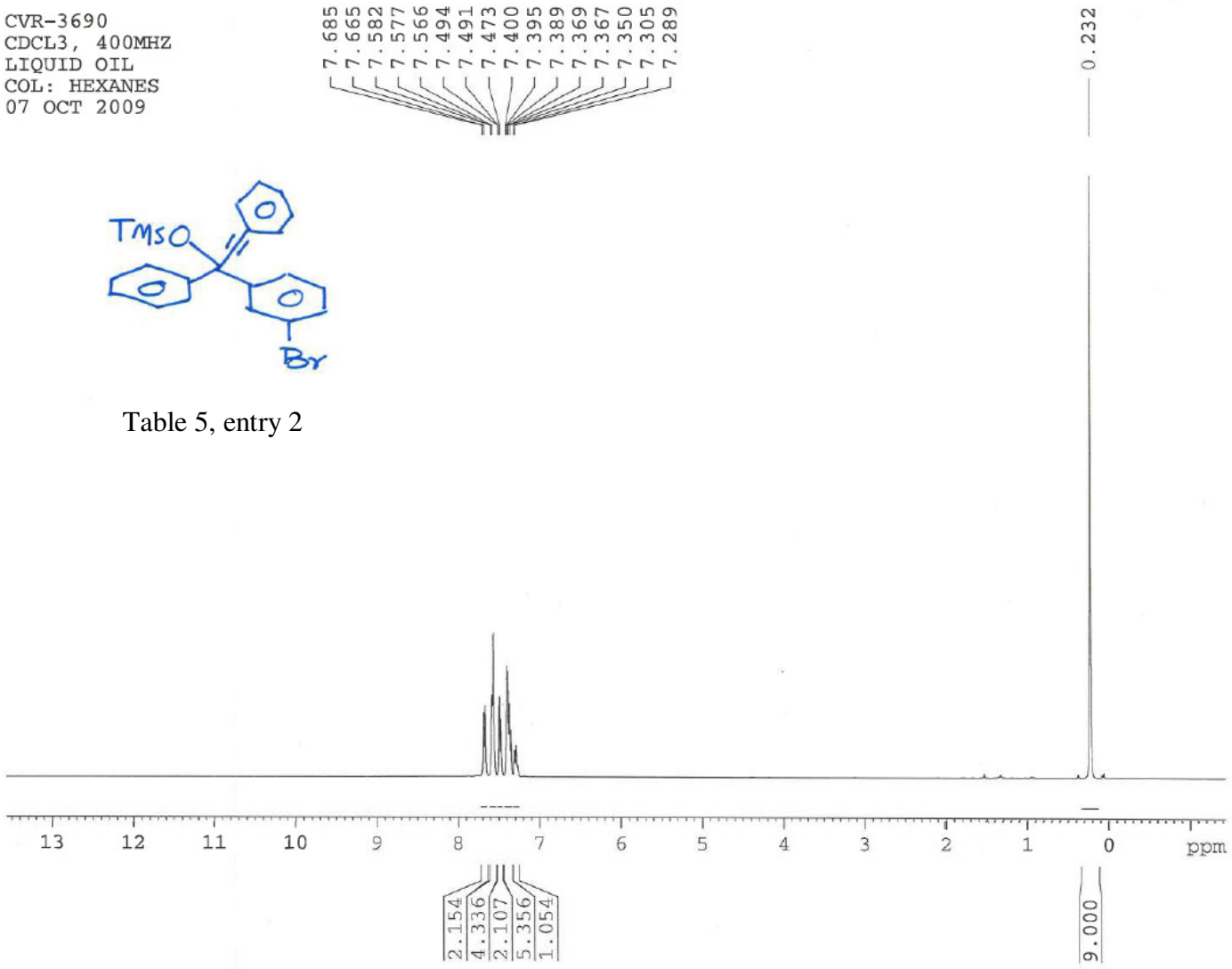


Table 5, entry 2

Manual Peak Matching Report
For Accurate Mass Determination

Theoretical mass	Experimental mass	PFK matching mass	Deviation*
434.07014	434.07124	430.97284	2.5 ppm

* The deviation is obtained from the following equation:

$$\text{deviation} = \frac{\text{experimental mass - theoretical mass}}{\text{nominal mass}}$$

Where nominal mass takes in account only ^{12}C, ^{1}H, ^{16}O, ^{14}N etc...

Theoretical mass correspond to the mass of the most abundant isotope peak

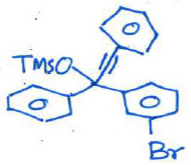


Table 5, entry 2

SPEC: fin084809 (12-OCT-09 16:21:43)
Samp: CVR-3690
Comm: 70 eV EI
Oper:
Base: 433.90
Peak: 1000.0 mmu
Study :
Masses: 50.01 > 650.00
Intensity: 3964275
REG #9 @ 0.68 min (EI +Q1MS LMR UP LR) (+25>32)

Scans : 1 > 35

Client: Venkat
#Peaks: 605
RIC : 29917173
4.0E+06

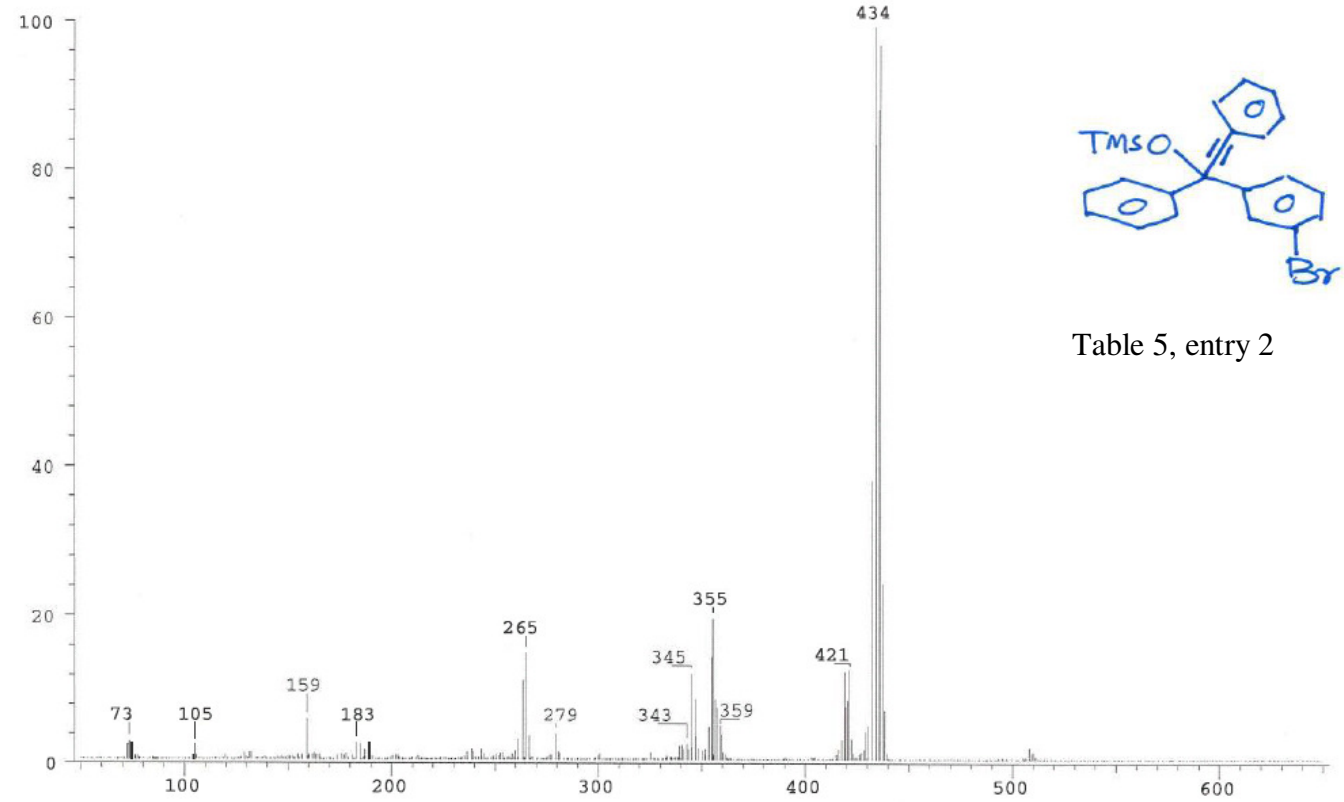


Table 5, entry 2

Date: Mon Oct 12 16:23:15 2009 ICIS: 8.3.0 SP1 for OSF1 (V4.0) build 97-324 from 20-Nov-97

LIST: fin084809 12-OCT-09 Elapse: 00:45.5 29
Samp: CVR-3690 Start : 16:21:43 35
Comm: 70 eV EI
Mode: EI +Q1MS LMR UP LR
Oper: Client: Venkat Inlet :
Base: 434.2 Inten : 186980 Masses: 50 > 650
Norm: 434.2 RIC : 2863564 #peaks: 622
Peak: 1000.00 mmu

35526

No.	Mass	Intensity	%RA	%RIC	Flags
1	159.	71936	38.47	2.51	F
2	263.	39630	21.19	1.38	F
3	263.	64005	34.23	2.24	F
4	265.	71952	38.48	2.51	F
5	265.	54336	29.06	1.90	F
6	344.	45827	24.51	1.60	F
7	345.	39557	21.16	1.38	F
8	346.	38918	20.81	1.36	F
9	354.	98594	52.73	3.44	F
10	355.	113532	60.72	3.96	FM
11	356.	52487	28.07	1.83	F
12	431.	38575	20.63	1.35	FM
13	432.	65920	35.26	2.30	F
14	433.	131132	70.13	4.58	F
15	434.	186980	100.00	6.53	F
16	435.	174904	93.54	6.11	F
17	436.	145600	77.87	5.08	F
18	437.	37572	20.09	1.31	FM

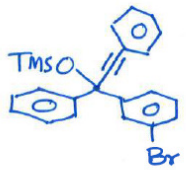


Table 5, entry 2

Date: Mon Oct 12 16:23:52 2009 ICIS: 8.3.0 SP1 for OSF1 (V4.0) build 97-324 from 20-Nov-97

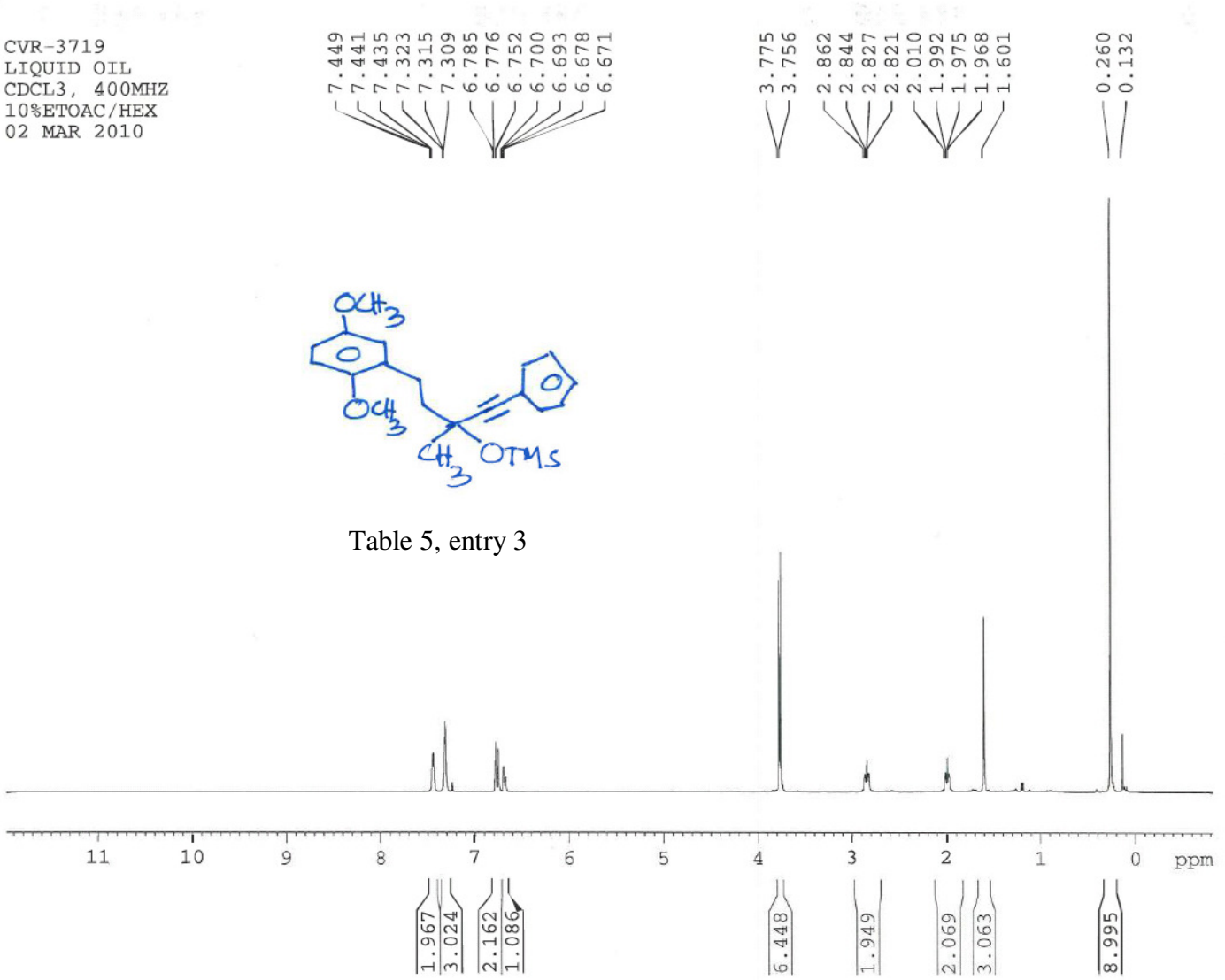


Table 5, entry 3

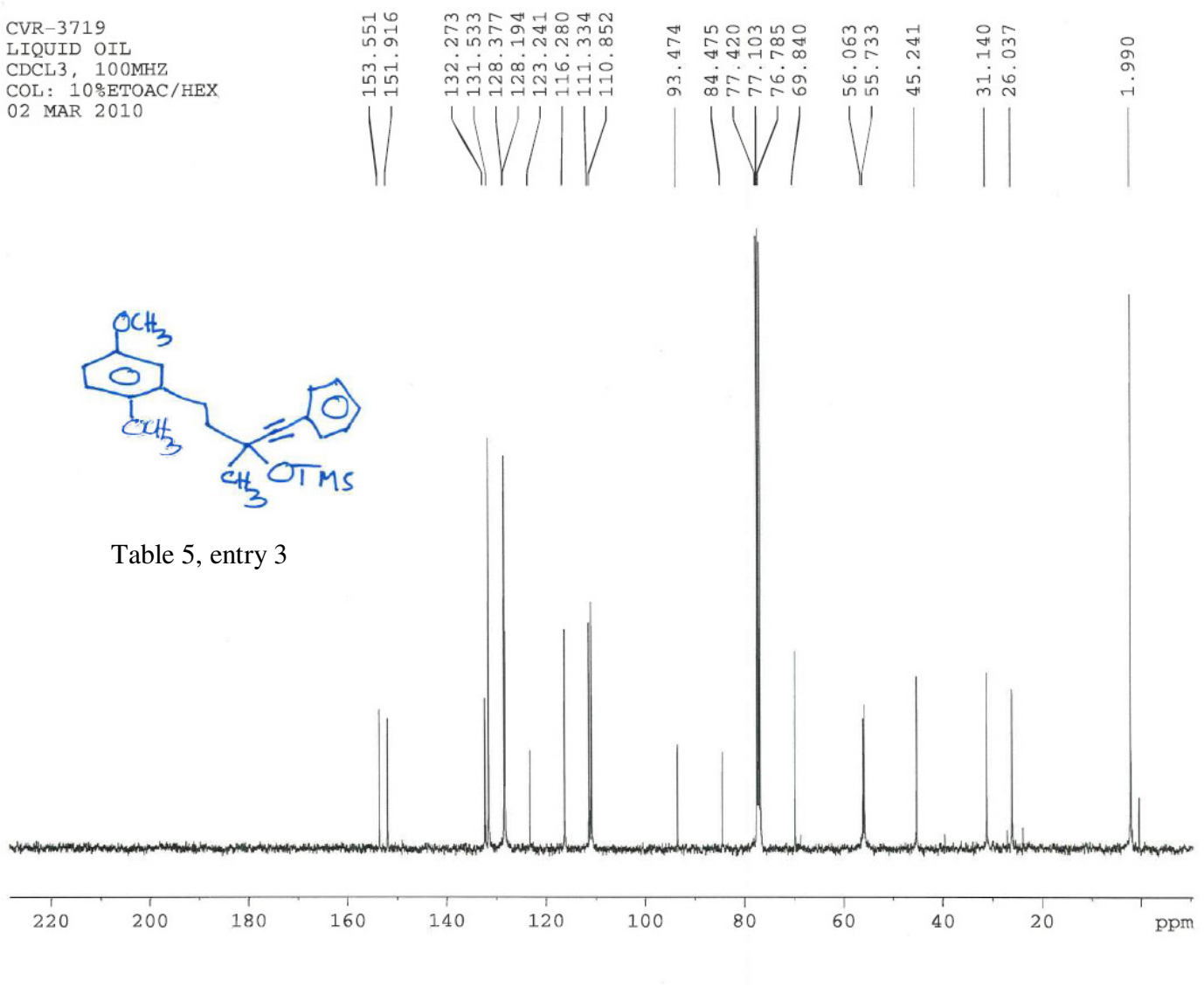


Table 5, entry 3

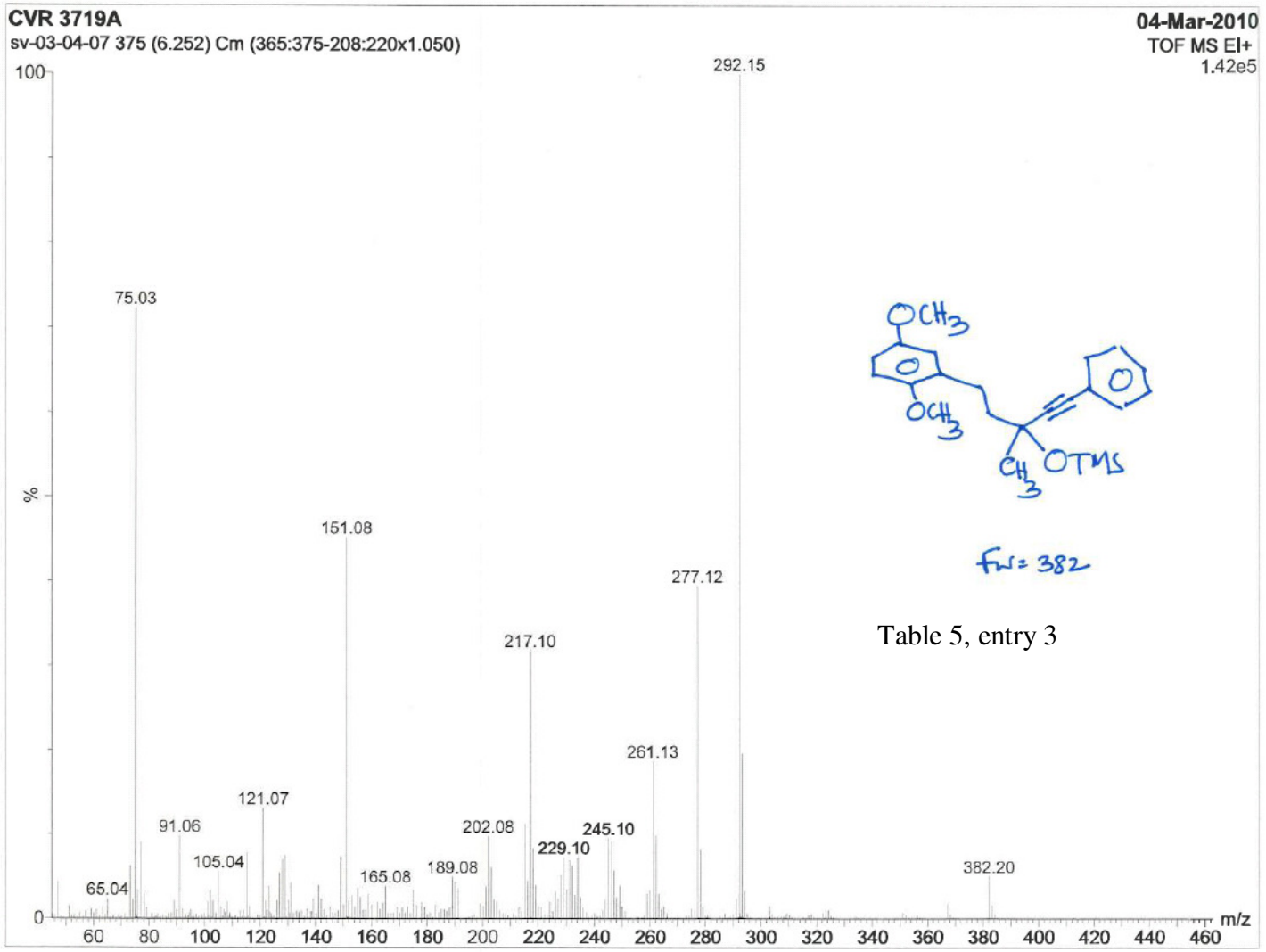
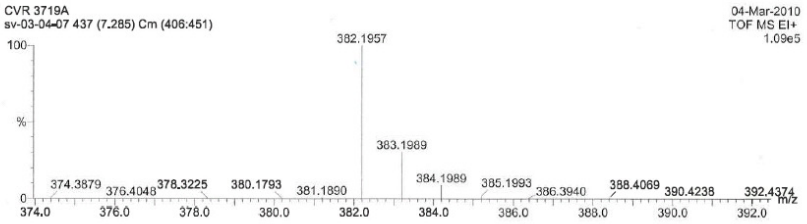


Table 5, entry 3

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
33 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)



Minimum:				-1.5		
Maximum:		5.0	10.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
382.1957	382.1964	-0.7	-1.9	10.0	1	C23 H30 O3 Si

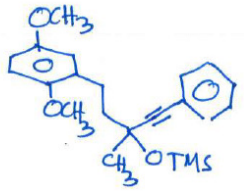


Table 5, entry 3

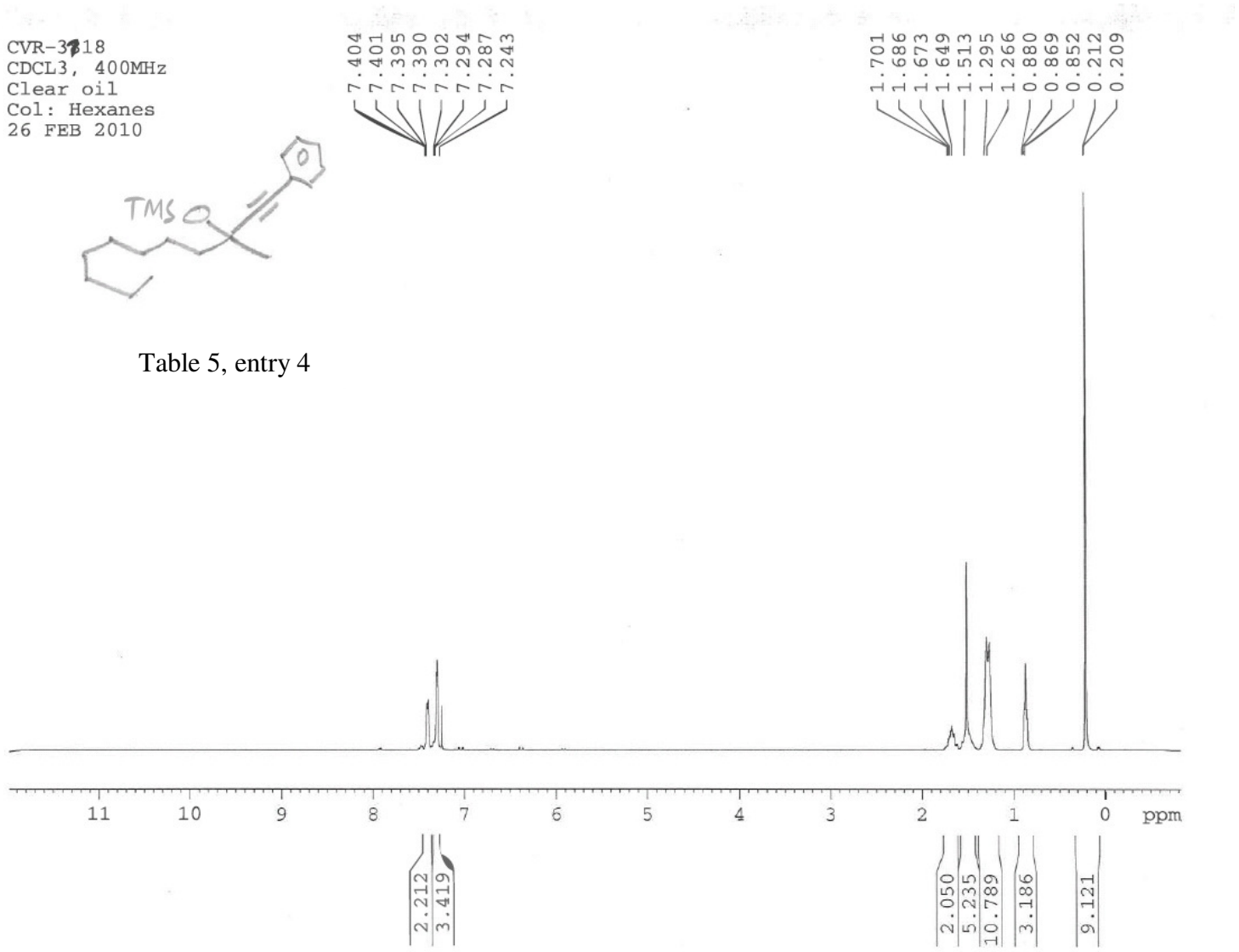


Table 5, entry 4

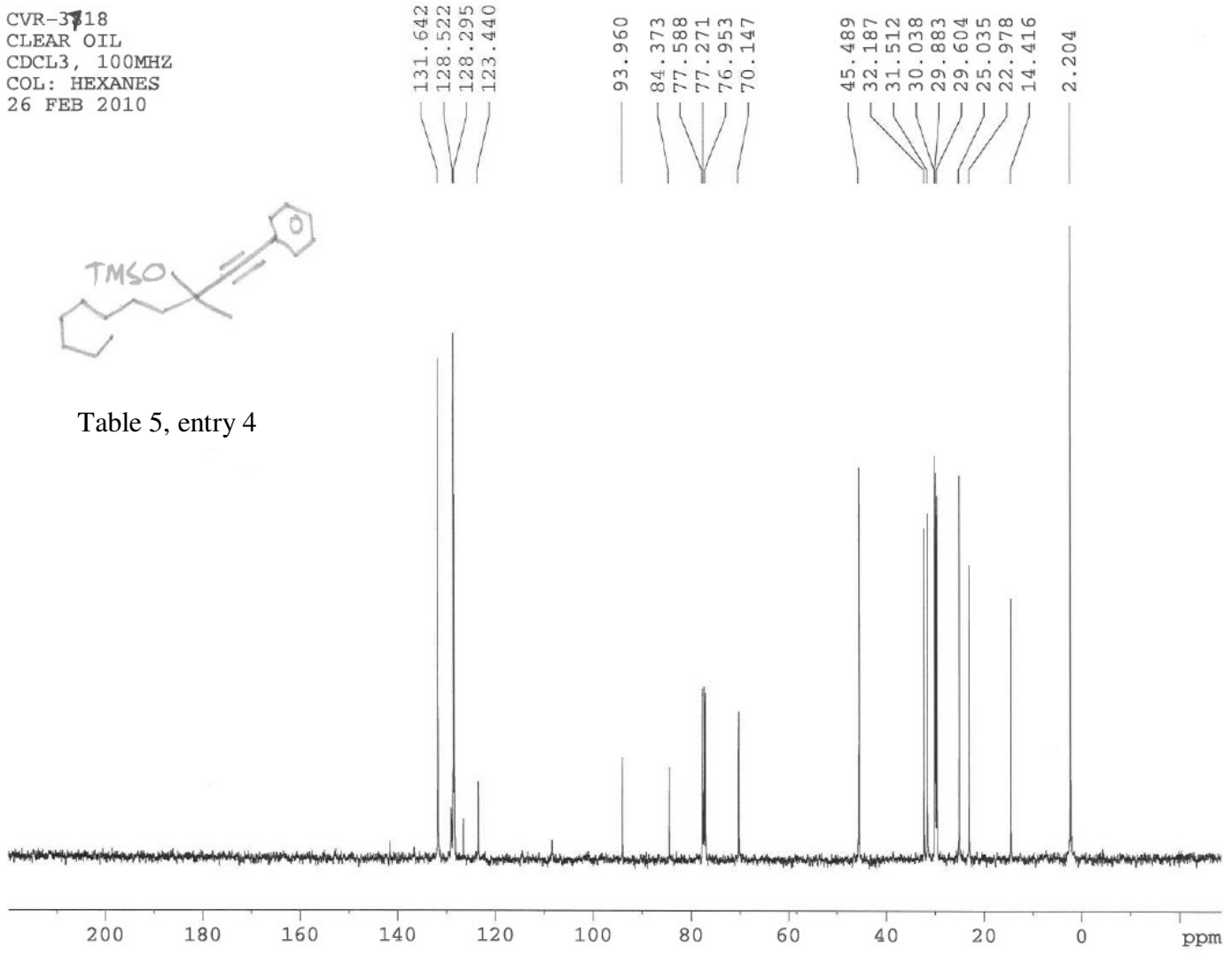


Table 5, entry 4

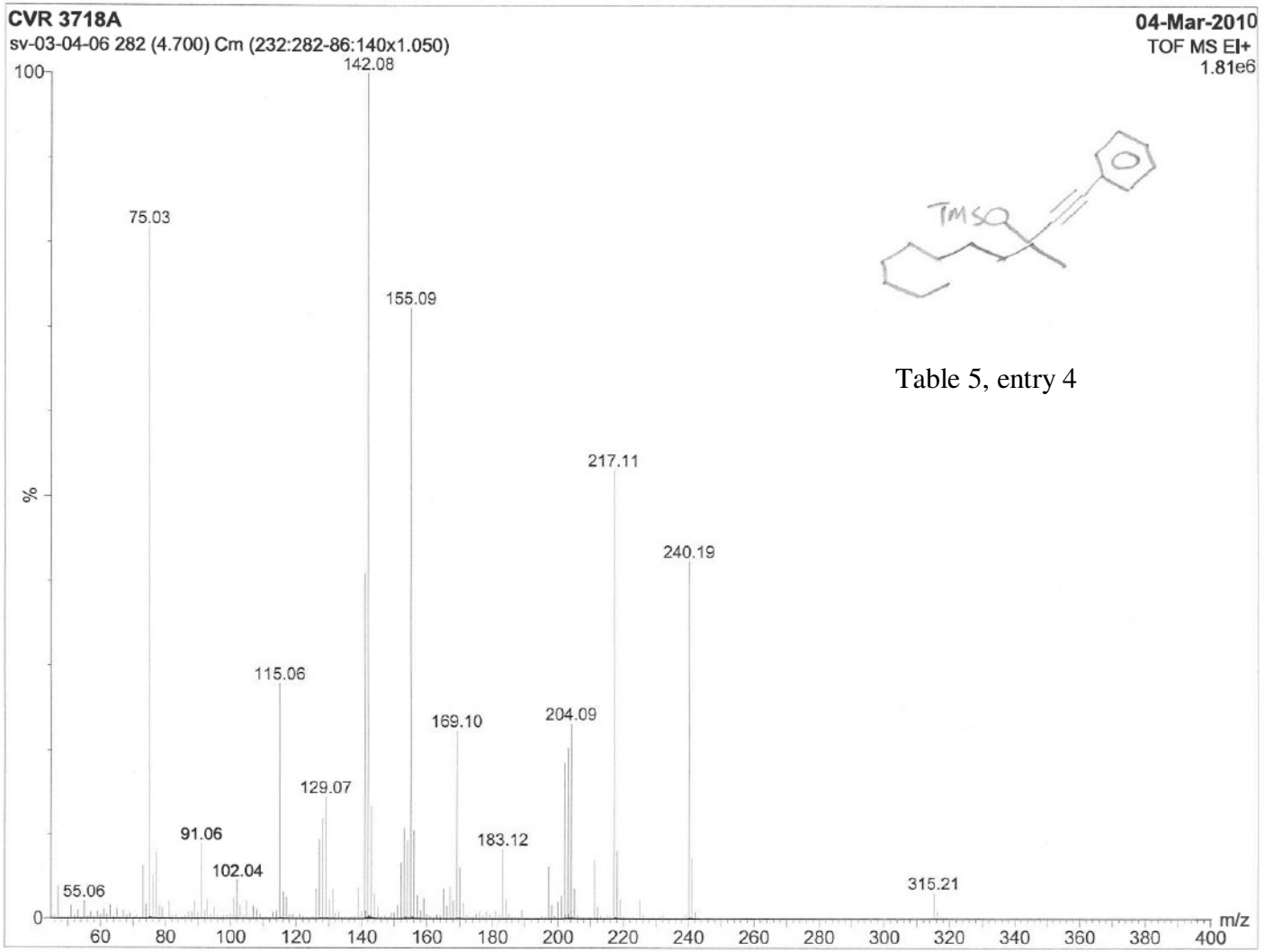


Table 5, entry 4

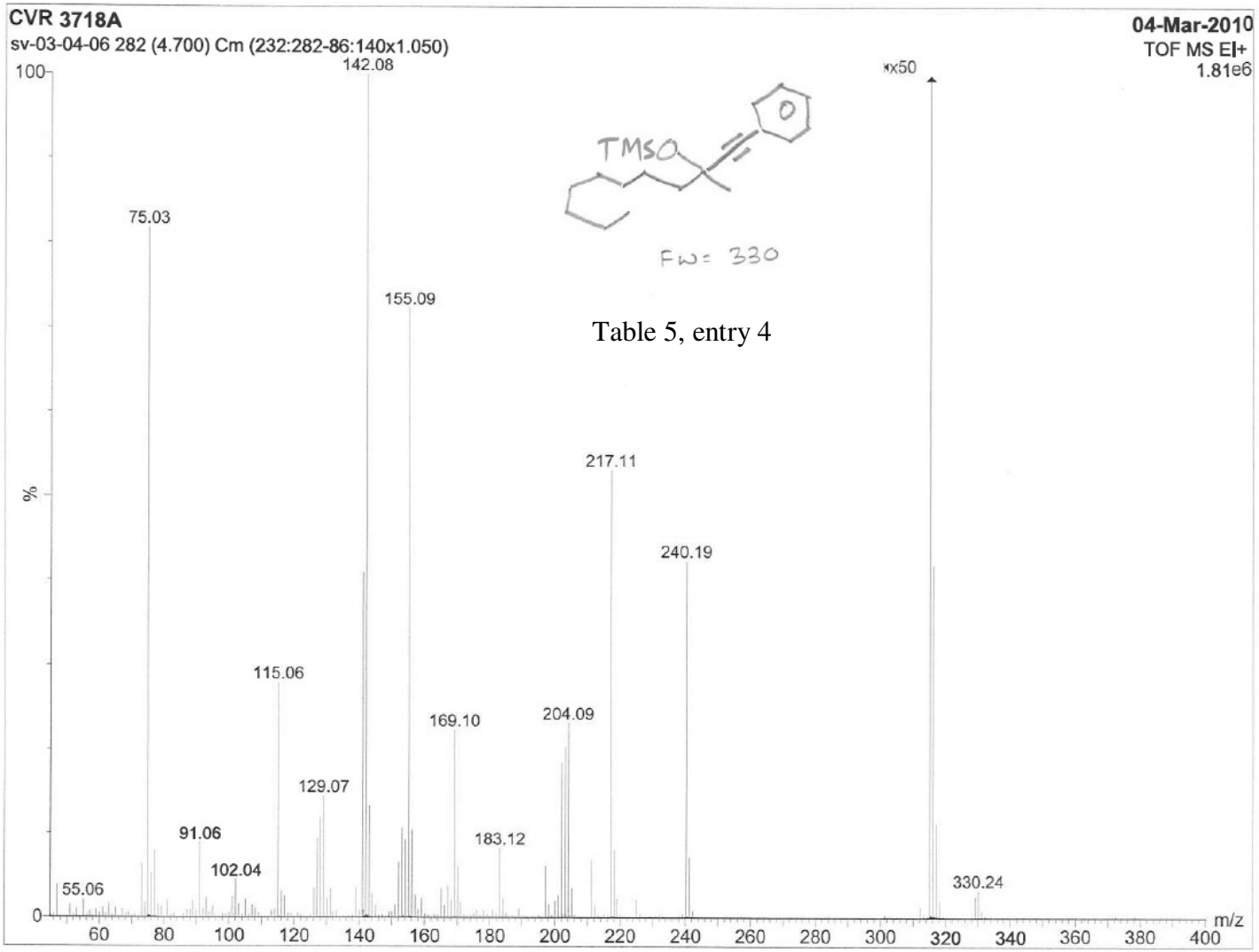


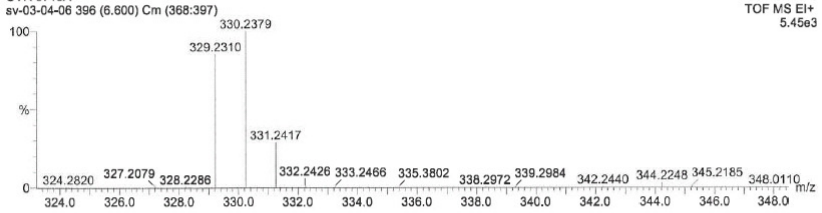
Table 5, entry 4

Elemental Composition Report **Page 1**

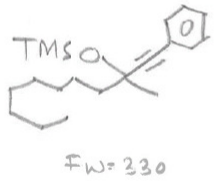
Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
9 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

CVR 3718A
sv-03-04-06 396 (6.600) Cm (368:397)
04-Mar-2010
TOF MS EI+
5.45e3



Minimum:				-1.5		
Maximum:		5.0	3.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
330.2379	330.2379	0.0	0.0	6.0	1	C21 H34 O Si



FW= 330

Table 5, entry 4

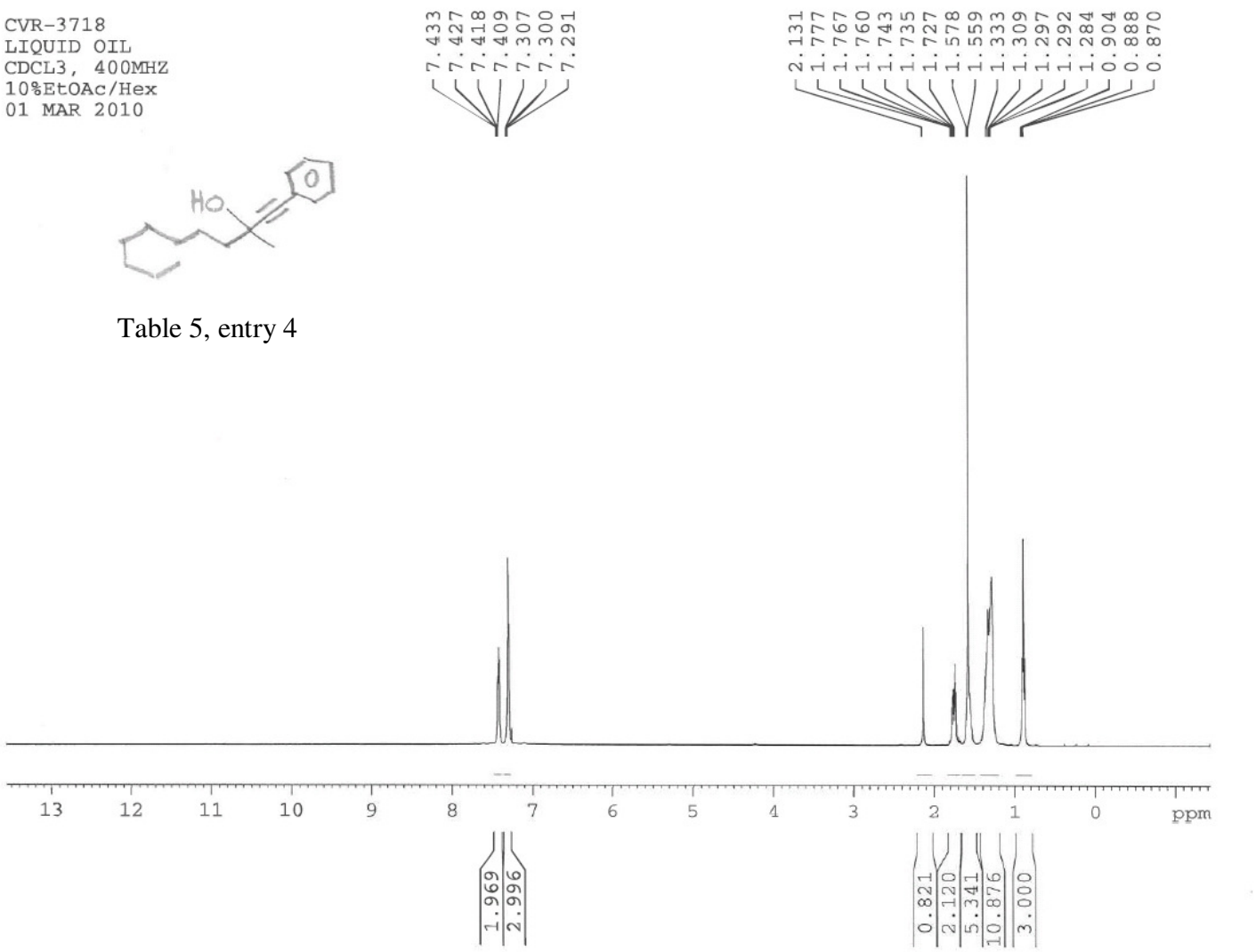


Table 5, entry 4

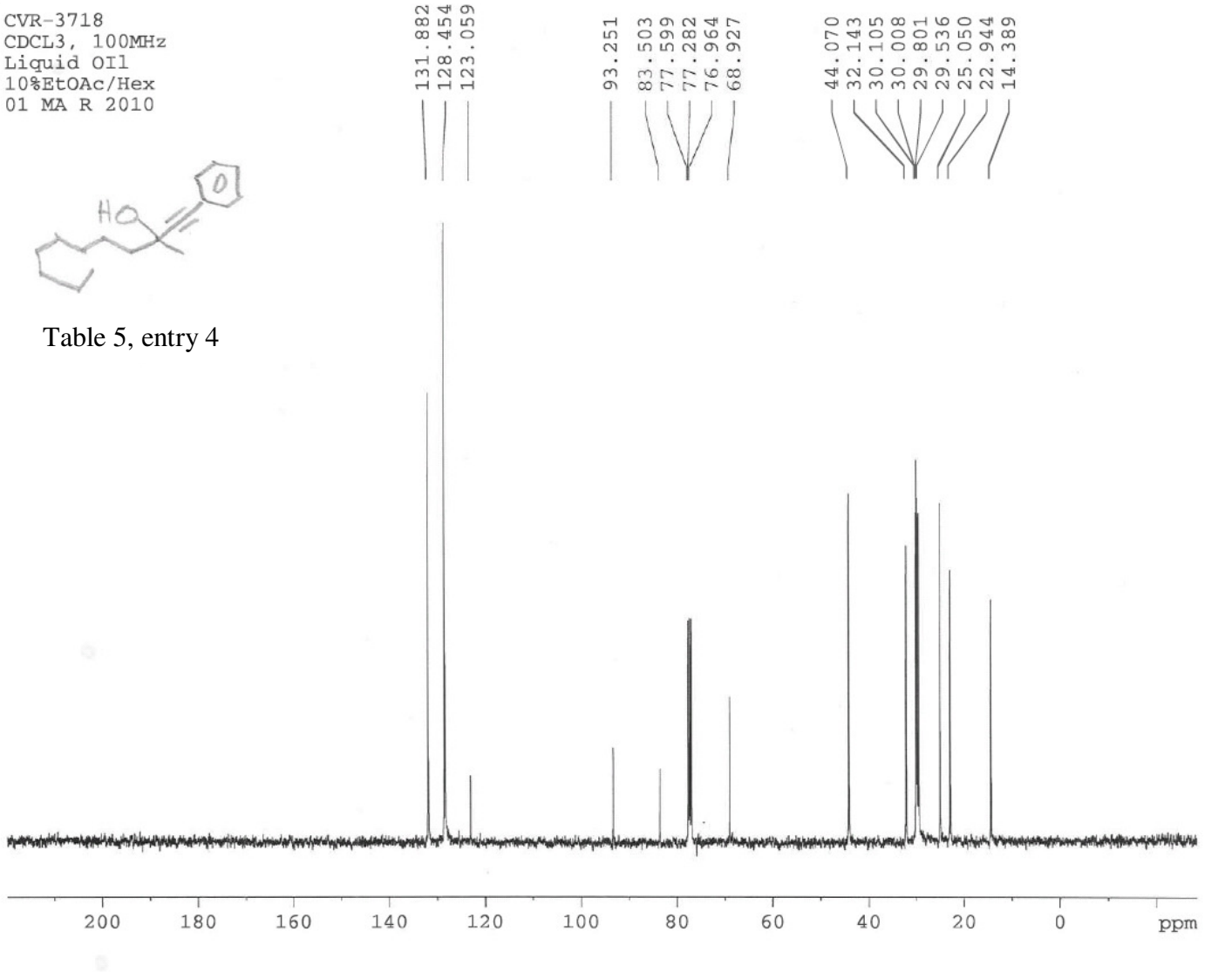


Table 5, entry 4

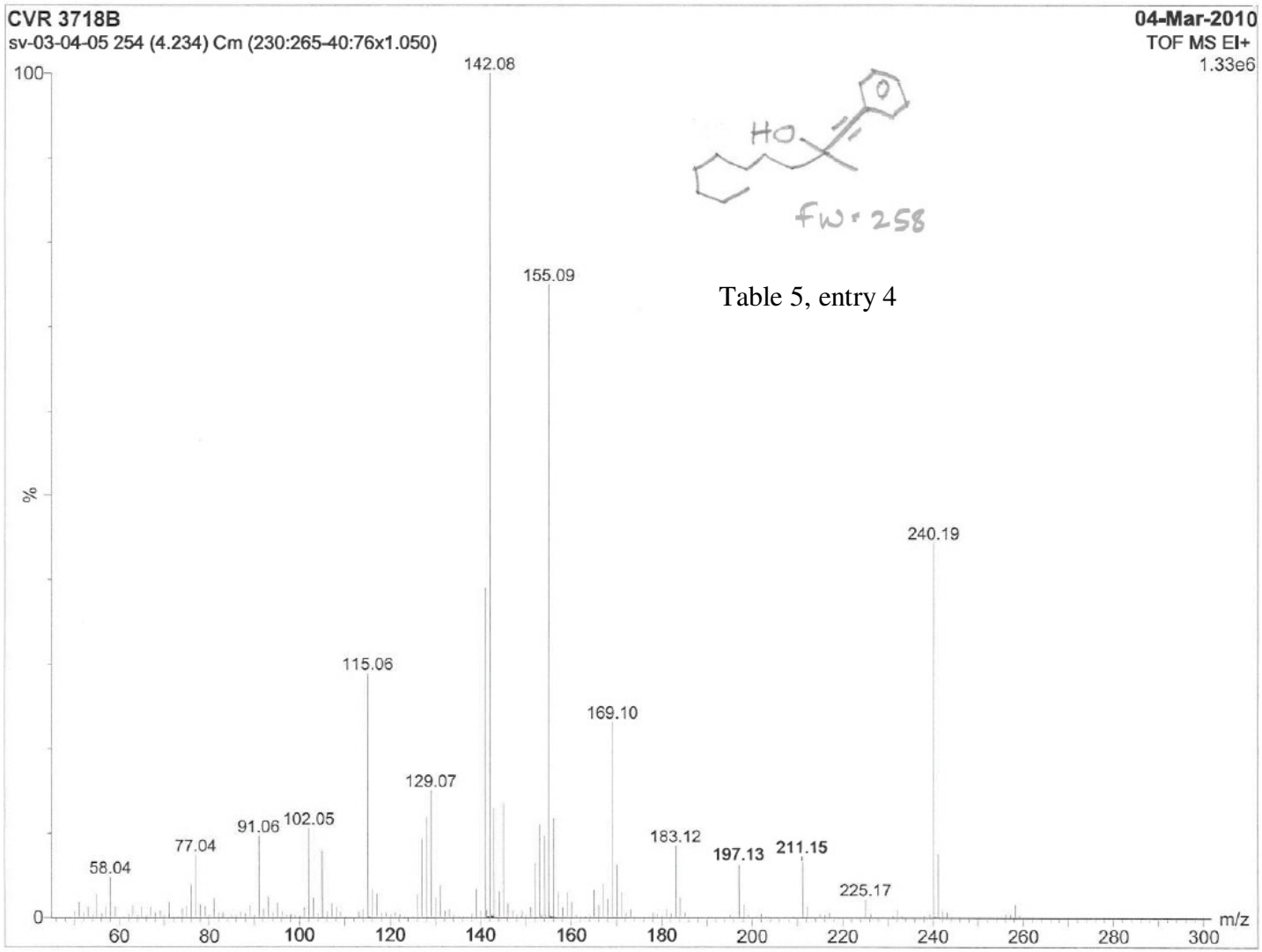


Table 5, entry 4

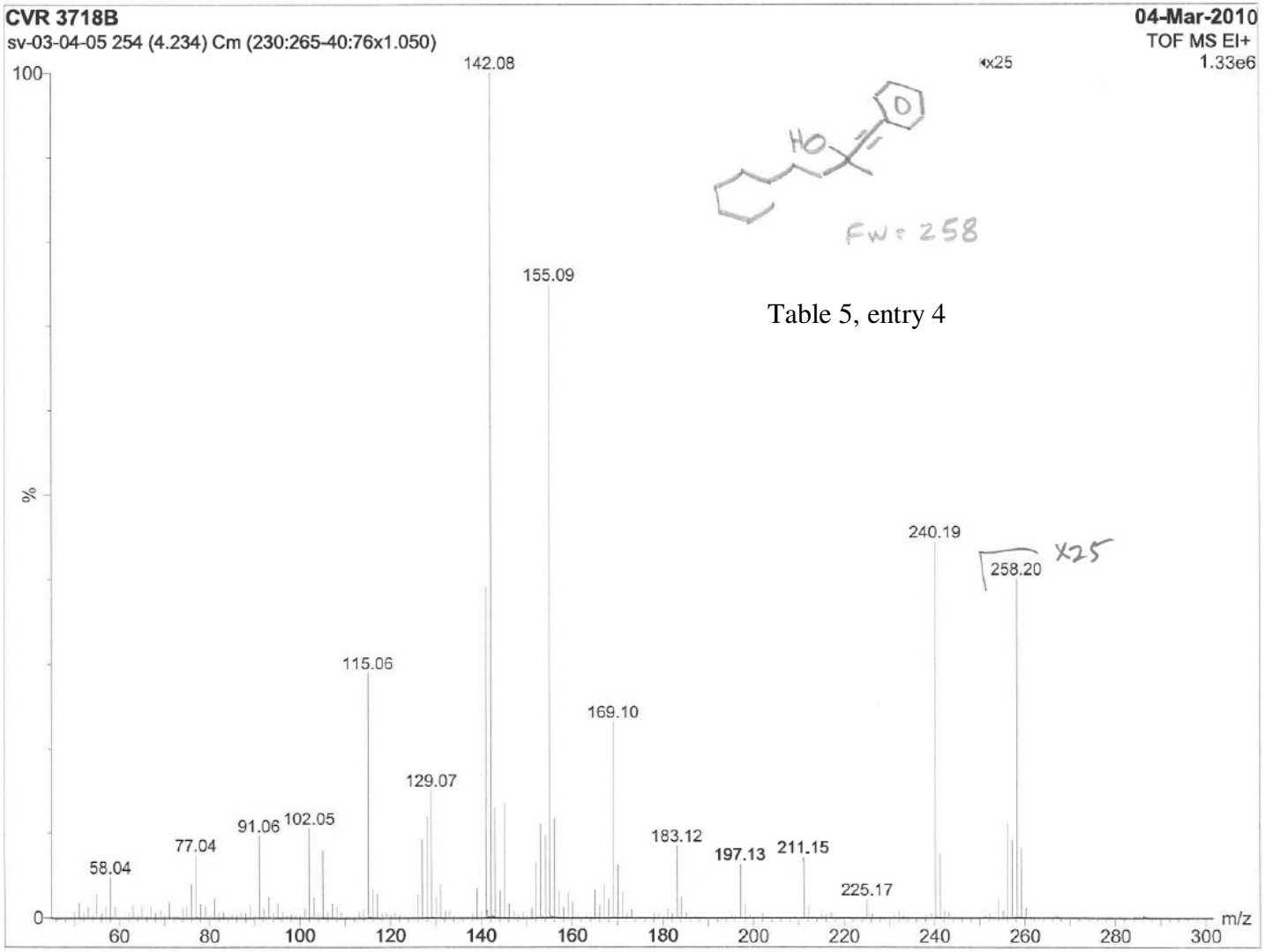


Table 5, entry 4

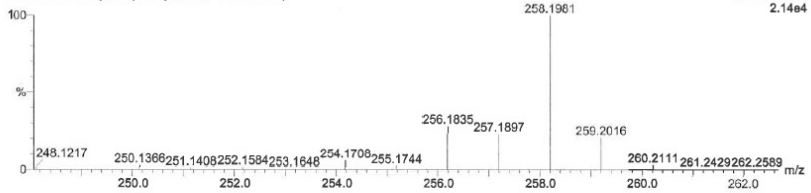
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
41 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

CVR 3718B
sv-03-04-05 254 (4.234) Cm (230:265-40:76x1.050)

04-Mar-2010
TOF MS EI+
2.14e4



Minimum:				-1.5		
Maximum:		5.0	3.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
258.1981	258.1984	-0.3	-1.0	6.0	1	C18 H26 O

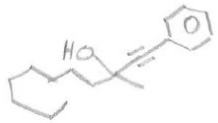


Table 5, entry 4