Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Protonated montmorillonite-mediated highly specific isomerization of oleanolic acid esters: application to the synthesis of $\Delta^{13(18)}$-CDDO-Me

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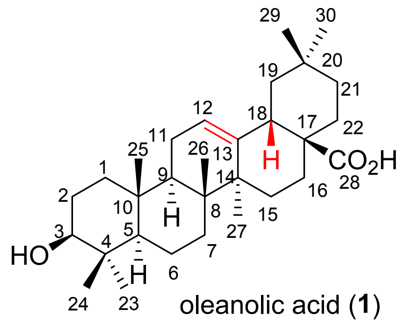
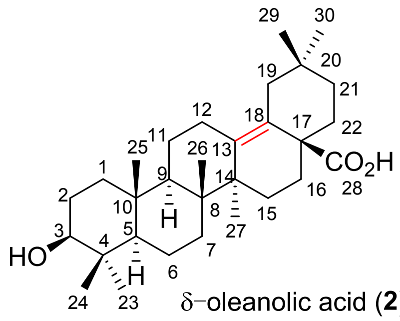
Table 1. Chemical shifts of specific H and C atoms of oleanolic acid (1) and δ-oleanolic acid (2)[a]



oleanolic acid (**1**)

^{13}C NMR (500 MHz, C_5D_5N)		^{1}H NMR (125 MHz, C_5D_5N)	
atom	δ_C	atom	δ_H
C-3	79.4	3β-H	3.42 (dd, *J* = 10.6, 5.5 Hz, 1H)
C-12	123.8	12-H	5.48 (t, *J* = 3.3 Hz, 1H)
C-13	146.1	18β-H	3.29 (dd, *J* = 13.8, 4.0 Hz, 1H)
C-18	43.3	11-H	2.07-2.20 (m, 2H)
C-28	181.4		



δ-oleanolic acid (**2**)

^{13}C NMR (500 MHz, C_5D_5N)		^{1}H NMR (125 MHz, C_5D_5N)	
atom	δ_C	atom	δ_H
C-3	79.4	3β-H	3.46 (dd, *J* = 10.1, 6.0 Hz, 1H)
C-12	25.7	12-H	2.84 (dd, *J* = 14.6, 2.0 Hz, 1H) 2.60 (d, *J* = 14.0 Hz, 1H)
C-13	139.2	19-H	2.24-2.26 (m, 1H) 1.91-1.95 (m, 1H)
C-18	130.6		
C-28	180.2		

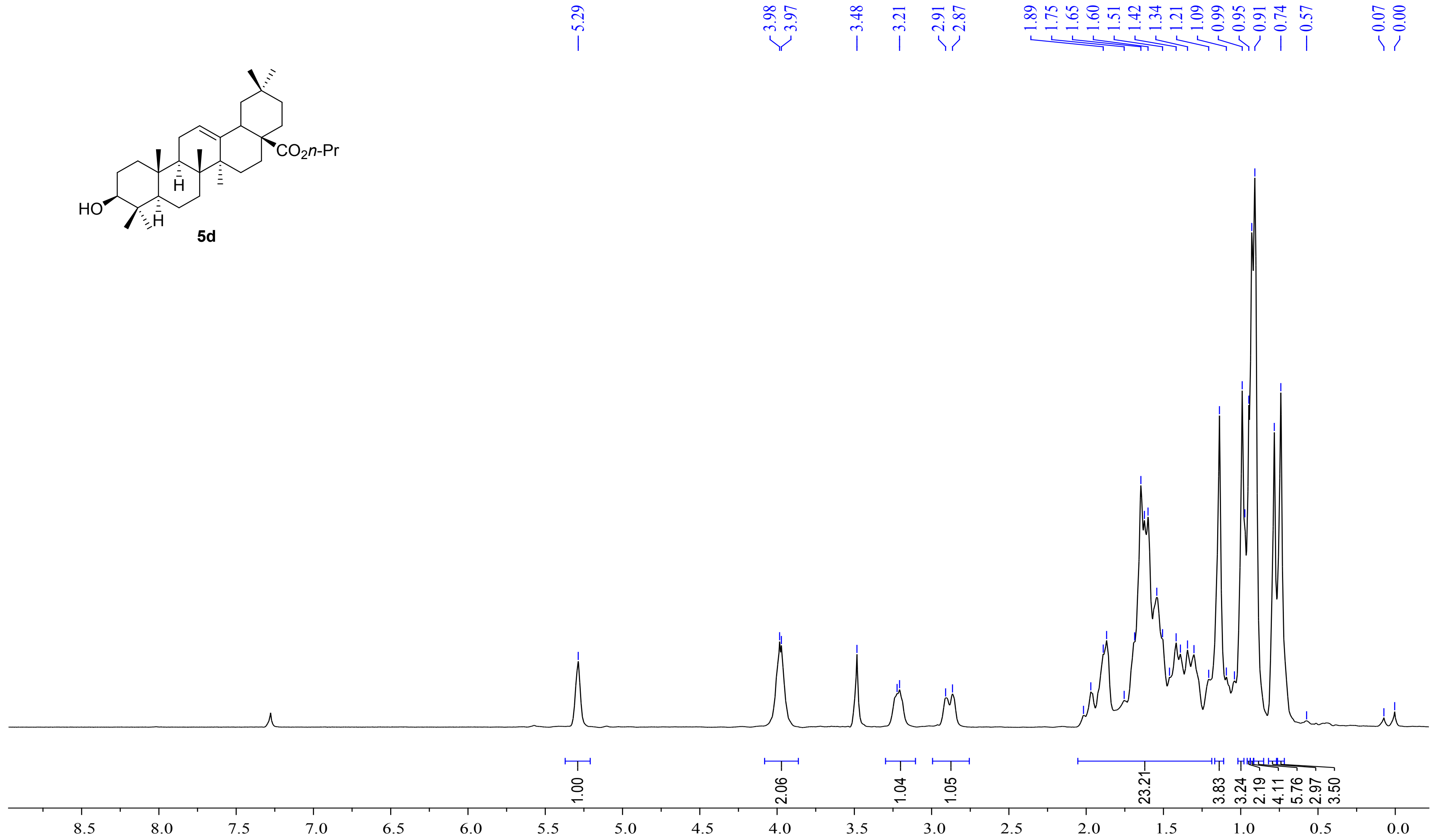
[a] In the ^{1}H NMR spectrum, the signal due to the olefinic proton resonating at 5.48 (t, *J* = 3.3 Hz, 1H) is characteristic of oleanolic acid; the signals due to the allylic protons resonating at 2.84 (dd, *J* = 14.6, 2.0 Hz, 1H) and 2.60 (d, *J* = 14.0 Hz, 1H) is characteristic of δ-oleanolic acid. In the ^{13}C NMR spectrum, the signals due to the olefinic carbons resonating at 123.8 and 146.1 is characteristic of oleanolic acid (**1**); the signals due to the olefinic carbons resonating at 130.6 and 139.2 is characteristic of δ-oleanolic acid (**2**).

^{1}H and ^{13}C NMR data of oleanolic acid (1) and δ-oleanolic acid (2) as following:

Oleanolic acid (1). ^{1}H NMR (500 MHz, C_5D_5N) δ 5.48 (t, J = 3.3 Hz, 1H), 3.42 (dd, J = 10.6, 5.5 Hz, 1H), 3.29 (dd, J = 13.8, 4.0 Hz, 1H), 2.07-2.20 (m, 2H), 2.00-2.06 (m, 1H), 1.93-1.96 (m, 3H), 1.78-1.83 (m, 4H), 1.68 (t, J = 8.9 Hz, 1H), 0.85-1.58 (m, 11H), 1.27 (s, 3H), 1.22 (s, 3H), 1.02 (s, 3H), 1.01 (s, 3H), 1.00 (s, 3H), 0.94 (s, 3H), 0.89 (s, 3H); ^{13}C NMR (125 MHz, C_5D_5N) δ 181.4, 146.1, 123.8, 79.4, 57.1, 49.4, 48.0, 47.8, 43.5, 43.3, 41.1, 40.6, 40.2, 38.7, 35.5, 34.6, 34.5, 34.5, 32.2, 30.0, 29.6, 29.4, 27.4, 25.1, 25.1, 25.0, 20.1, 18.7, 17.8, 16.8.

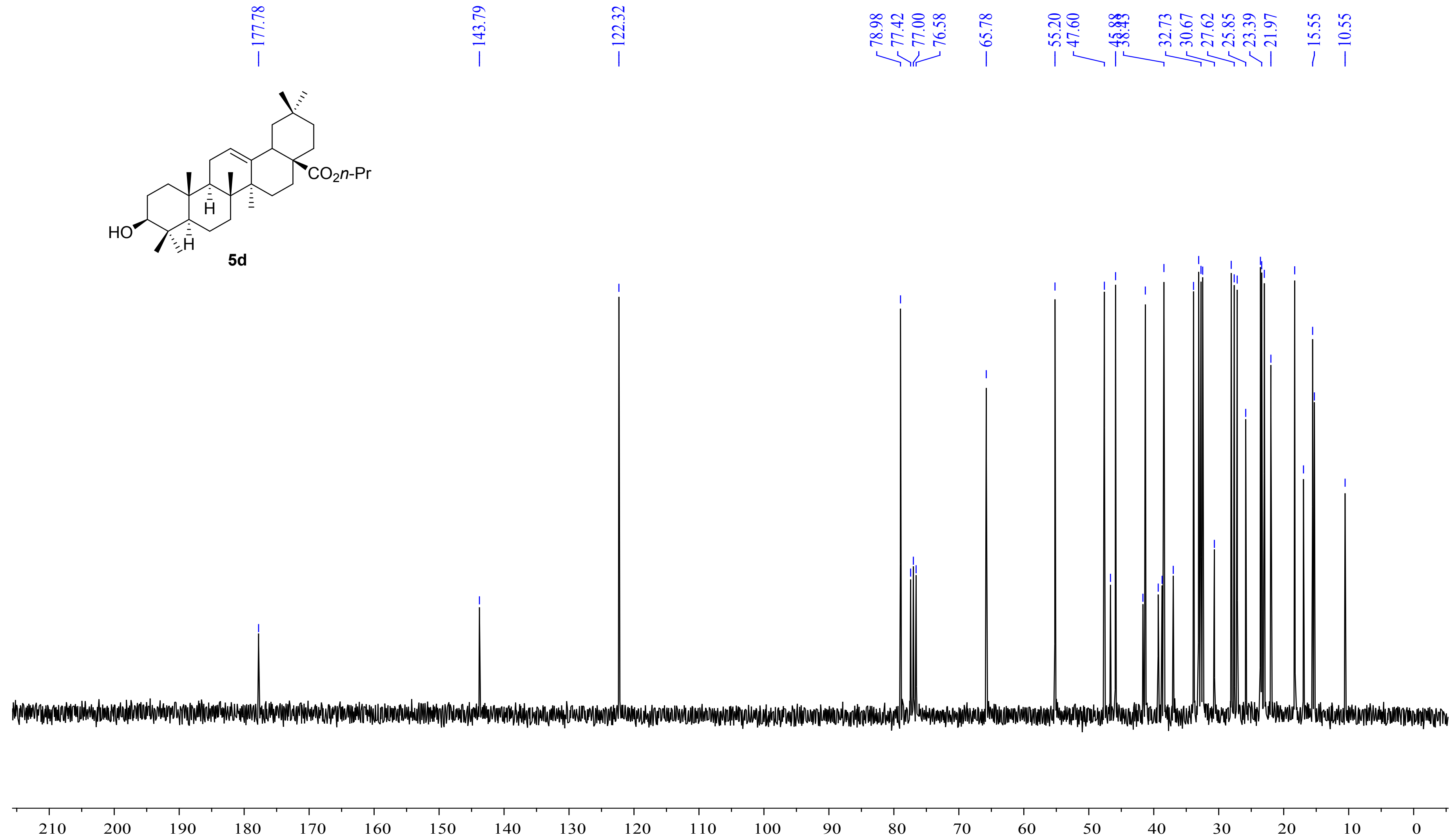
δ-oleanolic acid (2). ^{1}H NMR (500 MHz, C_5D_5N) δ 3.46 (dd, J = 10.1, 6.0 Hz, 1H), 2.84 (dd, J = 14.6, 2.0 Hz, 1H), 2.60 (d, J = 14.0 Hz, 1H), 2.52-2.55 (m, 1H), 2.24-2.26 (m, 1H), 2.18 (d, J = 13.9 Hz, 1H), 2.05 (t, J = 12.9 Hz, 1H), 1.91-1.95 (m, 1H), 1.84-1.89 (m, 2H), 0.87-1.73 (m, 15H), 1.24 (s, 3H), 1.22 (s, 3H), 1.14 (s, 3H), 1.00 (s, 3H), 0.95 (s, 3H), 0.89 (s, 3H), 0.84 (s, 3H); ^{13}C NMR (125 MHz, C_5D_5N) δ 180.2, 139.2, 130.6, 79.4, 57.2, 52.5, 50.1, 46.1, 43.1, 42.8, 40.7, 40.6, 39.0, 38.7, 37.7, 36.8, 34.9, 34.2, 33.6, 30.0, 29.5, 29.1, 26.9, 25.7, 23.4, 22.6, 20.1, 19.4, 17.9, 17.7.

^{1}H NMR of **5d**



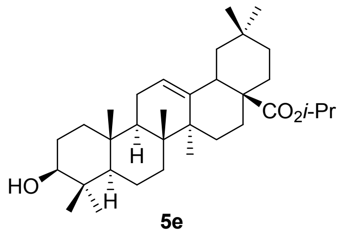
HO
H
H
CO2n-Pr
5d
5.29
3.98
3.97
3.48
3.21
2.91
2.87
1.89
1.75
1.65
1.60
1.51
1.42
1.34
1.21
1.09
0.99
0.95
0.91
0.74
0.57
0.07
0.00
1.00
2.06
1.04
1.05
23.21
3.83
3.24
2.19
4.11
5.76
2.97
3.50
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

^{13}C NMR of **5d**

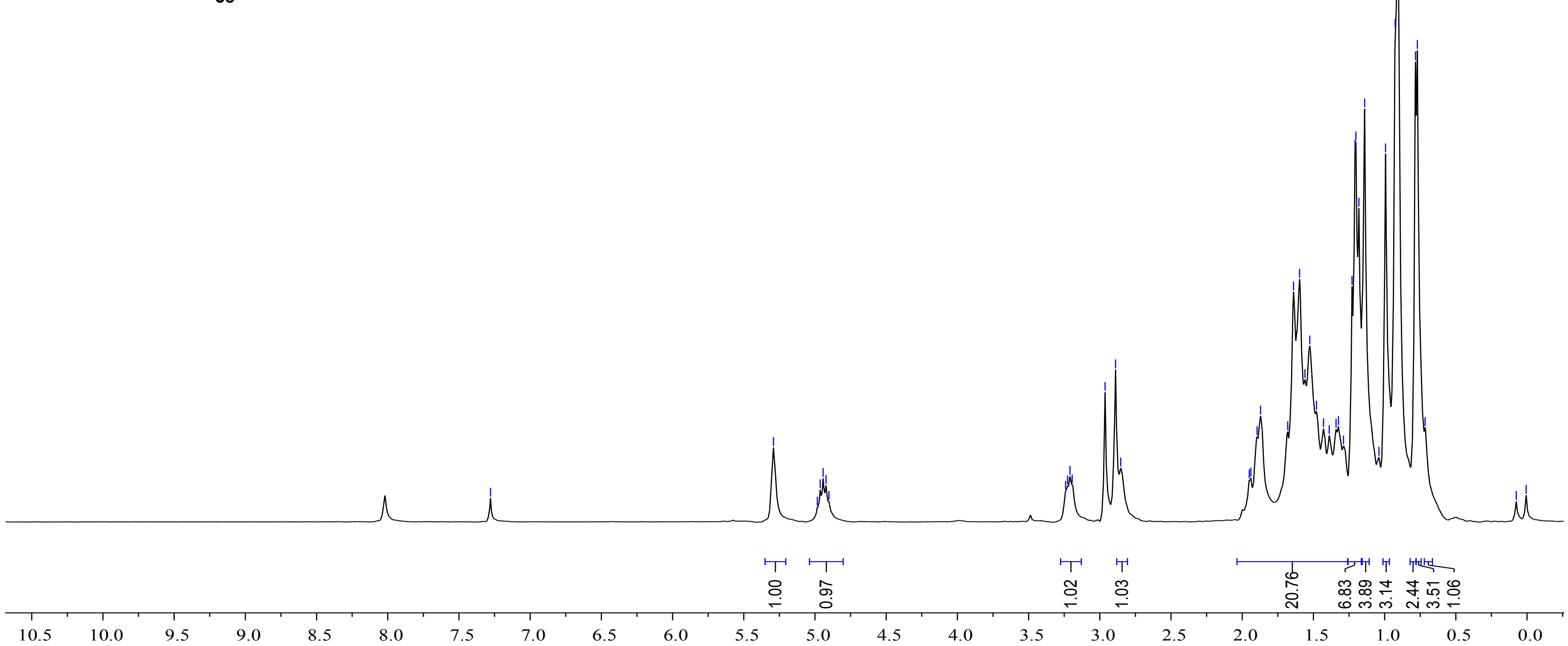


177.78
143.79
122.32
78.98
77.42
77.00
76.58
65.78
55.20
47.60
32.73
30.67
27.62
25.85
23.39
21.97
15.55
10.55
HO
H
H
CO2n-Pr
5d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

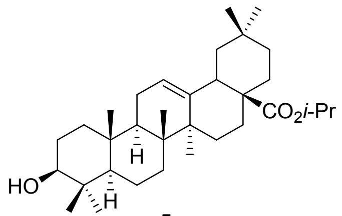
[1]H NMR of **5e**



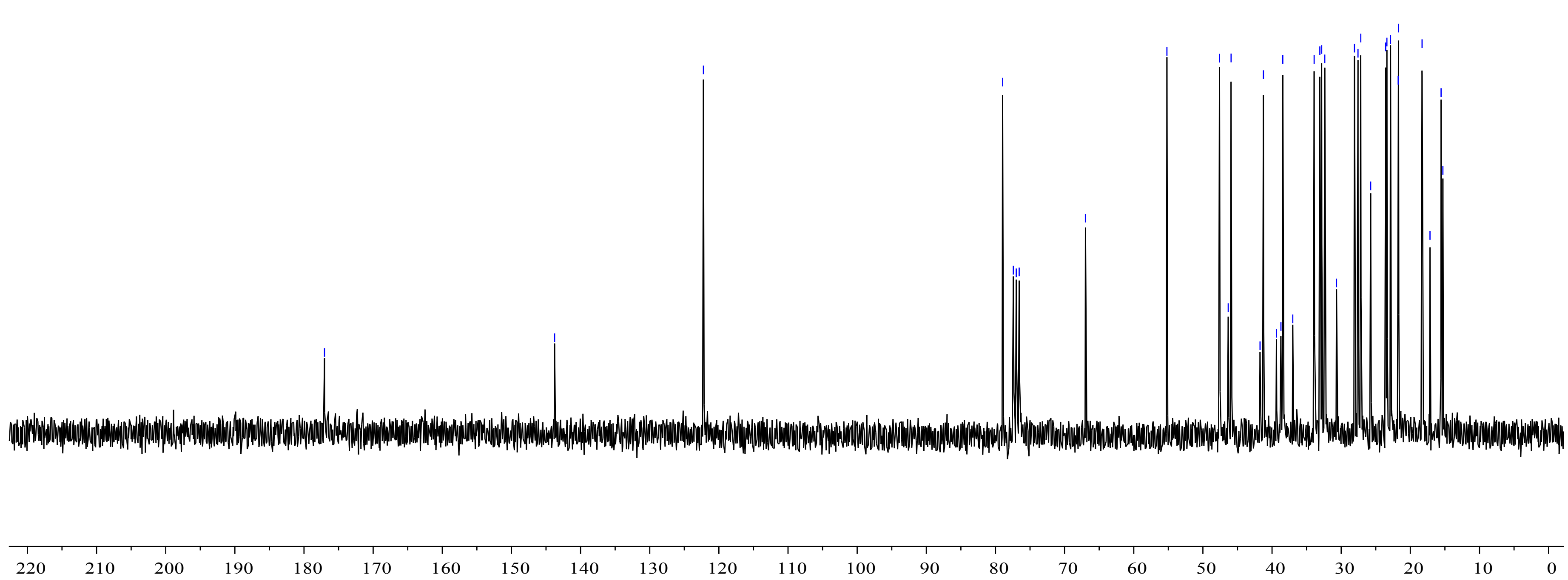
5e



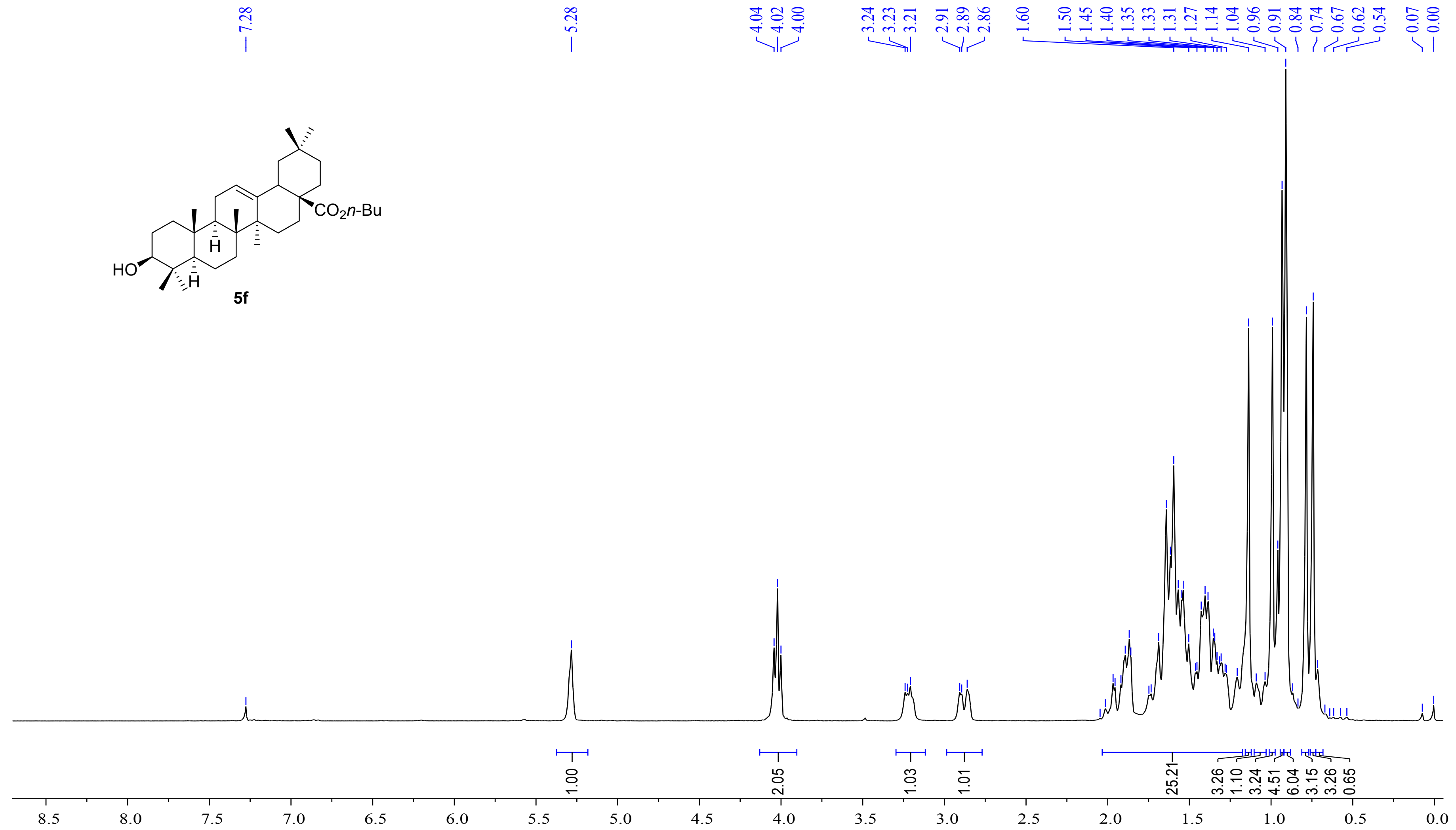
^{13}C NMR of **5e**



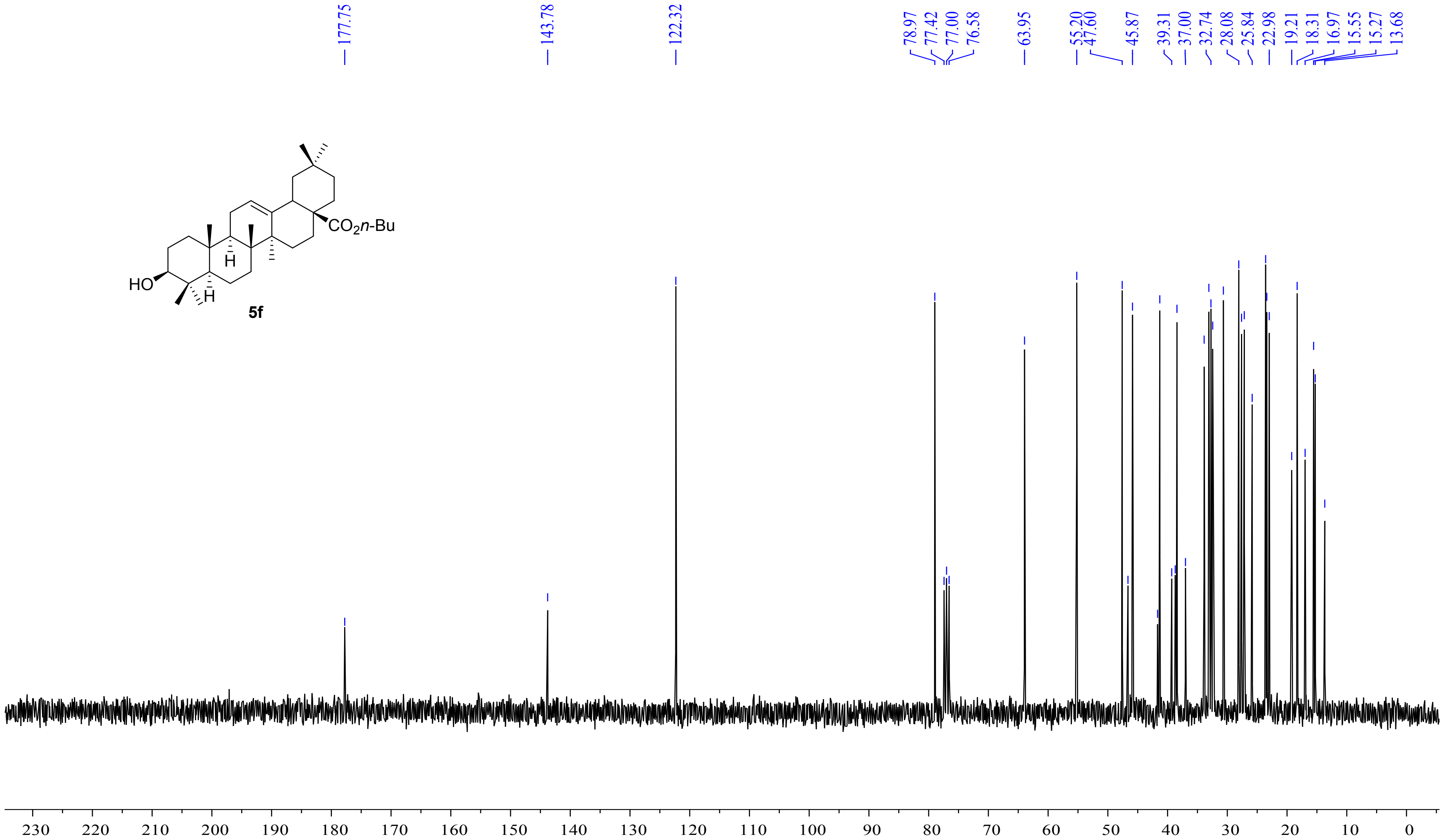
5e



[1]H NMR of **5f**

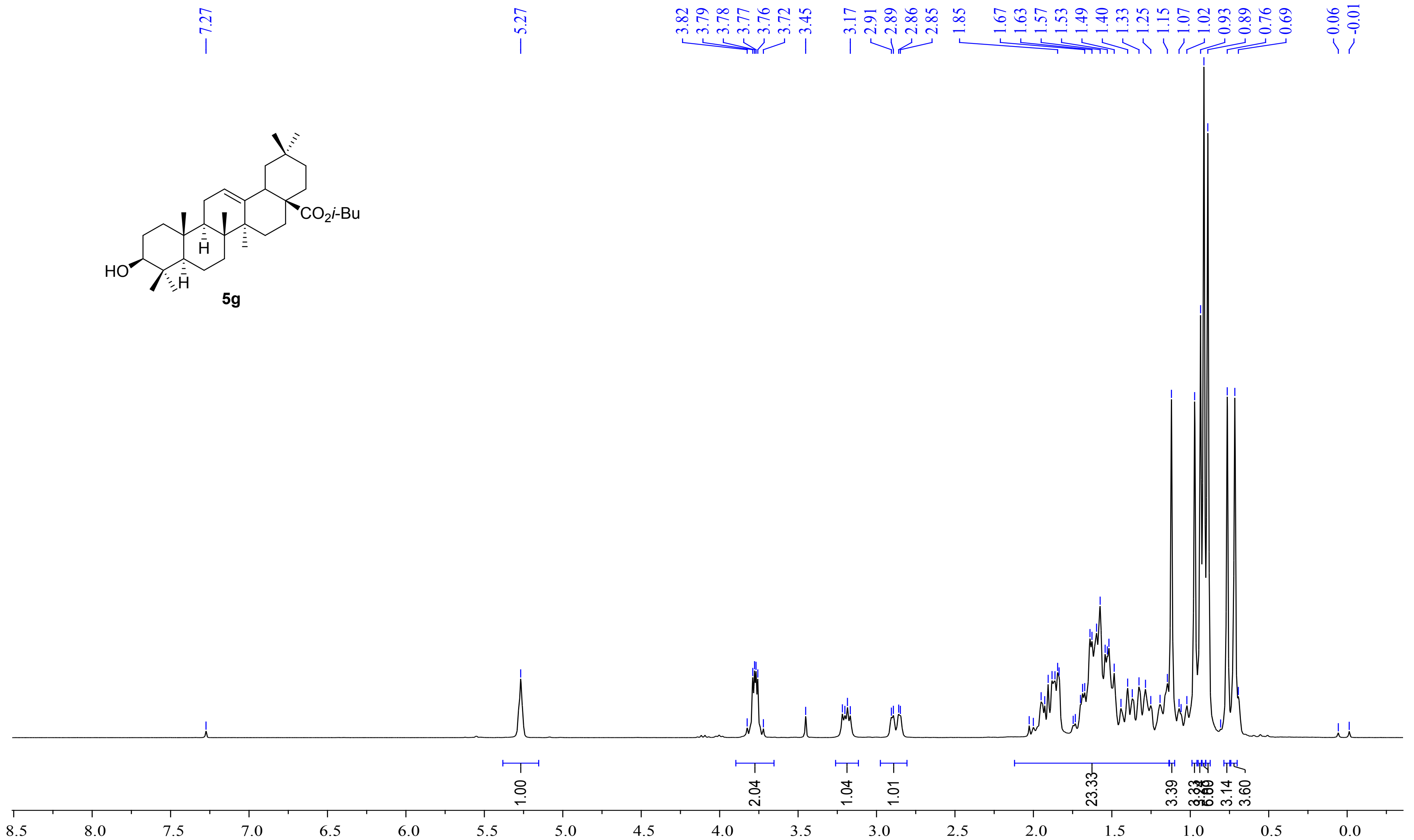


^{13}C NMR of **5f**



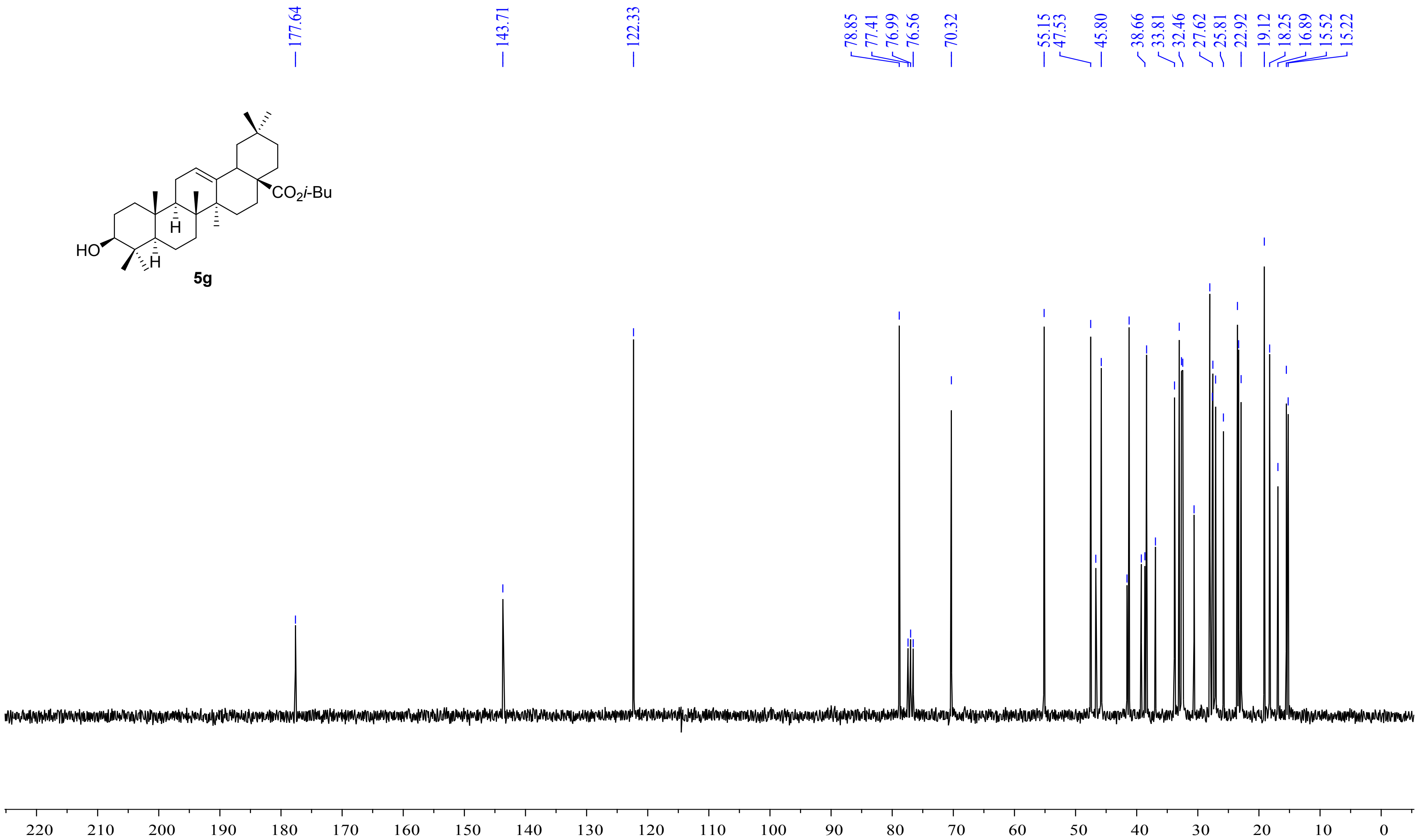
177.75
143.78
122.32
78.97
77.42
77.00
76.58
63.95
55.20
47.60
45.87
39.31
37.00
32.74
28.08
25.84
22.98
19.21
18.31
16.97
15.55
15.27
13.68
HO
H
H
CO2n-Bu
5f
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

^{1}H NMR of **5g**



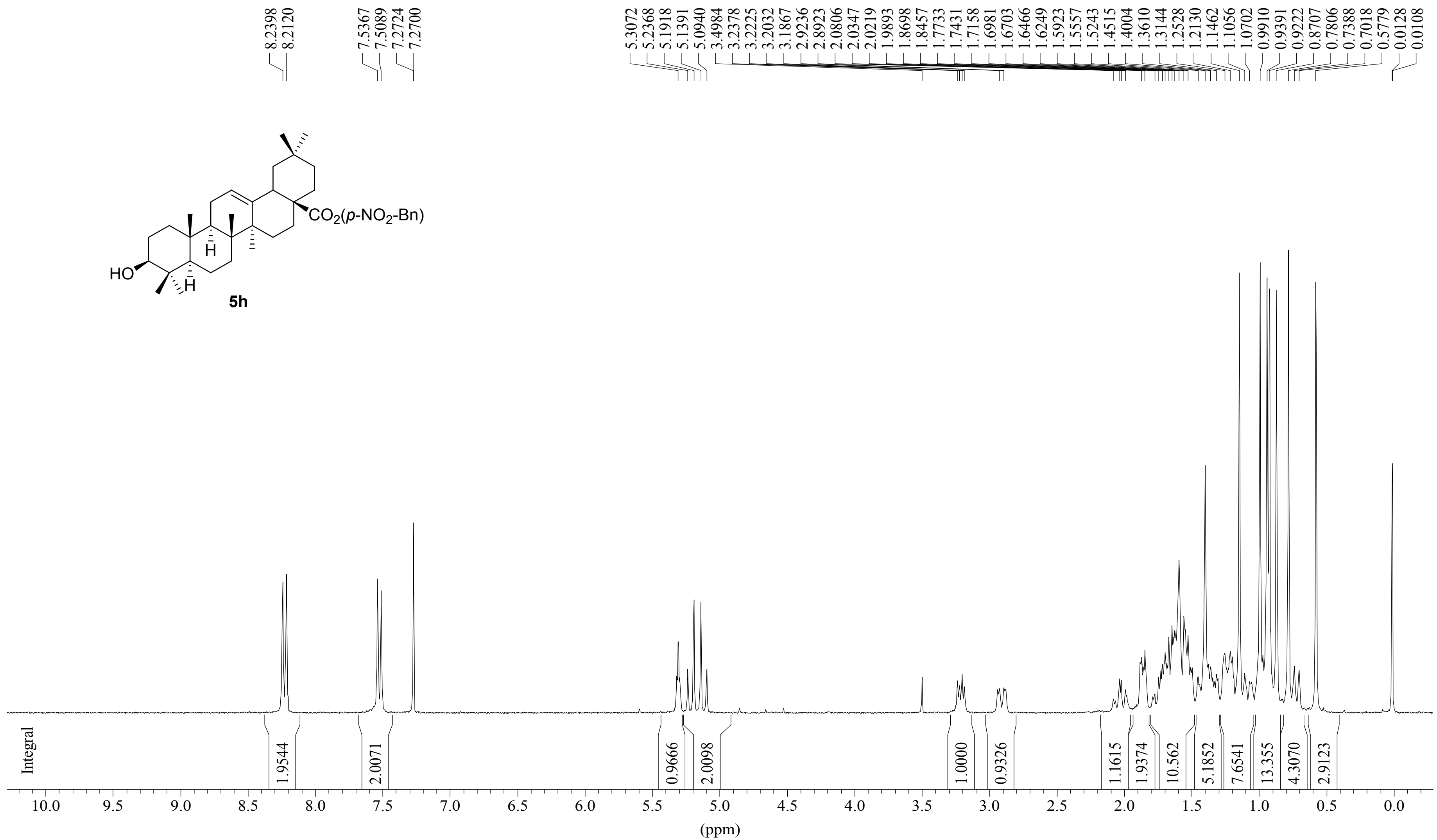
7.27
5.27
3.82 3.79 3.78 3.77 3.76 3.72 3.45
3.17 2.91 2.89 2.86 2.85
1.85 1.67 1.63 1.57 1.53 1.49 1.40 1.33 1.25 1.15 1.07 1.02 0.93 0.89 0.76 0.69
0.06 -0.01
HO
H
H
CO_2*i*-Bu
5g
1.00
2.04
1.04
1.01
23.33
3.39
3.14
3.60
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

^{13}C NMR of **5g**

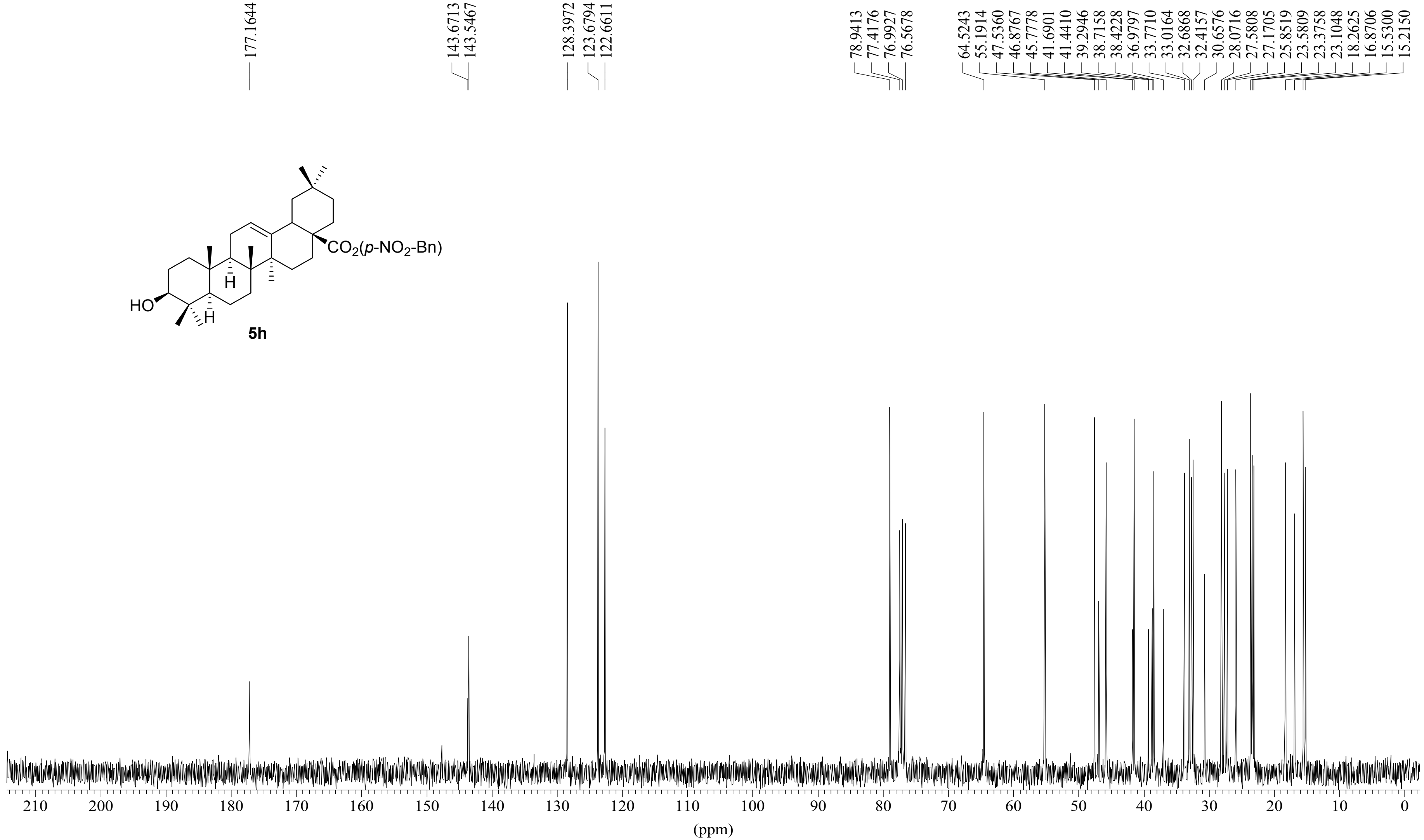


177.64
143.71
122.33
78.85
77.41
76.99
76.56
70.32
55.15
47.53
45.80
38.66
33.81
32.46
27.62
25.81
22.92
19.12
18.25
16.89
15.52
15.22
HO
H
H
CO2i-Bu
5g
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

^{1}H NMR of **5h**

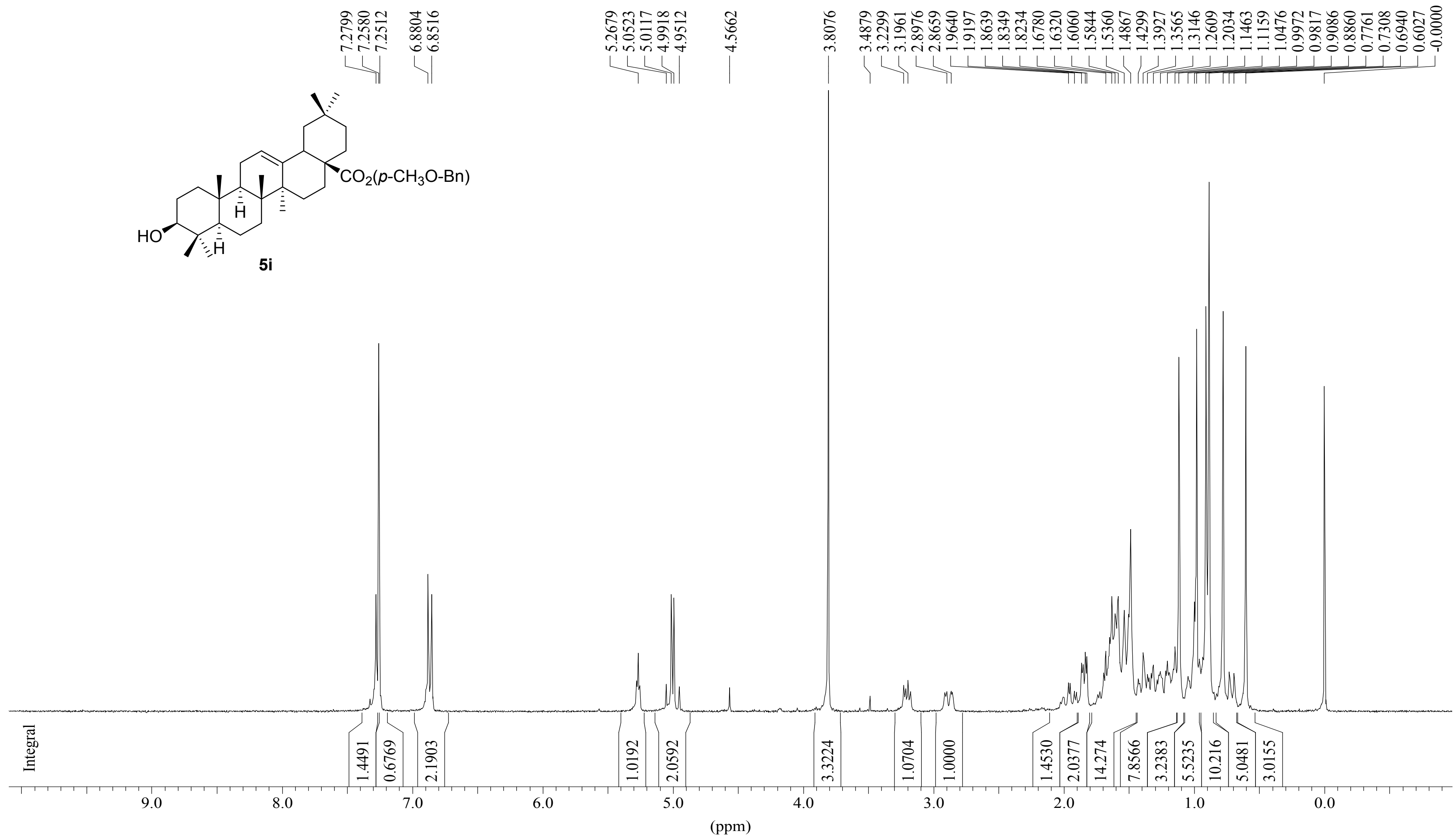

CO2(p-NO2-Bn)
HO
H
H
5h
8.2398
8.2120
7.5367
7.5089
7.2724
7.2700
5.3072
5.2368
5.1918
5.1391
5.0940
3.4984
3.2378
3.2225
3.2032
3.1867
2.9236
2.8923
2.0806
2.0347
2.0219
1.9893
1.8698
1.8457
1.7733
1.7431
1.7158
1.6981
1.6703
1.6466
1.6249
1.5923
1.5557
1.5243
1.4515
1.4004
1.3610
1.3144
1.2528
1.2130
1.1462
1.1056
1.0702
0.9910
0.9391
0.9222
0.8707
0.7806
0.7388
0.7018
0.5779
0.0128
0.0108
Integral
1.9544
2.0071
0.9666
2.0098
1.0000
0.9326
1.1615
1.9374
10.562
5.1852
7.6541
13.355
4.3070
2.9123
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

^{13}C NMR of **5h**



177.1644
143.6713
143.5467
128.3972
123.6794
122.6611
78.9413
77.4176
76.9927
76.5678
64.5243
55.1914
47.5360
46.8767
45.7778
41.6901
41.4410
39.2946
38.7158
38.4228
36.9797
33.7710
33.0164
32.6868
32.4157
30.6576
28.0716
27.5808
27.1705
25.8519
23.5809
23.3758
23.1048
18.2625
16.8706
15.5300
15.2150
HO
H
H
CO_2(*p*-NO_2-Bn)
5h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

^{1}H NMR of **5i**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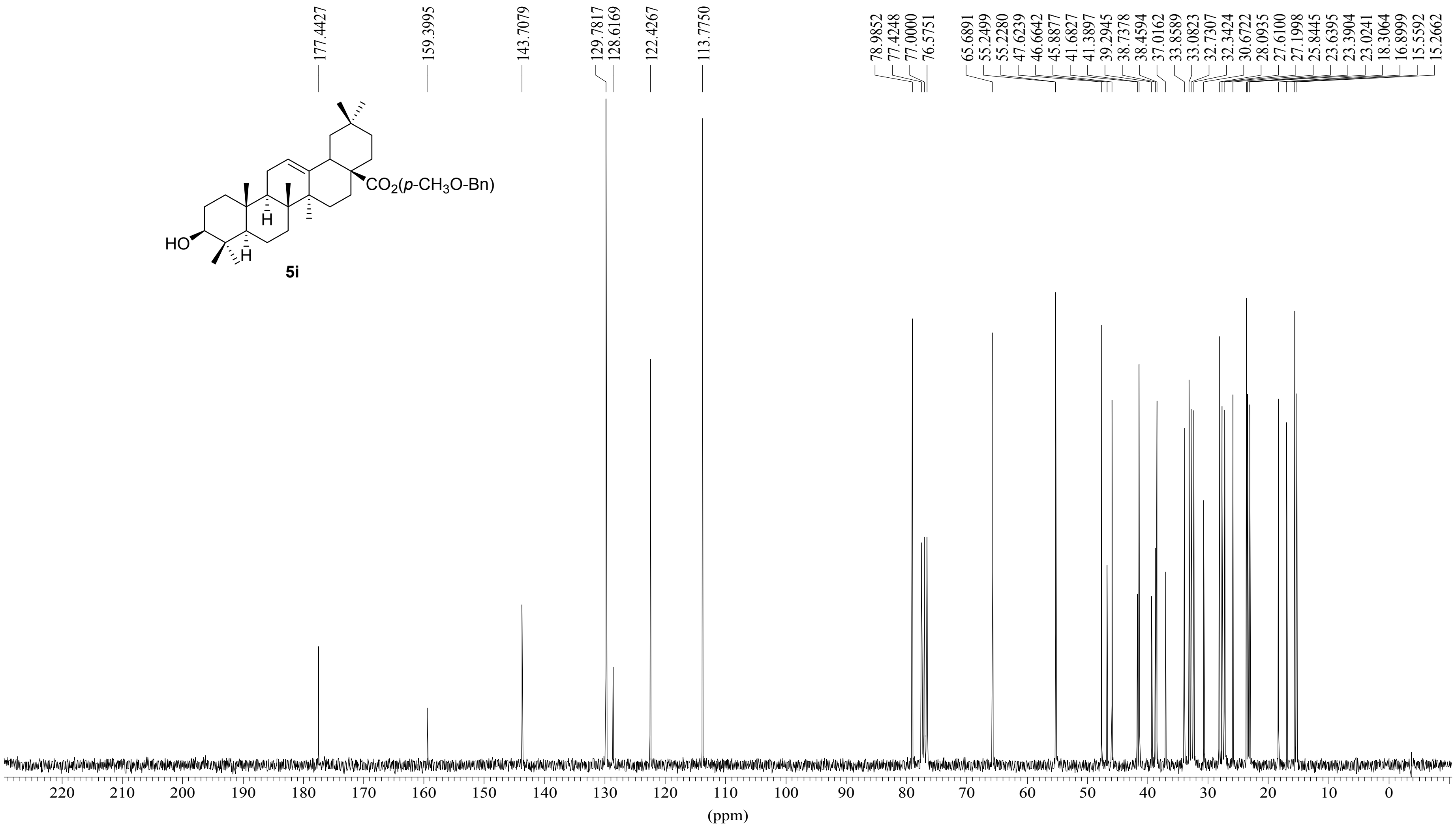
7.2512
6.8804
6.8516
5.2679
5.0523
5.0117
4.9918
4.9512
4.5662
3.8076
3.4879
3.2299
3.1961
2.8976
2.8659
1.9640
1.9197
1.8639
1.8349
1.8234
1.6780
1.6320
1.6060
1.5844
1.5360
1.4867
1.4299
1.3927
1.3565
1.3146
1.2609
1.2034
1.1463
1.1159
1.0476
0.9972
0.9817
0.9086
0.8860
0.7761
0.7308
0.6940
0.6027
-0.0000
HO
H
H
CO_2(*p*-CH_3O-Bn)
5i
Integral
1.4491
0.6769
2.1903
1.0192
2.0592
3.3224
1.0704
1.0000
1.4530
2.0377
14.274
7.8566
3.2383
5.5235
10.216
5.0481
3.0155
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

^{13}C NMR of **5i**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128.6169
122.4267
113.7750
78.9852
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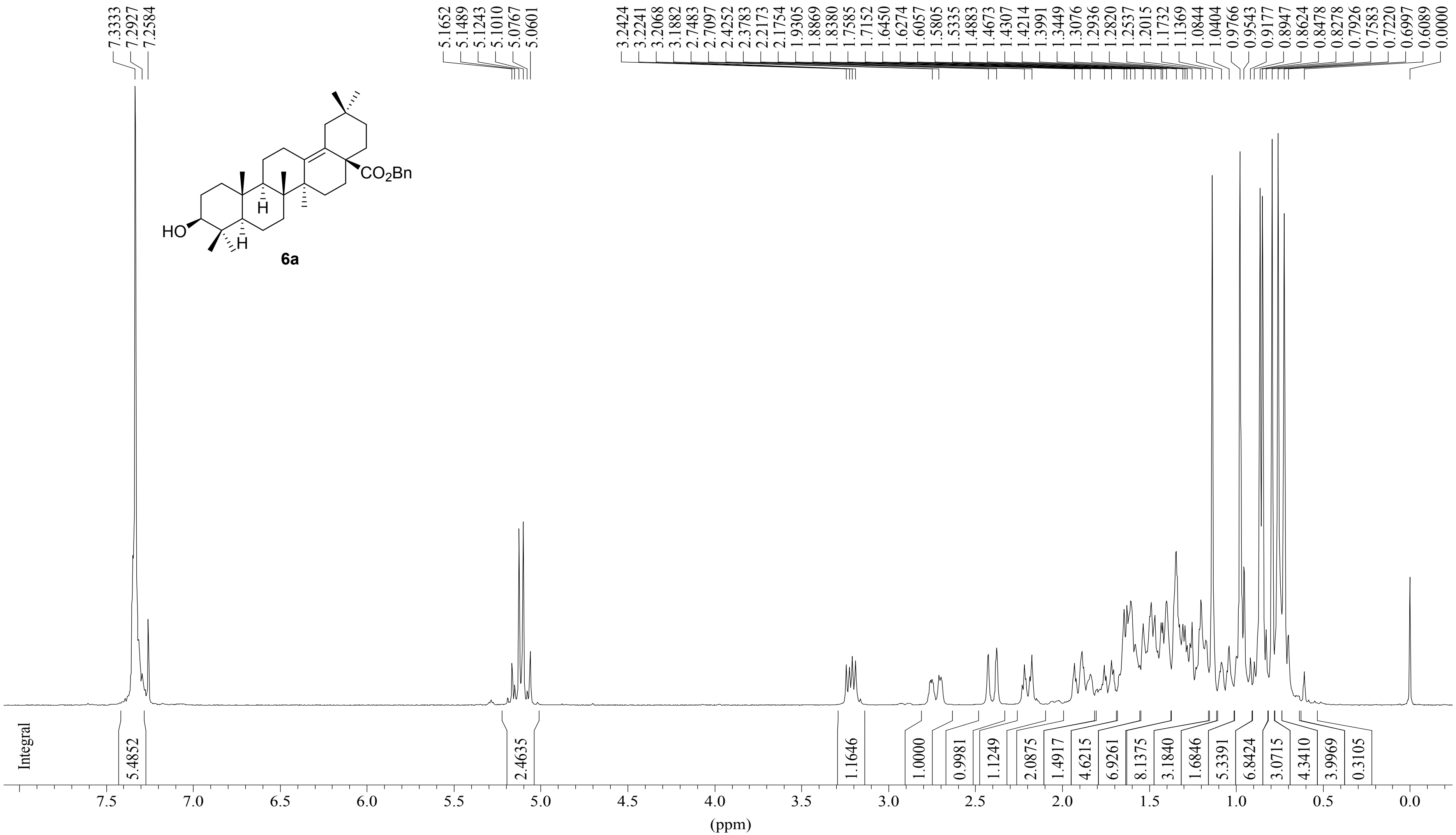
77.0000
76.5751
65.6891
55.2499
55.2280
47.6239
46.6642
45.8877
41.6827
41.3897
39.2945
38.7378
38.4594
37.0162
33.8589
33.0823
32.7307
32.3424
30.6722
28.0935
27.6100
27.1998
25.8445
23.6395
23.3904
23.0241
18.3064
16.8999
15.5592
15.2662
HO
H
H
CO_2(p-CH_3O-Bn)
5i
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

^{1}H NMR of **6a**


7.3333
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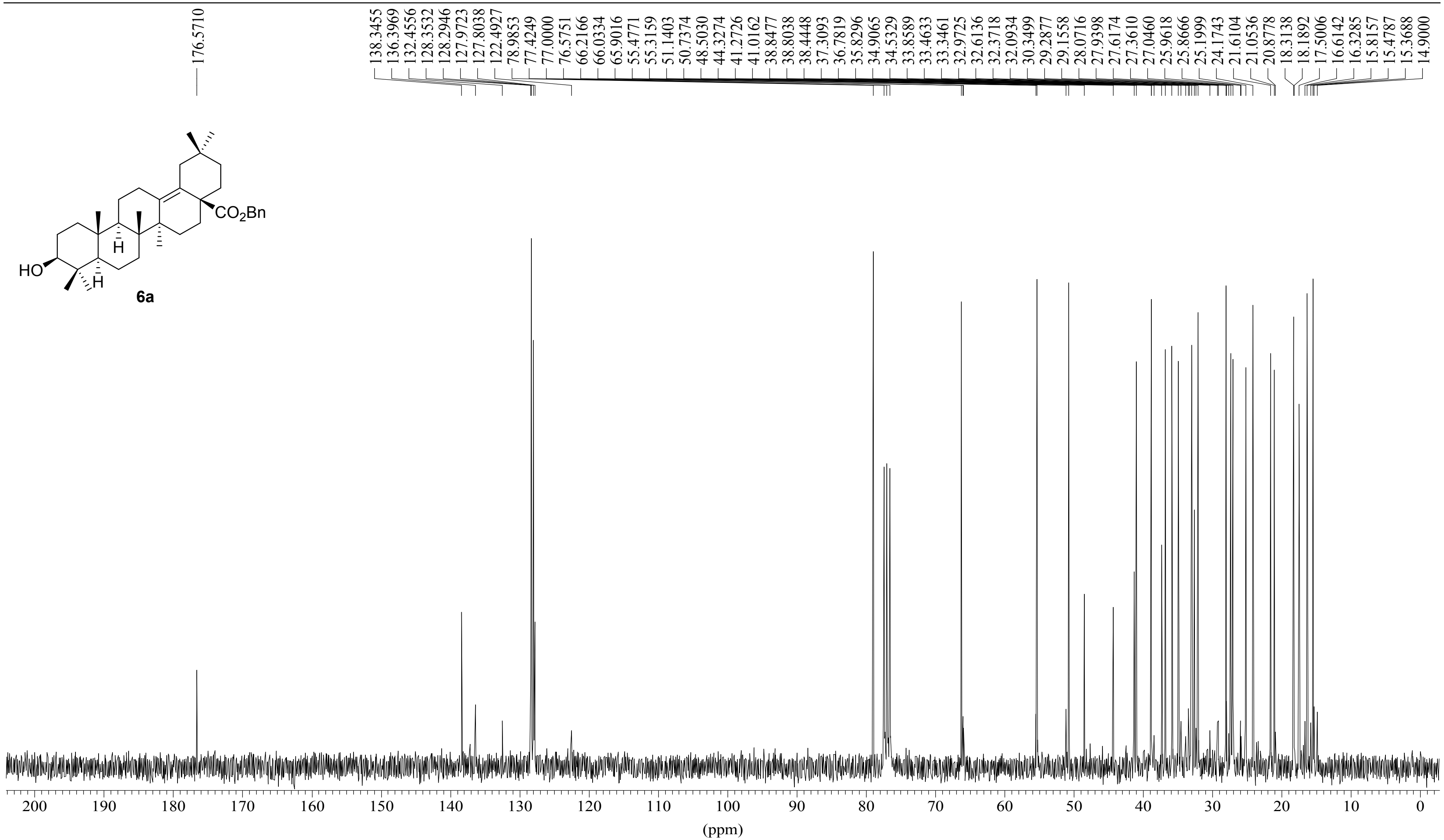
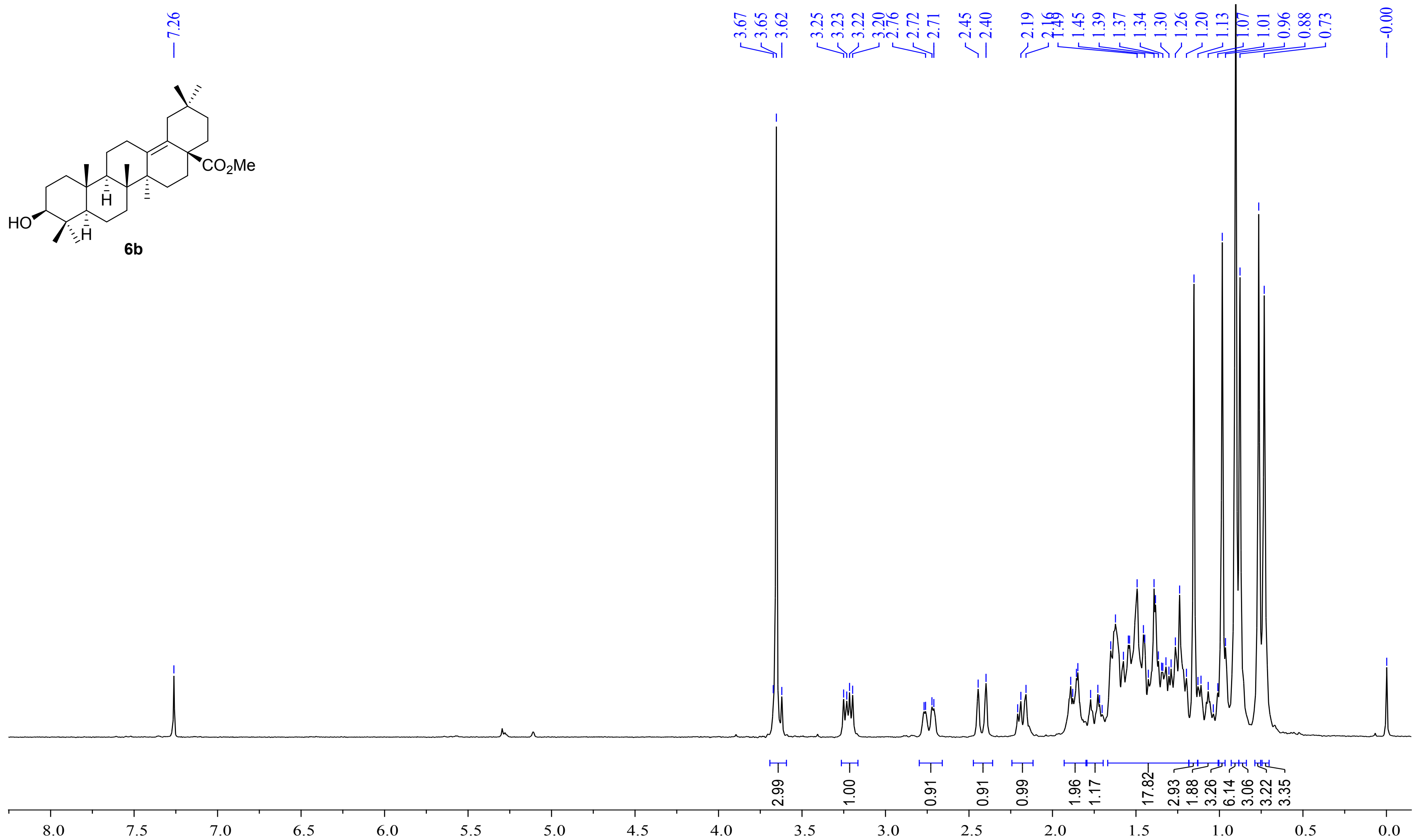
7.2584
5.1652
5.1489
5.1243
5.1010
5.0767
5.0601
3.2424
3.2241
3.2068
3.1882
2.7483
2.7097
2.4252
2.3783
2.2173
2.1754
1.9305
1.8869
1.8380
1.7585
1.7152
1.6450
1.6274
1.6057
1.5805
1.5335
1.4883
1.4673
1.4307
1.4214
1.3991
1.3449
1.3076
1.2936
1.2820
1.2537
1.2015
1.1732
1.1369
1.0844
1.0404
0.9766
0.9543
0.9177
0.8947
0.8624
0.8478
0.8278
0.7926
0.7583
0.7220
0.6997
0.6089
0.0000
CO_2Bn
HO
H
H
6a
Integral
5.4852
2.4635
1.1646
1.0000
0.9981
1.1249
2.0875
1.4917
4.6215
6.9261
8.1375
3.1840
1.6846
5.3391
6.8424
3.0715
4.3410
3.9969
0.3105
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

^{13}C NMR of **6a**

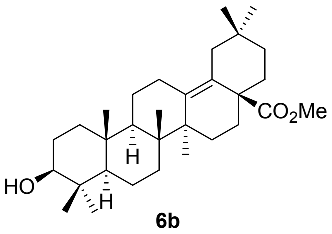

176.5710
138.3455
136.3969
132.4556
128.3532
128.2946
127.9723
127.8038
122.4927
78.9853
77.4249
77.0000
76.5751
66.2166
66.0334
65.9016
55.4771
55.3159
51.1403
50.7374
48.5030
44.3274
41.2726
41.0162
38.8477
38.8038
38.4448
37.3093
36.7819
35.8296
34.9065
34.5329
33.8589
33.4633
33.3461
32.9725
32.6136
32.3718
32.0934
30.3499
29.2877
29.1558
28.0716
27.9398
27.6174
27.3610
27.0460
25.9618
25.8666
25.1999
24.1743
21.6104
21.0536
20.8778
18.3138
18.1892
17.5006
16.6142
16.3285
15.8157
15.4787
15.3688
14.9000
CO2Bn
H
HO
H
6a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

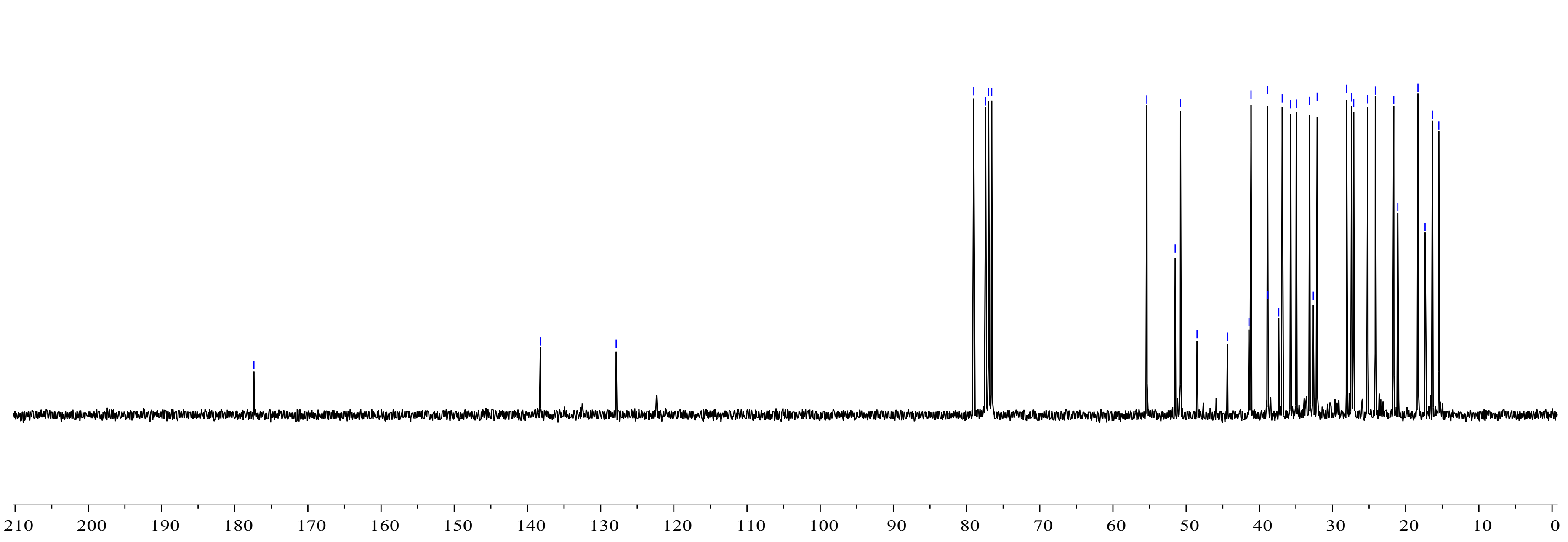
^{1}H NMR of **6b**



7.26
3.67
3.65
3.62
3.25
3.23
3.22
3.20
2.76
2.72
2.71
2.45
2.40
2.19
2.16
1.49
1.45
1.39
1.37
1.34
1.30
1.26
1.20
1.13
1.07
1.01
0.96
0.88
0.73
-0.00
HO
H
H
CO2Me
6b
2.99
1.00
0.91
0.91
0.99
1.96
1.17
17.82
2.93
1.88
3.26
6.14
3.06
3.22
3.35
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

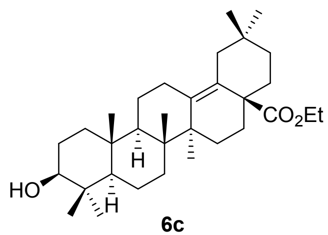
^{13}C NMR of **6b**



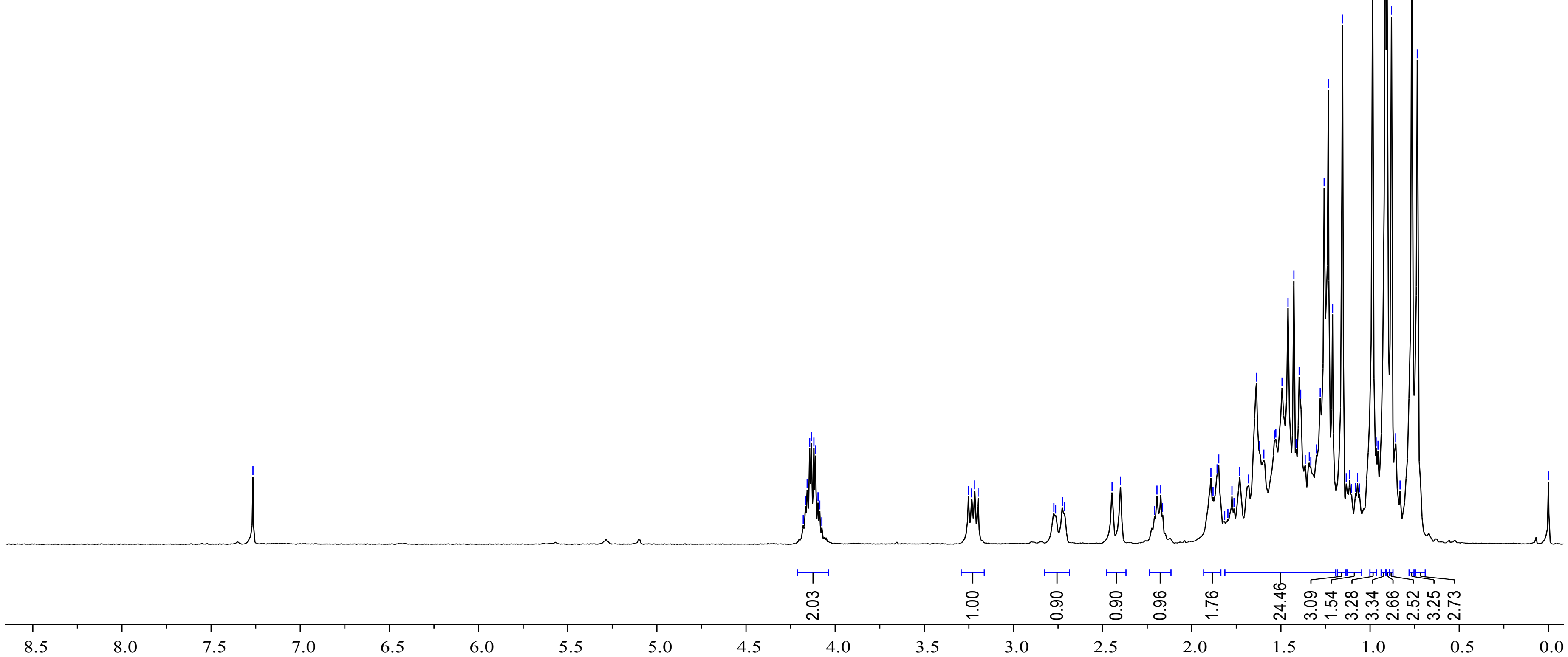


177.37
138.23
127.88
79.01
77.42
76.99
76.57
55.36
48.51
41.13
37.35
34.94
32.10
28.08
27.11
25.18
24.15
21.63
21.08
18.33
17.35
16.34
15.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

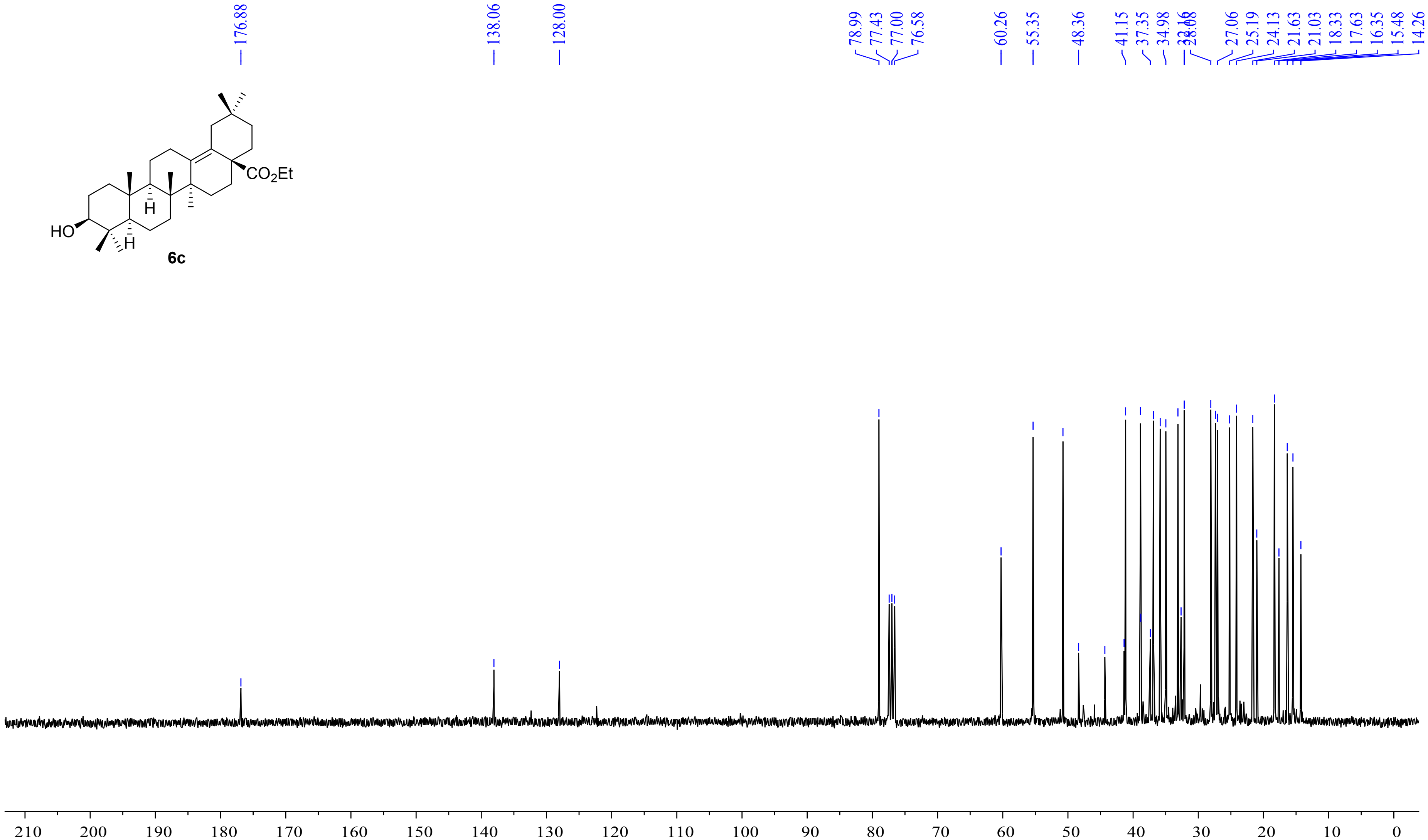
^{1}H NMR of **6c**



6c

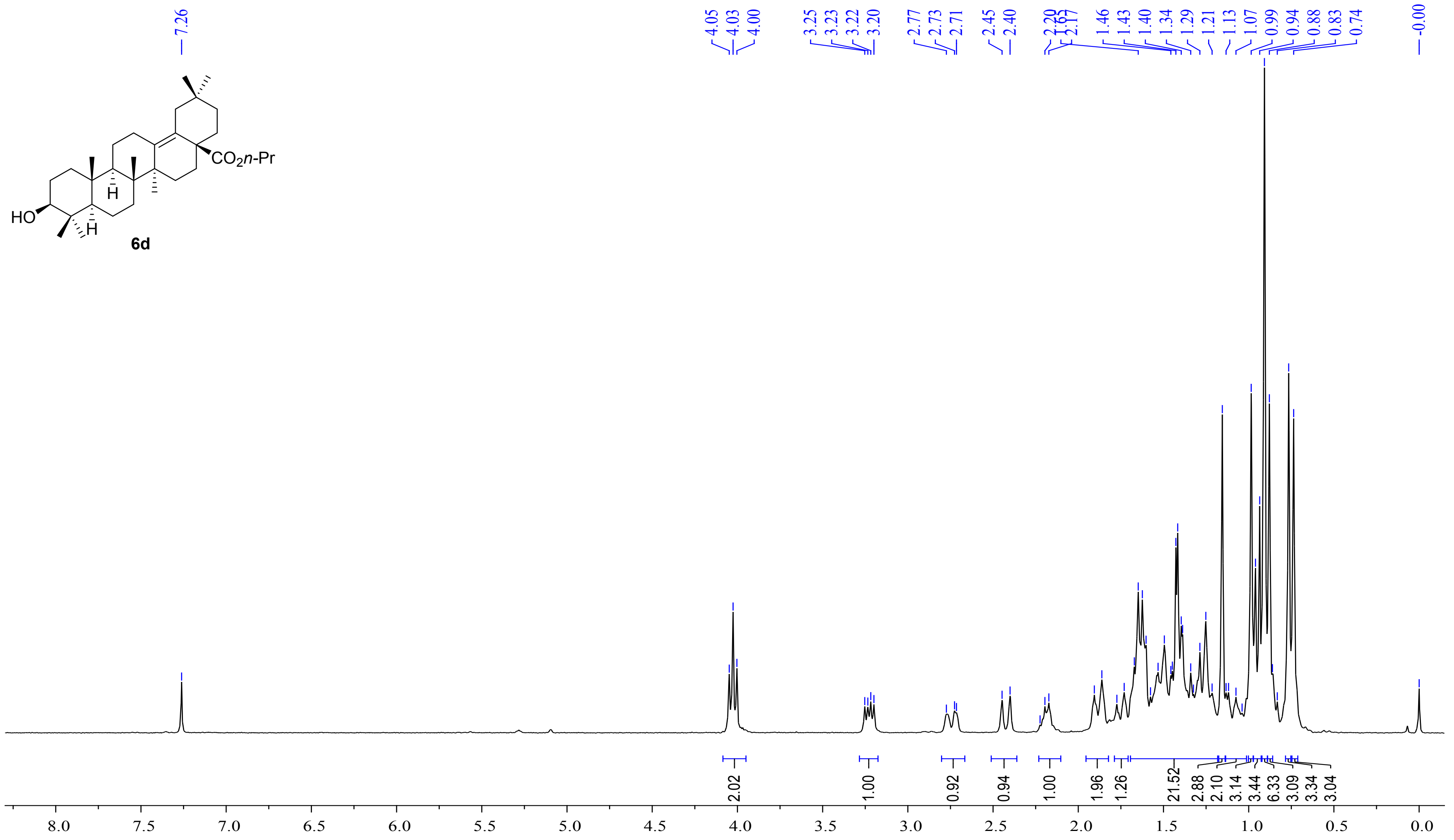


^{13}C NMR of **6c**



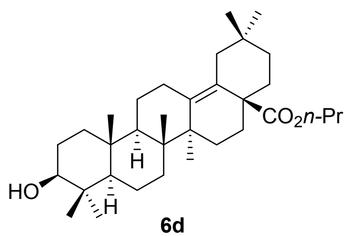
176.88
138.06
128.00
78.99
77.43
77.00
76.58
60.26
55.35
48.36
41.15
37.35
34.98
27.06
25.19
24.13
21.63
21.03
18.33
17.63
16.35
15.48
14.26
CO2Et
HO
H
H
6c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

^{1}H NMR of **6d**

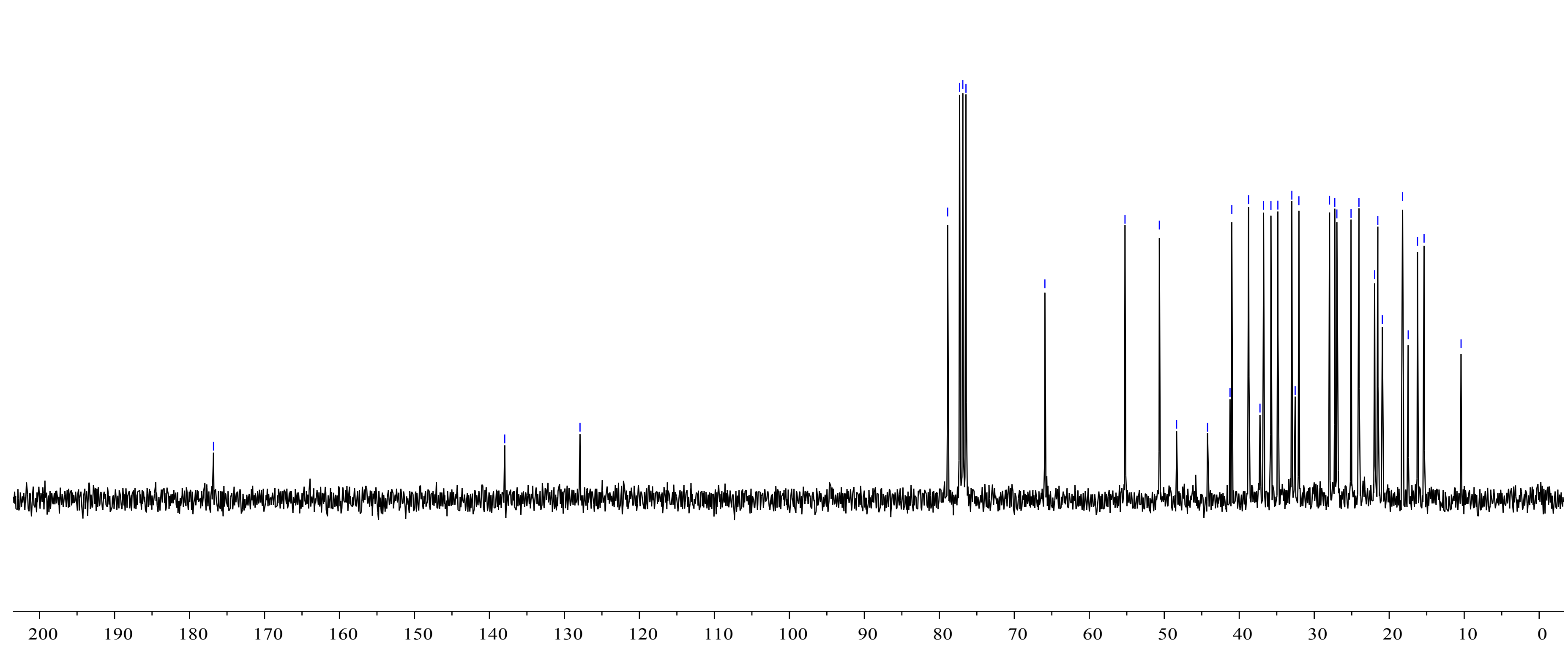


HO
H
H
CO2n-Pr
6d
7.26
4.05
4.03
4.00
3.25
3.23
3.22
3.20
2.77
2.73
2.71
2.45
2.40
2.20
1.65
2.17
1.46
1.43
1.40
1.34
1.29
1.21
1.13
1.07
0.99
0.94
0.88
0.83
0.74
-0.00
2.02
1.00
0.92
0.94
1.00
1.96
1.26
21.52
2.88
2.10
3.14
3.44
6.33
3.09
3.34
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

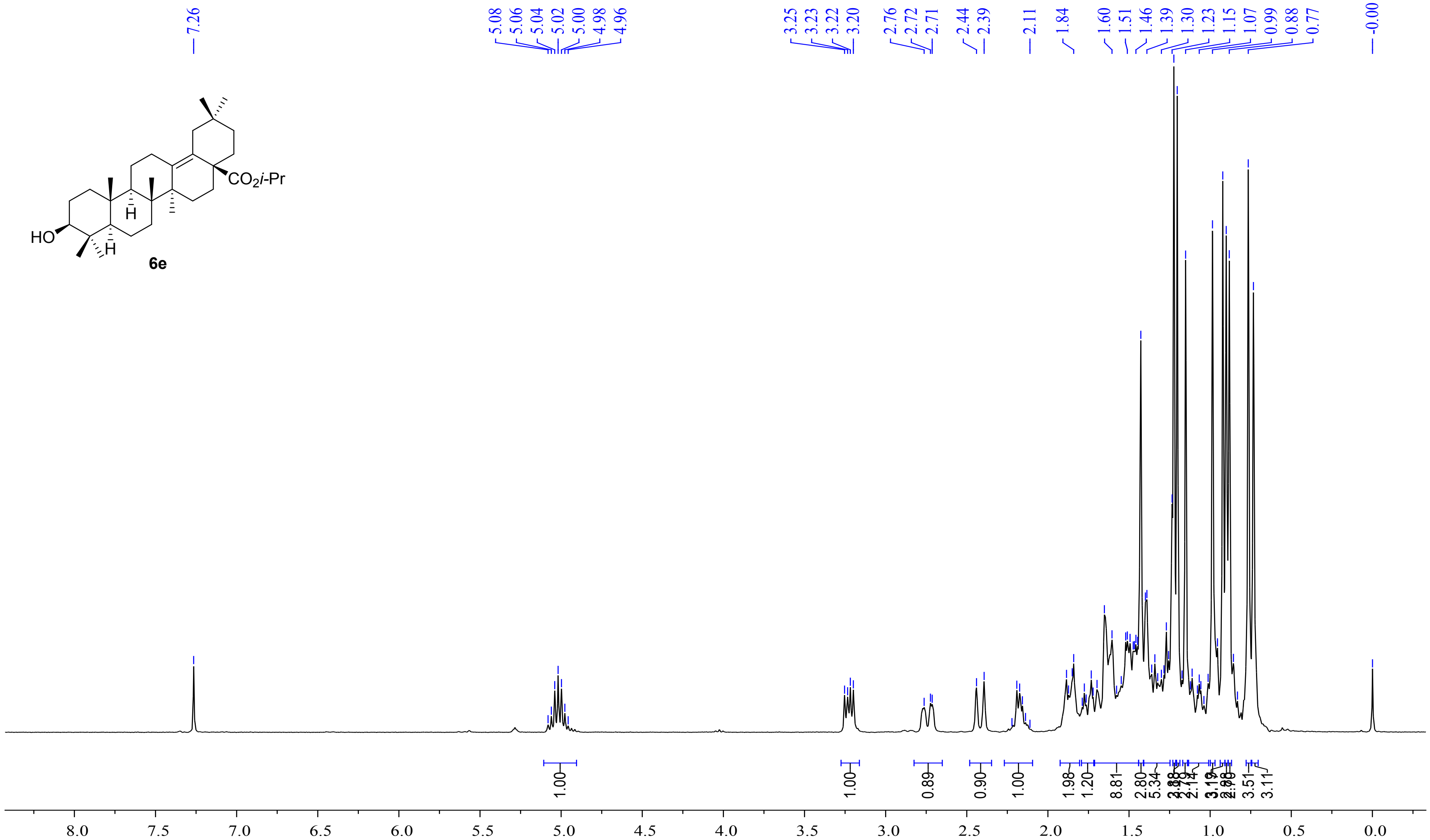
^{13}C NMR of **6d**



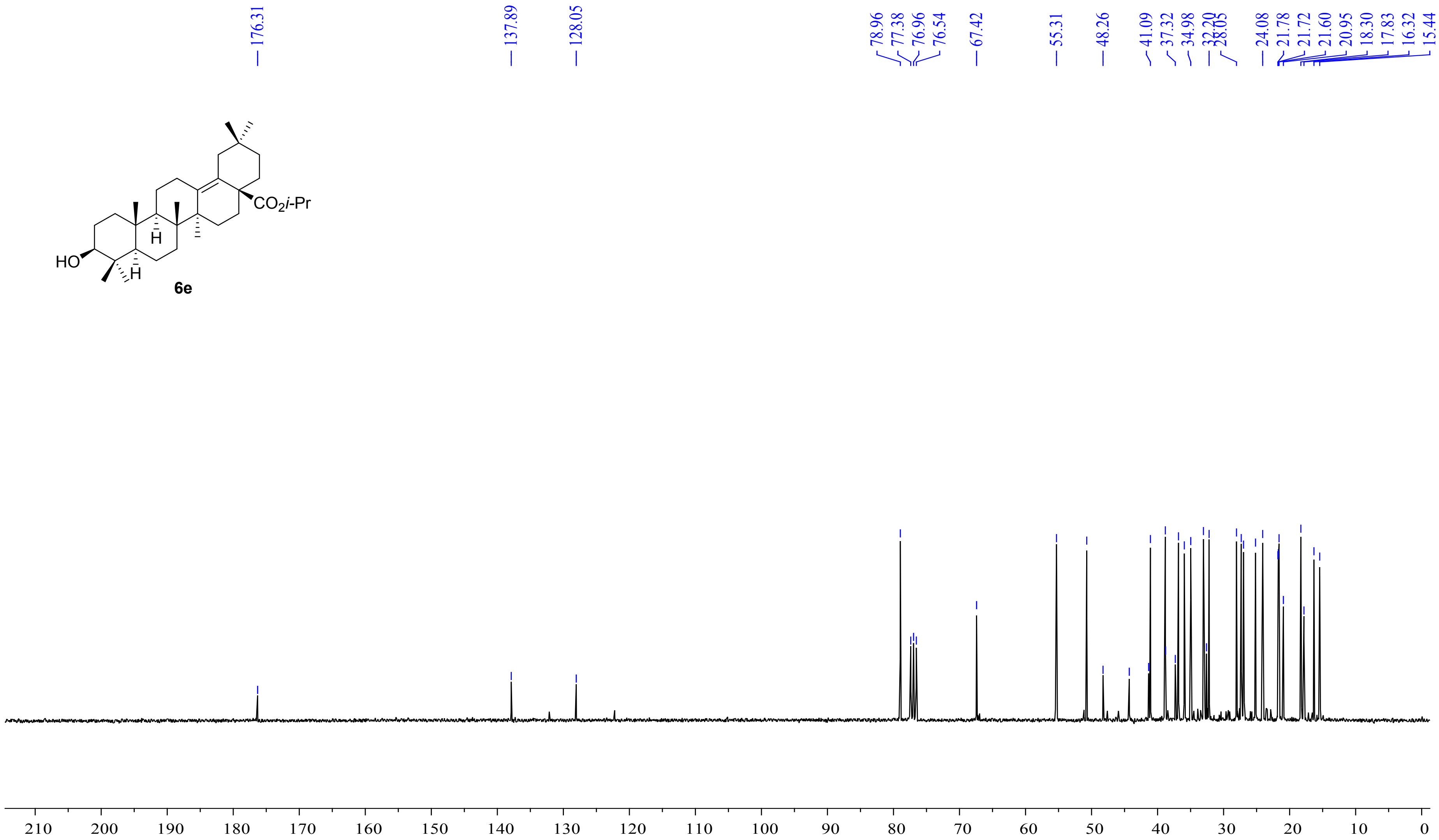
6d



^{1}H NMR of **6e**

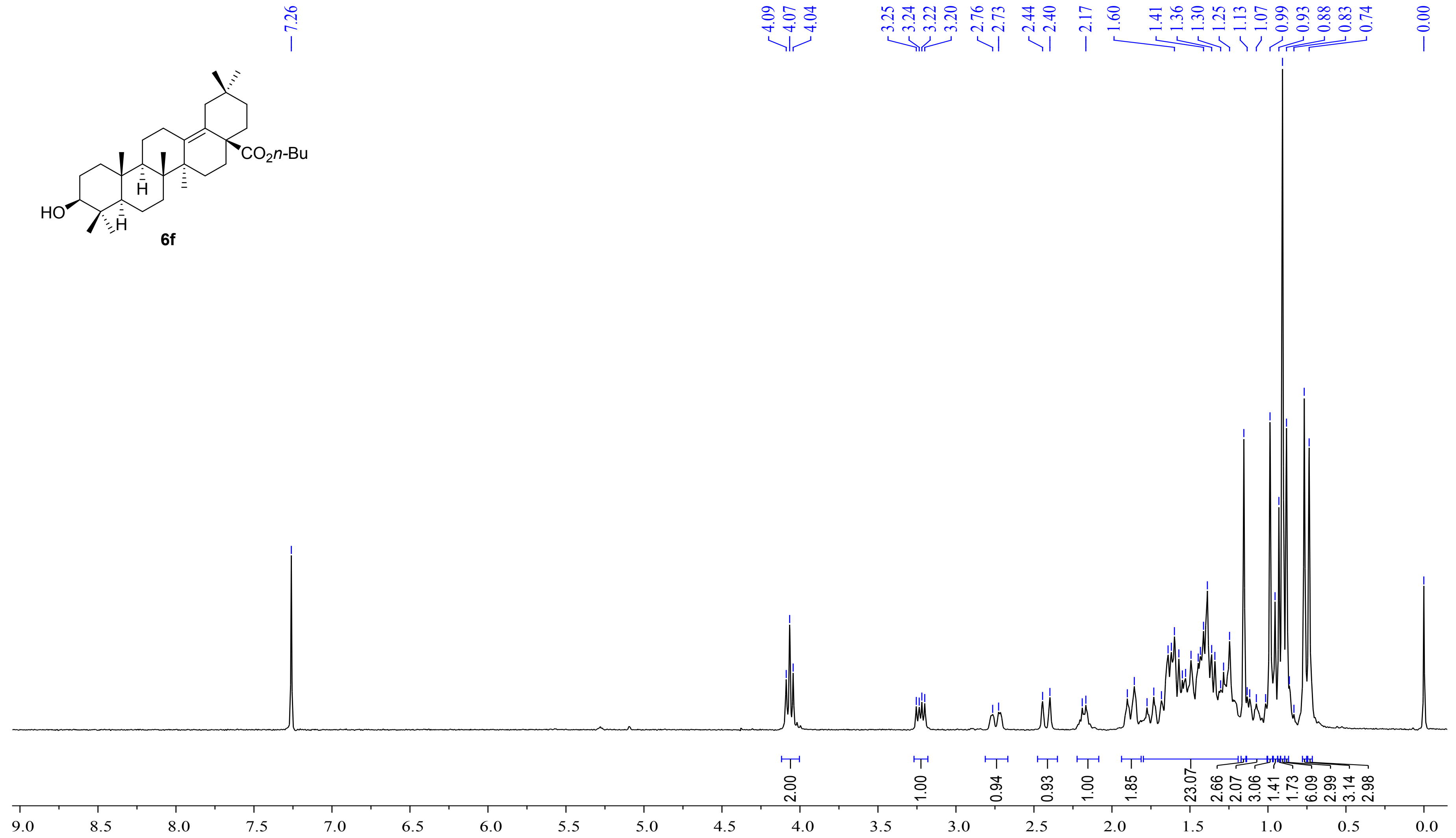


^{13}C NMR of **6e**

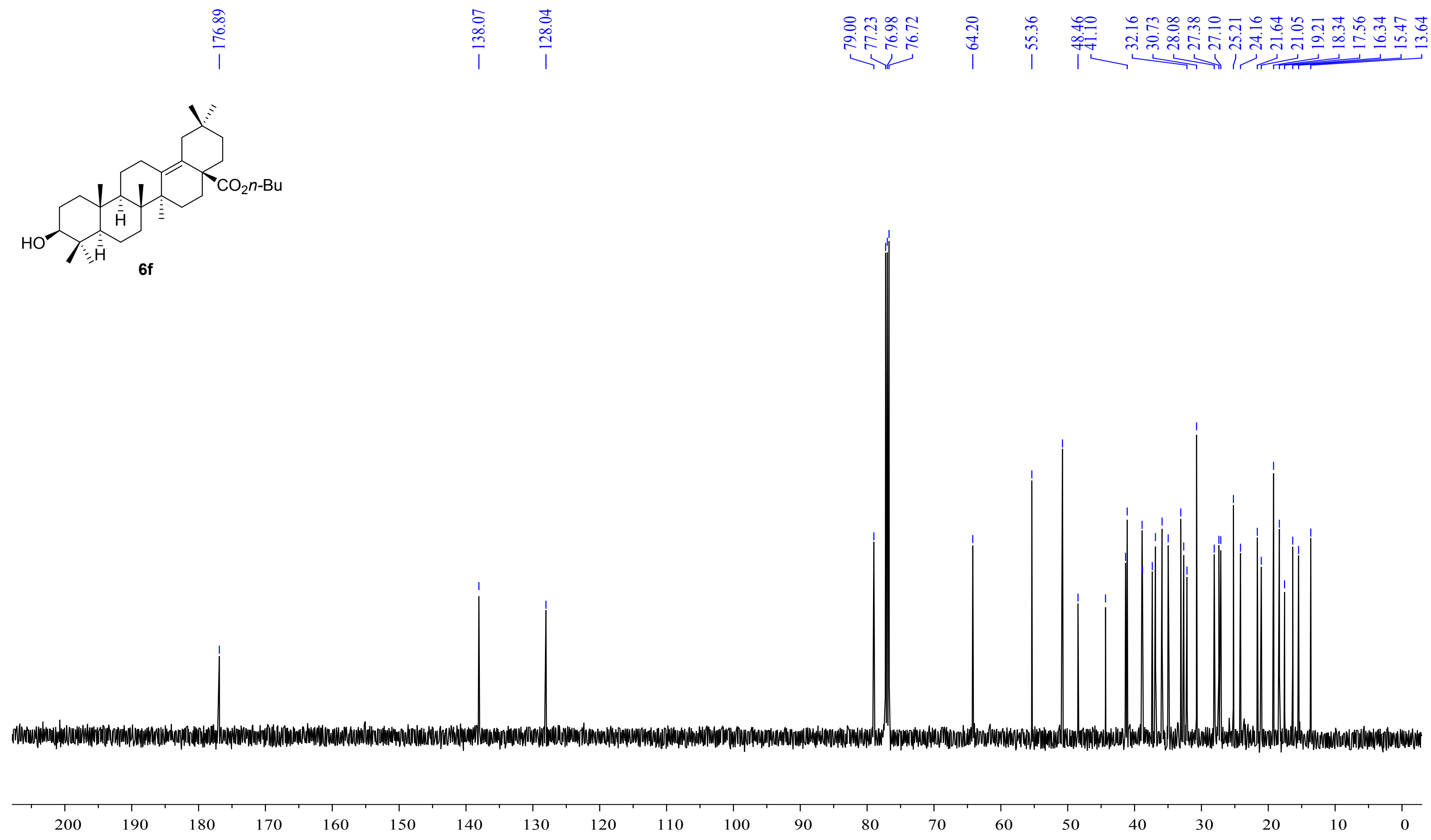


CO2i-Pr
HO
H
H
6e
176.31
137.89
128.05
78.96
77.38
76.96
76.54
67.42
55.31
48.26
41.09
37.32
34.98
32.20
28.05
24.08
21.78
21.72
21.60
20.95
18.30
17.83
16.32
15.44
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

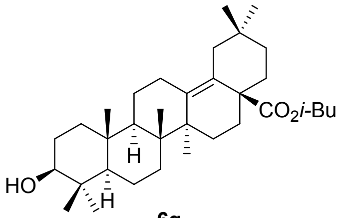
[1]H NMR of **6f**



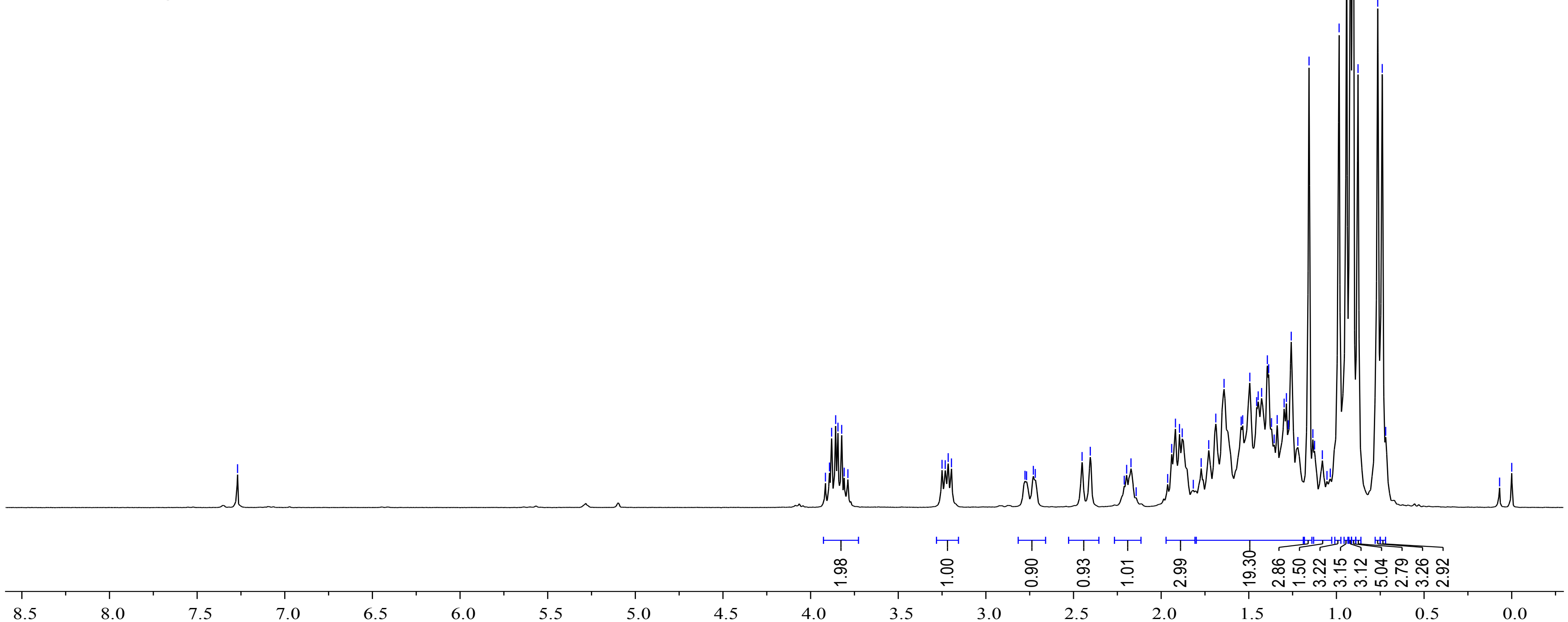
^{13}C NMR of **6f**


176.89
138.07
128.04
79.00
77.23
76.98
76.72
64.20
55.36
48.46
41.10
32.16
30.73
28.08
27.38
27.10
25.21
24.16
21.64
21.05
19.21
18.34
17.56
16.34
15.47
13.64
HO
H
H
CO_2*n*-Bu
6f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

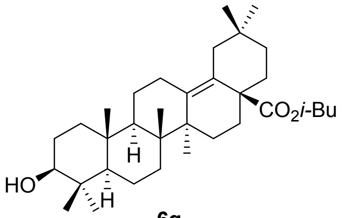
[1]H NMR of **6g**



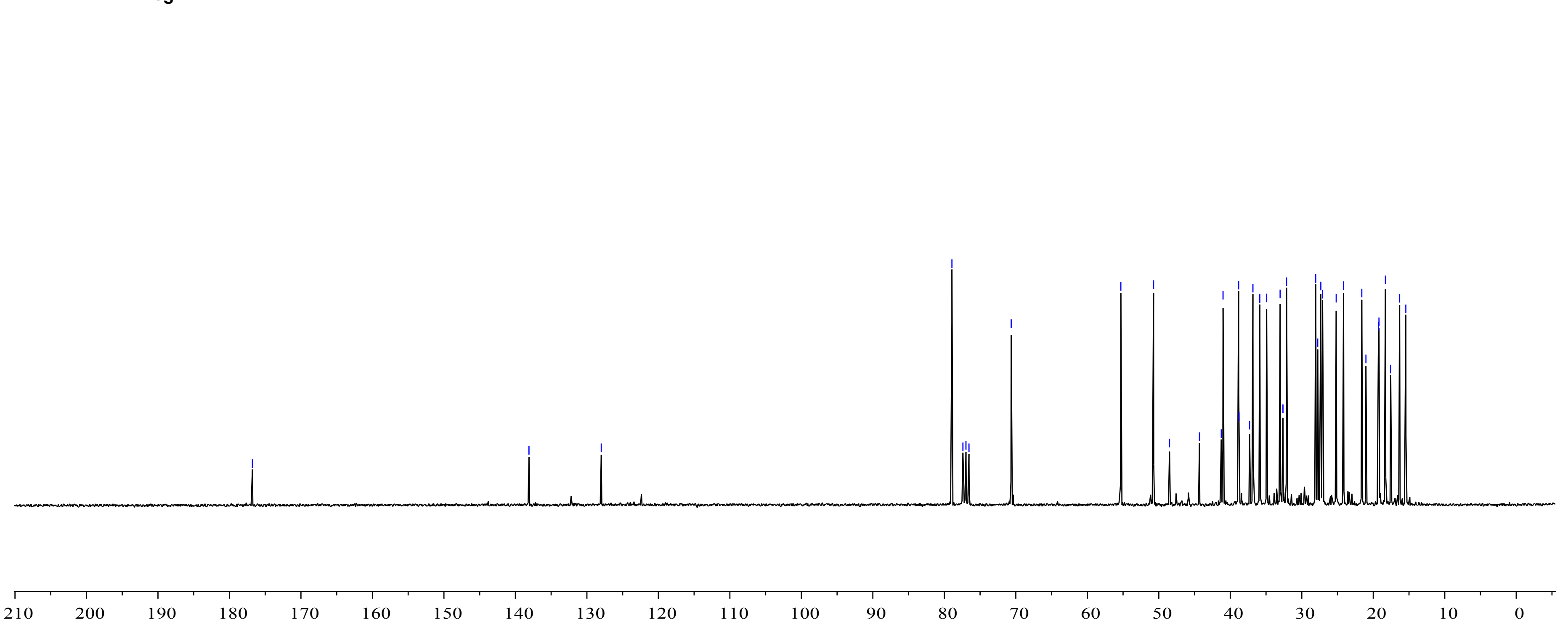
6g



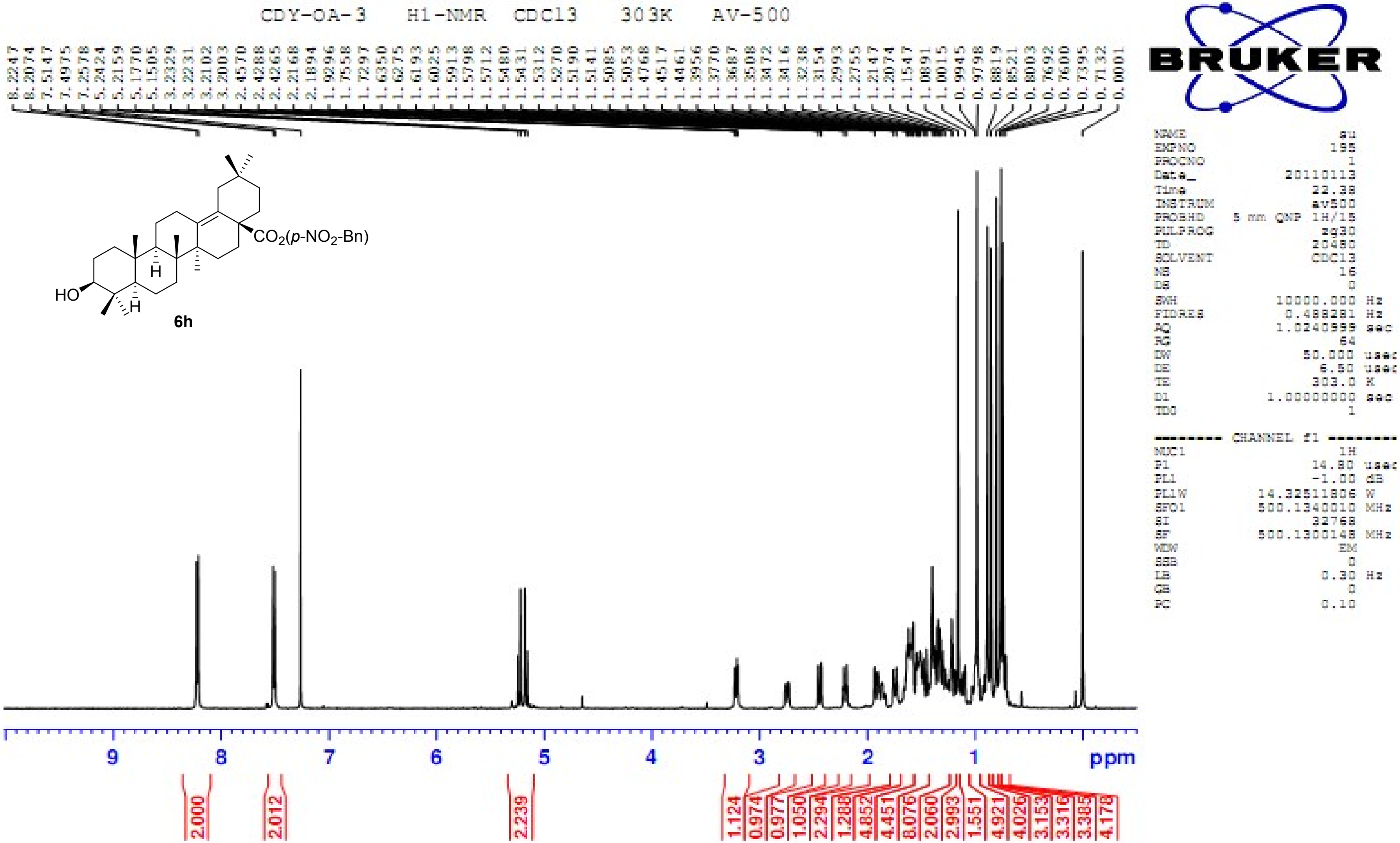
^{13}C NMR of **6g**



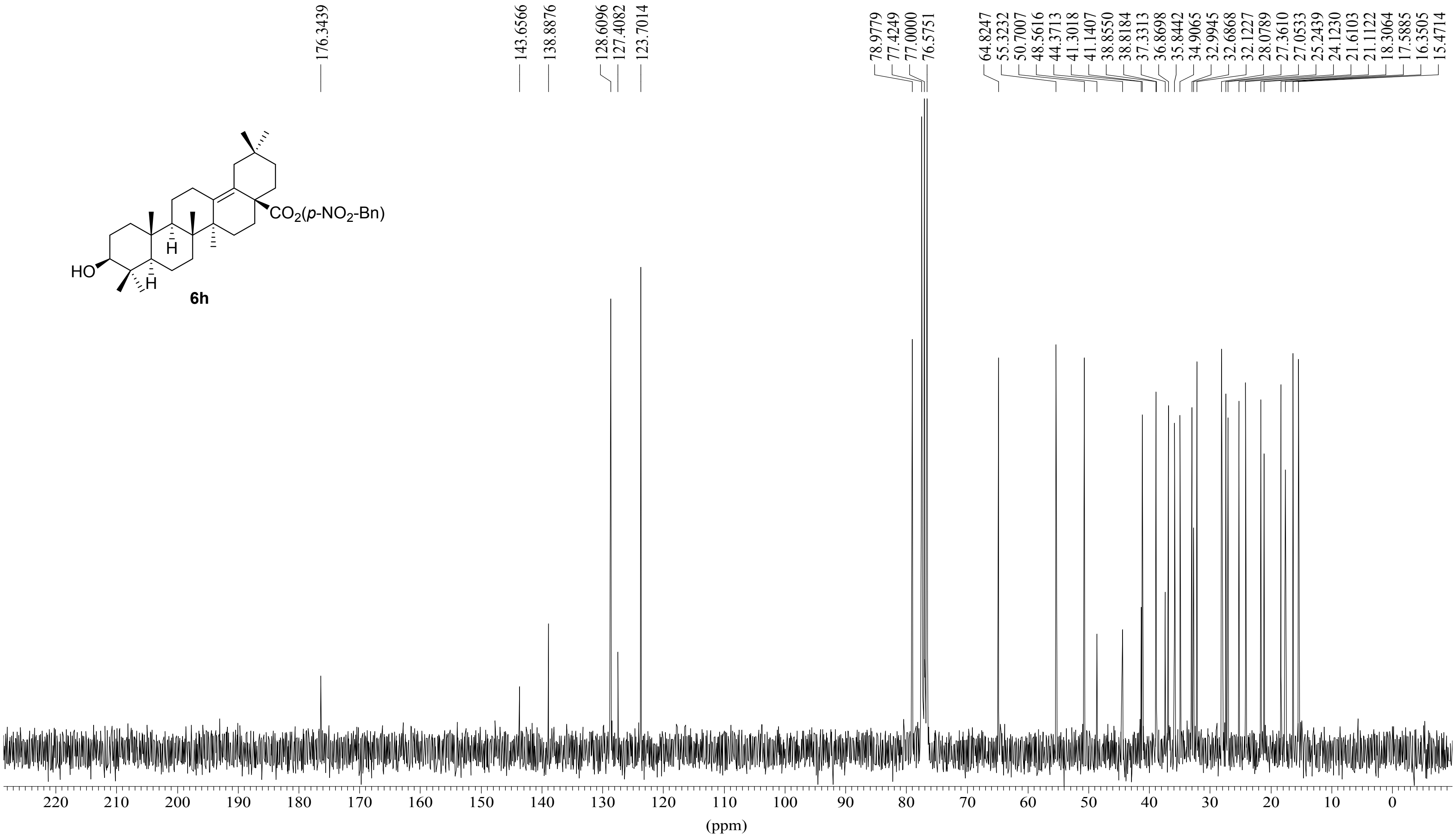
6g



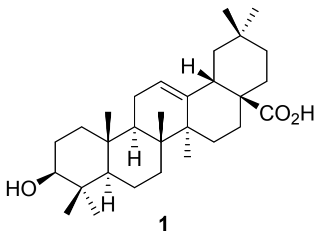
^{1}H NMR of **6h**

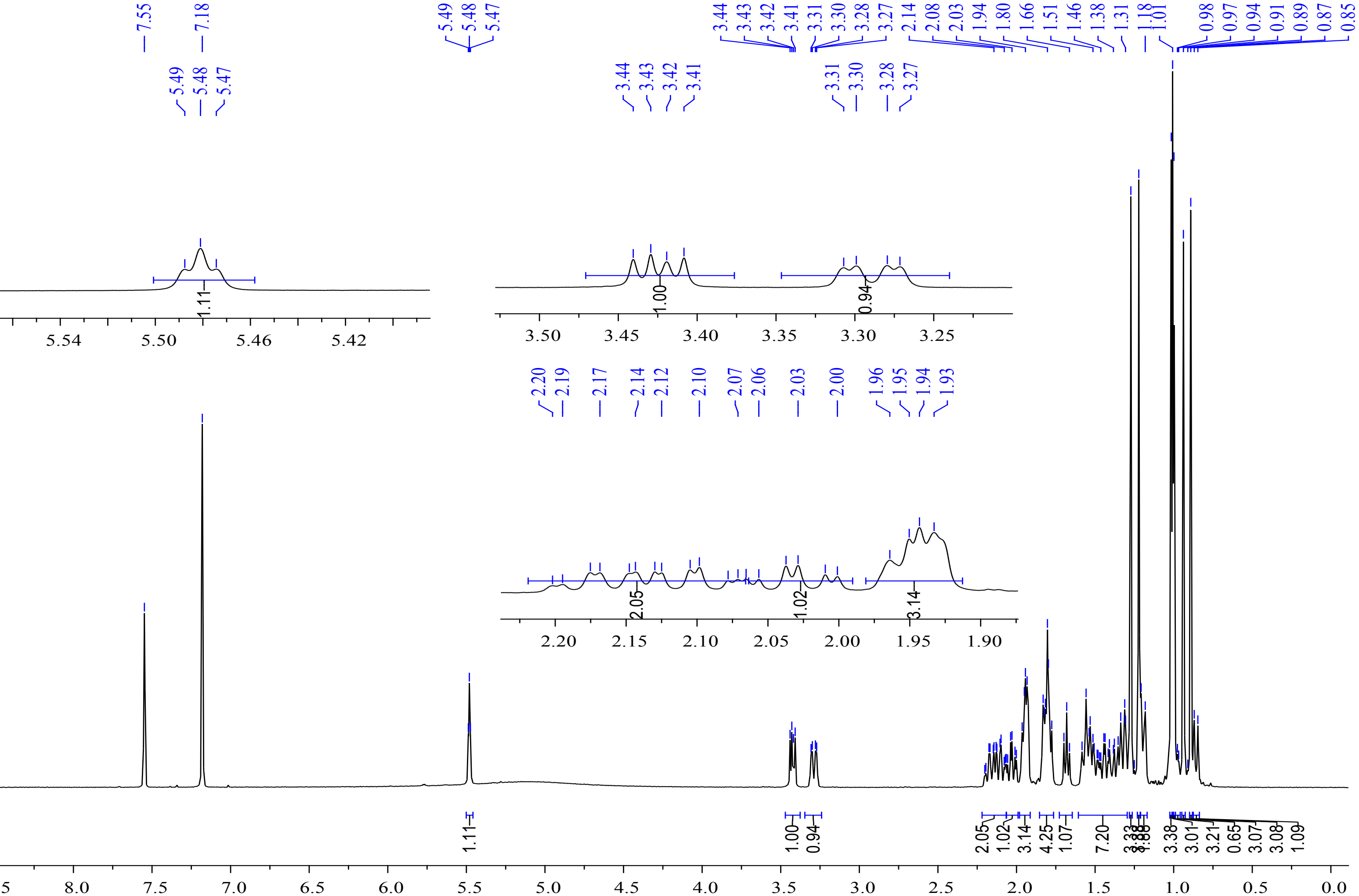


^{13}C NMR of **6h**

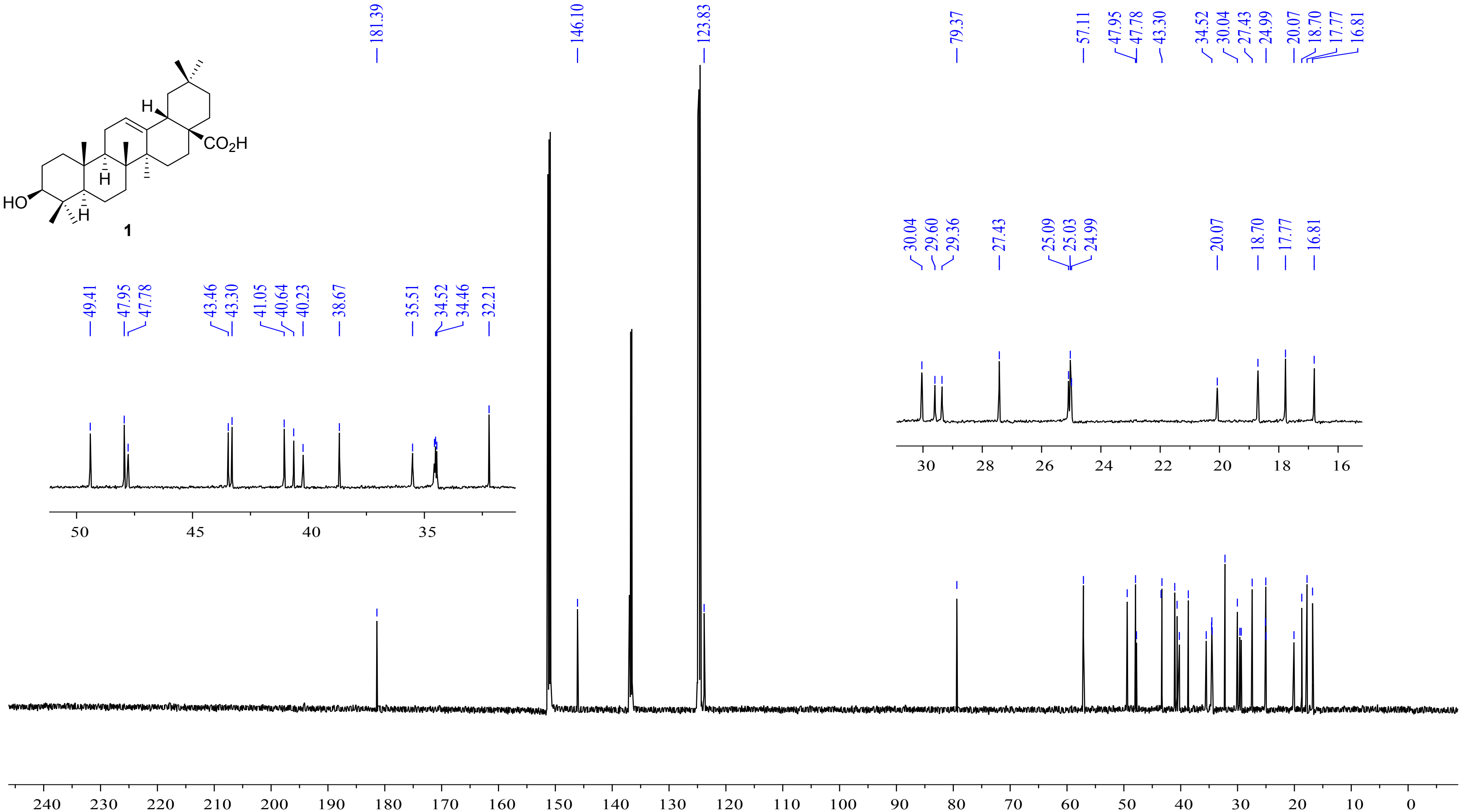

176.3439
143.6566
138.8876
128.6096
127.4082
123.7014
78.9779
77.4249
77.0000
76.5751
64.8247
55.3232
50.7007
48.5616
44.3713
41.3018
41.1407
38.8550
38.8184
37.3313
36.8698
35.8442
34.9065
32.9945
32.6868
32.1227
28.0789
27.3610
27.0533
25.2439
24.1230
21.6103
21.1122
18.3064
17.5885
16.3505
15.4714
HO
H
H
CO_2(*p*-NO_2-Bn)
6h
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

^{1}H NMR of **1**




8.69
7.55
7.18
5.49
5.48
5.47
3.44
3.43
3.42
3.41
3.31
3.30
3.28
3.27
2.14
2.08
2.03
1.94
1.80
1.66
1.51
1.46
1.38
1.31
1.18
1.01
0.98
0.97
0.94
0.91
0.89
0.87
0.85
5.58
5.54
5.50
5.46
5.42
1.11
3.50
3.45
3.40
3.35
3.30
3.25
1.00
0.94
2.20
2.19
2.17
2.14
2.12
2.10
2.07
2.06
2.03
2.00
1.96
1.95
1.94
1.93
2.15
2.10
2.05
2.00
1.95
1.90
2.05
1.02
3.14
4.25
1.07
7.20
3.33
3.38
3.01
3.21
0.65
3.07
3.08
1.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

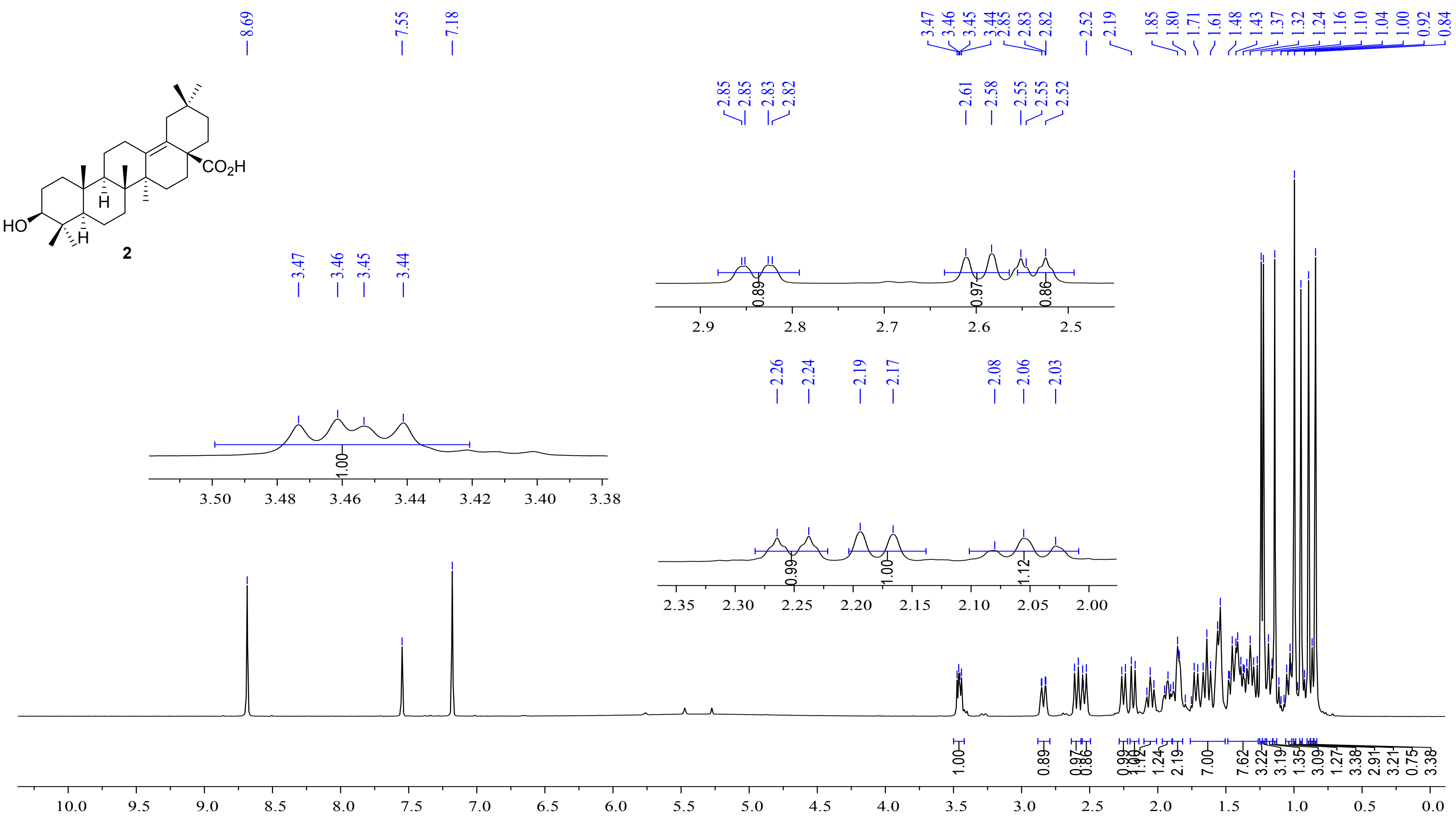
^{13}C NMR of **1**



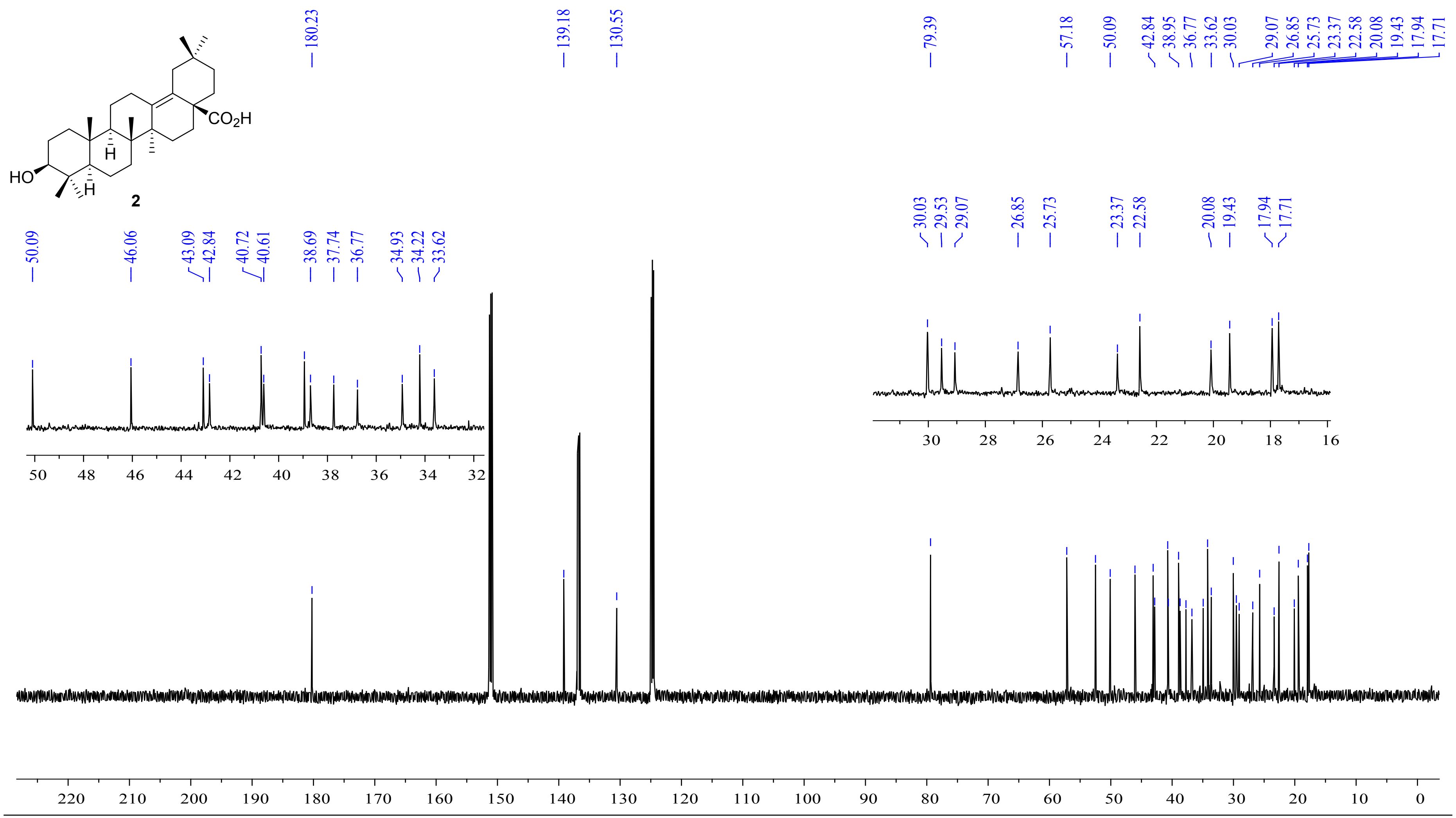
1

181.39
146.10
123.83
79.37
57.11
47.95
47.78
43.30
34.52
30.04
27.43
24.99
20.07
18.70
17.77
16.81
49.41
47.95
47.78
43.46
43.30
41.05
40.64
40.23
38.67
35.51
34.52
34.46
32.21
50
45
40
35
30.04
29.60
29.36
27.43
25.09
25.03
24.99
20.07
18.70
17.77
16.81
30
28
26
24
22
20
18
16
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

^{1}H NMR of **2**

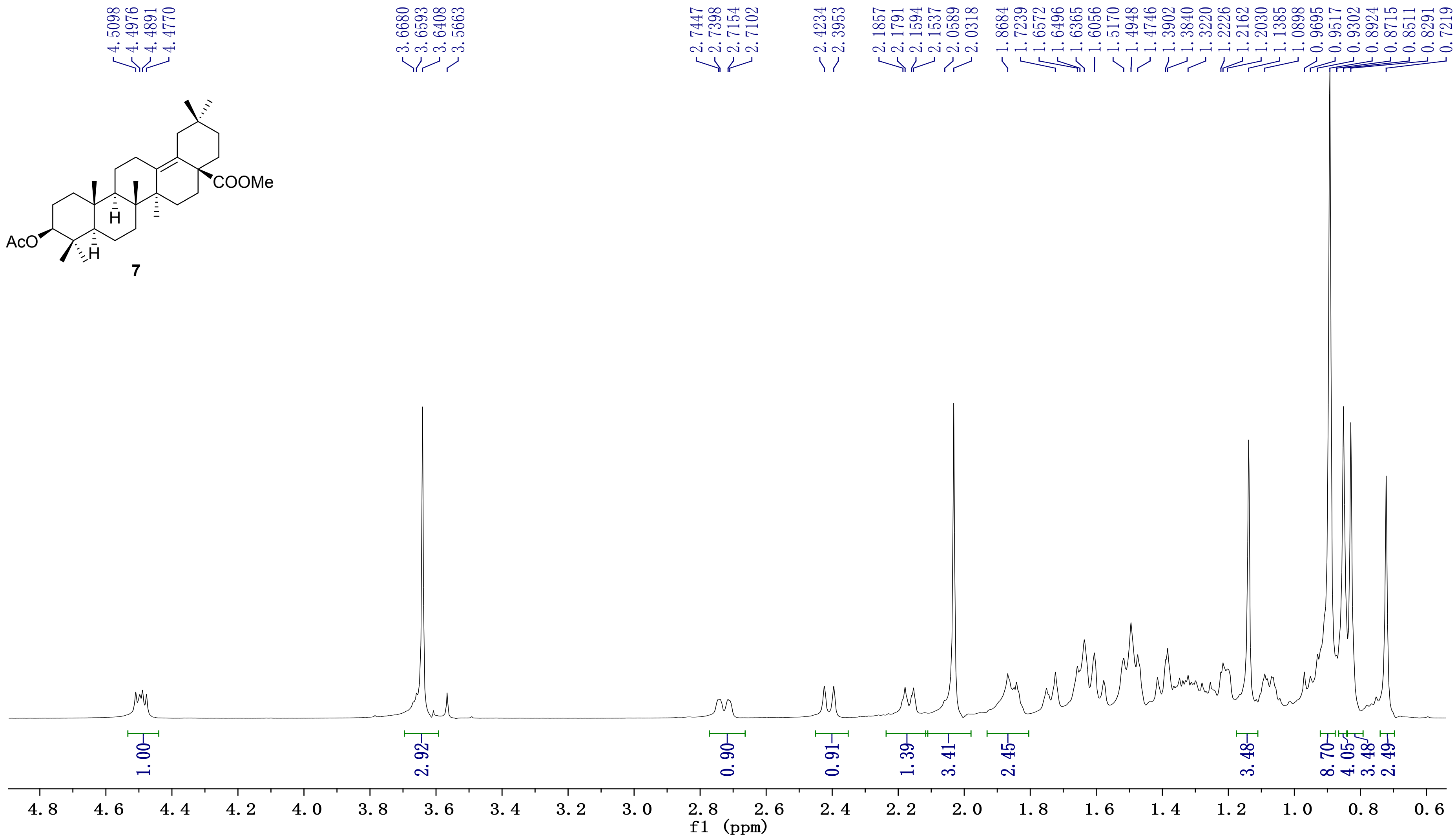


^{13}C NMR of **2**

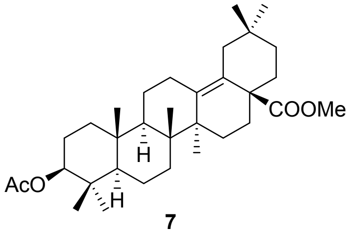


180.23
139.18
130.55
79.39
57.18
50.09
42.84
38.95
36.77
33.62
30.03
29.07
26.85
25.73
23.37
22.58
20.08
19.43
17.94
17.71
HO
H
H
CO_2H
2
50.09
46.06
43.09
42.84
40.72
40.61
38.69
37.74
36.77
34.93
34.22
33.62
30.03
29.53
29.07
26.85
25.73
23.37
22.58
20.08
19.43
17.94
17.71

^{1}H NMR of **7**

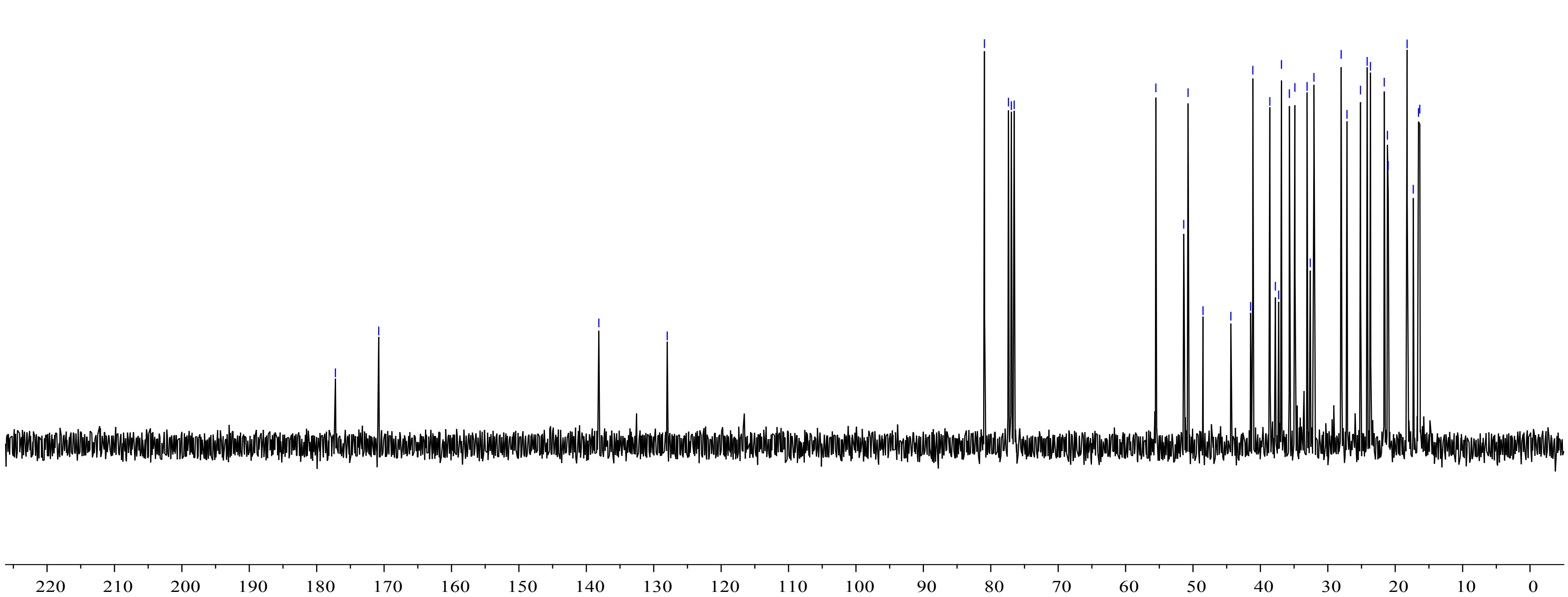

4.5098
4.4976
4.4891
4.4770
3.6680
3.6593
3.6408
3.5663
2.7447
2.7398
2.7154
2.7102
2.4234
2.3953
2.1857
2.1791
2.1594
2.1537
2.0589
2.0318
1.8684
1.7239
1.6572
1.6496
1.6365
1.6056
1.5170
1.4948
1.4746
1.3902
1.3840
1.3220
1.2226
1.2162
1.2030
1.1385
1.0898
0.9695
0.9517
0.9302
0.8924
0.8715
0.8511
0.8291
0.7219
AcO
H
H
COOMe
7
1.00
2.92
0.90
0.91
1.39
3.41
2.45
3.48
8.70
4.05
3.48
2.49
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
f1 (ppm)

^{13}C NMR of **7**



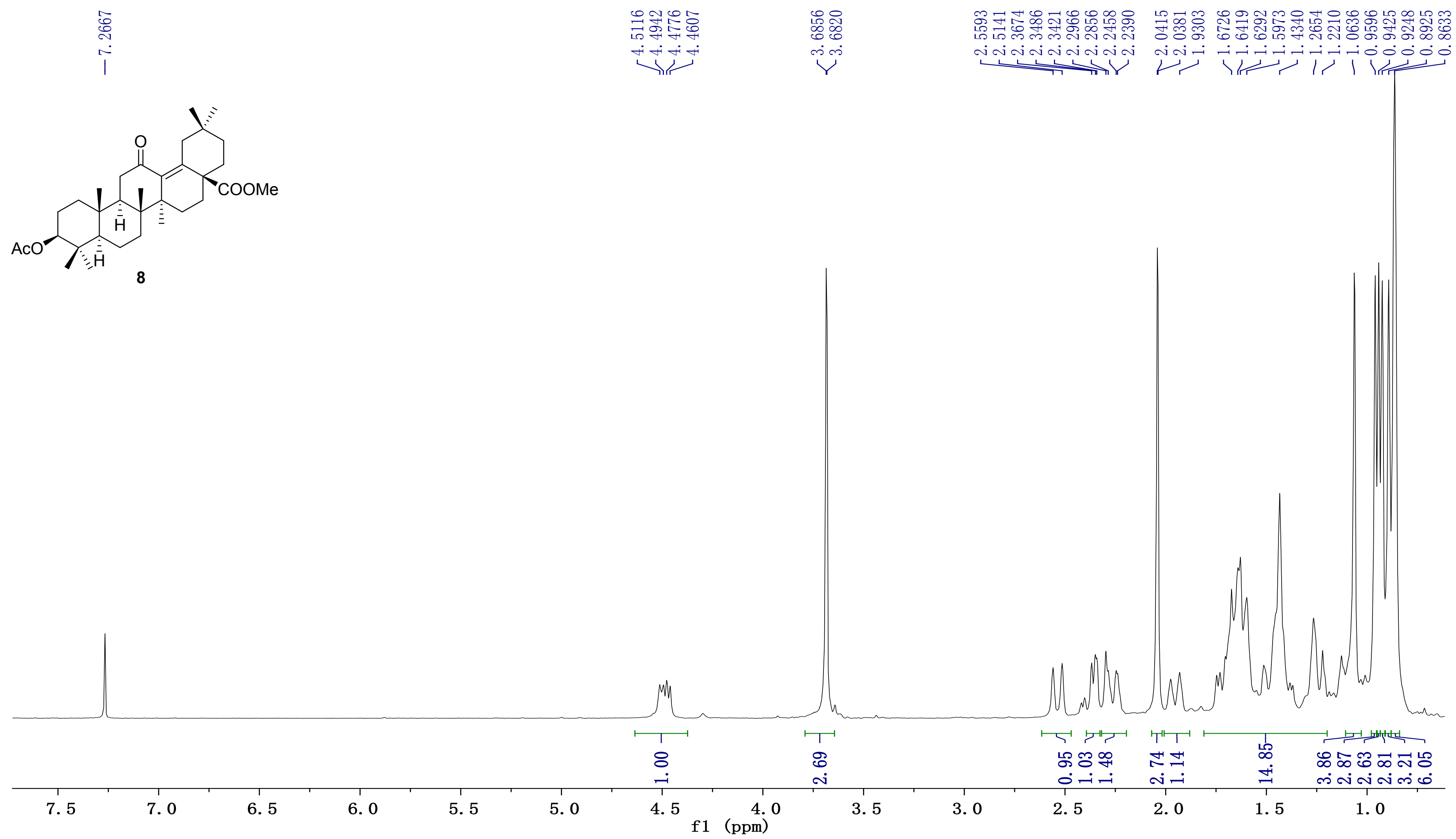
COOMe
AcO
H
H

7

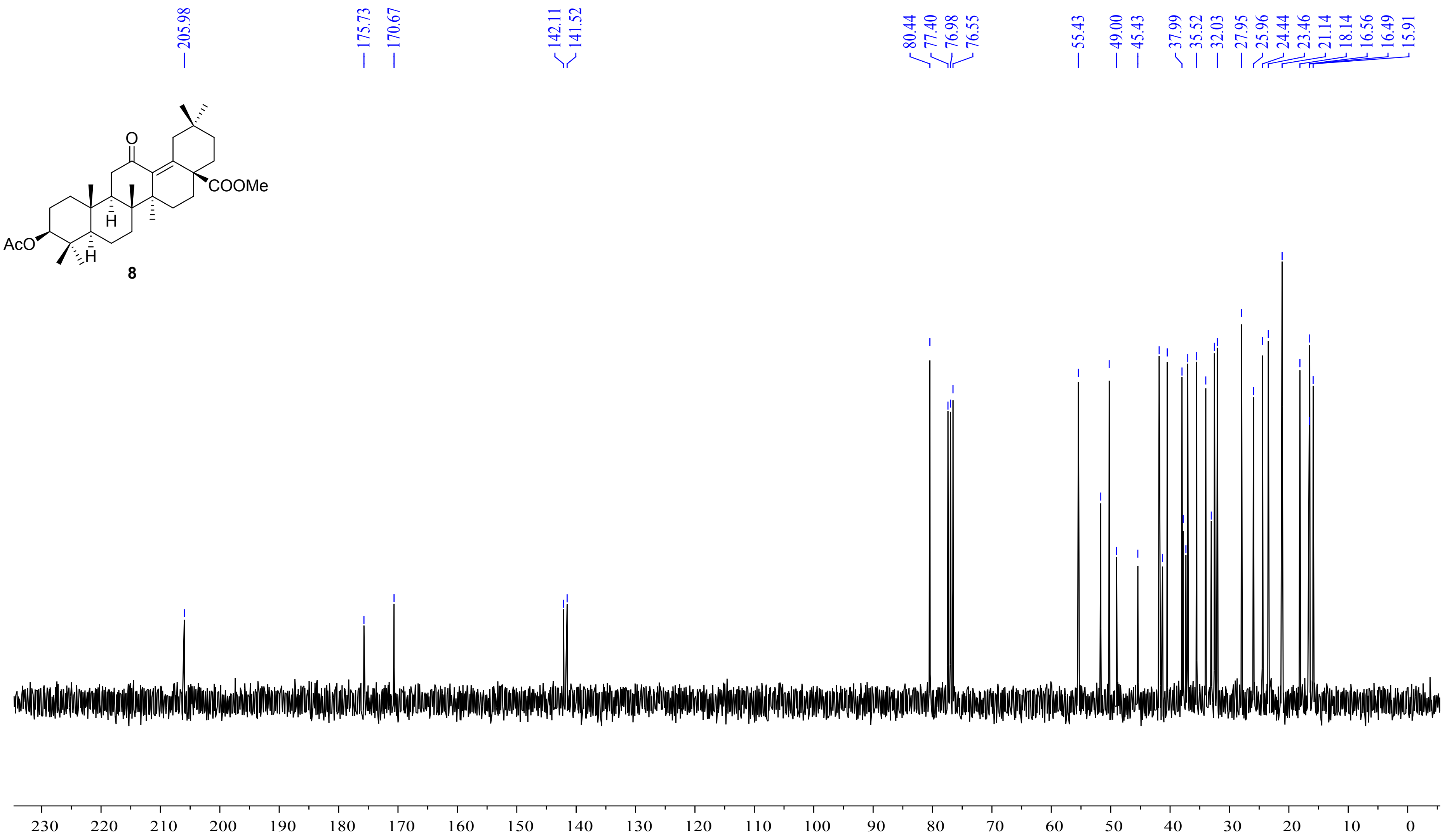


177.22
170.80
138.14
128.00
80.94
77.37
76.95
76.53
55.51
48.51
41.12
37.29
34.88
32.06
28.02
24.16
23.67
21.63
21.15
21.04
18.23
17.32
16.55
16.35
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

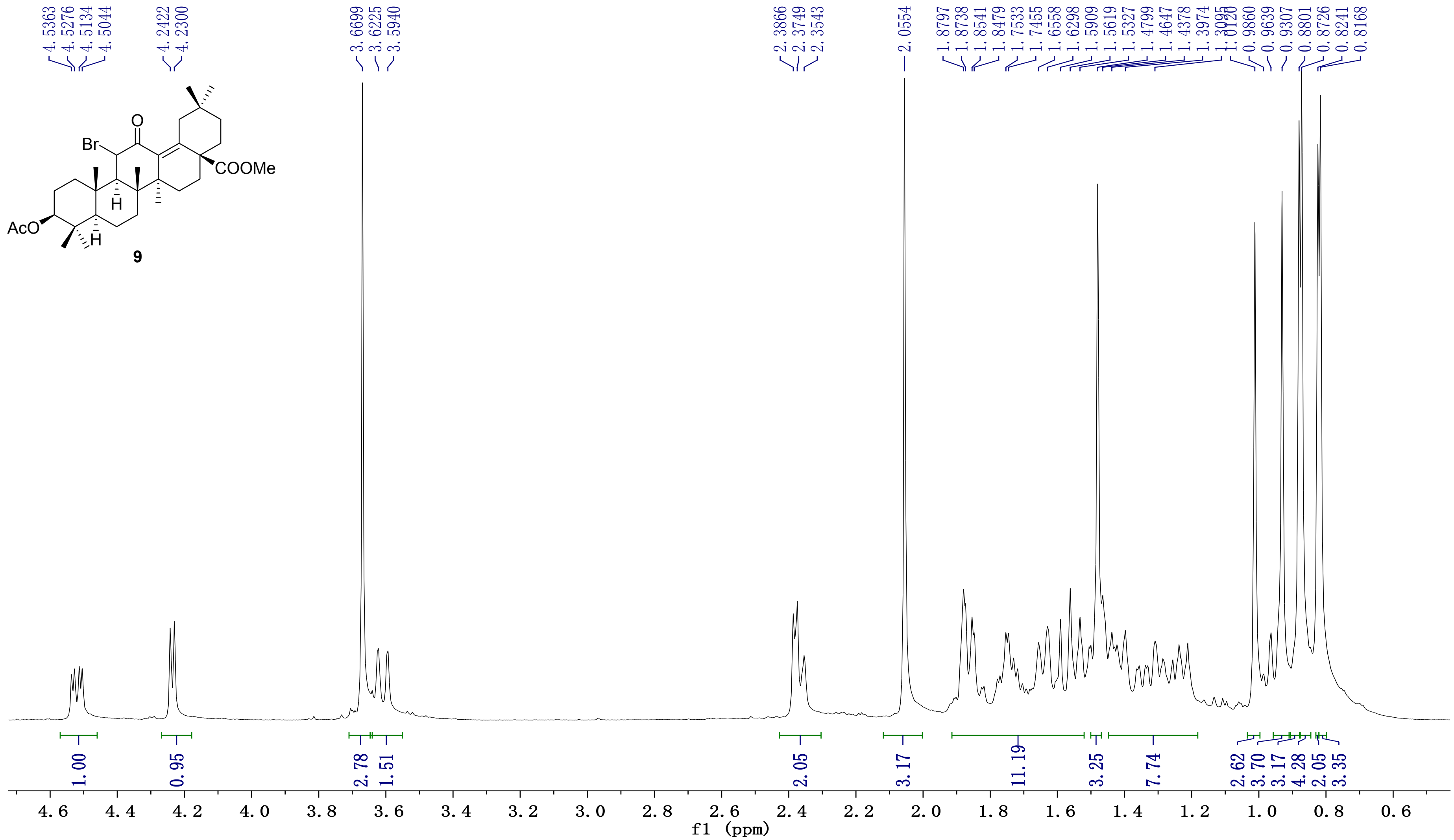
[1]H NMR of **8**


7.2667
4.5116
4.4942
4.4776
4.4607
3.6856
3.6820
2.5593
2.5141
2.3674
2.3486
2.3421
2.2966
2.2856
2.2458
2.2390
2.0415
2.0381
1.9303
1.6726
1.6419
1.6292
1.5973
1.4340
1.2654
1.2210
1.0636
0.9596
0.9425
0.9248
0.8925
0.8633
O
COOMe
H
AcO
H
8
1.00
2.69
0.95
1.03
1.48
2.74
1.14
14.85
3.86
2.87
2.63
2.81
3.21
6.05
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

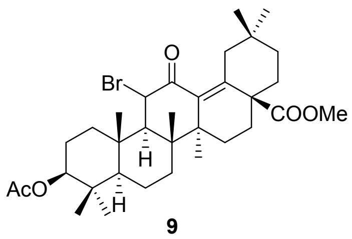
^{13}C NMR of **8**

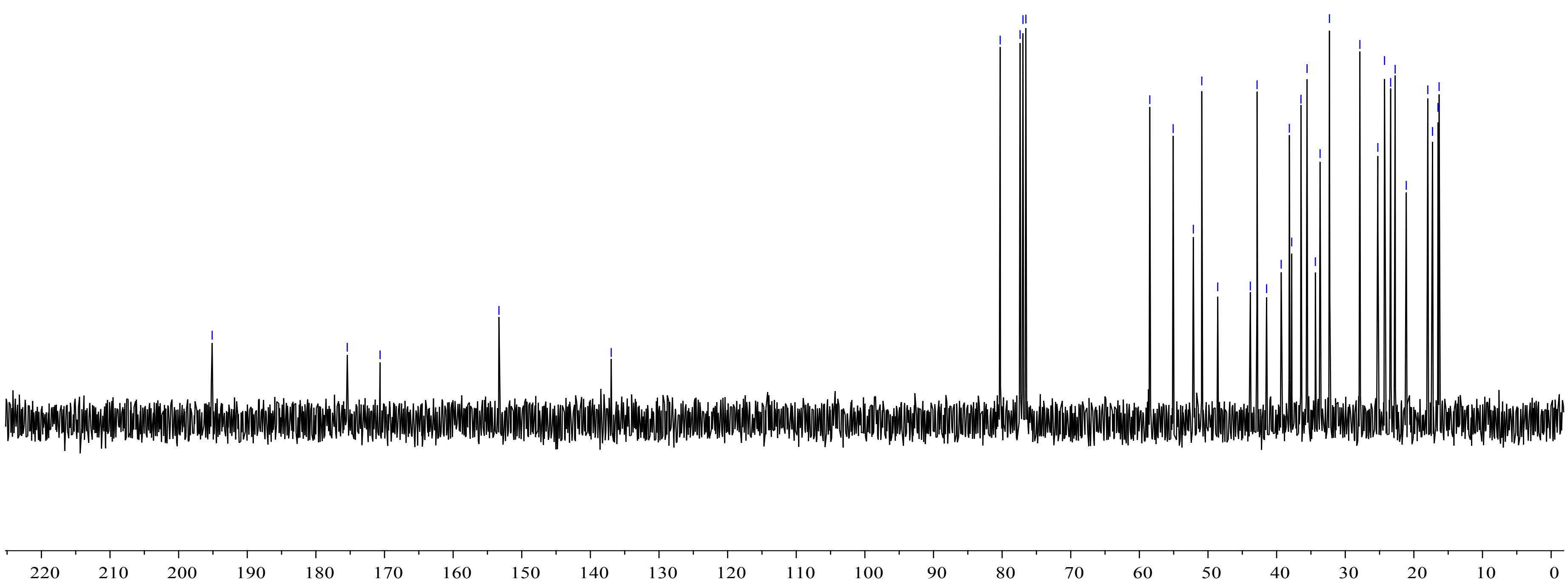

205.98
175.73
170.67
142.11
141.52
80.44
77.40
76.98
76.55
55.43
49.00
45.43
37.99
35.52
32.03
27.95
25.96
24.44
23.46
21.14
18.14
16.56
16.49
15.91
O
COOMe
H
AcO
H
8
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

^{1}H NMR of **9**

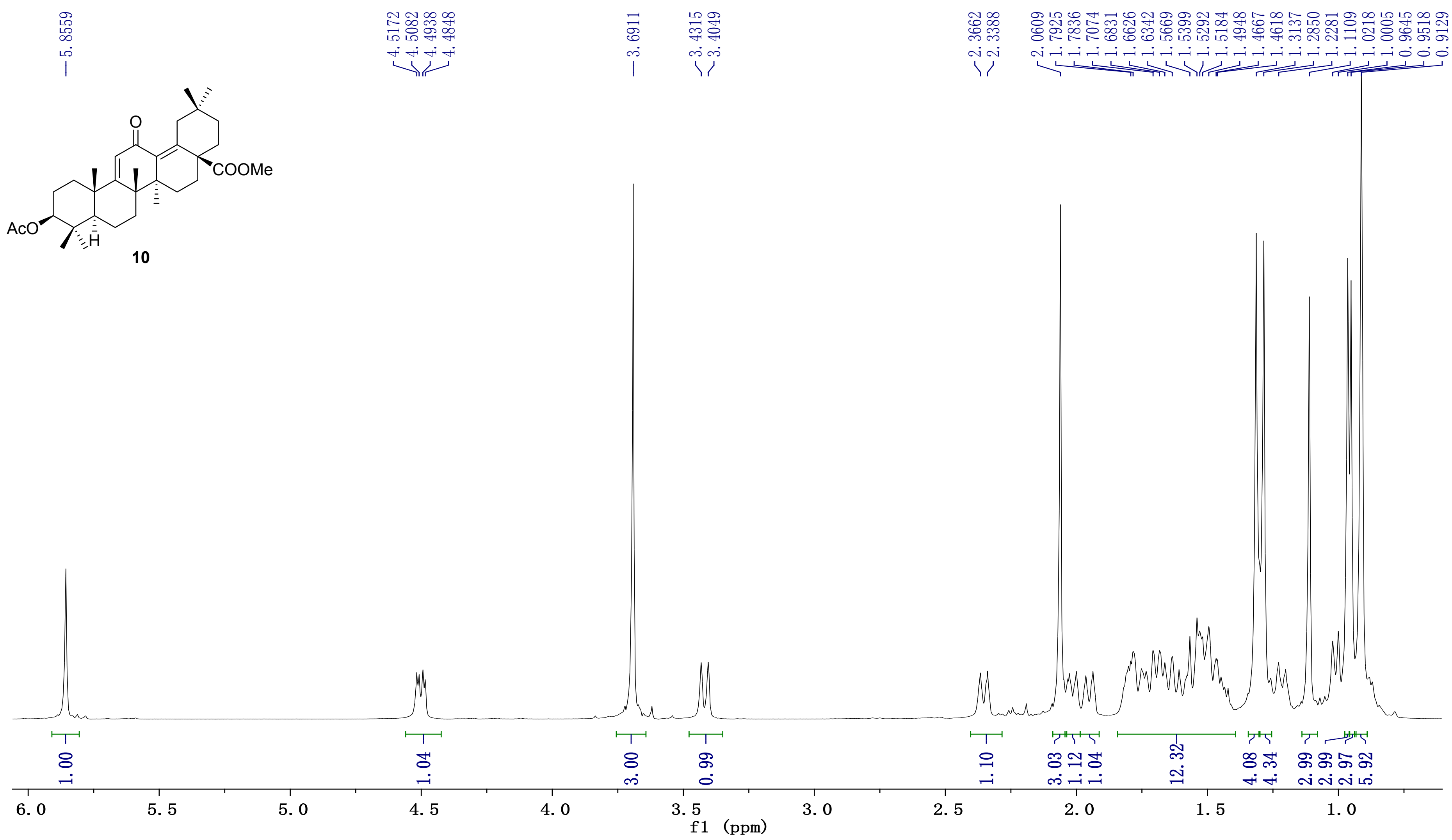


^{13}C NMR of **9**



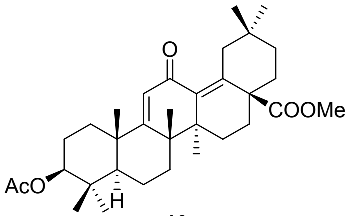

195.12
175.43
170.65
153.32
136.96
80.28
77.39
76.96
76.54
58.48
52.14
48.58
42.85
36.45
34.35
32.30
27.87
24.27
23.38
22.73
21.11
17.97
17.28
16.49
16.32
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

^{1}H NMR of **10**

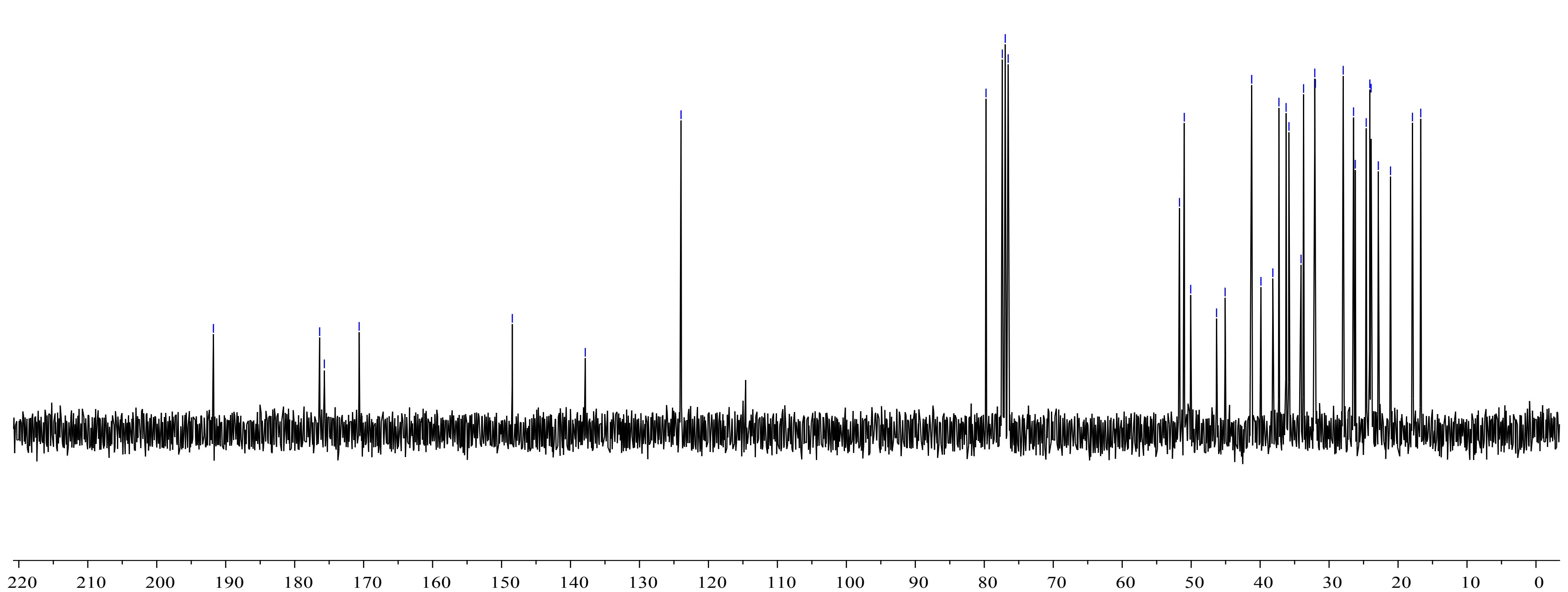


5.8559
4.5172
4.5082
4.4938
4.4848
3.6911
3.4315
3.4049
2.3662
2.3388
2.0609
1.7925
1.7836
1.7074
1.6831
1.6626
1.6342
1.5669
1.5399
1.5292
1.5184
1.4948
1.4667
1.4618
1.3137
1.2850
1.2281
1.1109
1.0218
1.0005
0.9645
0.9518
0.9129
O
COOMe
AcO
H
10
1.00
1.04
3.00
0.99
1.10
3.03
1.12
1.04
12.32
4.08
4.34
2.99
2.99
2.97
5.92
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

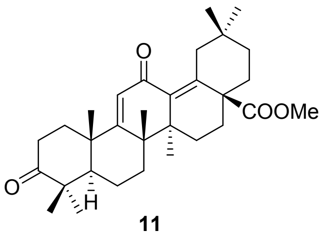
[13]C NMR of **10**



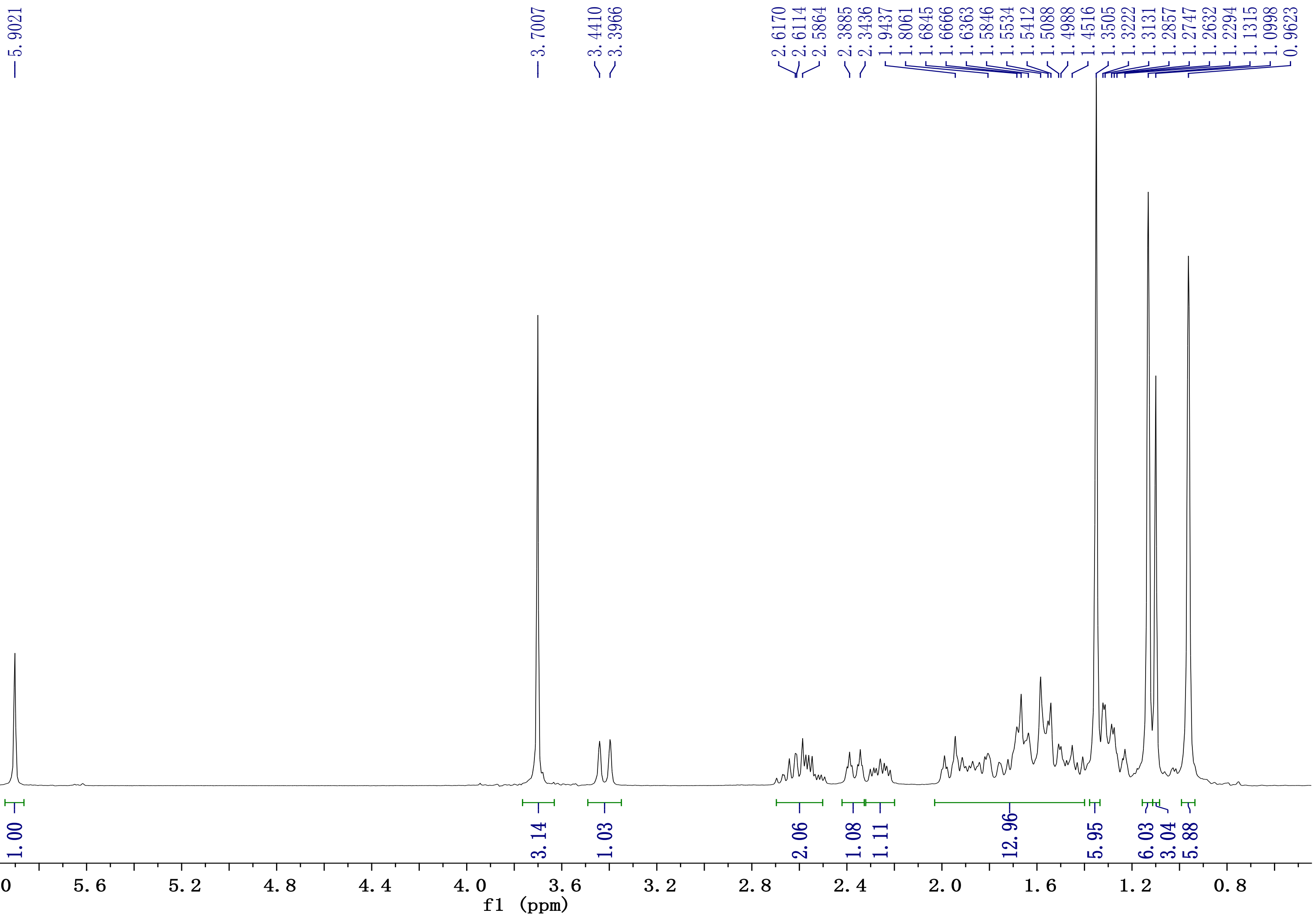
10



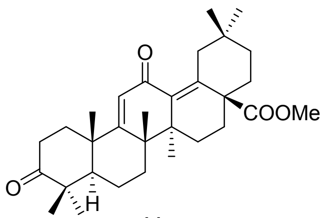
^{1}H NMR of **11**



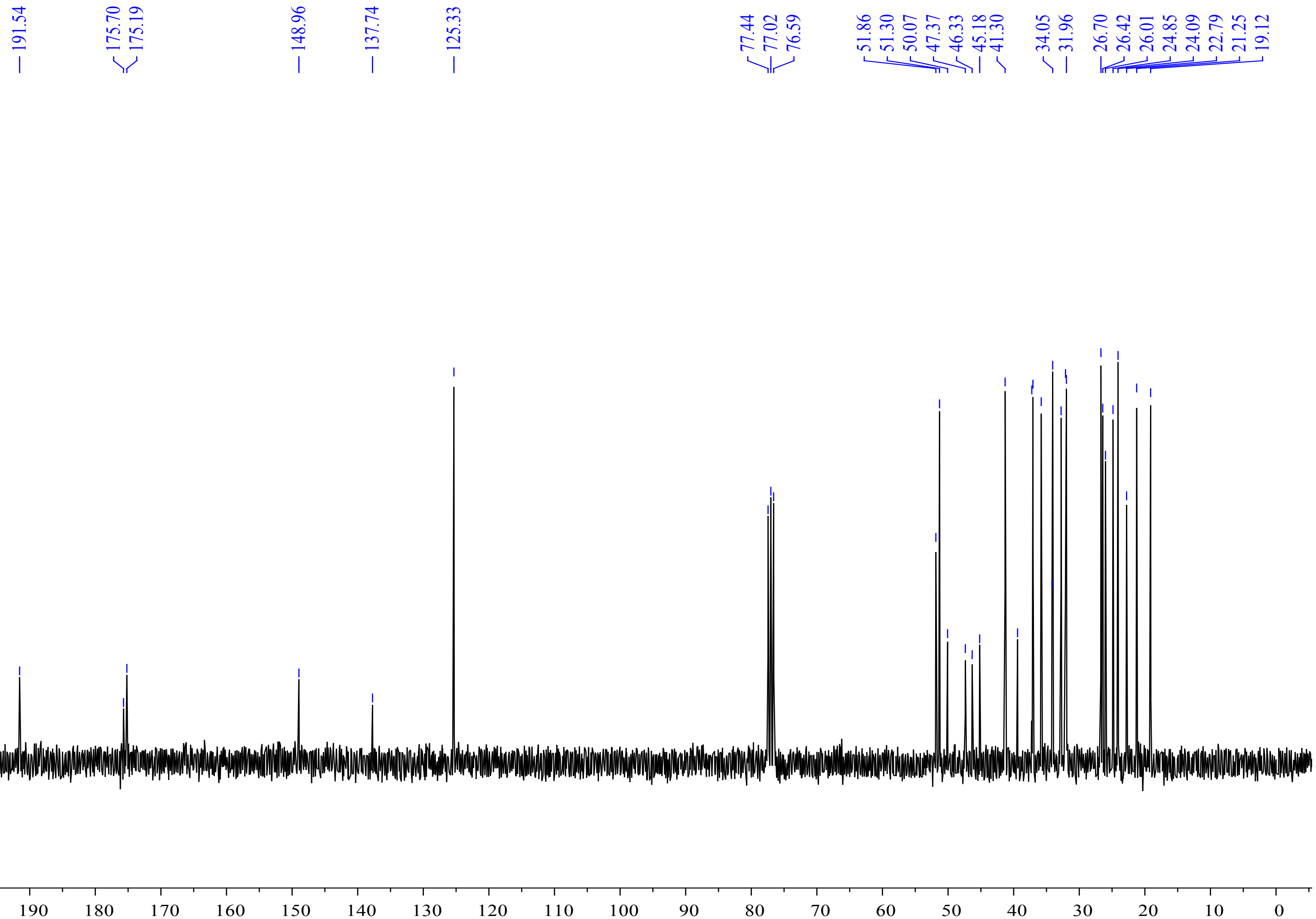
11



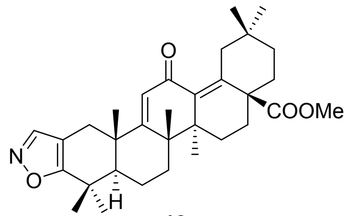
^{13}C NMR of **11**



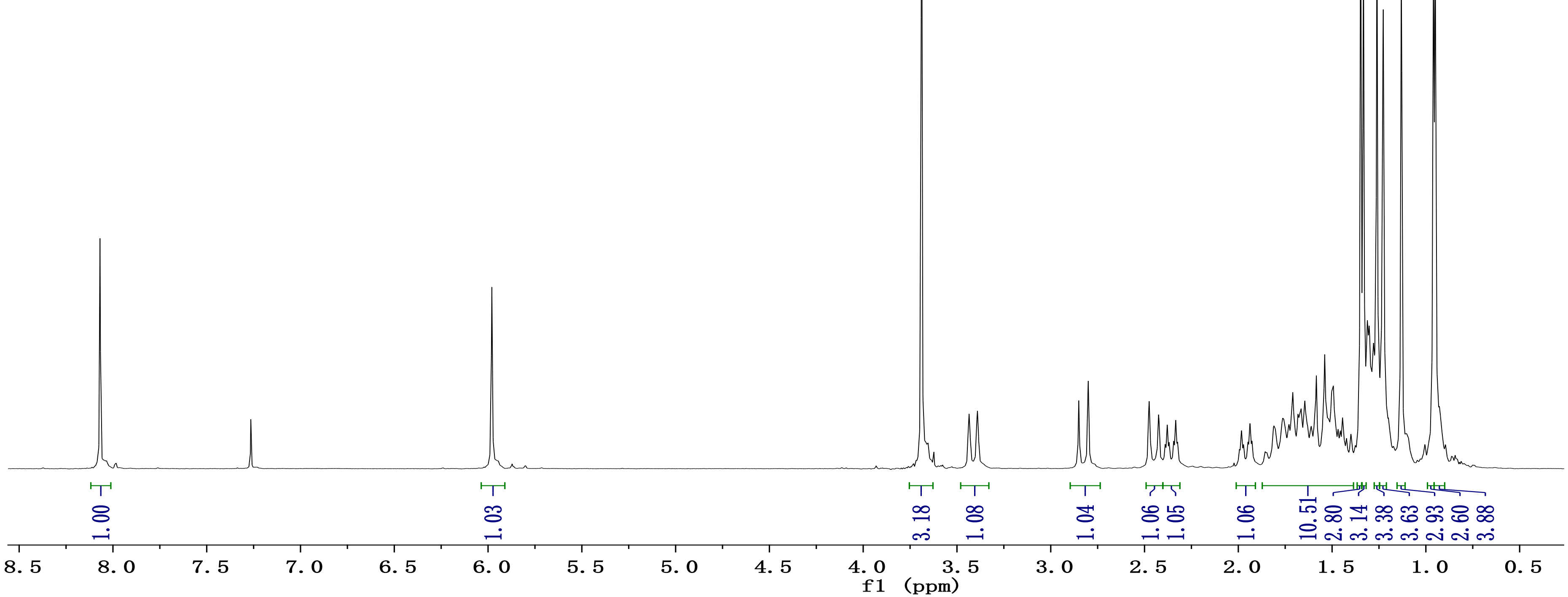
11



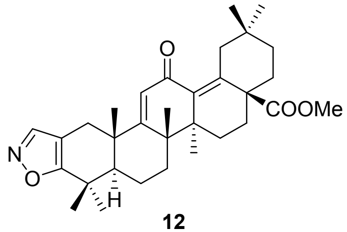
[1]H NMR of **12**



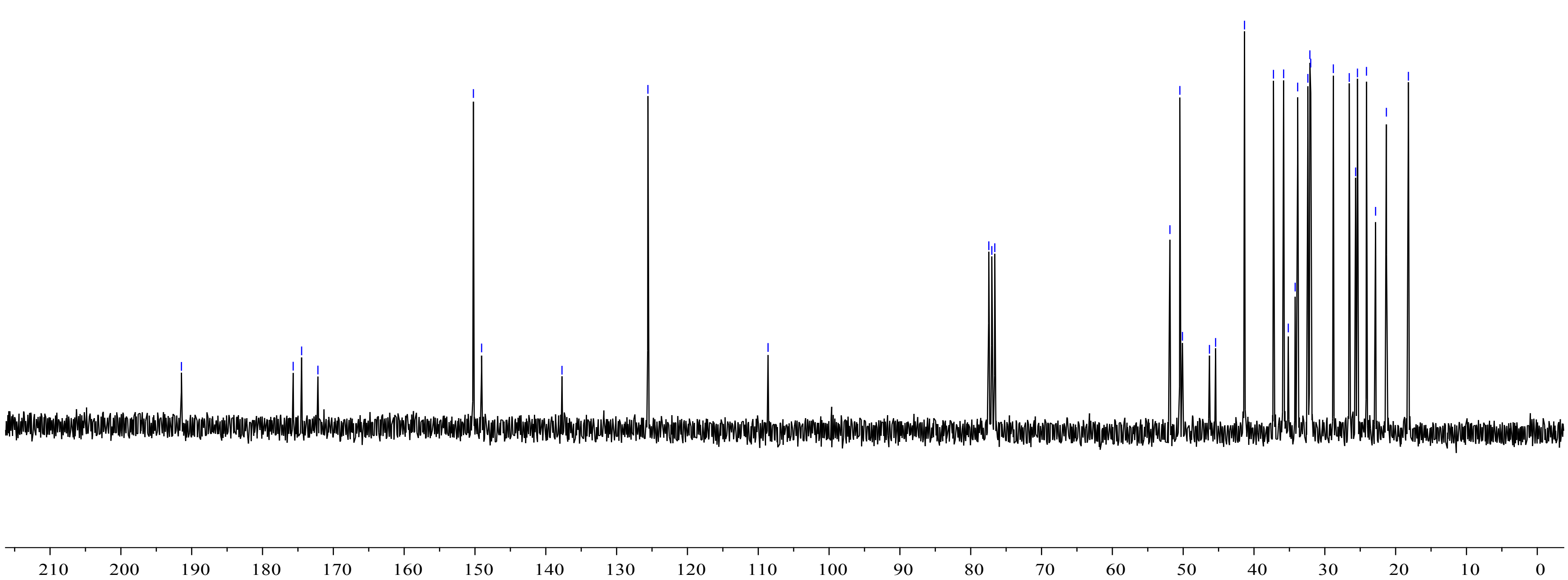
12



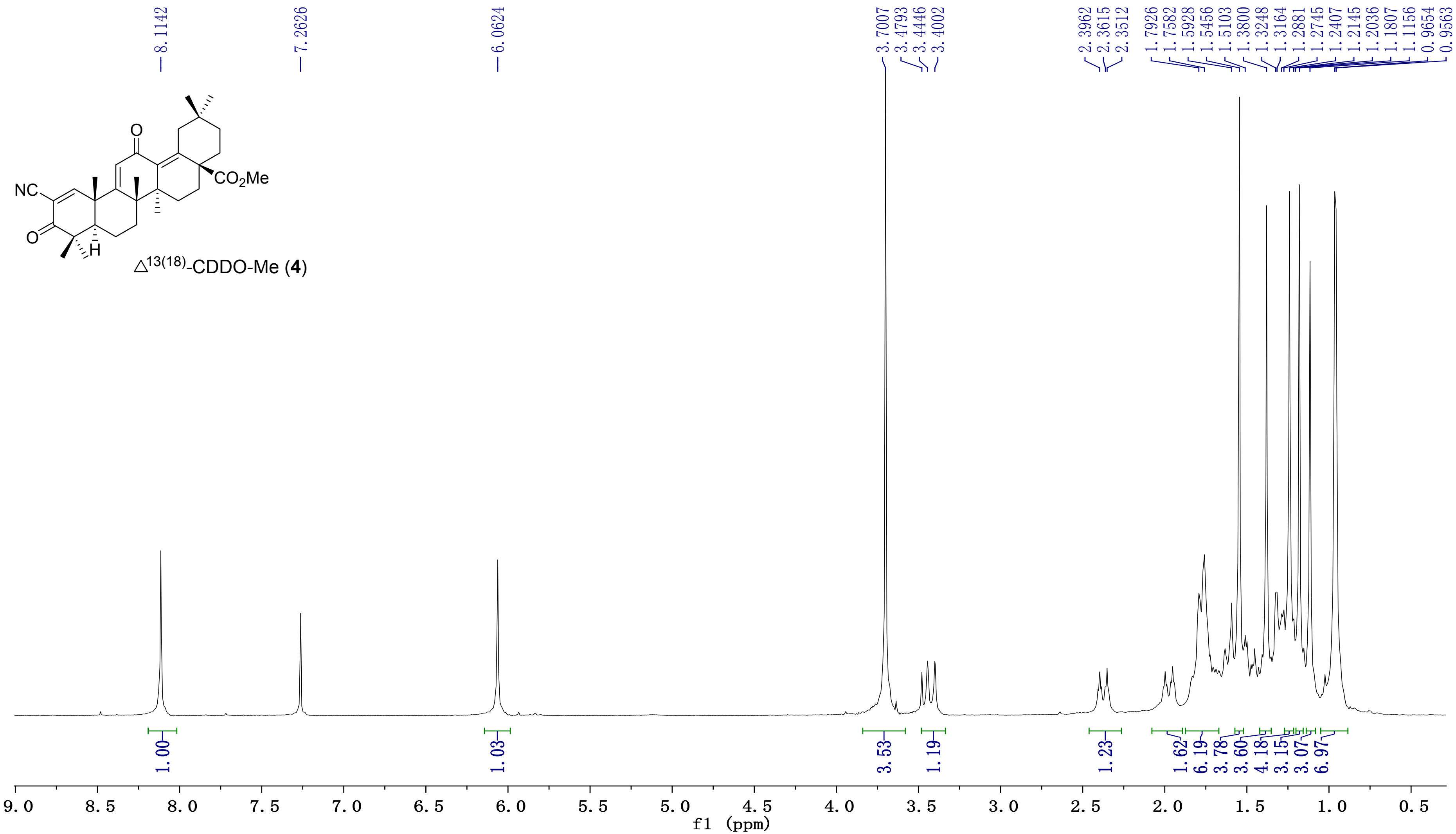
^{13}C NMR of **12**



12

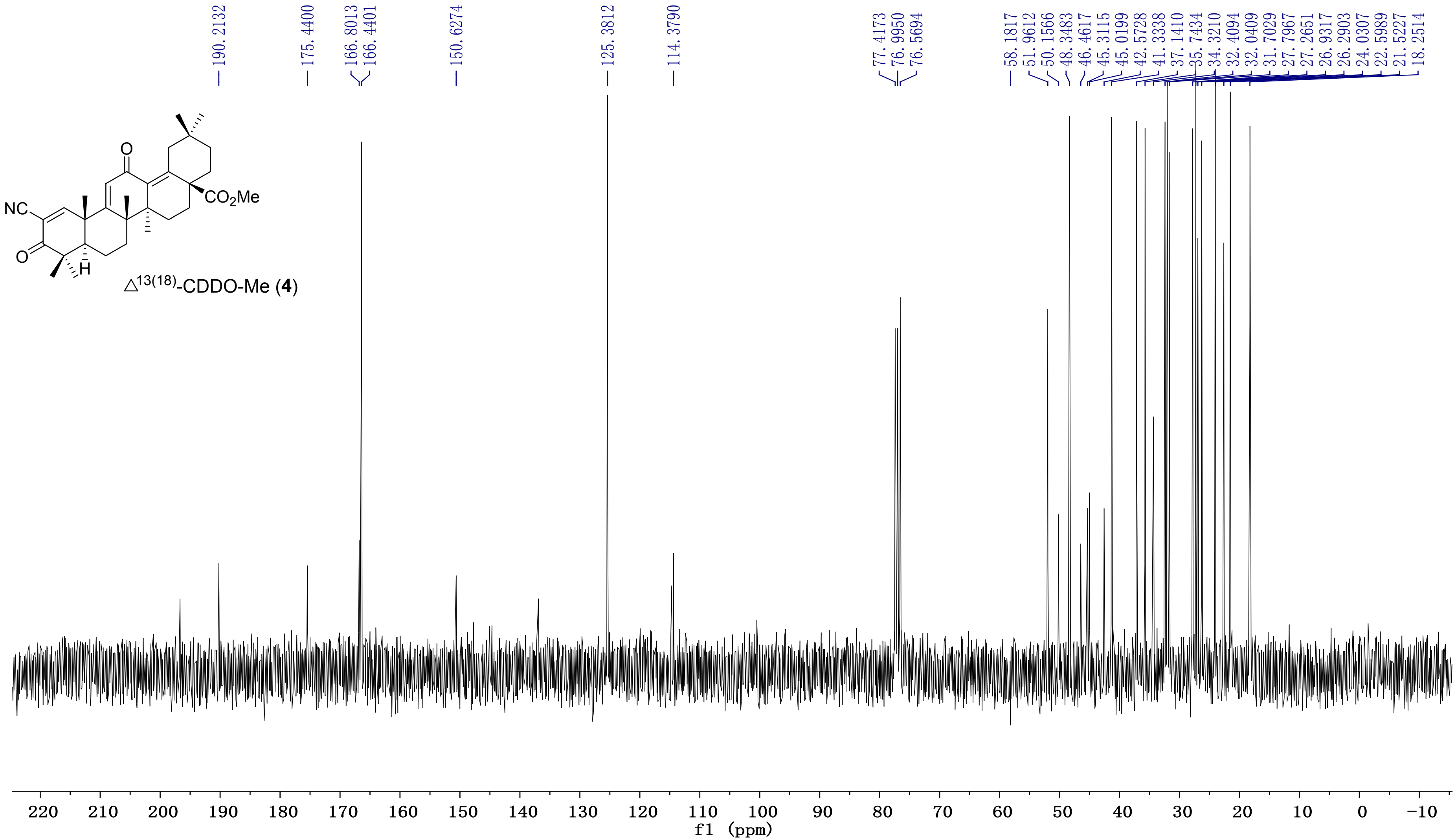


^{1}H NMR of **4**



8.1142
7.2626
6.0624
3.7007
3.4793
3.4446
3.4002
2.3962
2.3615
2.3512
1.7926
1.7582
1.5928
1.5456
1.5103
1.3800
1.3248
1.3164
1.2881
1.2745
1.2407
1.2145
1.2036
1.1807
1.1156
0.9654
0.9563
NC
O
O
H
CO_2Me
△13(18)-CDDO-Me (4)
1.00
1.03
3.53
1.19
1.23
1.62
6.19
3.78
3.60
4.18
3.15
3.07
6.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

[13]C NMR of **4**



△[13(18)]-CDDO-Me (**4**)