Supporting Information

Application of Mannich Bases to the Synthesis of Hydroxymethylated Isoflavonoids As Potential Antineoplastic Agents

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[d] Taras Shevchenko Kyiv National University, Kyiv 01601, Ukraine
[e] Lucille Parker Markey Cancer Center, University of Kentucky, Lexington, KY 40536-0509, USA
[f] Department of Urology, Elm & Carlton Streets, Roswell Park Cancer Institute, Buffalo, New York 14263, USA
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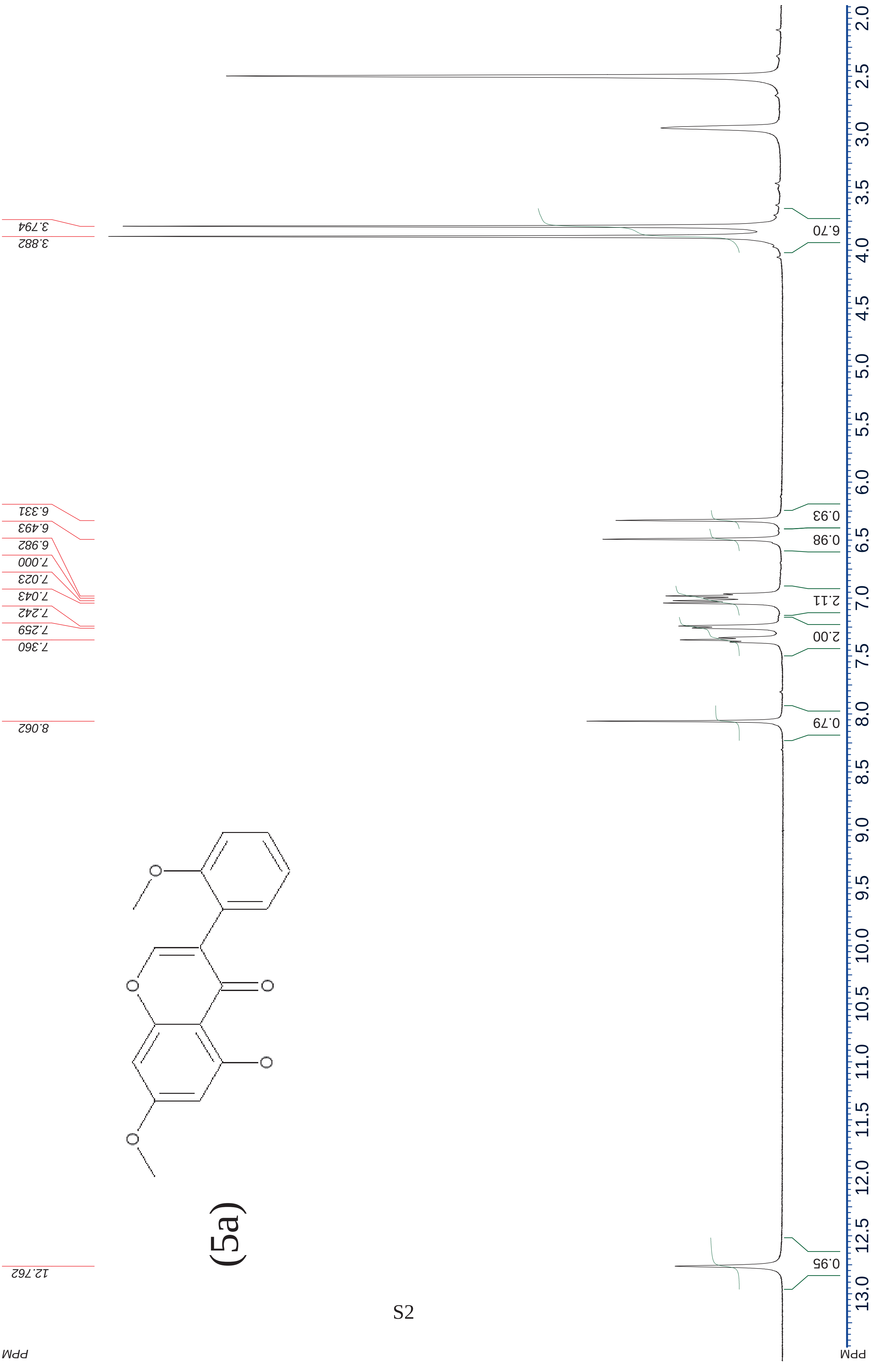
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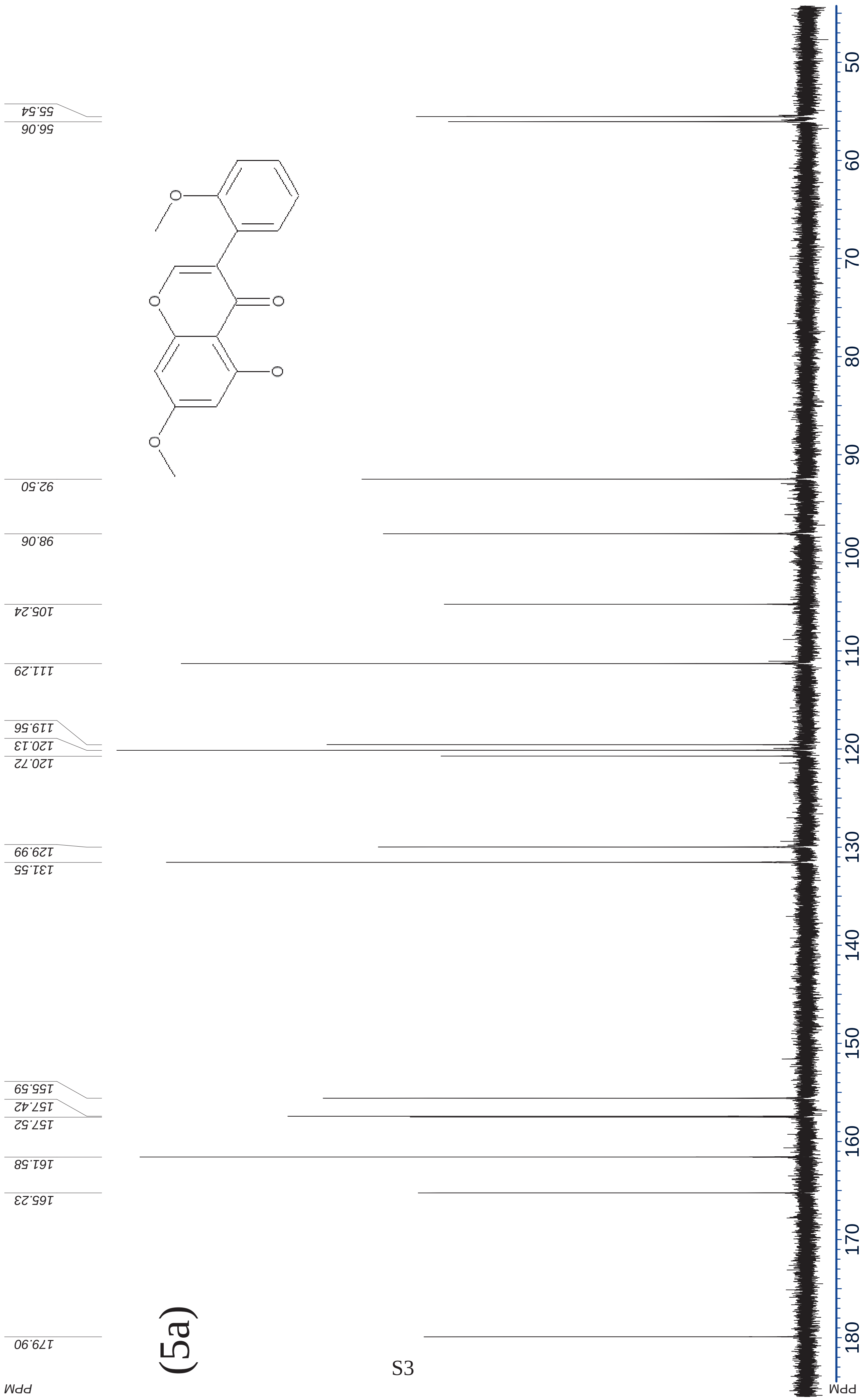
PPM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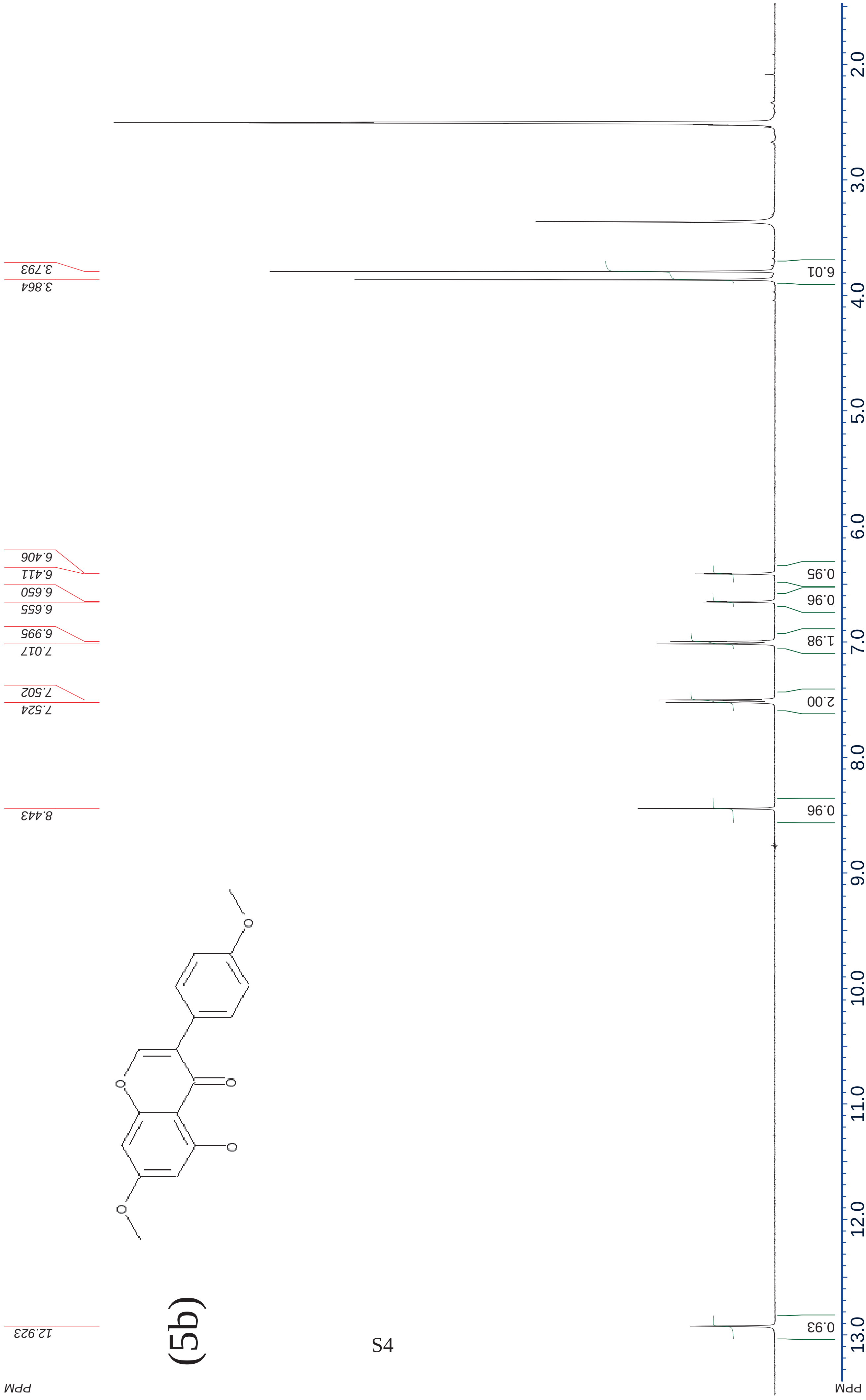
PPM

(5a)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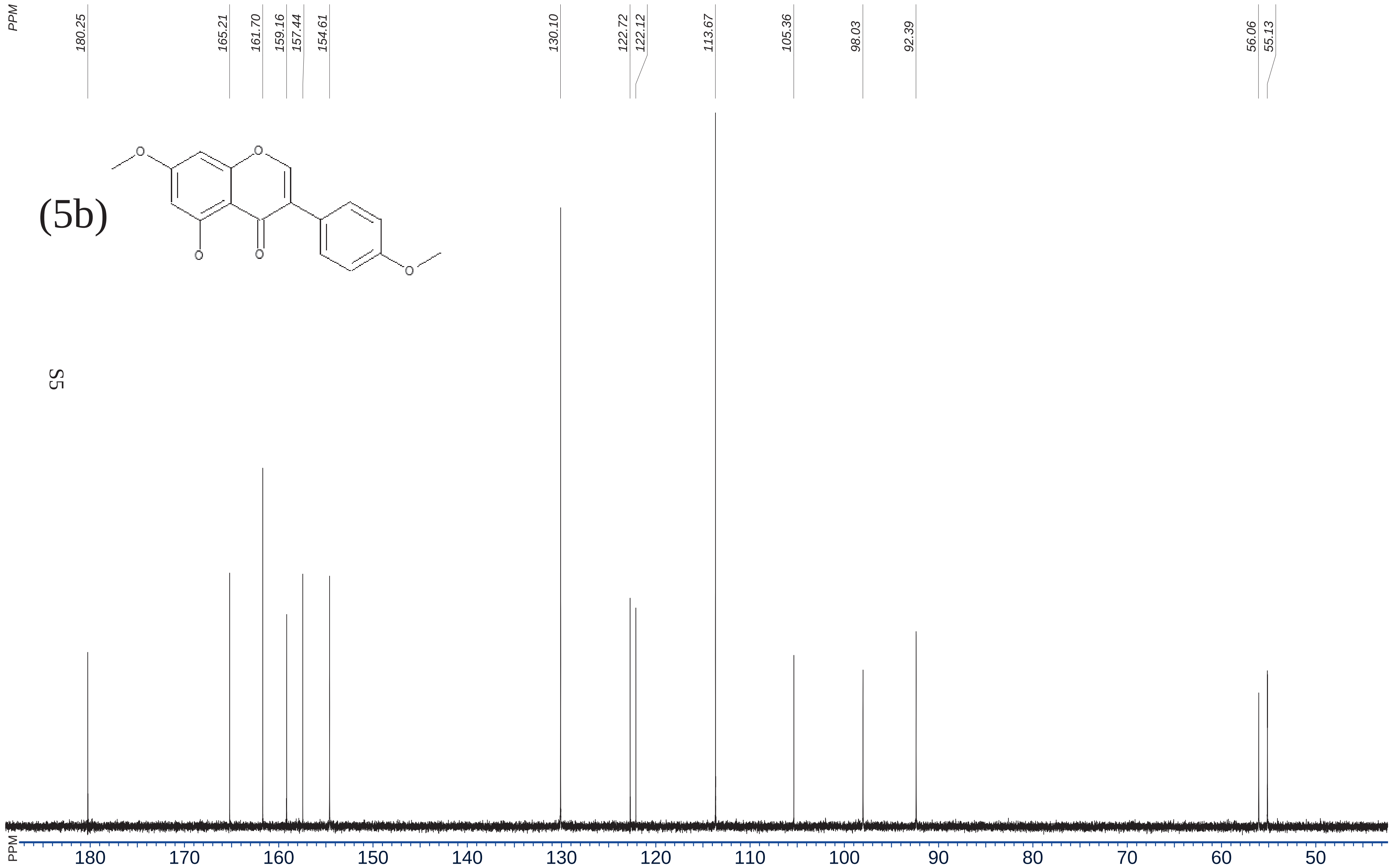
PPM

(5b)

(5b)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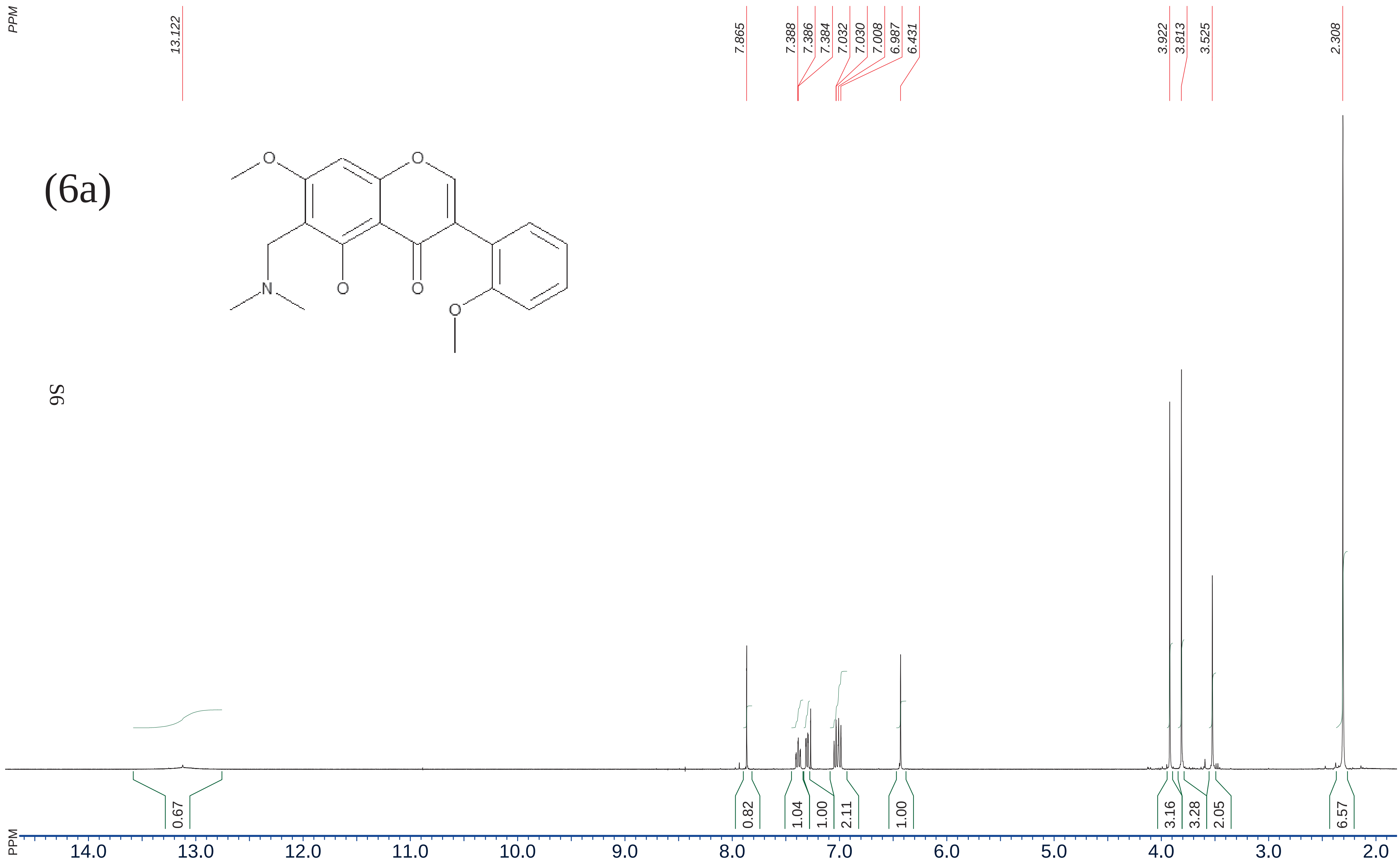
PPM

(6a)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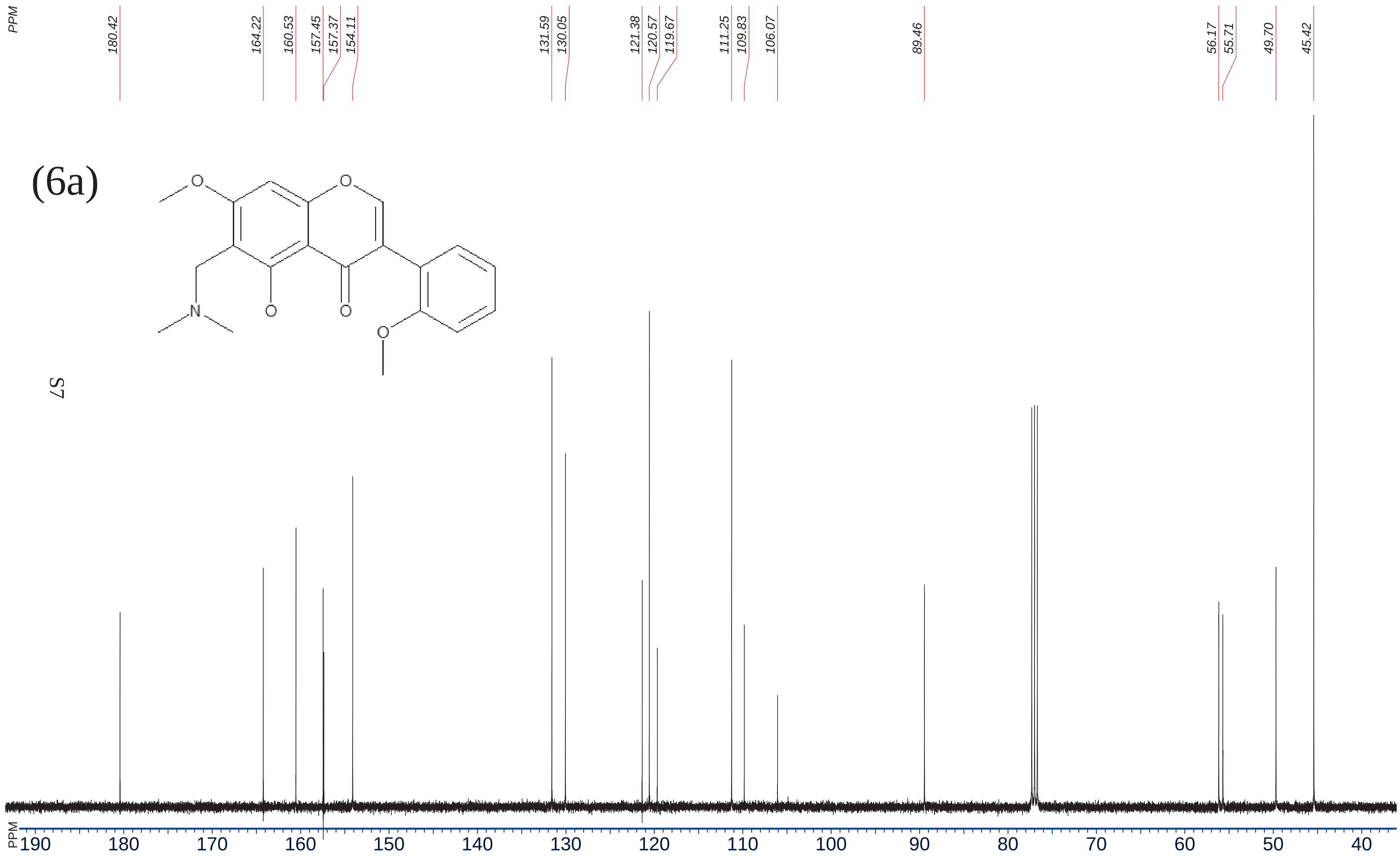
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O
O
N
O
O
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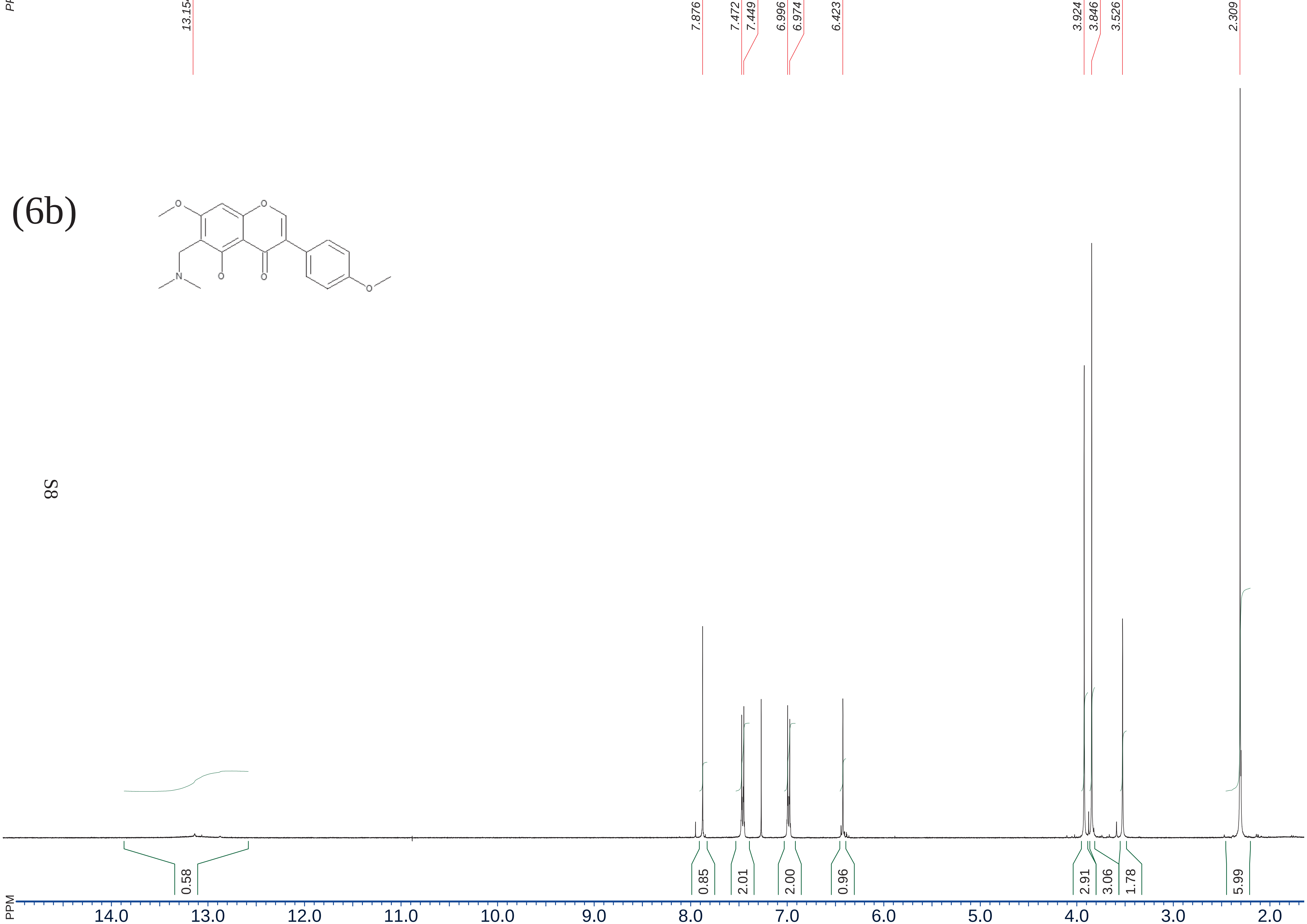
(6b)



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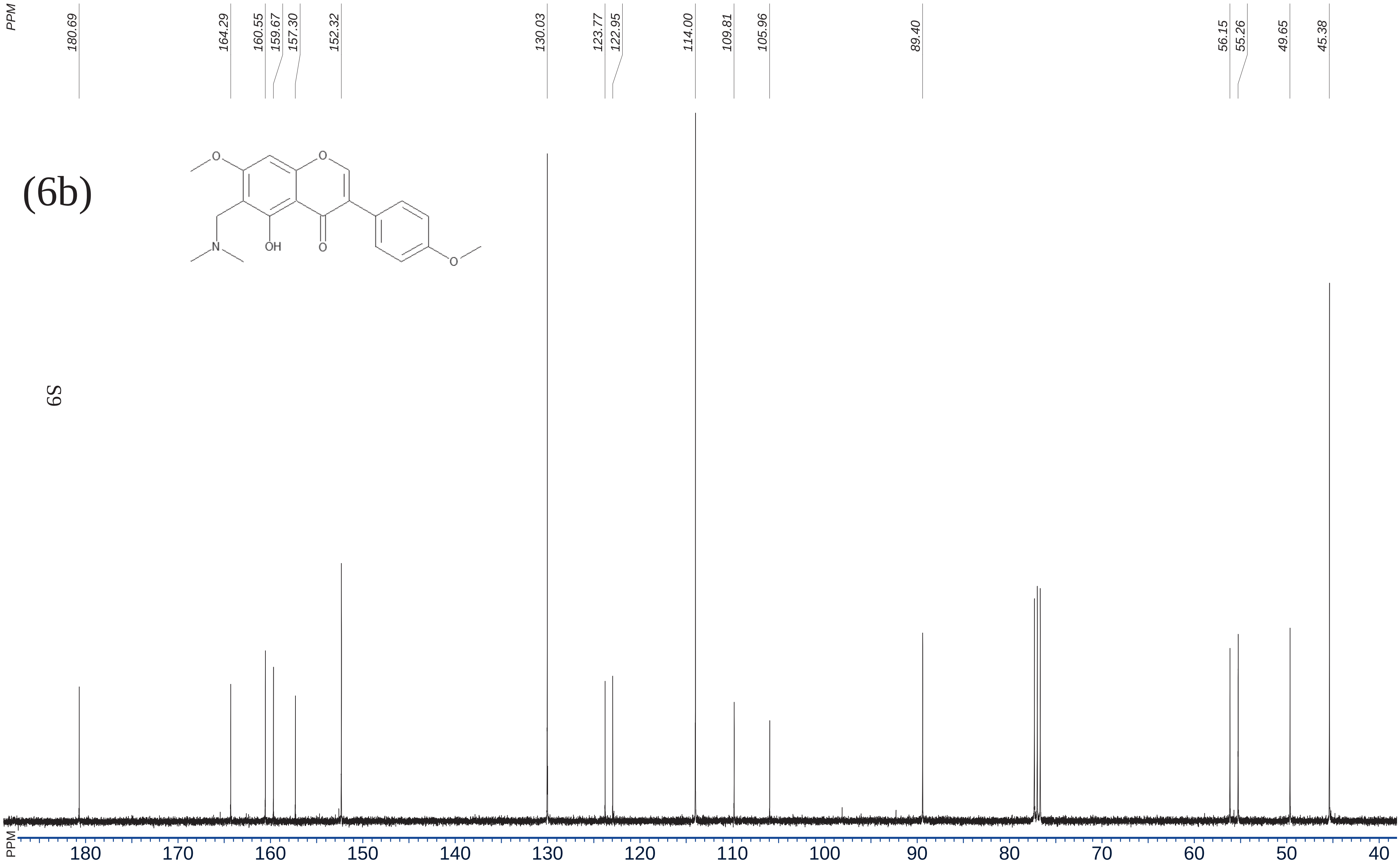
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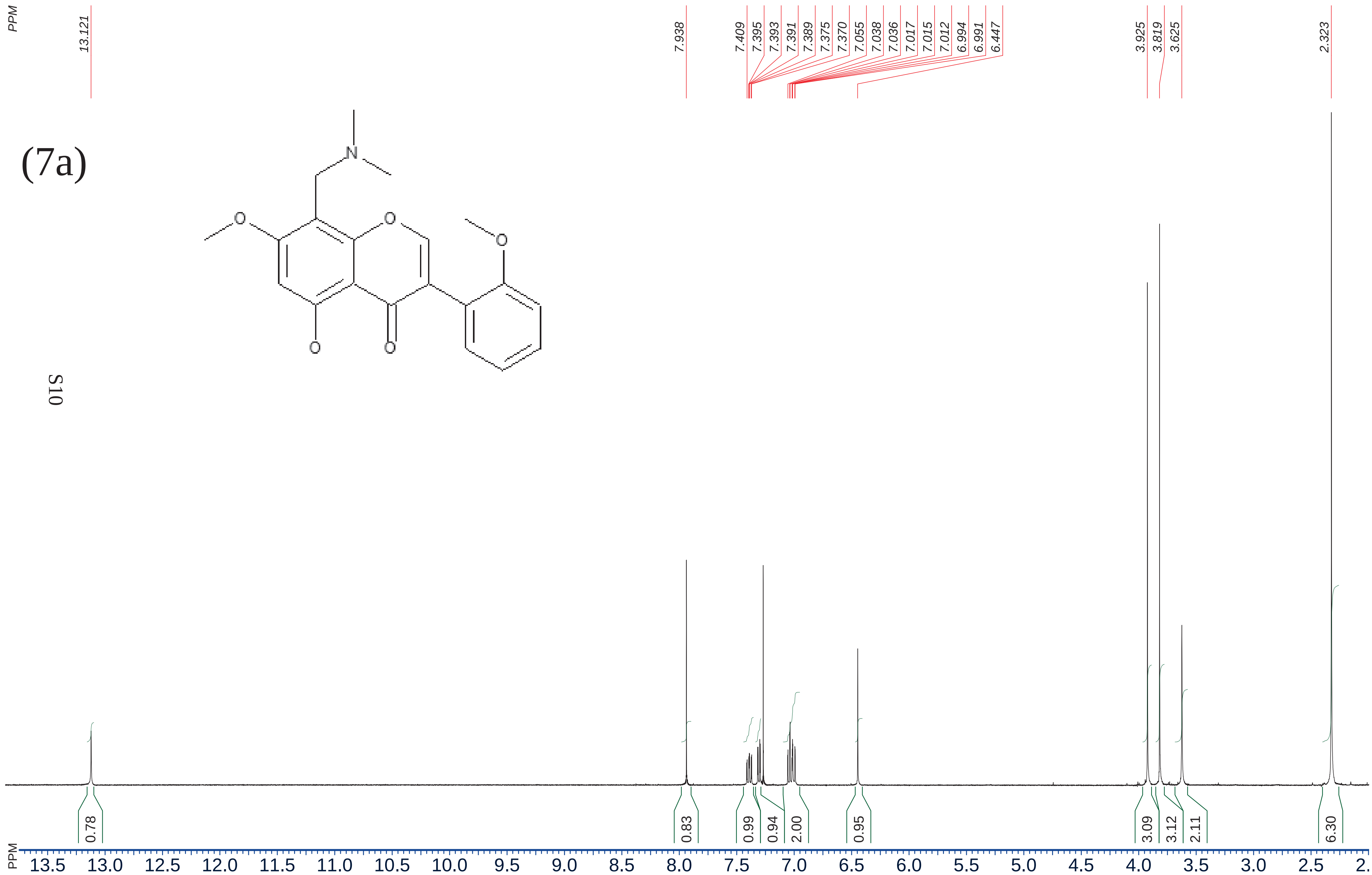
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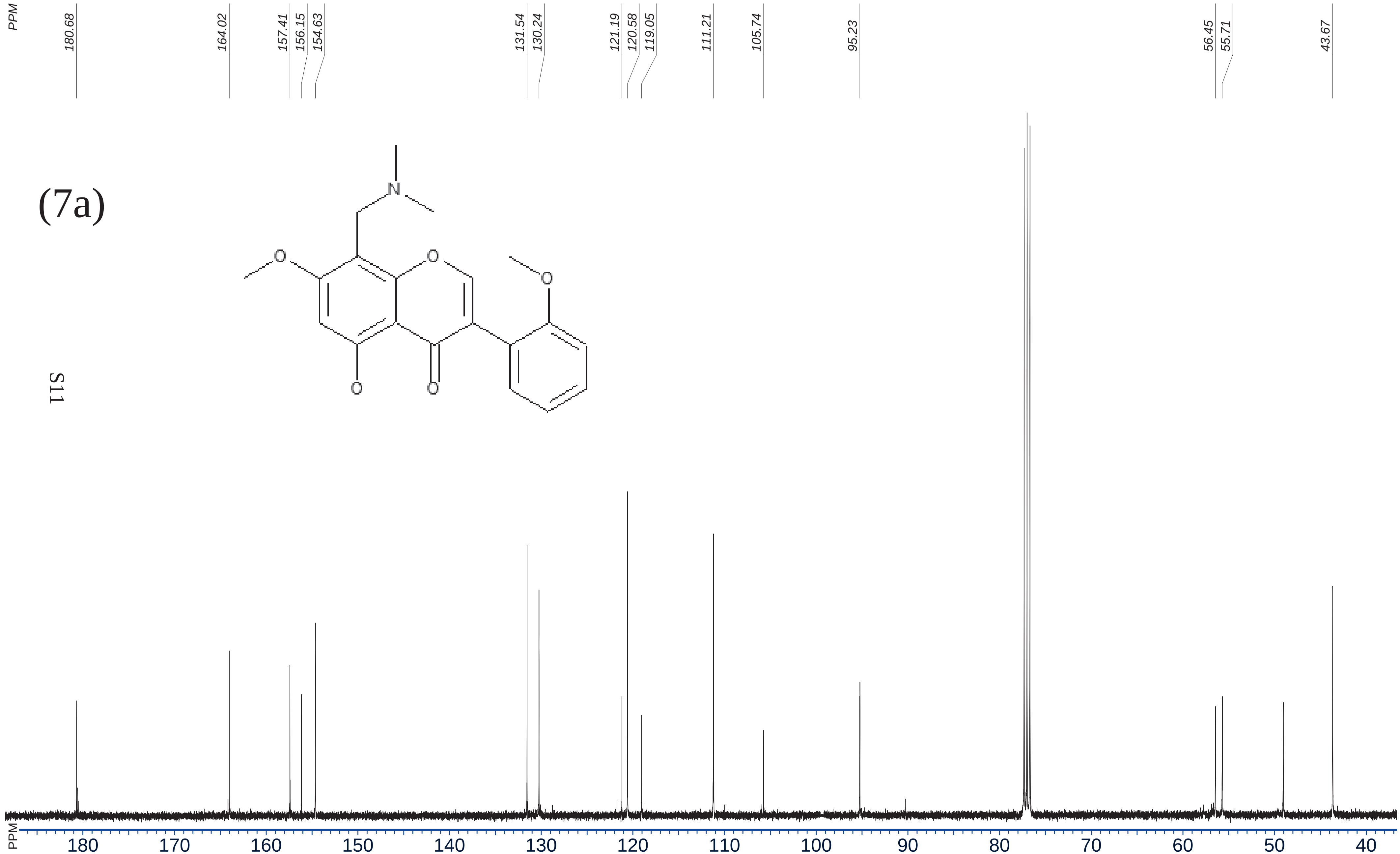
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PPM

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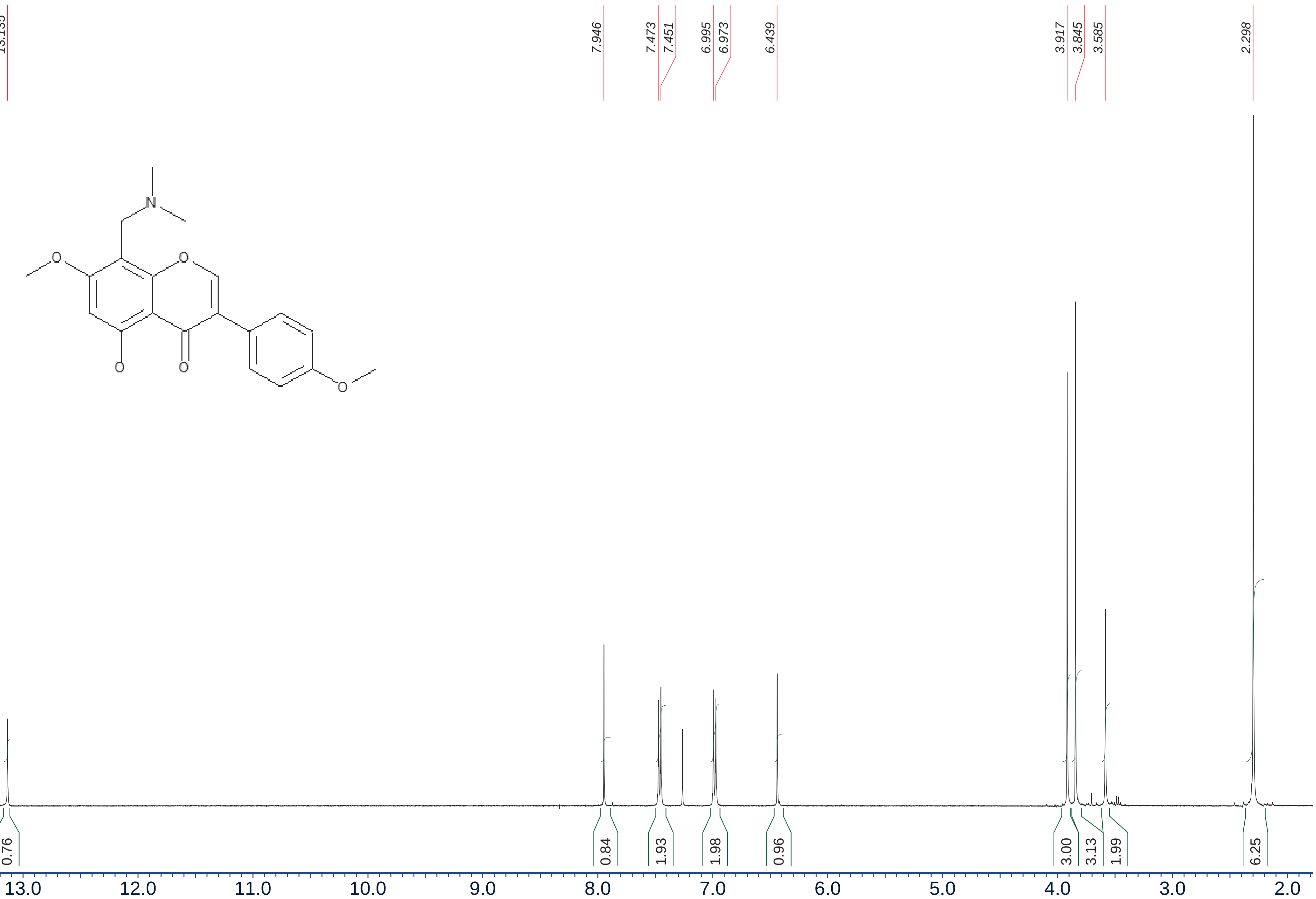
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2.0

(7b)


PPM
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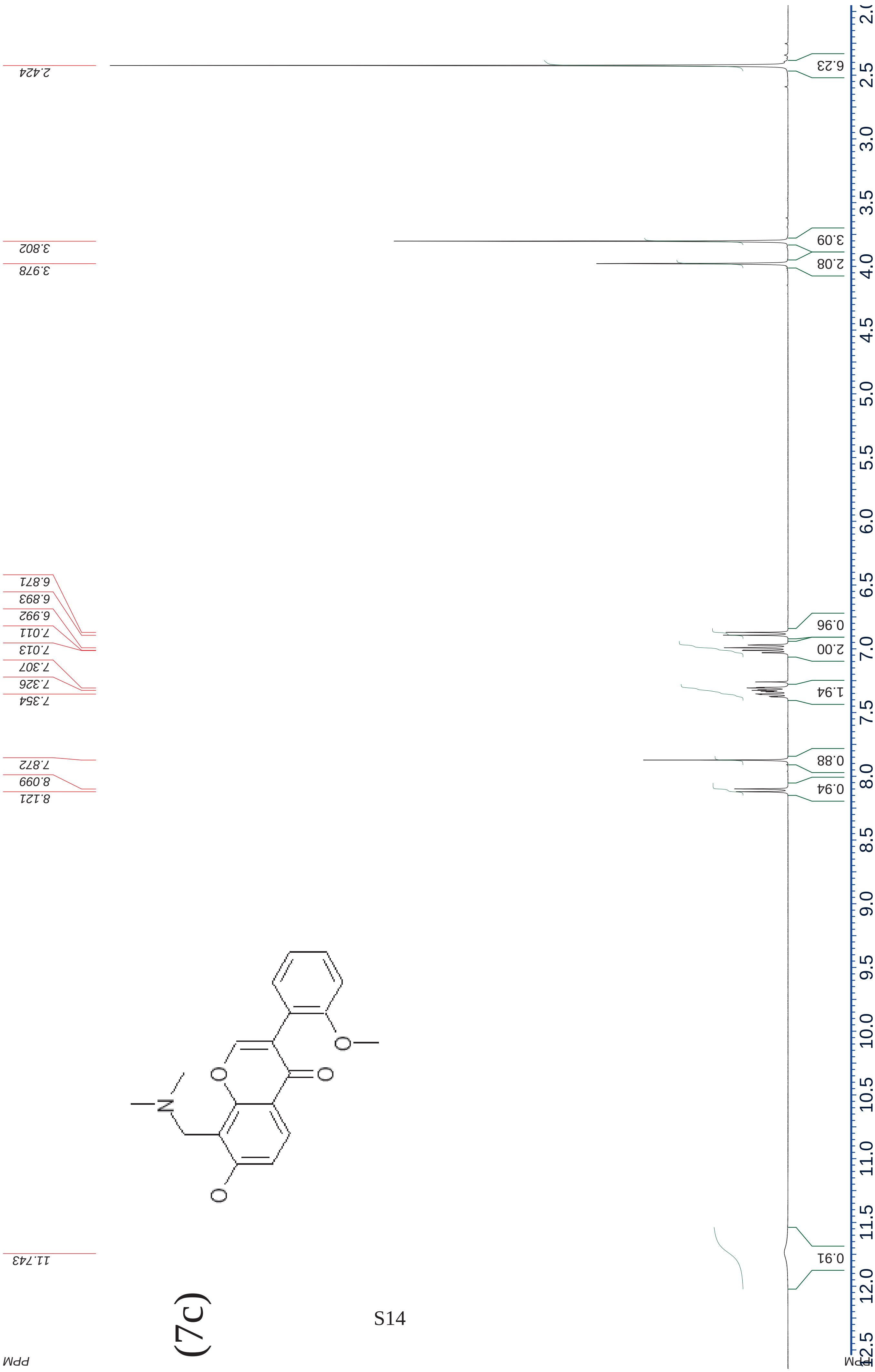
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0.94
0.91

(7c)


PPM
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129.65
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122.22
121.06
120.54
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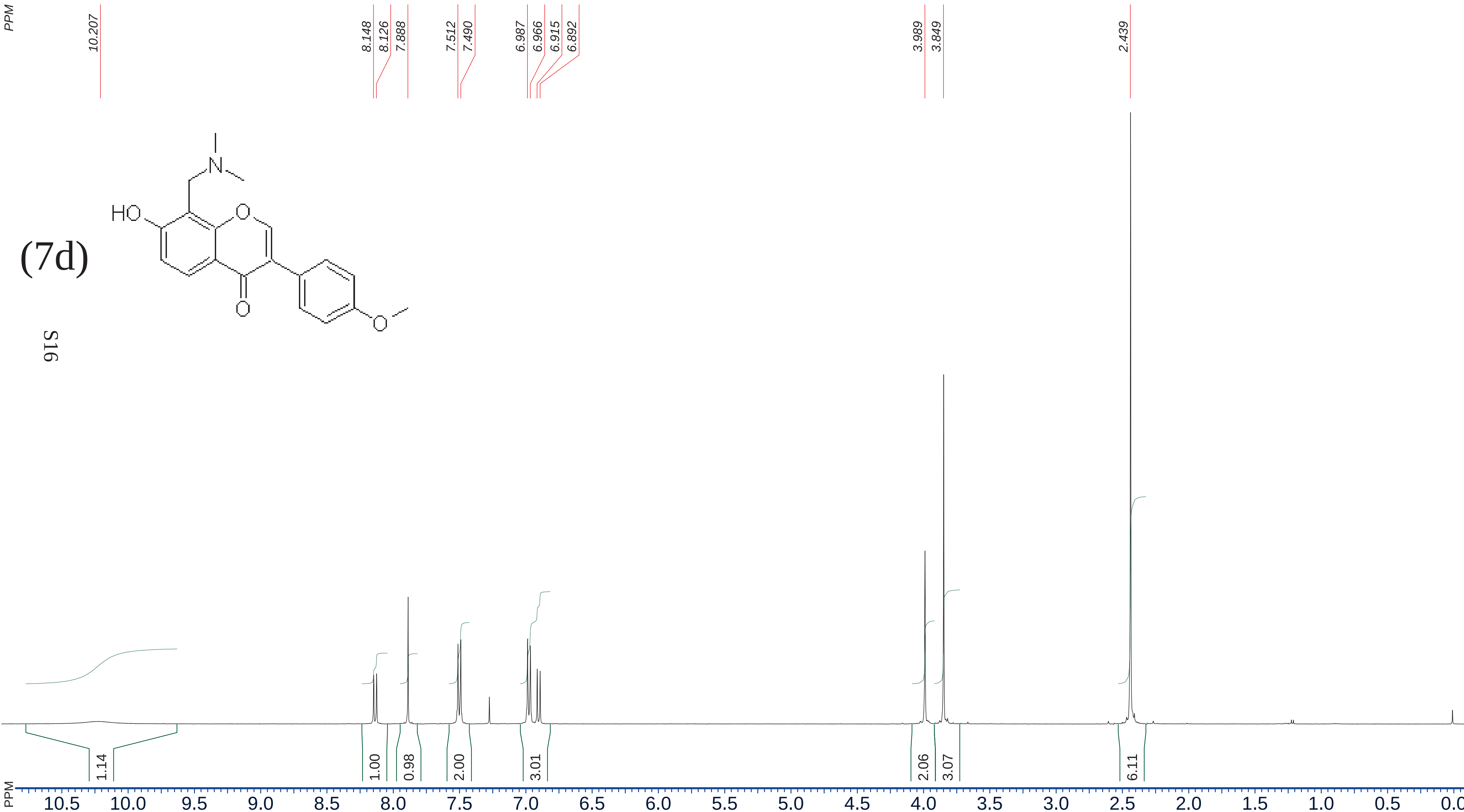
(7c)

(7d)



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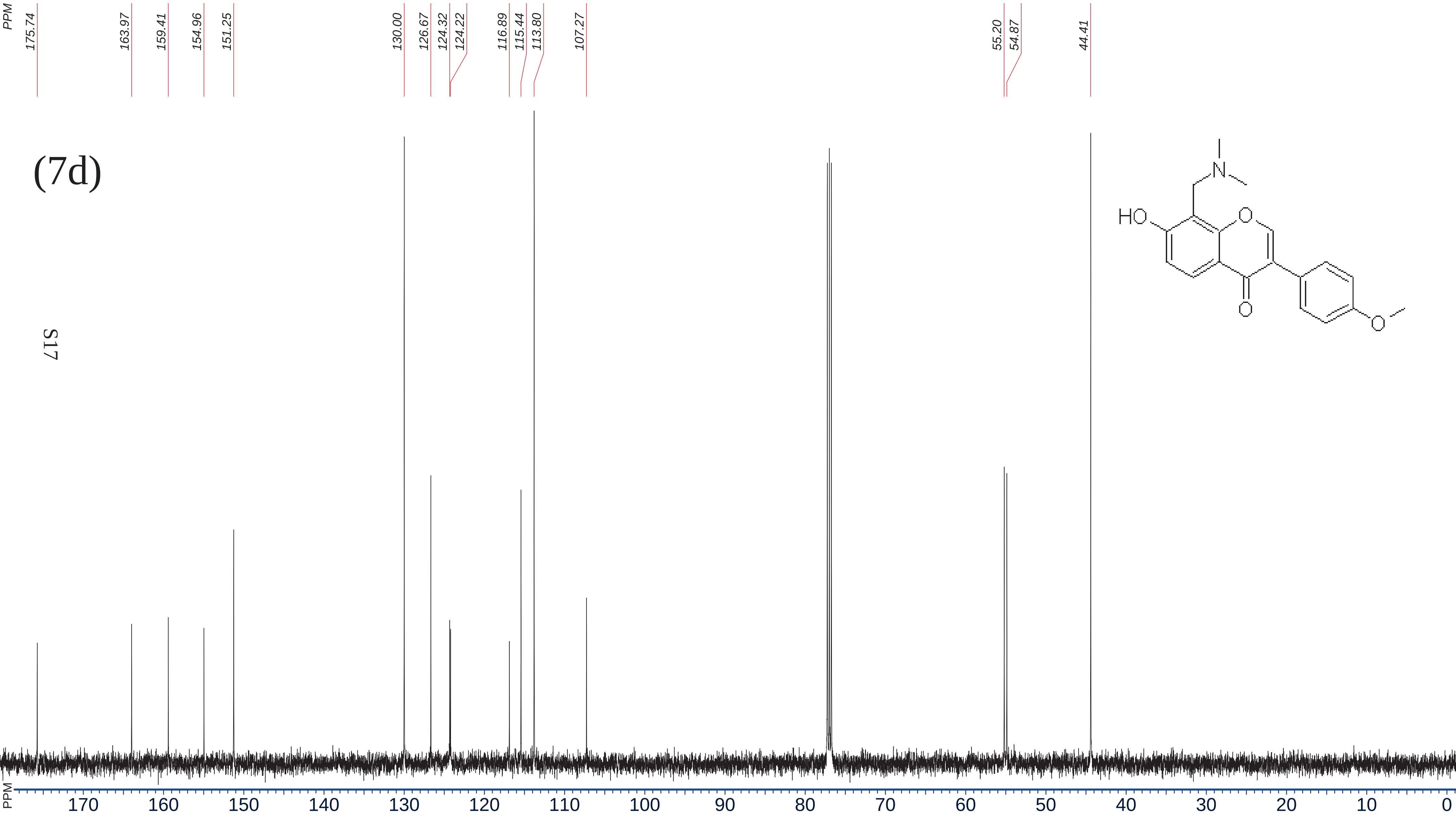
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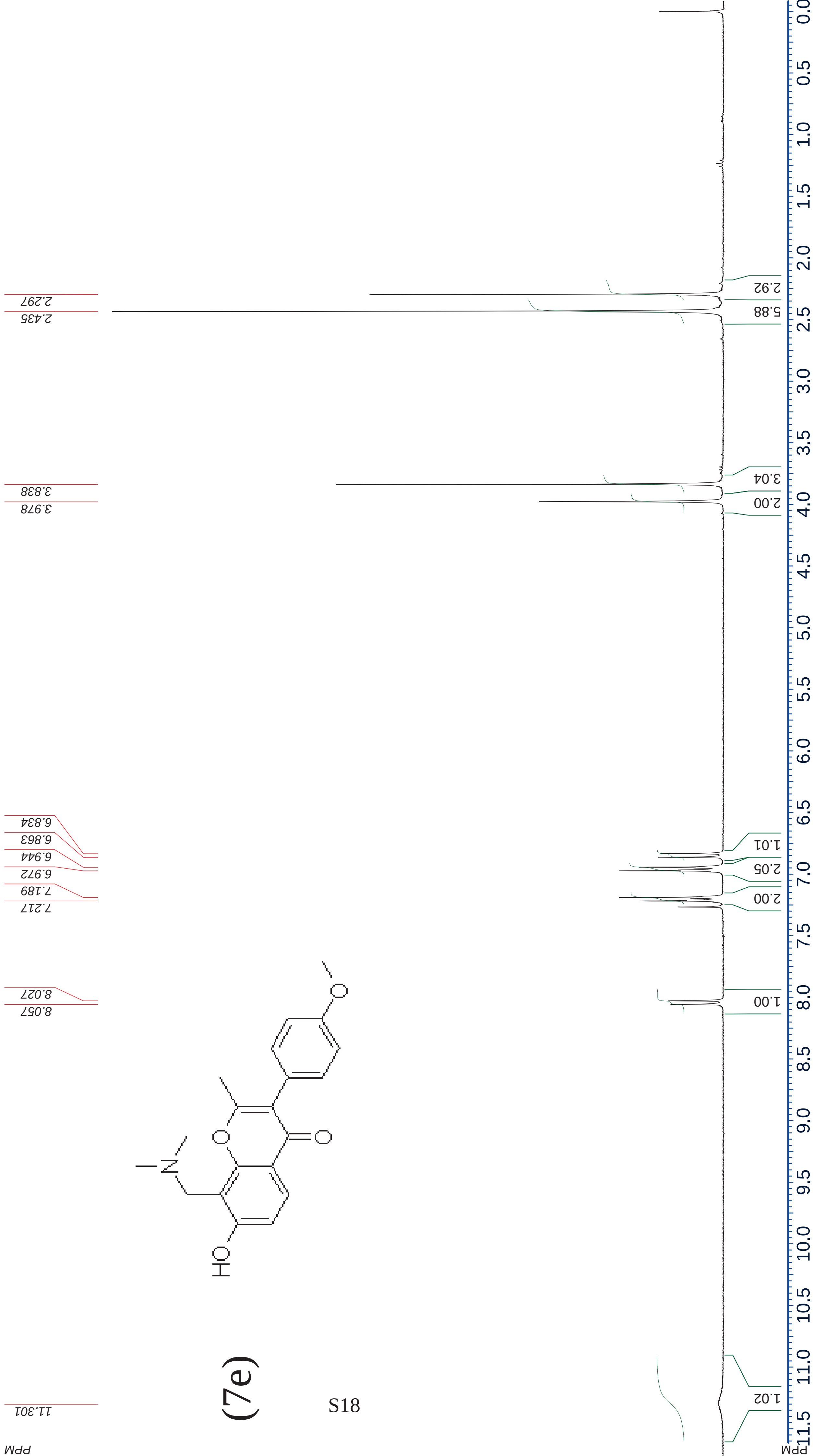

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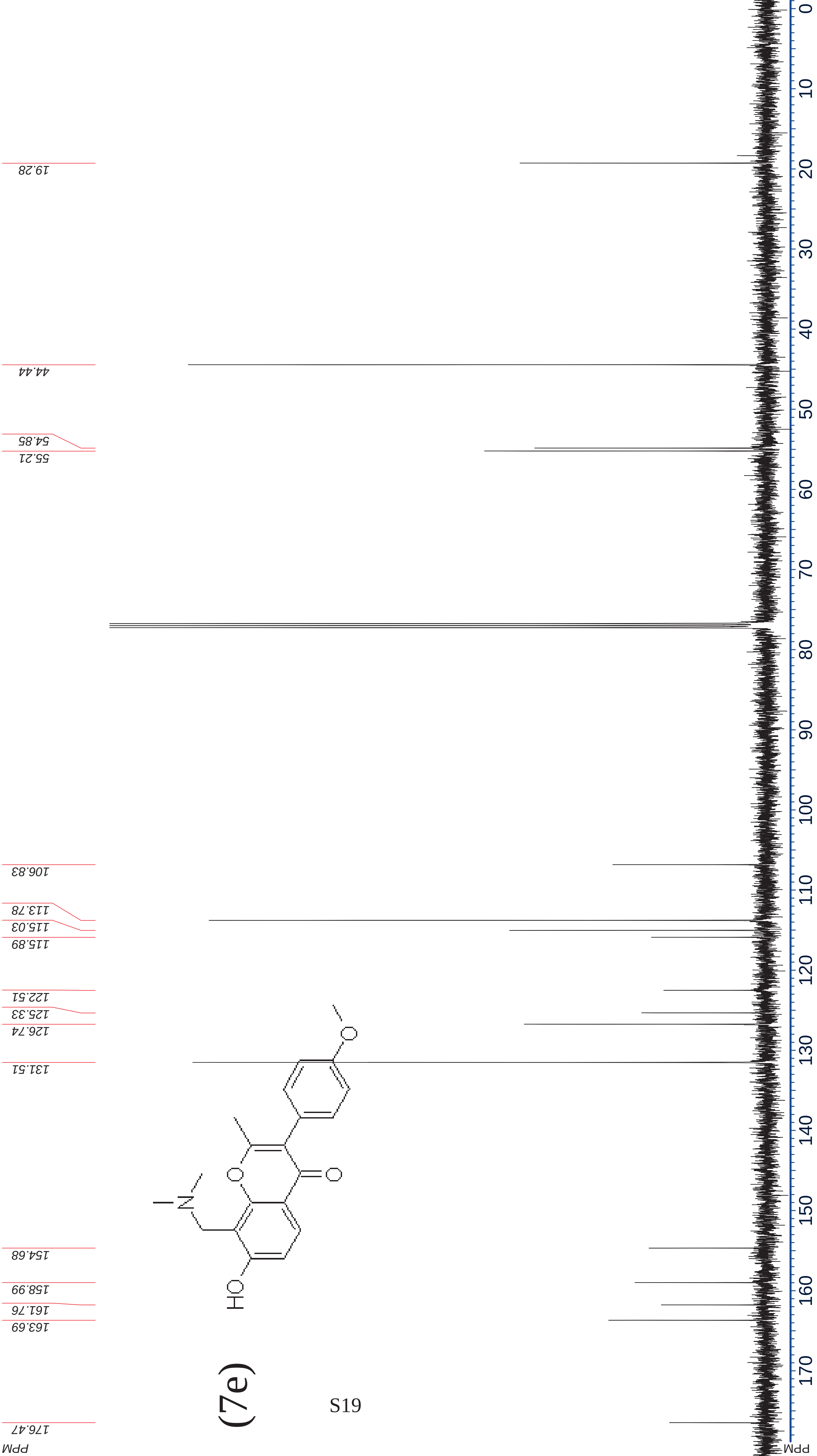
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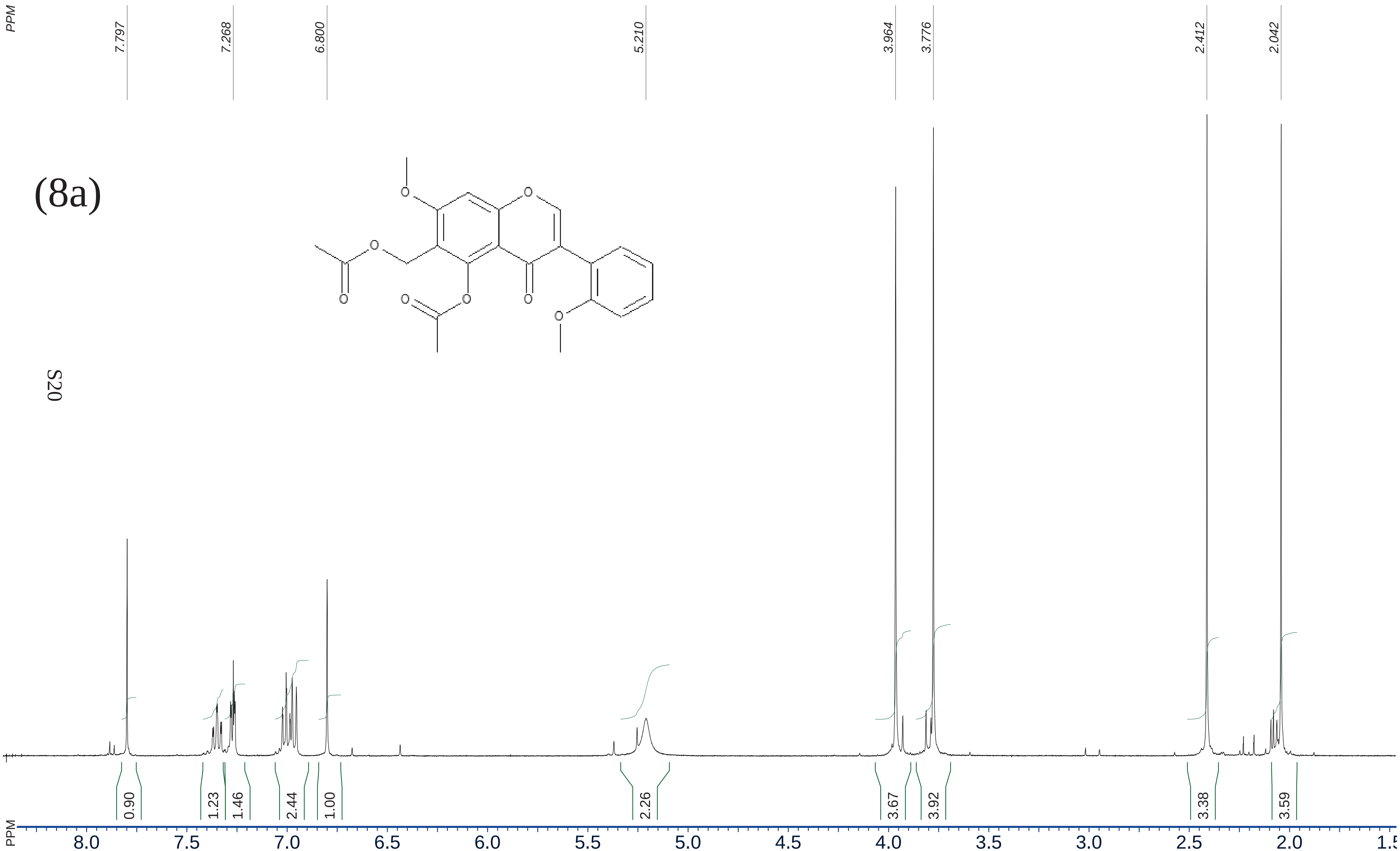
(7e)

(8a)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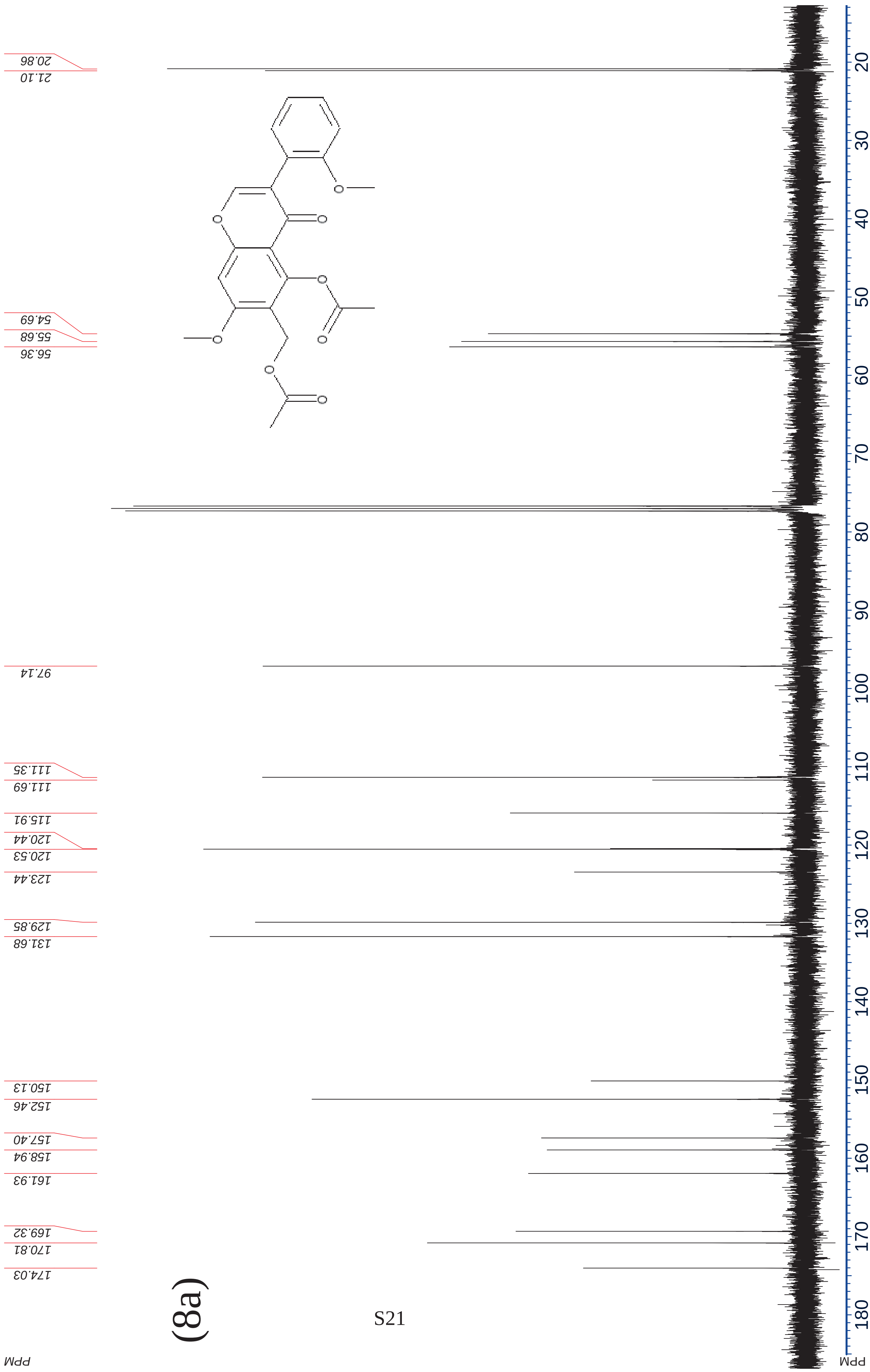
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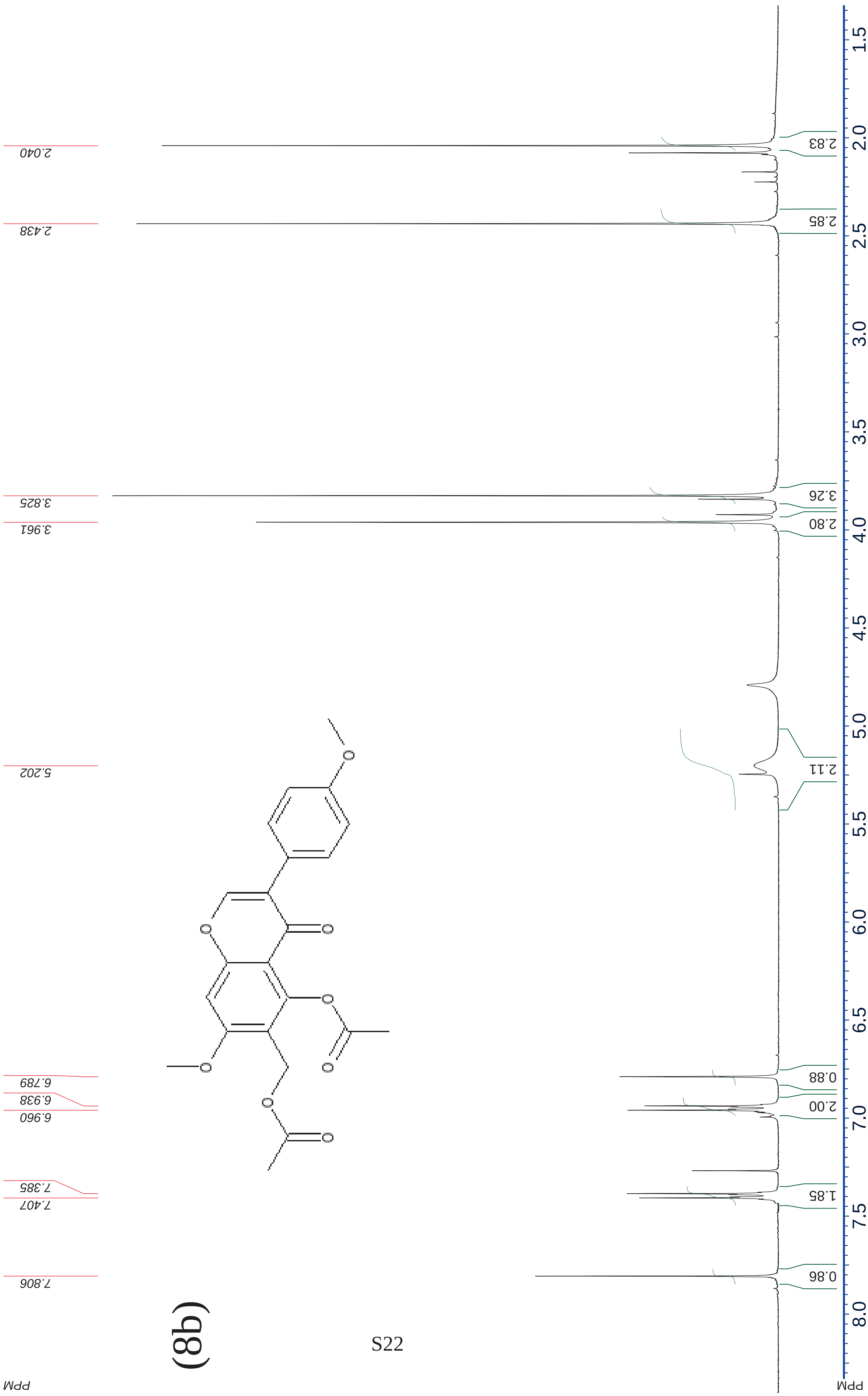
PPM

(8a)



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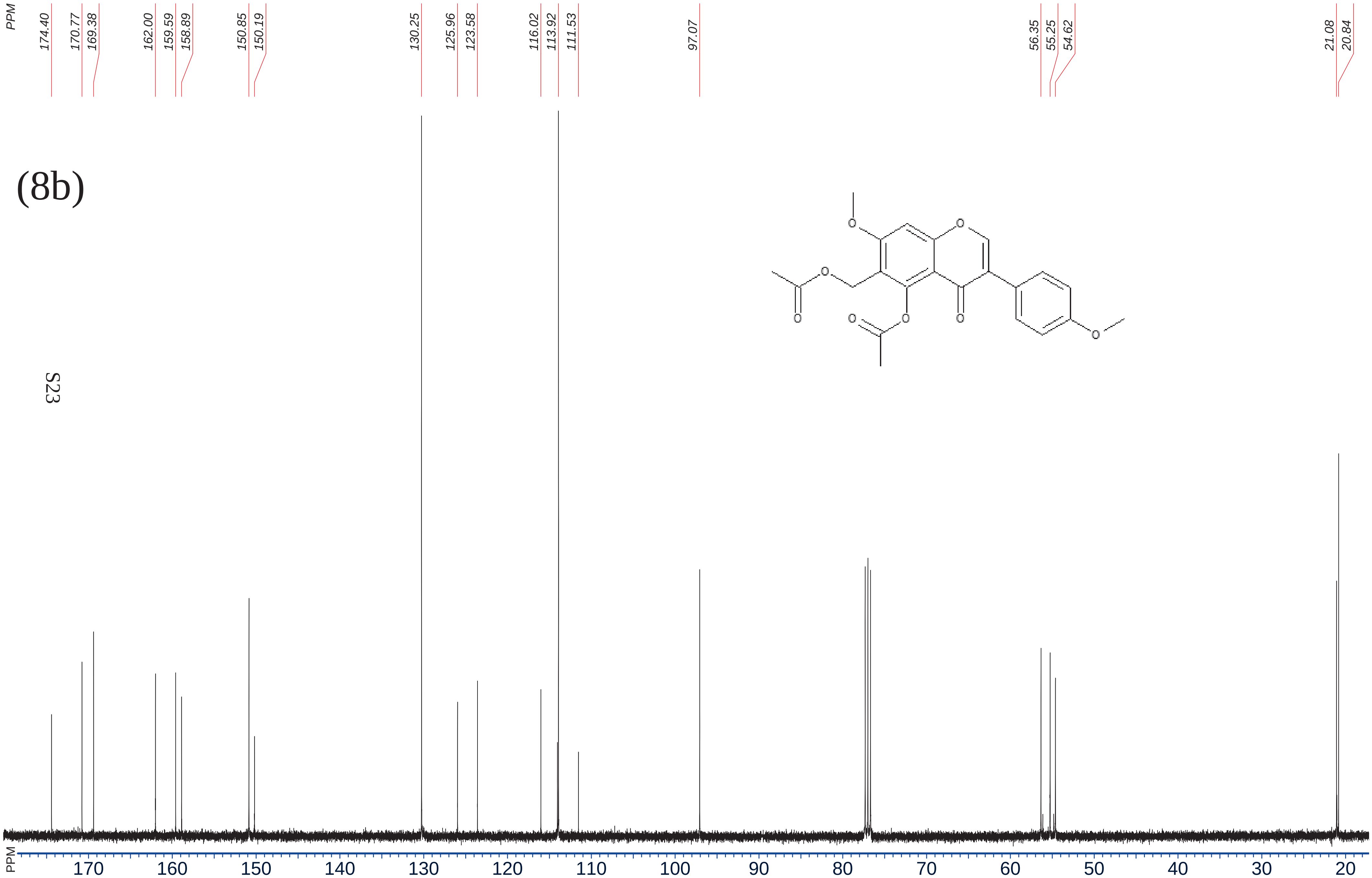
(8b)

(8b)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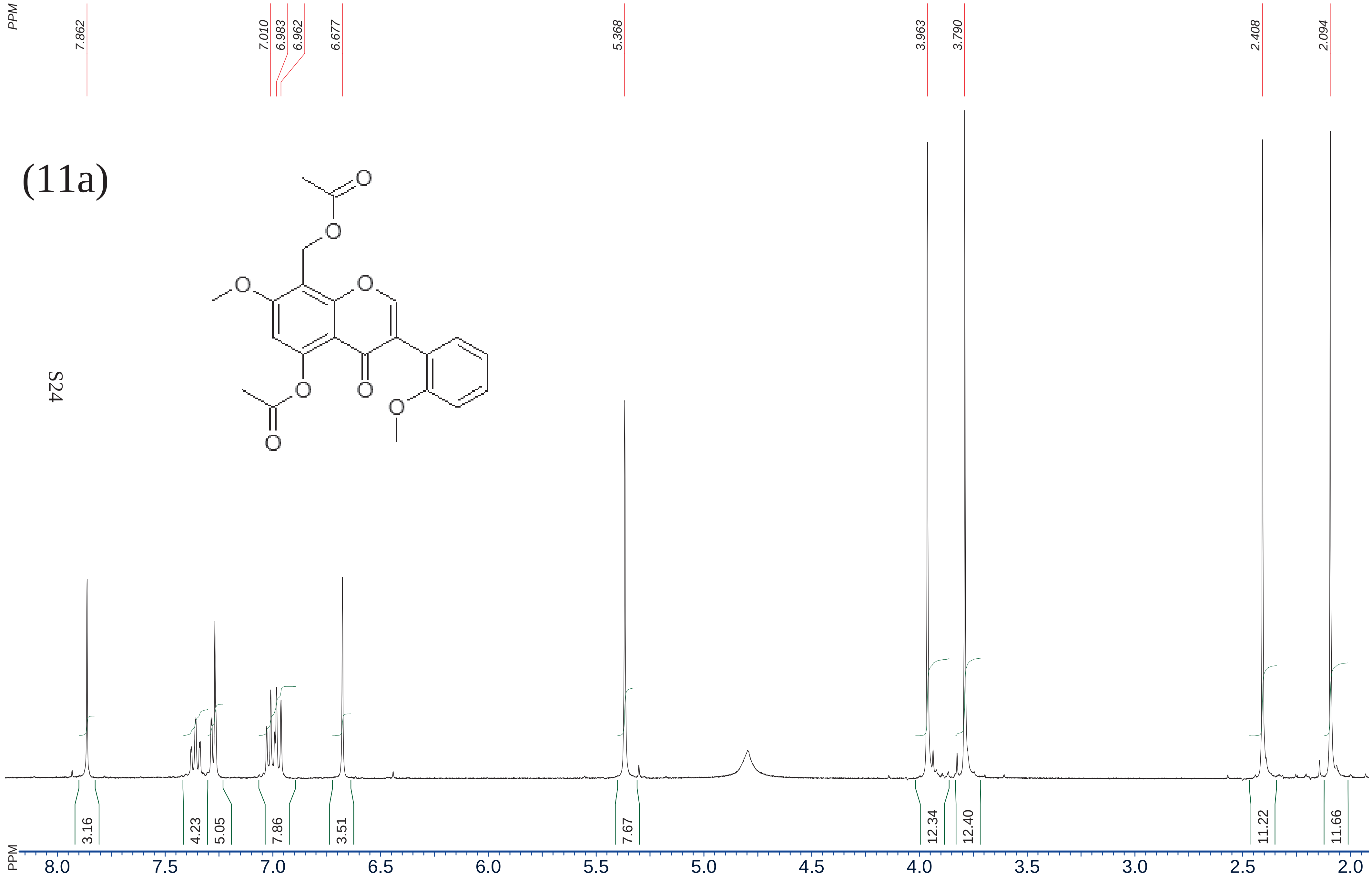
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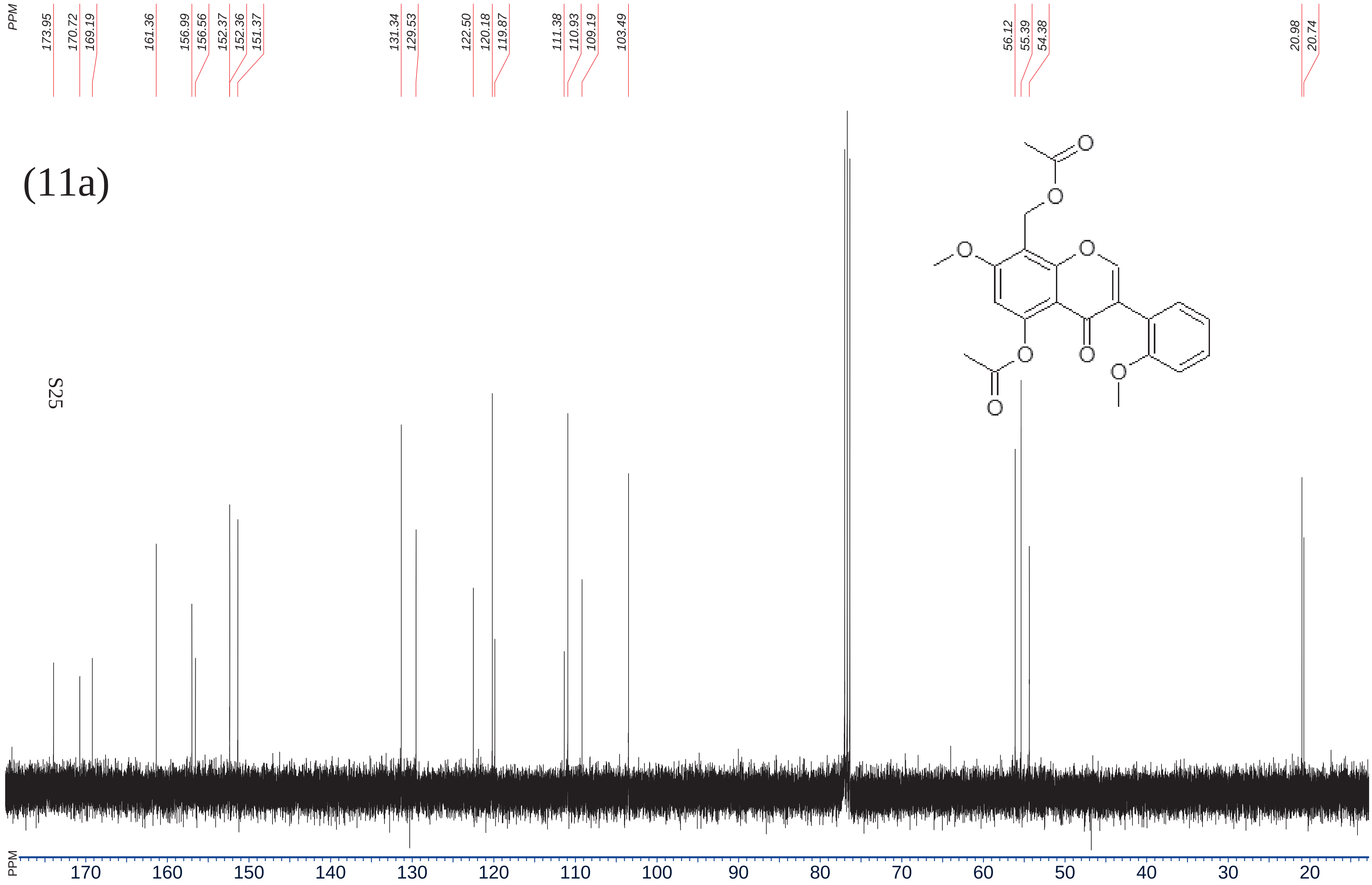
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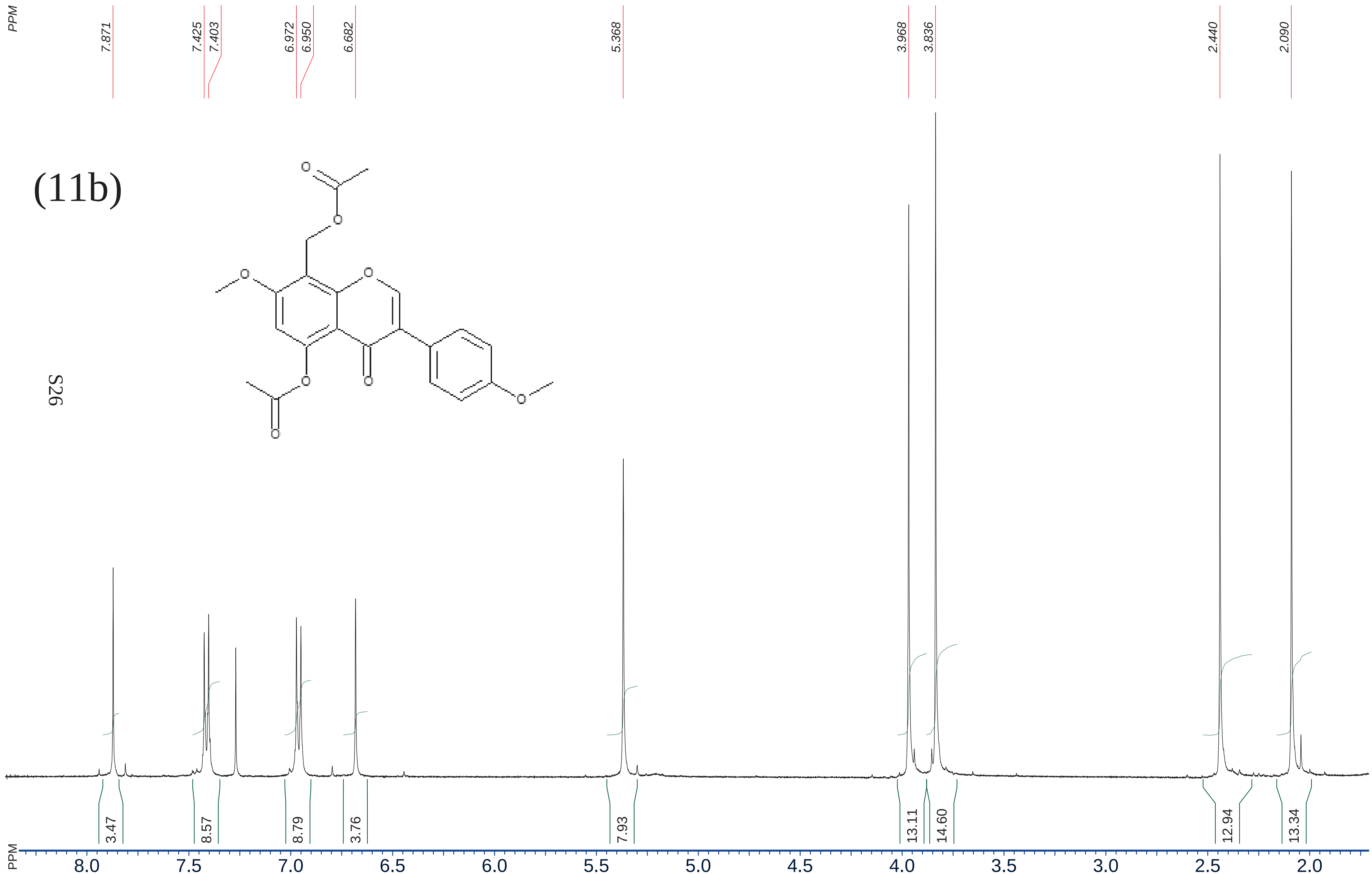

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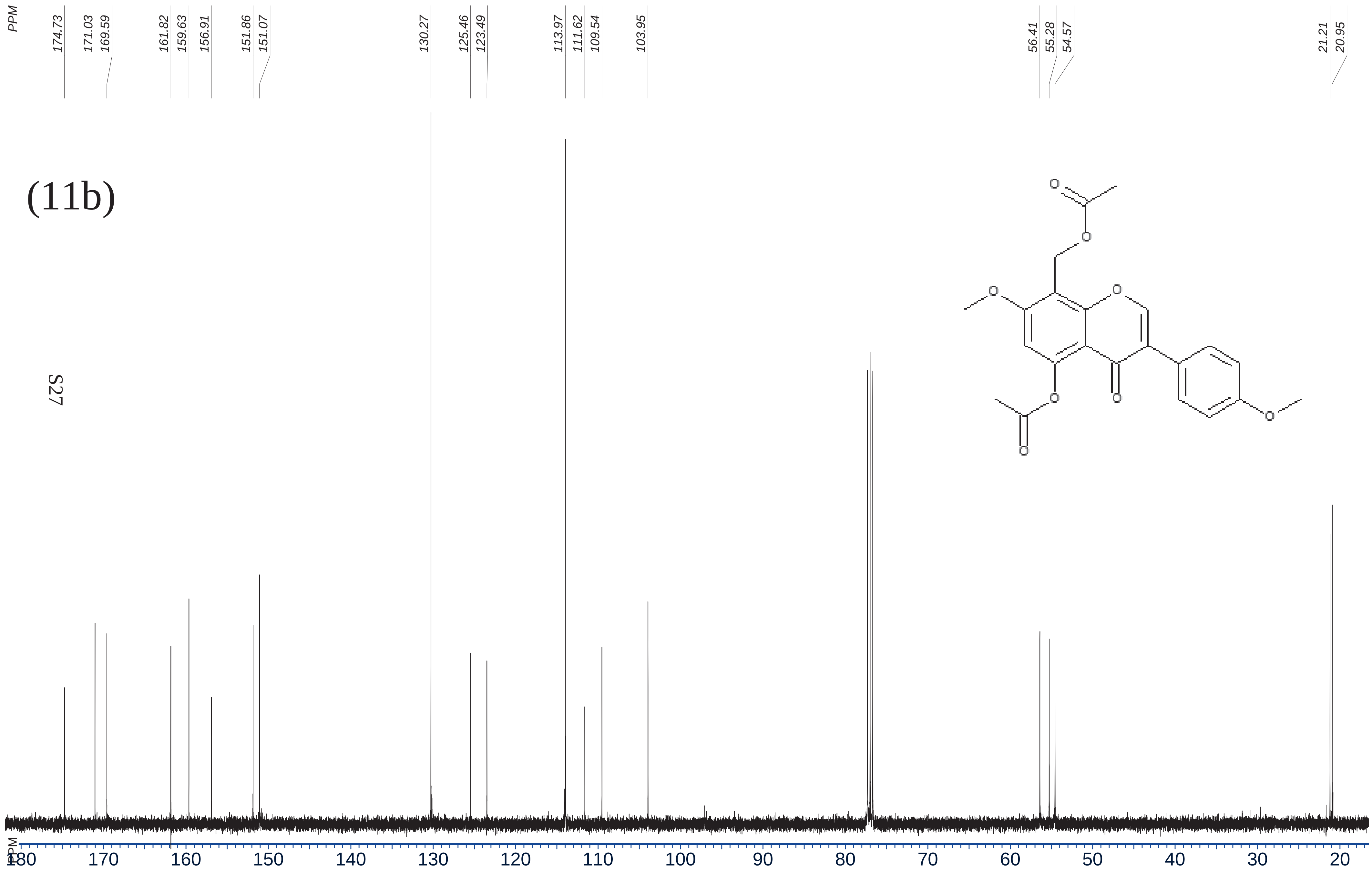
(11b)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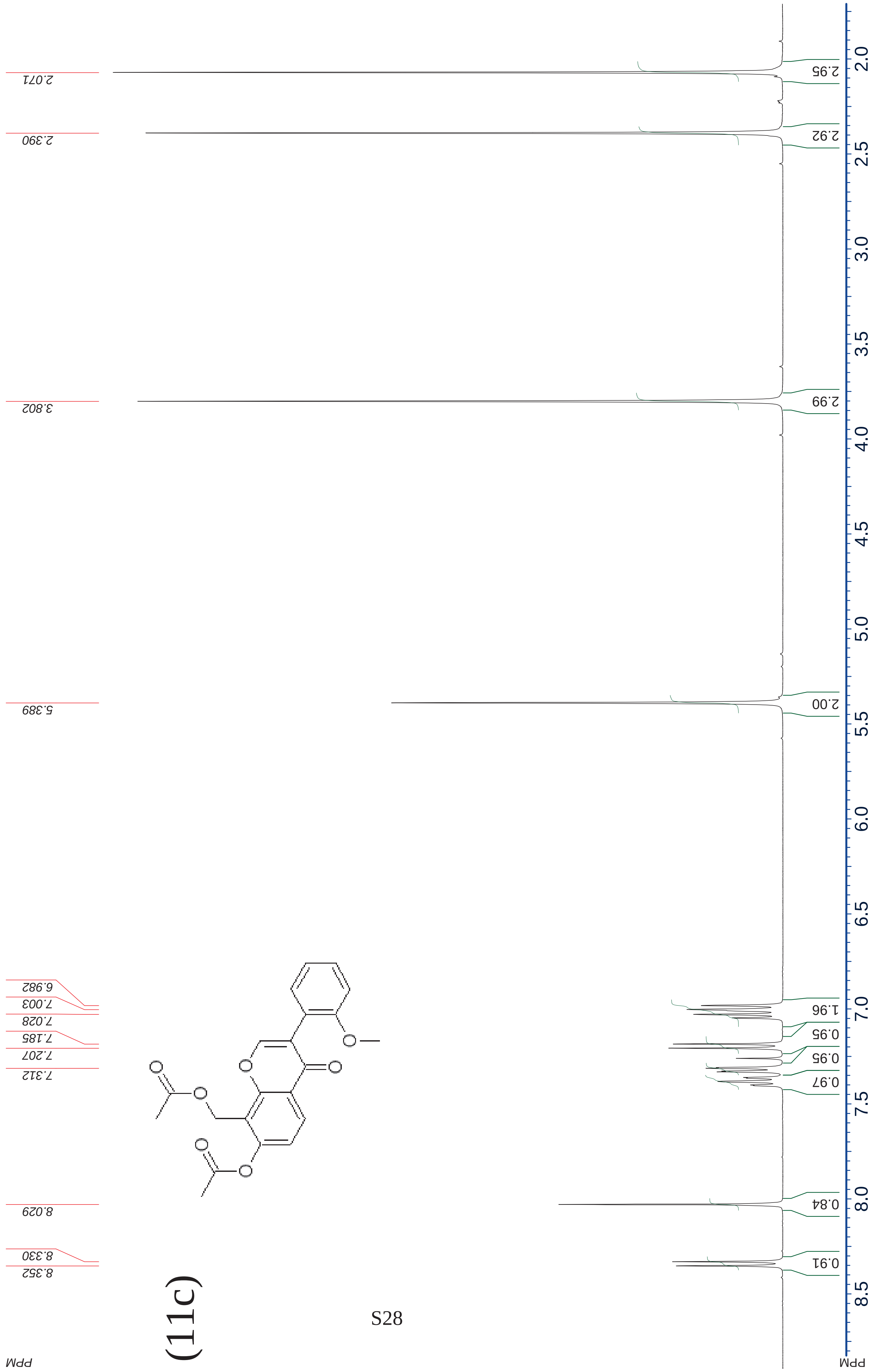
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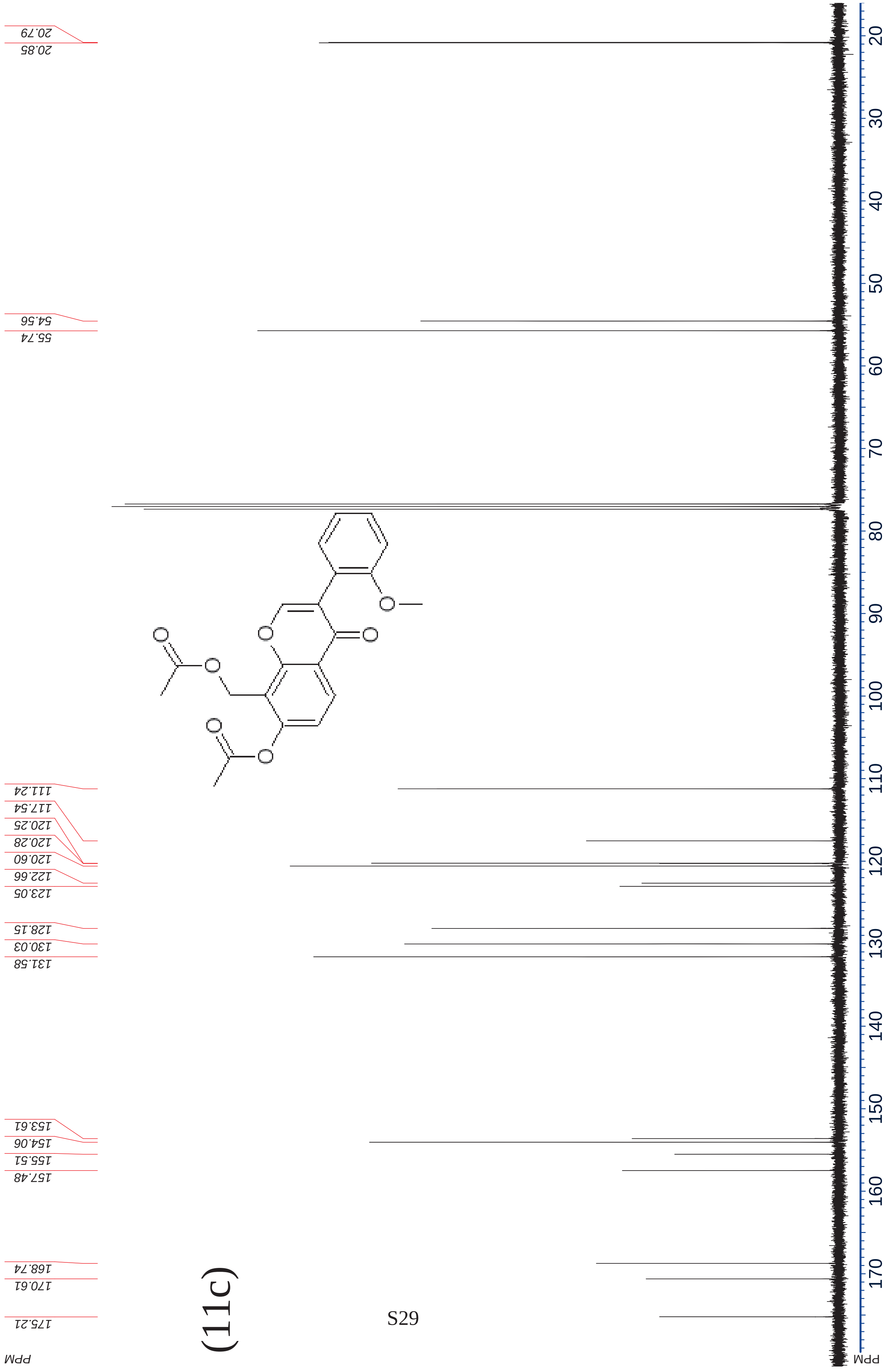
(11c)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175.21
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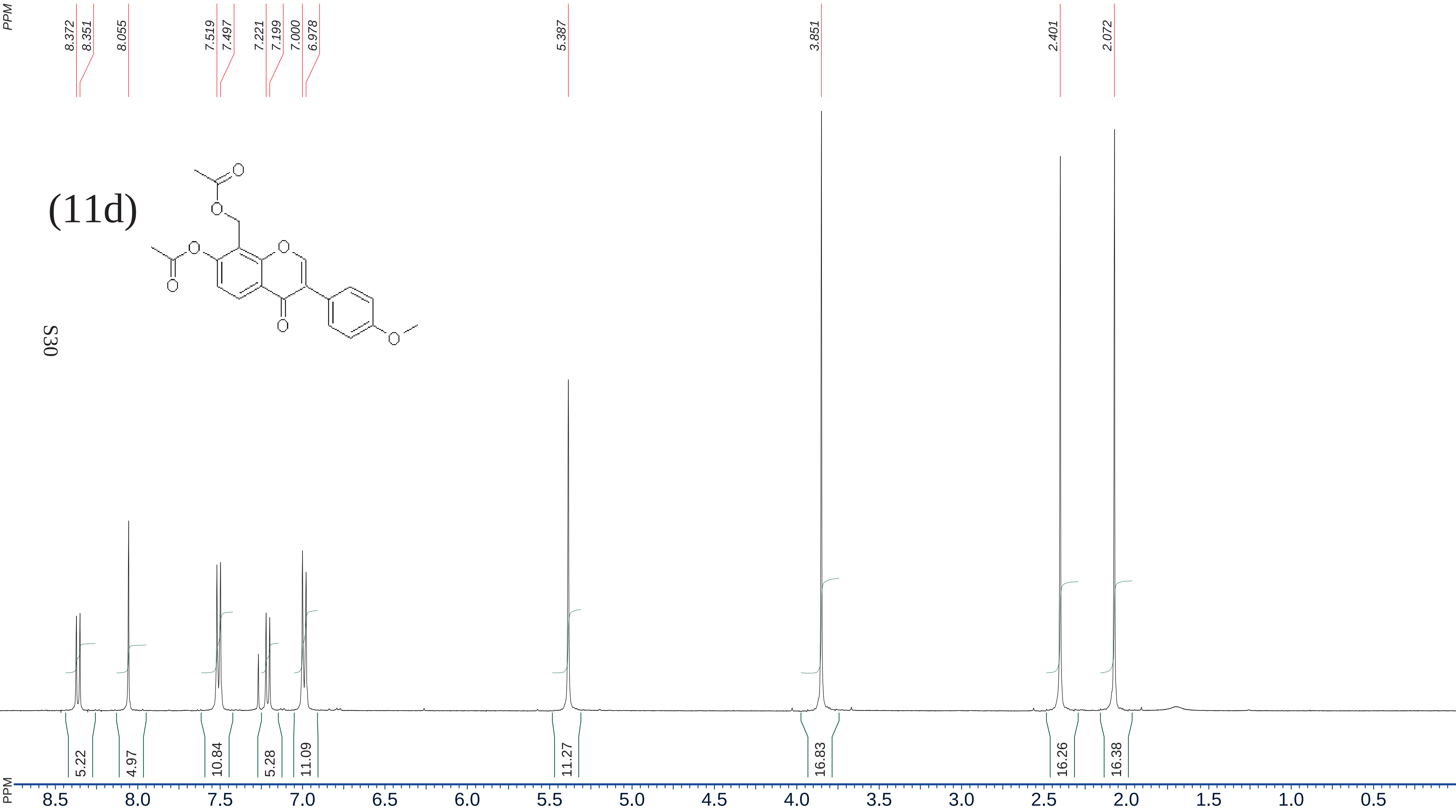
(11c)

(11d)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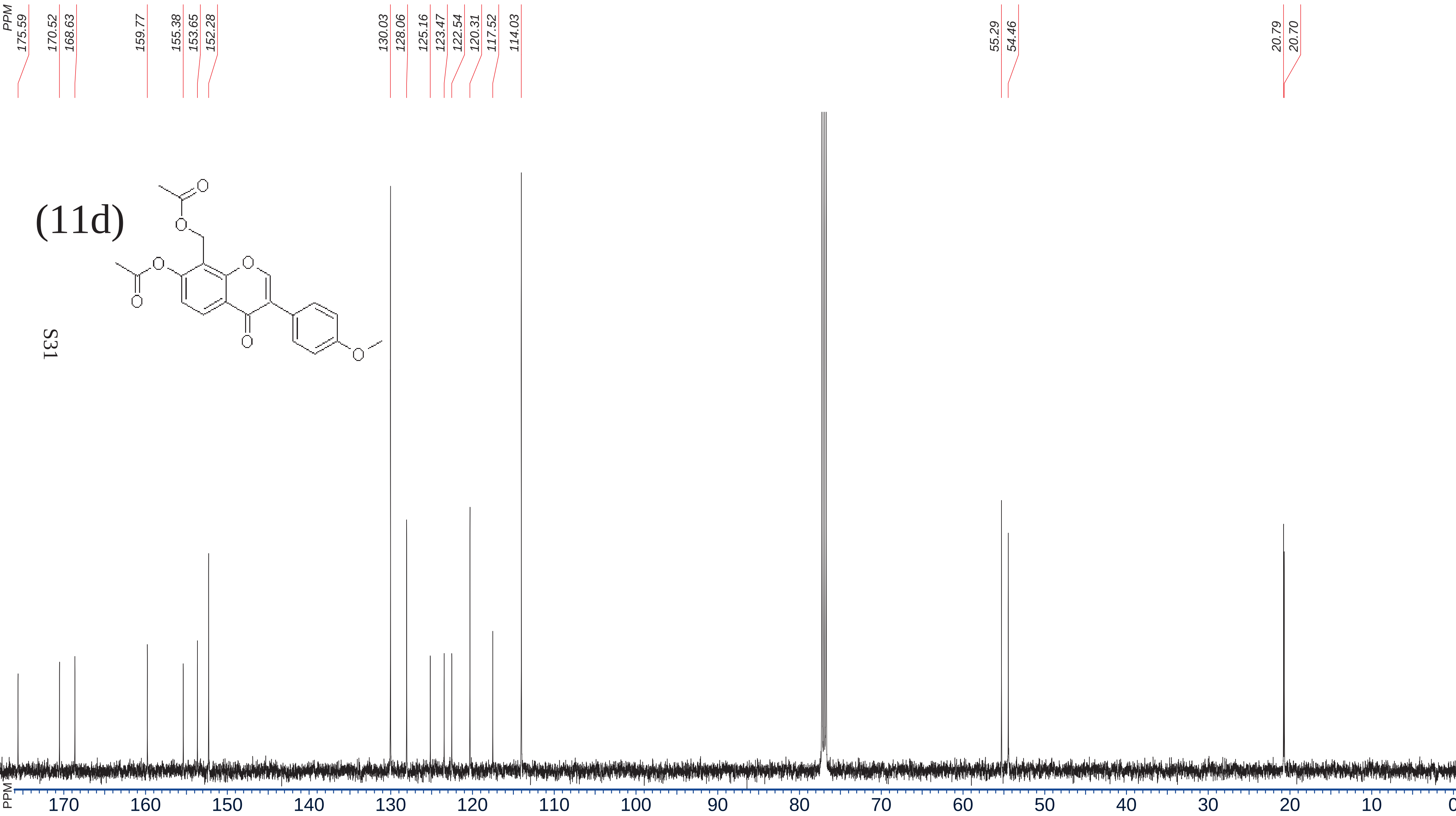
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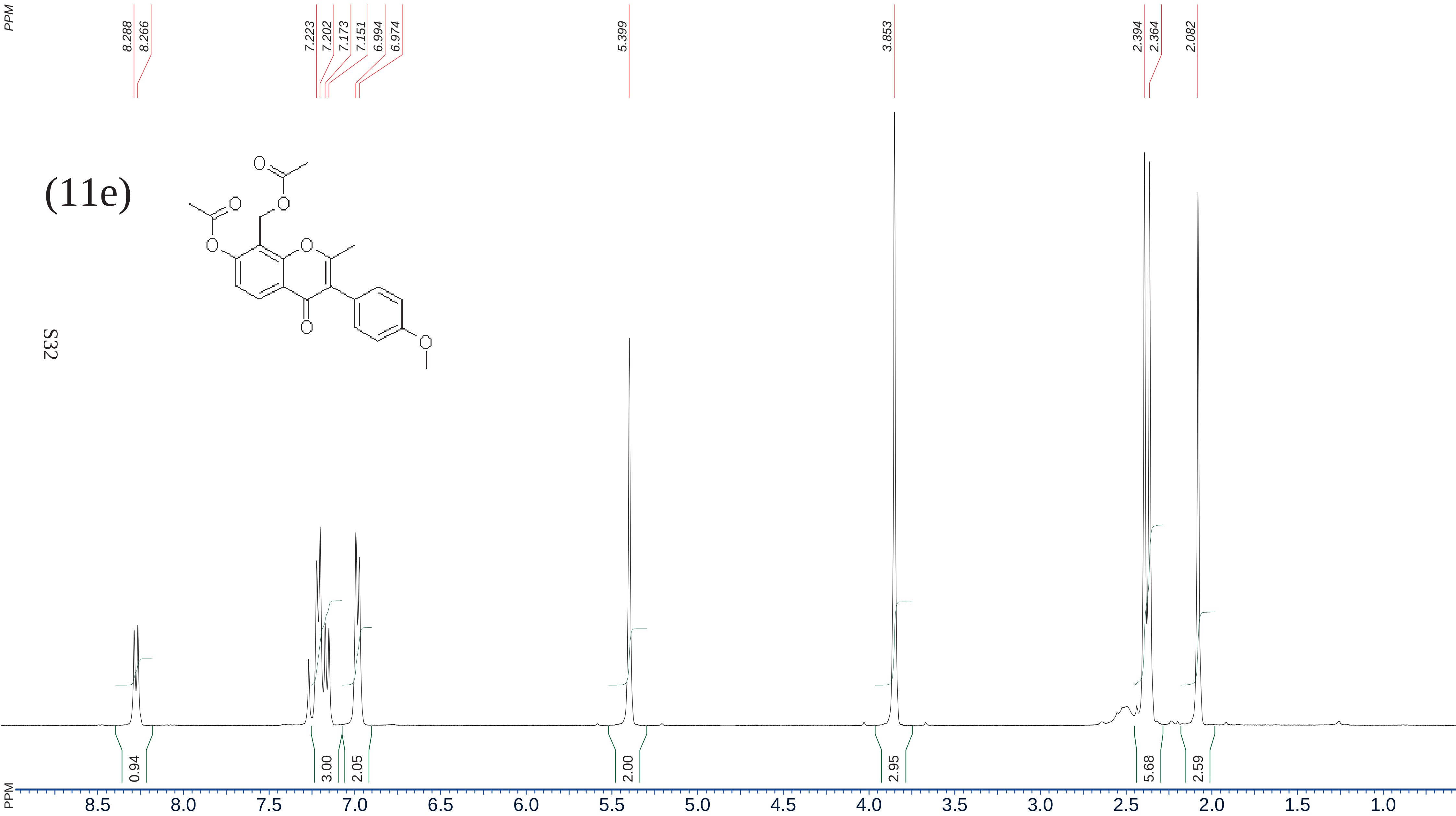
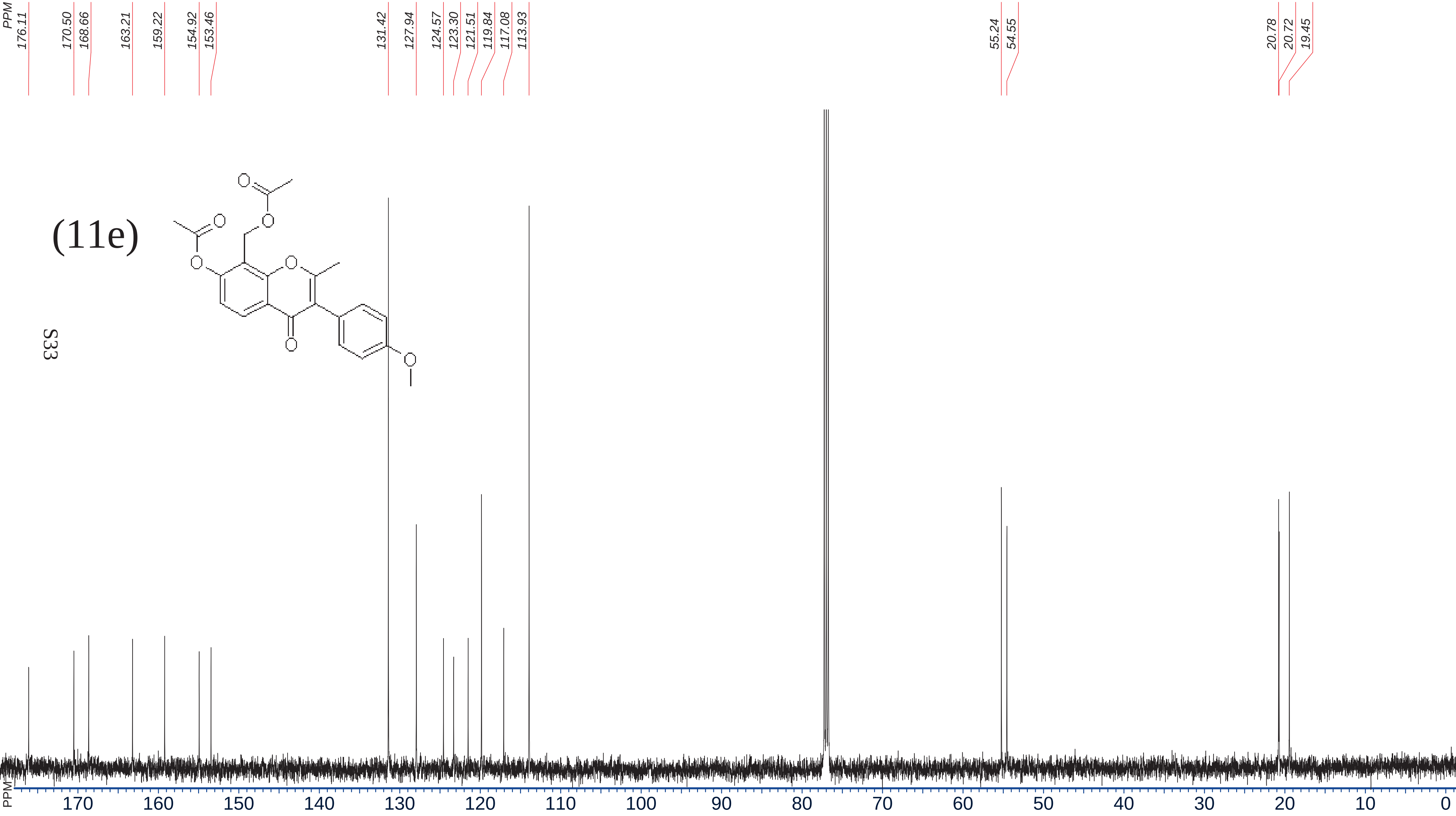
PPM

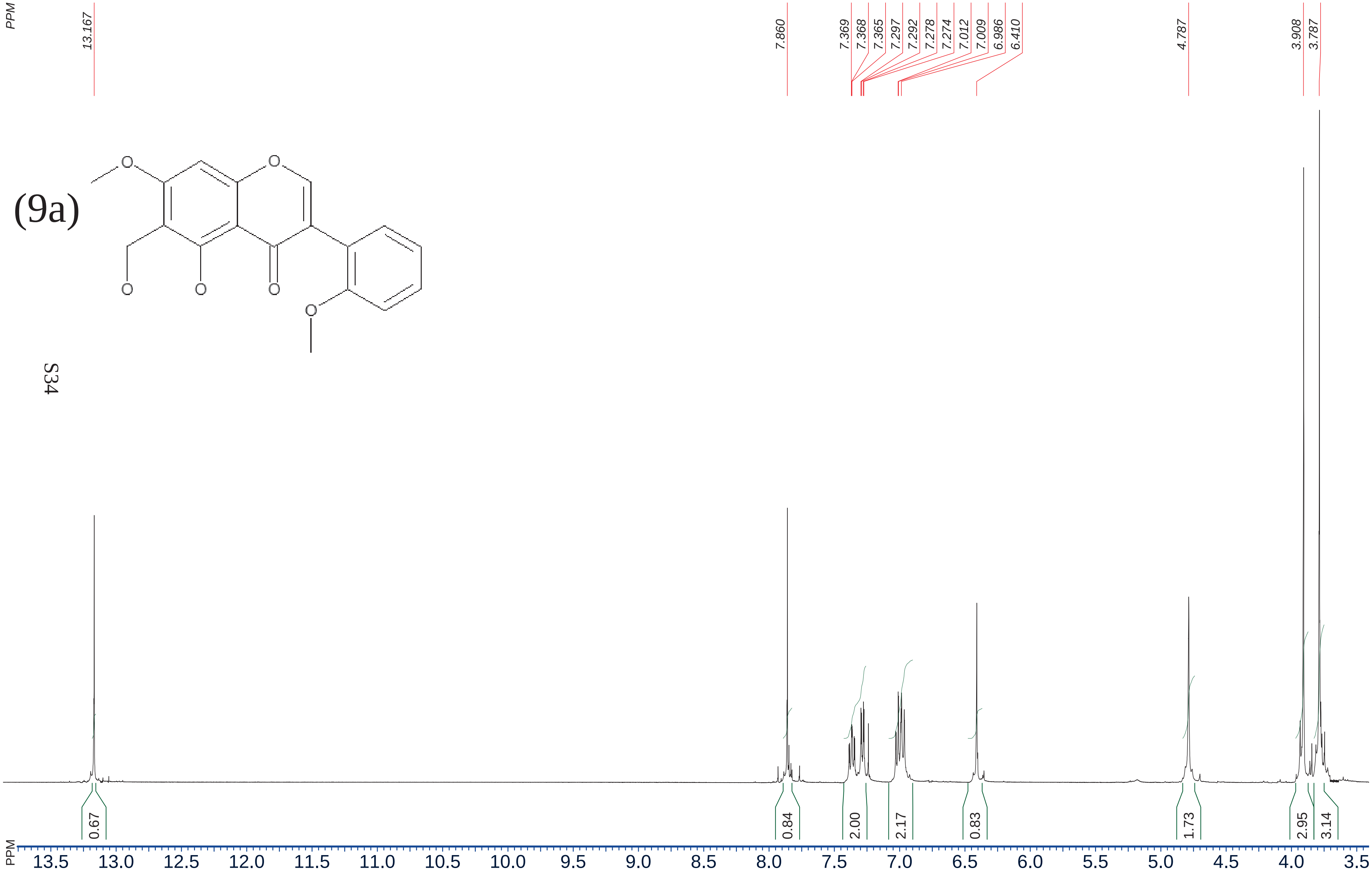
(11e)

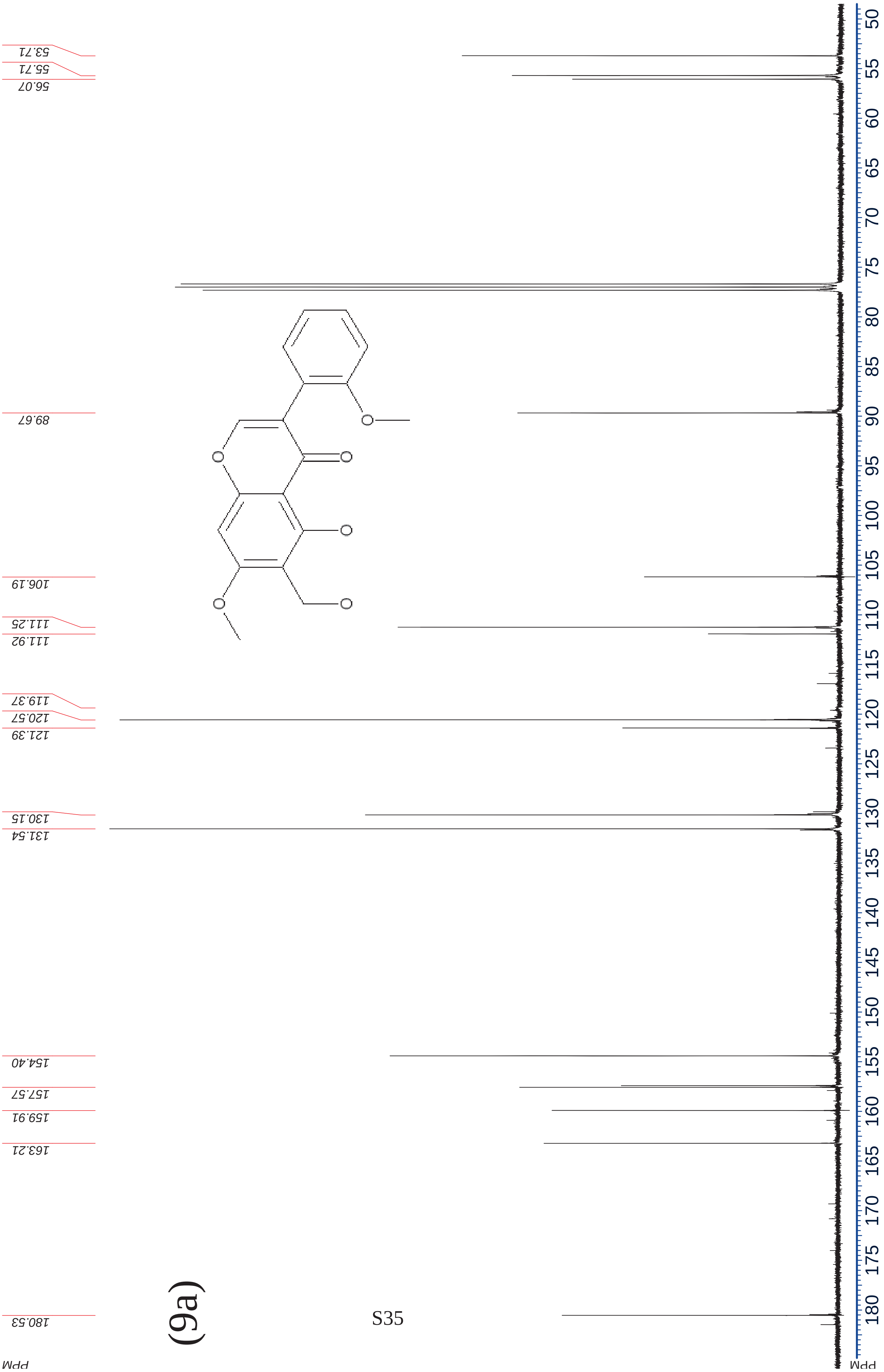

PPM
8.288
8.266
7.223
7.202
7.173
7.151
6.994
6.974
5.399
3.853
2.394
2.364
2.082
0.94
3.00
2.05
2.00
2.95
5.68
2.59
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
PPM

(11e)


PPM
176.11
170.50
168.66
163.21
159.22
154.92
153.46
131.42
127.94
124.57
123.30
121.51
119.84
117.08
113.93
55.24
54.55
20.78
20.72
19.45
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

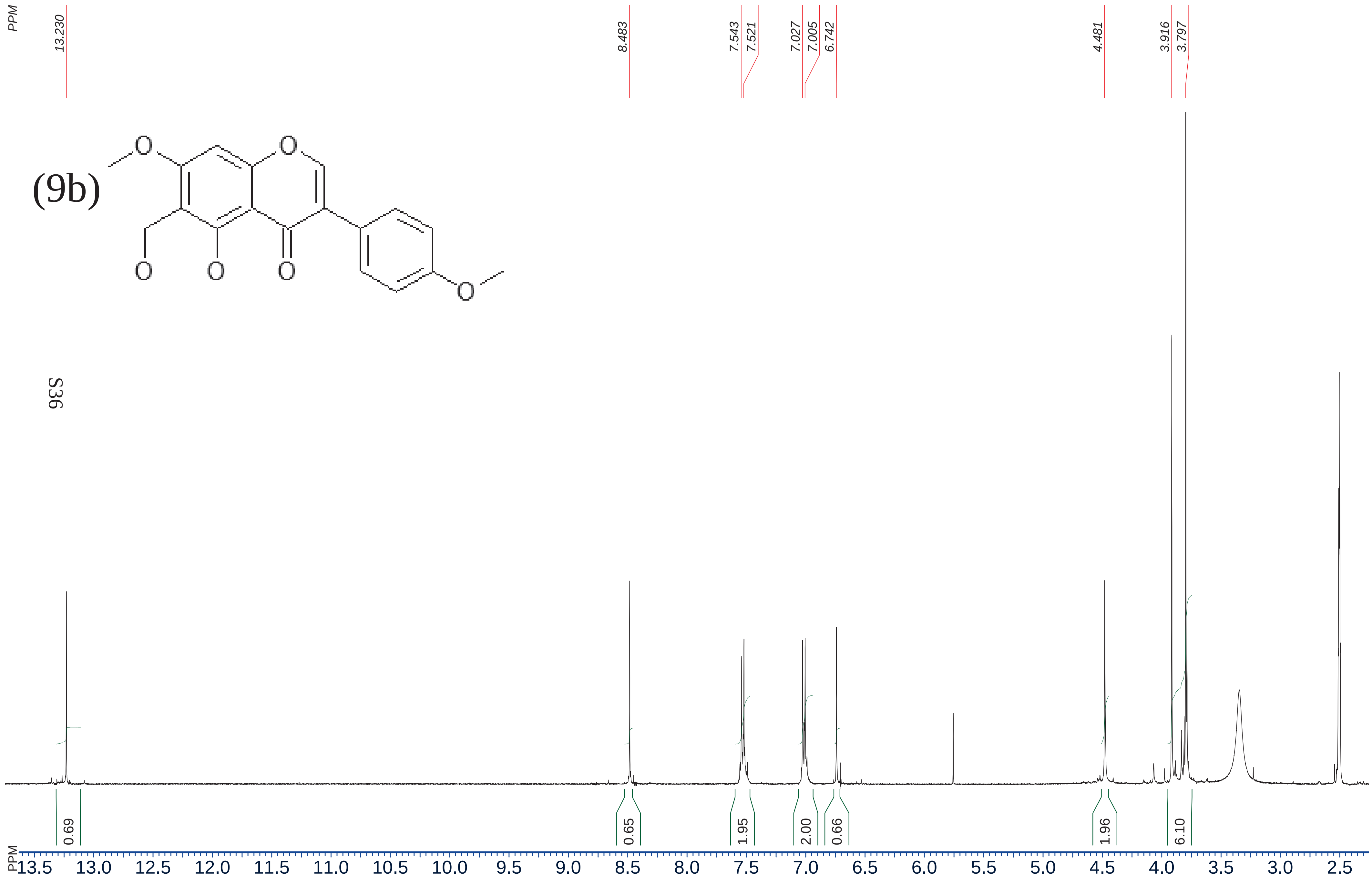
(9a)

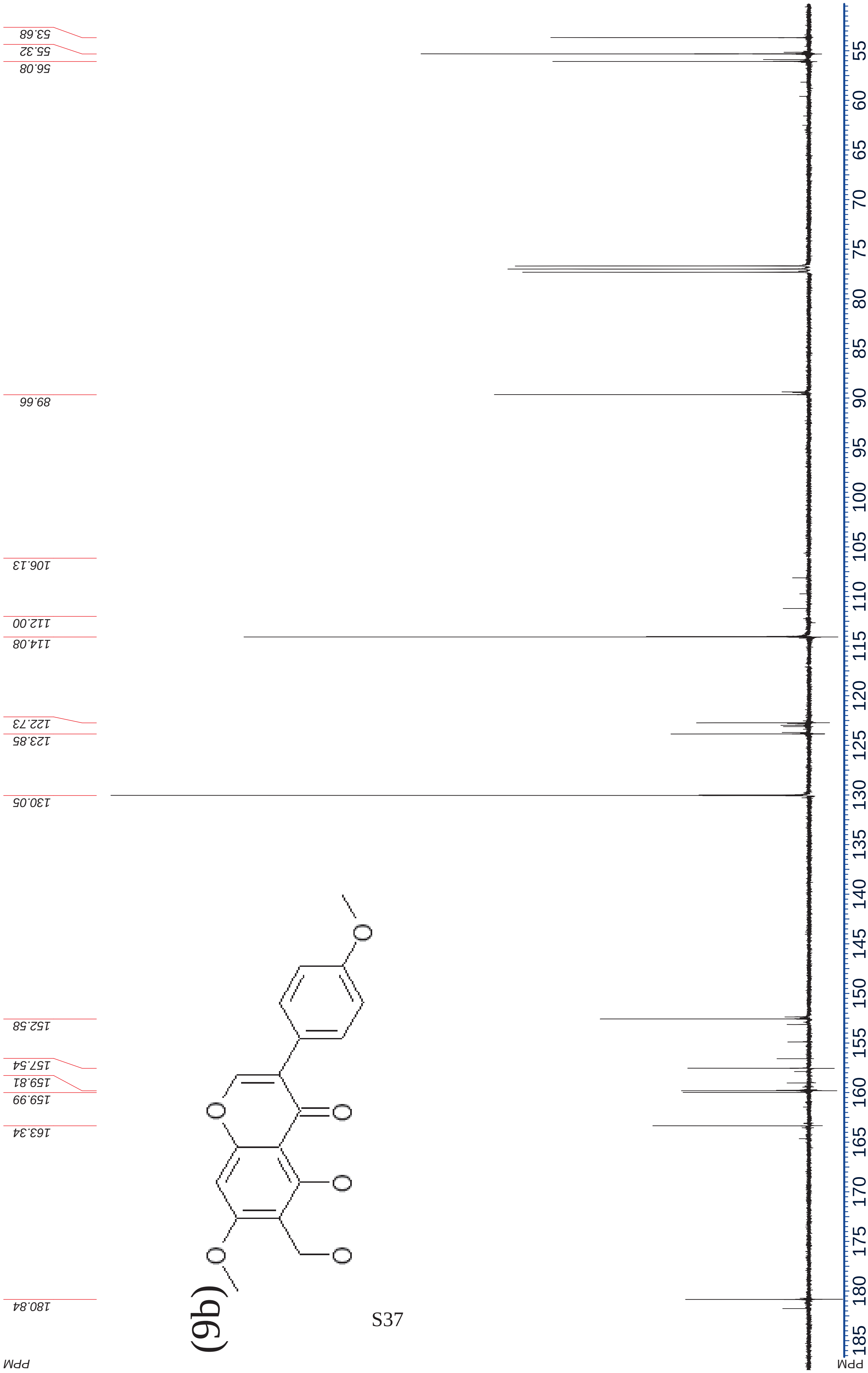

PPM
13.167
7.860
7.369
7.368
7.365
7.297
7.292
7.278
7.274
7.012
7.009
6.986
6.410
4.787
3.908
3.787
0.67
0.84
2.00
2.17
0.83
1.73
2.95
3.14
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5
PPM


53.71
55.71
56.07
89.67
106.19
111.25
111.92
119.37
120.57
121.39
130.15
131.54
154.40
157.57
159.91
163.21
180.53
PPM

(9a)

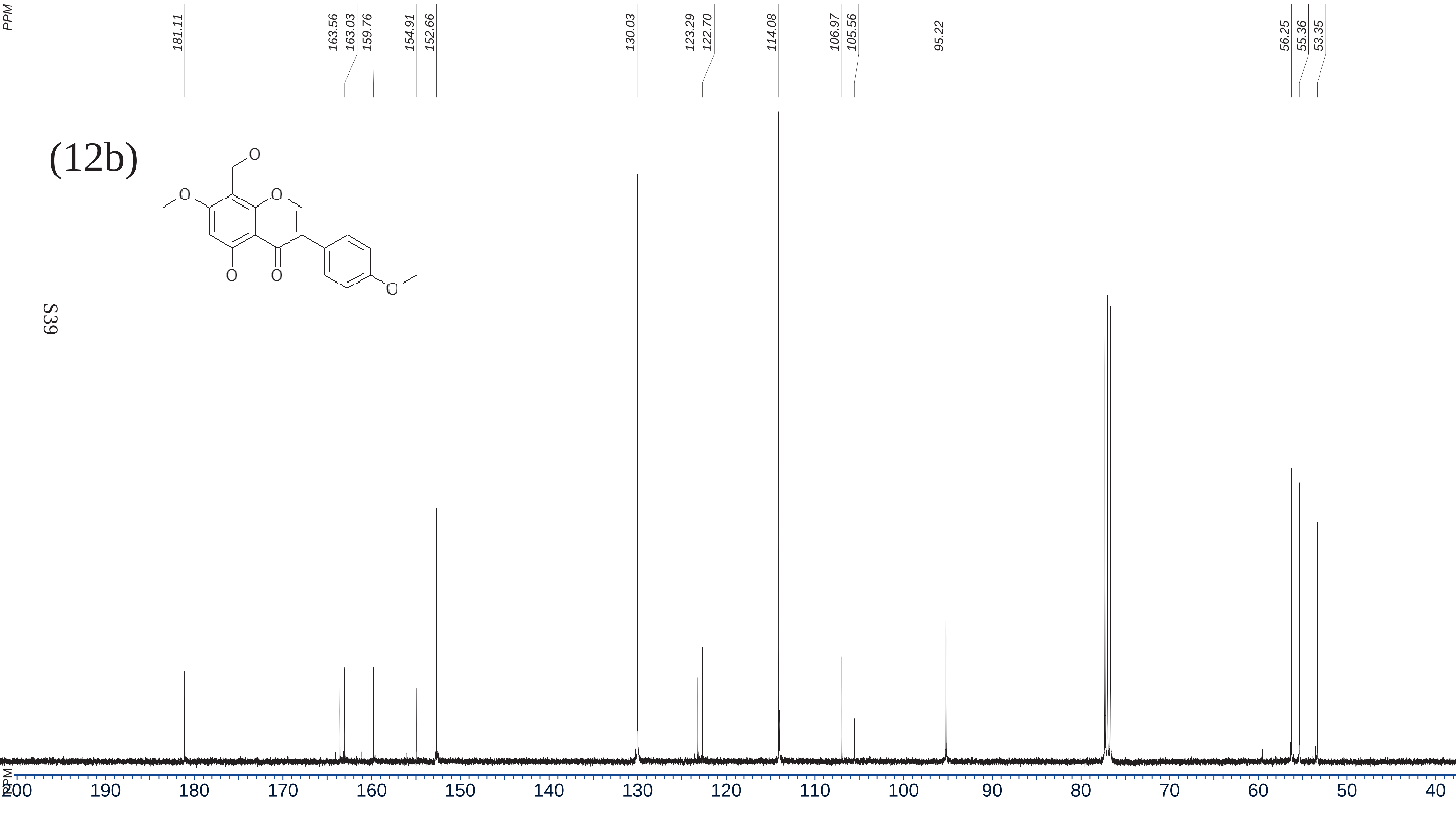
(9b)


13.230
8.483
7.543
7.521
7.027
7.005
6.742
4.481
3.916
3.797
0.69
0.65
1.95
2.00
0.66
1.96
6.10
PPM
13.5 13.0 12.5 12.0 11.5 11.0 10.5 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


53.68
55.32
56.08
89.66
106.13
112.00
114.08
122.73
123.85
130.05
152.58
157.54
159.81
159.99
163.34
180.84
PPM
(9b)

(12b)

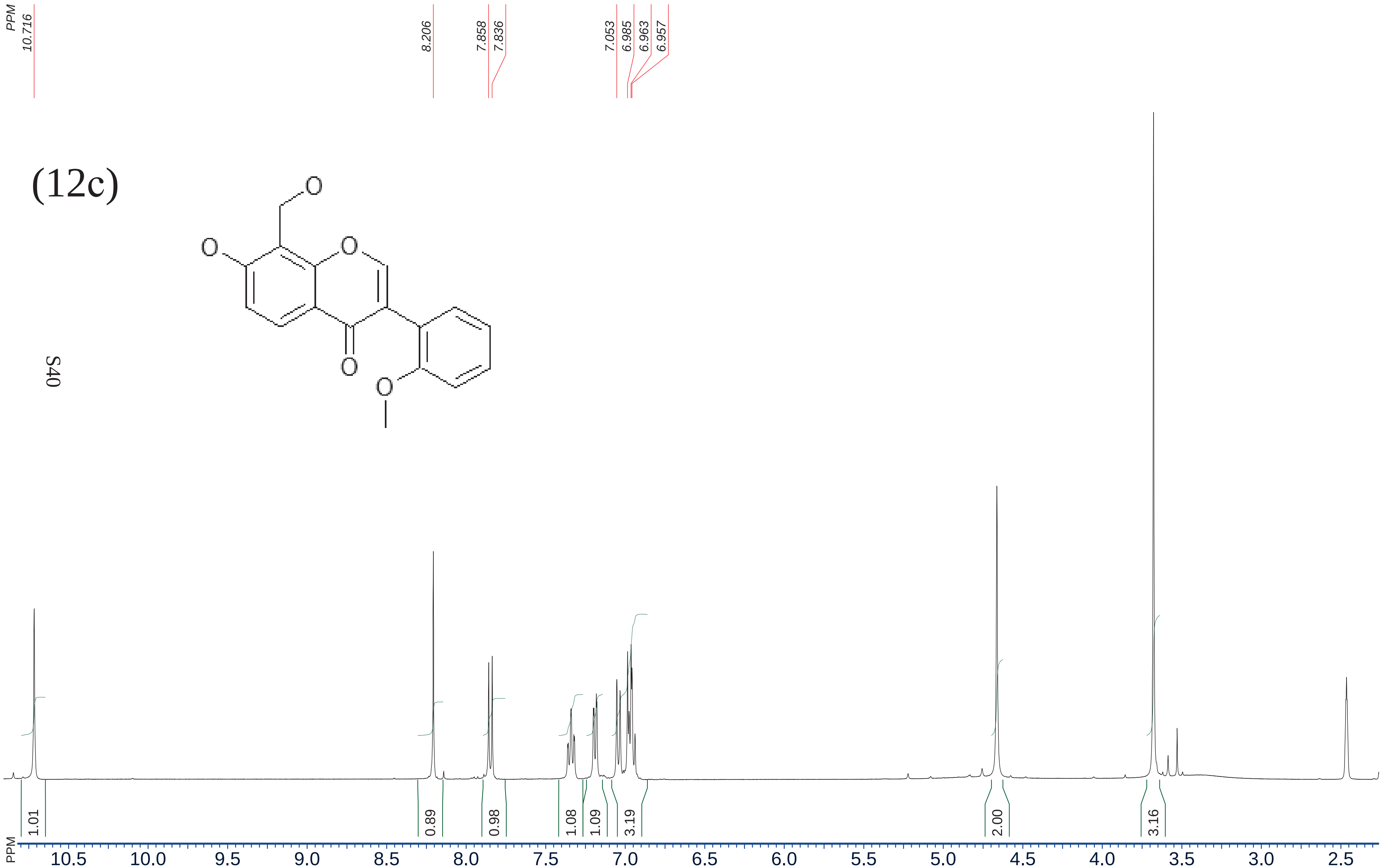

PPM
13.136
7.927
7.466
7.444
6.994
6.972
6.433
4.852
3.948
3.844
0.95
0.86
2.10
2.00
1.06
2.00
2.91
3.18
PPM
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5



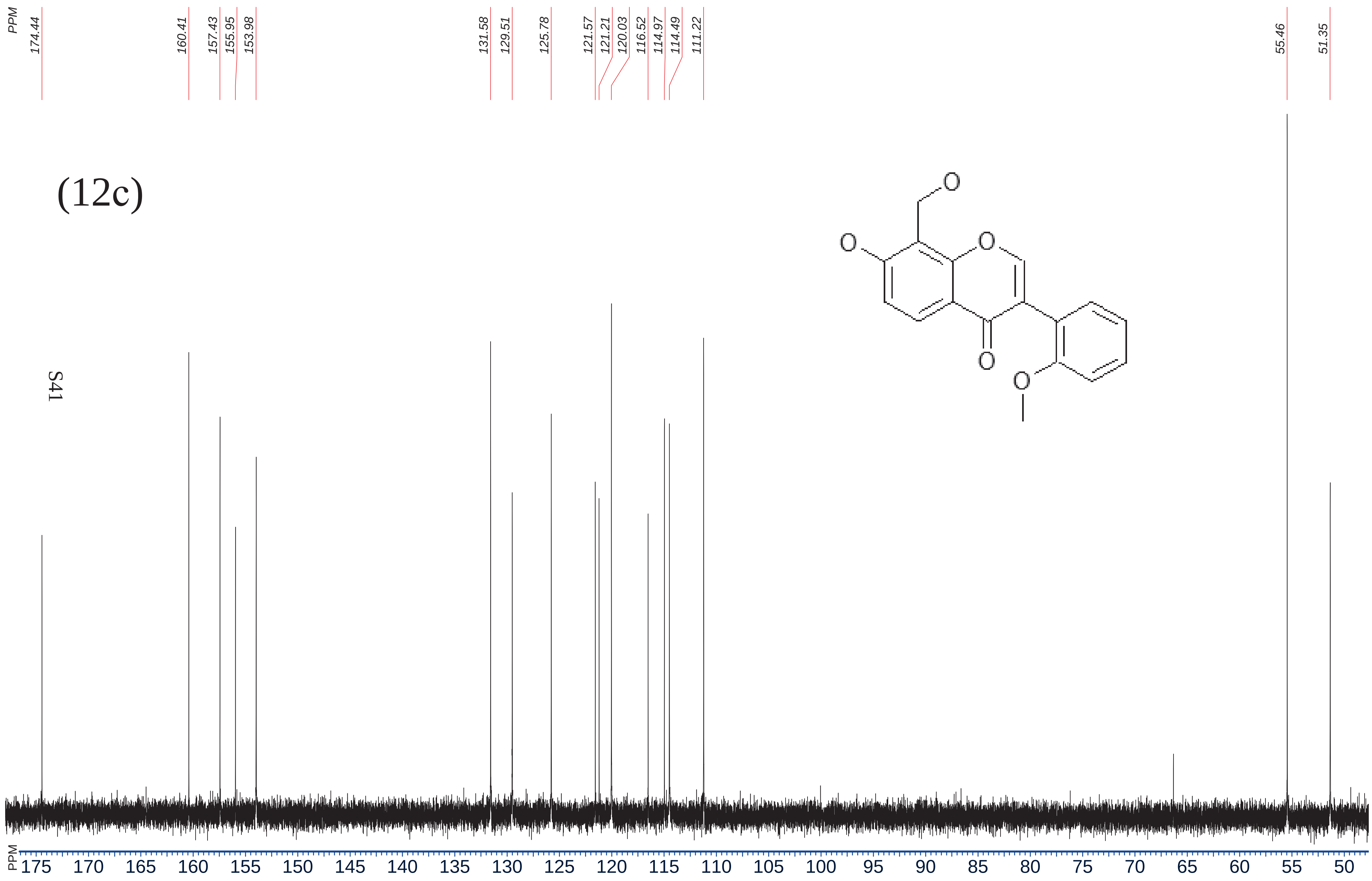
PPM
181.11
163.56
163.03
159.76
154.91
152.66
130.03
123.29
122.70
114.08
106.97
105.56
95.22
56.25
55.36
53.35
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40

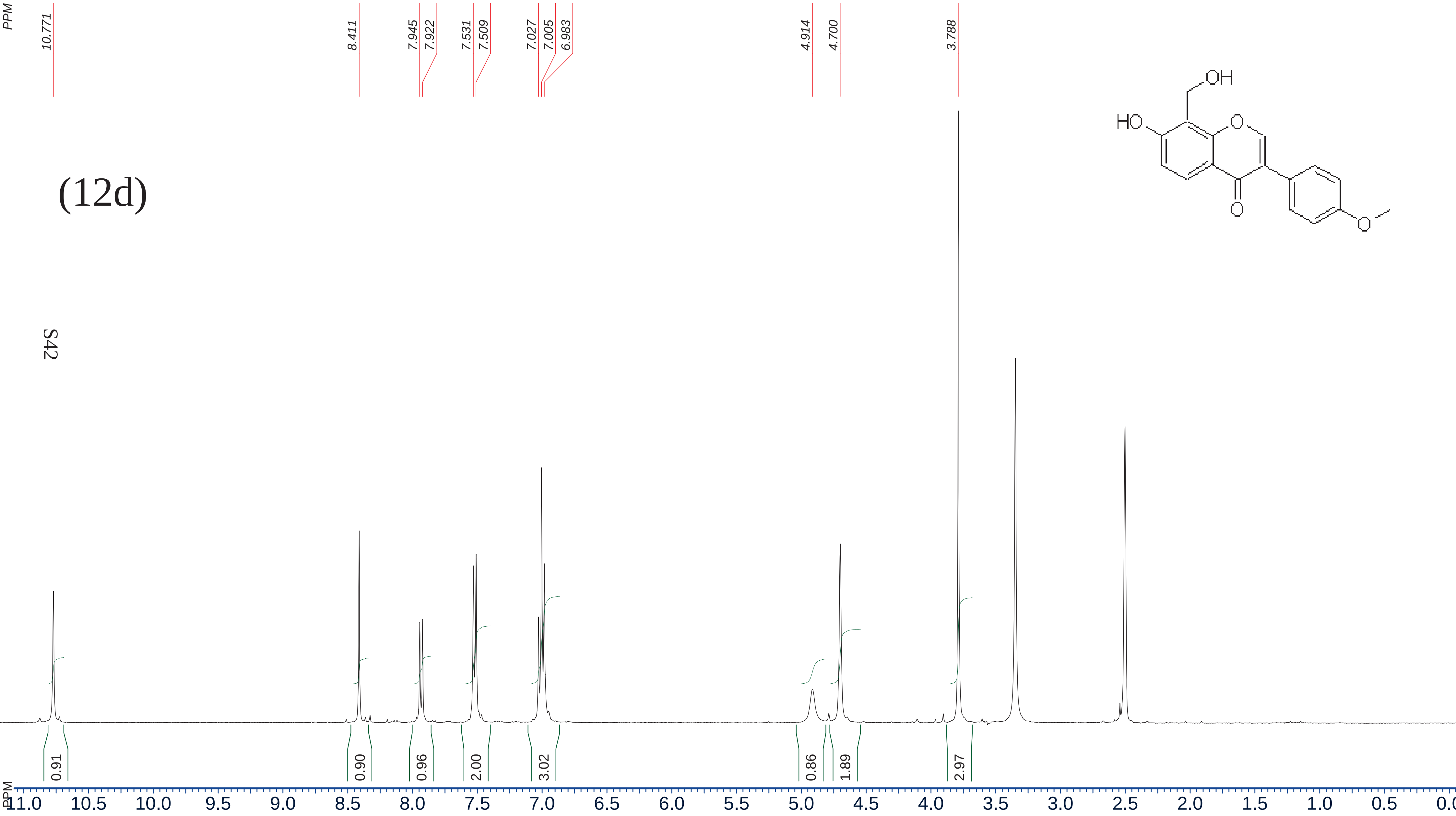
(12b)

(12c)


PPM
10.716
8.206
7.858
7.836
7.053
6.985
6.963
6.957
1.01
0.89
0.98
1.08
1.09
3.19
2.00
3.16
10.5
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

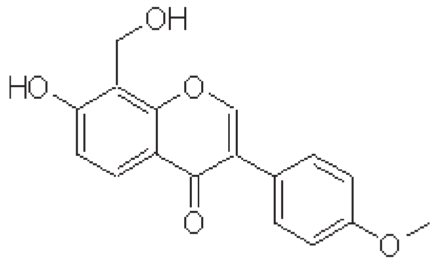
(12c)

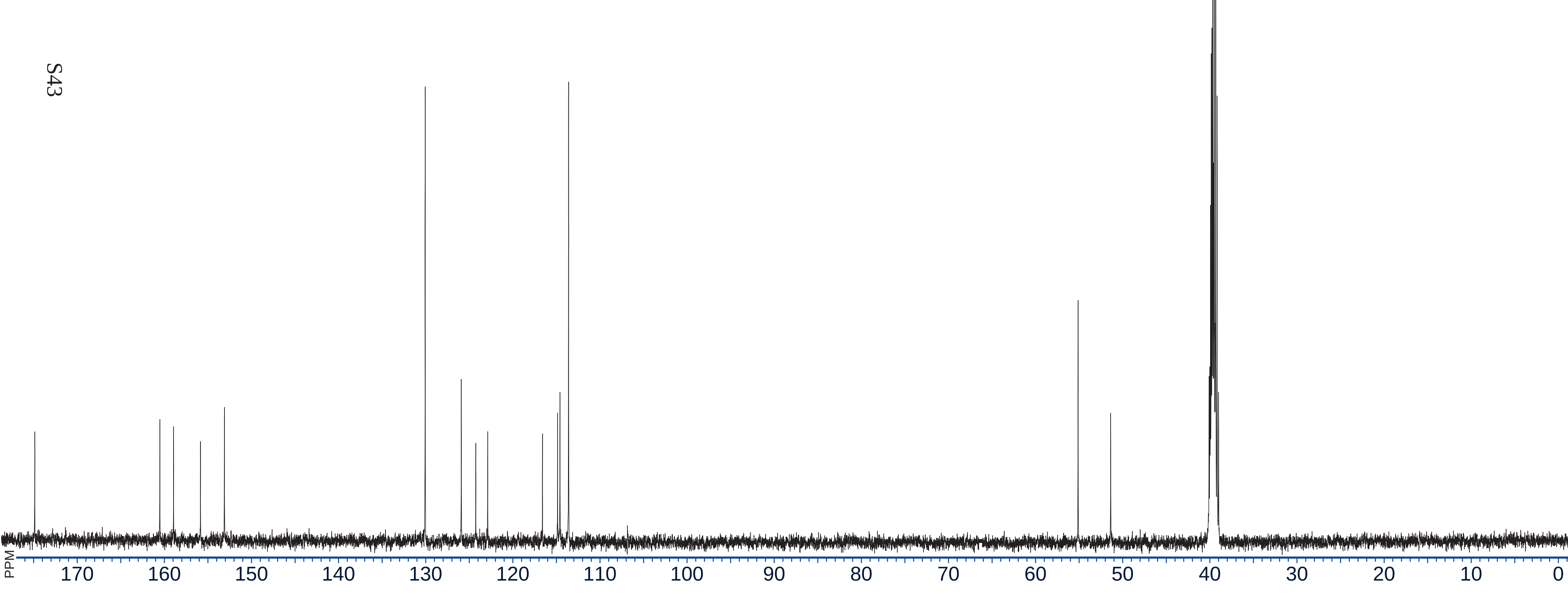

PPM
174.44
160.41
157.43
155.95
153.98
131.58
129.51
125.78
121.57
121.21
120.03
116.52
114.97
114.49
111.22
55.46
51.35
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50


PPM
10.771
8.411
7.945
7.922
7.531
7.509
7.027
7.005
6.983
4.914
4.700
3.788
HO
OH
O
O
O
0.91
0.90
0.96
2.00
3.02
0.86
1.89
2.97
11.0
10.5
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

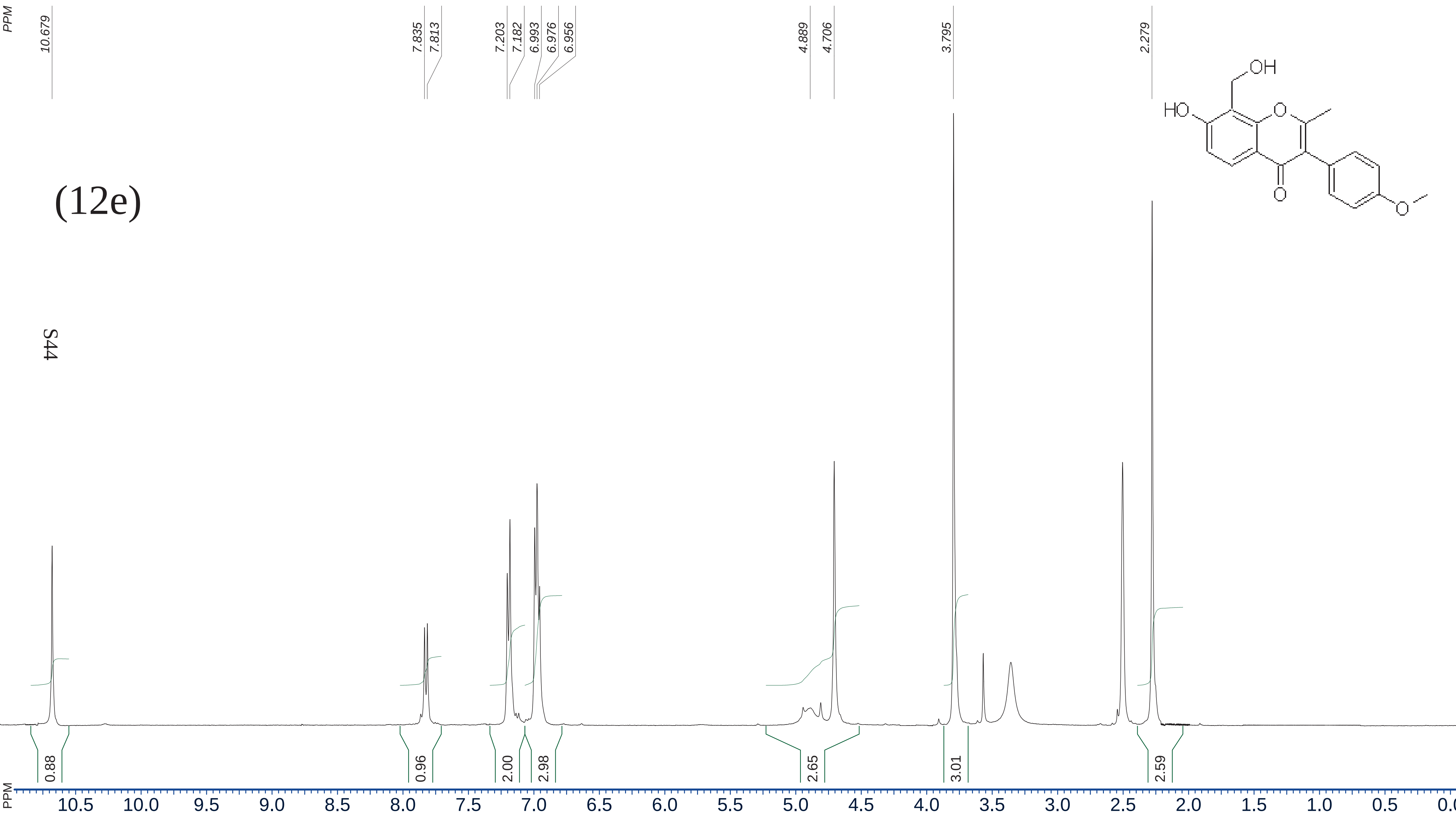
(12d)

(12d)



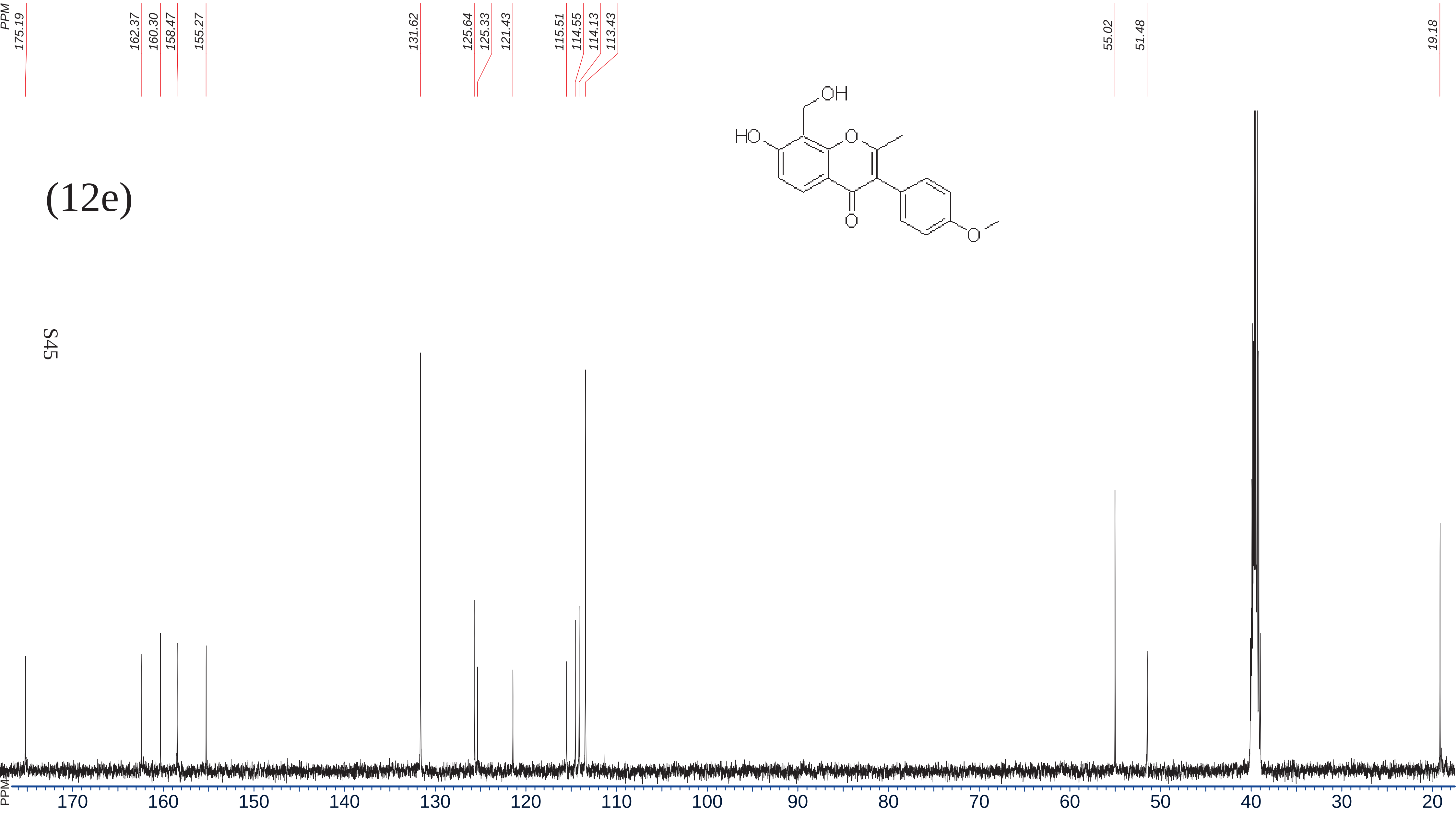

PPM
174.87
160.51
158.94
155.85
153.10
130.06
125.91
124.25
122.88
116.60
114.87
114.59
113.60
55.13
51.39
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

(12e)

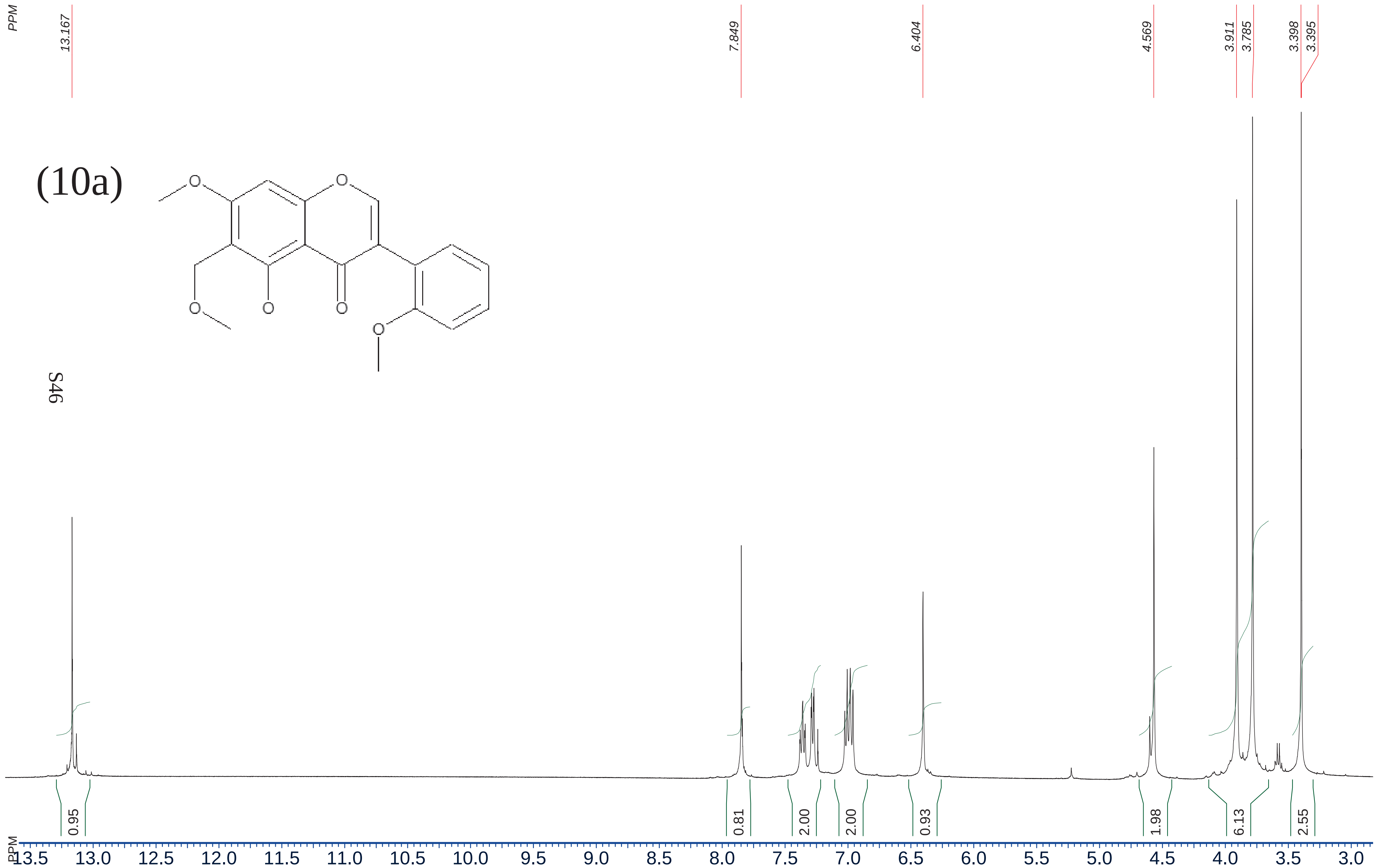


PPM
10.679
7.835
7.813
7.203
7.182
6.993
6.976
6.956
4.889
4.706
3.795
2.279
HO
OH
O
O
0.88
0.96
2.00
2.98
2.65
3.01
2.59
PPM
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

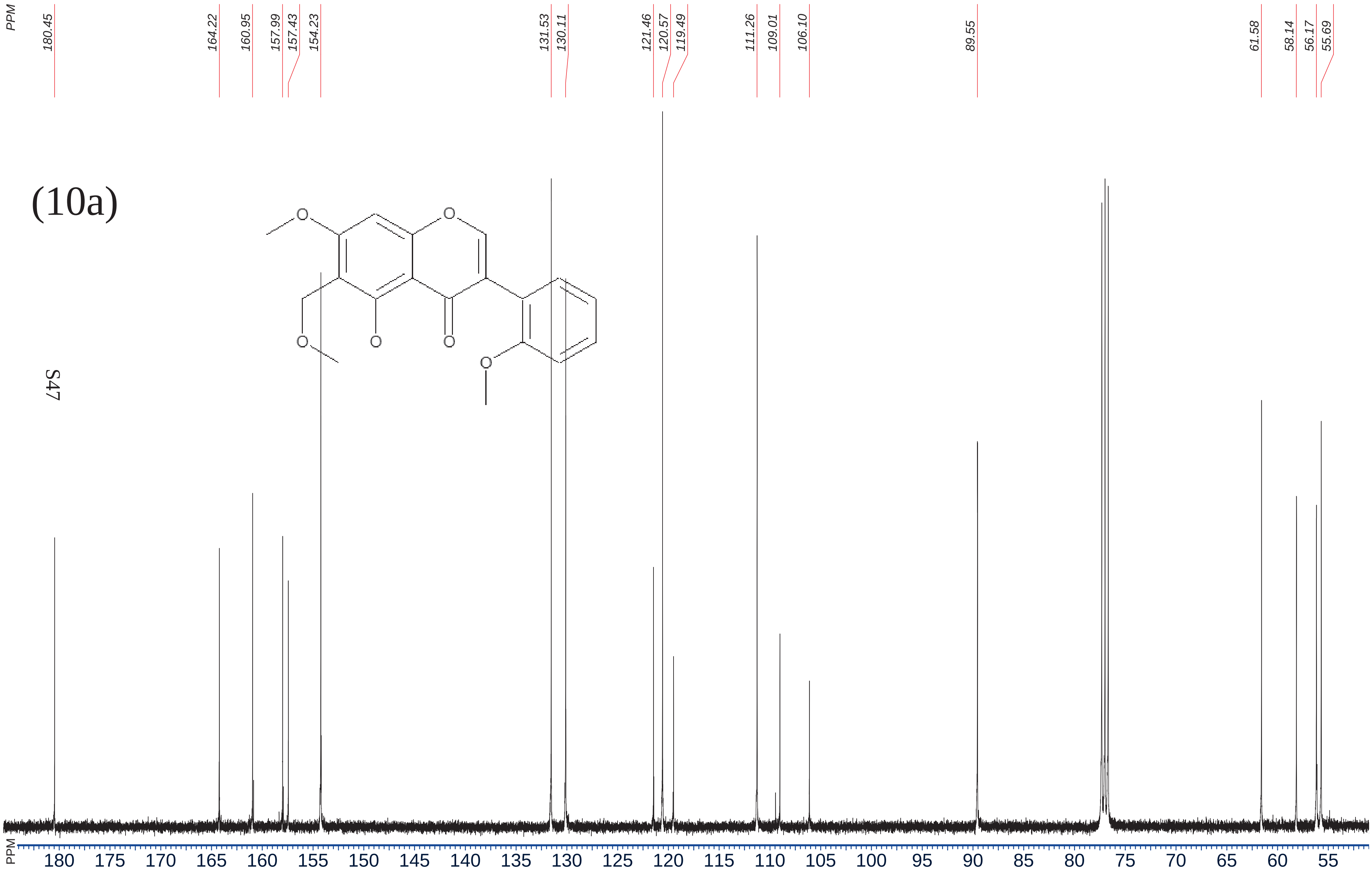
(12e)

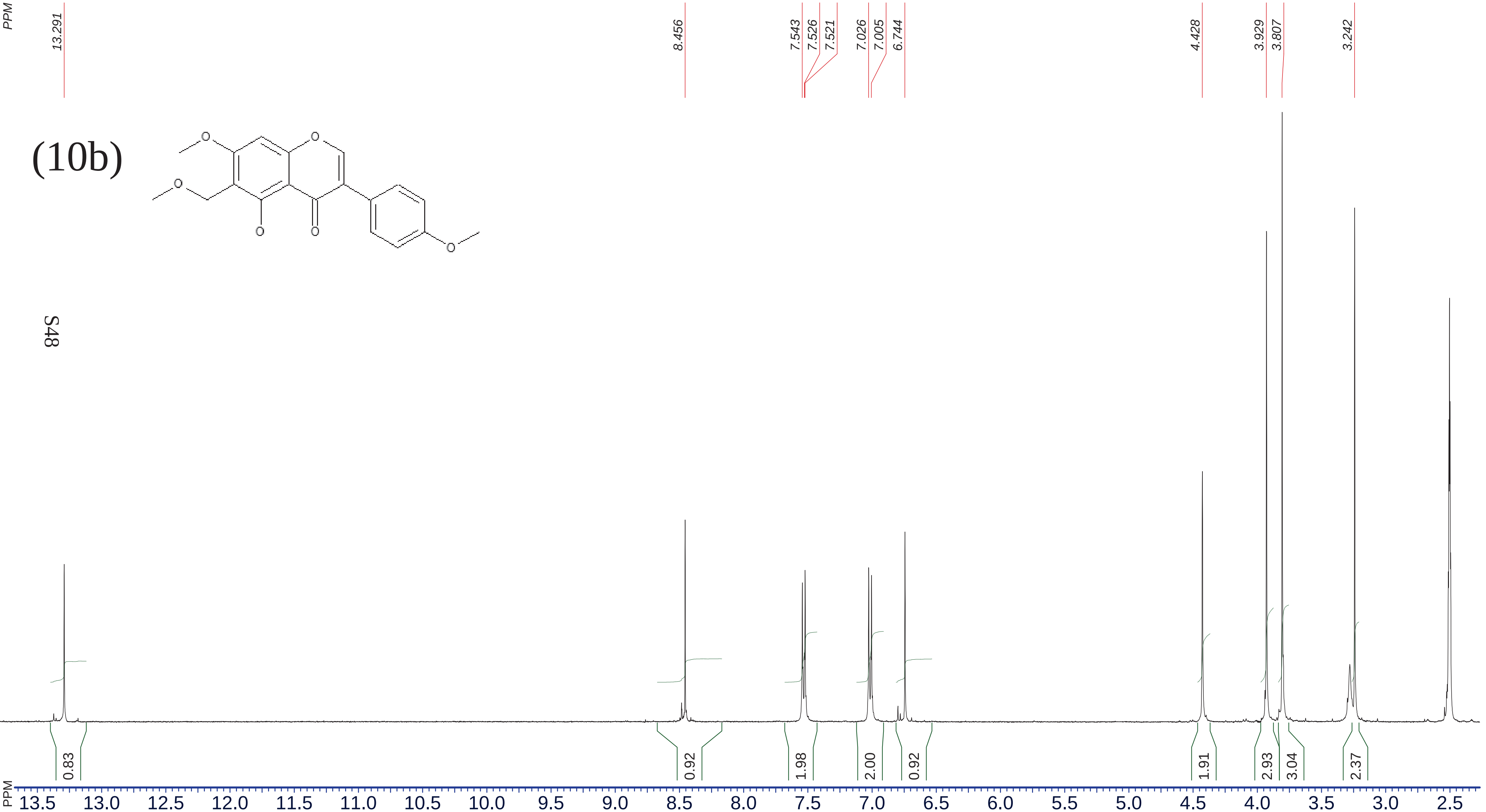

PPM
175.19
162.37
160.30
158.47
155.27
131.62
125.64
125.33
121.43
115.51
114.55
114.13
113.43
55.02
51.48
19.18
OH
HO
O
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
PPM

(10a)

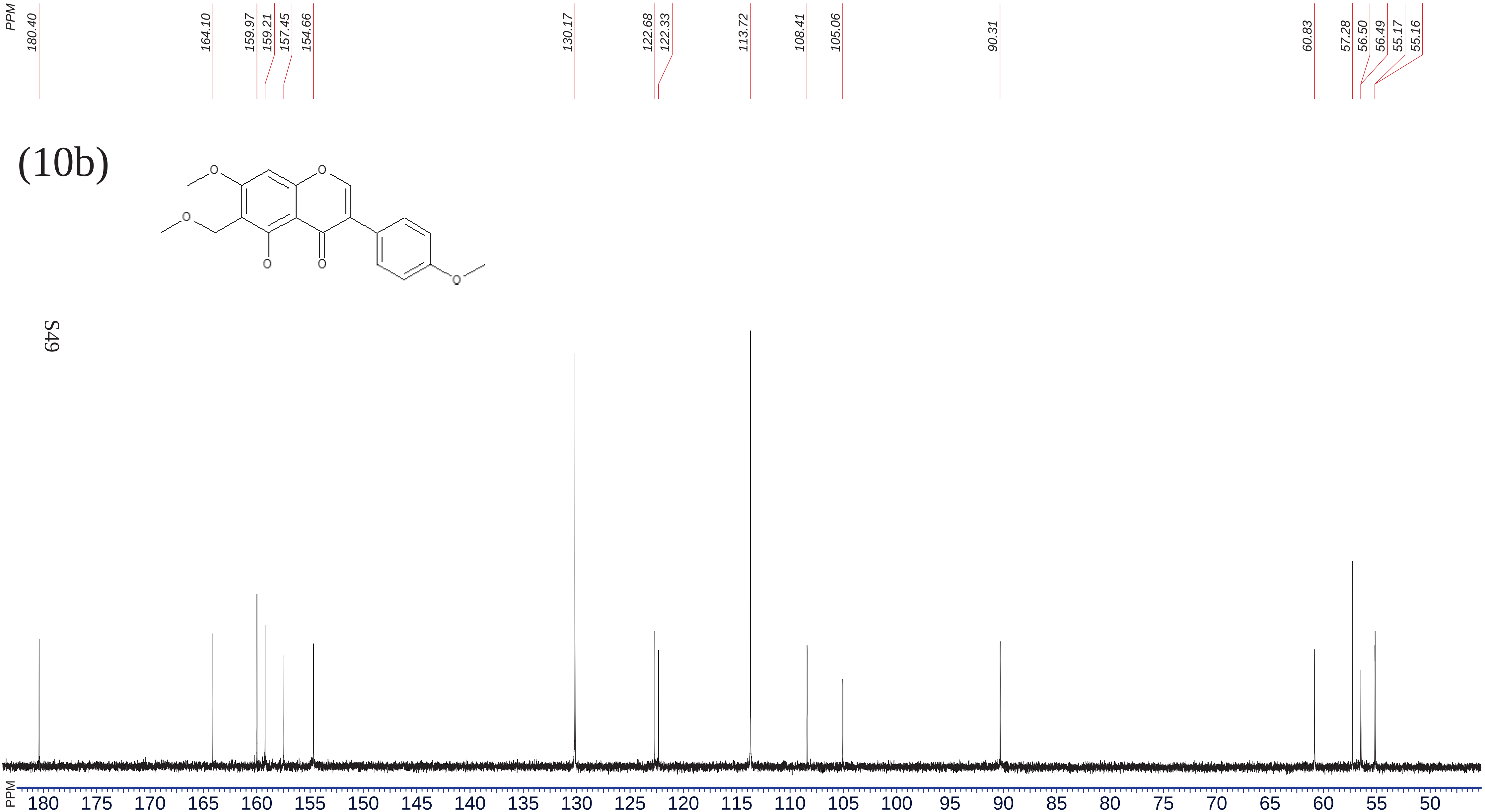

PPM
13.167
7.849
6.404
4.569
3.911
3.785
3.398
3.395
0.95
0.81
2.00
2.00
0.93
1.98
6.13
2.55
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0

(10a)


PPM
180.45
164.22
160.95
157.99
157.43
154.23
131.53
130.11
121.46
120.57
119.49
111.26
109.01
106.10
89.55
61.58
58.14
56.17
55.69
PPM
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55

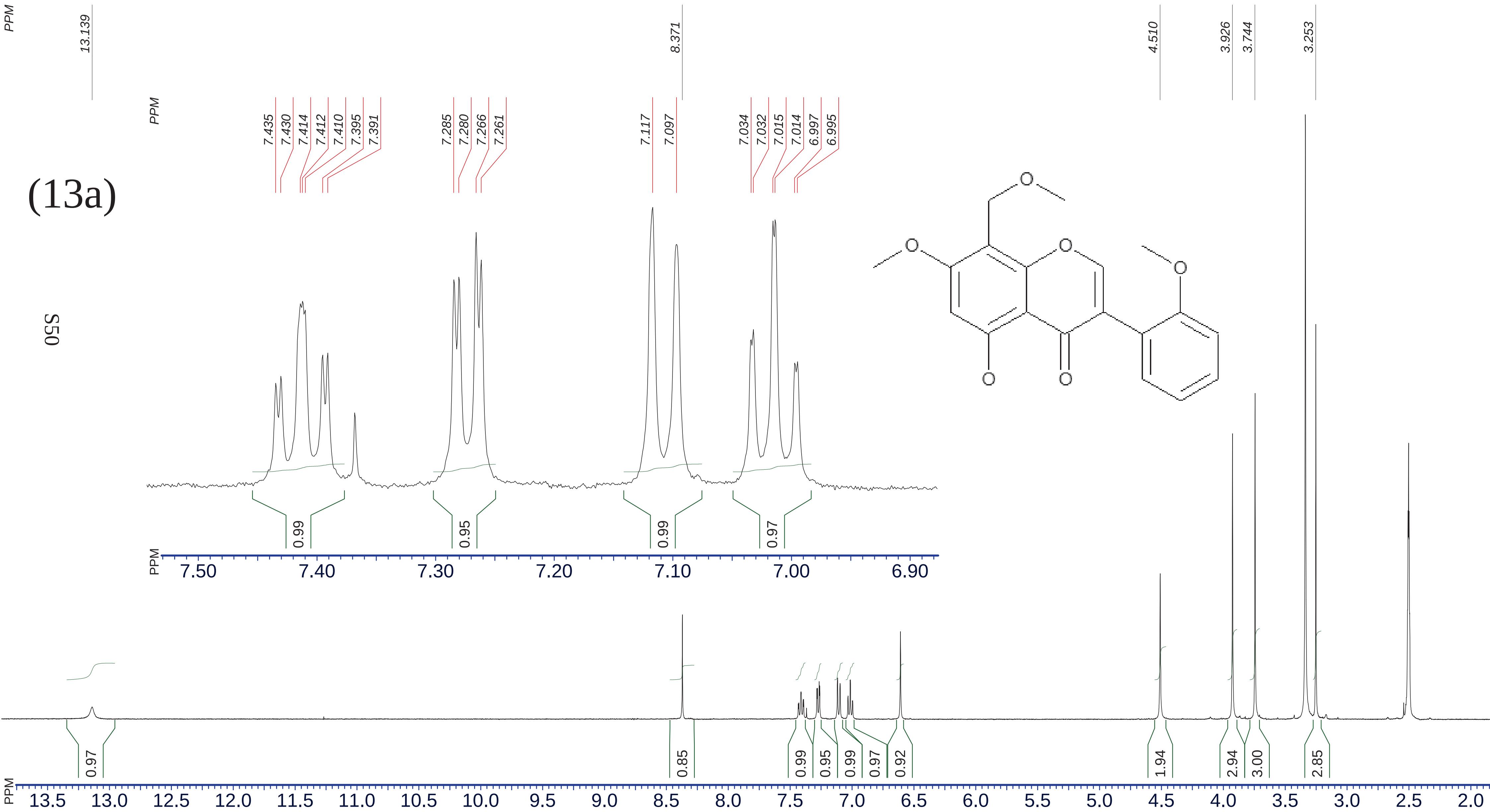

PPM
13.291
8.456
7.543
7.526
7.521
7.026
7.005
6.744
4.428
3.929
3.807
3.242
0.83
0.92
1.98
2.00
0.92
1.91
2.93
3.04
2.37
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
PPM

(10b)


PPM
180.40
164.10
159.97
159.21
157.45
154.66
130.17
122.68
122.33
113.72
108.41
105.06
90.31
60.83
57.28
56.50
56.49
55.17
55.16
PPM
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50

(10b)

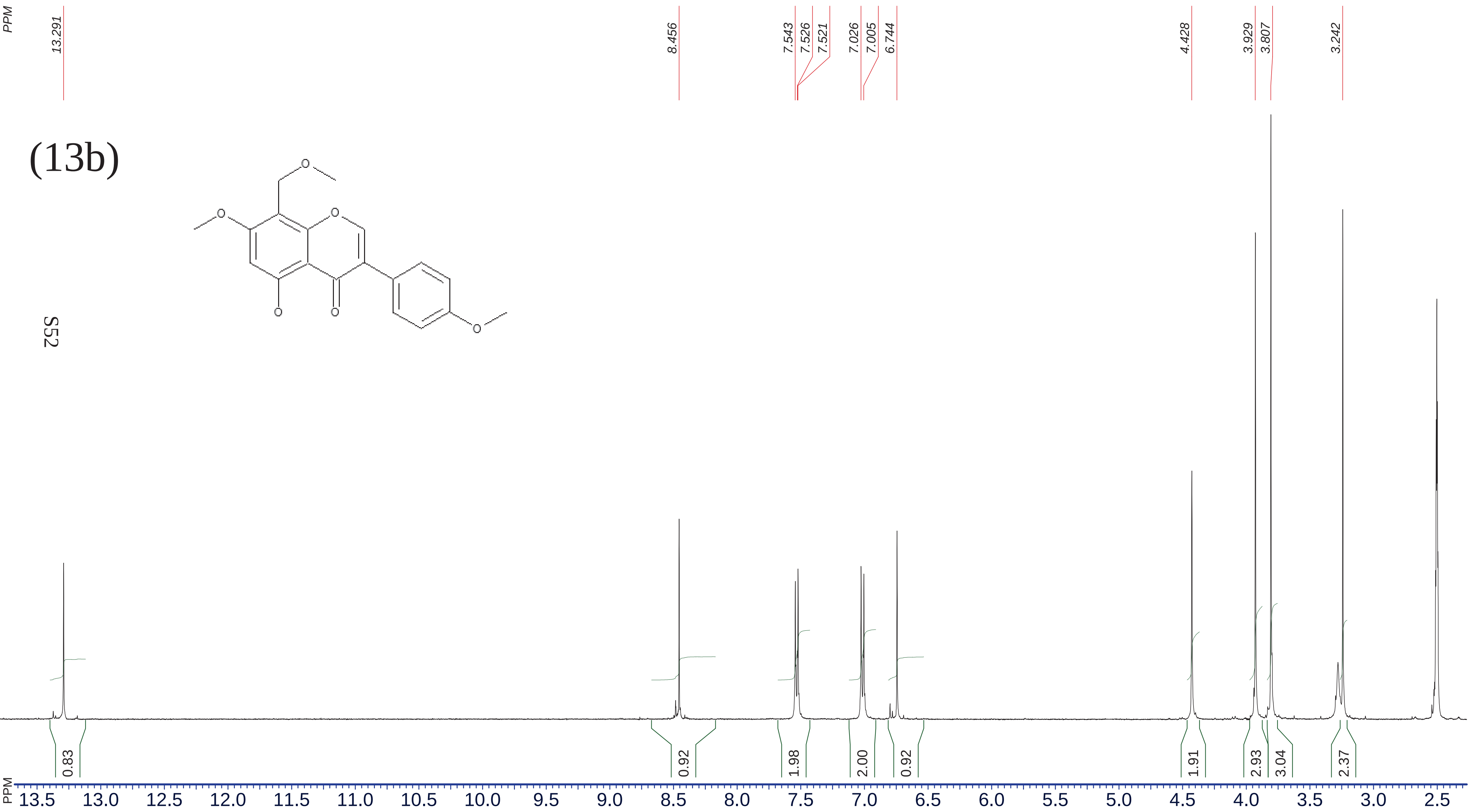
(13a)


PPM
13.139
8.371
4.510
3.926
3.744
3.253
7.435
7.430
7.414
7.412
7.410
7.395
7.391
7.285
7.280
7.266
7.261
7.117
7.097
7.034
7.032
7.015
7.014
6.997
6.995
0.99
0.95
0.99
0.97
7.50
7.40
7.30
7.20
7.10
7.00
6.90
0.97
0.85
0.99
0.95
0.99
0.97
0.92
1.94
2.94
3.00
2.85
13.5
13.0
12.5
12.0
11.5
11.0
10.5
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

(13a)


PPM
180.10
163.65
162.04
157.30
155.57
155.31
131.45
129.88
120.28
120.04
119.37
111.23
104.46
104.03
95.24
60.89
60.89
57.23
56.49
55.52
PPM
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40

(13b)


PPM
13.291
8.456
7.543
7.526
7.521
7.026
7.005
6.744
4.428
3.929
3.807
3.242
0.83
0.92
1.98
2.00
0.92
1.91
2.93
3.04
2.37
PPM
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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5.0
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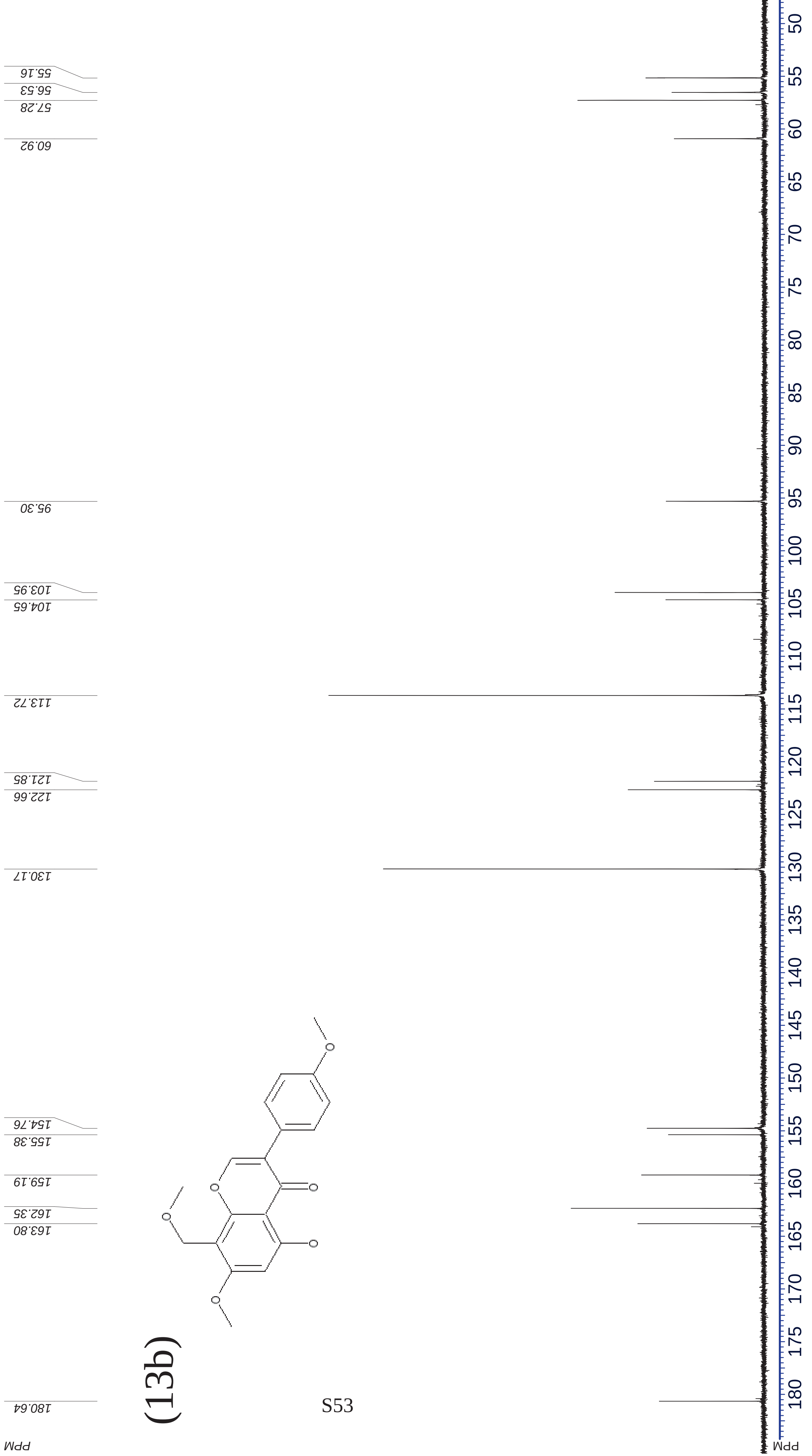
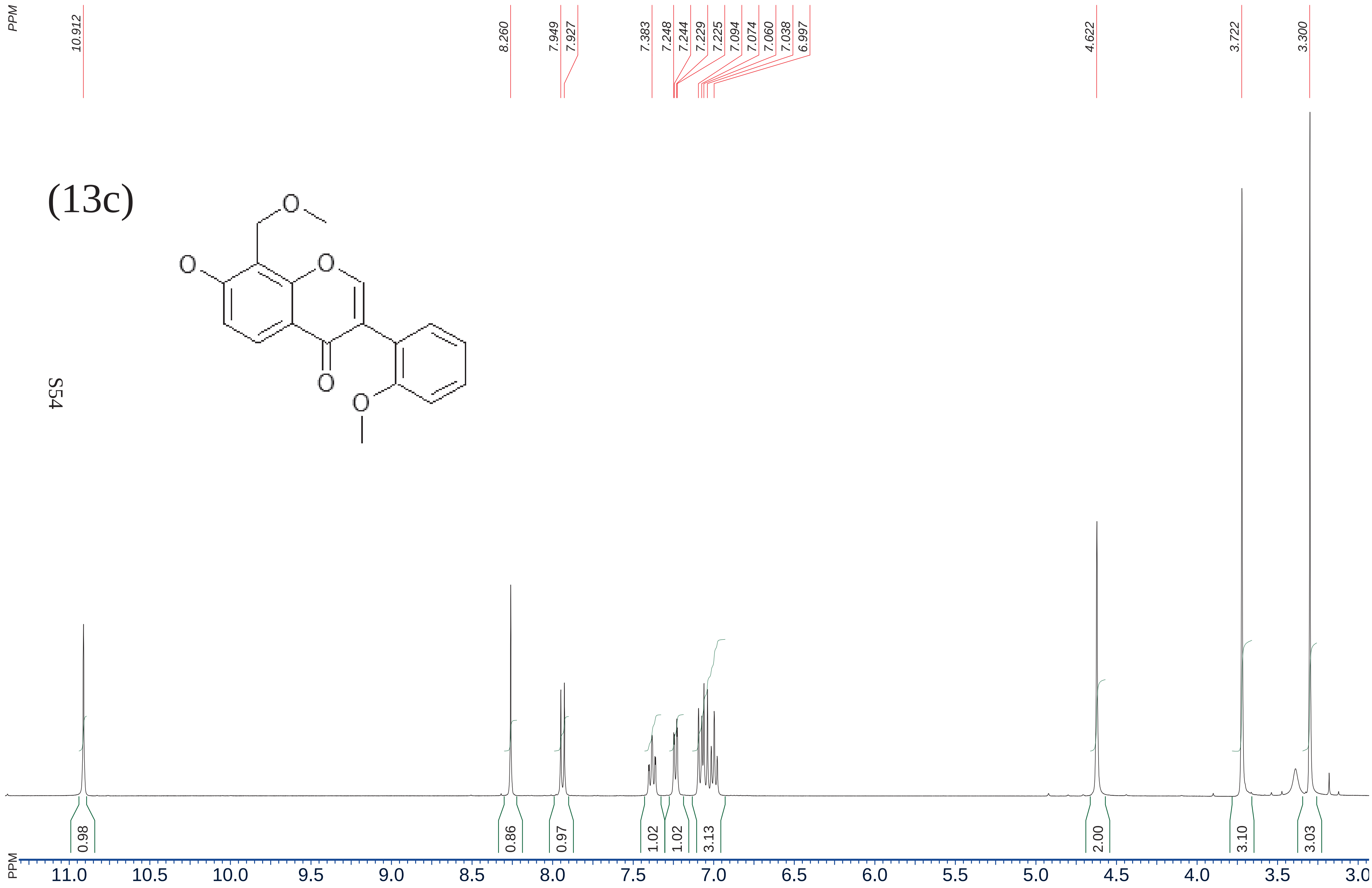
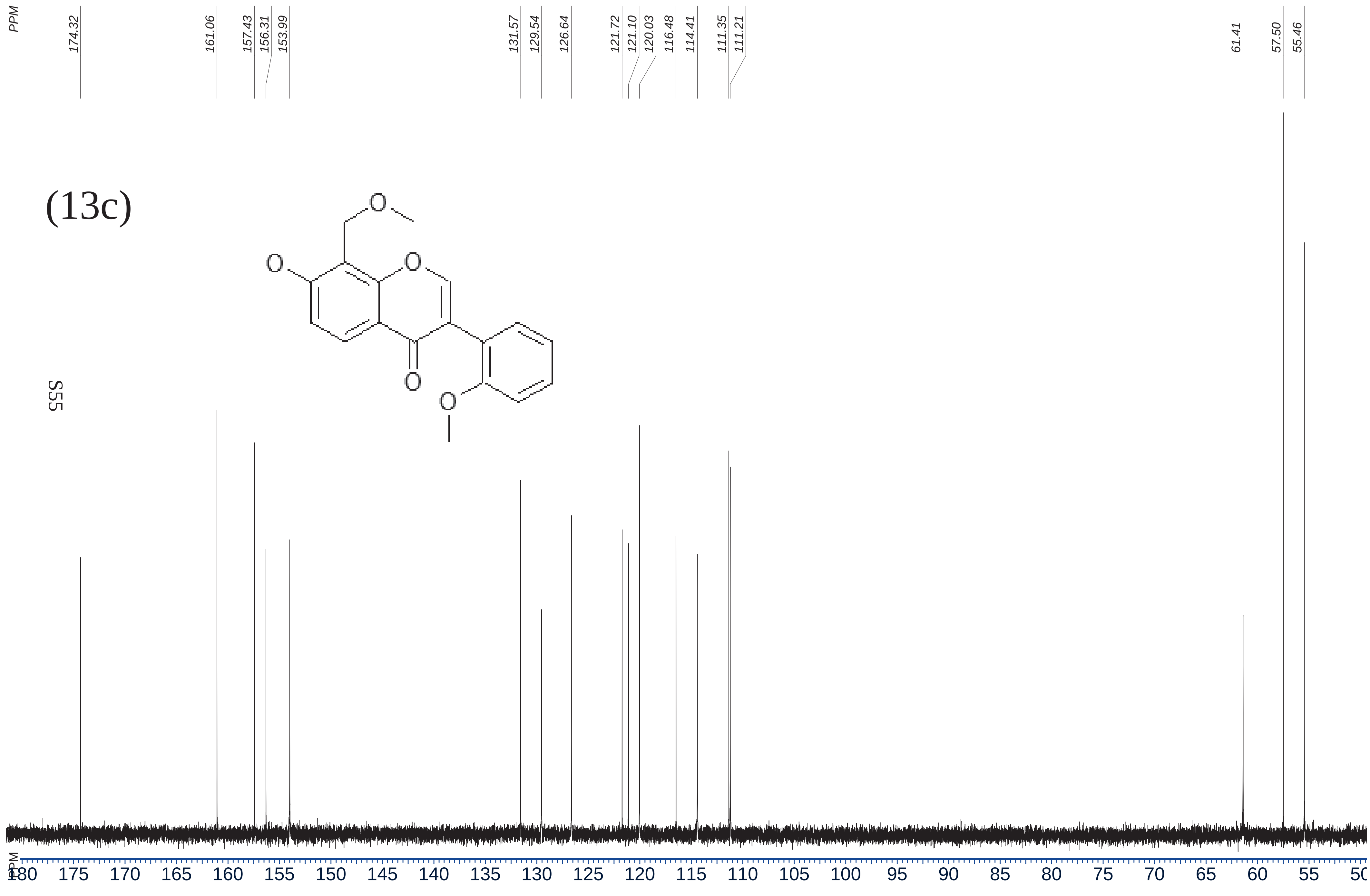
4.0
3.5
3.0
2.5


55.16
56.53
57.28
60.92
95.30
103.95
104.65
113.72
121.85
122.66
130.17
154.76
155.38
159.19
162.35
163.80
180.64
PPM
50
55
60
65
70
75
80
85
90
95
100
105
110
115
120
125
130
135
140
145
150
155
160
165
170
175
180
PPM

(13b)

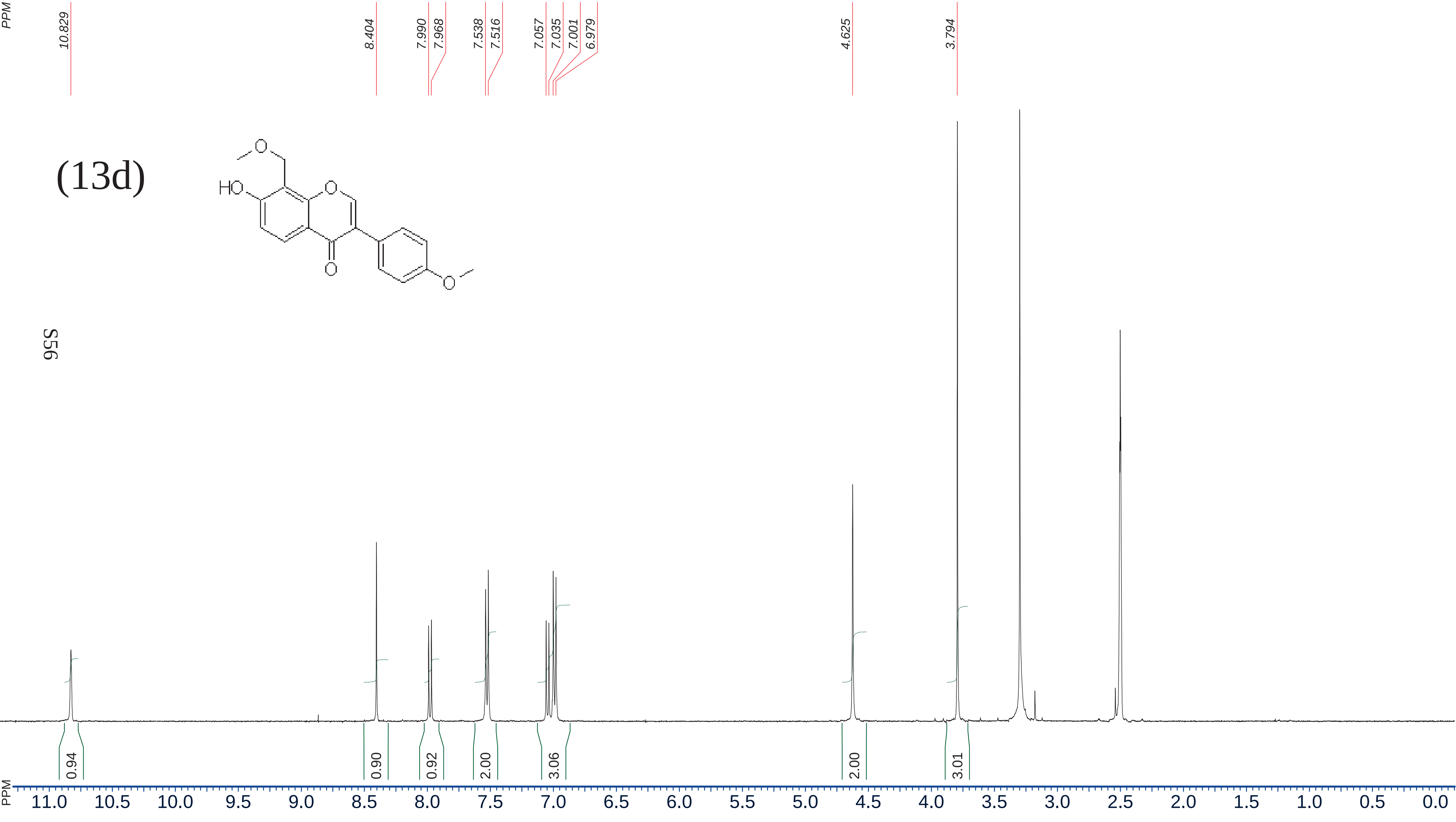
(13c)


PPM
10.912
8.260
7.949
7.927
7.383
7.248
7.244
7.229
7.225
7.094
7.074
7.060
7.038
6.997
4.622
3.722
3.300
0.98
0.86
0.97
1.02
1.02
3.13
2.00
3.10
3.03
PPM
11.0
10.5
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

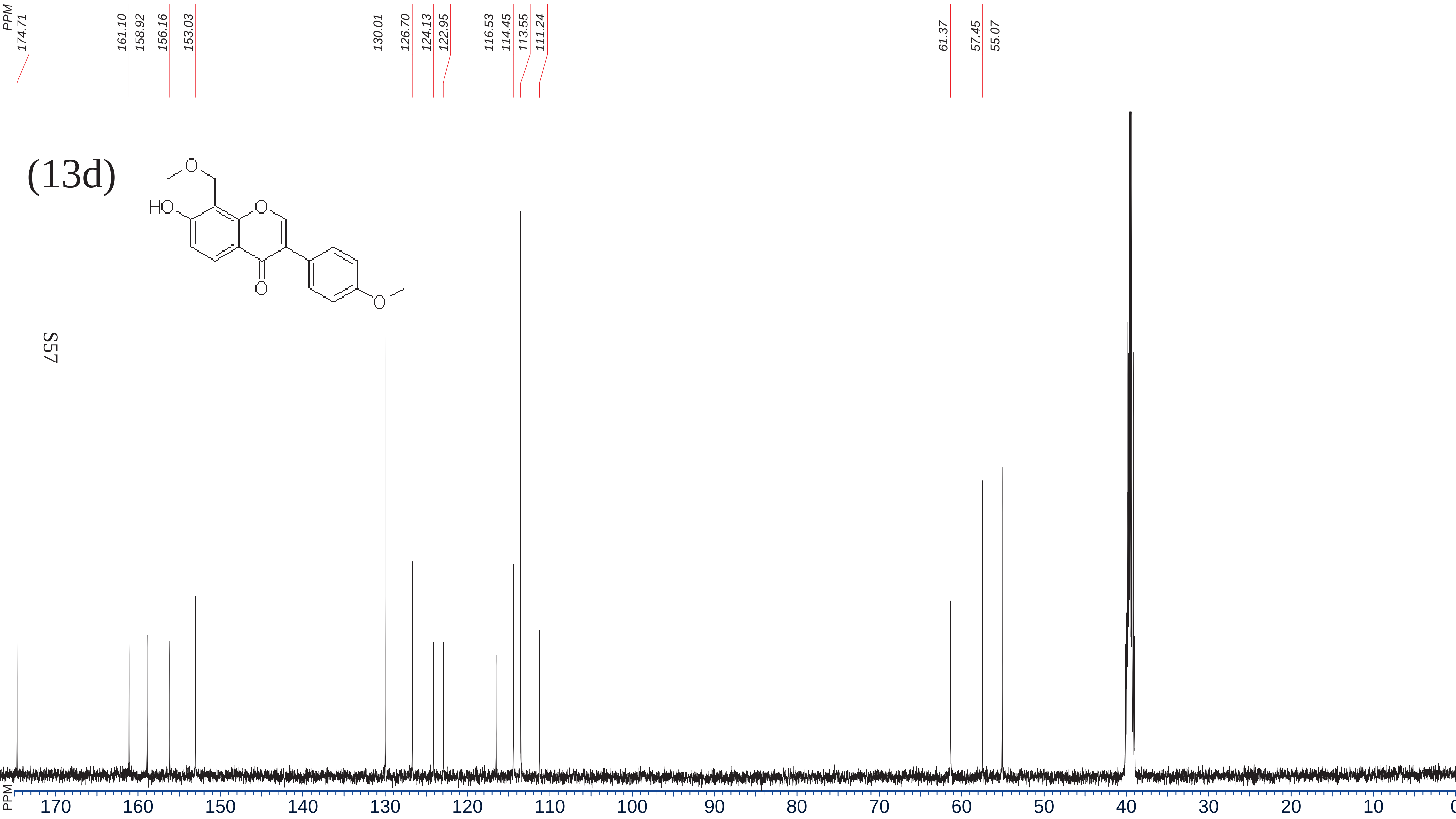

PPM
174.32
161.06
157.43
156.31
153.99
131.57
129.54
126.64
121.72
121.10
120.03
116.48
114.41
111.35
111.21
61.41
57.50
55.46
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
PPM

(13c)

(13d)

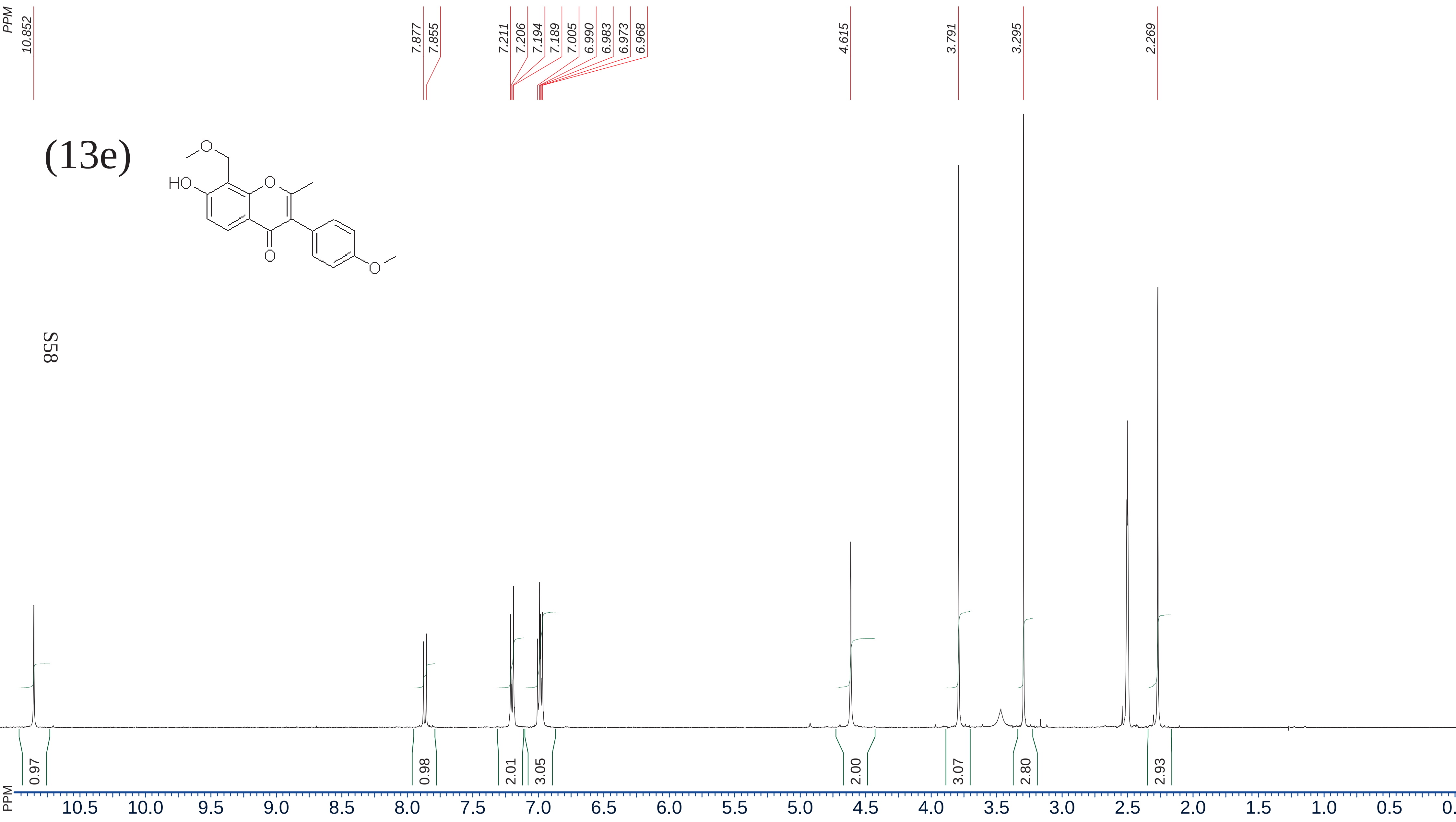

HO
PPM
10.829
8.404
7.990
7.968
7.538
7.516
7.057
7.035
7.001
6.979
4.625
3.794
0.94
0.90
0.92
2.00
3.06
2.00
3.01
PPM
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

(13d)

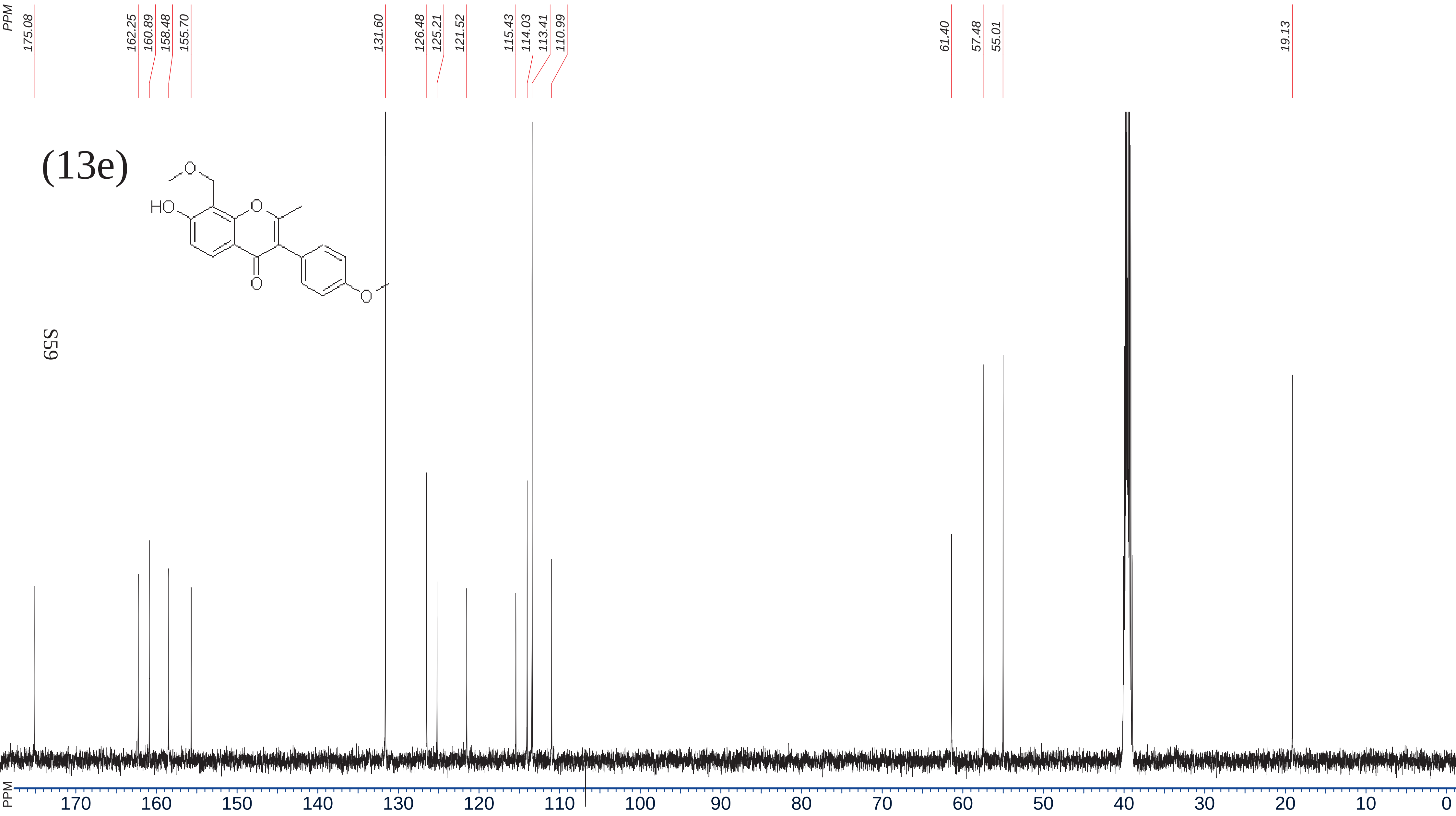


PPM
174.71
161.10
158.92
156.16
153.03
130.01
126.70
124.13
122.95
116.53
114.45
113.55
111.24
61.37
57.45
55.07
HO
O
PPM
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

(13e)

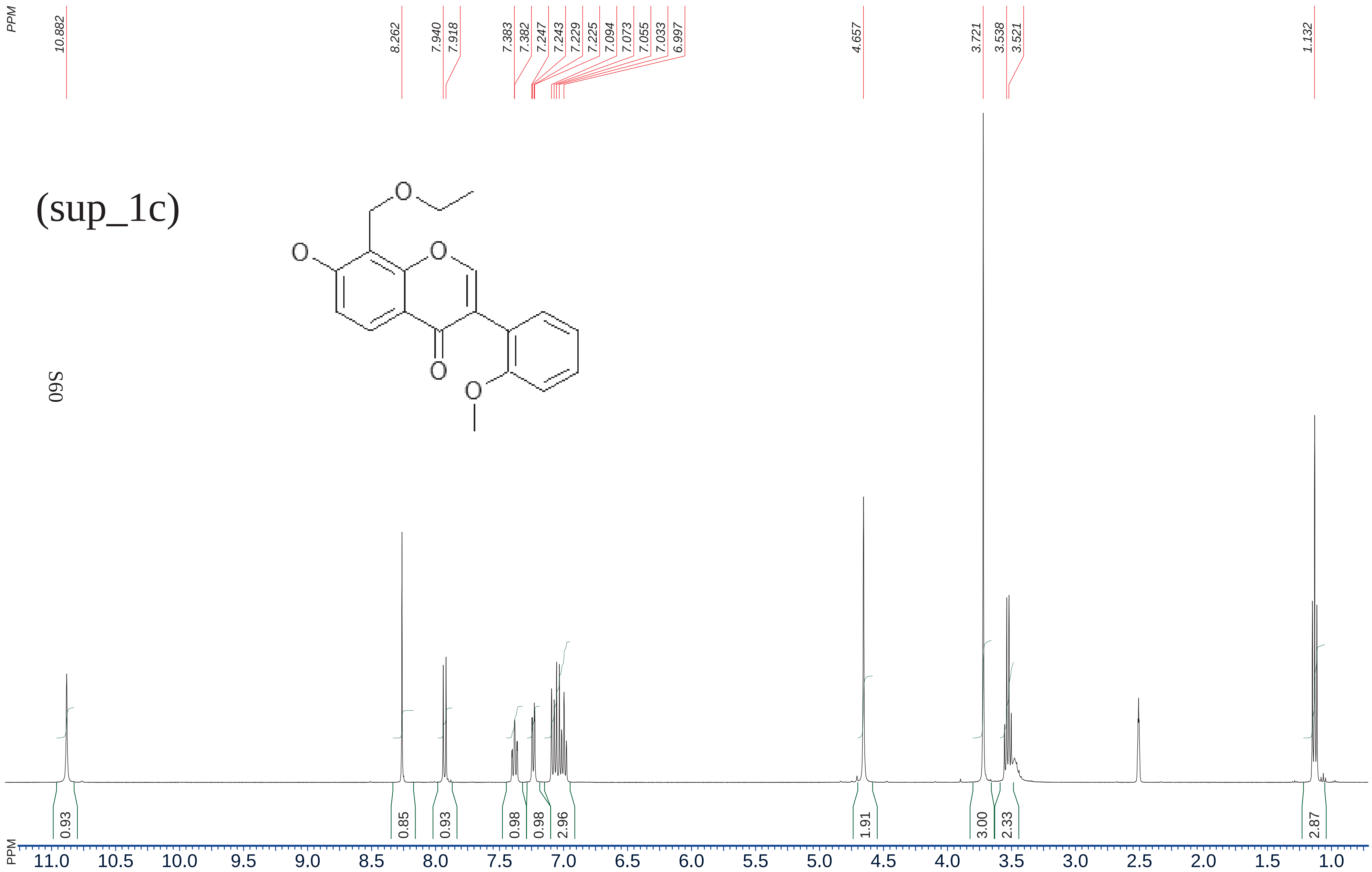

PPM
10.852
7.877
7.855
7.211
7.206
7.194
7.189
7.005
6.990
6.983
6.973
6.968
4.615
3.791
3.295
2.269
HO
O
0.97
0.98
2.01
3.05
2.00
3.07
2.80
2.93
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

(13e)

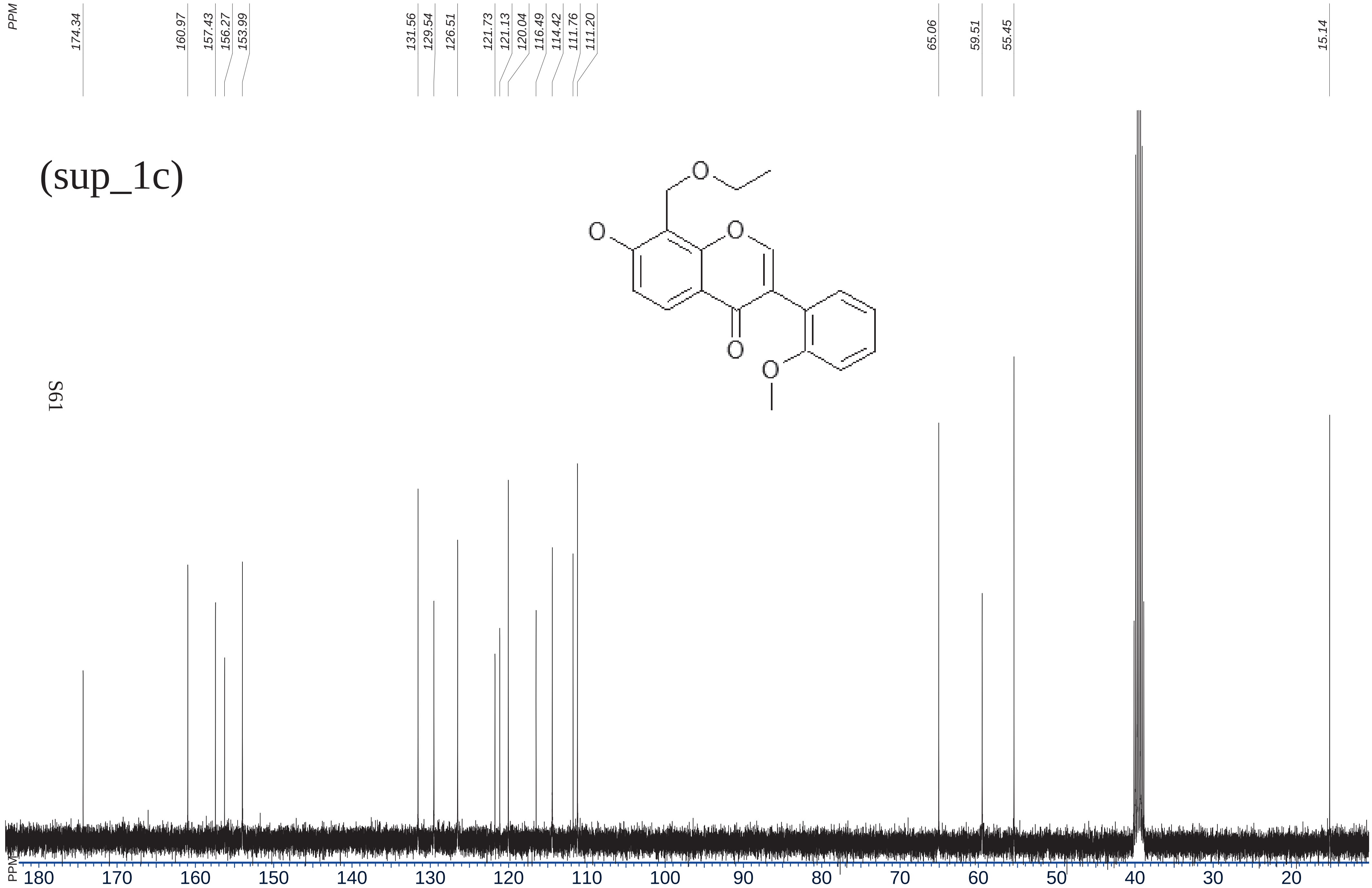


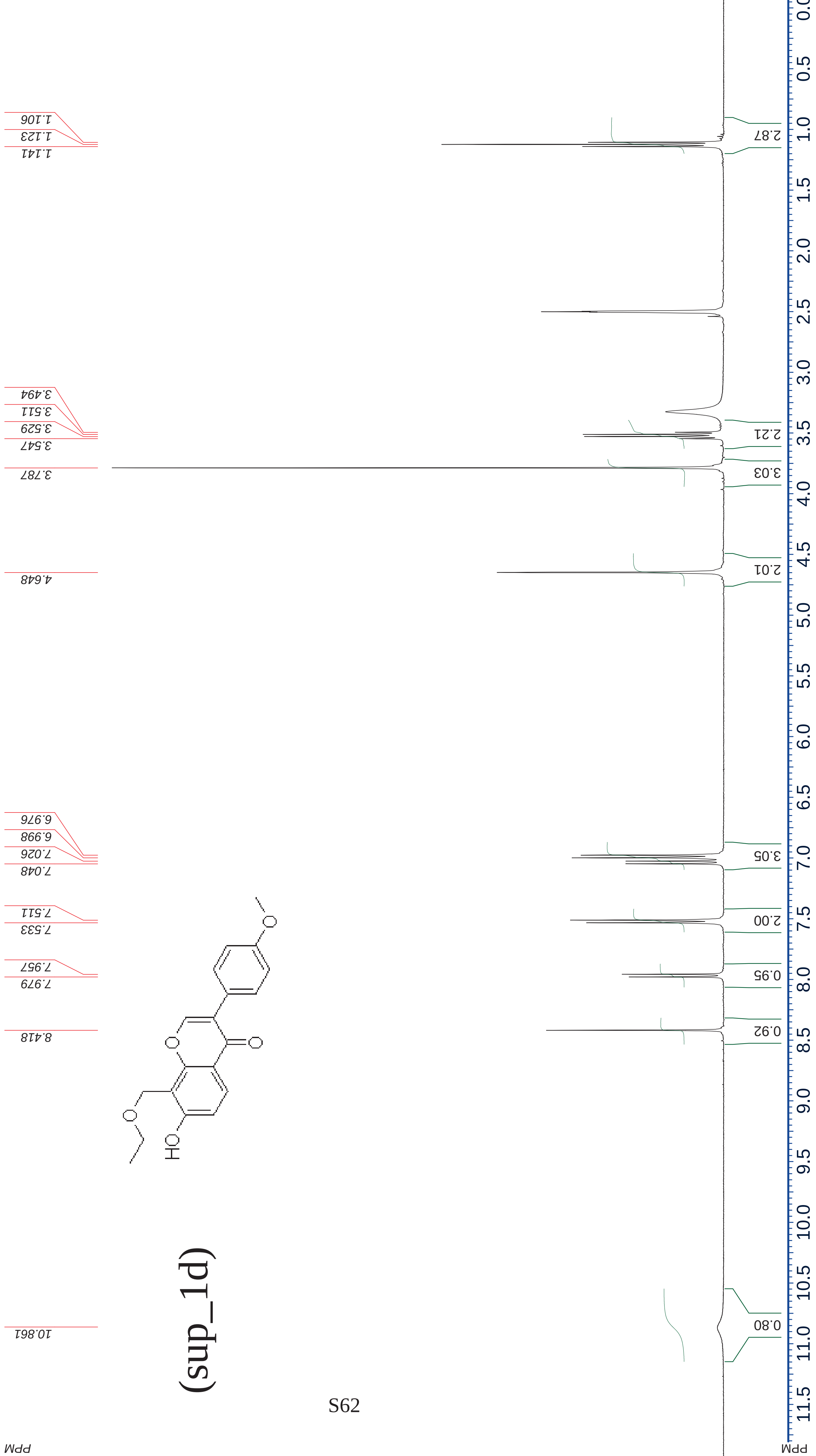
PPM
175.08
162.25
160.89
158.48
155.70
131.60
126.48
125.21
121.52
115.43
114.03
113.41
110.99
61.40
57.48
55.01
19.13
HO
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
PPM

(sup_1c)


PPM
10.882
8.262
7.940
7.918
7.383
7.382
7.247
7.243
7.229
7.225
7.094
7.073
7.055
7.033
6.997
4.657
3.721
3.538
3.521
1.132
0.93
0.85
0.93
0.98
0.98
2.96
1.91
3.00
2.33
2.87
PPM
11.0
10.5
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

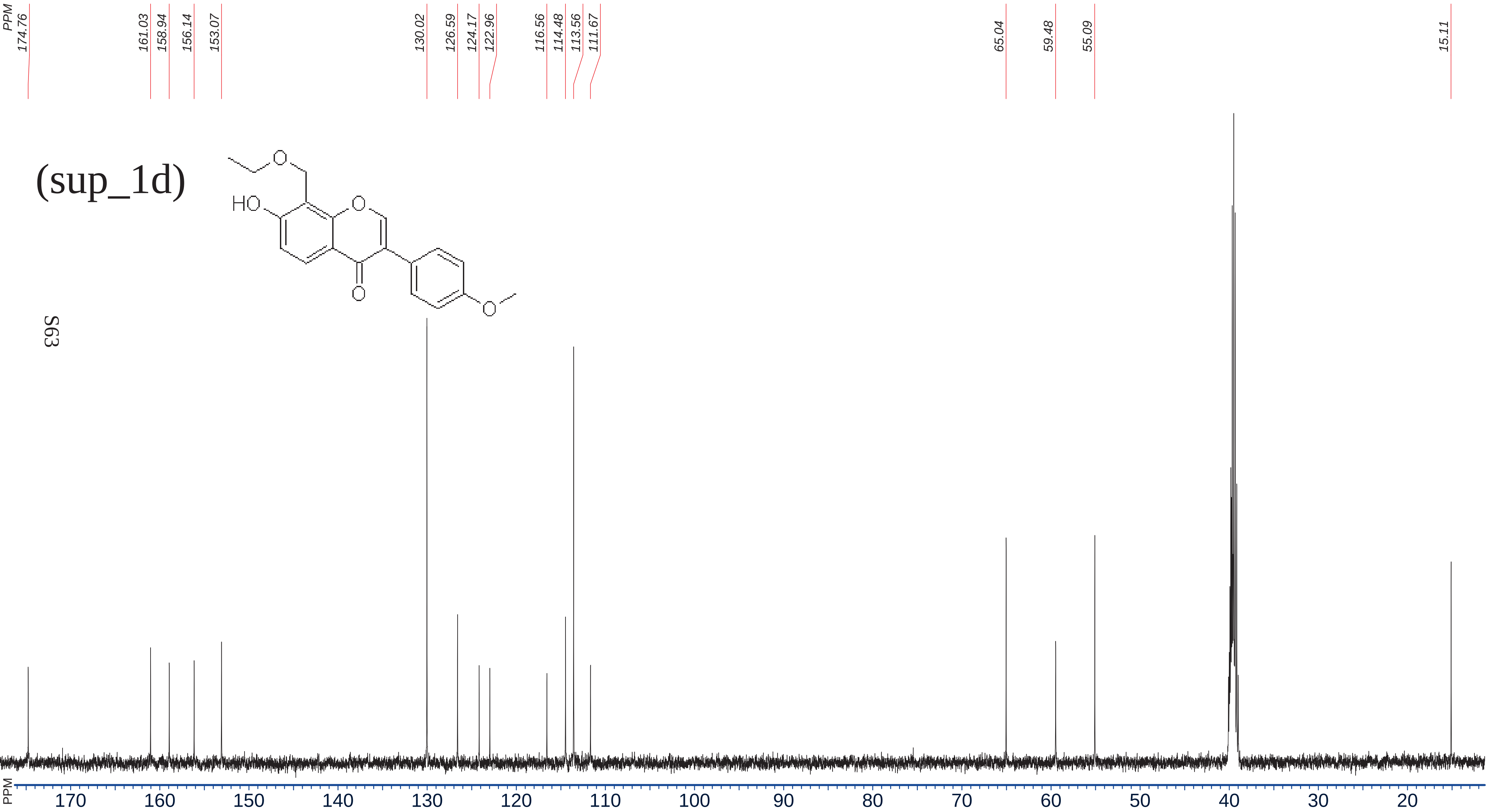
(sup_1c)


PPM
174.34
160.97
157.43
156.27
153.99
131.56
129.54
126.51
121.73
121.13
120.04
116.49
114.42
111.76
111.20
65.06
59.51
55.45
15.14
O
O
O
O
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
PPM

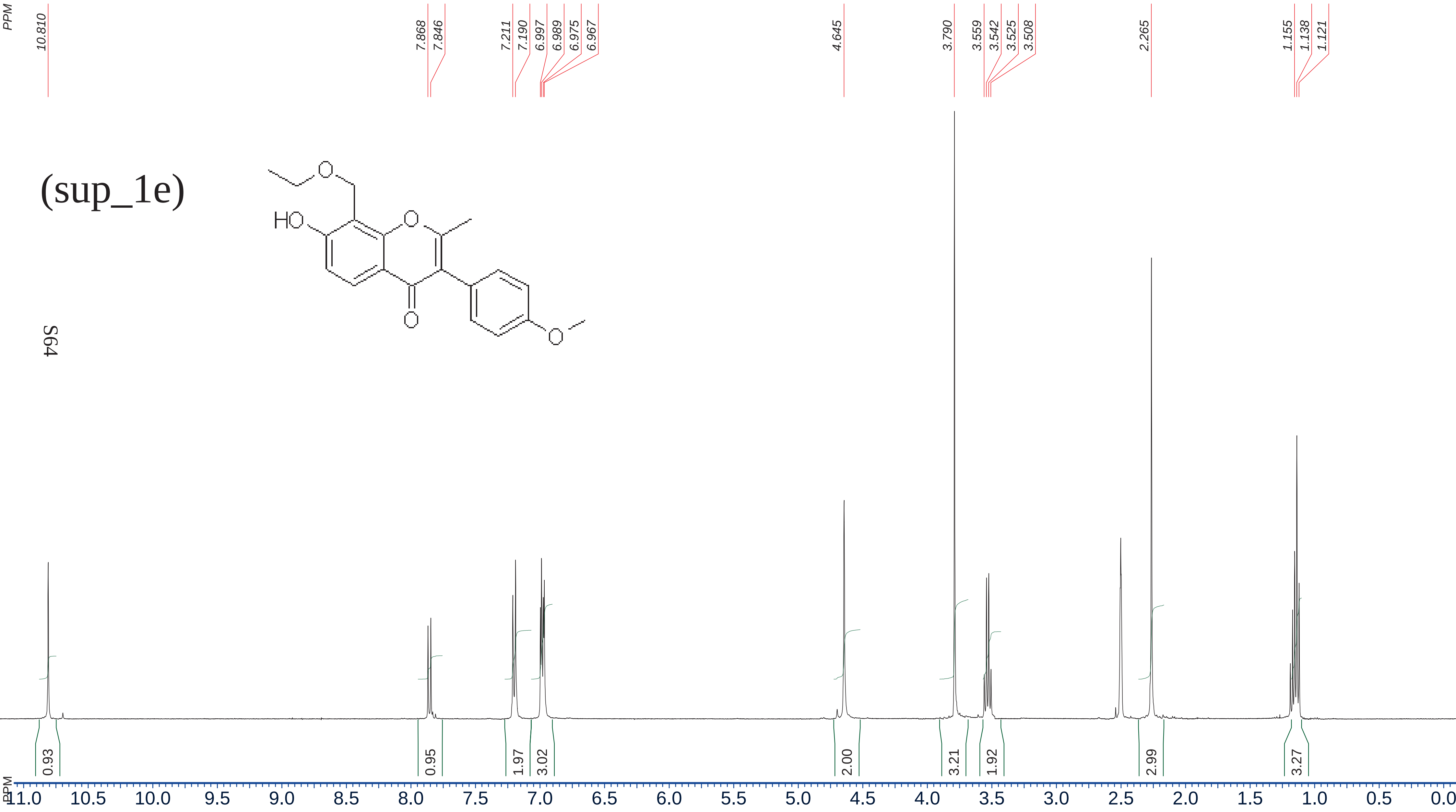

1.106
1.123
1.141
3.494
3.511
3.529
3.547
3.787
4.648
6.976
6.998
7.026
7.048
7.511
7.533
7.957
7.979
8.418
10.861
2.87
2.21
3.03
2.01
3.05
2.00
0.95
0.92
0.80
PPM
OH

(sup_1d)

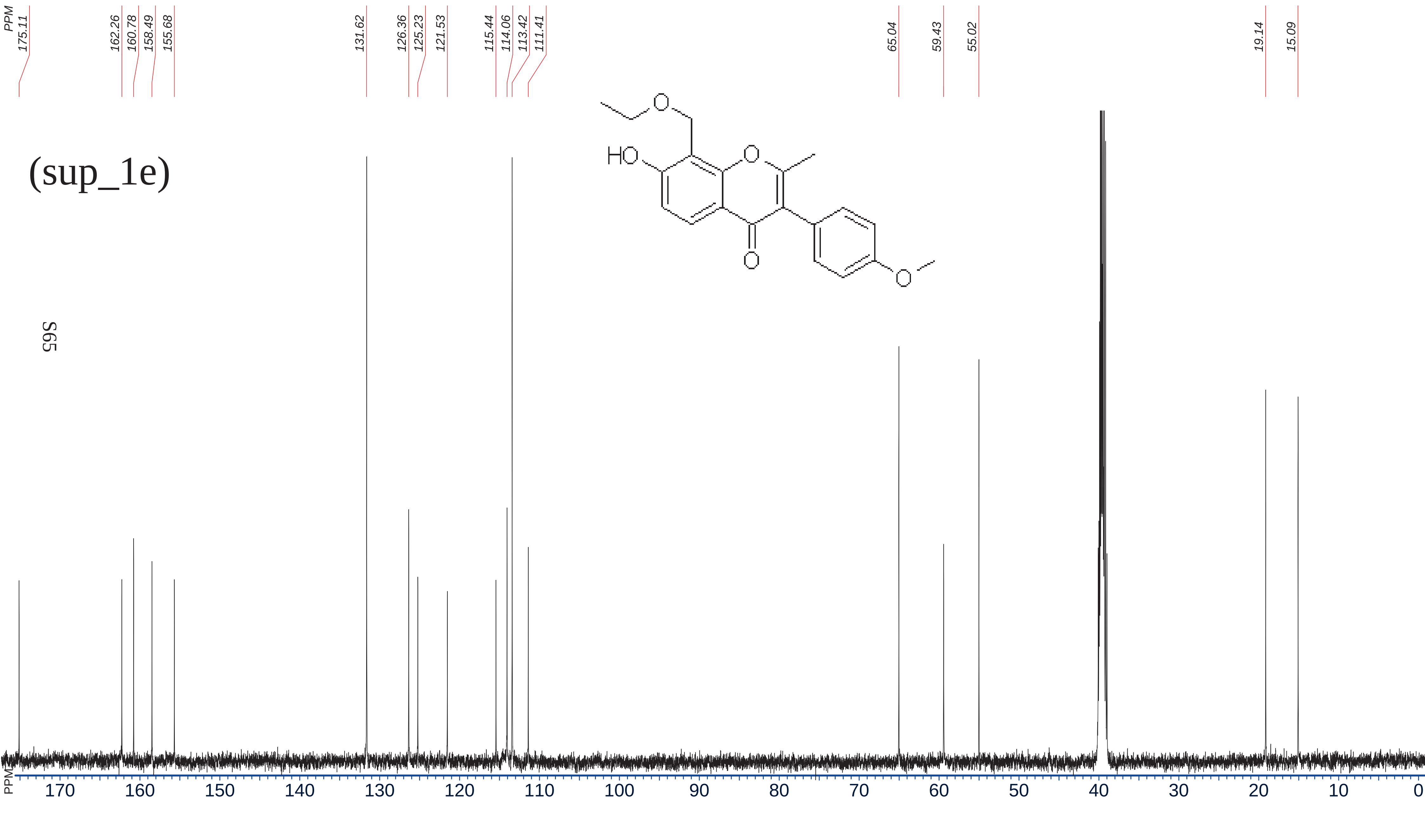
(sup_1d)

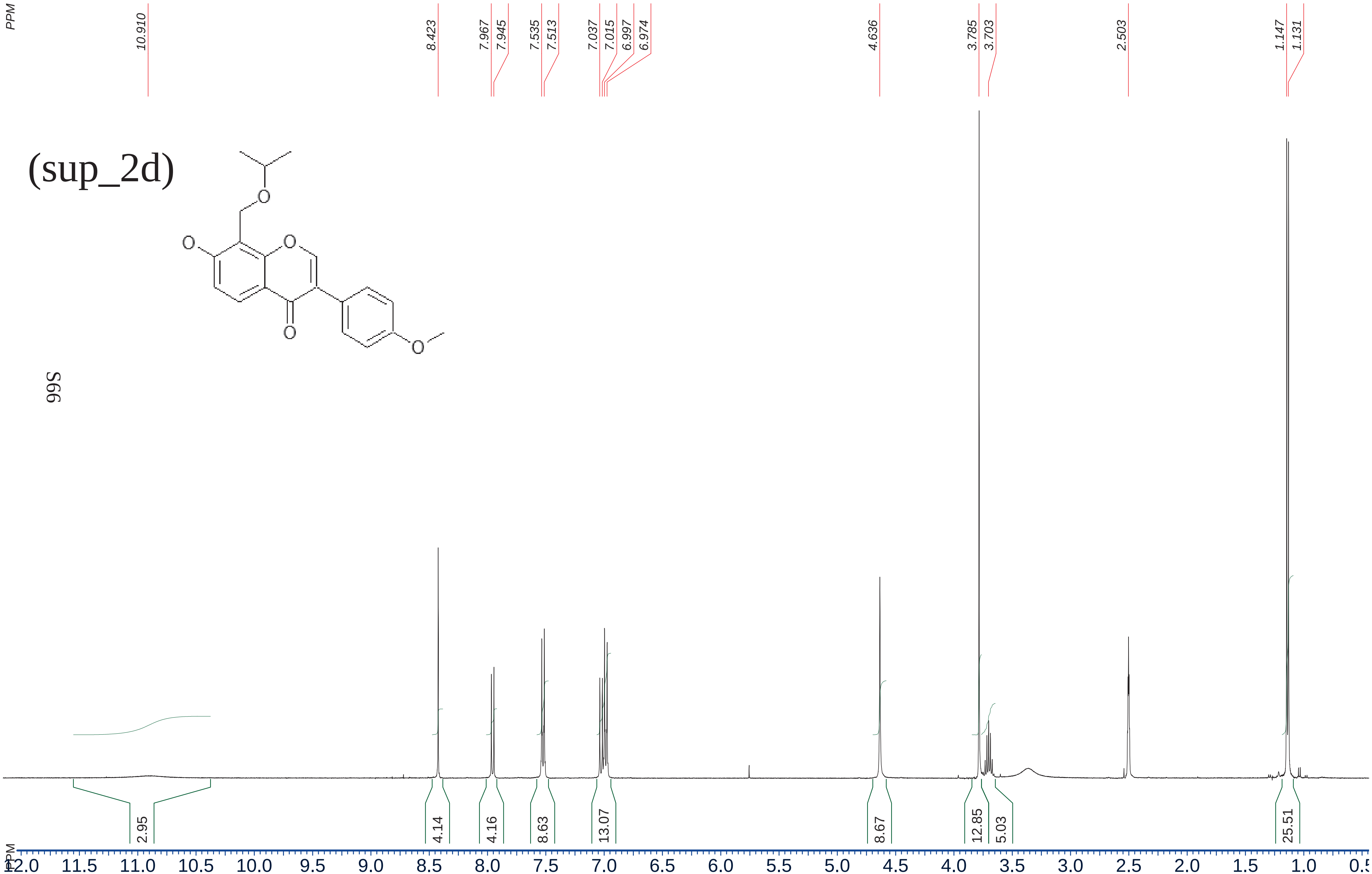

PPM
174.76
161.03
158.94
156.14
153.07
130.02
126.59
124.17
122.96
116.56
114.48
113.56
111.67
65.04
59.48
55.09
15.11
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
PPM

(sup_1e)


PPM
10.810
7.868
7.846
7.211
7.190
6.997
6.989
6.975
6.967
4.645
3.790
3.559
3.542
3.525
3.508
2.265
1.155
1.138
1.121
HO
O
0.93
0.95
1.97
3.02
2.00
3.21
1.92
2.99
3.27
11.0 10.5 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

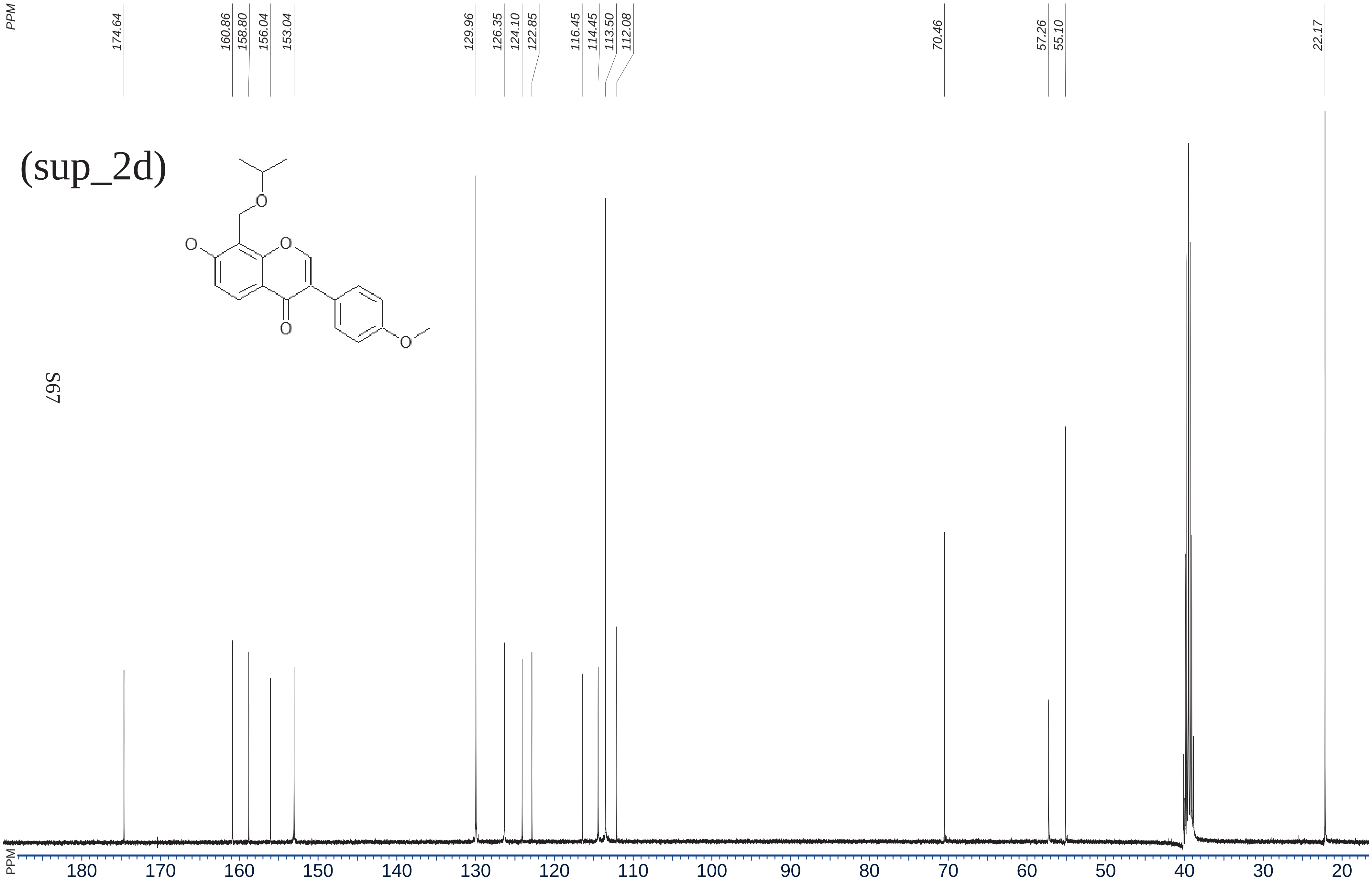
(sup_1e)


PPM
175.11
162.26
160.78
158.49
155.68
131.62
126.36
125.23
121.53
115.44
114.06
113.42
111.41
65.04
59.43
55.02
19.14
15.09
HO
O
O
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM

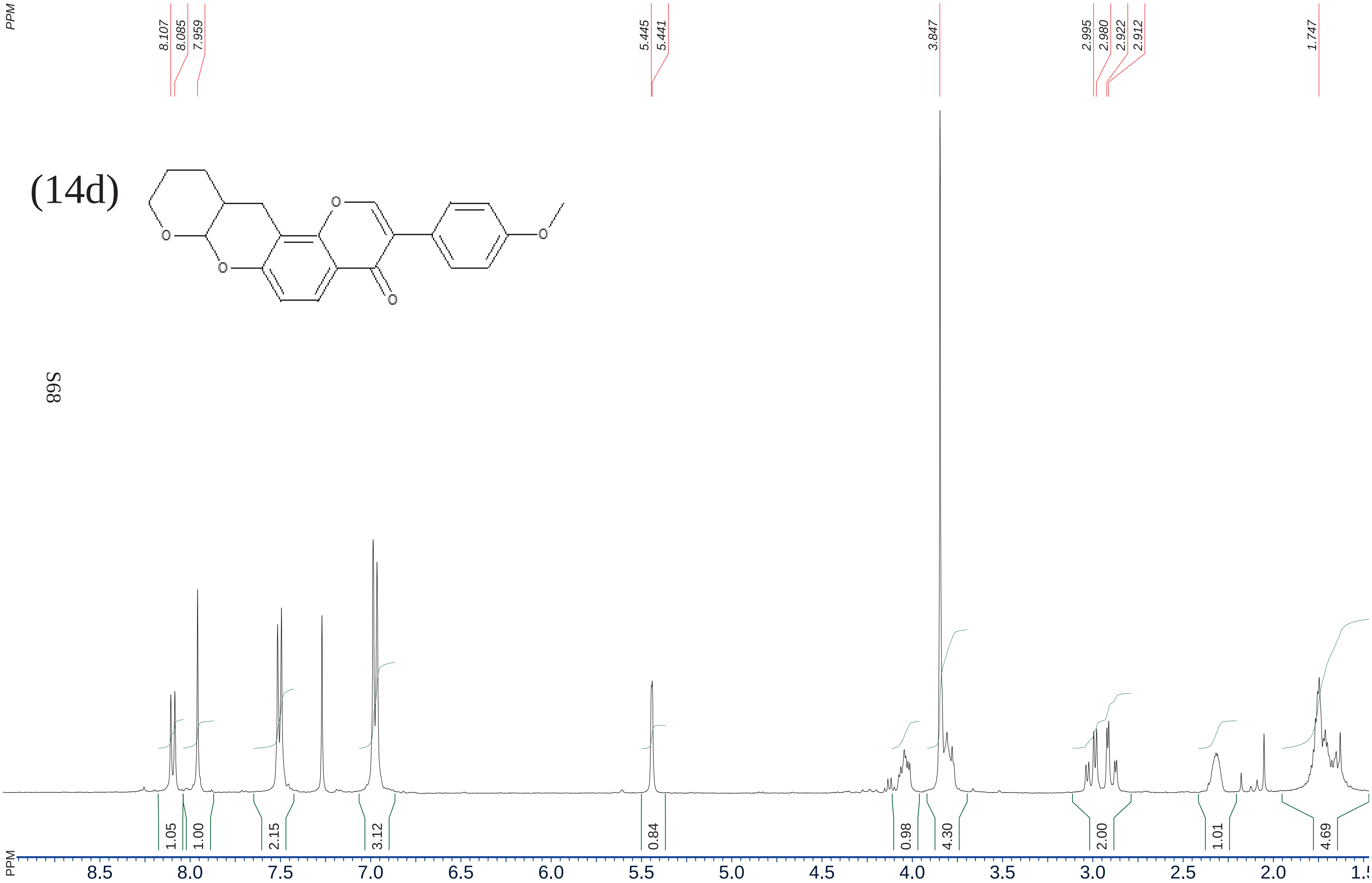

PPM
10.910
8.423
7.967
7.945
7.535
7.513
7.037
7.015
6.997
6.974
4.636
3.785
3.703
2.503
1.147
1.131
2.95
4.14
4.16
8.63
13.07
8.67
12.85
5.03
25.51
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
PPM

(sup_2d)

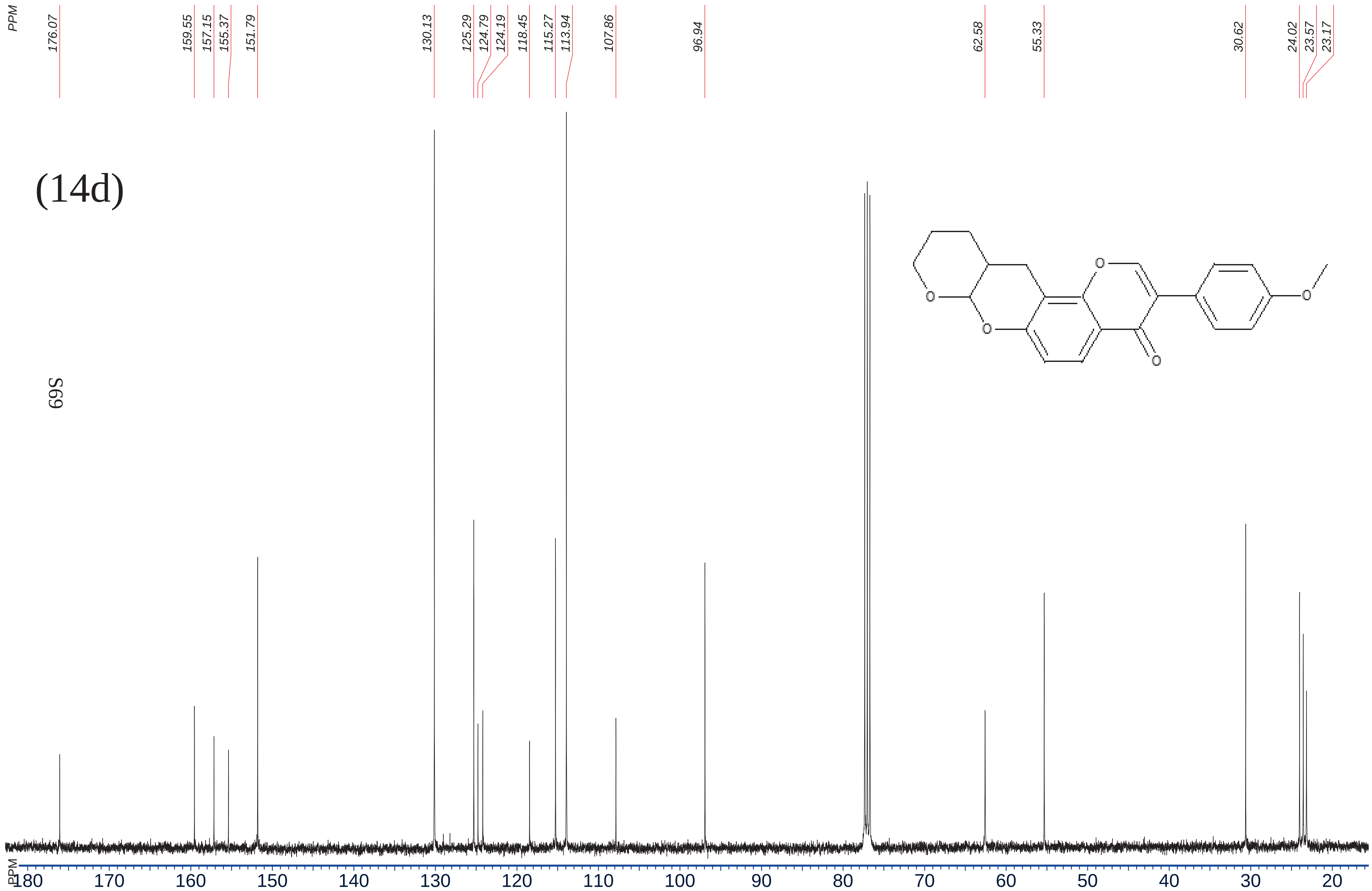
(sup_2d)


PPM
174.64
160.86
158.80
156.04
153.04
129.96
126.35
124.10
122.85
116.45
114.45
113.50
112.08
70.46
57.26
55.10
22.17
PPM
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20

(14d)


PPM
8.107
8.085
7.959
5.445
5.441
3.847
2.995
2.980
2.922
2.912
1.747
1.05
1.00
2.15
3.12
0.84
0.98
4.30
2.00
1.01
4.69
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
PPM

(14d)



PPM
176.07
159.55
157.15
155.37
151.79
130.13
125.29
124.79
124.19
118.45
115.27
113.94
107.86
96.94
62.58
55.33
30.62
24.02
23.57
23.17
O
O
O
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
PPM