SUPPORTING INFORMATION

Propargylic and Allenic Carbocycle Synthesis through Palladium-Catalyzed Dearomatization Reaction

Bo Peng,[†] Xiujuan Feng,[†] Xin Zhang,[‡] Sheng Zhang,[†] and Ming Bao*,[†]

[†]*State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116012, China*

[‡]*School Environmental Science &Technology, Dalian University of Technology, Dalian 116023, China*

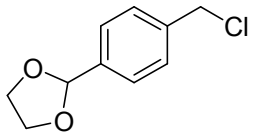
xiujuan.feng@163.com (X. J. Feng), mingbao@dlut.edu.cn (M. Bao).

Table of Contents

General. All experiments were carried out under standard Schlenk techniques. Solvents were dried and degassed before use by standard procedures. The starting materials **1a**, **1b**, **1c**, **1d**, **1e**, **1f** and **1q** are commercially available. Compounds **1g**,[1] **1i**,[2] **1l**,[3] and **3a-d**[4] have appeared in the literatures.

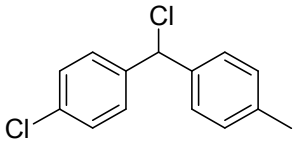
Preparation and spectral data of benzylic chlorides

2-(4-(Chloromethyl)phenyl)-1,3-dioxolane (1h).



To a solution of PPh_3 (288.2 mg, 1.1 mmol) in CCl_4 (3 mL) at room temperature was added 4-(1,3-dioxolan-2-yl)benzyl alcohol (180.2 mg, 1.0 mmol). After the mixture was stirred at 50 ºC for 30 minutes, the solvent was removed under a reduced pressure, and the residue was purified with basic alumina column to give **1h** as colorless oil in 95% yield (188.1 mg). It is worth noting that the deprotection reaction of the acetal moiety could readily take place when NCS/PPh_3 or PCl_3/CH_2Cl_2 was employed as a chlorination reagent. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 8.0 Hz, 2H), 7.38 (d, J = 8.4 Hz, 2H), 5.79 (s, 1H), 4.56 (s, 2H), 4.08 (t, J = 3.6 Hz, 2H), 4.01 (t, J = 3.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.5, 138.4, 128.7, 126.9, 103.4, 65.4, 45.9; IR (neat) 2886, 1721, 1389, 1267, 1083, 743, 679 cm^{-1}; HRMS (EI) calcd for $C_{10}H_{10}O_2Cl$: 197.0369 $[M-H]^+$; found: 197.0375.

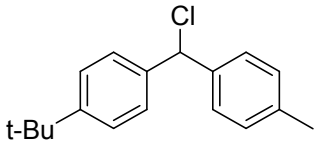
4-Chloro-4'-methyl-benzhydryl chloride (1j).



To a solution of 4-chloro-4'-methylbenzhydrol (232.3 mg, 1.0 mmol) in dichloromethane (3.0 mL) at 0 ºC was added $SOCl_2$ (2.0 equiv). After the temperature was enhanced to room temperature slowly and stirred for 8 h, the solvent and excess $SOCl_2$ were removed under reduced pressure, and the residue obtained was dissolved in dichloromethane (10 mL). The solution was washed with dilute aqueous bicarbonate and dried over magnesium sulfate. Then the solvent was removed under reduced pressure to give pure product **1j** as a brown solid in 98% yield (245.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J

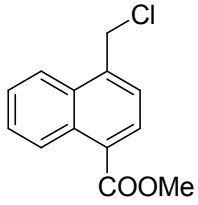
= 8.8 Hz, 2H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.06 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 138.2, 137.7, 133.8, 129.3, 129.1, 128.6, 127.6, 64.4, 21.1; IR (neat) 1904, 1594, 1488, 1089, 1014, 799, 763, 741 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{12}Cl_2$: 250.0316 $[M]^+$; found: 250.0310.

4-Methyl-4'-*tert*-butyl-benzhydryl chloride (1k).



Compound **1k** was prepared according to the procedure for the synthesis of **1j**. Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 6H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.08 (s, 1H), 2.31 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 138.51, 138.46, 137.9, 129.3, 127.8, 127.6, 125.6, 64.4, 34.7, 31.5, 21.3; IR (neat) 2962, 1907, 1511, 1409, 1363, 1108, 768, 578 cm^{-1}; HRMS (EI) calcd for $C_{18}H_{21}Cl$: 272.1332 $[M]^+$; found: 272.1338.

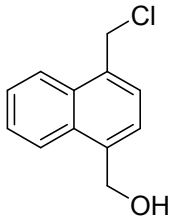
Methyl 4-(chloromethyl)-1-naphthoate (1m).



To a mixture of methyl 4-hydroxymethyl-1-naphthoate (216.2 mg, 1.0 mmol) and *N*-chlorosuccinimide (NCS, 145.6 mg, 1.1 mmol) in dichloromethane (50 mL) at -20 ºC was added a solution of PPh_3 (288.0 mg, 1.1 mmol) in dichloromethane (15 mL) through a drop funnel slowly. After the mixture was stirred at -20 ºC for 10 minutes, the reaction temperature was allowed to enhance to room temperature slowly. And then the solvent was removed under reduced pressure, and the residue was purified by silica gel column chromatography (eluent: hexane/ethyl acetate = 10/1) to give **1m** as a colorless oil in 85% yield (199.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94-8.91 (m, 1H), 8.17-8.15(m, 1H), 8.08 (d, *J* = 7.2 Hz, 1H), 7.64-7.62 (m, 2H), 7.53 (d, *J* = 7.2 Hz, 1H), 5.02 (s, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 137.8, 131.6, 131.3, 129.3, 128.6, 127.7, 126.9, 126.6, 126.2, 123.9, 52.3, 43.9; IR

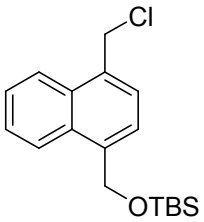
(neat) 2950, 1716, 1592, 1285, 1127, 1012, 809, 717 cm^{-1}. HRMS (EI) calcd for $C_{13}H_{11}O_2Cl$: 234.0448 $[M]^+$; found: 234.0454.

(4-(Chloromethyl)naphthalen-1-yl)methanol (1n).



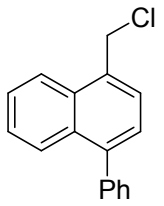
Compound **1n** was prepared according to the procedure for the synthesis of **1m**. Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.0 Hz, 1H), 8.15 (d, J = 8.0 Hz, 1H), 7.64-7.57 (m, 2H), 7.49(d, J = 1.6 Hz, 1H), 7.47 (d, J = 1.8 Hz, 1H), 5.14 (d, J = 3.6 Hz, 2H), 5.04 (s, 2H), 1.78 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.0, 133.4, 131.6, 131.4, 127.3, 126.7, 126.6, 124.5, 124.46, 124.41, 63.5, 44.6; IR (neat) 3272, 3175, 2902, 1452, 1345, 1256, 1162, 1071, 835, 690 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{11}OCl$: 206.0498 $[M]^+$; found: 206.0504.

***tert*-Butyl((4-(chloromethyl)naphthalen-1-yl)methoxy)-dimethylsilane (1o).**



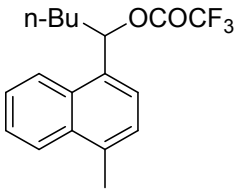
Compound **1o** was prepared according to the procedure for the synthesis of **1m**. Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8 Hz, 1H), 8.05 (d, J = 8 Hz, 1H), 7.60-7.52 (m, 4H), 5.24 (s, 2H), 5.06 (s, 2H), 1.02 (s, 9H), 0.18 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.7, 132.4, 131.3, 131.2, 127.6, 126.5, 126.2, 124.5, 124.1, 123.2, 63.3, 44.9, 26.1, 18.6, -5.1; IR (neat) 2954, 2855, 1517, 1470, 1256, 1114, 837, 778, 754 cm^{-1}. HRMS (EI) calcd for $C_{11}H_{12}$: $C_{18}H_{25}OSiCl$: 320.1363 $[M]^+$; found: 320.1355.

1-(Chloromethyl)-4-phenylnaphthalene (1p).



Compound **1p** was prepared according to the procedure for the synthesis of **1m**. Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.62-7.58 (m, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.50-7.41 (m, 6H), 7.36 (d, J = 7.2 Hz, 1H), 5.08 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$,): δ 142.0, 140.3, 132.4, 132.2, 131.3, 130.0, 128.3, 127.4, 127.2, 127.1, 126.5, 126.3, 126.2, 123.8, 44.7; IR (neat) 3056, 1583, 1514, 1392, 1257, 1030, 938, 844, 768, 728, 703 cm^{-1}; HRMS (EI) calcd for $C_{17}H_{13}Cl$: 252.0706 $[M]^+$; found: 252.0711.

1-(4-Methylnaphthalen-1-yl)pentyl 2,2,2-trifluoroacetate (1r).



To a solution of 1-(4-methylnaphthalen-1-yl)pentan-1-ol (228.3 mg, 1.0 mmol) in dichloromethane (3.0 mL) at -20 ºC was added trifluoroacetic anhydride (231.5 mg, 1.1 mmol). Then the reaction temperature was allowed to enhance to room temperature slowly. And then the solvent was removed under reduced pressure, and the residue was purified by silica gel column chromatography (eluent: hexane/ethyl acetate = 10/1) to give **1r** as a colorless oil in 71% yield (230.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.04 (m, 2H), 7.59-7.54 (m, 2H), 7.44 (d, J = 3.6 Hz, 1H), 7.32 (d, J = 7.2 Hz, 1H), 6.63 (dd, J = 4.0, 2.8 Hz, 1H), 2.69 (s, 3H), 2.19-2.08 (m, 2H), 1.43-1.30 (m, 4H), 0.88 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 156.8, 135.6, 132.9, 132.5, 130.2, 126.3, 126.1, 125.8, 125.2, 123.9, 123.2, 116.1, 113.3, 78.4, 35.6, 27.8, 22.3, 19.7, 13.8; IR (neat) 2933, 2864, 1784, 1458, 1380, 1221, 1160, 832, 777, 755 cm^{-1} HRMS (EI) calcd for $C_{18}H_{19}O_2F_3$: 324.1337 $[M]^+$; found: 324.1327.

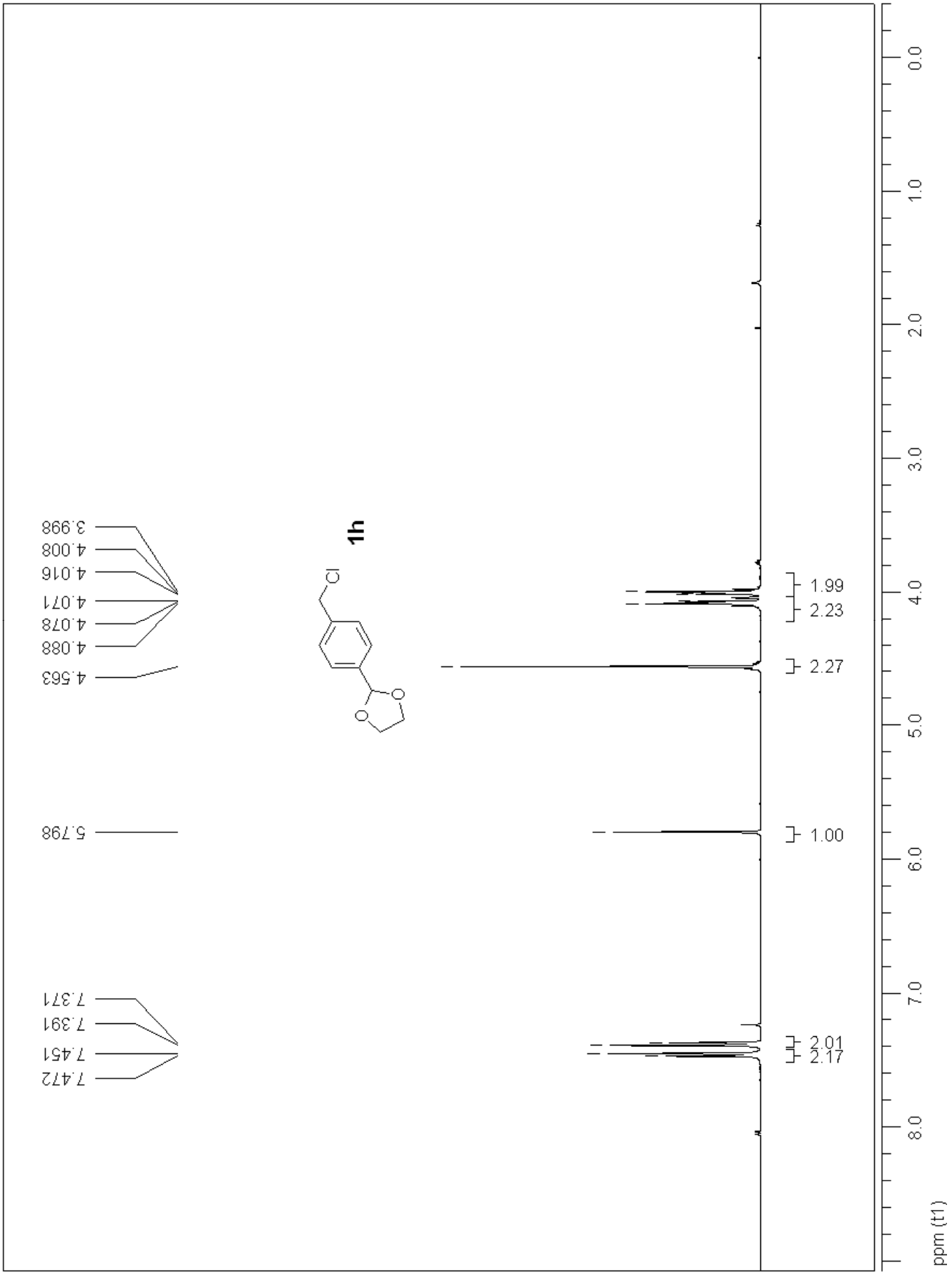
References:

(1) Roberto, F.; Kamil, M.; Andres, J. *J. Am. Chem. Soc.* **2005**, *127*, 9271–9276.

(2) Royals, E. E.; Prasad, R. N. *J. Am. Chem. Soc.* **1955**, *77*, 1696–1697.

(3) Staley, S. W.; Dustman, C. K. *J. Am. Chem. Soc.* **1981**, *103*, 4297–4302.

(4) Lu, S.; Xu, Z.; Bao, M.; Yamamoto, Y. *Angew. Chem. Int. Ed.* 2008, *47*, 4366–4369.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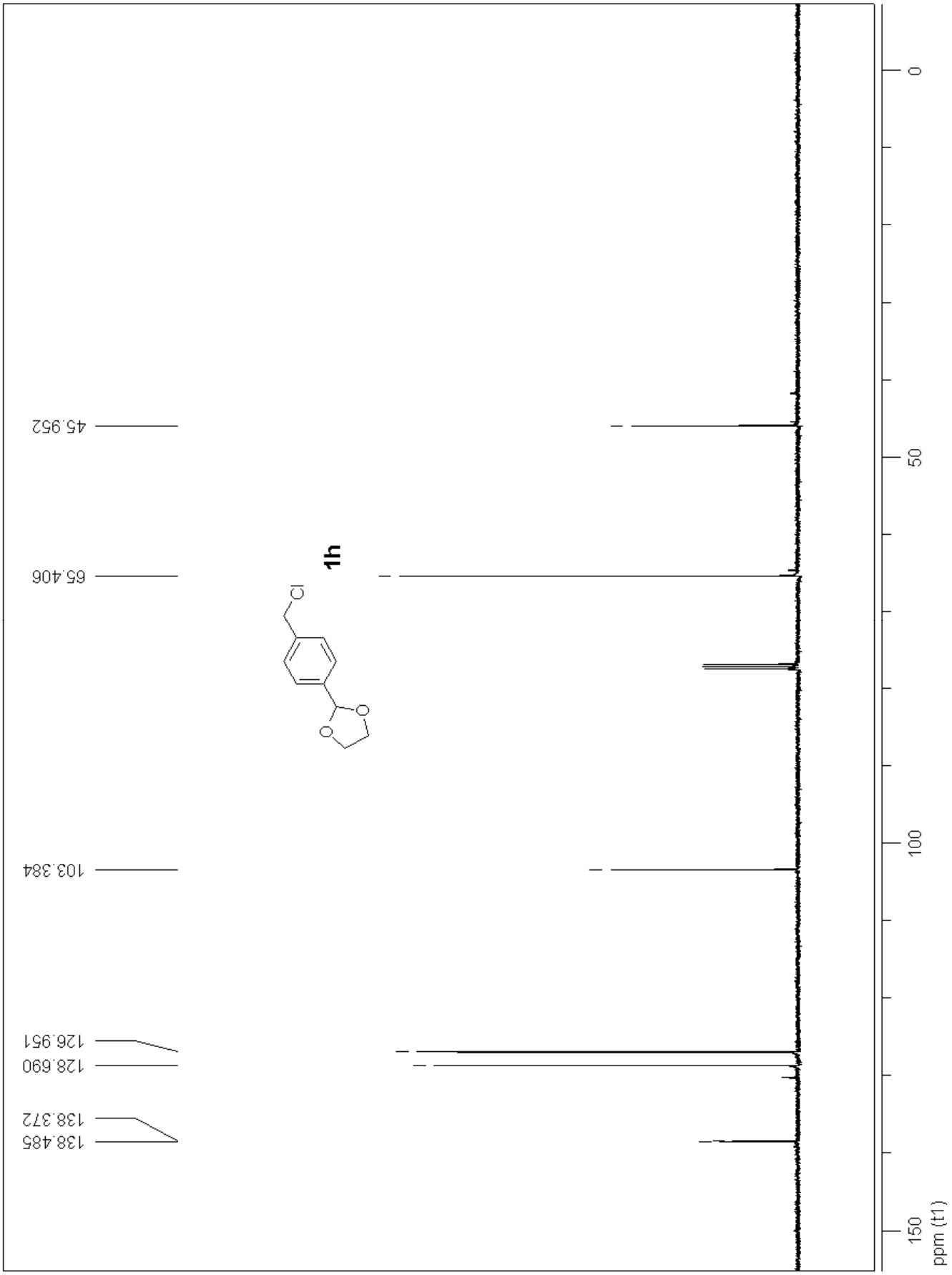
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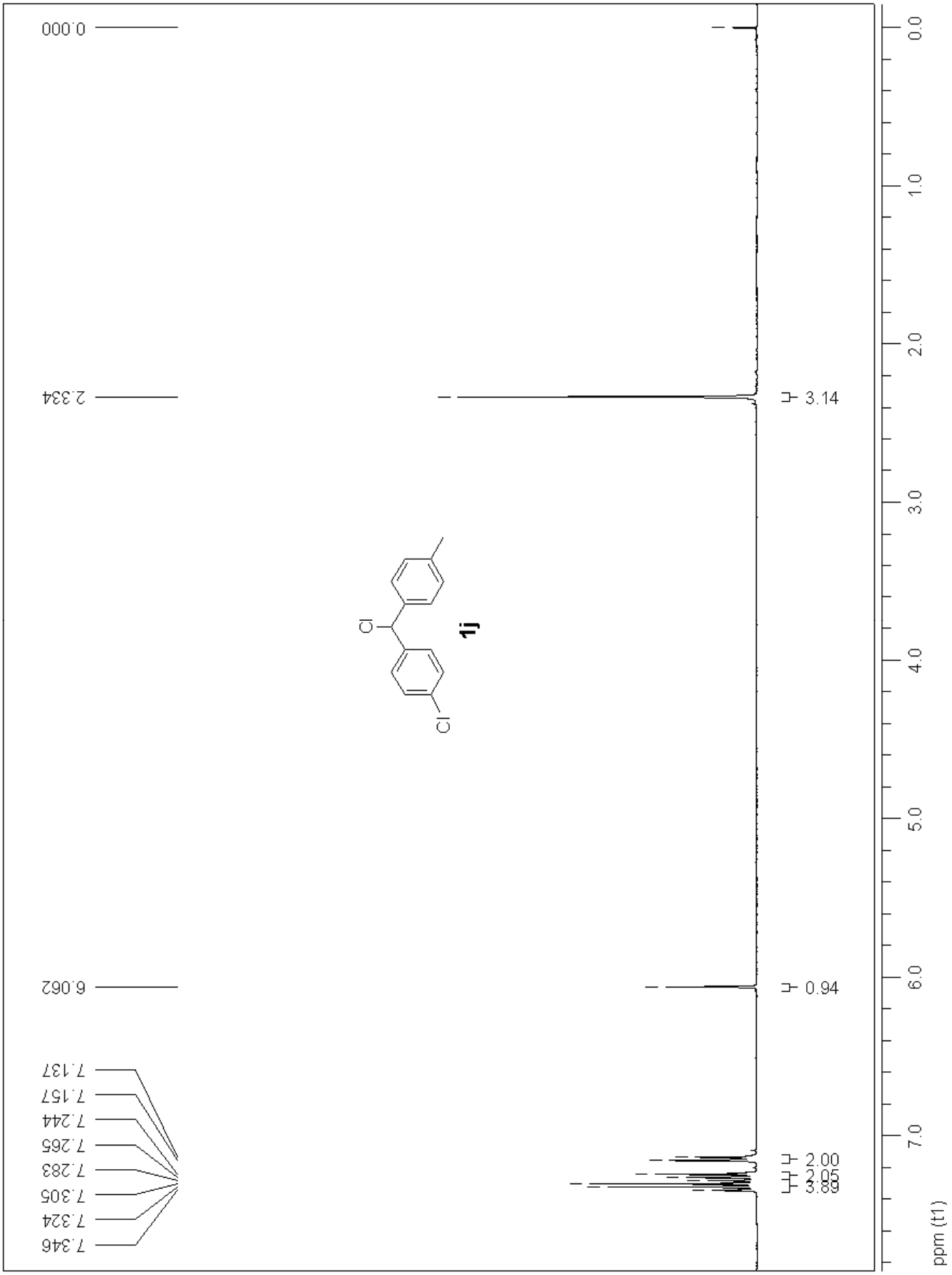
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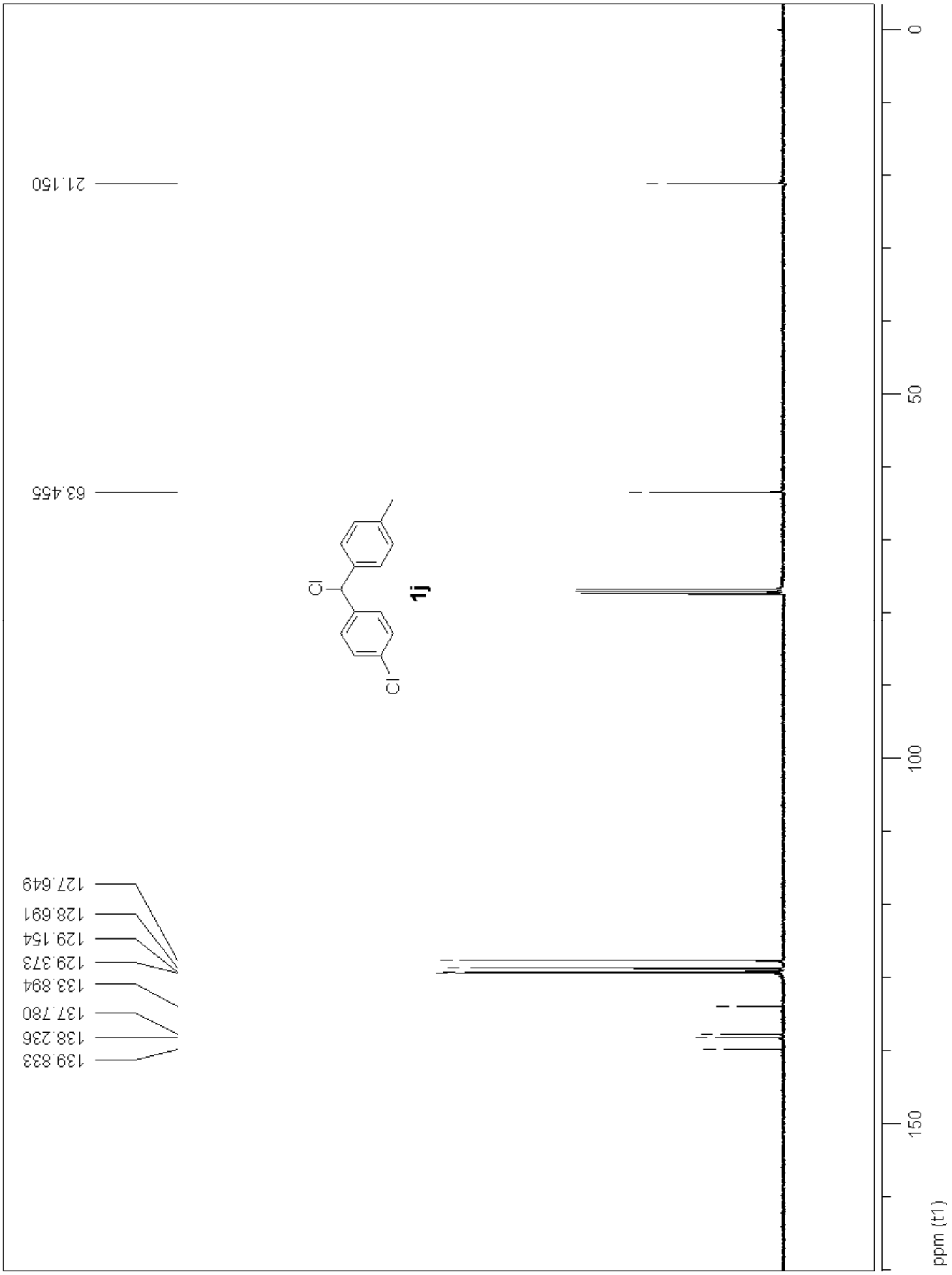
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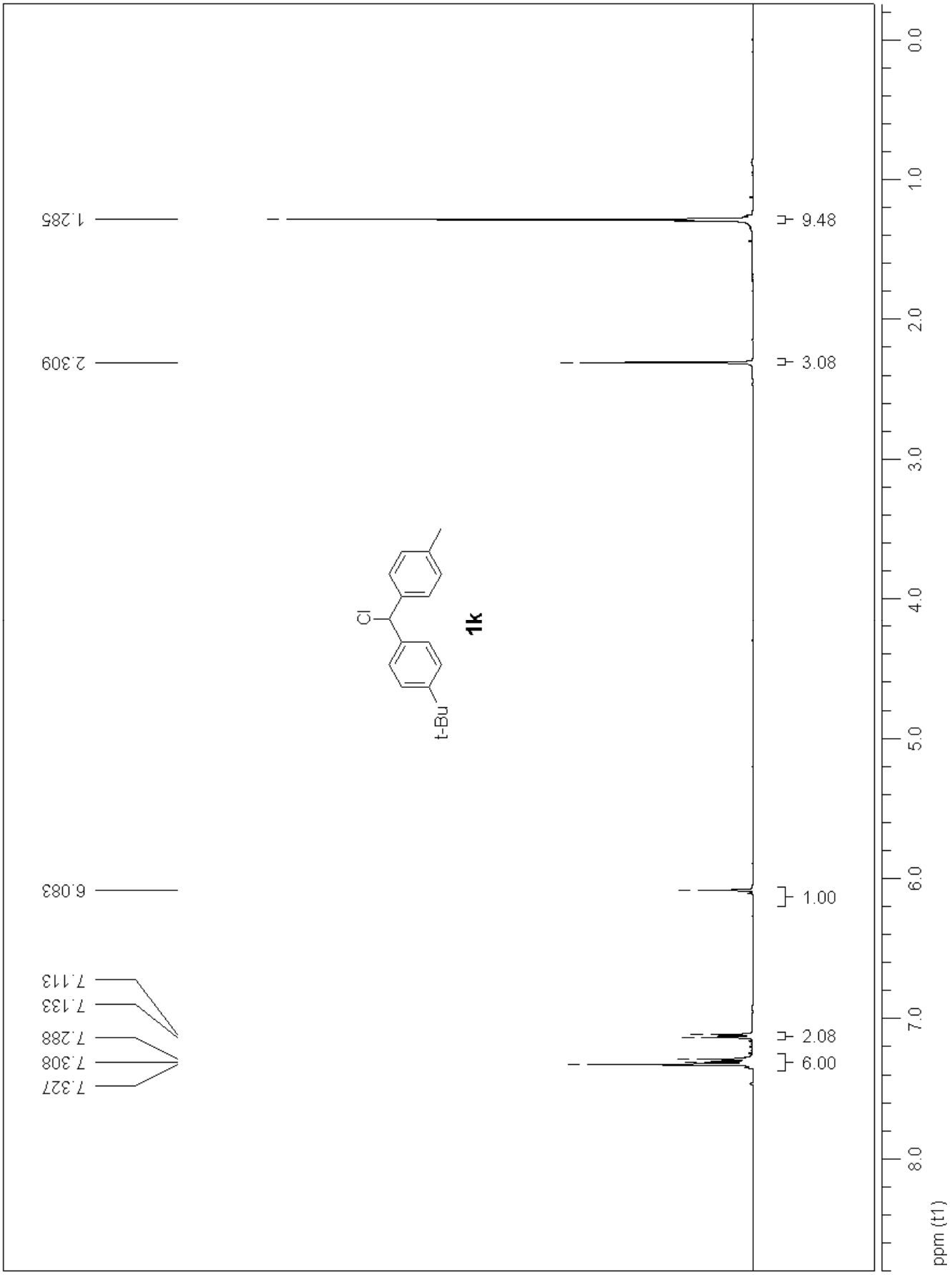
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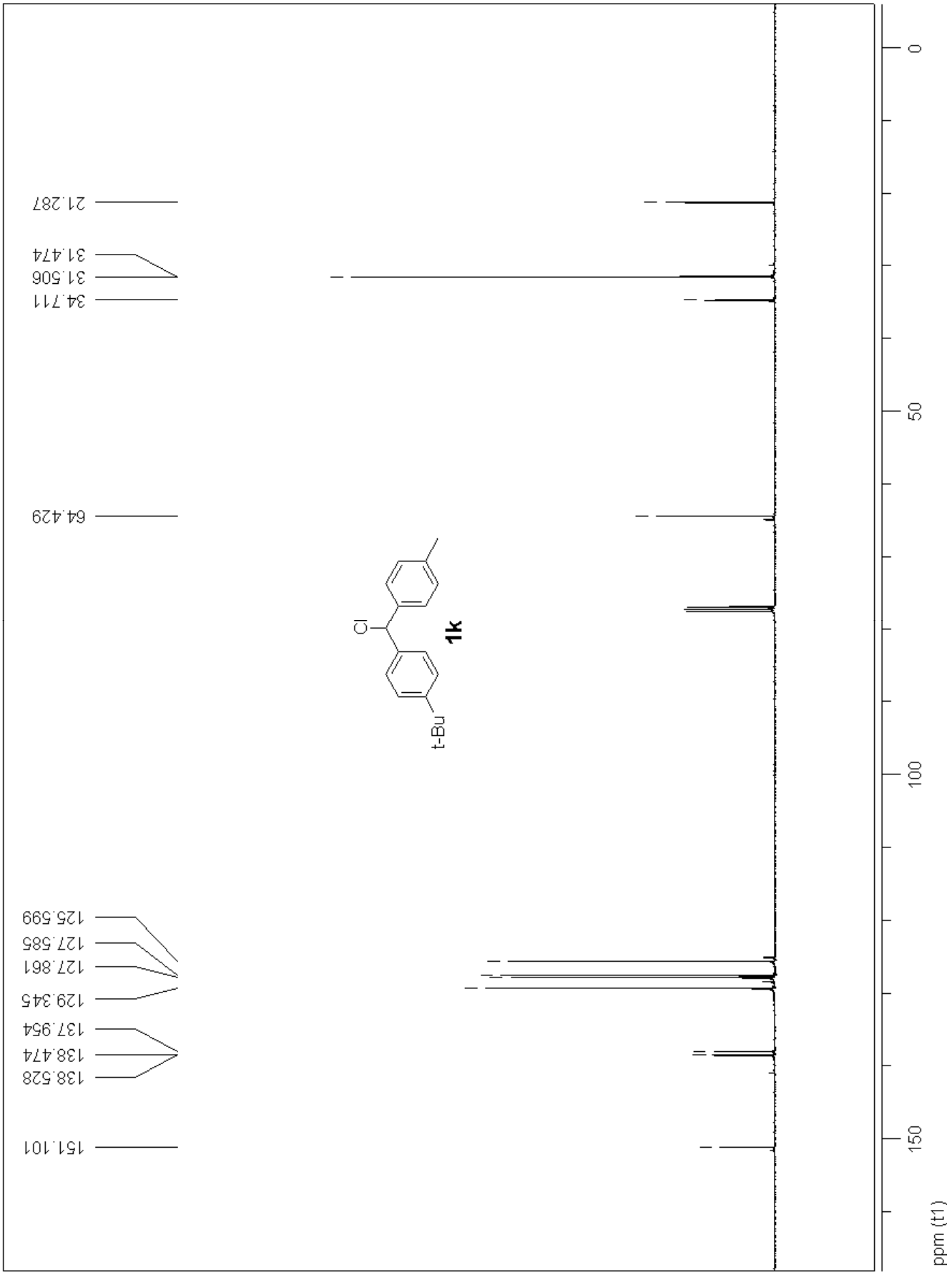
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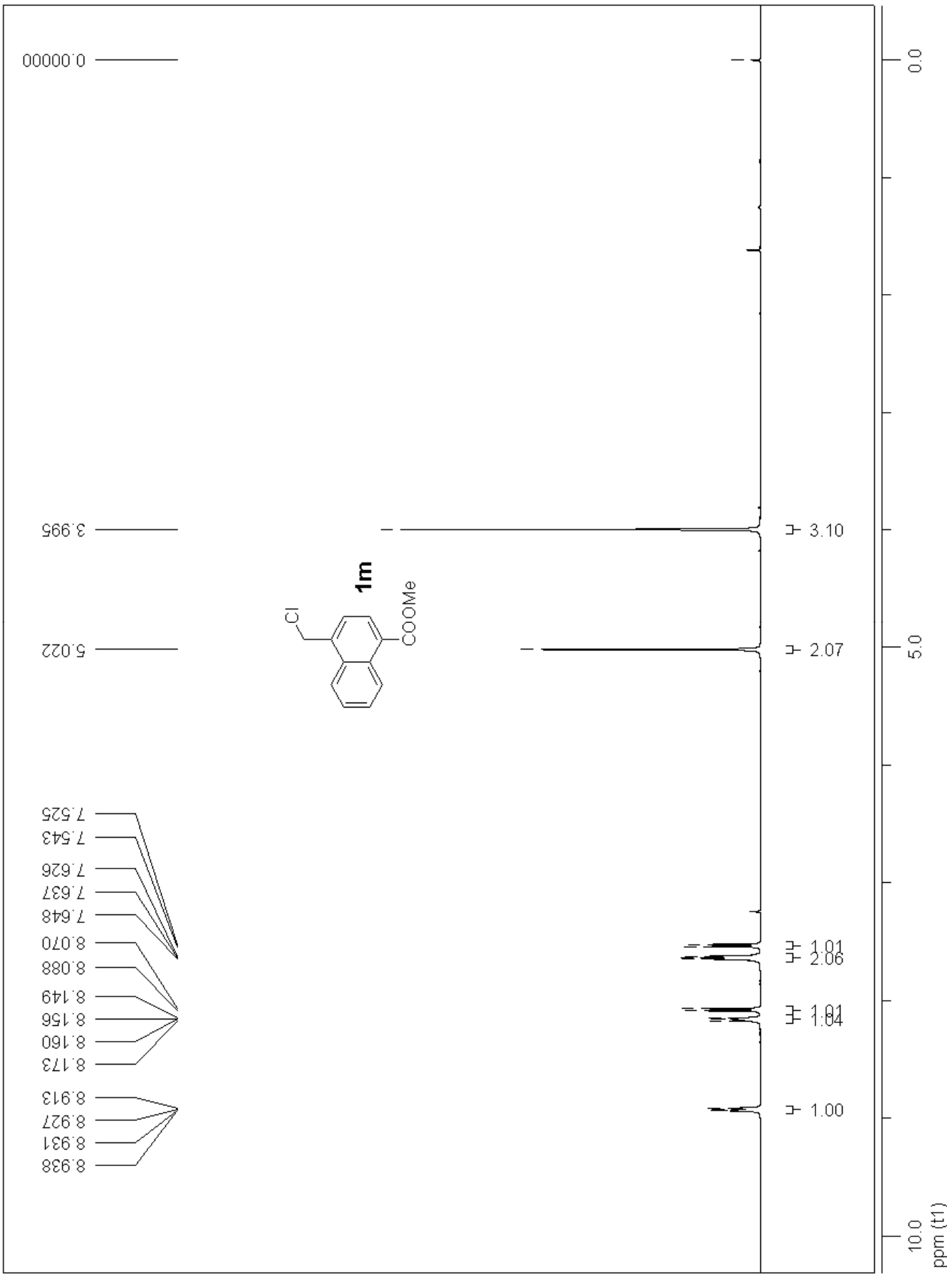
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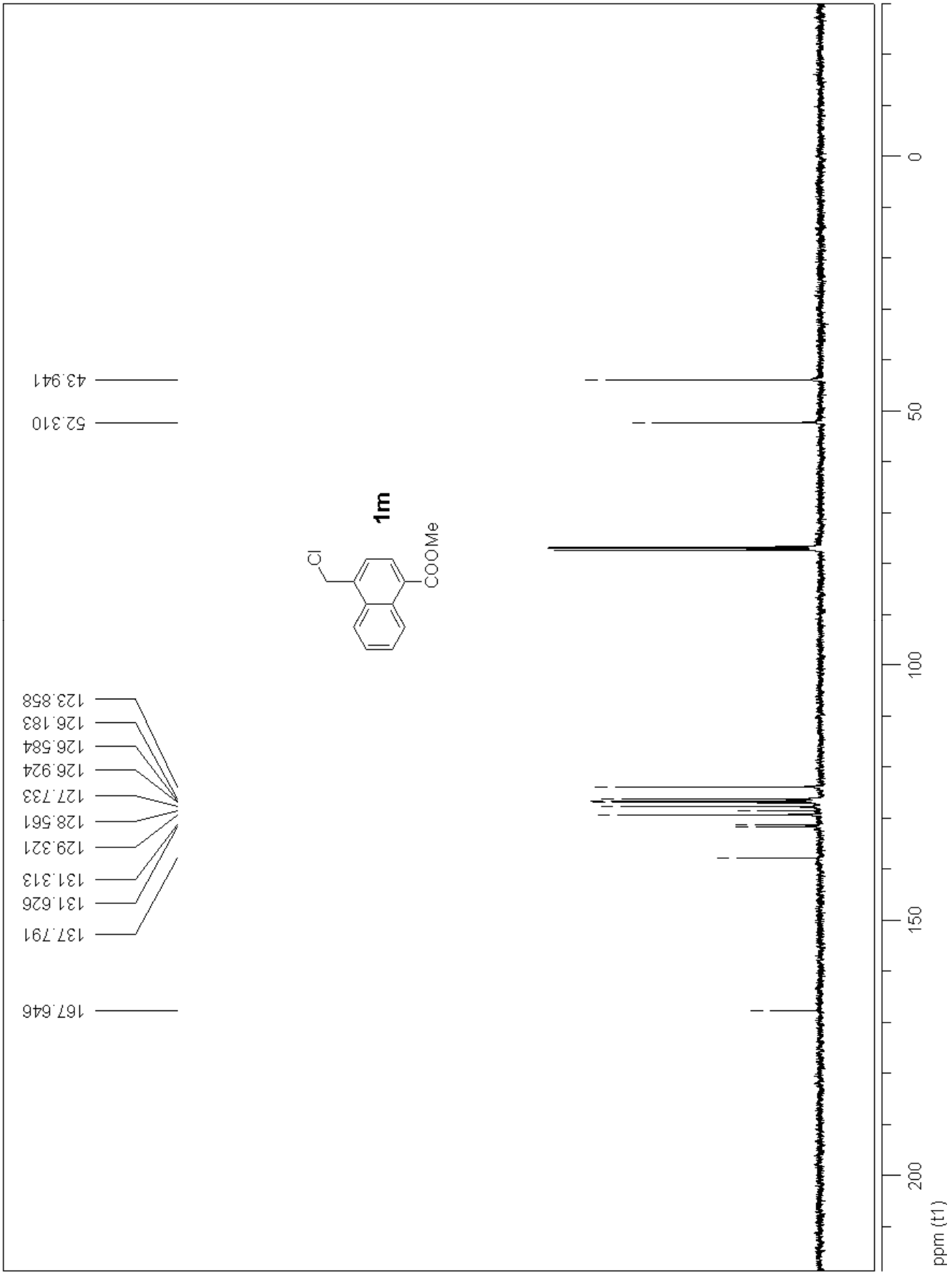
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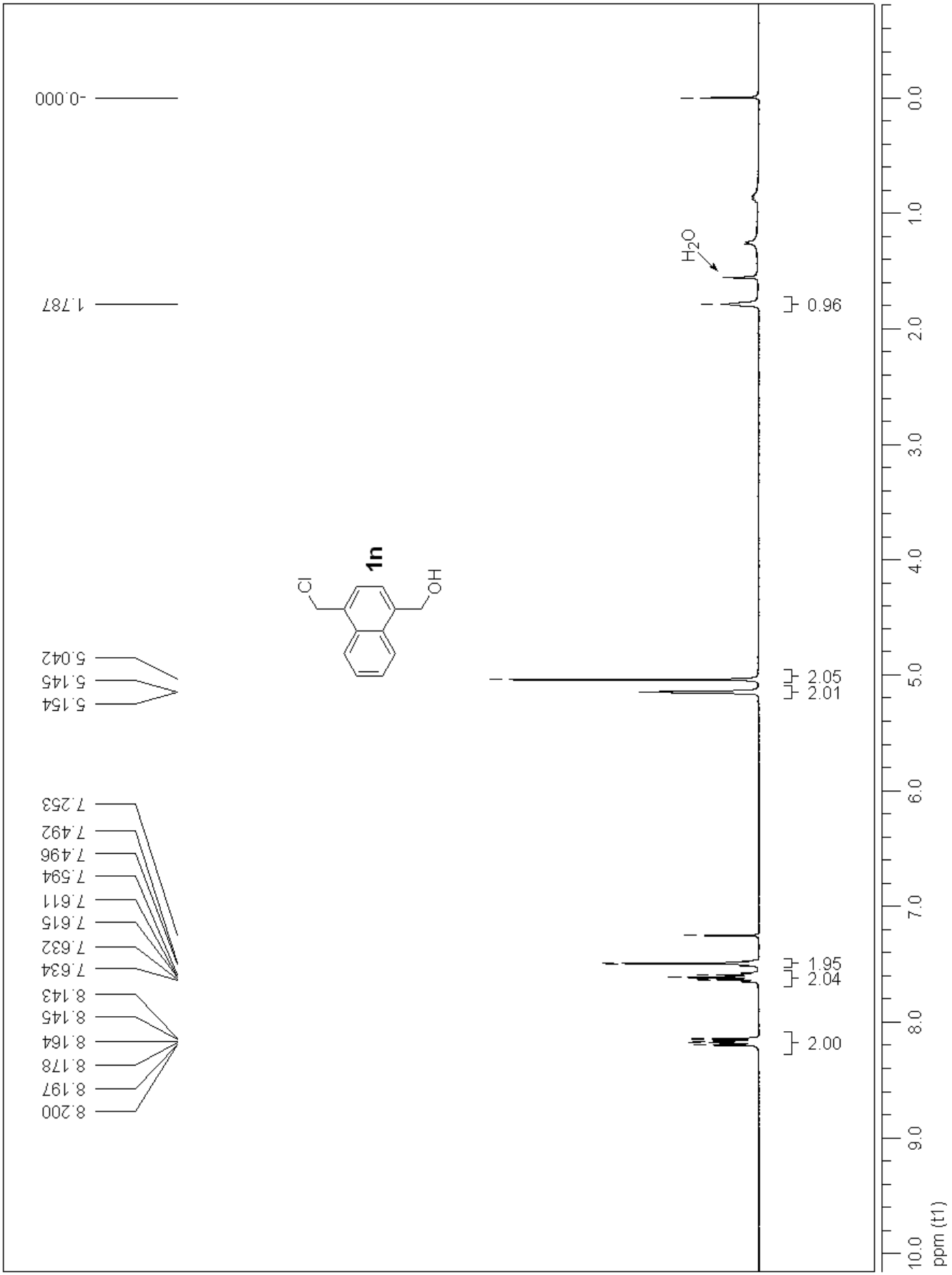
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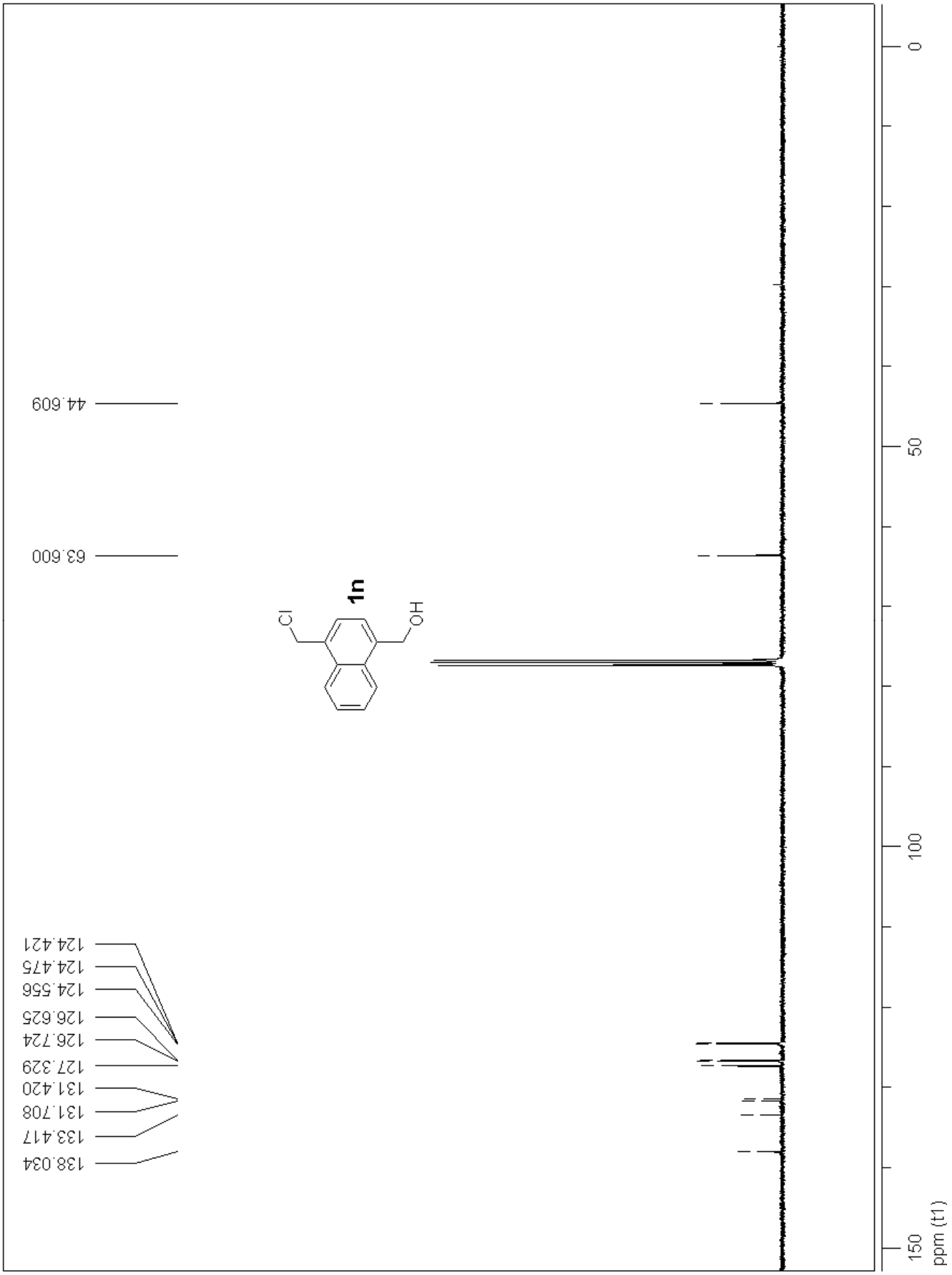
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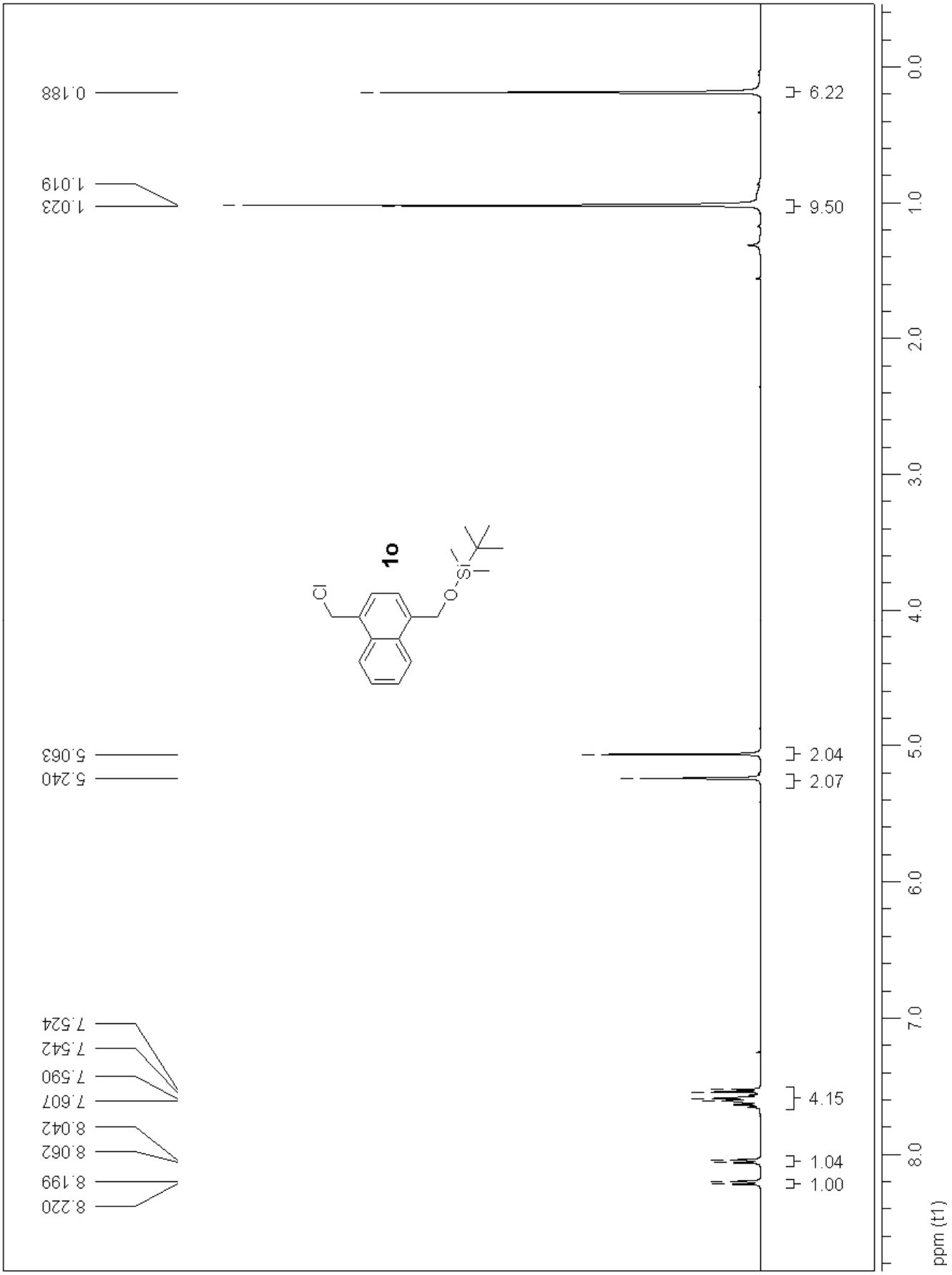
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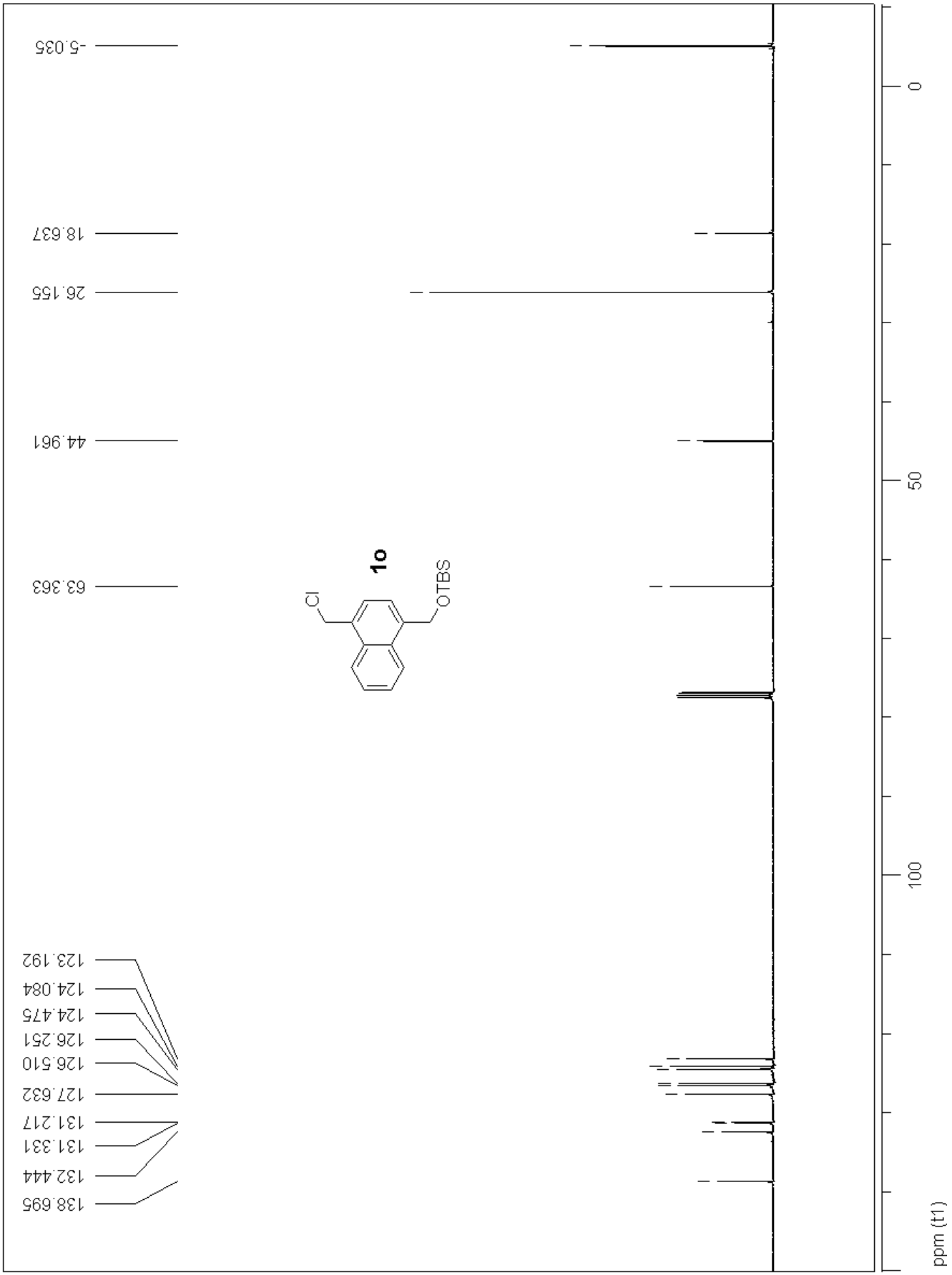
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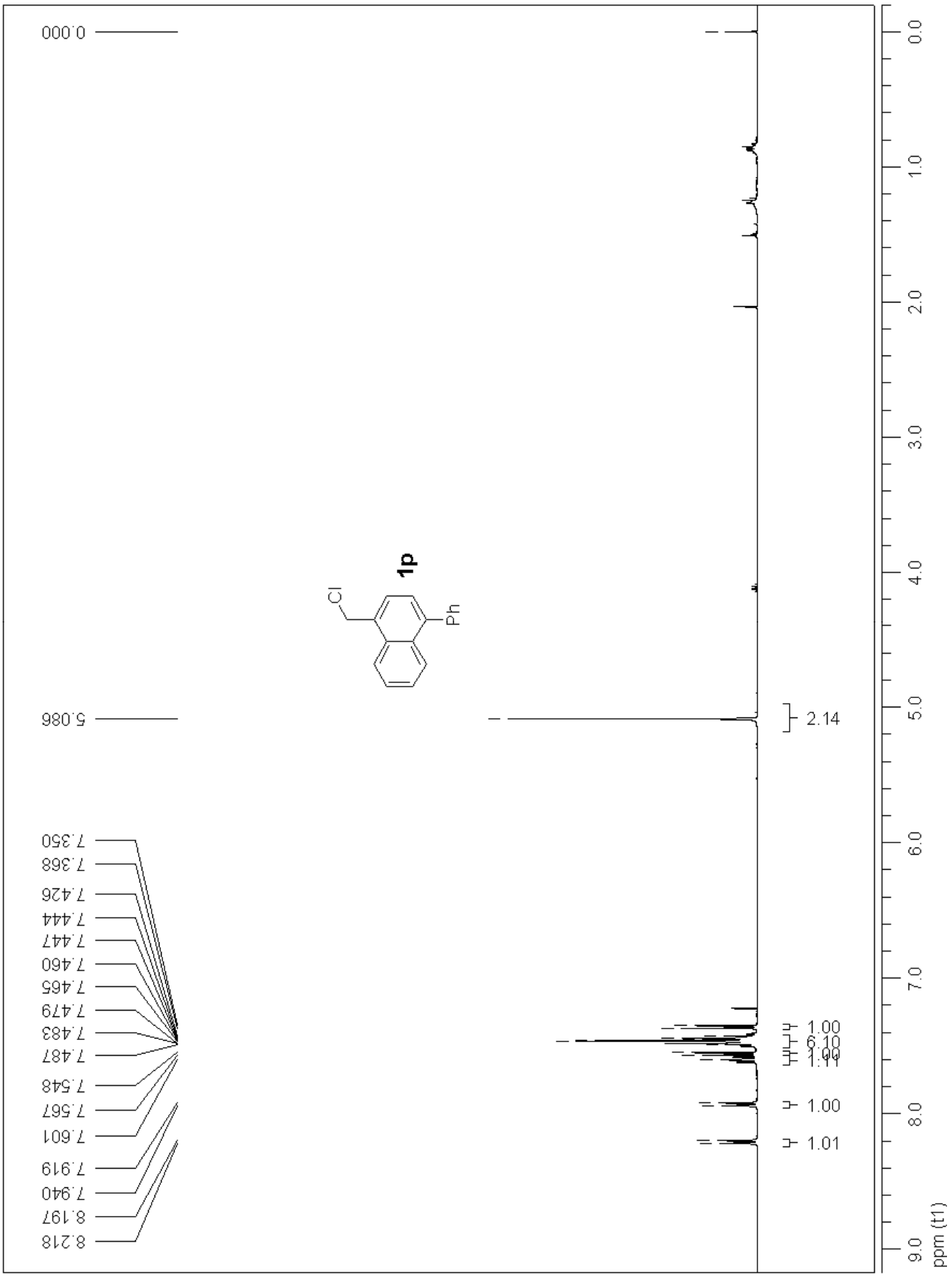
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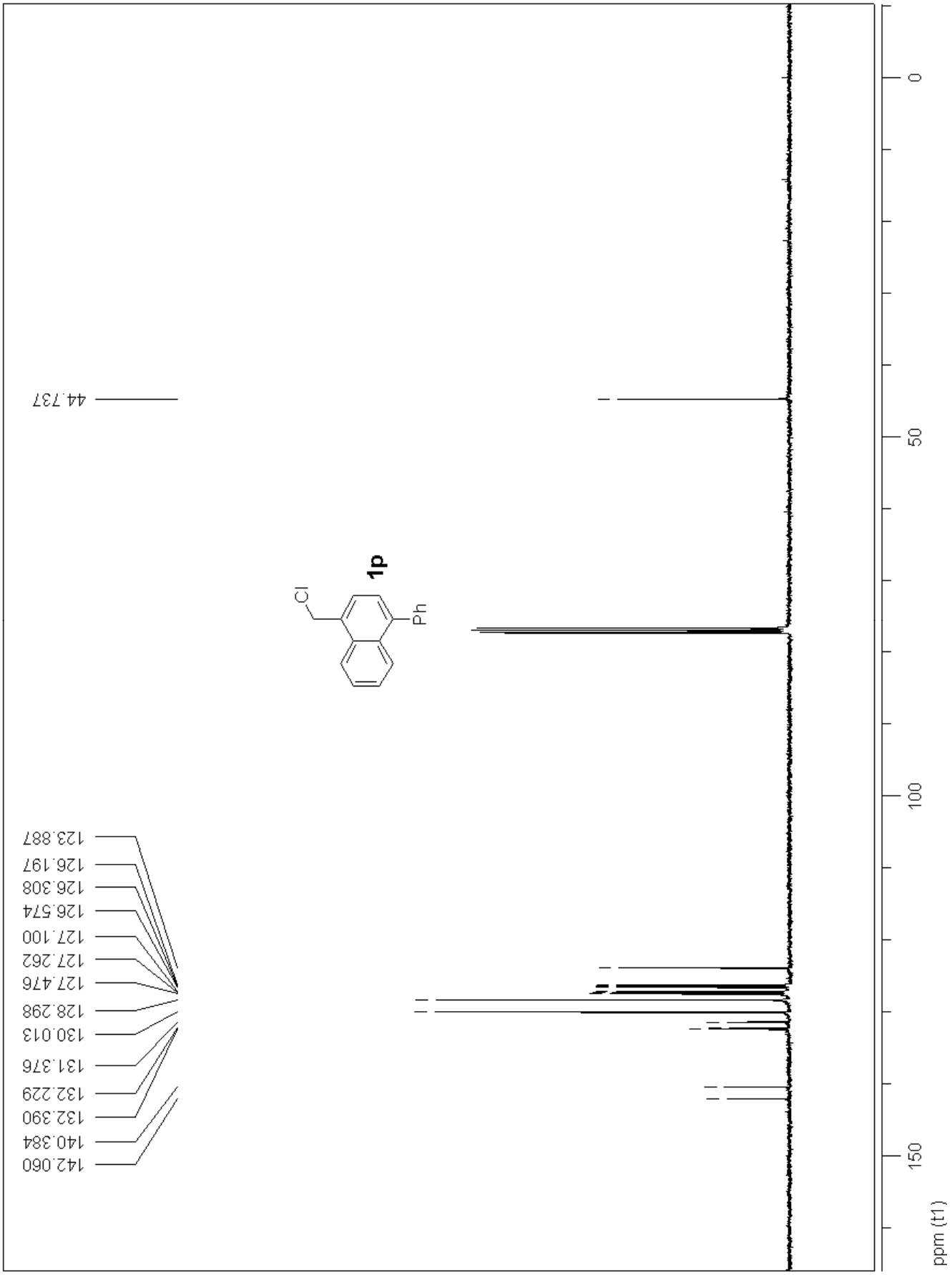
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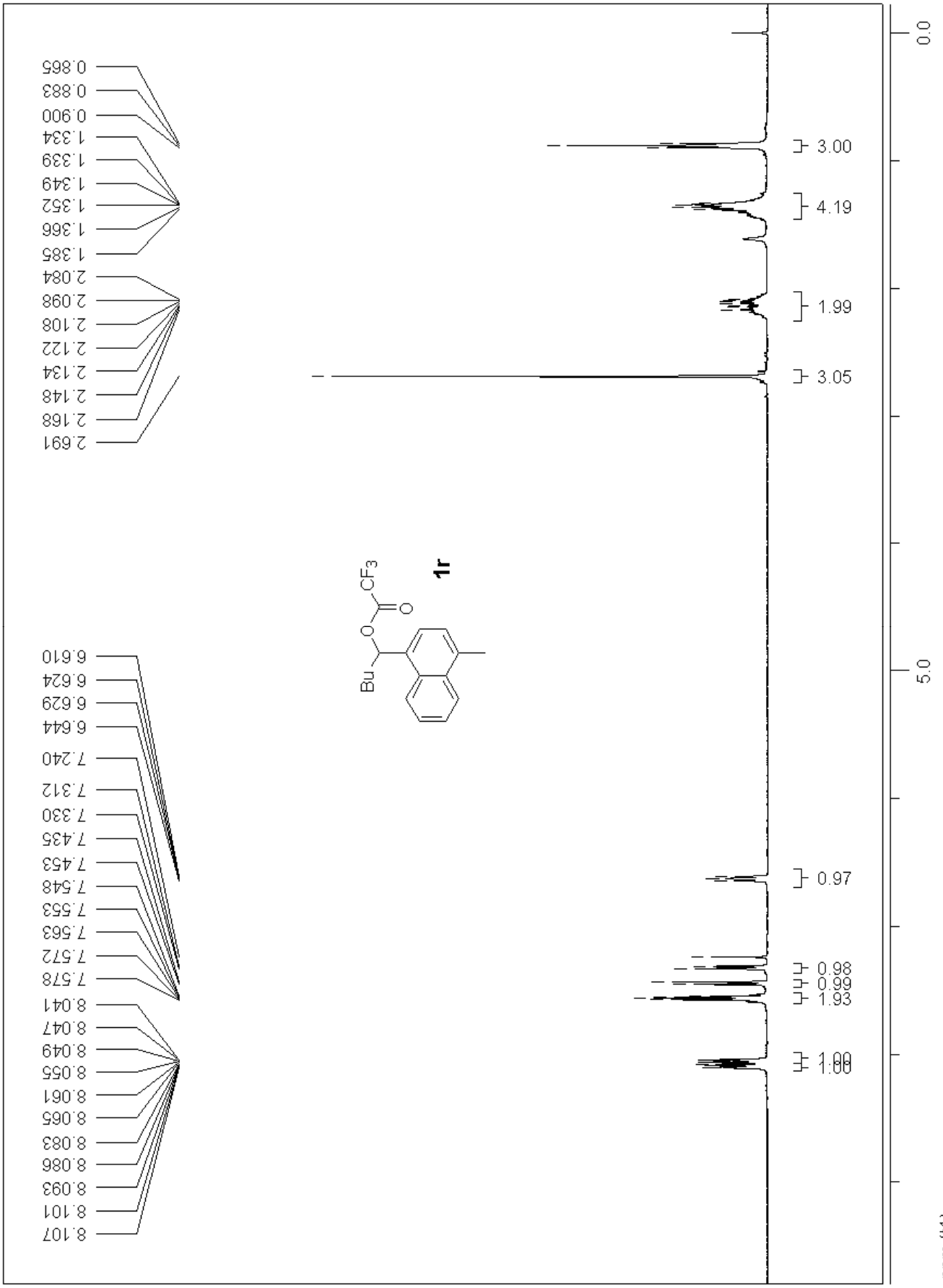
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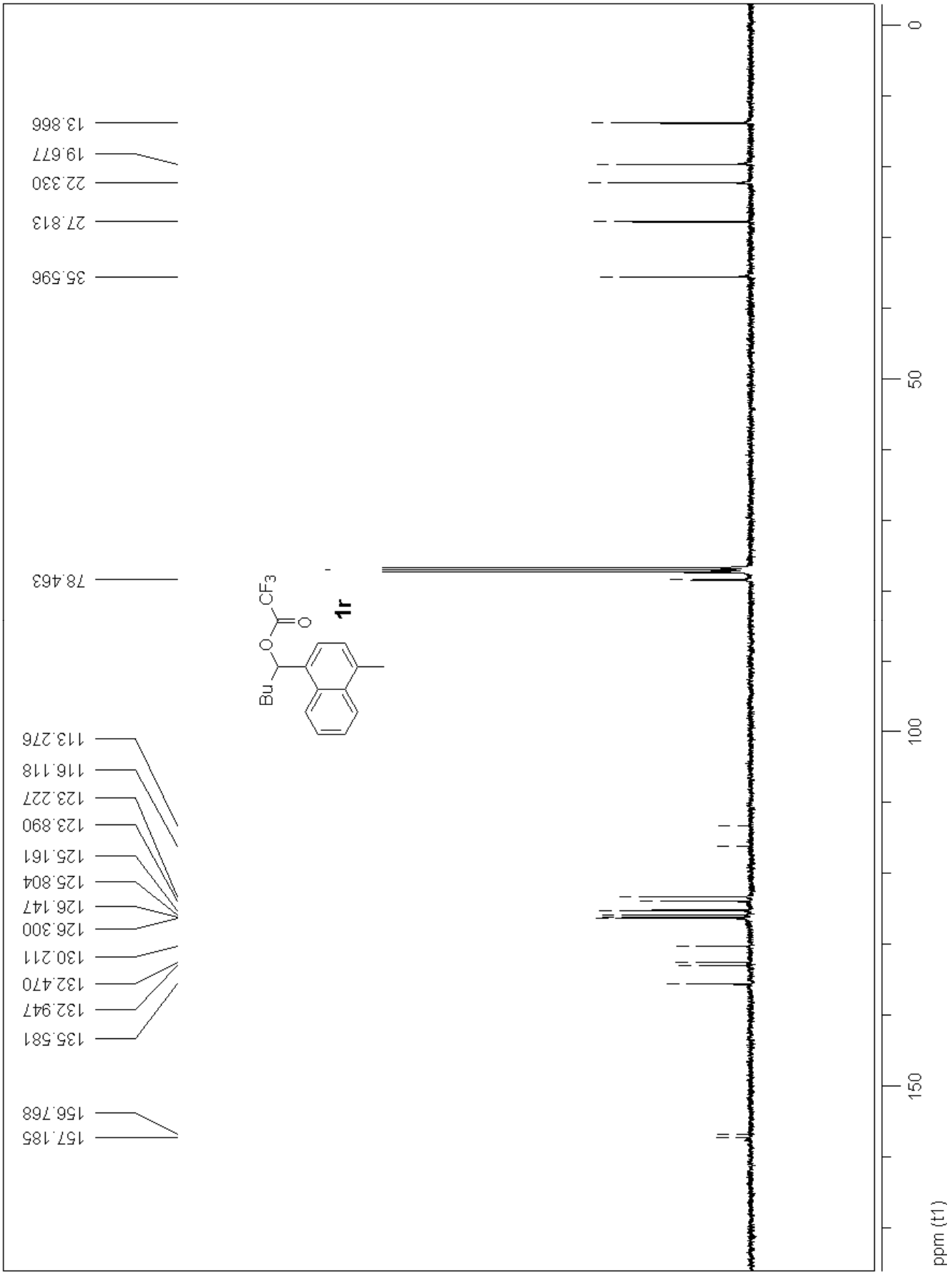
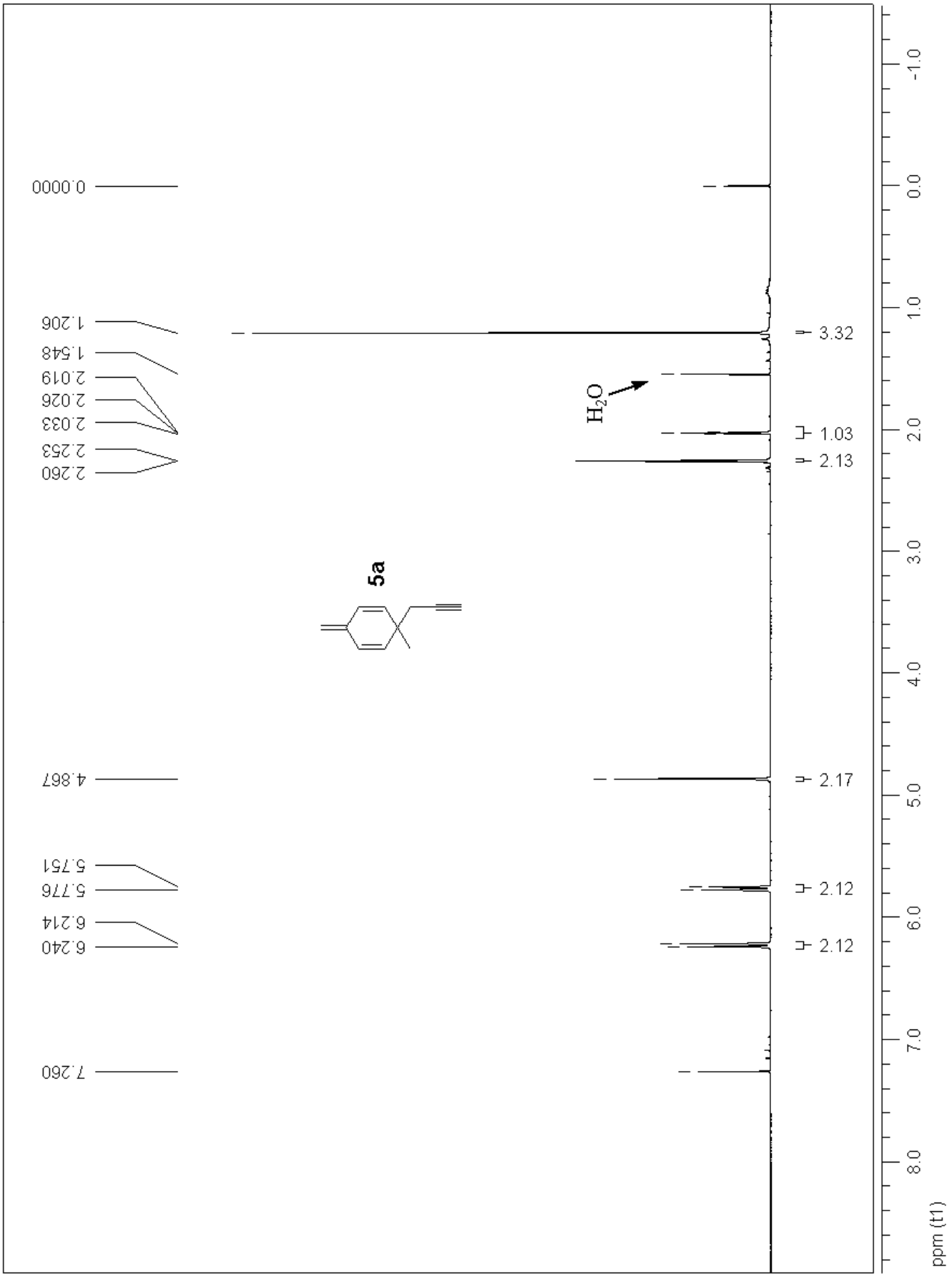
1.339
1.349
1.352
1.366
1.385
2.084
2.098
2.108
2.122
2.134
2.148
2.168
2.691
6.610
6.624
6.629
6.644
7.240
7.312
7.330
7.435
7.453
7.548
7.553
7.563
7.572
7.578
8.041
8.047
8.049
8.055
8.061
8.065
8.083
8.086
8.093
8.101
8.107
Bu
O
CF3
O
1r
3.00
4.19
1.99
3.05
0.97
0.98
0.99
1.93
1.00
1.00
0.0
5.0
ppm (t1)


13.866
19.677
22.330
27.813
35.596
78.463
113.276
116.118
123.227
123.890
125.161
125.804
126.147
126.300
130.211
132.470
132.947
135.581
156.768
157.185
Bu
O
O
CF3
1r
0
50
100
150
ppm (t1)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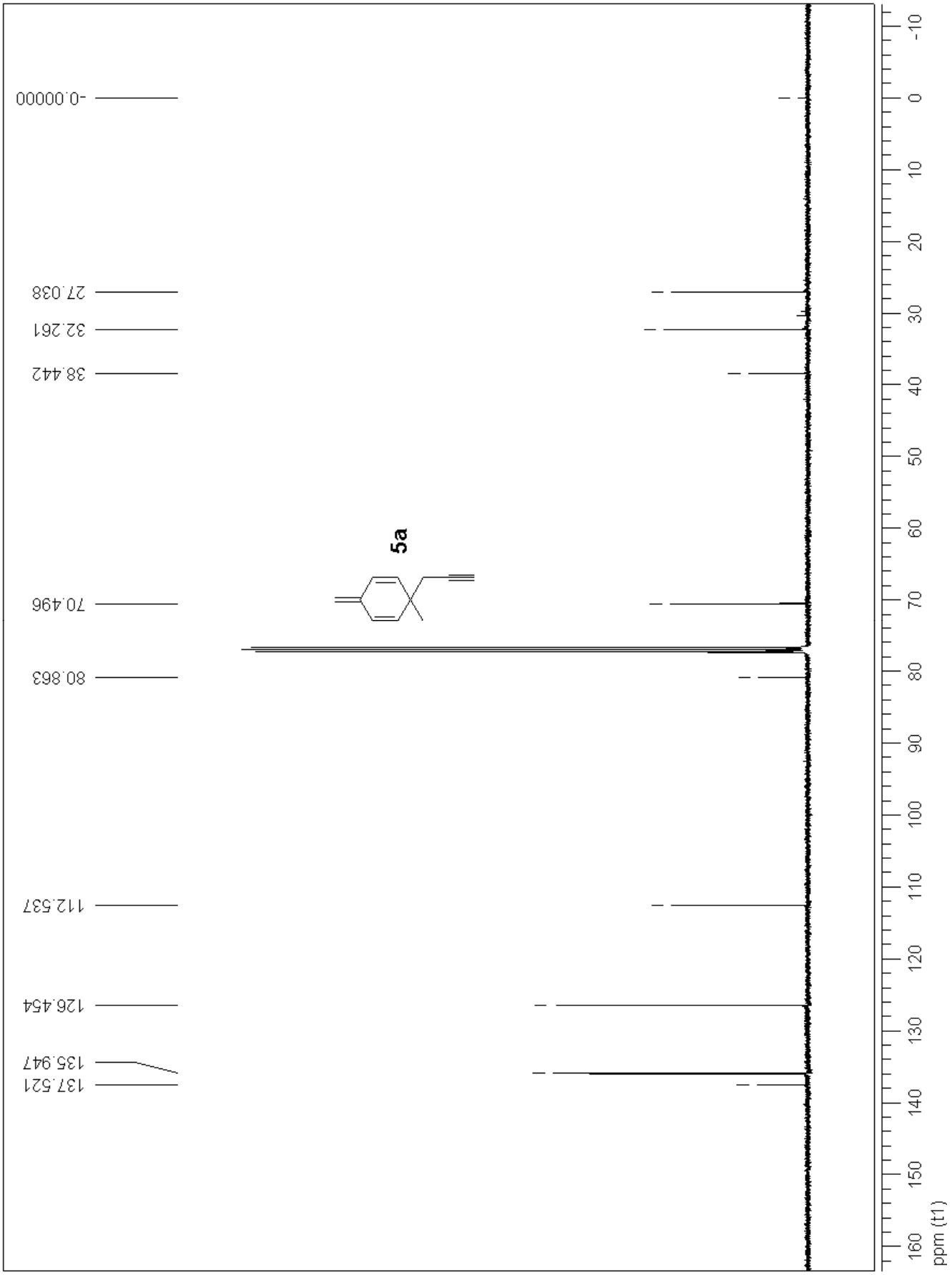
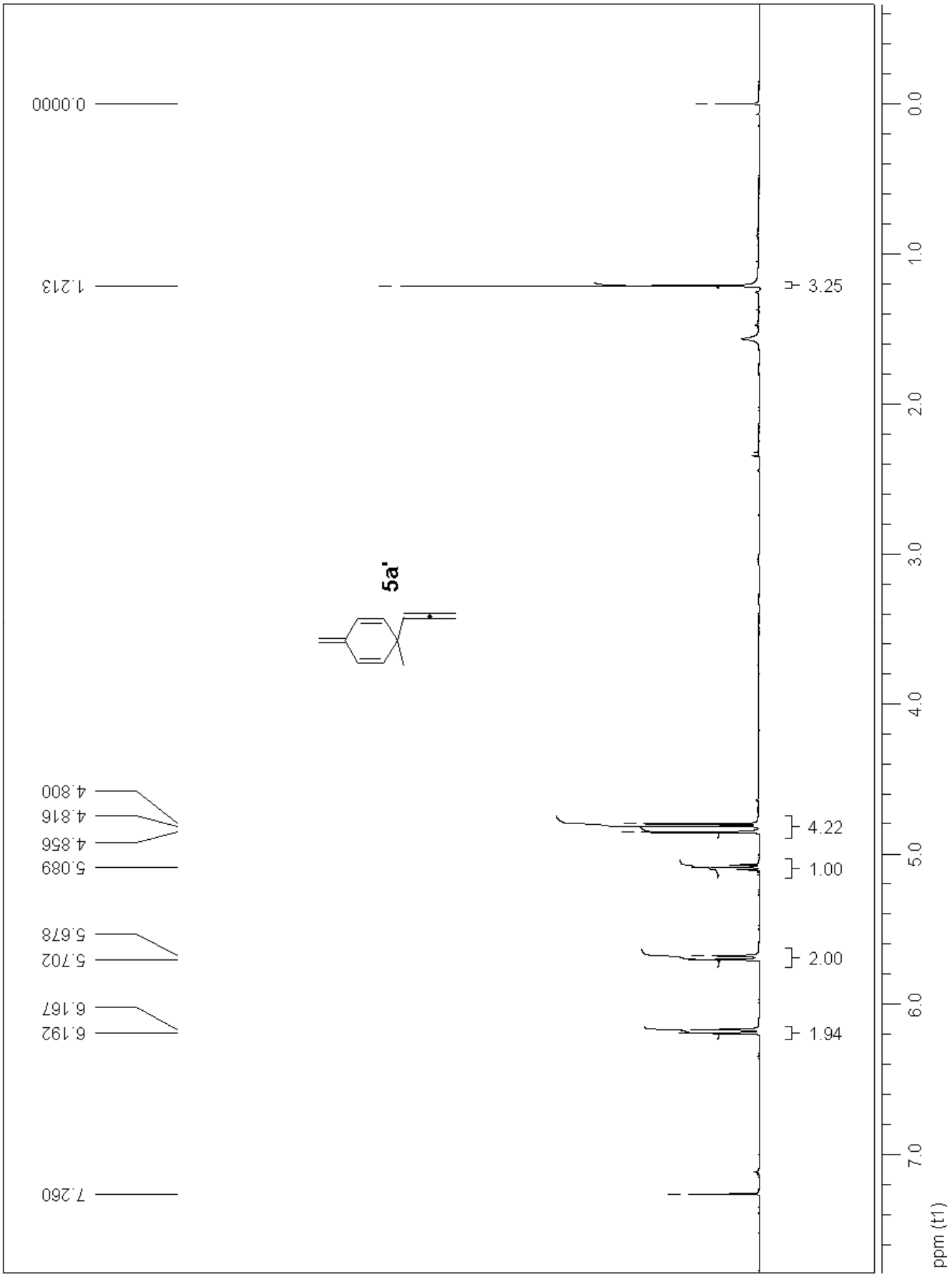
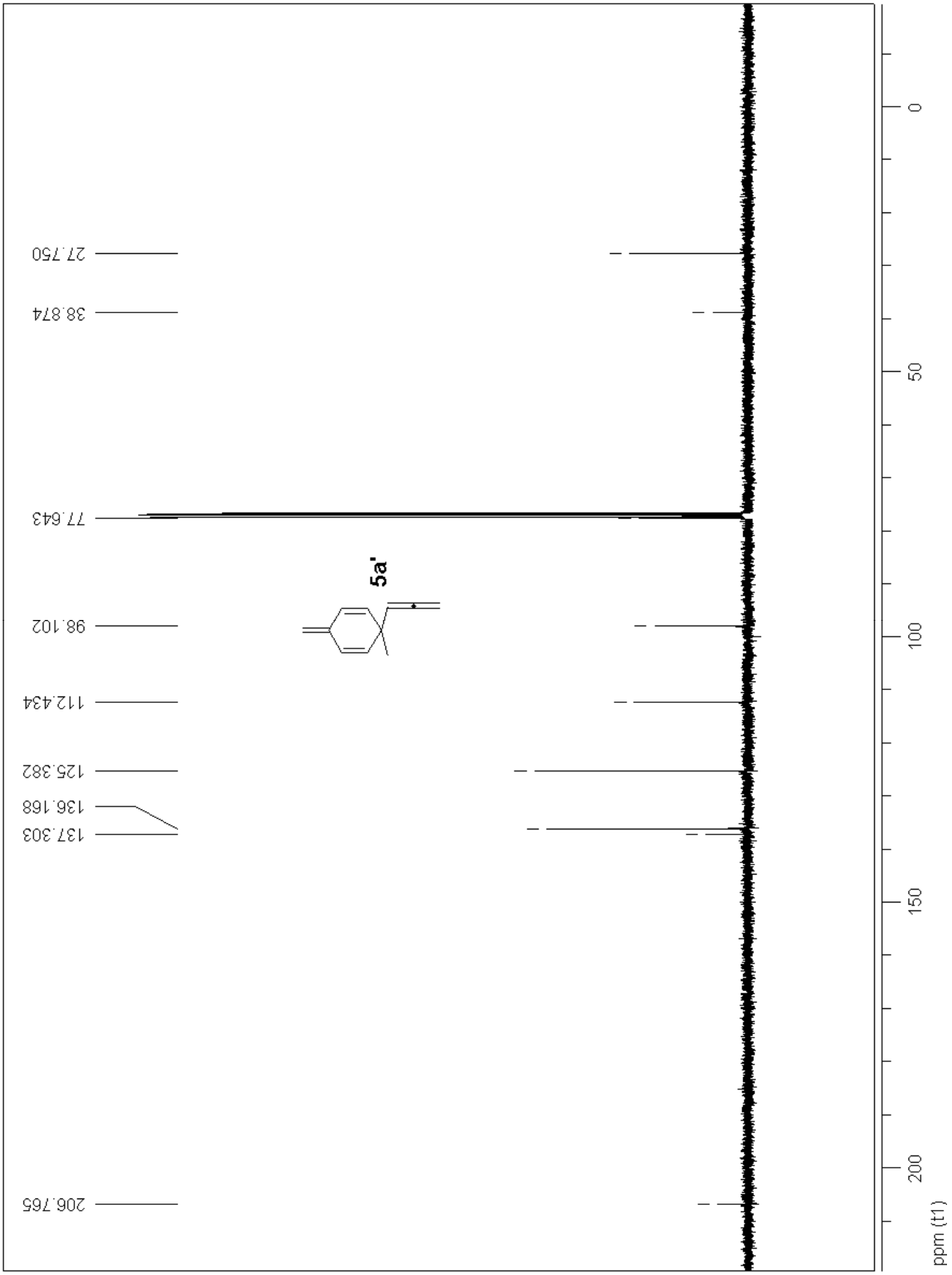
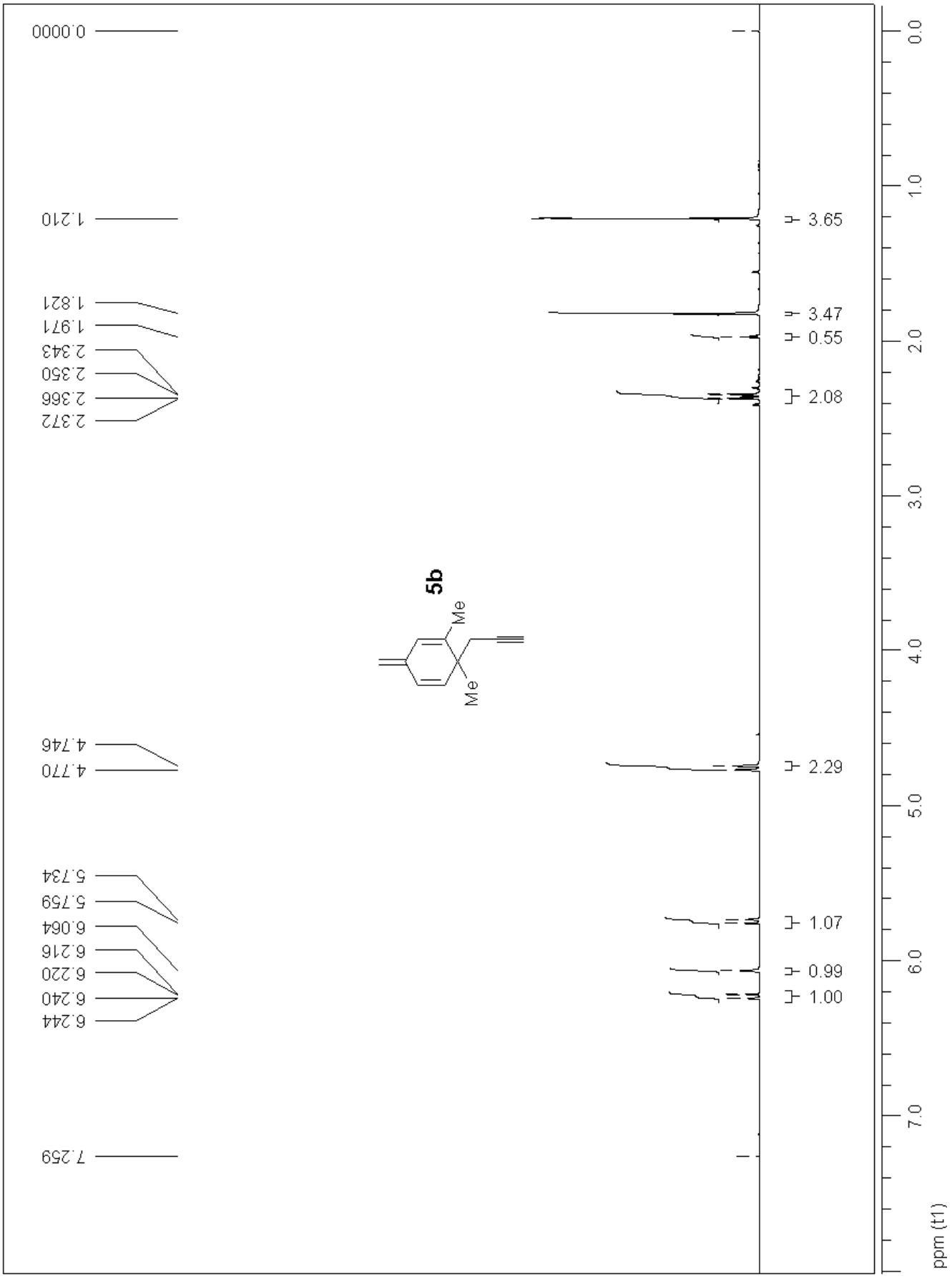
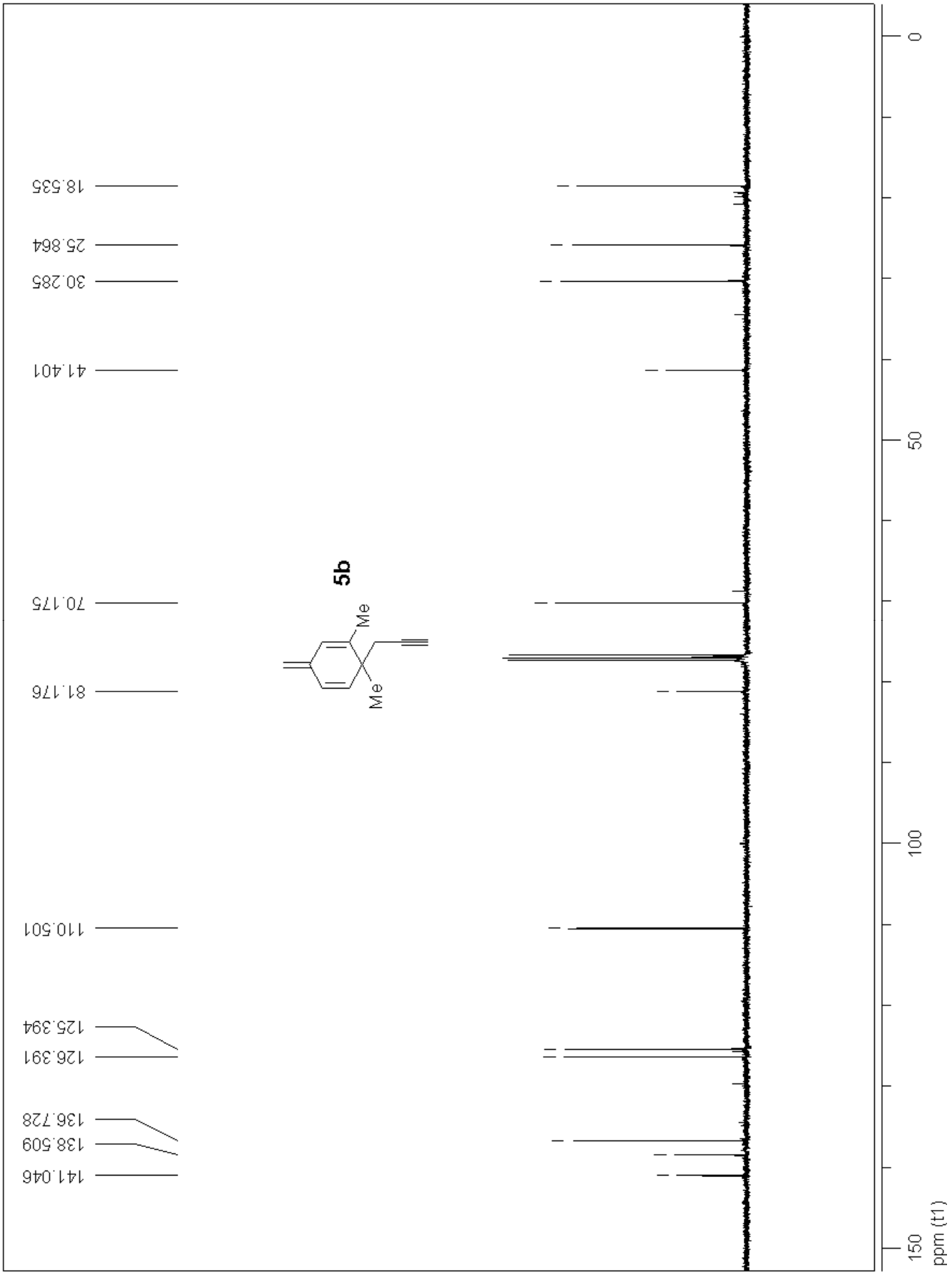
1.206
1.548
2.019
2.026
2.033
2.253
2.260
4.867
5.751
5.776
6.214
6.240
7.260
5a
H2O
3.32
1.03
2.13
2.17
2.12
2.12
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)

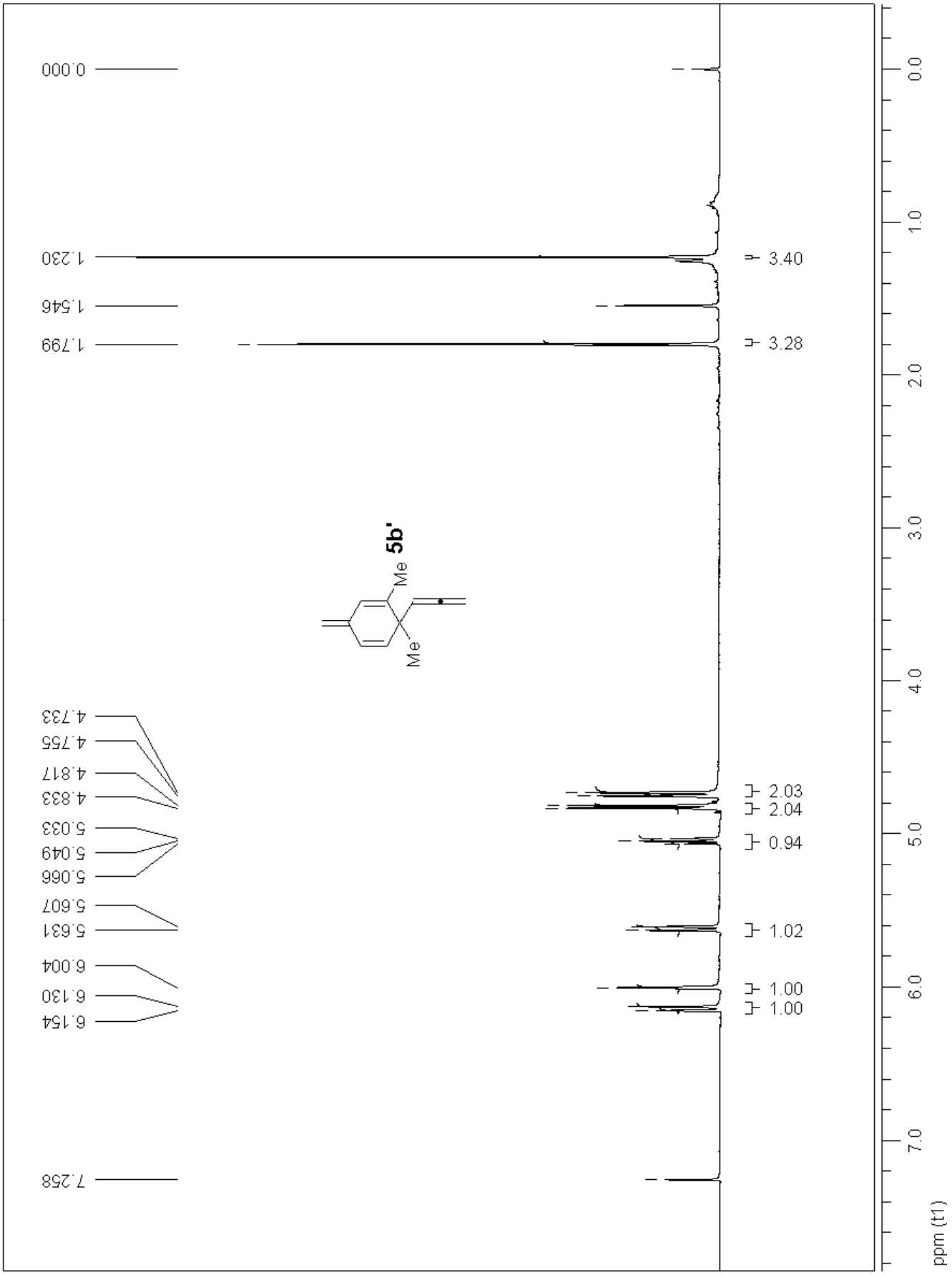

5a
-0.00000
27.038
32.261
38.442
70.496
80.863
112.537
126.454
135.947
137.521
ppm (t1)

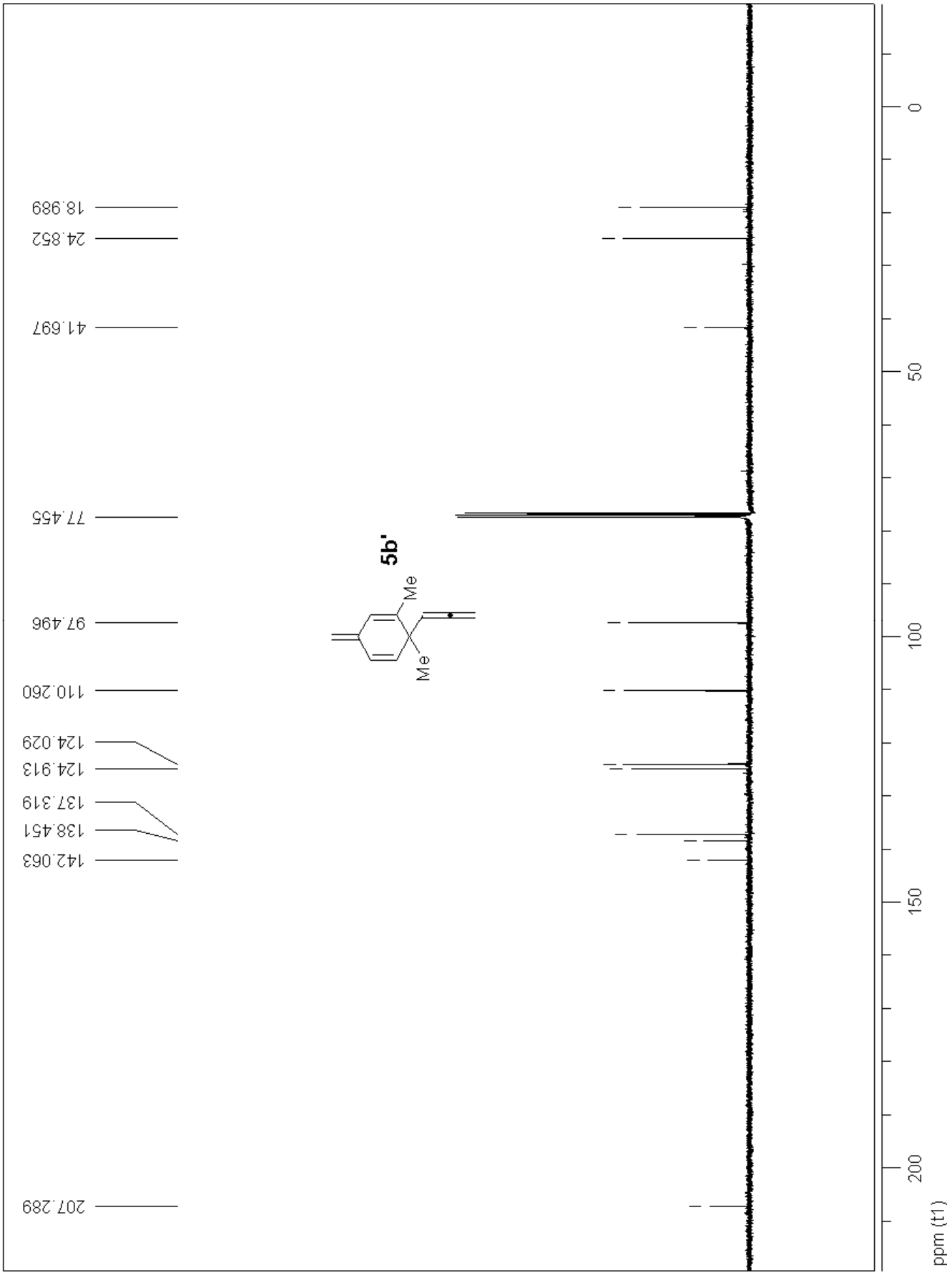

0.0000
1.213
7.260
6.192
6.167
5.702
5.678
5.089
4.856
4.816
4.800
3.25
4.22
1.00
2.00
1.94
5a'
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ppm (t1)

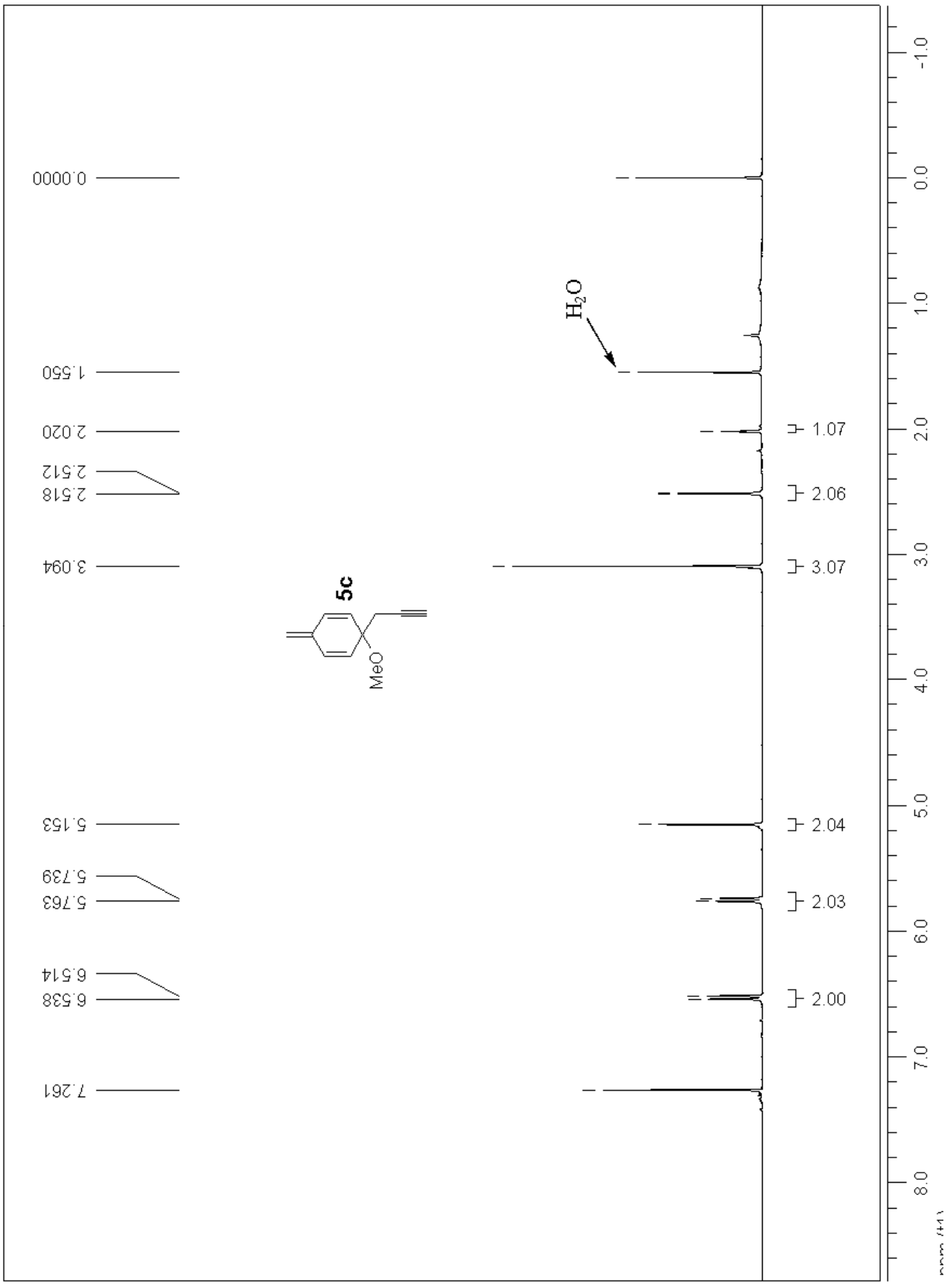

27.750
38.874
77.643
5a'
98.102
112.434
125.382
136.168
137.303
206.765
0
50
100
150
200
ppm (t1)

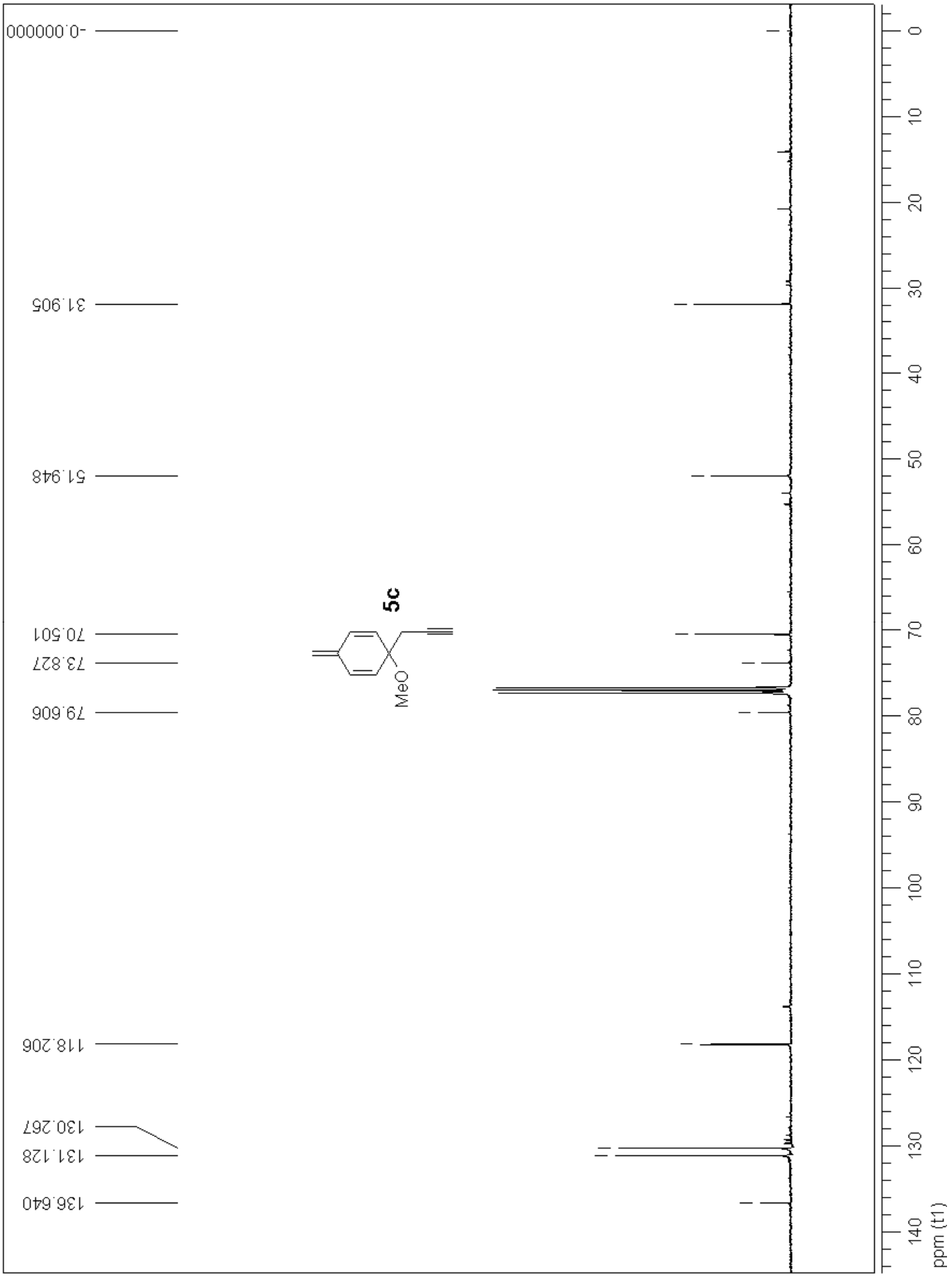

0.0000
1.210
1.821
1.971
2.343
2.350
2.366
2.372
4.746
4.770
5.734
5.759
6.064
6.216
6.220
6.240
6.244
7.259
5b
Me
Me
3.65
3.47
0.55
2.08
2.29
1.07
0.99
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ppm (f1)

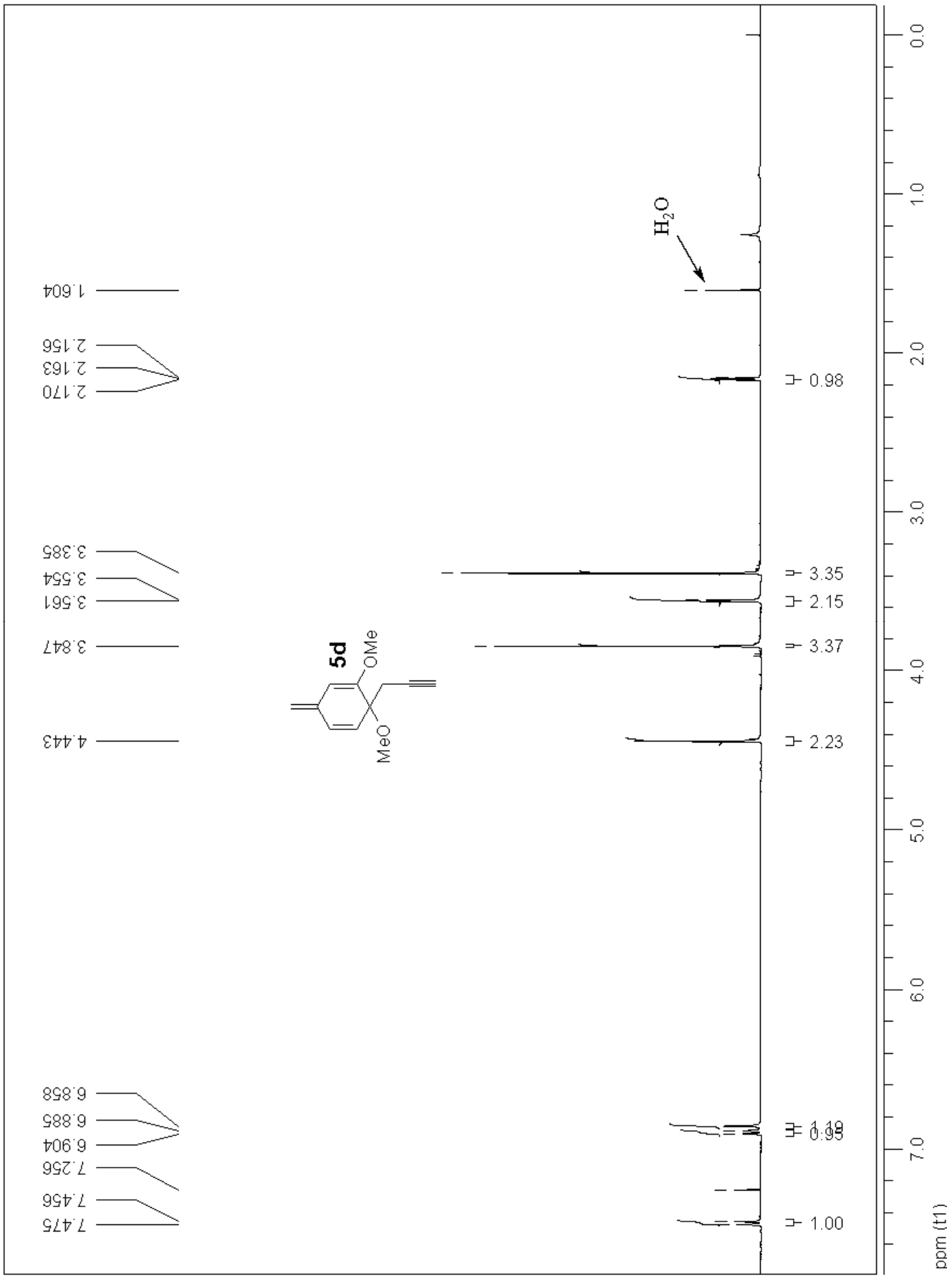

18.535
25.864
30.285
41.401
70.175
81.176
110.501
125.394
126.391
136.728
138.509
141.046
5b
Me
Me
0
50
100
150
ppm (t1)

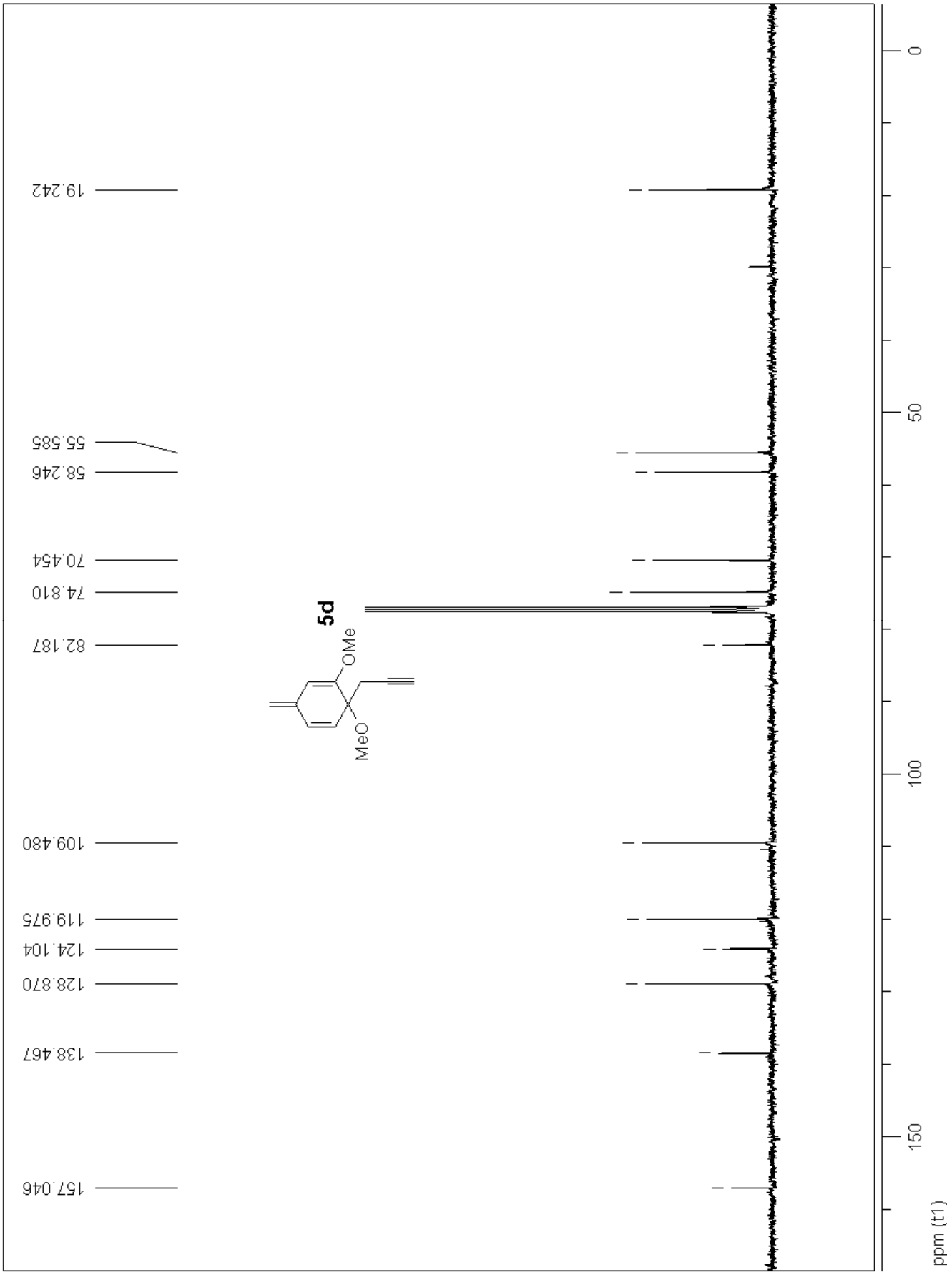

0.000
1.230
1.546
1.799
4.733
4.755
4.817
4.833
5.033
5.049
5.066
5.607
5.631
6.004
6.130
6.154
7.258
3.40
3.28
2.03
2.04
0.94
1.02
1.00
1.00
5b'
Me
Me
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ppm (t1)

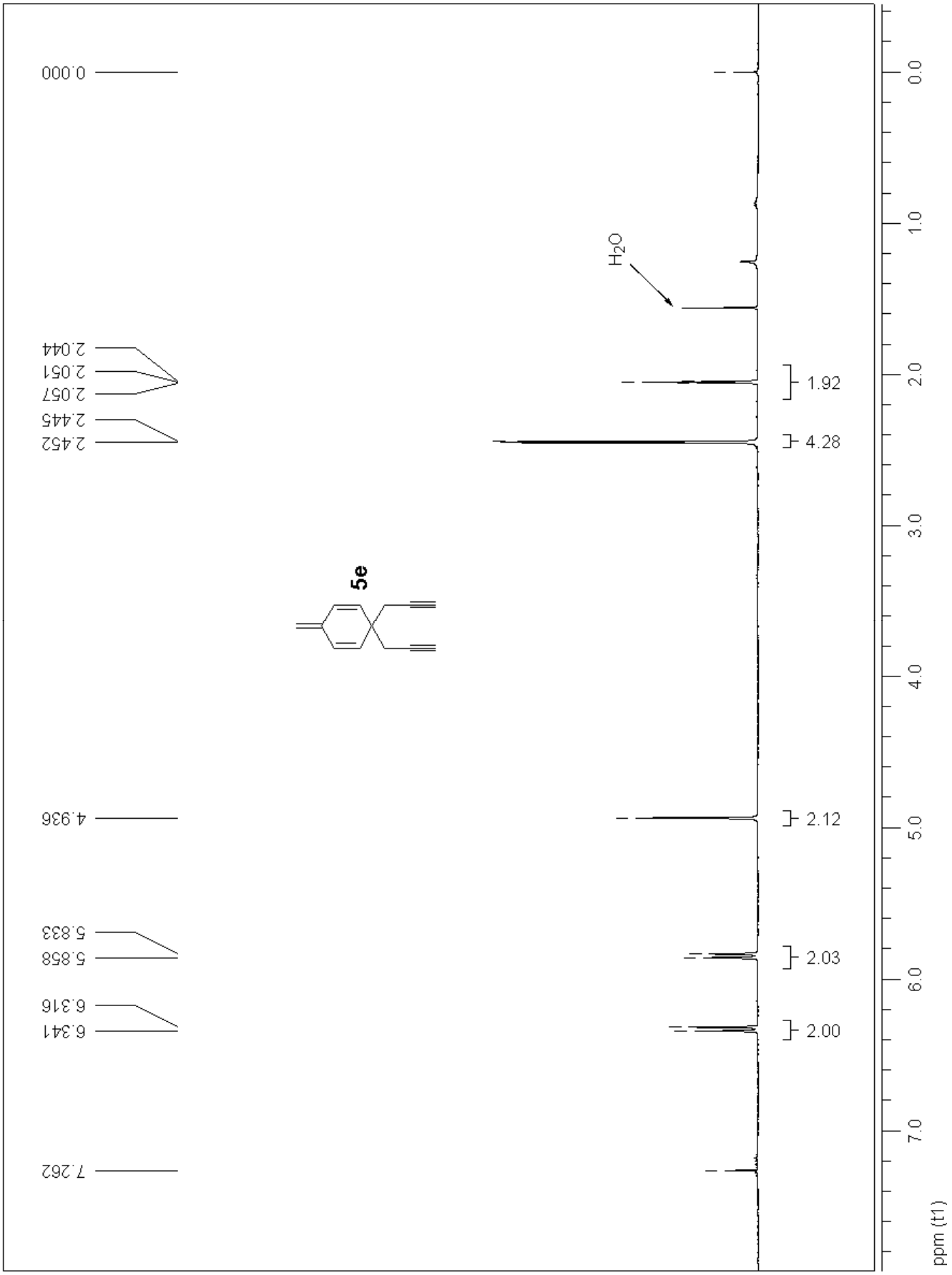

18.989
24.852
41.697
77.455
97.496
110.260
124.029
124.913
137.319
138.451
142.063
207.289
5b'
Me
Me
0
50
100
150
200
ppm (t1)

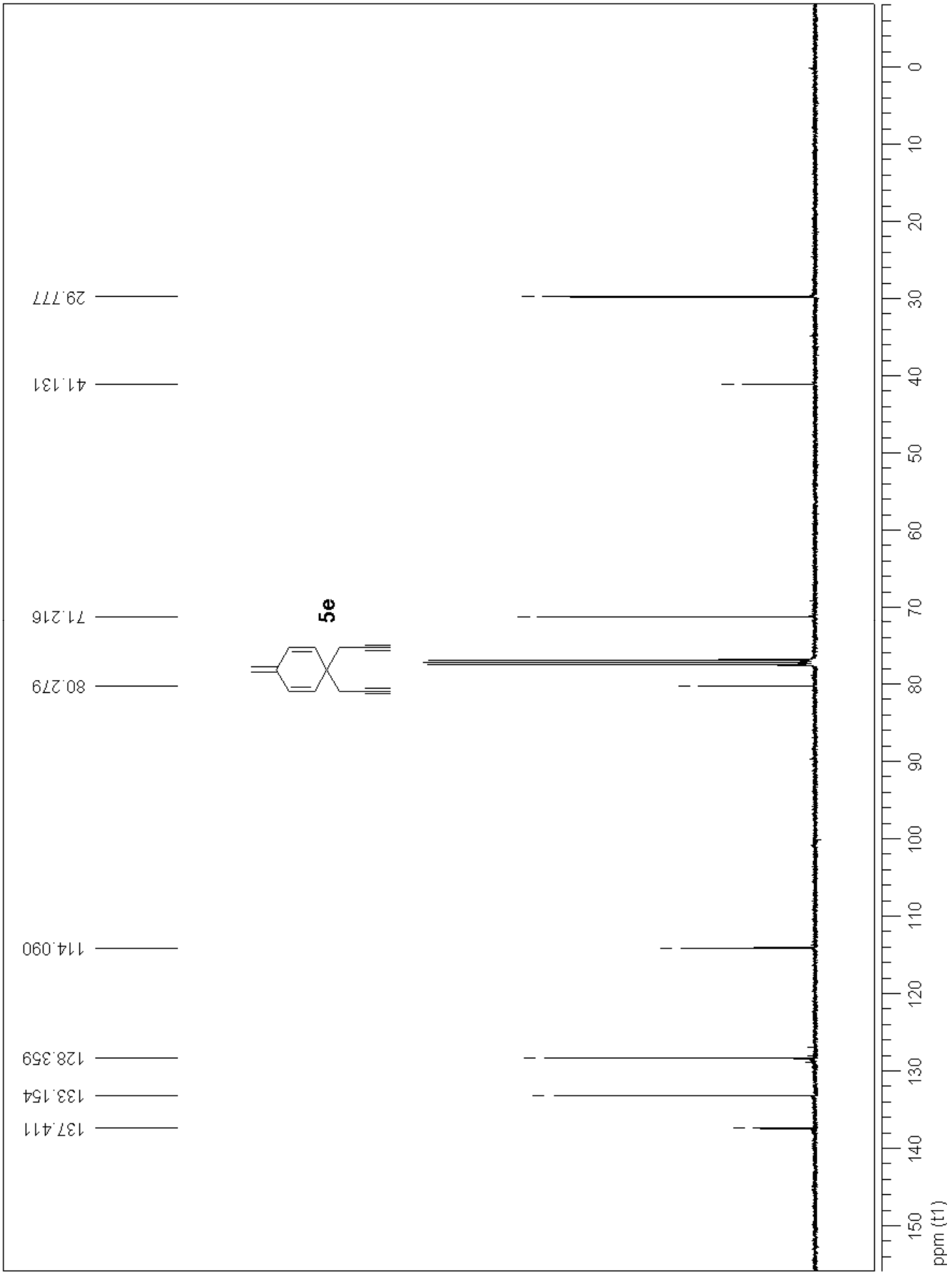

0.0000
1.550
2.020
2.512
2.518
3.094
5.153
5.739
5.763
6.514
6.538
7.261
H_2O
5c
MeO
1.07
2.06
3.07
2.04
2.03
2.00
-1.0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0

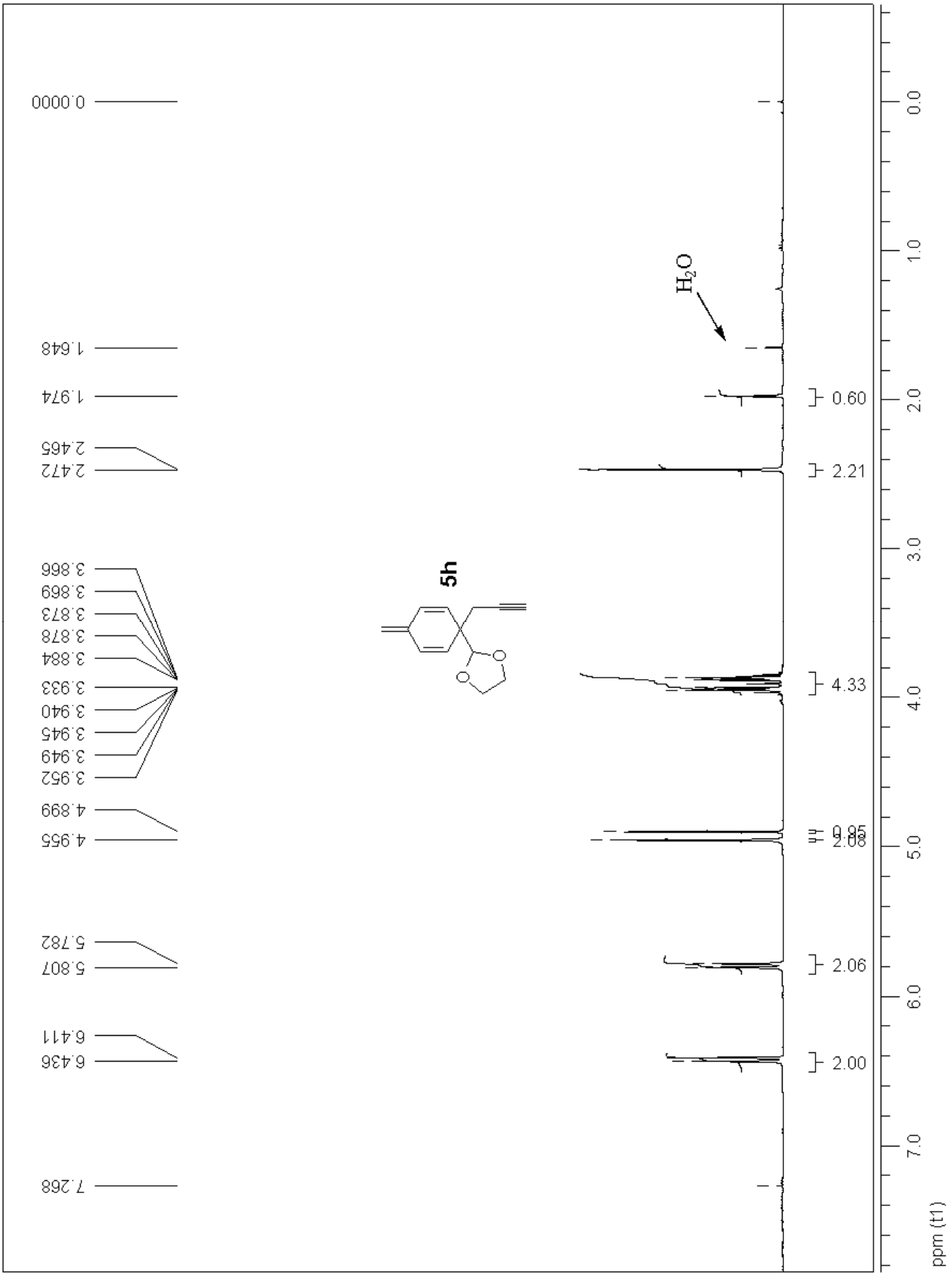

-0.000000
31.905
51.948
70.501
73.827
79.606
118.206
130.267
131.128
136.640
5c
MeO
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm (t1)

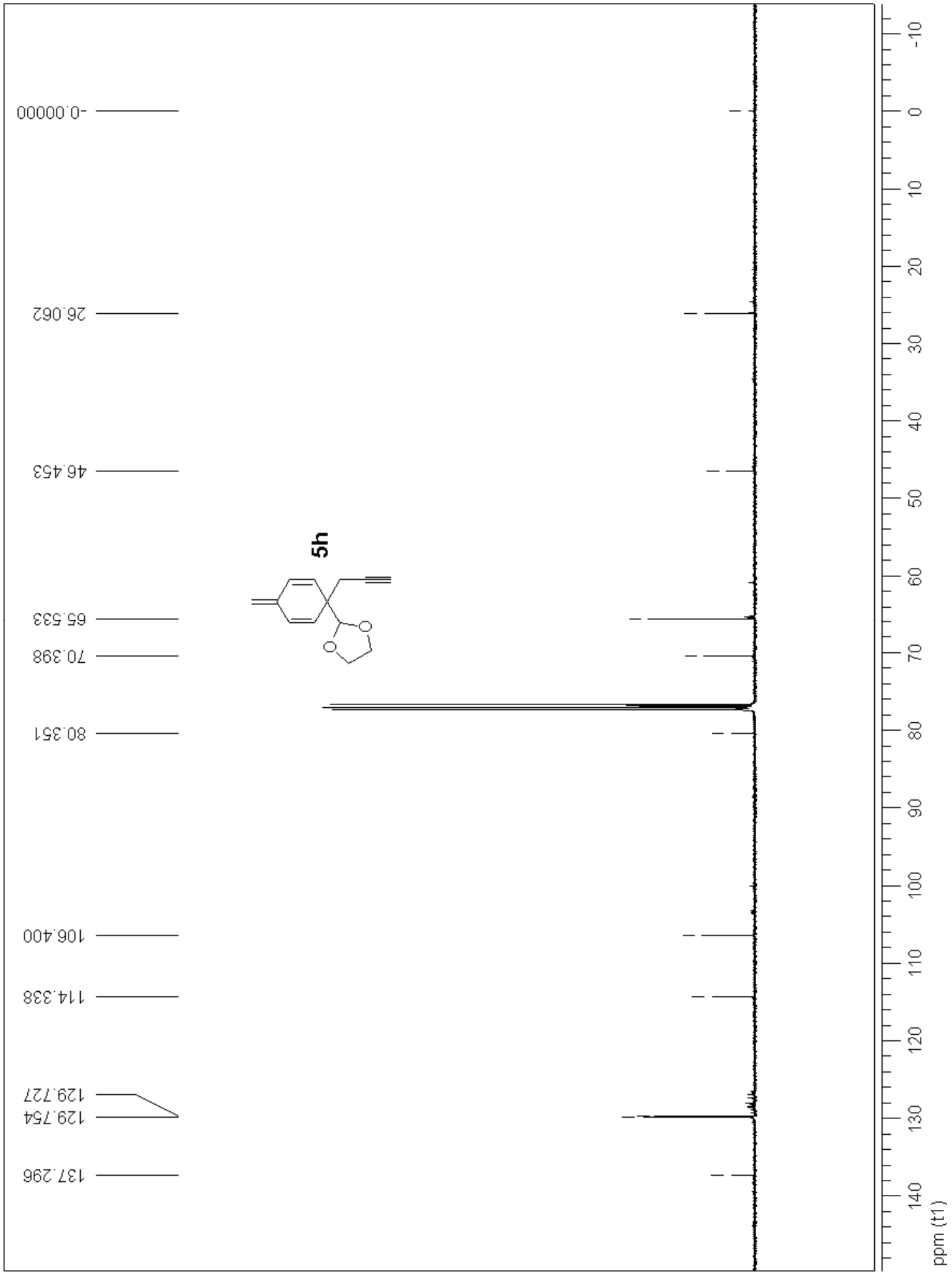

5d
OMe
MeO
H_2O
1.604
2.156
2.163
2.170
3.385
3.554
3.561
3.847
4.443
6.858
6.885
6.904
7.256
7.456
7.475
0.98
3.35
2.15
3.37
2.23
1.00
ppm (f1)

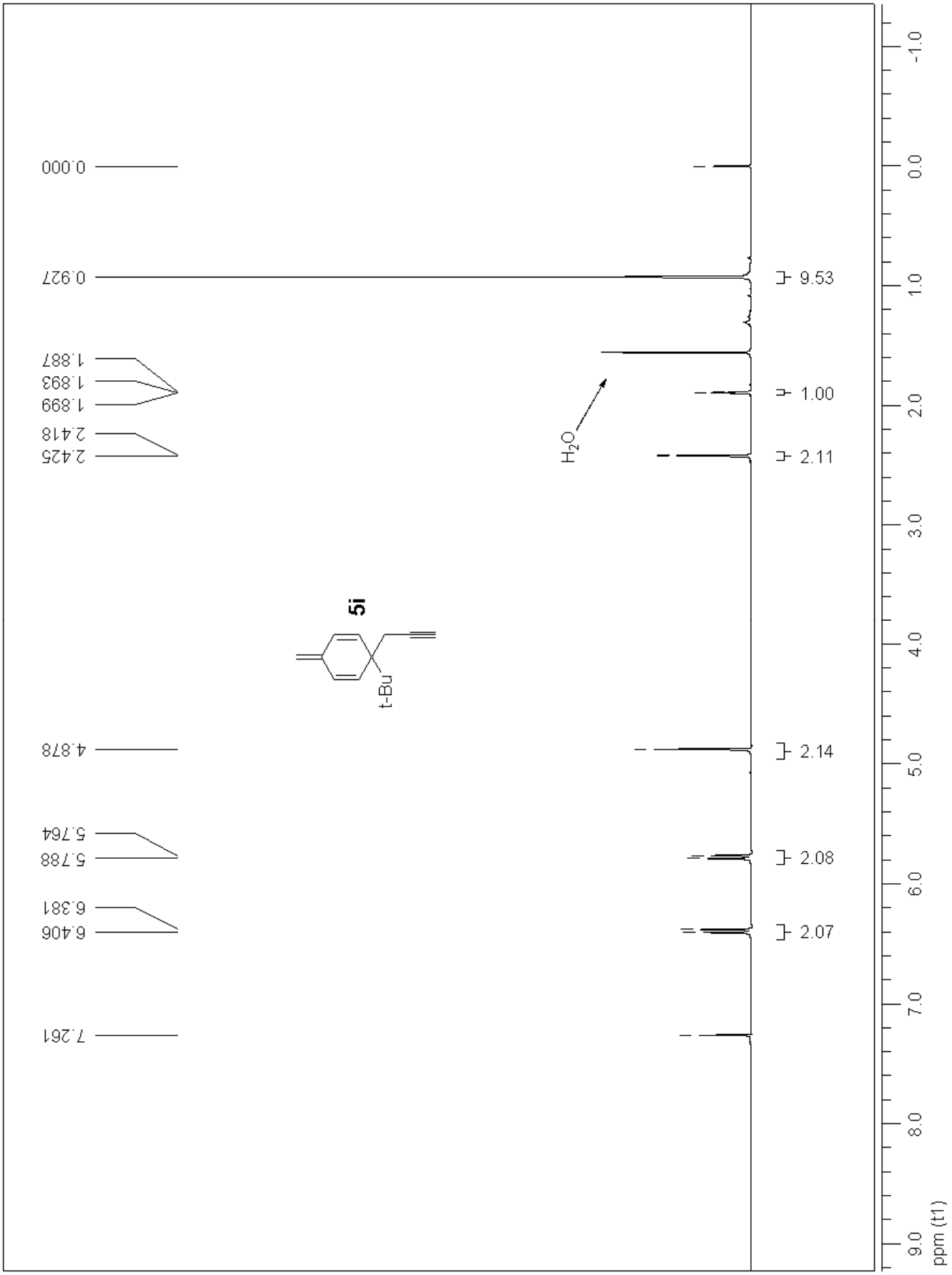

5d
OMe
MeO
157.046
138.467
128.870
124.104
119.975
109.480
82.187
74.810
70.454
58.246
55.585
19.242
0
50
100
150
ppm (t1)

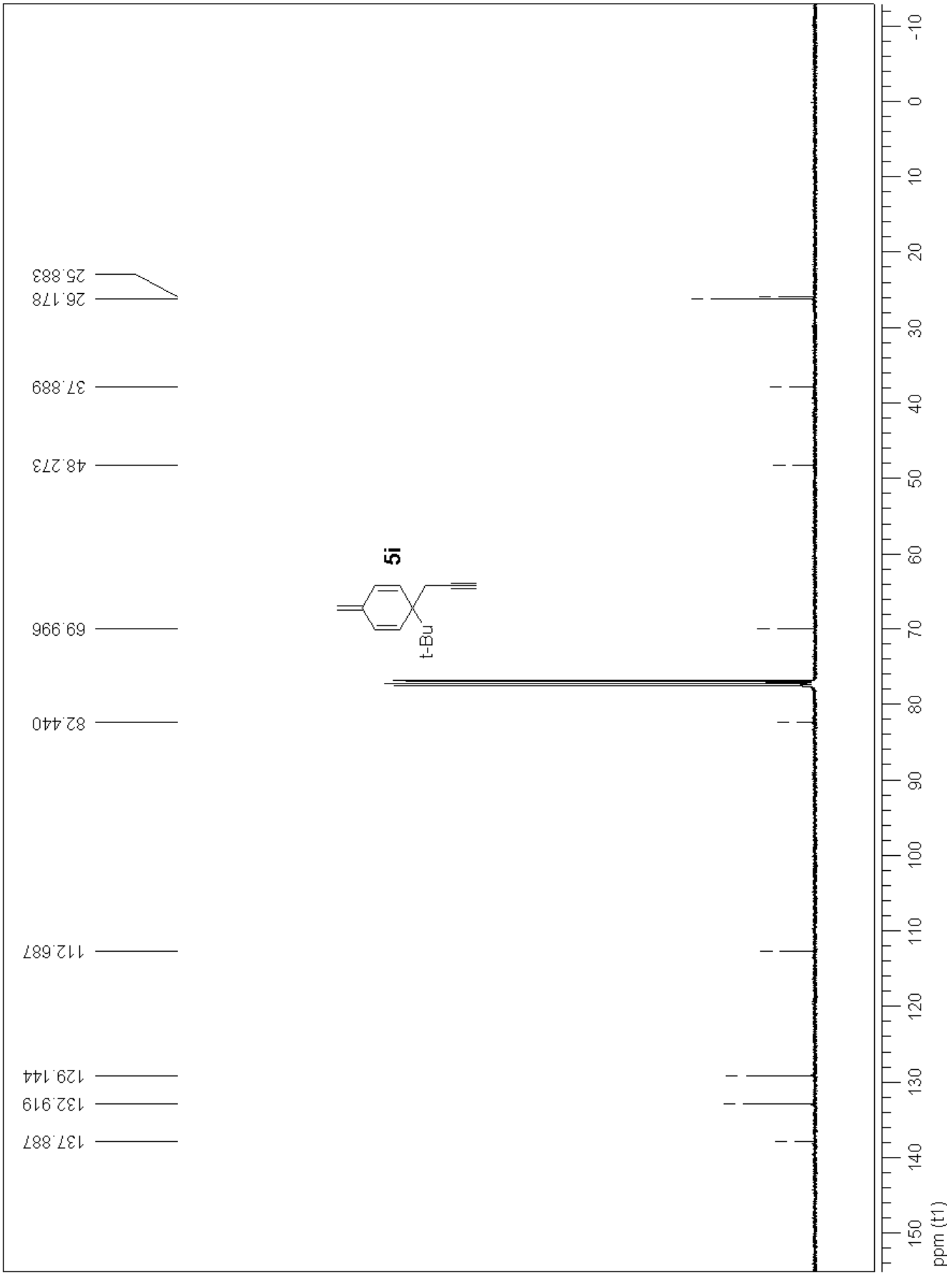

0.000
2.044
2.051
2.057
2.445
2.452
4.936
5.833
5.858
6.316
6.341
7.262
5e
H2O
1.92
4.28
2.12
2.03
2.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ppm (t1)

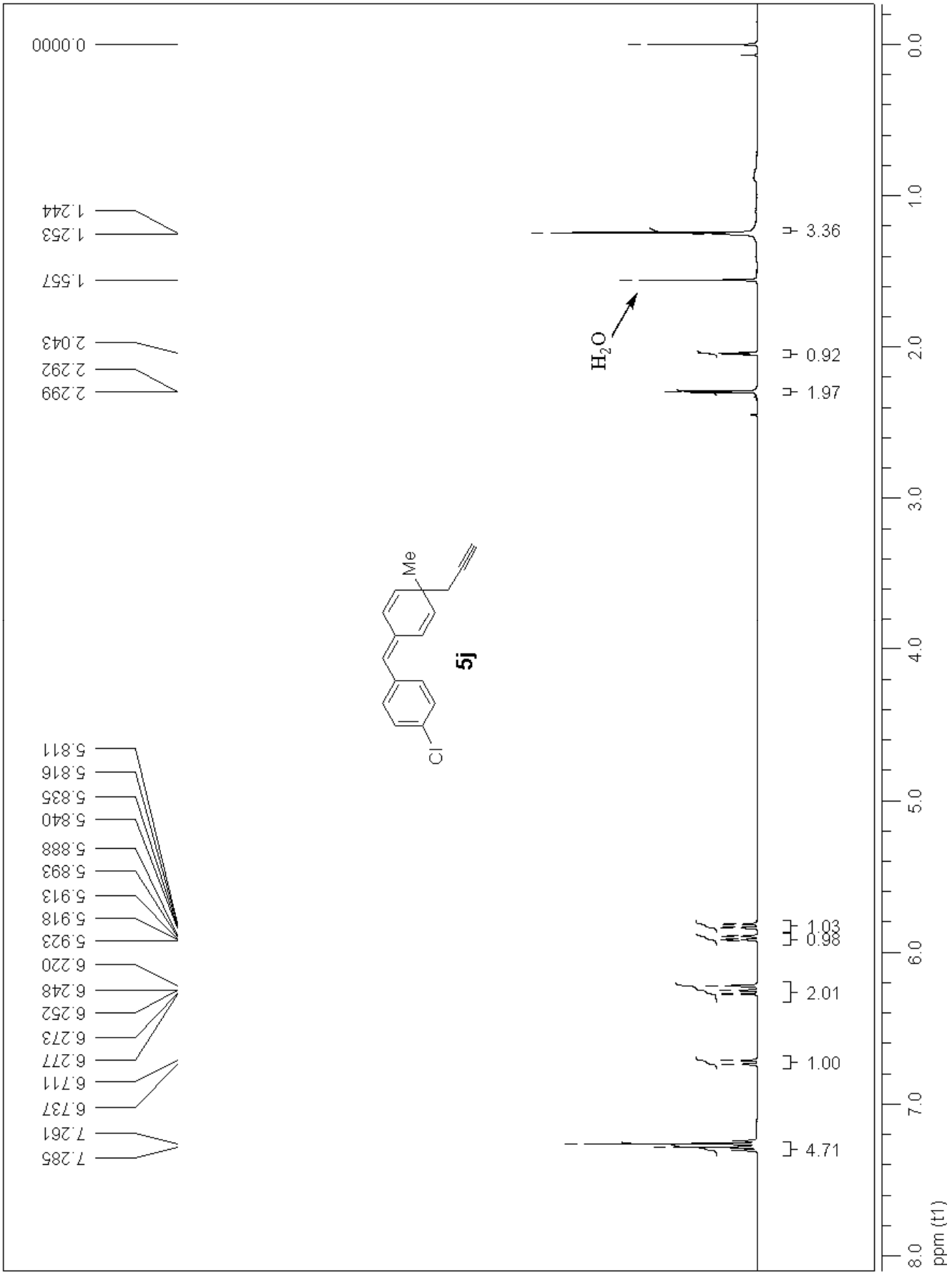

5e
29.777
41.131
71.216
80.279
114.090
128.359
133.154
137.411
ppm (t1)

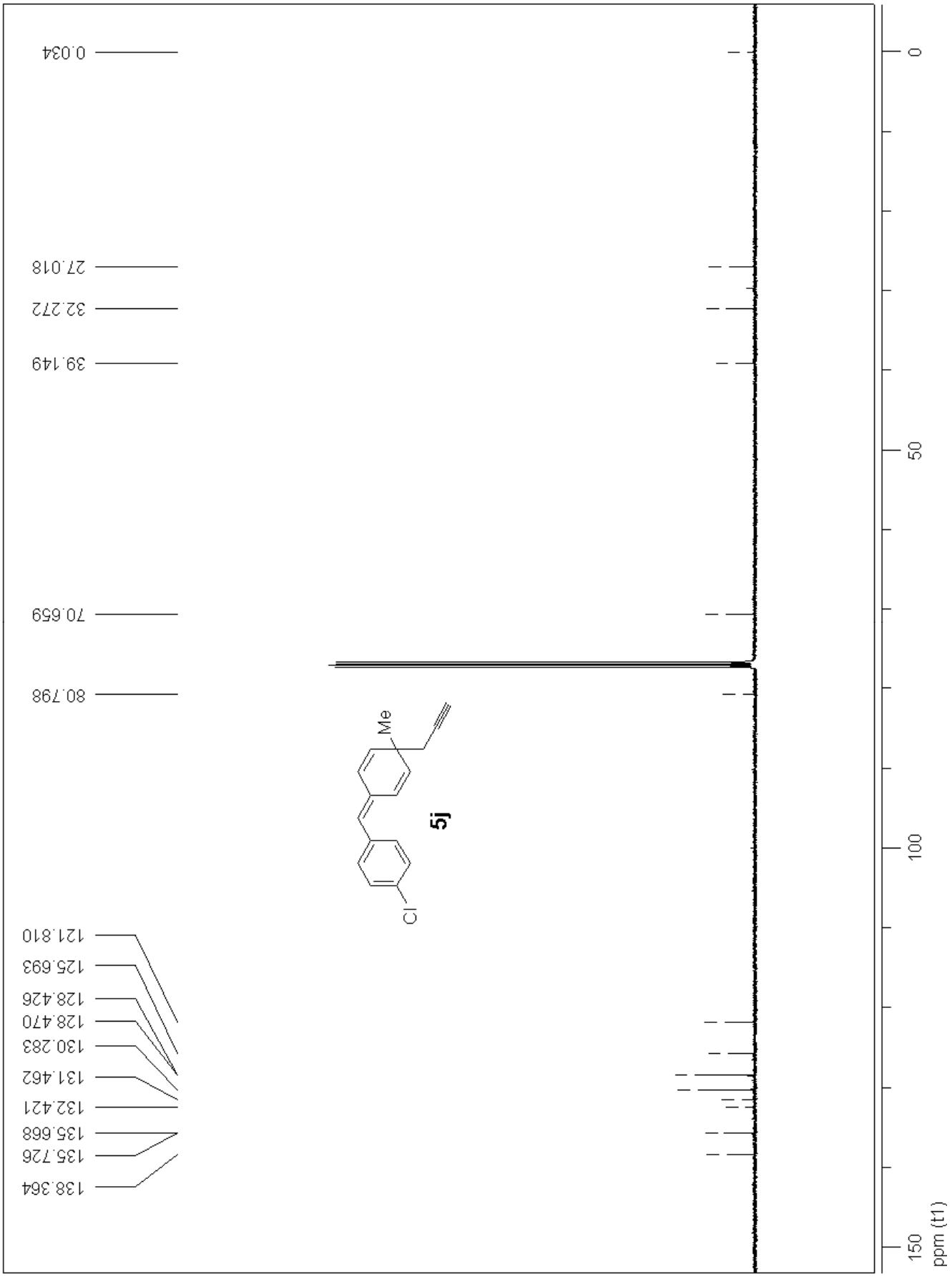

0.0000
1.648
1.974
2.465
2.472
3.866
3.869
3.873
3.878
3.884
3.933
3.940
3.945
3.949
3.952
4.899
4.955
5.782
5.807
6.411
6.436
7.268
5h
H2O
0.60
2.21
4.33
0.85
2.08
2.06
2.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
ppm (t1)

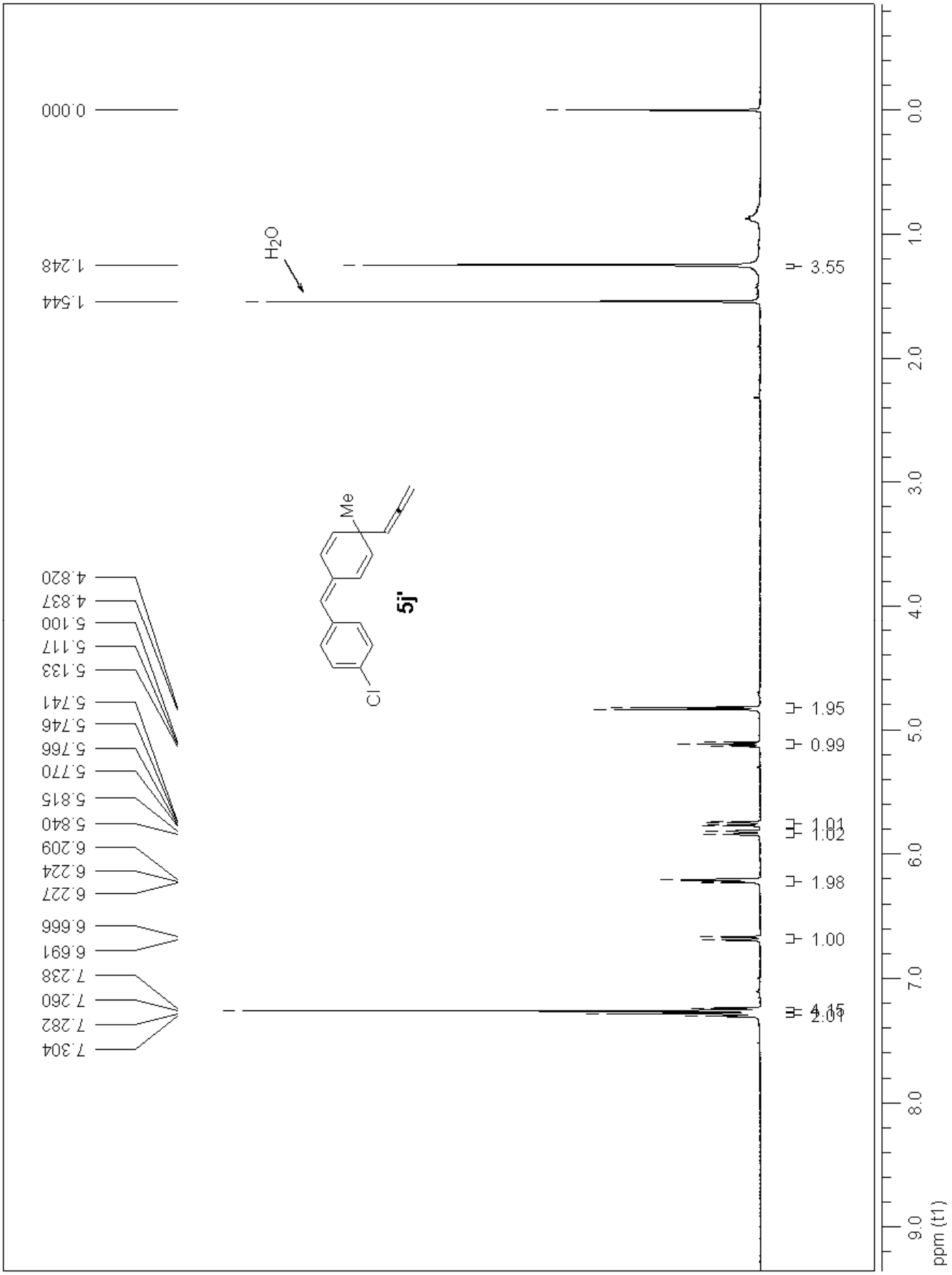

5h
-0.00000
26.062
46.453
65.533
70.398
80.351
106.400
114.338
129.727
129.754
137.296
ppm (t1)

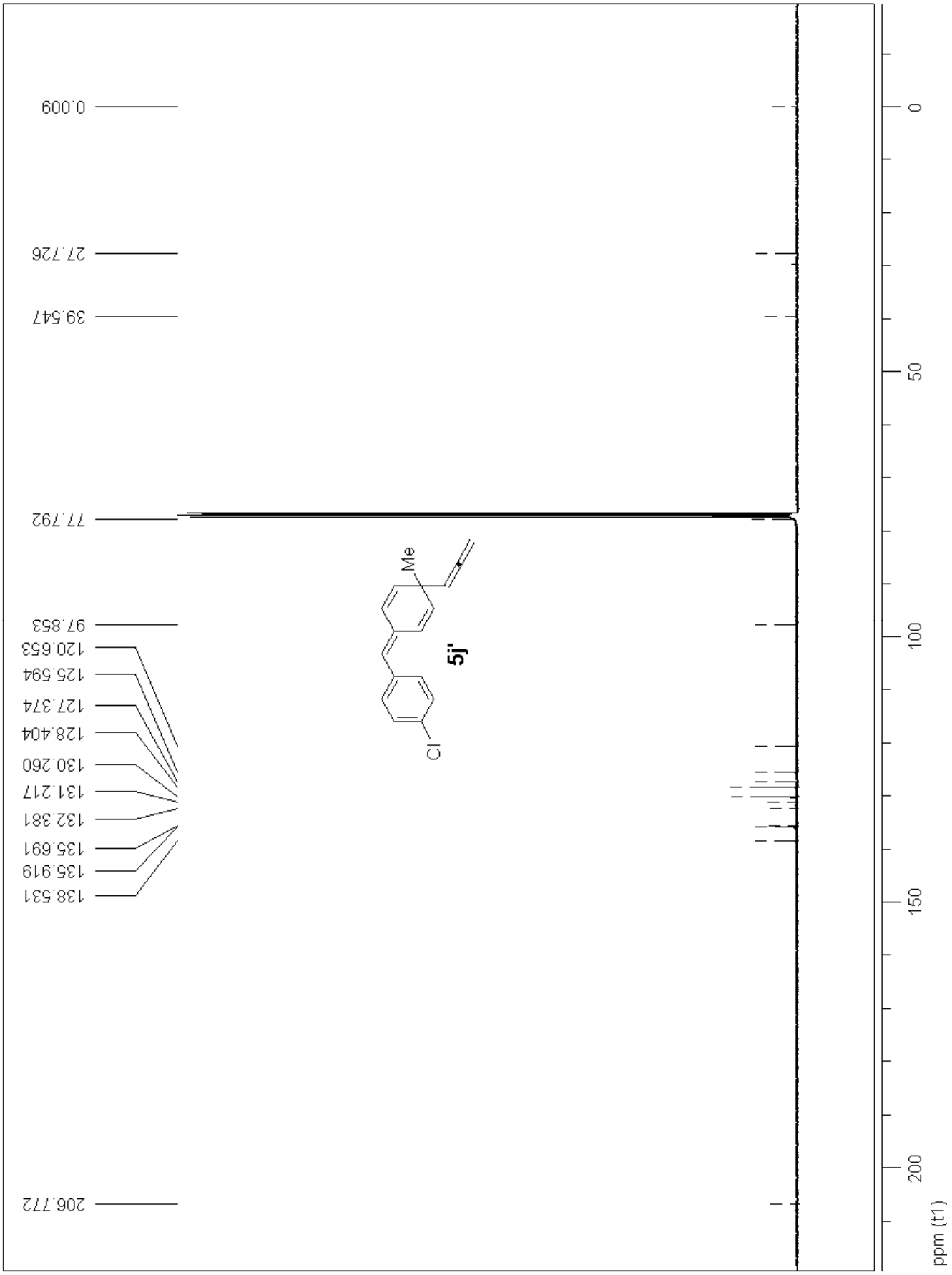

0.000
0.927
1.887
1.893
1.899
2.418
2.425
4.878
5.764
5.788
6.381
6.406
7.261
9.53
1.00
2.11
2.14
2.08
2.07
H_2O
5i
t-Bu
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (t1)

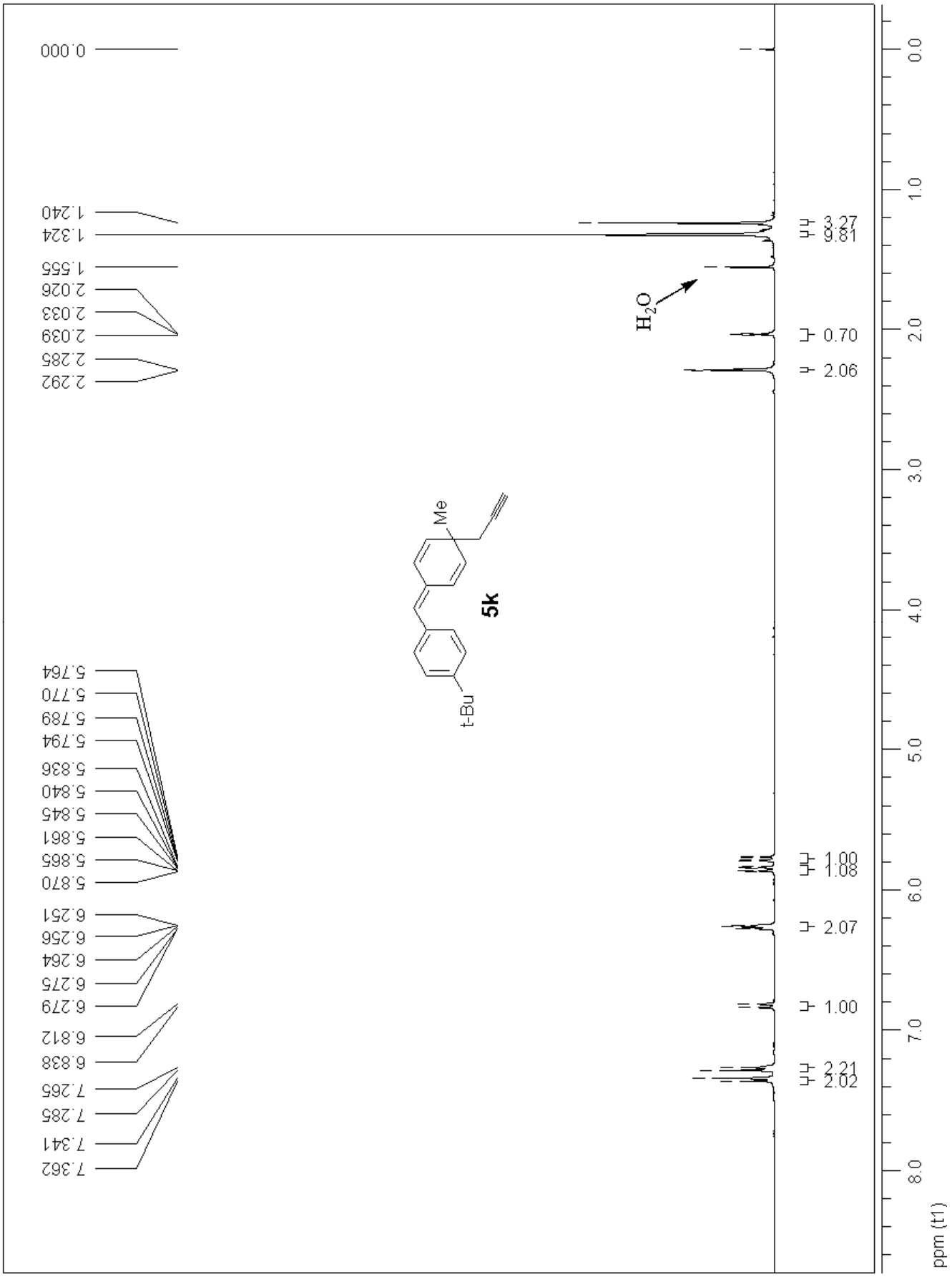

25.883
26.178
37.889
48.273
69.996
82.440
112.687
129.144
132.919
137.887
5i
t-Bu
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
ppm (f1)

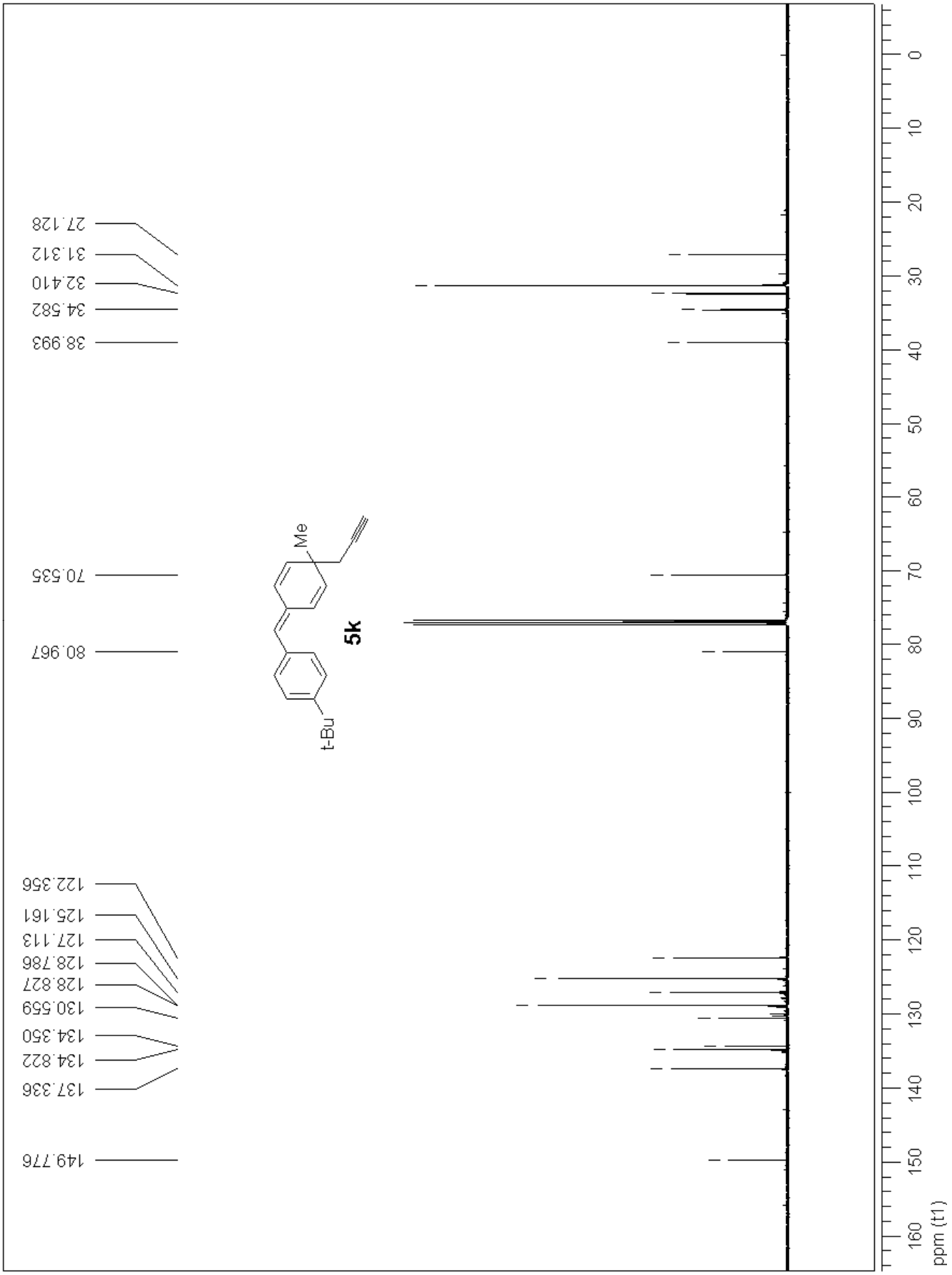

0.0000
1.244
1.253
1.557
2.043
2.292
2.299
5.811
5.816
5.835
5.840
5.888
5.893
5.913
5.918
5.923
6.220
6.248
6.252
6.273
6.277
6.711
6.737
7.261
7.285
Me
Cl
5j
H2O
3.36
0.92
1.97
1.03
0.98
2.01
1.00
4.71
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

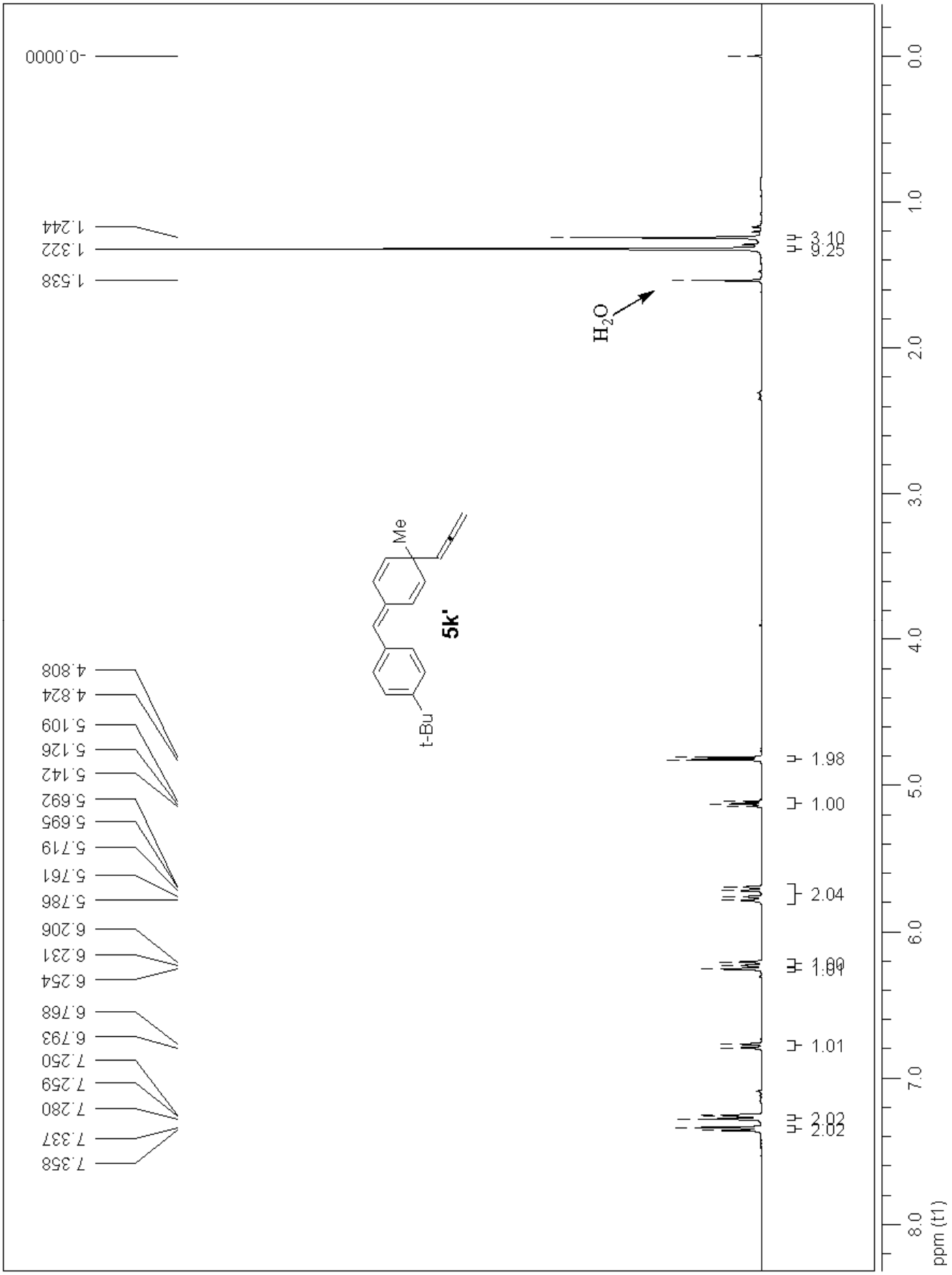

0.034
27.018
32.272
39.149
70.659
80.798
121.810
125.693
128.426
128.470
130.283
131.462
132.421
135.668
135.726
138.364
Me
Cl
5j
0
50
100
150
ppm (t1)

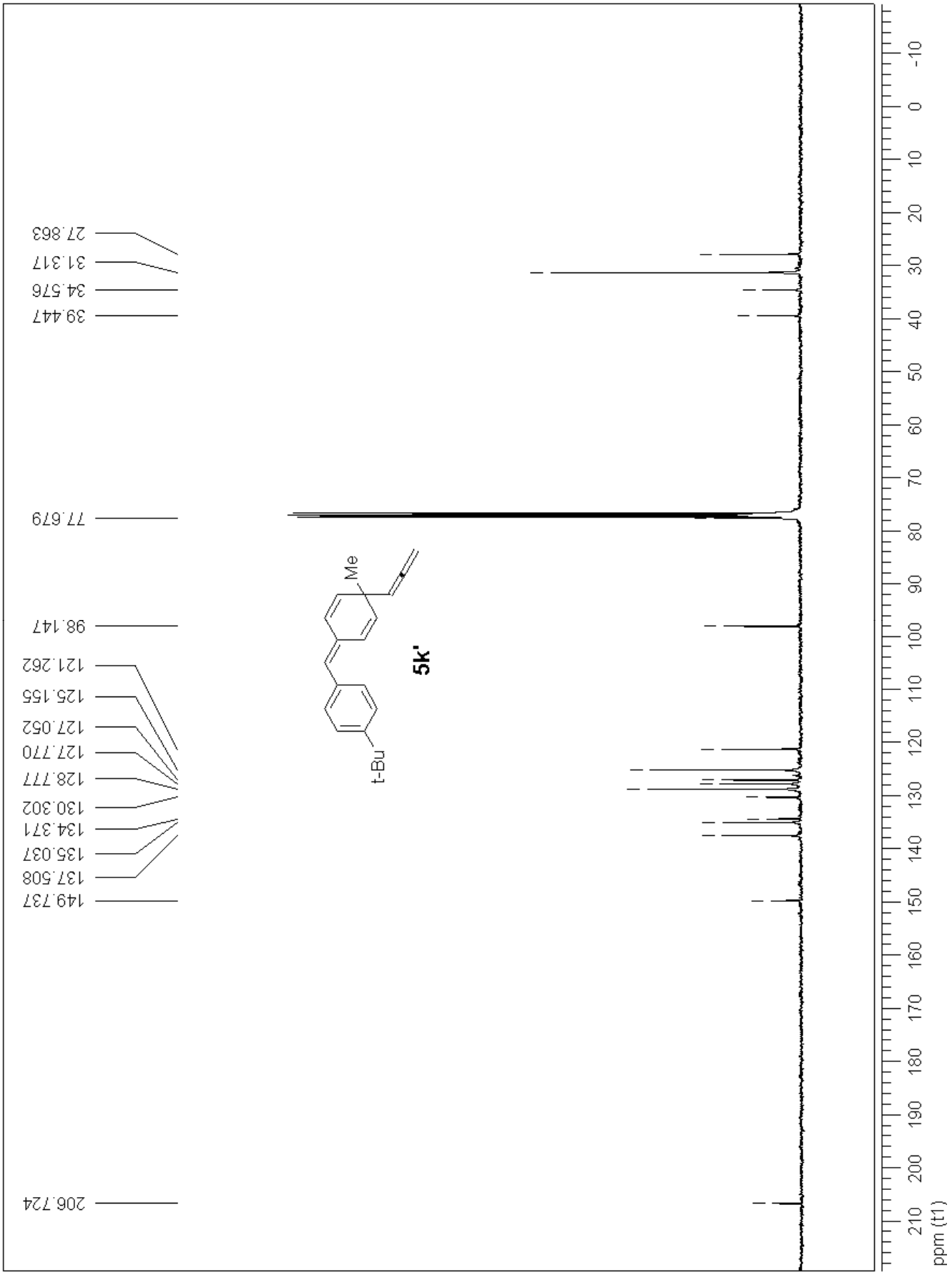

0.000
1.248
1.544
4.820
4.837
5.100
5.117
5.133
5.741
5.746
5.766
5.770
5.815
5.840
6.209
6.224
6.227
6.666
6.691
7.238
7.260
7.282
7.304
H2O
Me
Cl
5j'
3.55
1.95
0.99
1.01
1.02
1.98
1.00
4.15
2.04
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
ppm (t1)

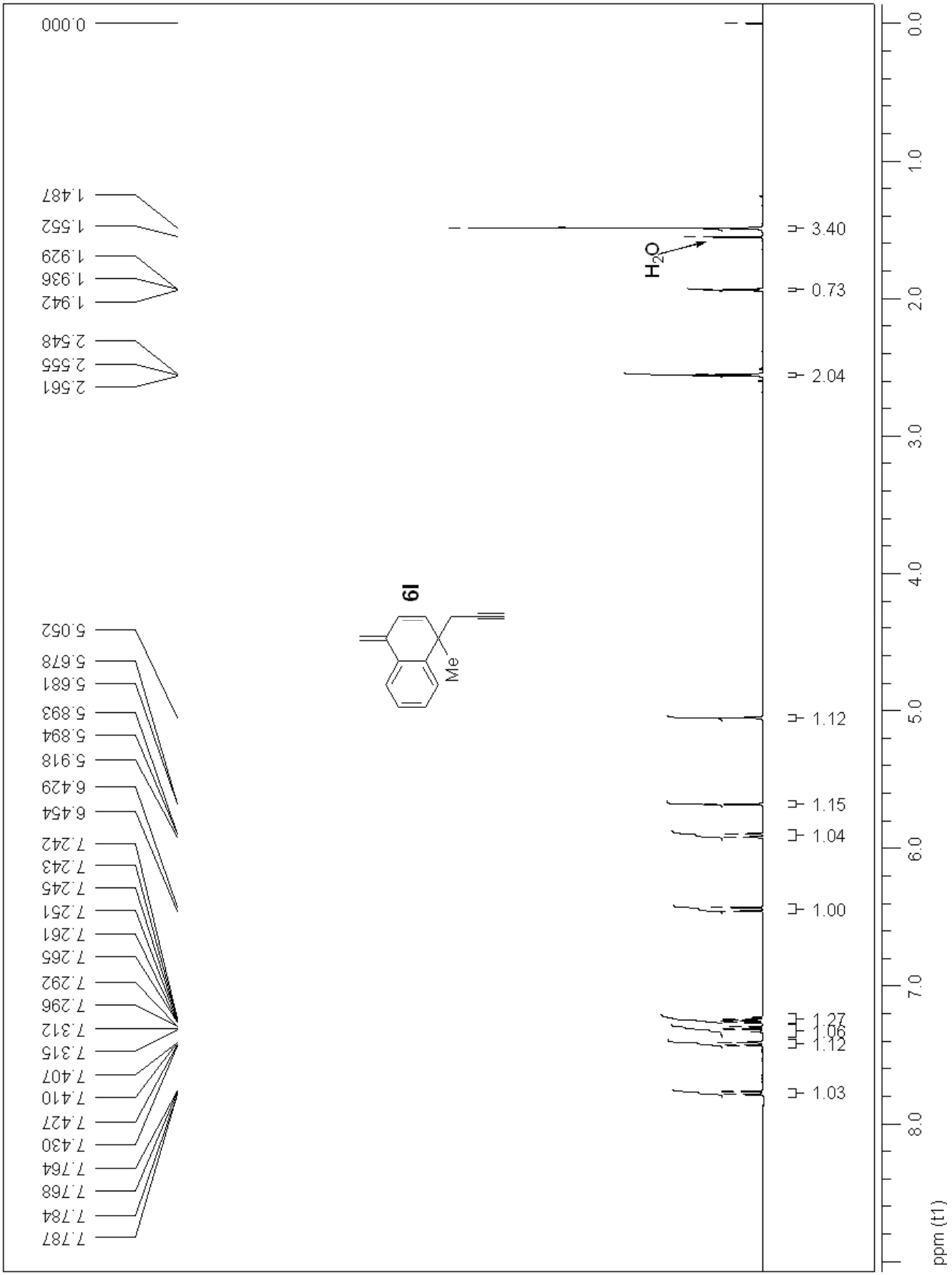

0.009
27.726
39.547
77.792
97.853
120.653
125.594
127.374
128.404
130.260
131.217
132.381
135.691
135.919
138.531
206.772
Me
Cl
5j'
0
50
100
150
200
ppm (t1)


0.000
1.240
1.324
1.555
2.026
2.033
2.039
2.285
2.292
5.764
5.770
5.789
5.794
5.836
5.840
5.845
5.861
5.865
5.870
6.251
6.256
6.264
6.275
6.279
6.812
6.838
7.265
7.285
7.341
7.362
Me
t-Bu
5k
H_2O
3.27
9.81
0.70
2.06
1.00
1.08
2.07
1.00
2.21
2.02
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)


27.128
31.312
32.410
34.582
38.993
70.535
80.967
122.356
125.161
127.113
128.786
128.827
130.559
134.350
134.822
137.336
149.776
Me
t-Bu
5k
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
ppm (t1)


-0.0000
1.244
1.322
1.538
4.808
4.824
5.109
5.126
5.142
5.692
5.695
5.719
5.761
5.786
6.206
6.231
6.254
6.768
6.793
7.250
7.259
7.280
7.337
7.358
H2O
Me
t-Bu
5k'
3.10
9.25
1.98
1.00
2.04
1.00
1.01
2.02
2.02
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)


206.724
149.737
137.508
135.037
134.371
130.302
128.777
127.770
127.052
125.155
121.262
98.147
77.679
39.447
34.576
31.317
27.863
Me
t-Bu
5k'
ppm (t1)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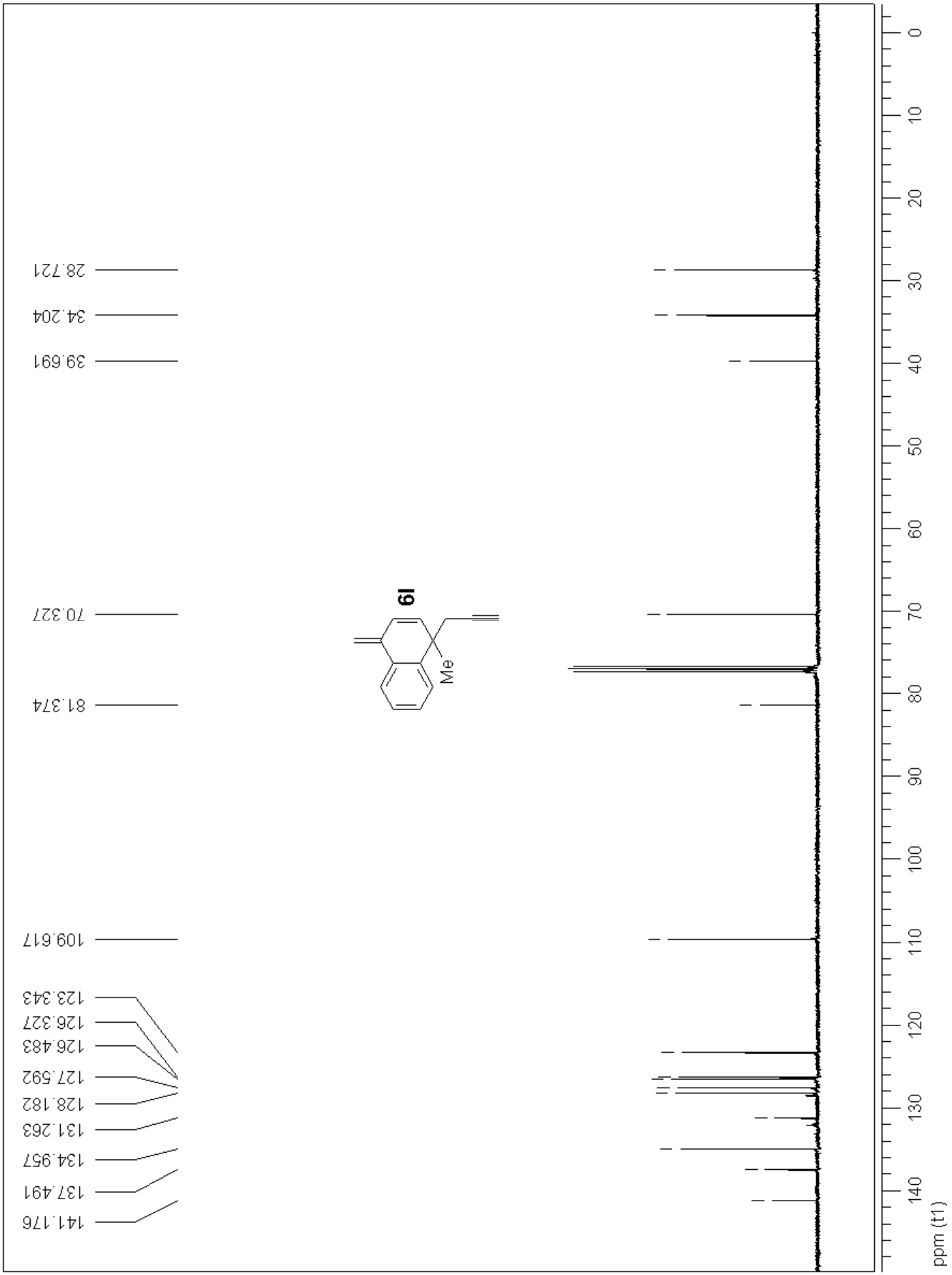
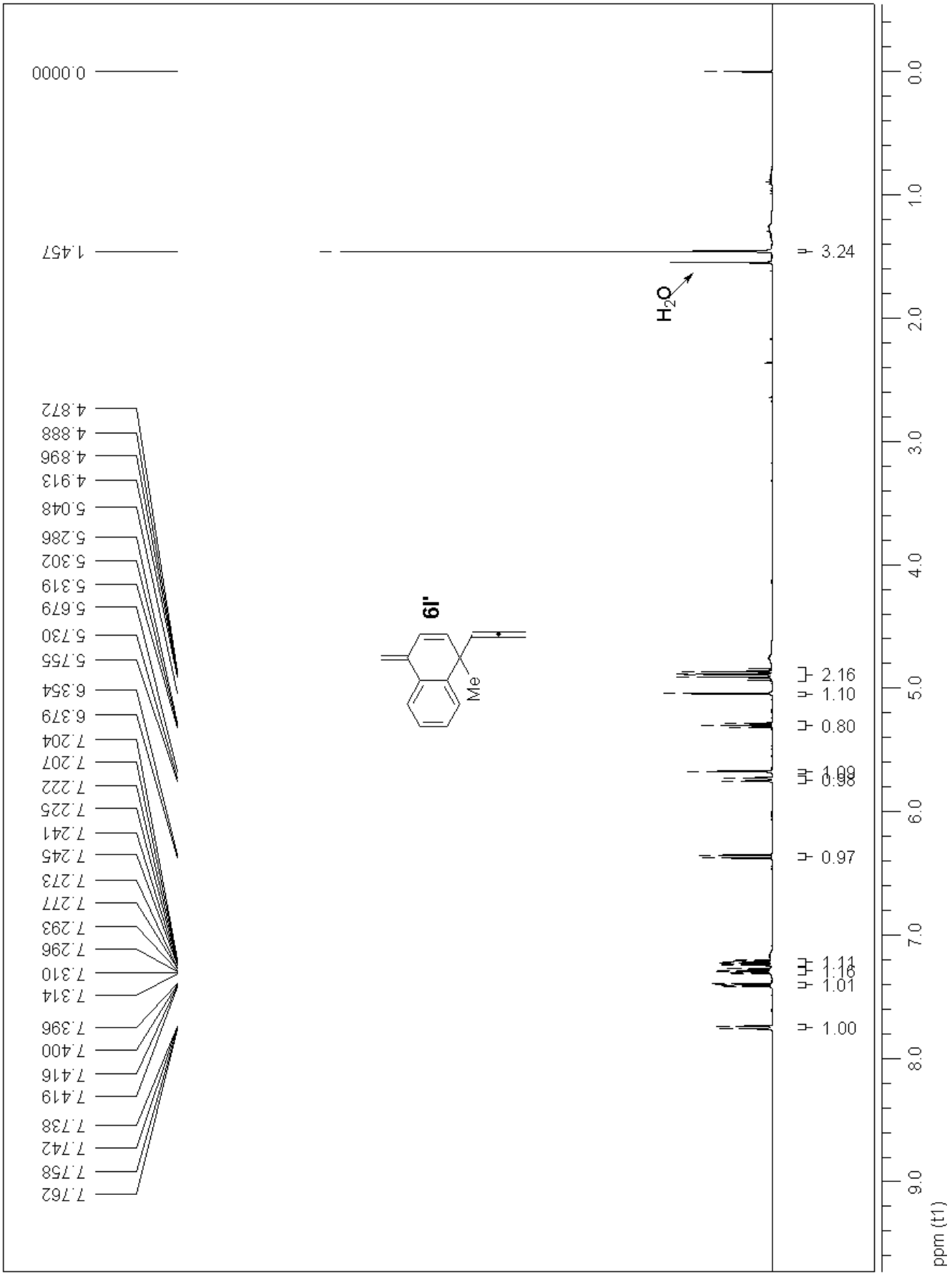
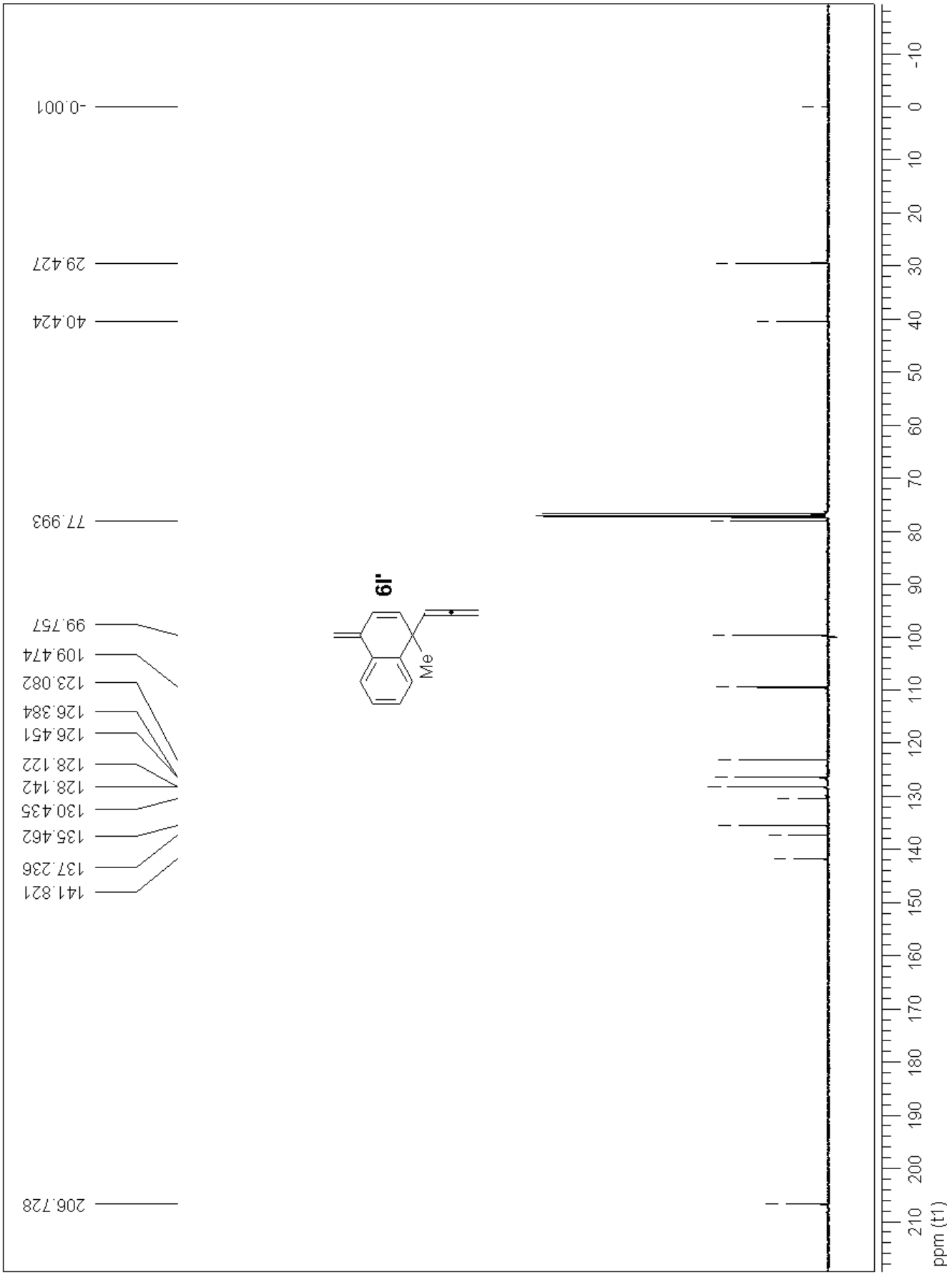
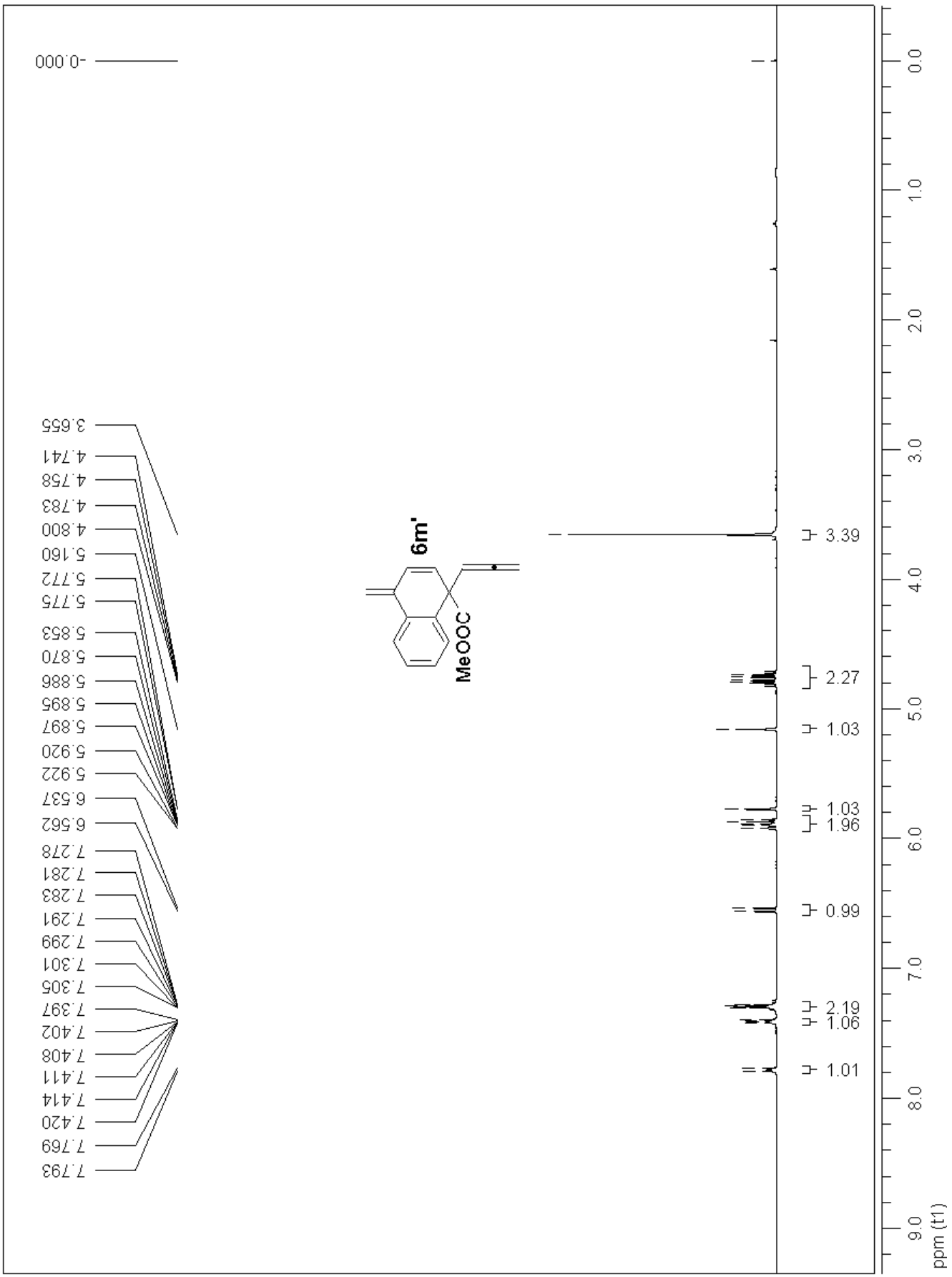
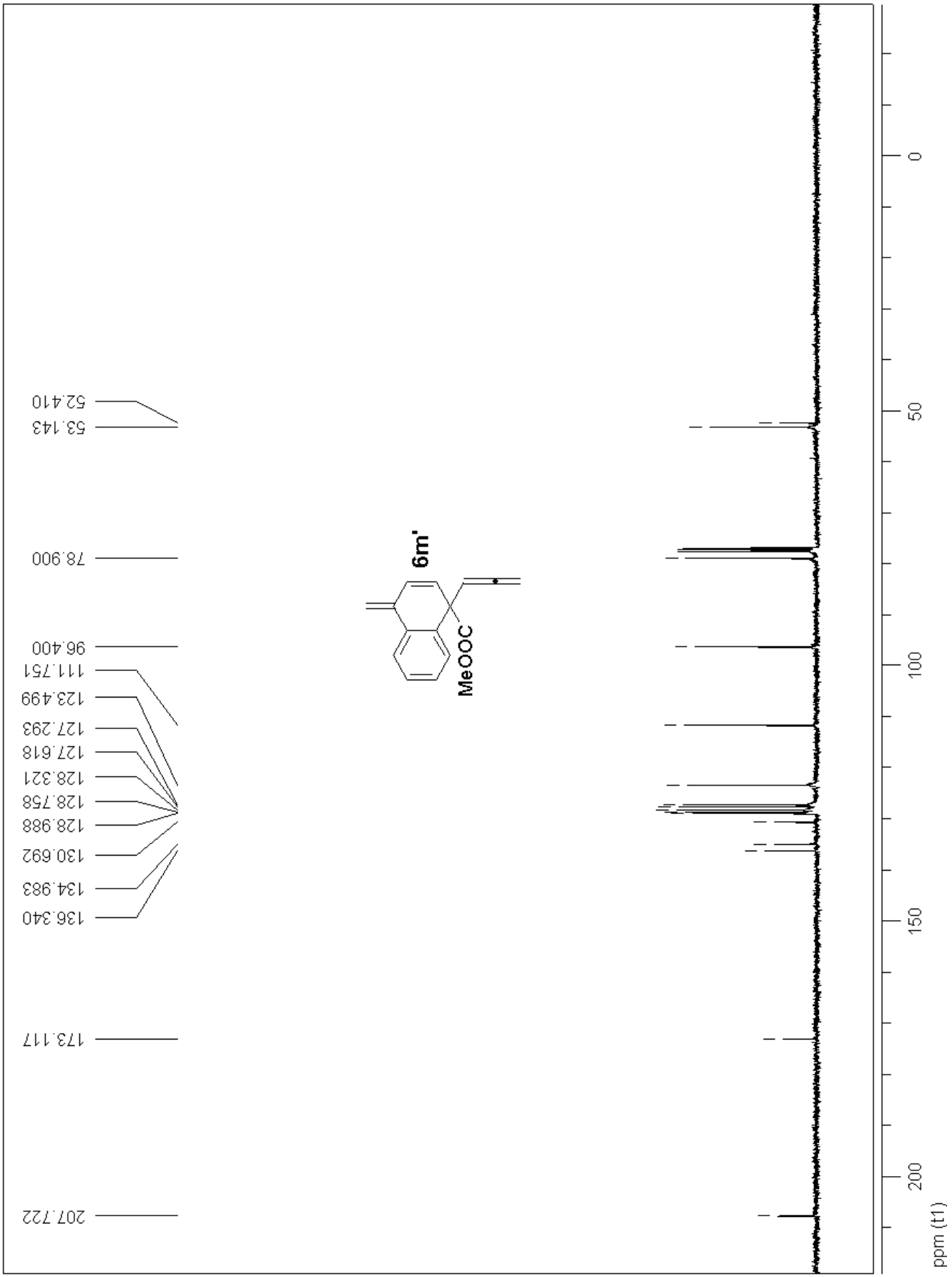
1.487
1.552
1.929
1.936
1.942
2.548
2.555
2.561
5.052
5.678
5.681
5.893
5.894
5.918
6.429
6.454
7.242
7.243
7.245
7.251
7.261
7.265
7.292
7.296
7.312
7.315
7.407
7.410
7.427
7.430
7.764
7.768
7.784
7.787
6l
Me
H2O
3.40
0.73
2.04
1.12
1.15
1.04
1.00
1.27
1.06
1.12
1.03
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

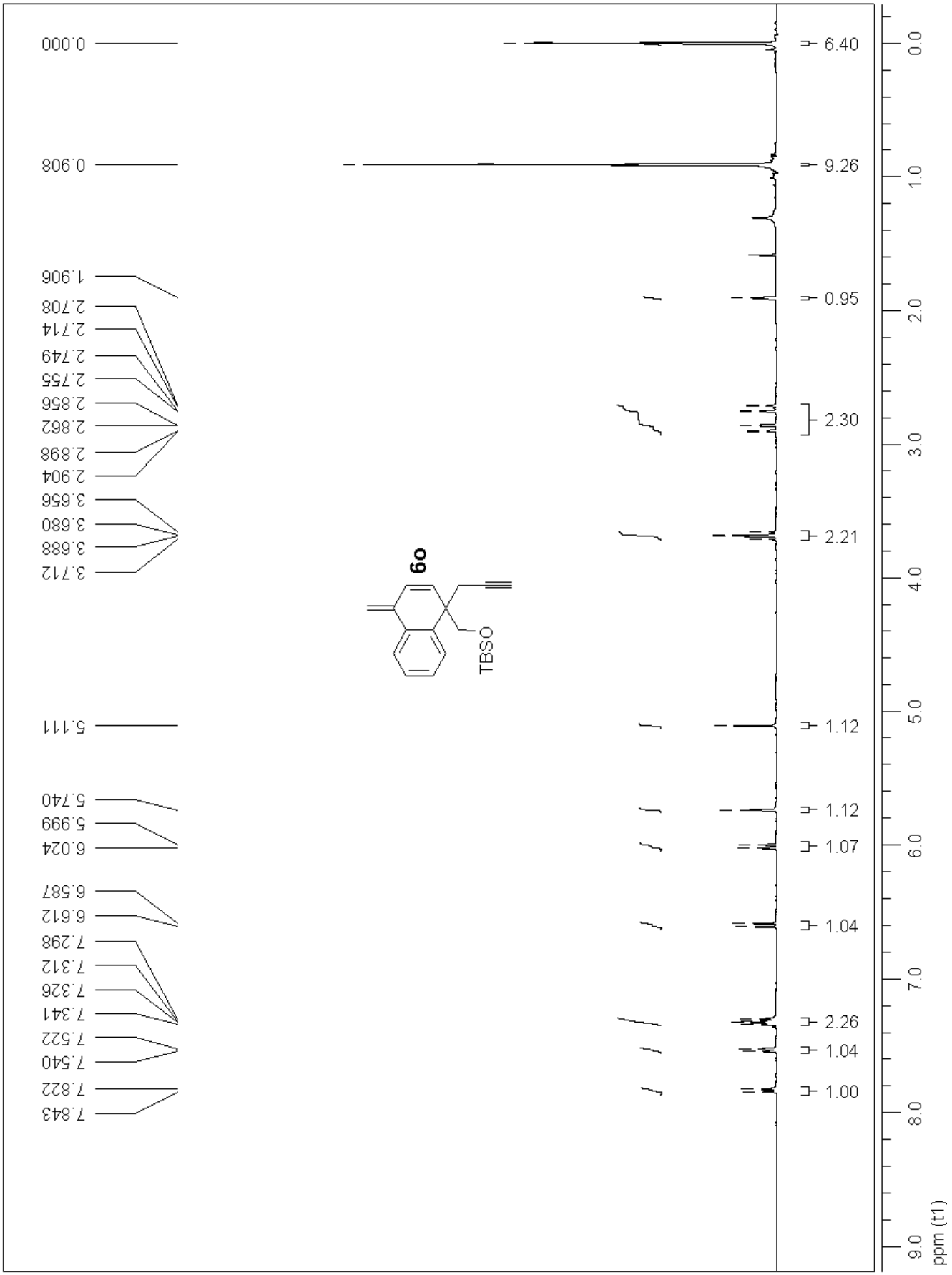

28.721
34.204
39.691
70.327
81.374
109.617
123.343
126.327
126.483
127.592
128.182
131.263
134.957
137.491
141.176
6l
Me
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm (f1)

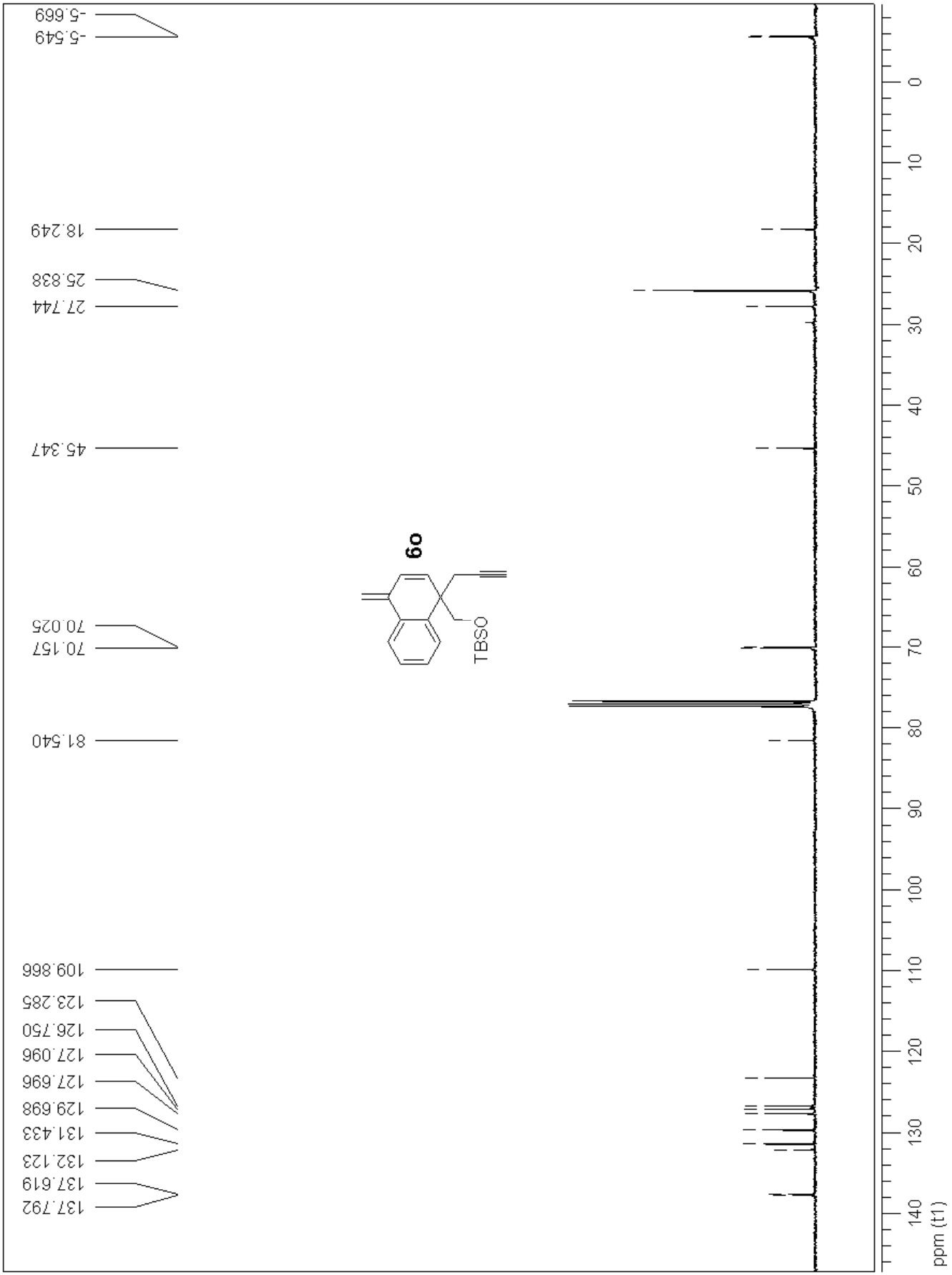

0.0000
1.457
4.872
4.888
4.896
4.913
5.048
5.286
5.302
5.319
5.679
5.730
5.755
6.354
6.379
7.204
7.207
7.222
7.225
7.241
7.245
7.273
7.277
7.293
7.296
7.310
7.314
7.396
7.400
7.416
7.419
7.738
7.742
7.758
7.762
6l'
Me
H2O
3.24
2.16
1.10
0.80
1.09
0.98
0.97
1.14
1.16
1.01
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
ppm (f1)

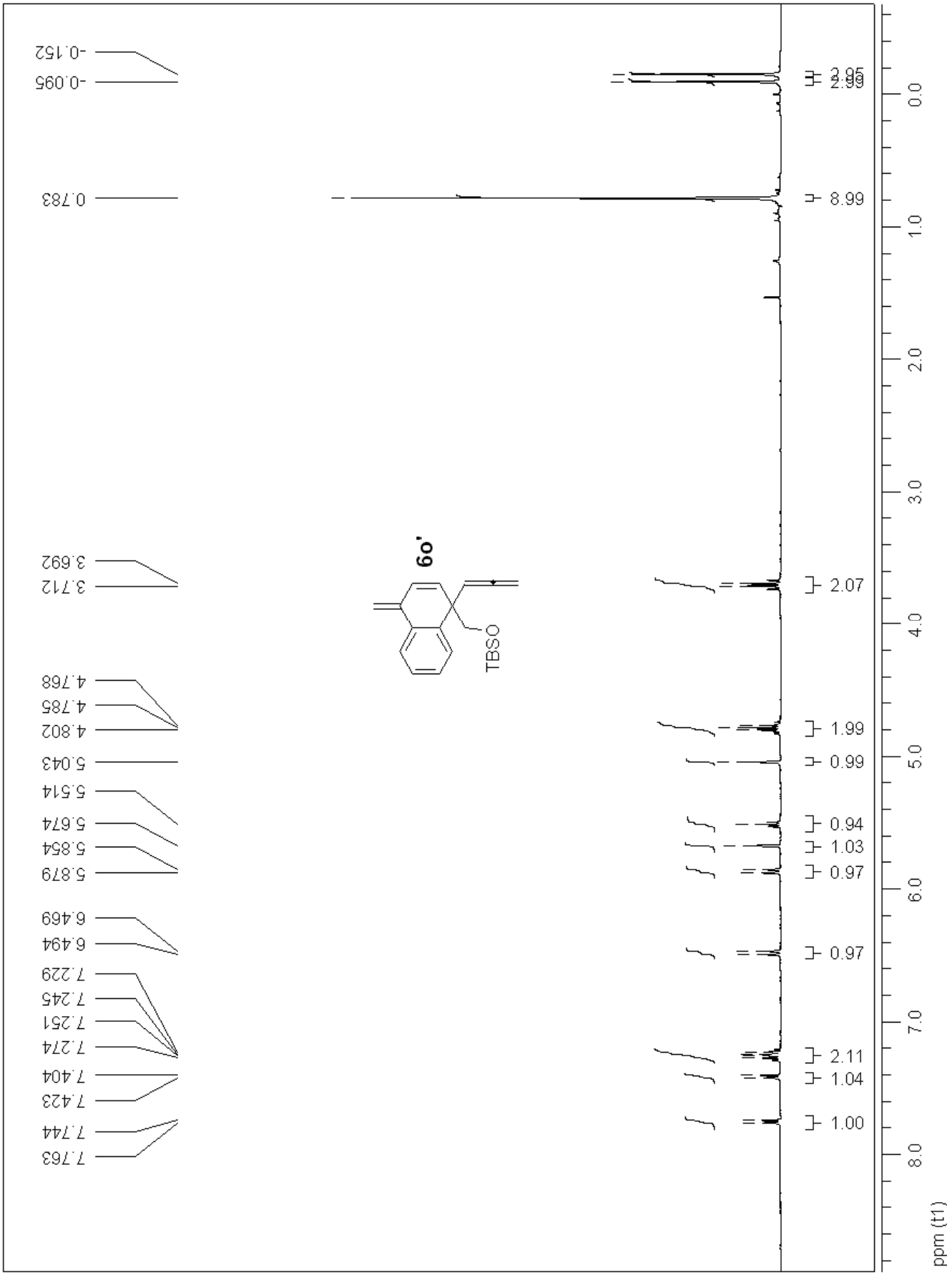

6l'
Me
206.728
141.821
137.236
135.462
130.435
128.142
128.122
126.451
126.384
123.082
109.474
99.757
77.993
40.424
29.427
-0.001
ppm (t1)

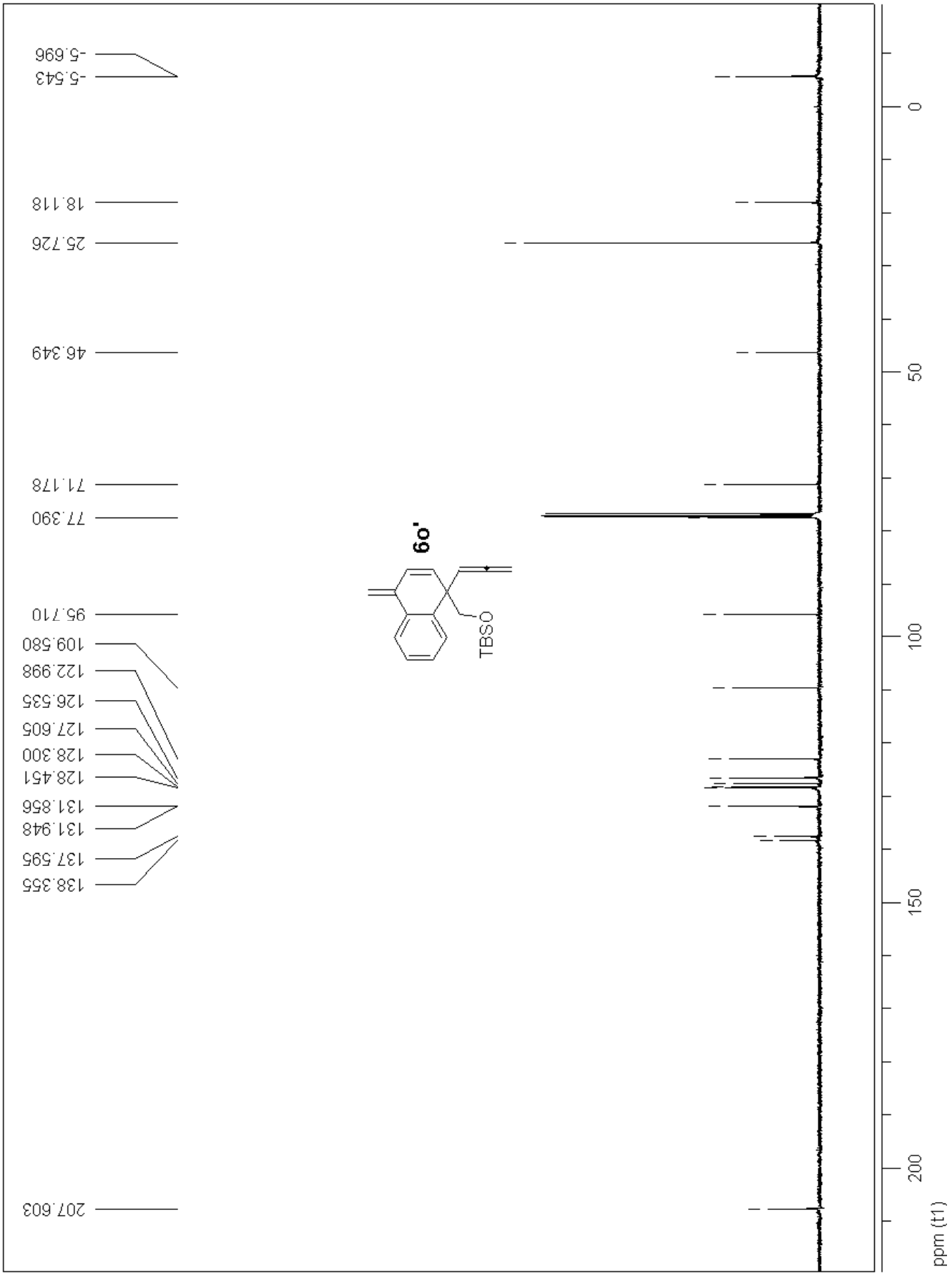

6m'
MeOOC
3.39
2.27
1.03
1.03
1.96
0.99
2.19
1.06
1.01
ppm (f1)

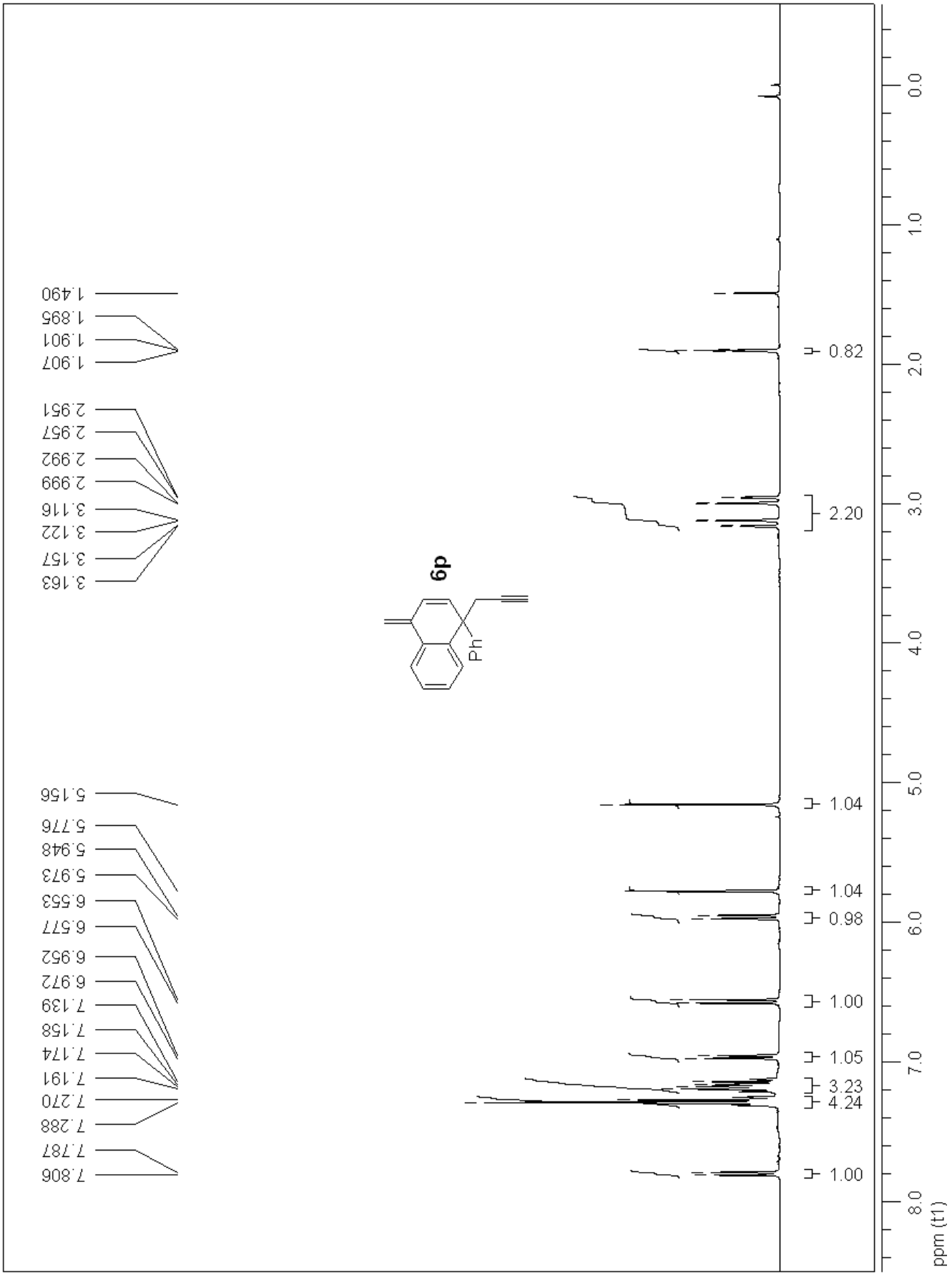

6m'
MeOOC
207.722
173.117
136.340
134.983
130.692
128.988
128.758
128.321
127.618
127.293
123.499
111.751
96.400
78.900
53.143
52.410
200
150
100
50
0
ppm (t1)

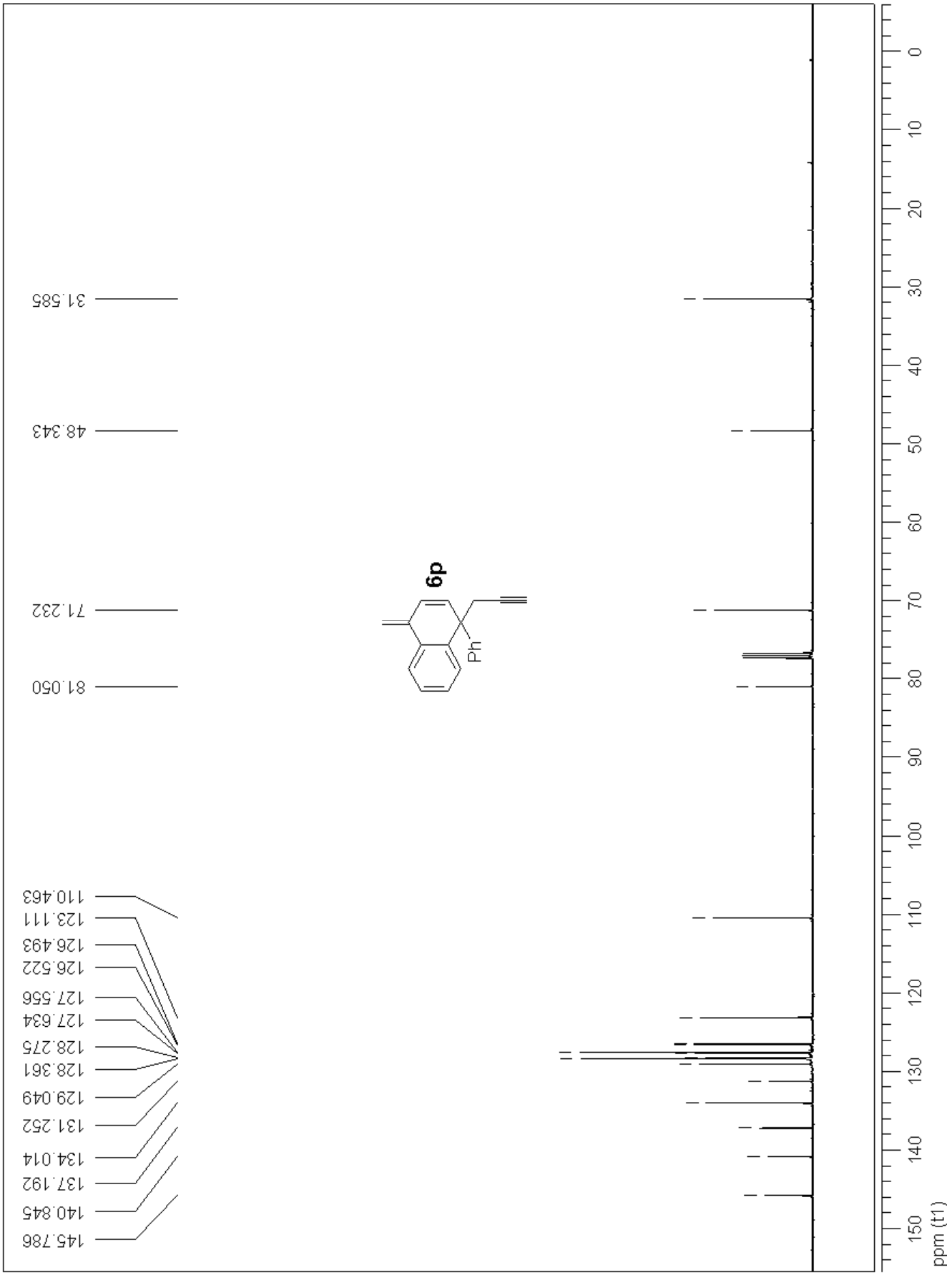

0.000
0.908
1.906
2.708
2.714
2.749
2.755
2.856
2.862
2.898
2.904
3.656
3.680
3.688
3.712
5.111
5.740
5.999
6.024
6.587
6.612
7.298
7.312
7.326
7.341
7.522
7.540
7.822
7.843
6.40
9.26
0.95
2.30
2.21
1.12
1.12
1.07
1.04
2.26
1.04
1.00
6o
TBSO
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
ppm (t1)

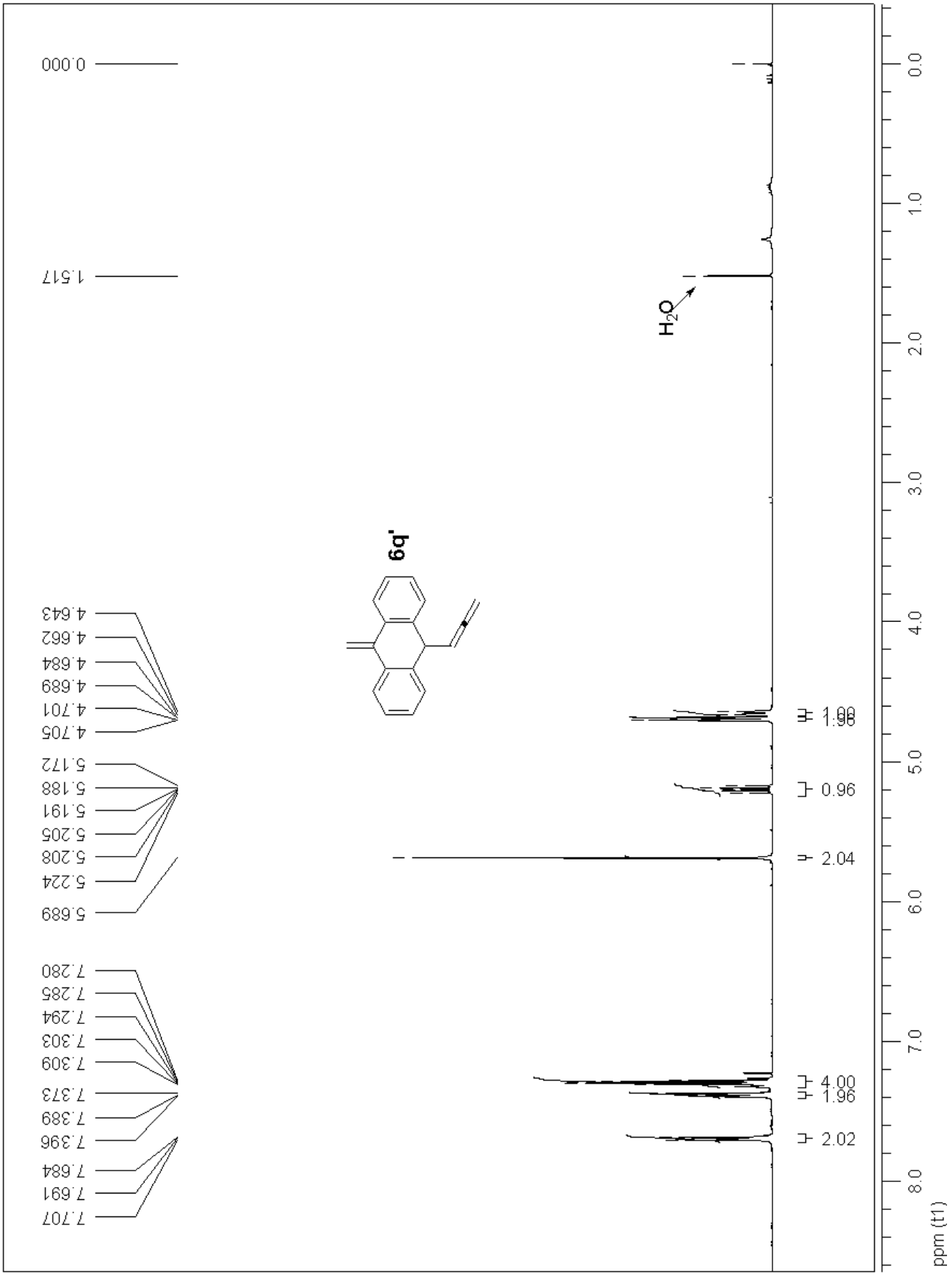

-5.669
-5.549
18.249
25.838
27.744
45.347
70.025
70.157
81.540
109.866
123.285
126.750
127.096
127.696
129.698
131.433
132.123
137.619
137.792
6o
TBSO
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm (f1)

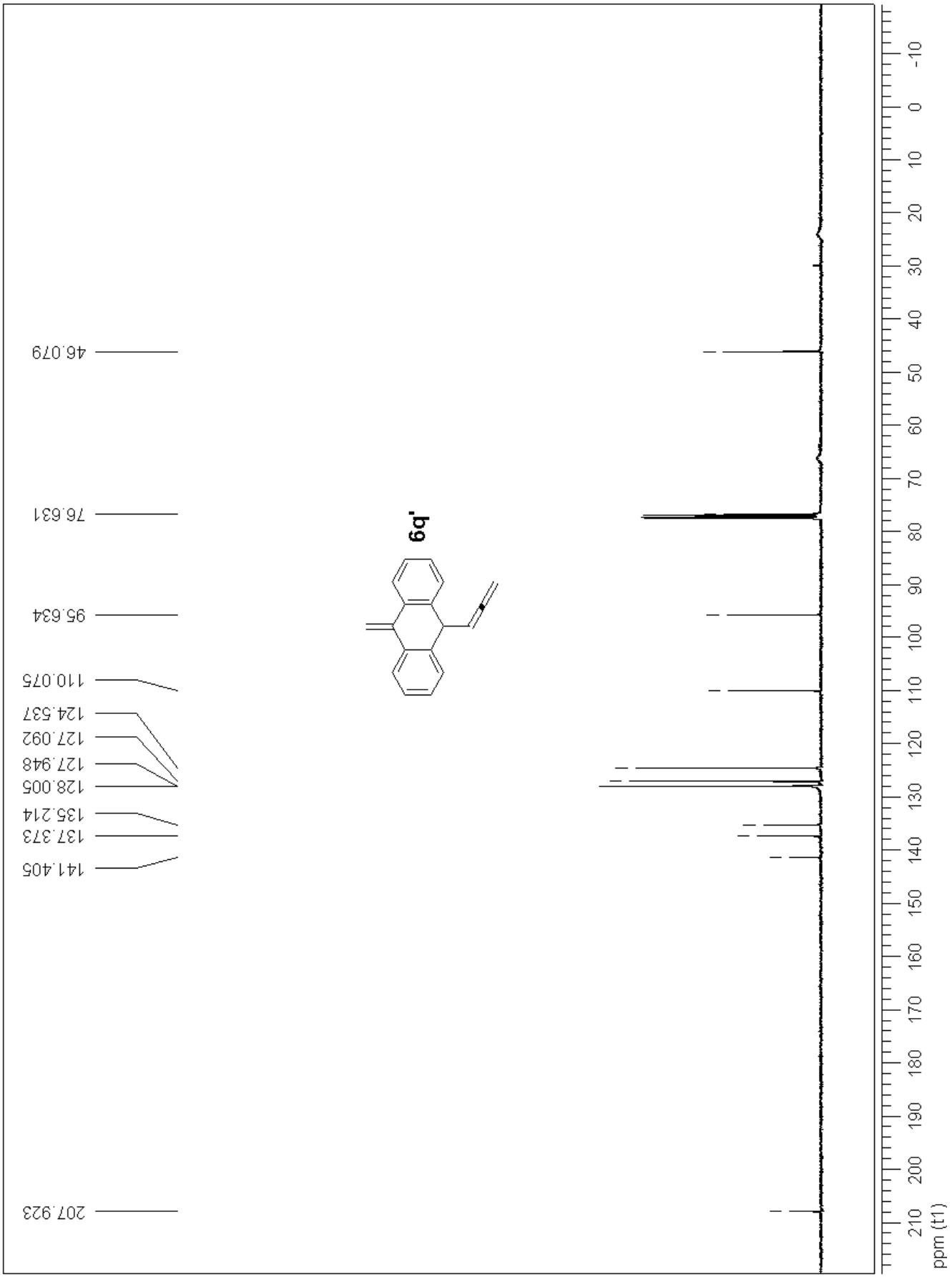

-0.152
-0.095
0.783
3.692
3.712
4.768
4.785
4.802
5.043
5.514
5.674
5.854
5.879
6.469
6.494
7.229
7.245
7.251
7.274
7.404
7.423
7.744
7.763
6o'
TBSO
2.95
2.99
8.99
2.07
1.99
0.99
0.94
1.03
0.97
0.97
2.11
1.04
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

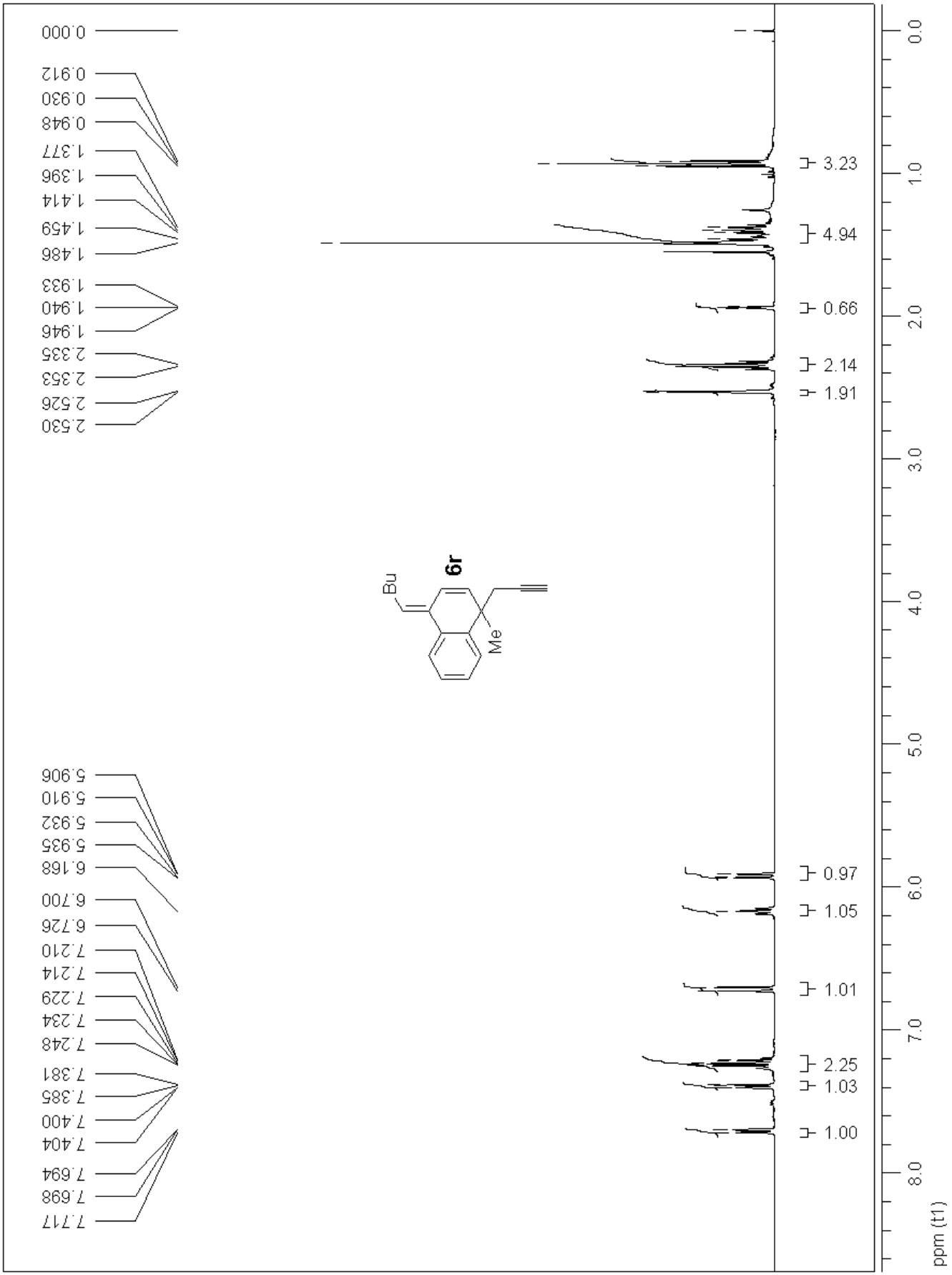

-5.696
-5.543
18.118
25.726
46.349
71.178
77.390
95.710
109.580
122.998
126.535
127.605
128.300
128.451
131.856
131.948
137.595
138.355
207.603
6o'
TBSO
0
50
100
150
200
ppm (t1)

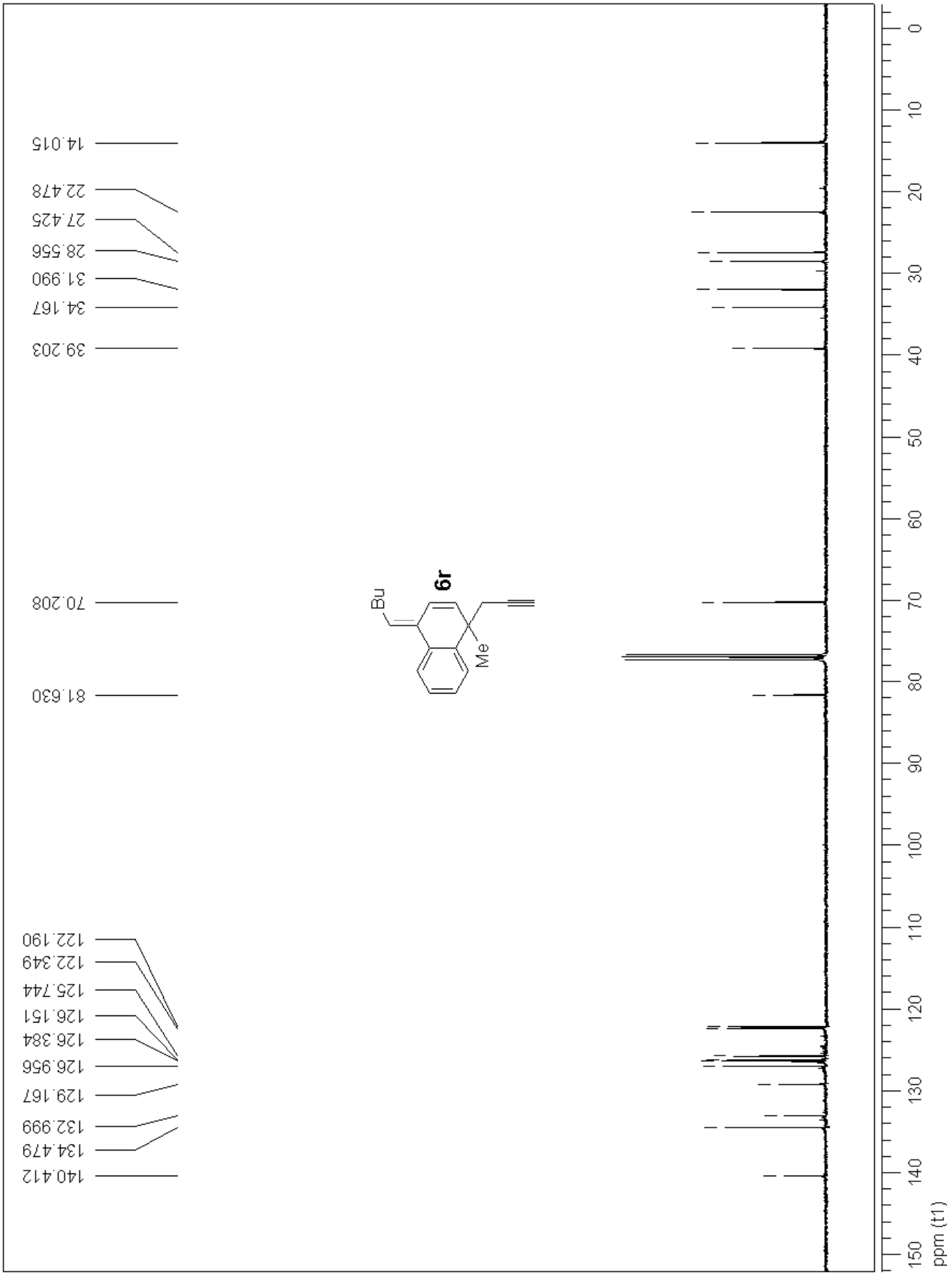

1.490
1.895
1.901
1.907
2.951
2.957
2.992
2.999
3.116
3.122
3.157
3.163
5.156
5.776
5.948
5.973
6.553
6.577
6.952
6.972
7.139
7.158
7.174
7.191
7.270
7.288
7.787
7.806
6p
Ph
1.00
1.04
1.04
0.98
1.00
1.05
3.23
4.24
1.00
0.82
2.20
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

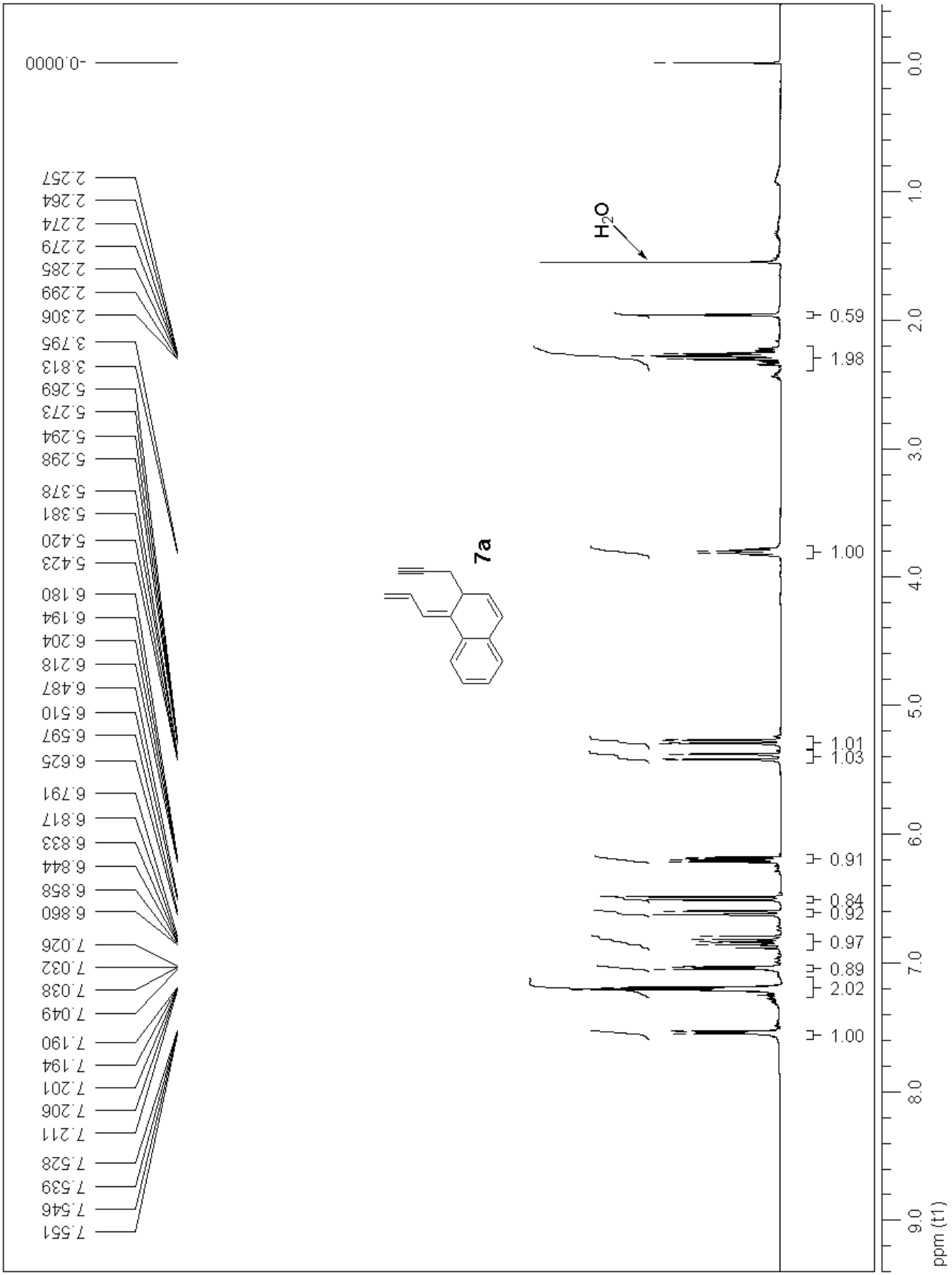

6p
Ph
31.585
48.343
71.232
81.050
110.463
123.111
126.493
126.522
127.556
127.634
128.275
128.361
129.049
131.252
134.014
137.192
140.845
145.786
ppm (t1)

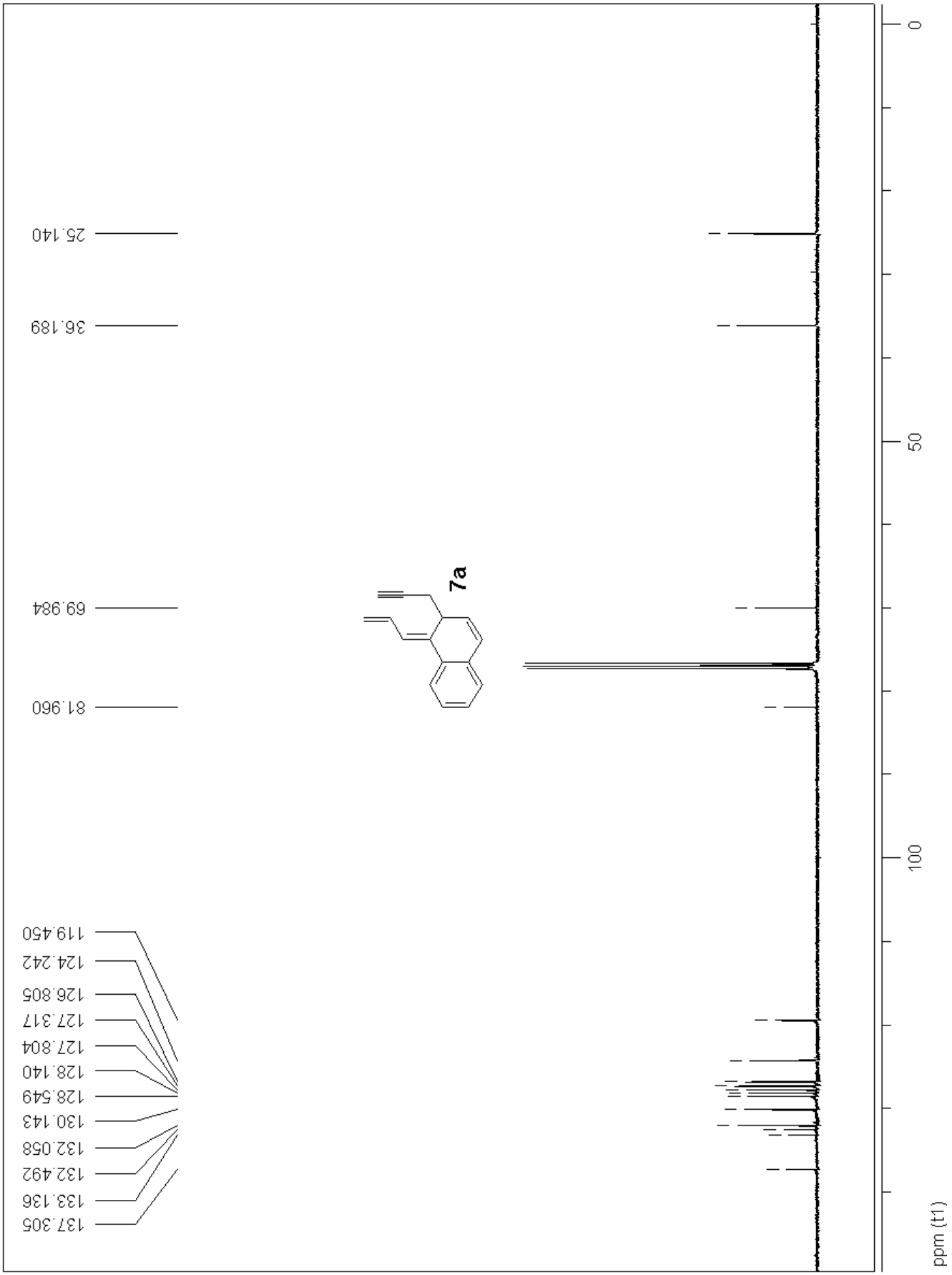

0.000
1.517
4.643
4.662
4.684
4.689
4.701
4.705
5.172
5.188
5.191
5.205
5.208
5.224
5.689
7.280
7.285
7.294
7.303
7.309
7.373
7.389
7.396
7.684
7.691
7.707
6q'
H_2O
1.00
1.98
0.96
2.04
4.00
1.96
2.02
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

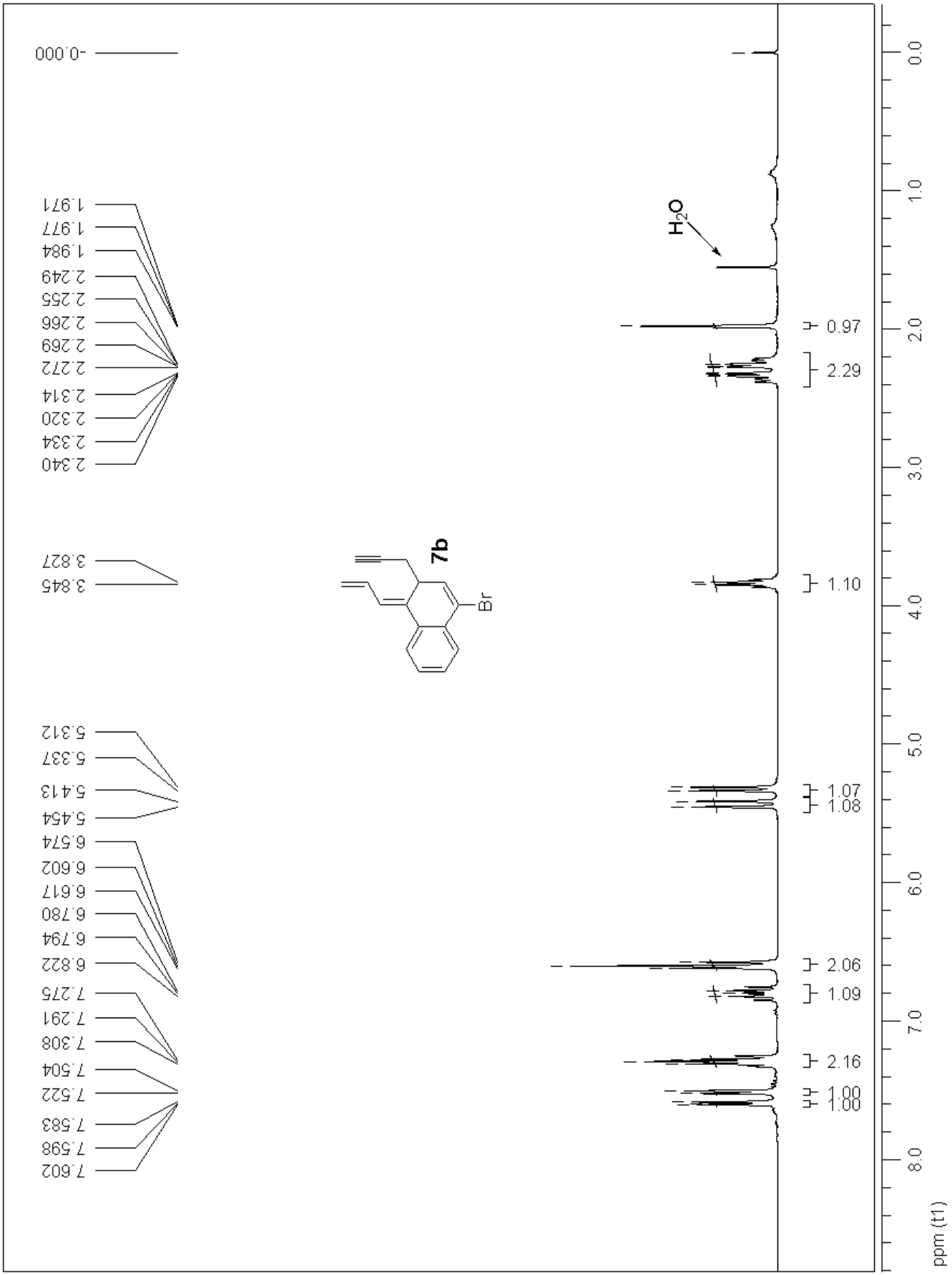

6q'
207.923
141.405
137.373
135.214
128.005
127.948
127.092
124.537
110.075
95.634
76.631
46.079
ppm (t1)

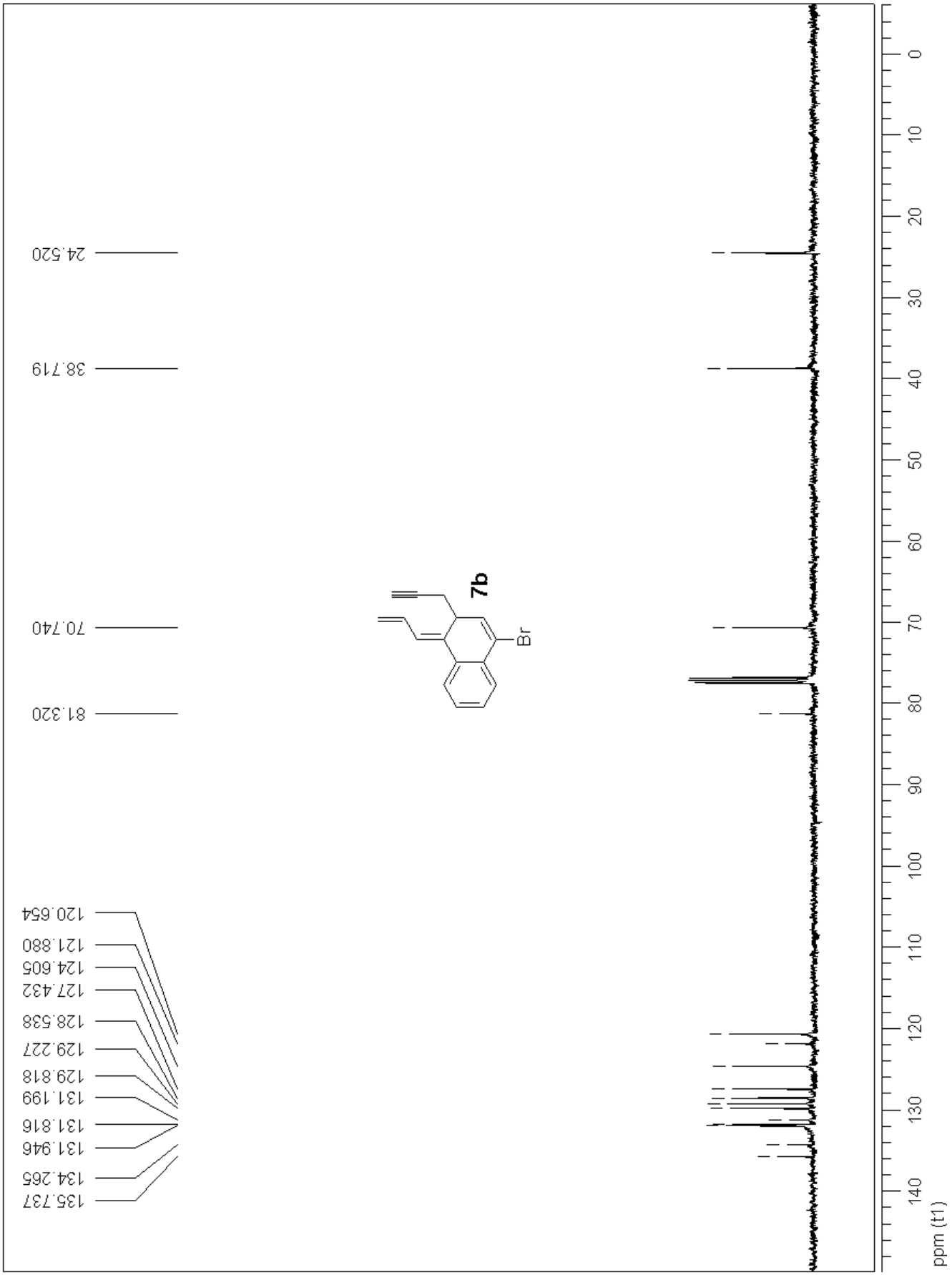

0.000
0.912
0.930
0.948
1.377
1.396
1.414
1.459
1.486
1.933
1.940
1.946
2.335
2.353
2.526
2.530
5.906
5.910
5.932
5.935
6.168
6.700
6.726
7.210
7.214
7.229
7.234
7.248
7.381
7.385
7.400
7.404
7.694
7.698
7.717
Bu
6r
Me
3.23
4.94
0.66
2.14
1.91
0.97
1.05
1.01
2.25
1.03
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (f1)

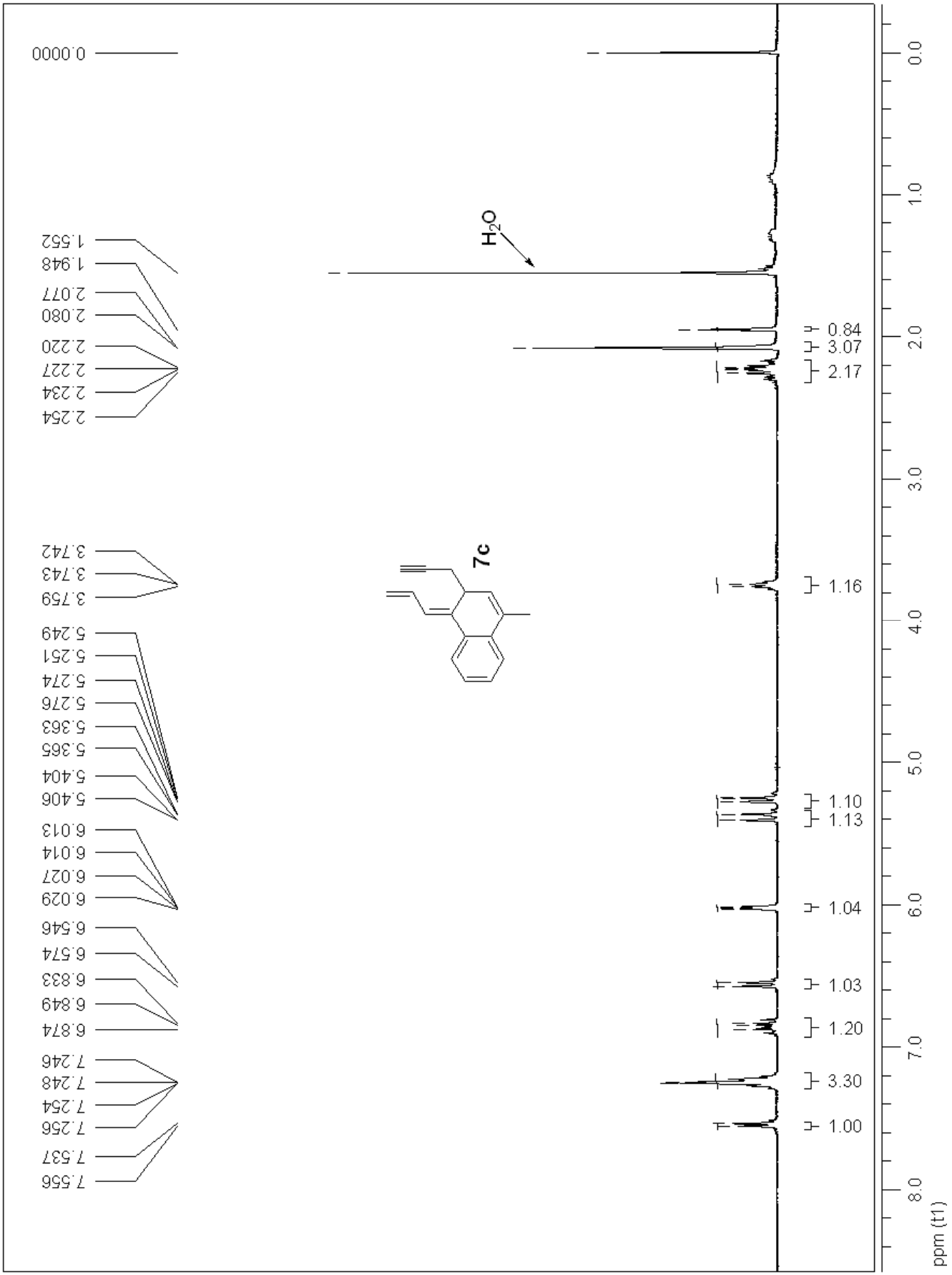

14.015
22.478
27.425
28.556
31.990
34.167
39.203
70.208
81.630
122.190
122.349
125.744
126.151
126.384
126.956
129.167
132.999
134.479
140.412
Bu
Me
6r
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
ppm (f1)

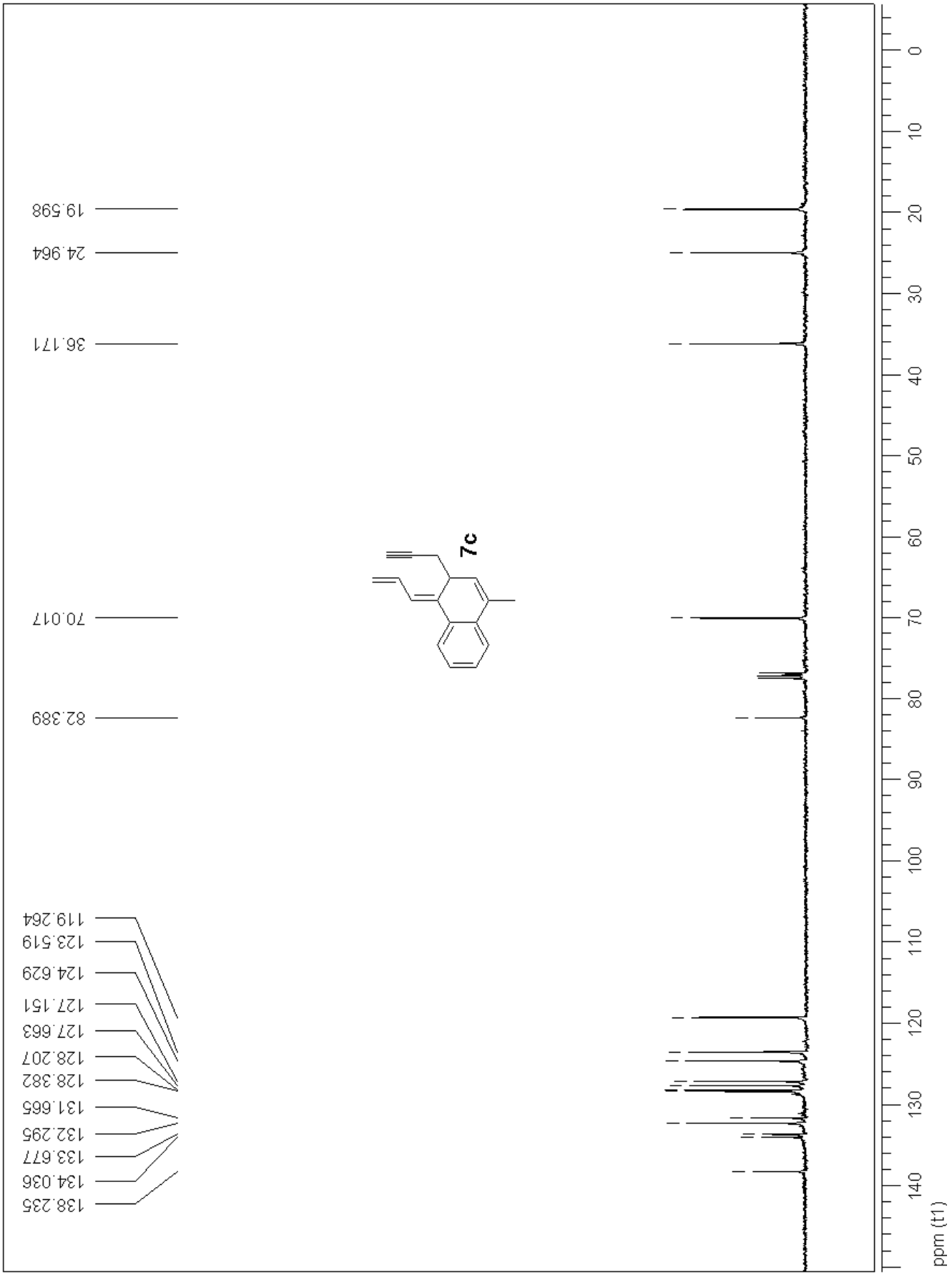

0.0000
2.257
2.264
2.274
2.279
2.285
2.299
2.306
3.795
3.813
5.269
5.273
5.294
5.298
5.378
5.381
5.420
5.423
6.180
6.194
6.204
6.218
6.487
6.510
6.597
6.625
6.791
6.817
6.833
6.844
6.858
6.860
7.026
7.032
7.038
7.049
7.190
7.194
7.201
7.206
7.211
7.528
7.539
7.546
7.551
H2O
7a
0.59
1.98
1.00
1.01
1.03
0.91
0.84
0.92
0.97
0.89
2.02
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
ppm (f1)

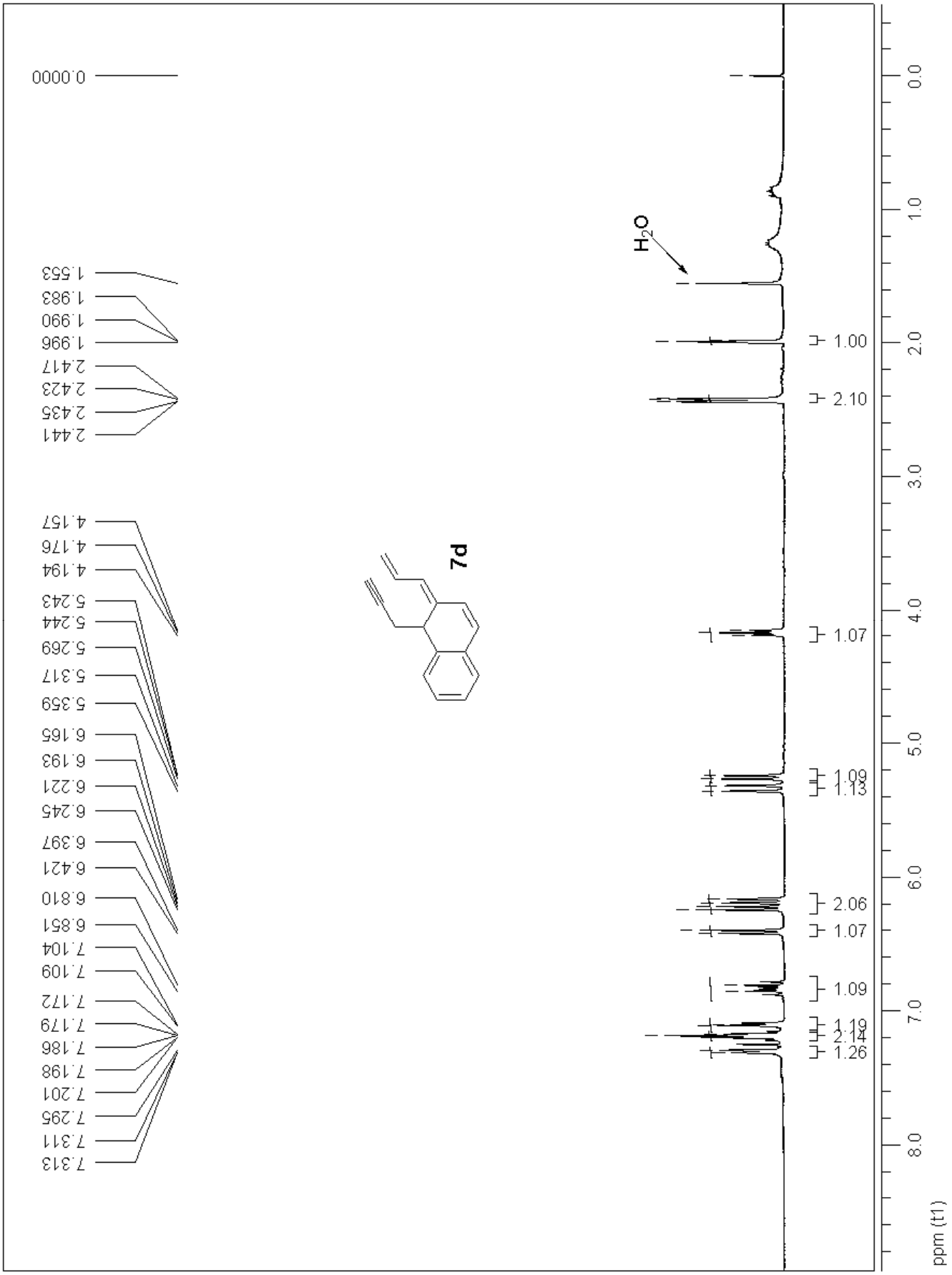

7a
25.140
36.189
69.984
81.960
119.450
124.242
126.805
127.317
127.804
128.140
128.549
130.143
132.058
132.492
133.136
137.305
0
50
100
ppm (t1)


-0.000
1.971
1.977
1.984
2.249
2.255
2.266
2.269
2.272
2.314
2.320
2.334
2.340
3.827
3.845
5.312
5.337
5.413
5.454
6.574
6.602
6.617
6.780
6.794
6.822
7.275
7.291
7.308
7.504
7.522
7.583
7.598
7.602
7b
Br
H2O
0.97
2.29
1.10
1.07
1.08
2.06
1.09
2.16
1.00
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

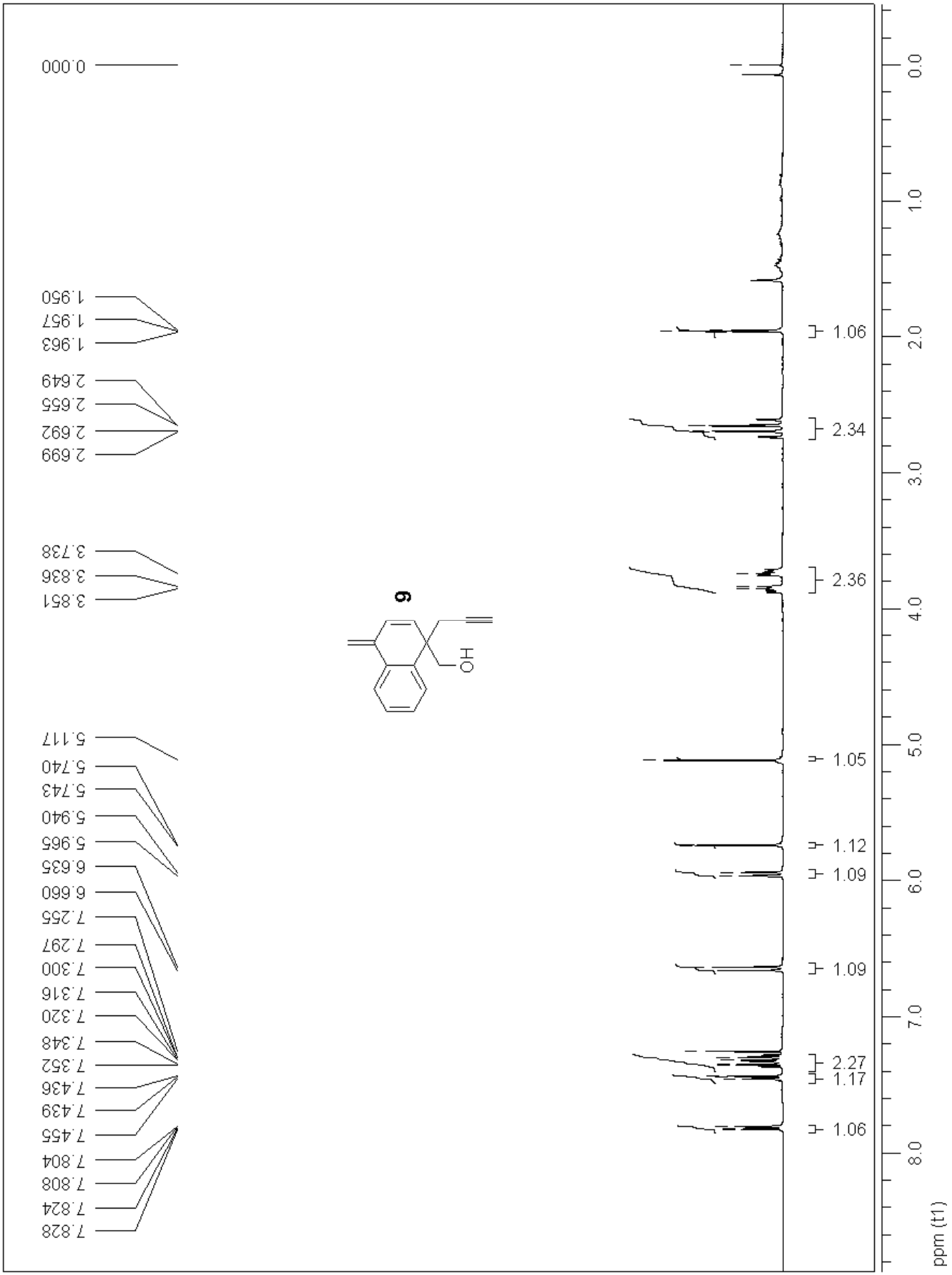

24.520
38.719
70.740
81.320
120.654
121.880
124.605
127.432
128.538
129.227
129.818
131.199
131.816
131.946
134.265
135.737
7b
Br
ppm (t1)

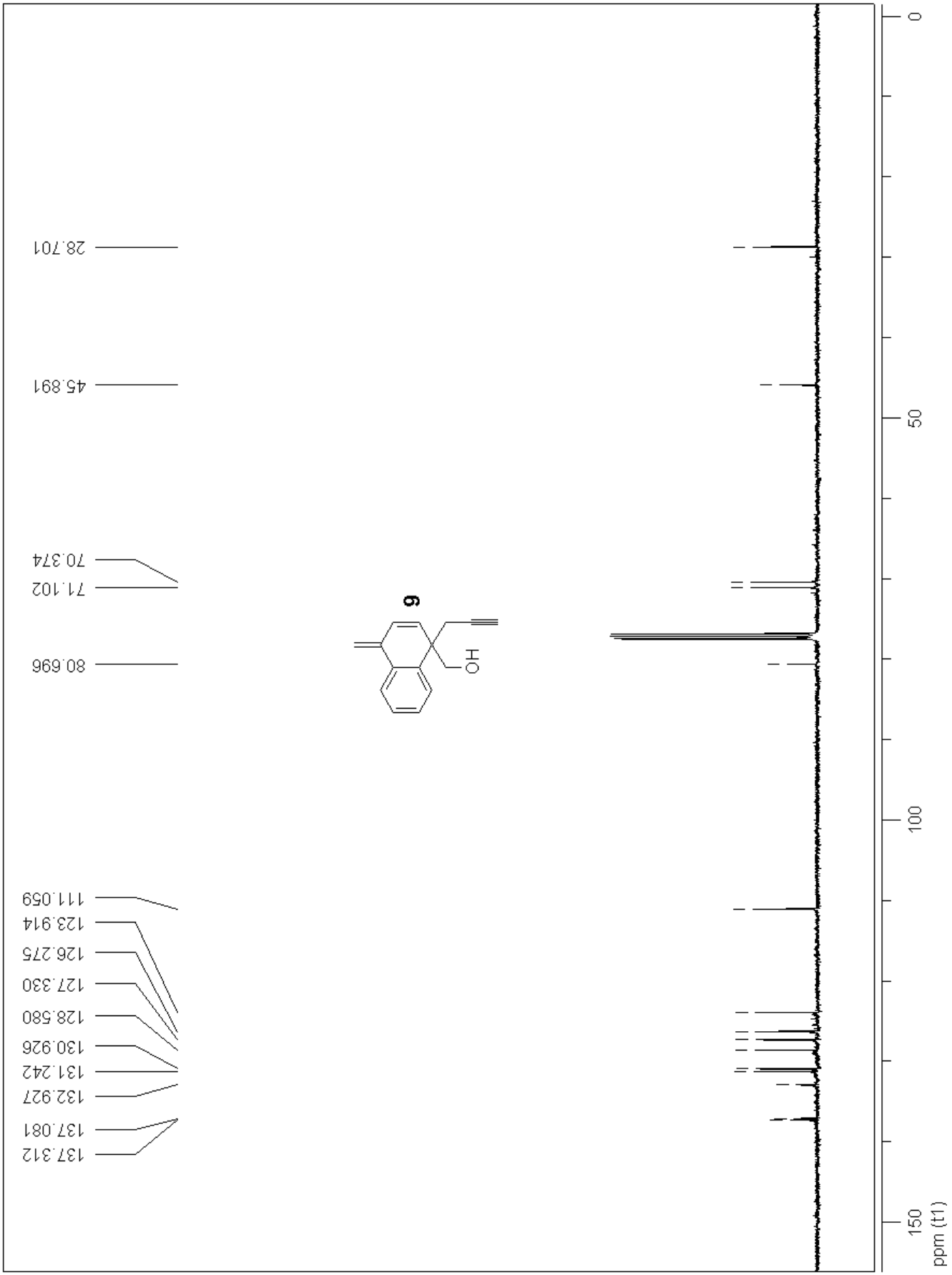

0.0000
1.552
1.948
2.077
2.080
2.220
2.227
2.234
2.254
3.742
3.743
3.759
5.249
5.251
5.274
5.276
5.363
5.365
5.404
5.406
6.013
6.014
6.027
6.029
6.546
6.574
6.833
6.849
6.874
7.246
7.248
7.254
7.256
7.537
7.556
H2O
7c
0.84
3.07
2.17
1.16
1.10
1.13
1.04
1.03
1.20
3.30
1.00
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)


19.598
24.964
36.171
70.017
82.389
119.264
123.519
124.629
127.151
127.663
128.207
128.382
131.665
132.295
133.677
134.036
138.235
7c
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm (f1)


0.0000
1.553
1.983
1.990
1.996
2.417
2.423
2.435
2.441
4.157
4.176
4.194
5.243
5.244
5.269
5.317
5.359
6.165
6.193
6.221
6.245
6.397
6.421
6.810
6.851
7.104
7.109
7.172
7.179
7.186
7.198
7.201
7.295
7.311
7.313
7d
H2O
1.00
2.10
1.07
1.09
1.13
2.06
1.07
1.09
1.19
2.14
1.26
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)

29.281
40.157
71.307
82.357
119.347
127.044
127.127
127.235
127.418
128.785
129.336
131.186
132.328
132.880
137.040
138.920
7d
0
50
100
ppm (t1)


0.000
1.950
1.957
1.963
2.649
2.655
2.692
2.699
3.738
3.836
3.851
5.117
5.740
5.743
5.940
5.965
6.635
6.660
7.255
7.297
7.300
7.316
7.320
7.348
7.352
7.436
7.439
7.455
7.804
7.808
7.824
7.828
6
OH
1.06
2.34
2.36
1.05
1.12
1.09
1.09
2.27
1.17
1.06
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
ppm (t1)


137.312
137.081
132.927
131.242
130.926
128.580
127.330
126.275
123.914
111.059
80.696
71.102
70.374
45.891
28.701
9
OH
0
50
100
150
ppm (f1)