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

Electronic Supplementary Information

Divergent Synthesis of Biflavonoids Yields Novel Inhibitors of the Aggregation of Amyloid β (1-42)

Tze Han Sum,[a] Tze Jing Sum,[a] Súil Collins,[a,b] Warren R. J. D. Galloway,[a] David G. Twigg,[a] Florian Hollfelder[b] and David R. Spring*[a]

[a]Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK. Email: spring@ch.cam.ac.uk

[b]Department of Biochemistry, University of Cambridge, 80 Tennis Court Road, Cambridge, CB2 1GA UK.

Contents:

Table ESI 1: Comments on the behaviour of the library compounds in the ThT assay. See manuscript for assay details. See **Figure ESI 1** and **Figure ESI 2** for data.

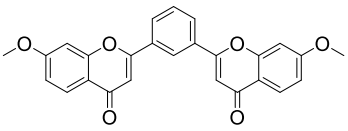
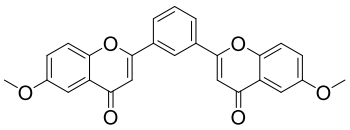
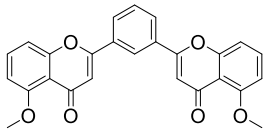
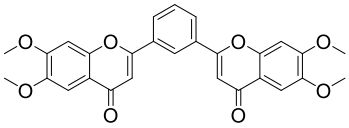
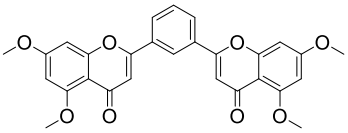
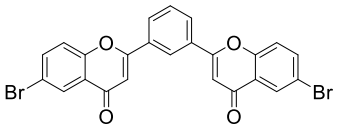
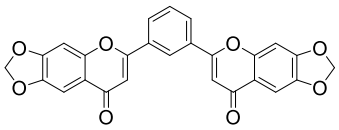
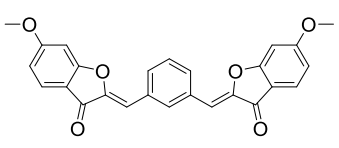
Compound	Comments on behaviour in assay
 **27**	Overly fluorescent
 **28**	Inactive/poor activity
 **29**	Inactive/poor activity
 **30**	Inactive/poor activity
 **31**	Overly fluorescent
 **32**	Inactive/poor activity
 **33**	Moderate activity
 **34**	Moderate activity

Table ESI 1 continued:

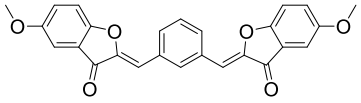
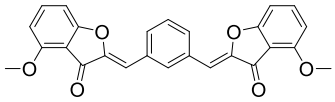
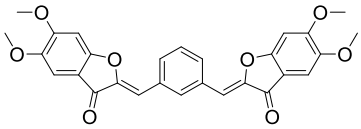
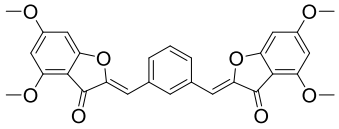
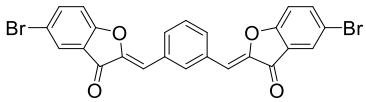
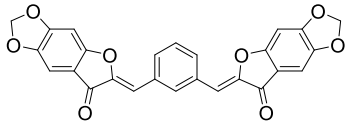
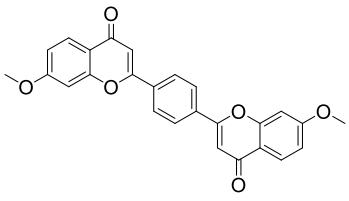
Compound	Comments on behaviour in assay
 **35**	Inactive/poor activity
 **36**	Inactive/poor activity
 **37**	Sparingly soluble
 **38**	Moderate activity
 **39**	Inactive/poor activity
 **40**	Inactive/poor activity
 **46**	Inactive/ poor activity

Table ESI 1 continued:

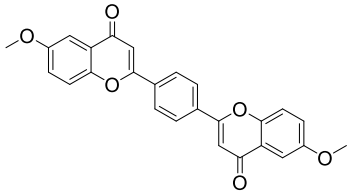
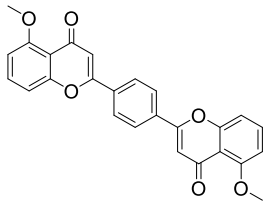
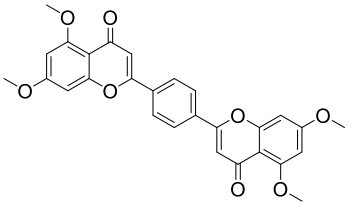
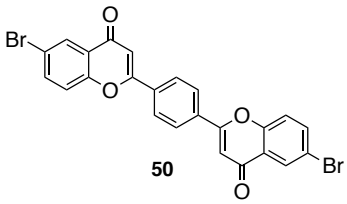
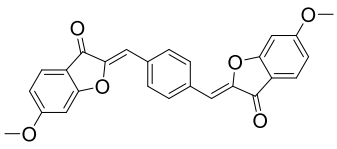
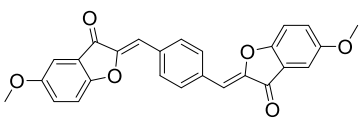
Compound	Comments on behaviour in assay
 **47**	Inactive/poor activity
 **48**	Inactive/poor activity
 **49**	Overly fluorescent
 **50**	Inactive/poor activity
 **51**	Moderate activity
 **52**	Moderate activity

Table ESI 1 continued:

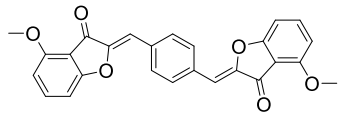
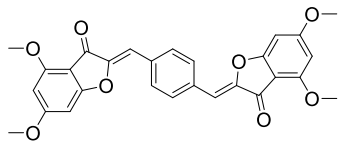
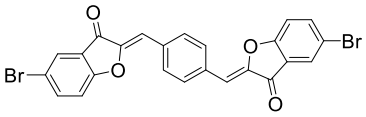
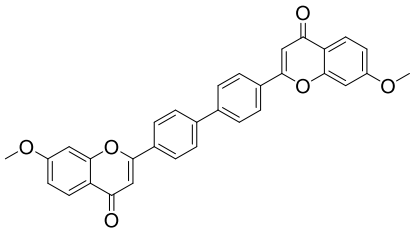
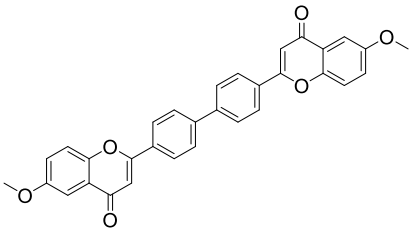
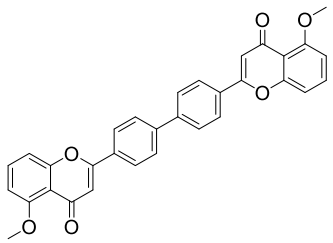
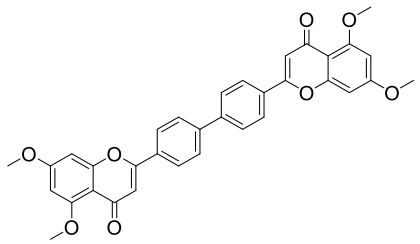
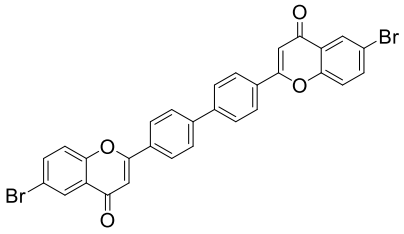
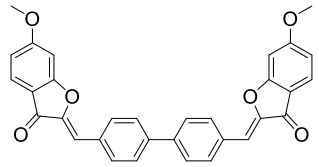
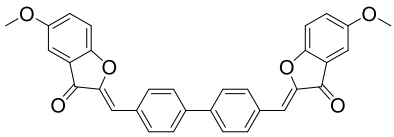
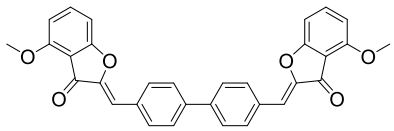
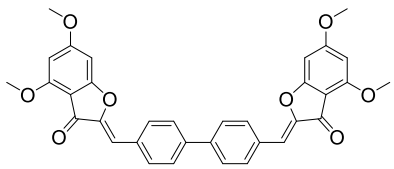
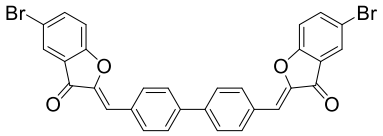
Compound	Comments on behaviour in assay
 **53**	Inactive/poor activity
 **54**	Sparingly soluble
 **55**	Moderate activity
 **61**	Overly fluorescent
 **62**	Inactive/poor activity
 **63**	Inactive/poor activity

Table ESI 1 continued:

Compound	Comments on behaviour in assay
 **64**	Overly fluorescent
 **65**	Overly fluorescent
 **66**	Moderate activity
 **67**	Moderate activity
 **68**	Moderate activity
 **69**	Sparingly soluble
 **70**	Moderate activity

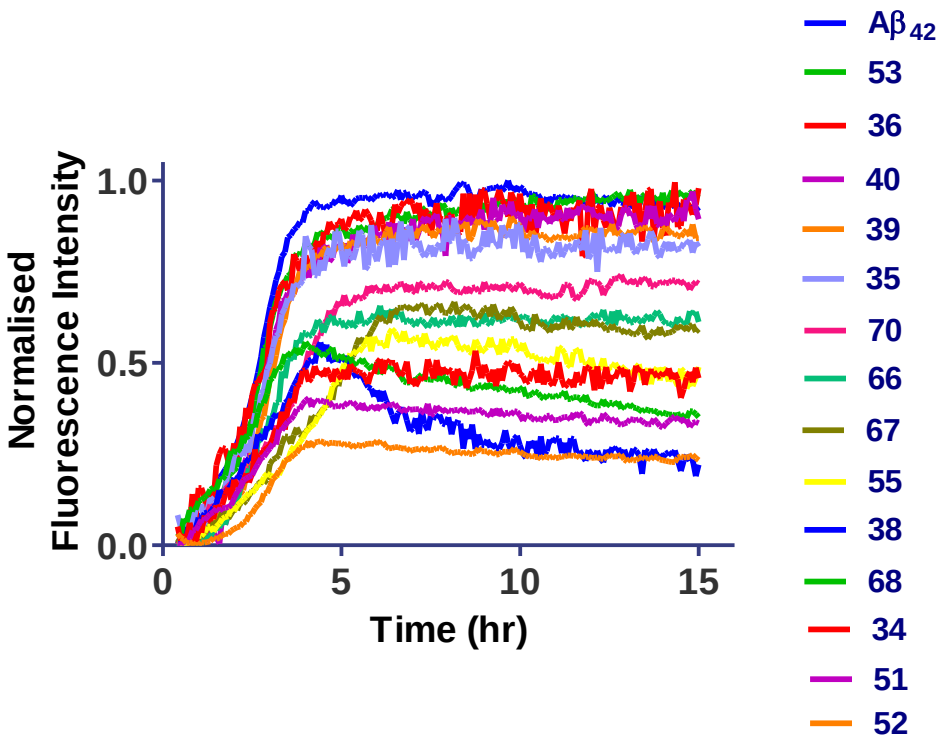


Figure ESI 1: $A\beta_{42}$ aggregation profiles in the ThT assay with the addition of biaurones (50 µM). $A\beta_{42}$ curve represent the time course of $A\beta_{42}$ aggregation alone (initial concentration of 10 µM $A\beta_{42}$ peptide).

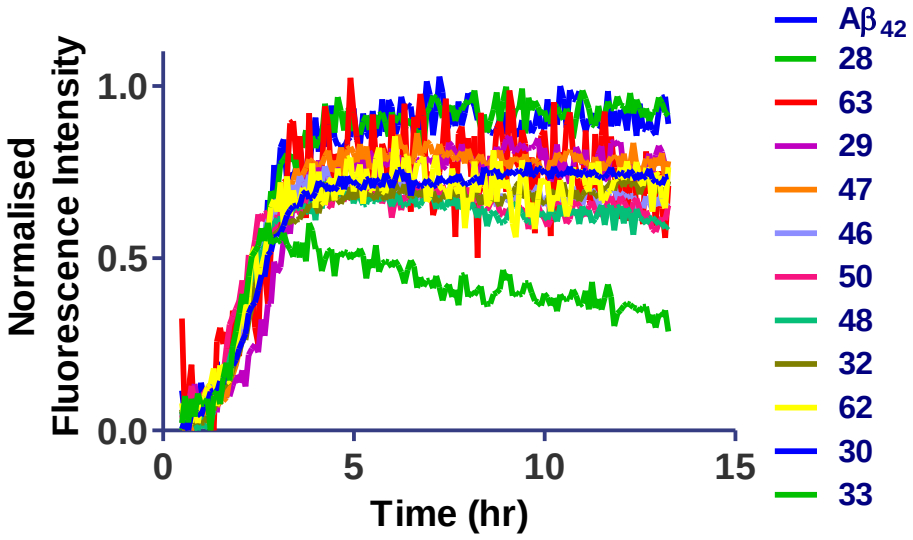
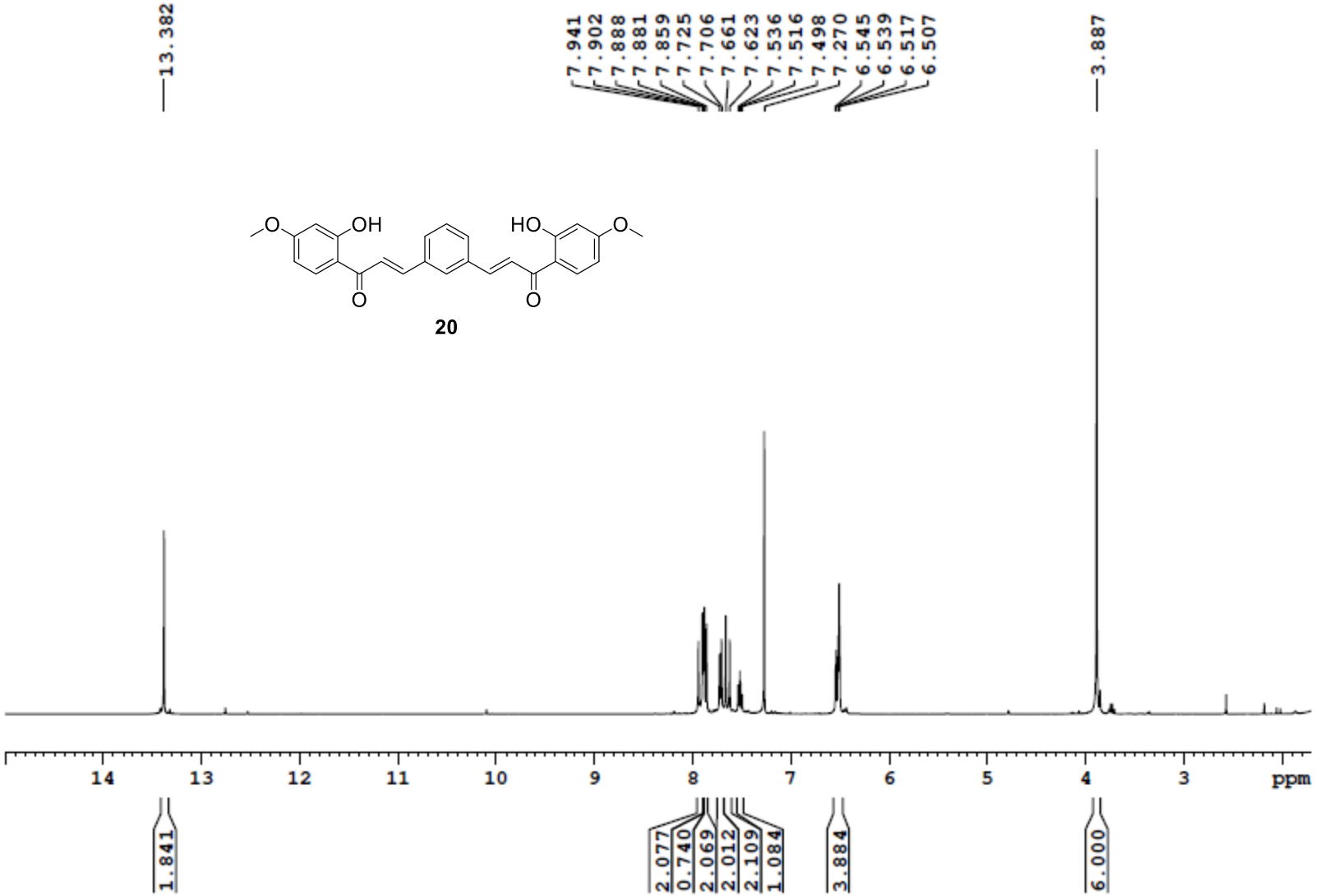


Figure ESI 2: $A\beta_{42}$ aggregation profiles in the ThT assay with the addition of biflavones (50 µM). $A\beta_{42}$ curve represent the time course of $A\beta_{42}$ aggregation alone (initial concentration of 10 µM $A\beta_{42}$ peptide). Overly fluorescent compounds have been omitted.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7.881
7.859
7.725
7.706
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7.623
7.536
7.516
7.498
7.270
6.545
6.539
6.517
6.507
3.887
O
OH
HO
O
O
O
20
14
13
12
11
10
9
8
7
6
5
4
3
ppm
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0.740
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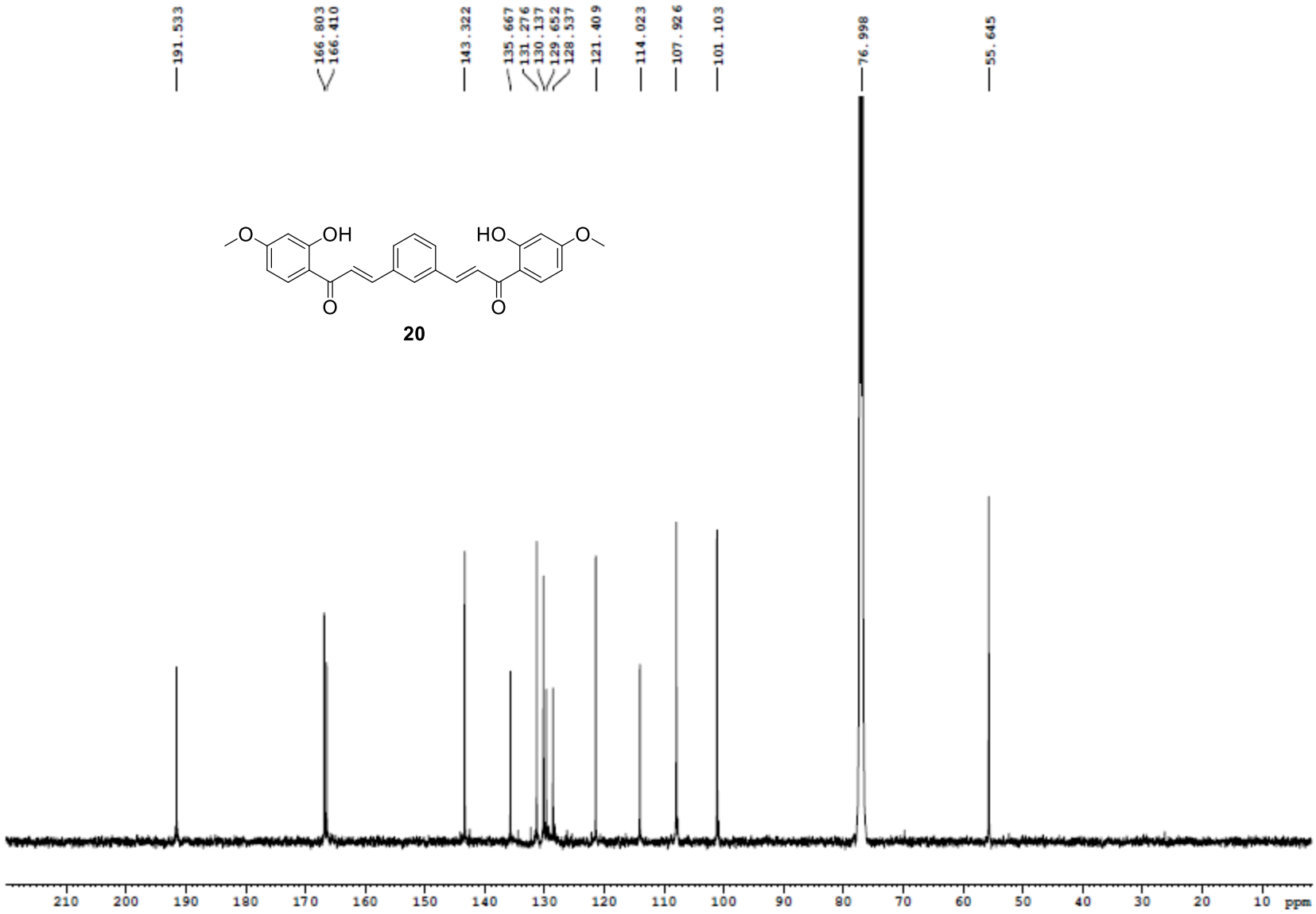
2.012
2.109
1.084
3.884
6.000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101.103
76.998
55.645
OH
HO
O
O
O
O
20
210
200
190
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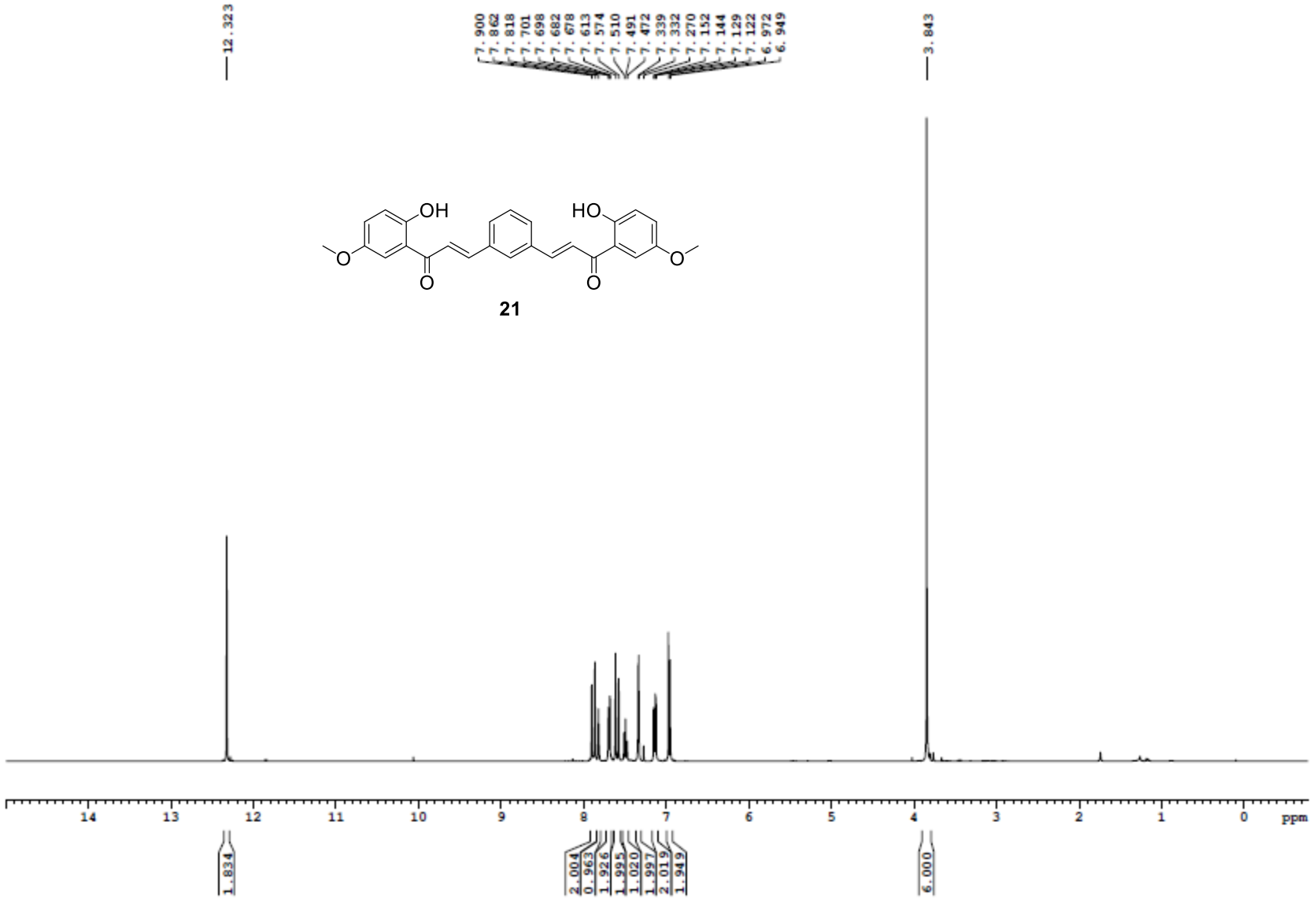
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.900
7.862
7.818
7.701
7.698
7.682
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7.472
7.339
7.332
7.270
7.152
7.144
7.129
7.122
6.972
6.949
3.843
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HO
O
O
O
O
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14
13
12
11
10
9
8
7
6
5
4
3
2
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1.020
1.997
2.019
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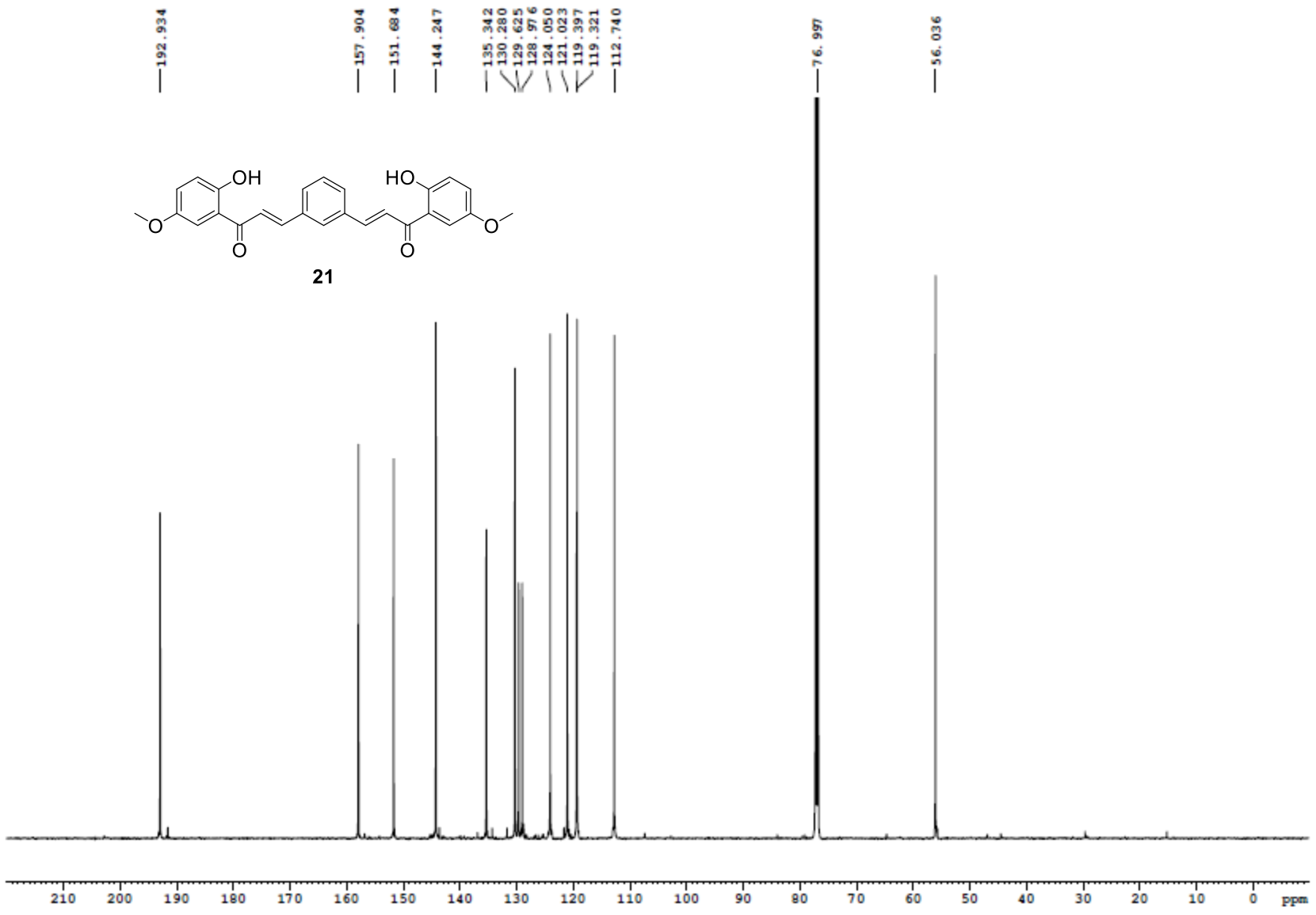
6.000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157.904
151.684
144.247
135.342
130.280
129.625
128.976
124.050
121.023
119.397
119.321
112.740
76.997
56.036
OH
HO
O
O
O
O
21
210
200
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140
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120
110
100
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80
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60
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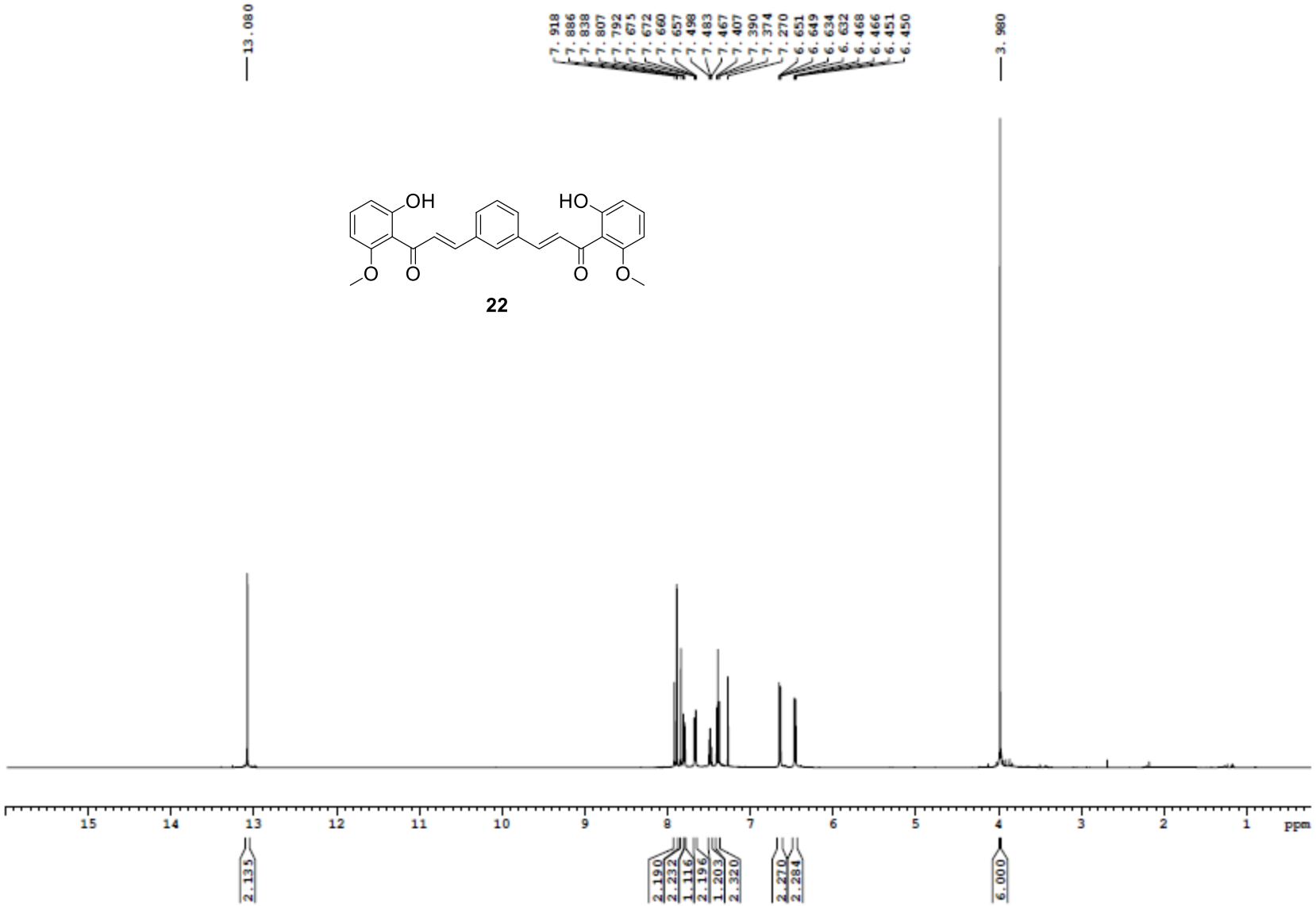
20
10
0
ppm


13.080
7.918
7.886
7.838
7.807
7.792
7.675
7.672
7.660
7.657
7.498
7.483
7.467
7.407
7.390
7.374
7.270
6.651
6.649
6.634
6.632
6.468
6.466
6.451
6.450
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HO
O
O
O
O
22
15
14
13
12
11
10
9
8
7
6
5
4
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2.284
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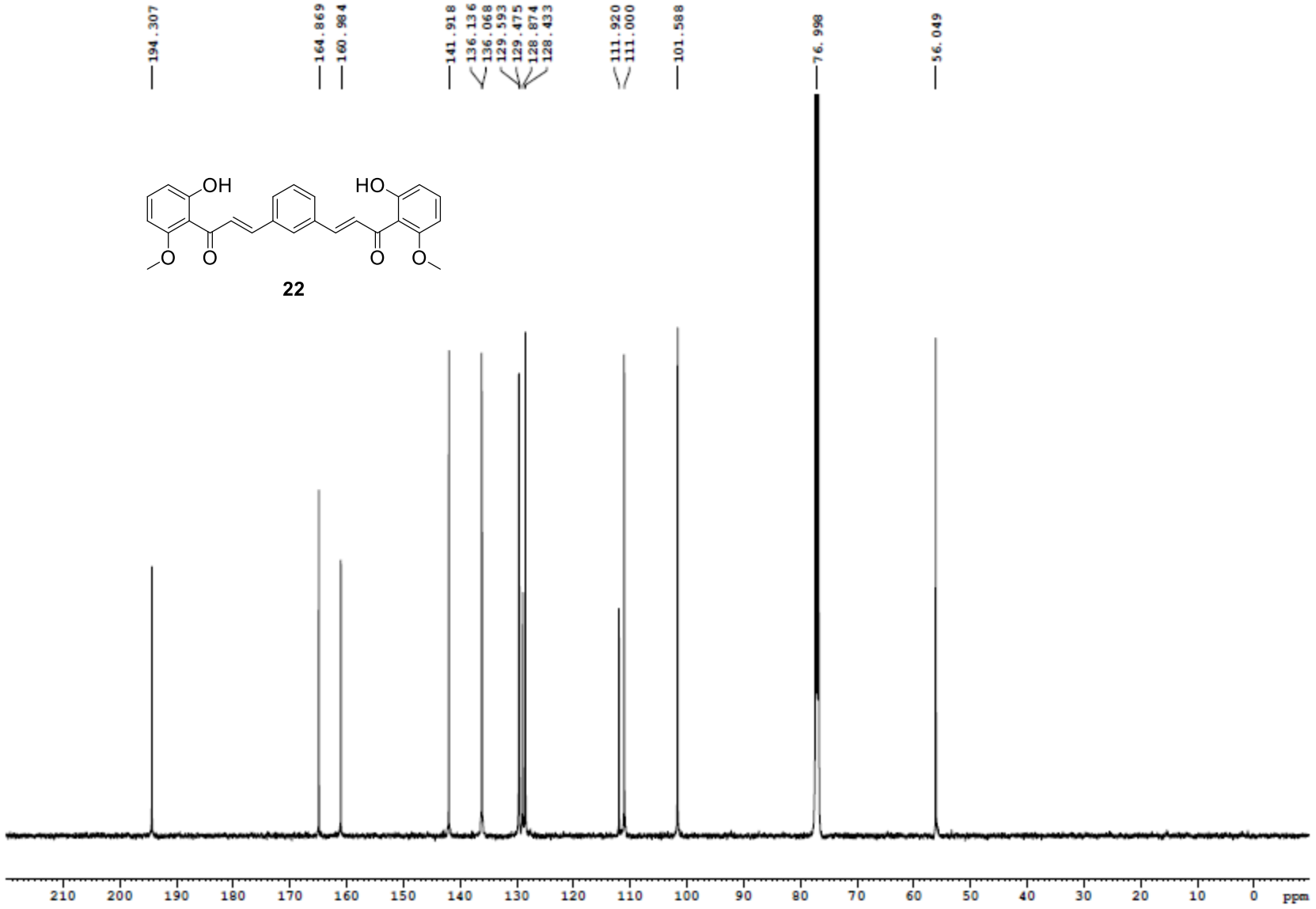
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164.869
160.984
141.918
136.136
136.068
129.593
129.475
128.874
128.433
111.920
111.000
101.588
76.998
56.049
OH
HO
O
O
O
O
22
210
200
190
180
170
160
150
140
130
120
110
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90
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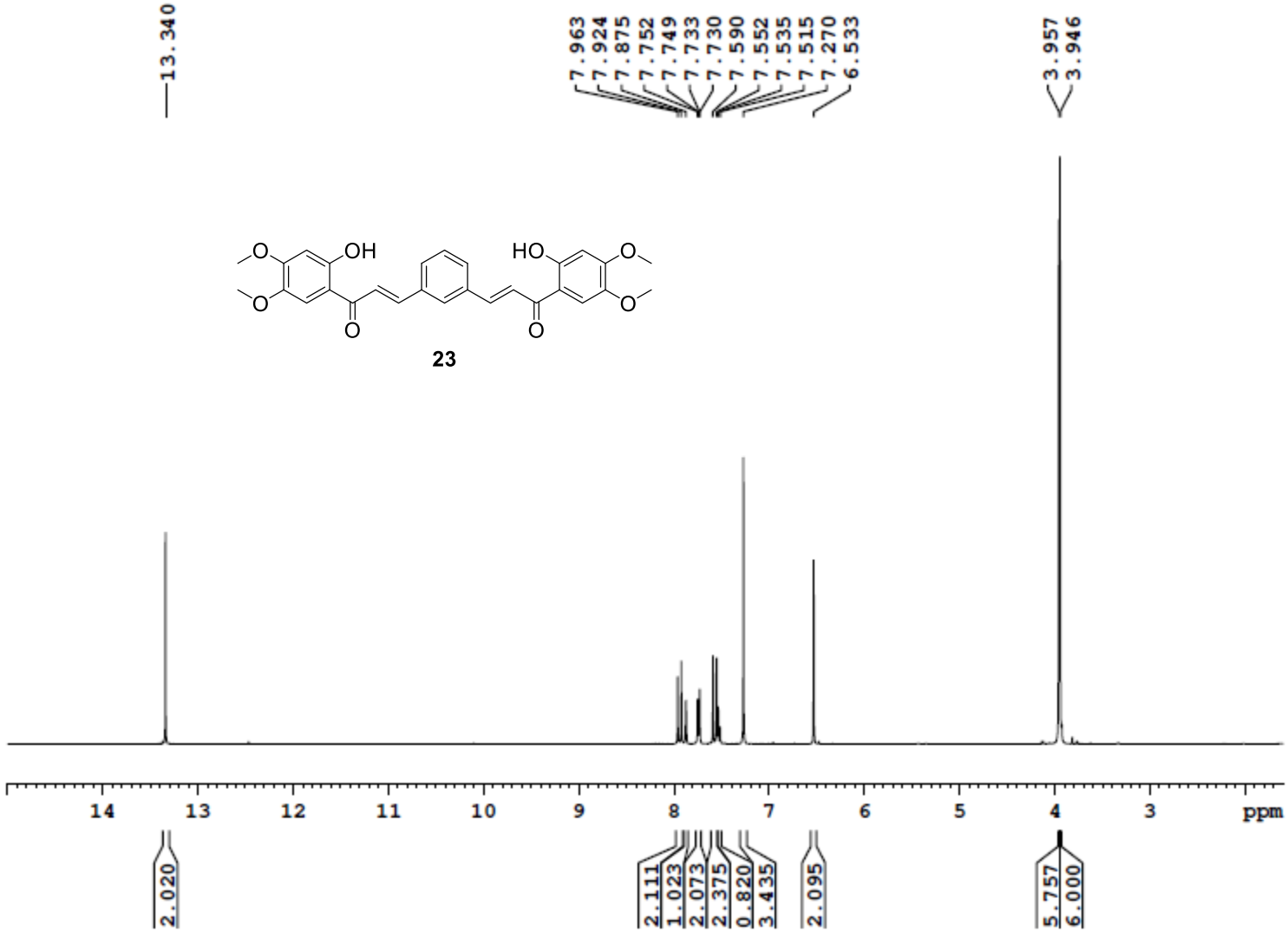
70
60
50
40
30
20
10
0
ppm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13
12
11
10
9
8
7
6
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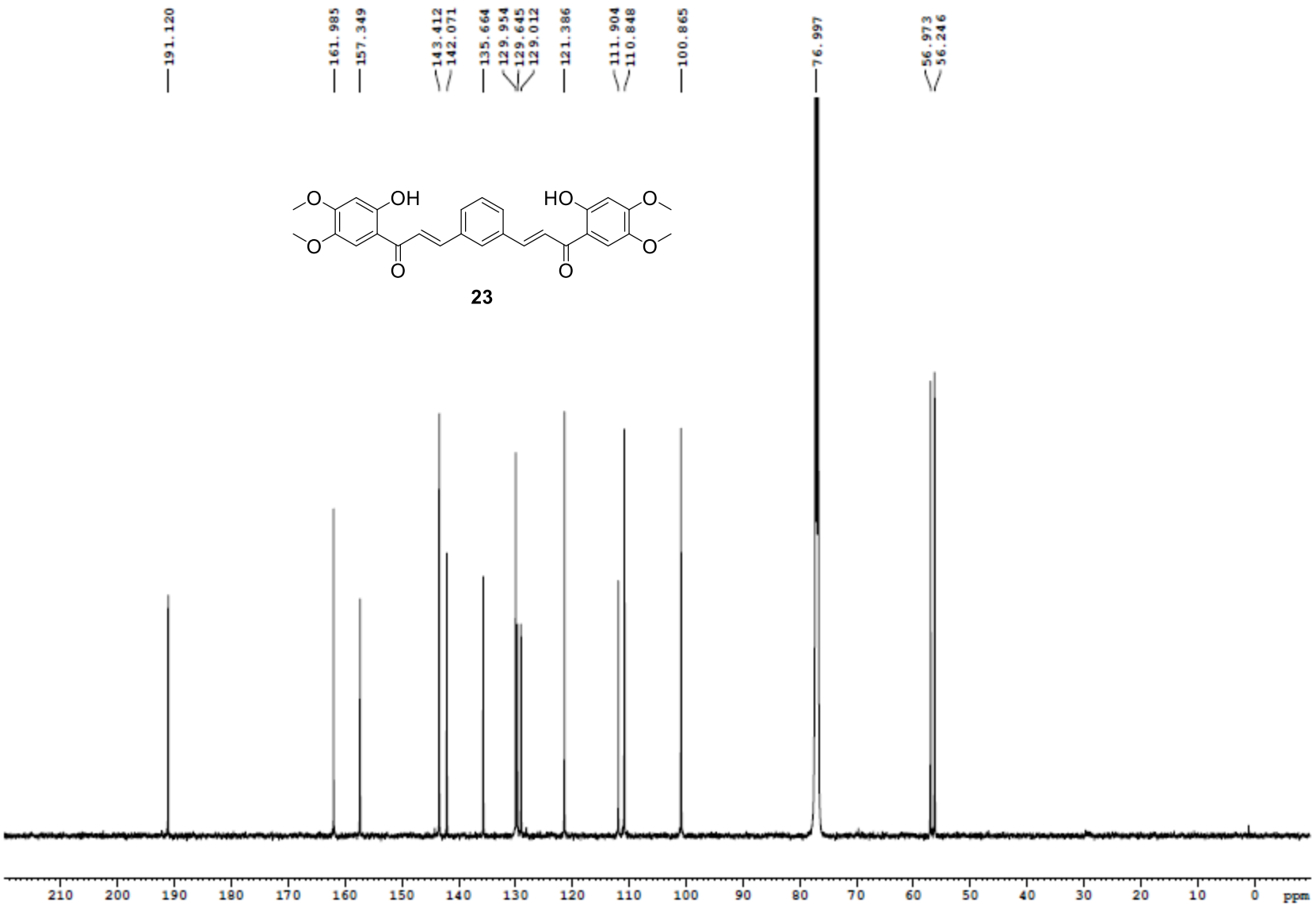
6.000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157.349
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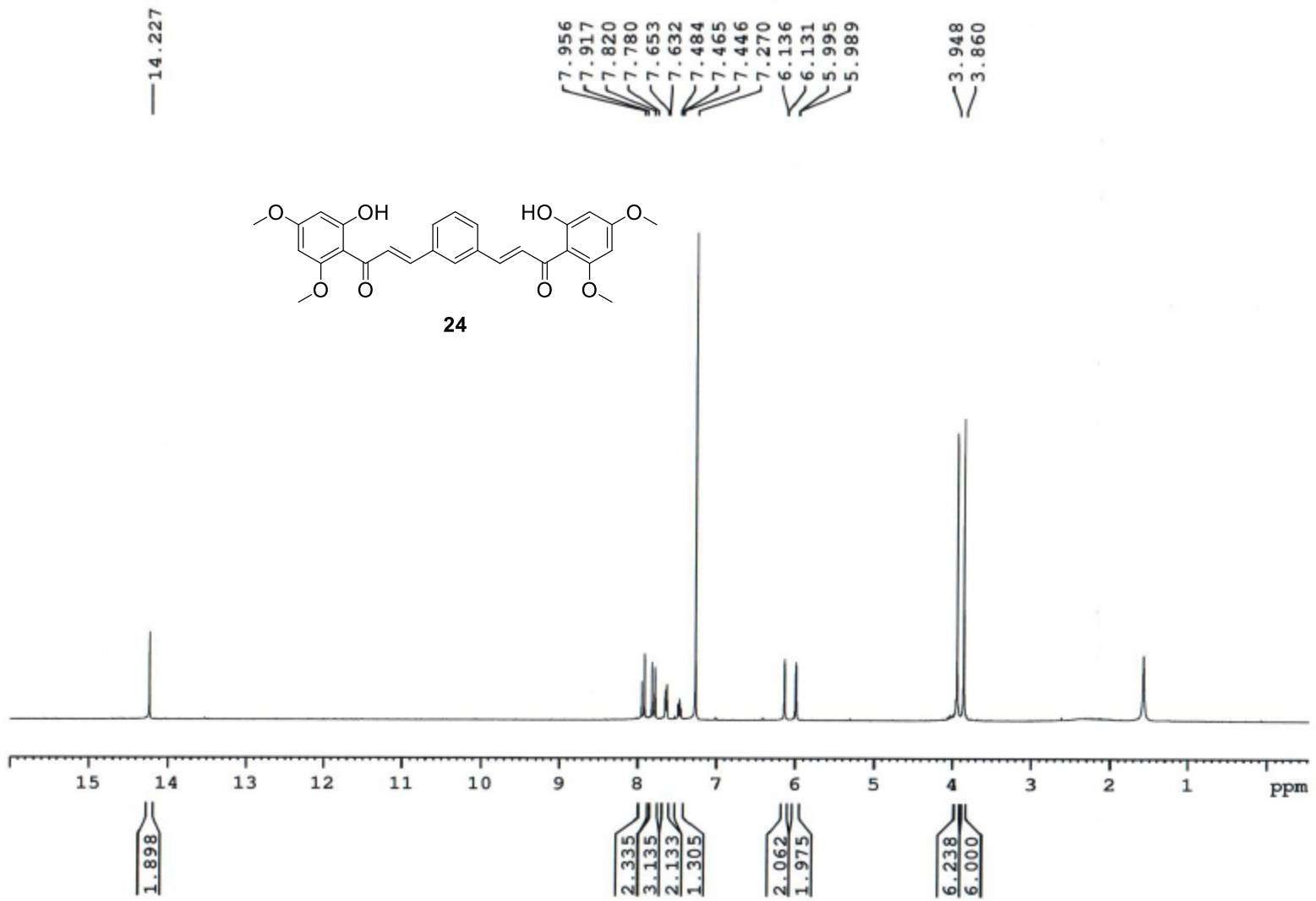
100.865
76.997
56.973
56.246
OH
HO
O
O
O
O
O
O
23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.632
7.484
7.465
7.446
7.270
6.136
6.131
5.995
5.989
3.948
3.860
O
OH
HO
O
O
O
O
O
24
15
14
13
12
11
10
9
8
7
6
5
4
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ppm
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3.135
2.133
1.305
2.062
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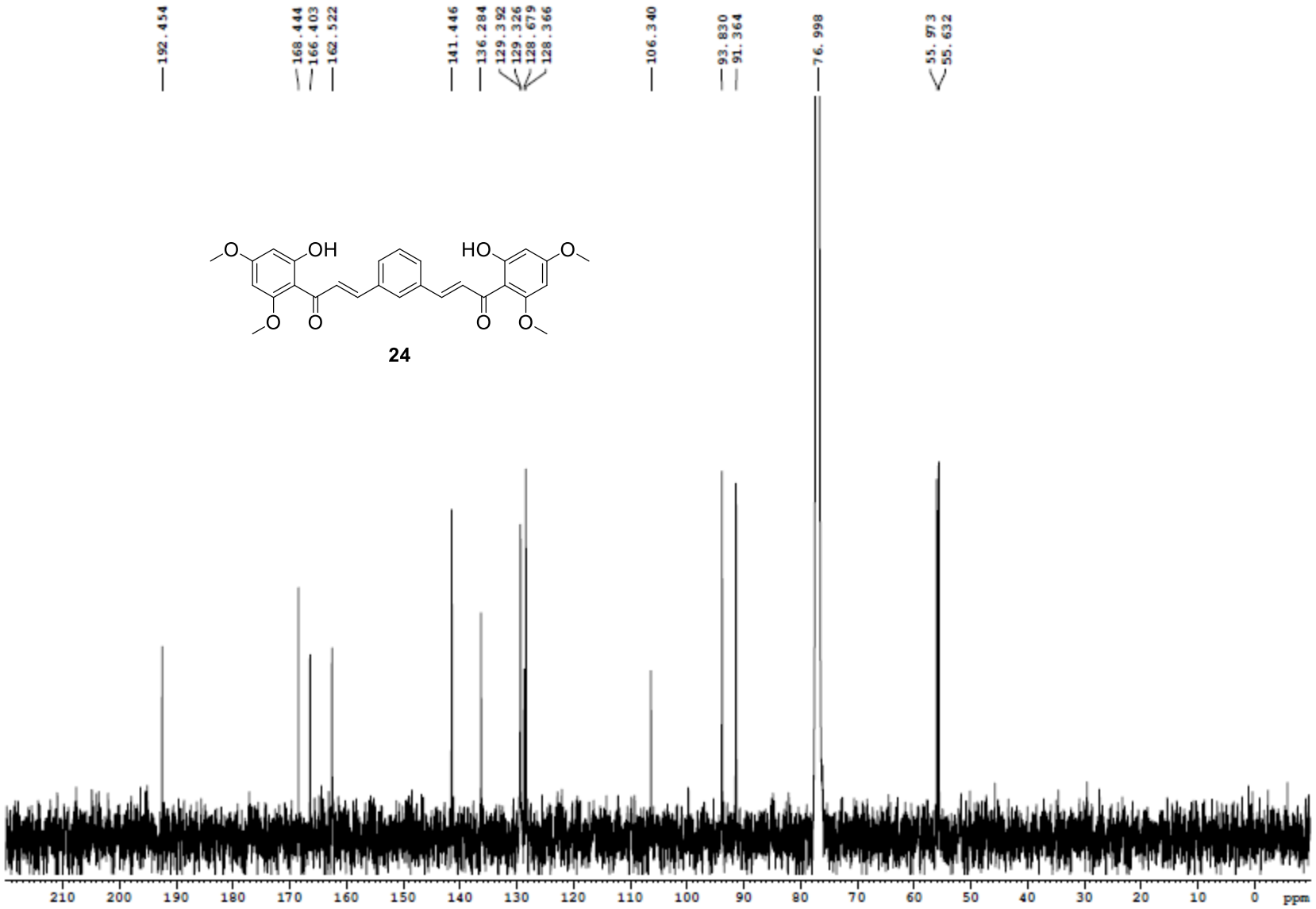
6.238
6.000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129.392
129.326
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91.364
76.998
55.973
55.632
O
OH
HO
O
O
O
O
O
24
210
200
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140
130
120
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100
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60
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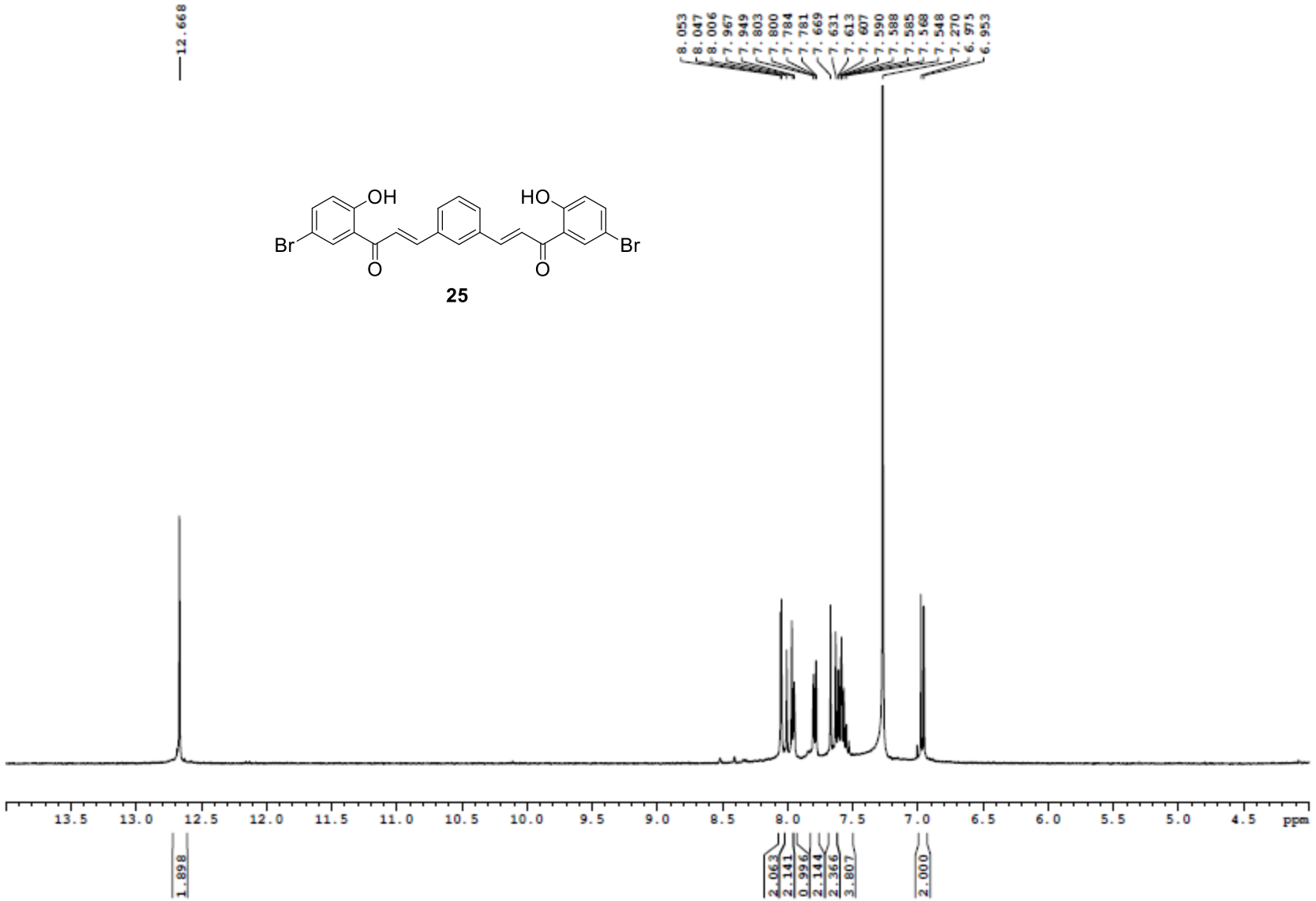
ppm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7.800
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7.781
7.669
7.631
7.613
7.607
7.590
7.588
7.585
7.568
7.548
7.270
6.975
6.953
OH
HO
Br
Br
O
O
25
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13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.5
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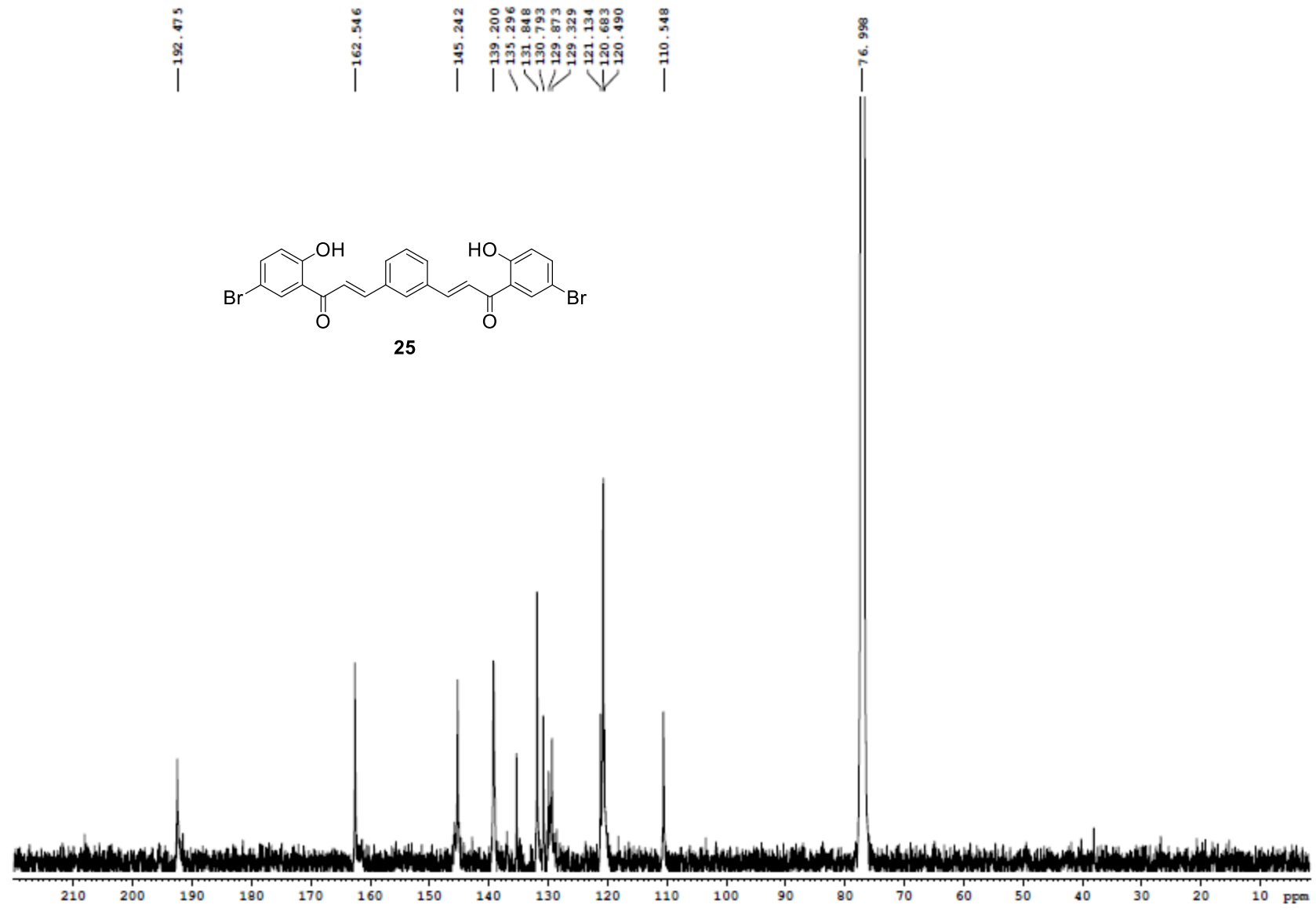
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130.793
129.873
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120.683
120.490
110.548
76.998
OH
HO
Br
Br
O
O
25
210
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150
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110
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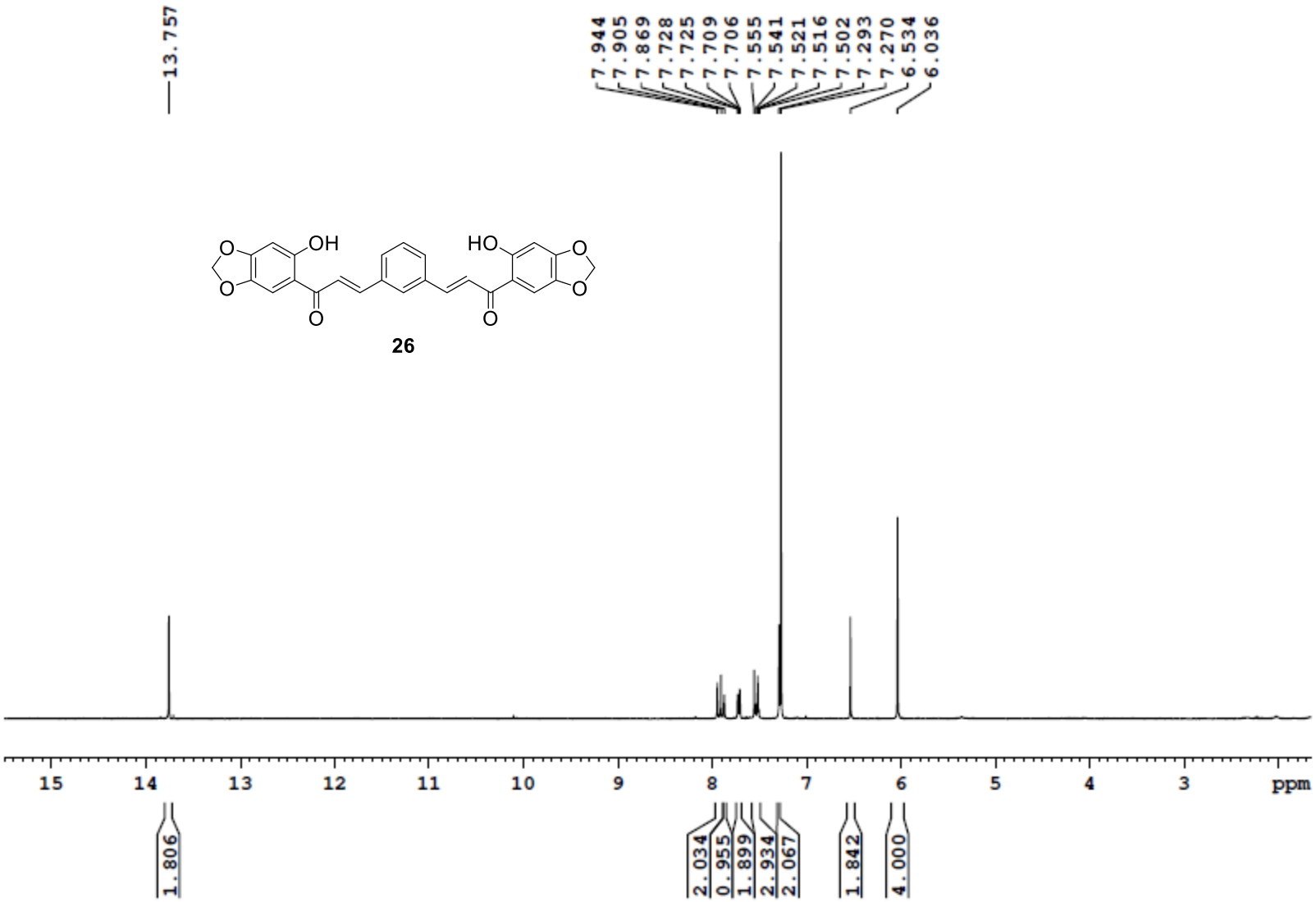
10
ppm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7.905
7.869
7.728
7.725
7.709
7.706
7.555
7.541
7.521
7.516
7.502
7.293
7.270
6.534
6.036
OH
HO
O
O
O
O
O
O
26
15
14
13
12
11
10
9
8
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3
ppm
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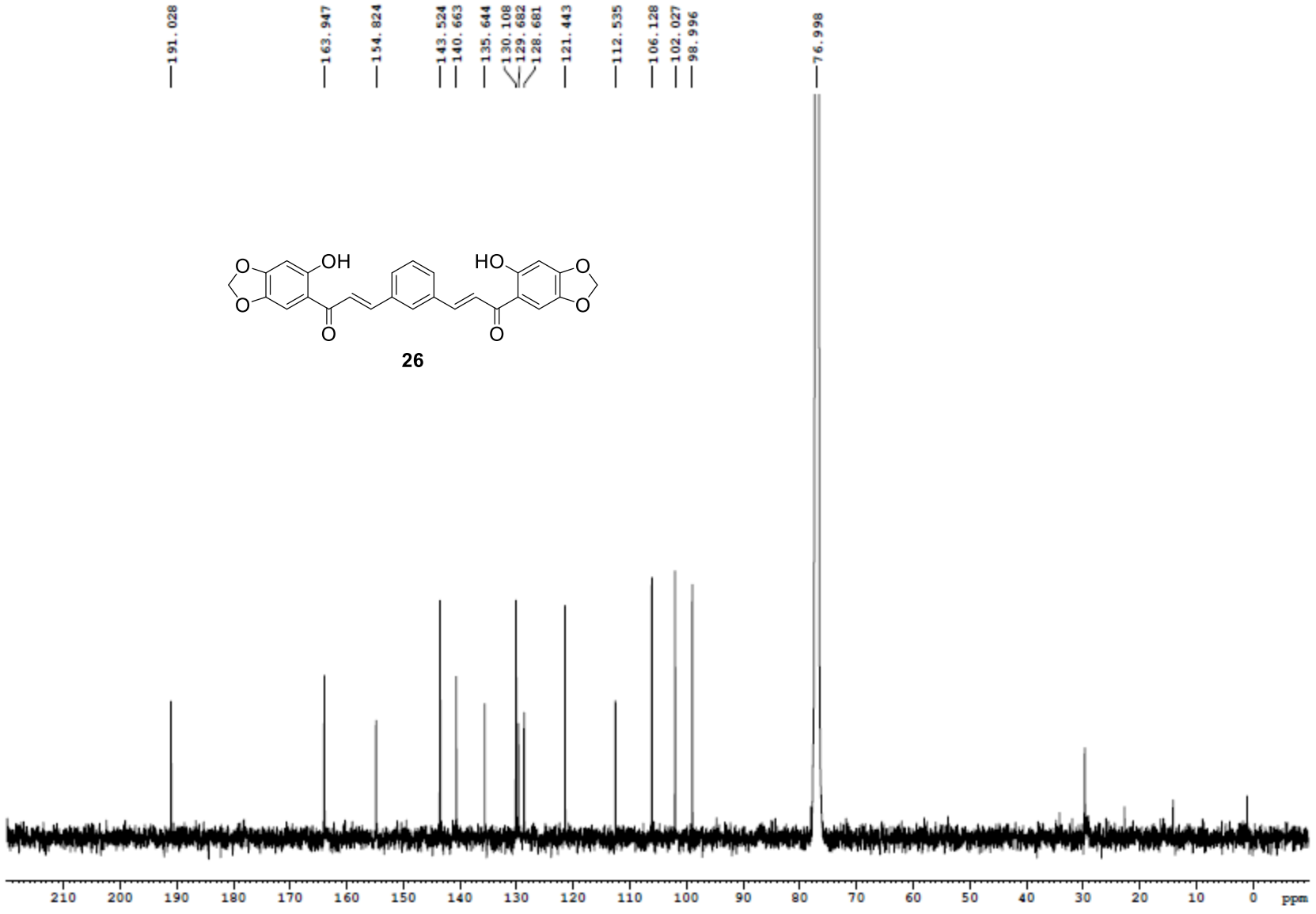
4.000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130.108
129.682
128.681
121.443
112.535
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102.027
98.996
76.998
OH
HO
O
O
O
O
O
O
210
200
190
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130
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50
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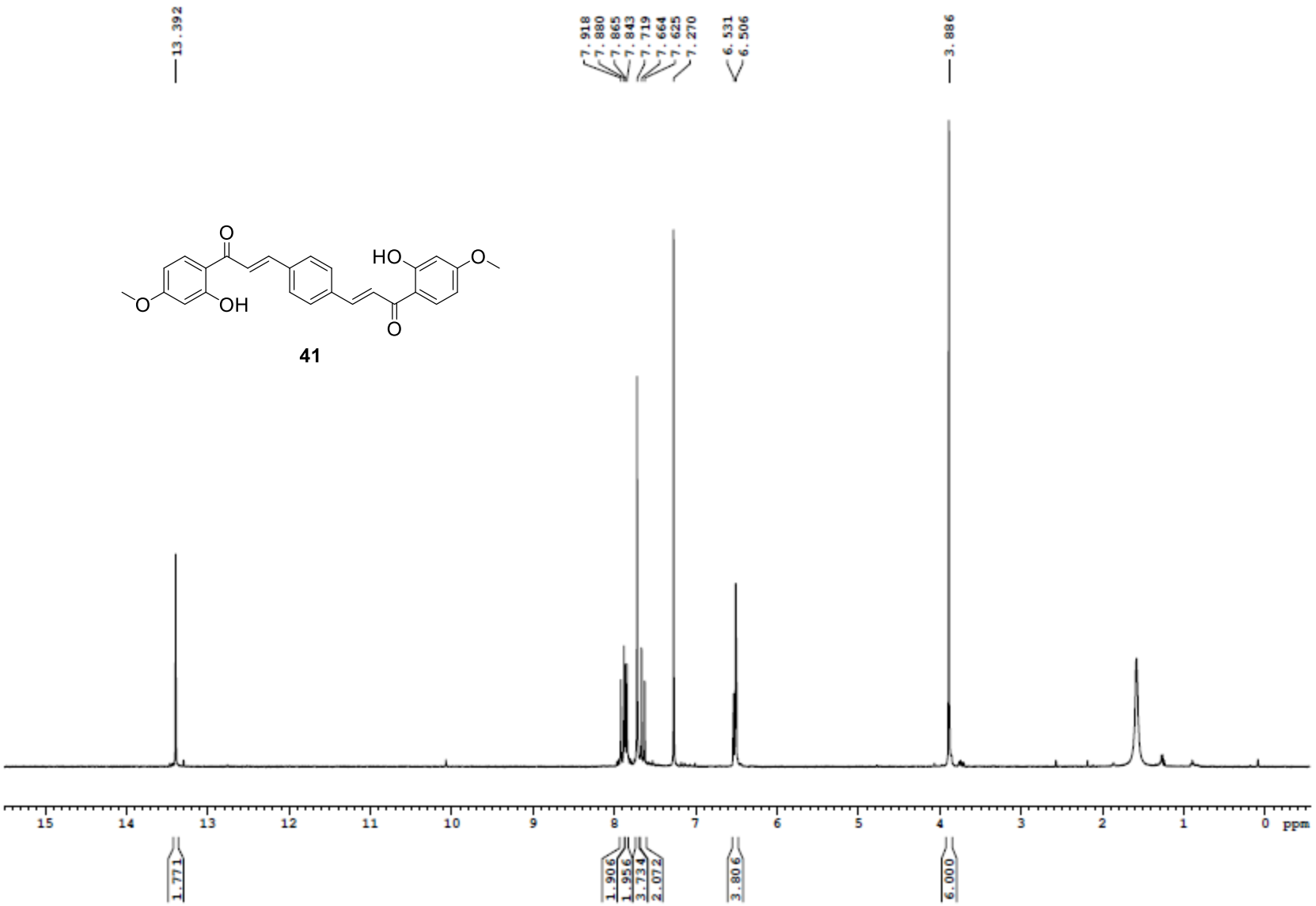
10
0
ppm

26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7.880
7.865
7.843
7.719
7.664
7.625
7.270
6.531
6.506
3.886
O
HO
O
O
OH
O
41
15
14
13
12
11
10
9
8
7
6
5
4
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2
1
0
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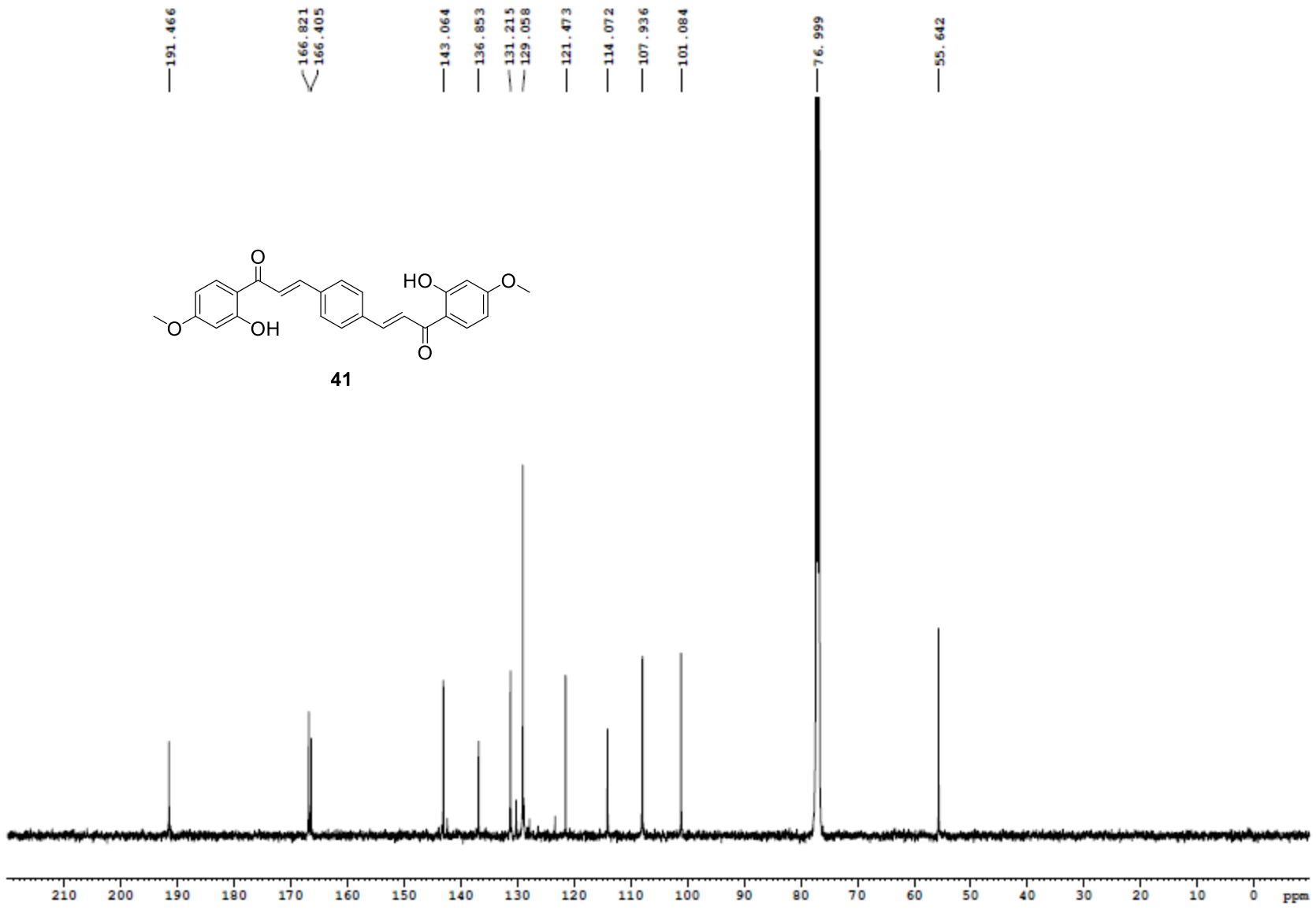
1.906
1.956
3.734
2.072
3.806
6.000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166.405
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131.215
129.058
121.473
114.072
107.936
101.084
76.999
55.642
O
HO
O
O
OH
O
41
210
200
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160
150
140
130
120
110
100
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80
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60
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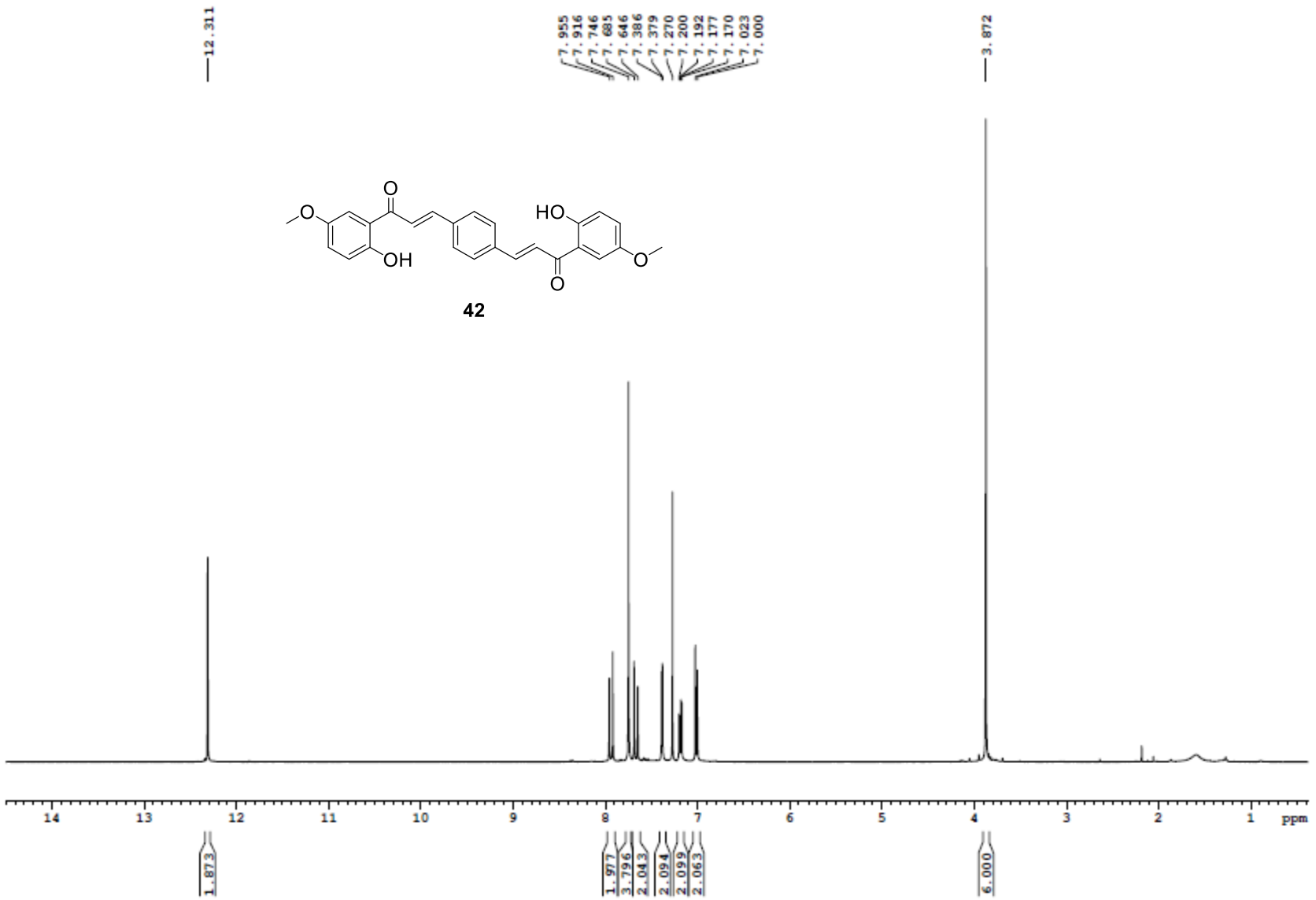
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7.916
7.746
7.685
7.646
7.386
7.379
7.270
7.200
7.192
7.177
7.170
7.023
7.000
3.872
O
O
HO
OH
O
O
42
14
13
12
11
10
9
8
7
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ppm
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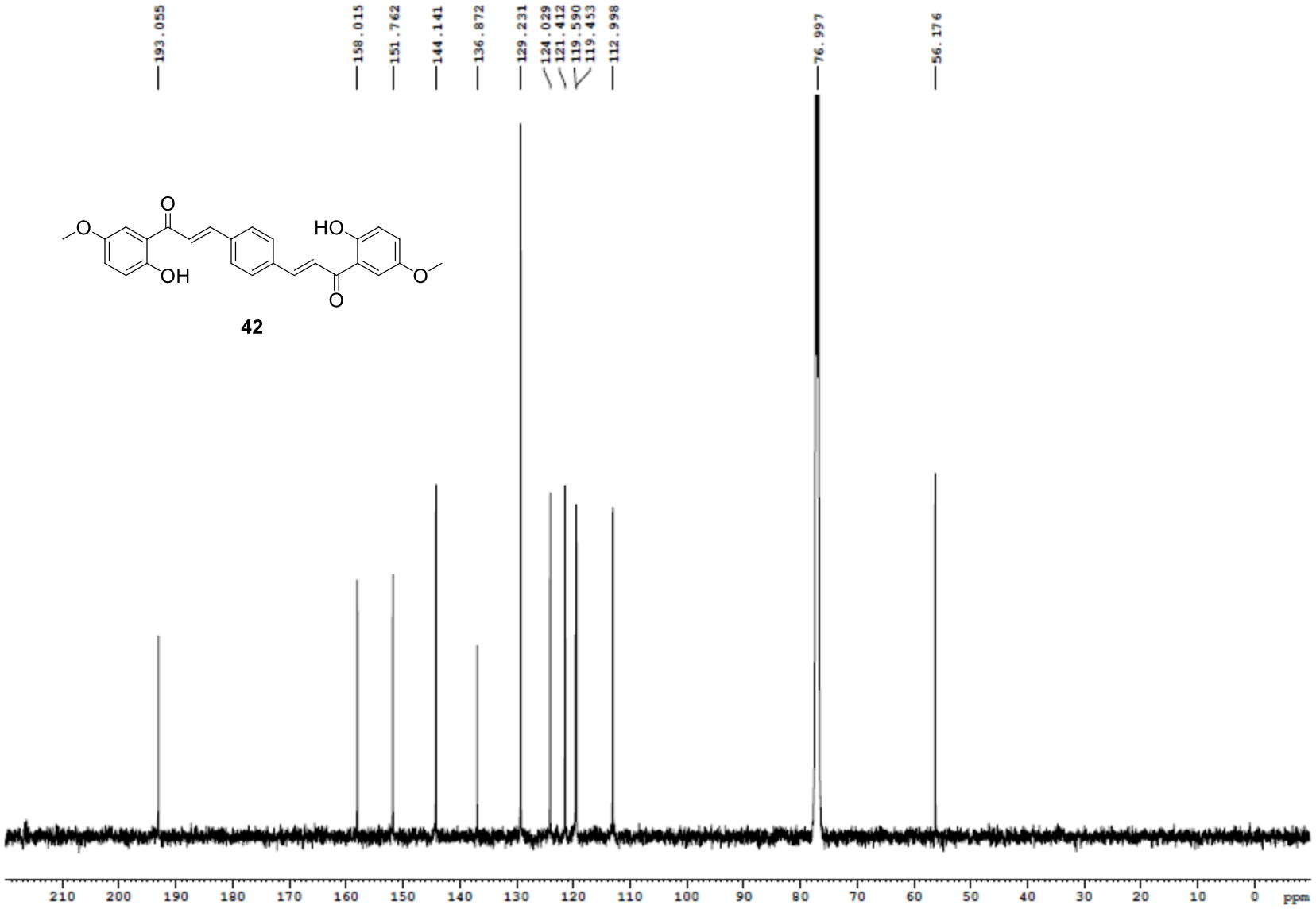
3.796
2.043
2.094
2.099
2.063
6.000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158.015
151.762
144.141
136.872
129.231
124.029
121.412
119.590
119.453
112.998
76.997
56.176
O
O
OH
HO
O
O
42
210
200
190
180
170
160
150
140
130
120
110
100
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80
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60
50
40
30
20
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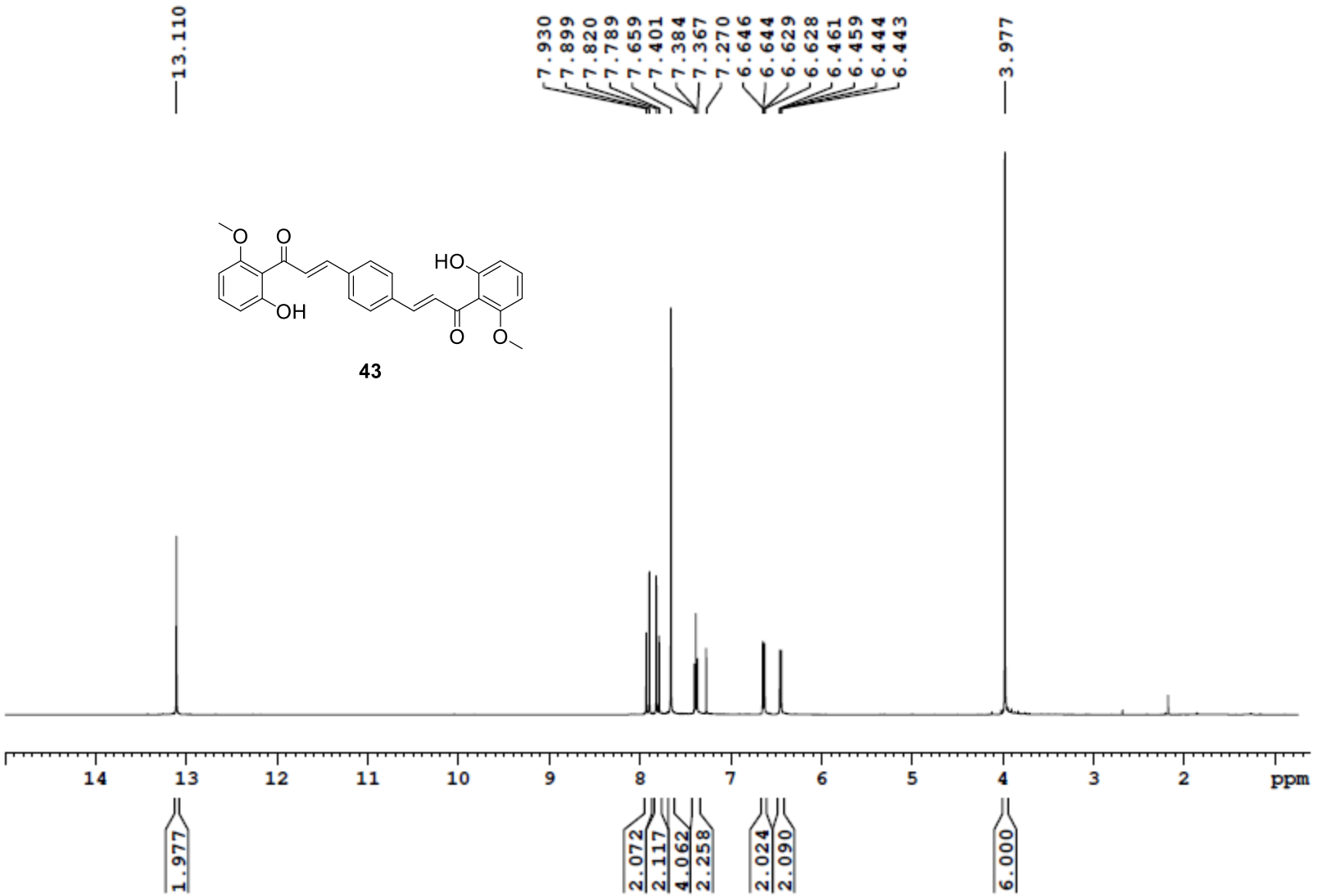
0
ppm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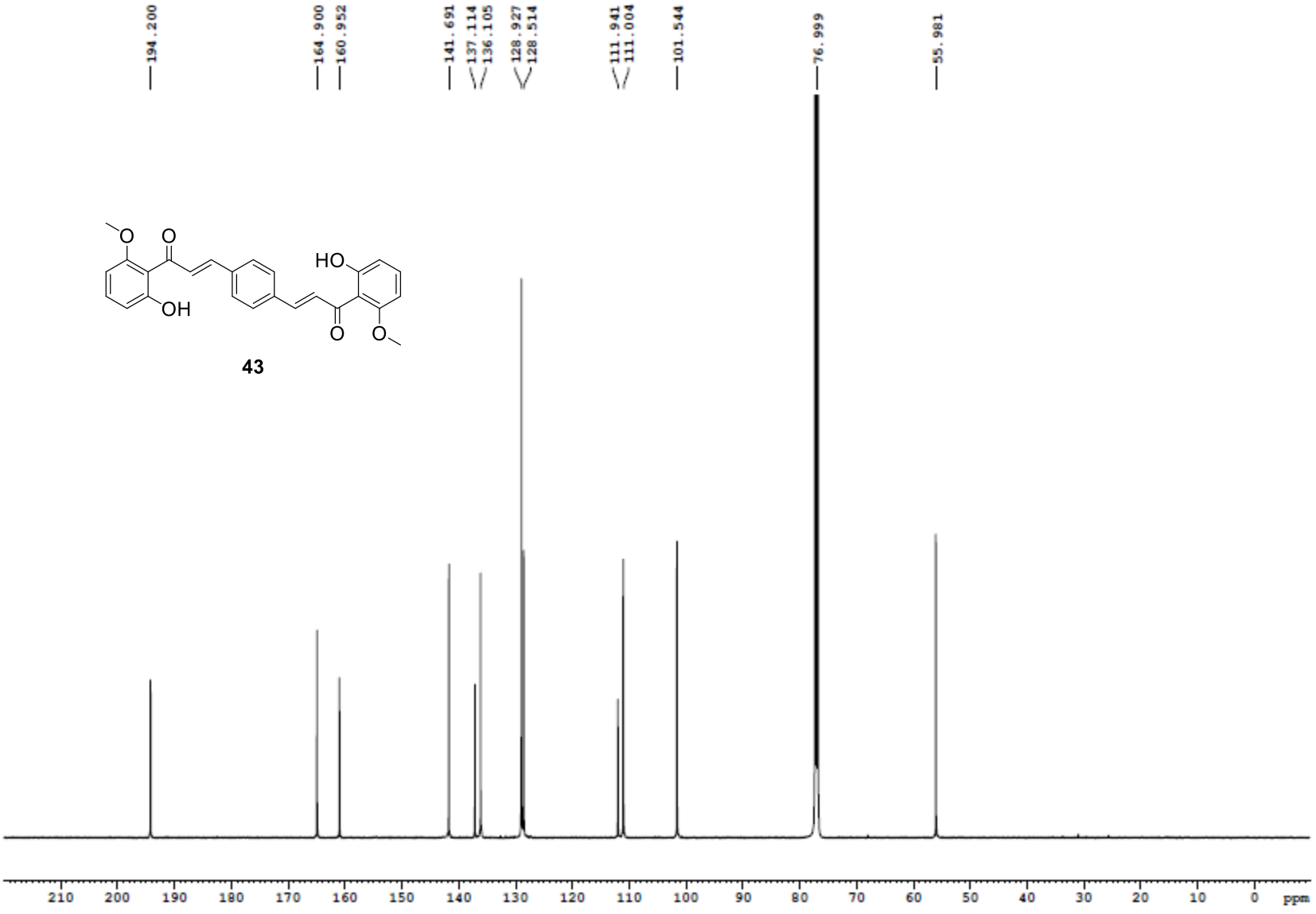
7.899
7.820
7.789
7.659
7.401
7.384
7.367
7.270
6.646
6.644
6.629
6.628
6.461
6.459
6.444
6.443
3.977
O
O
HO
OH
O
O
14
13
12
11
10
9
8
7
6
5
4
3
2
ppm
1.977
2.072
2.117
4.062
2.258
2.024
2.090
6.000

43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136.105
128.927
128.514
111.941
111.004
101.544
76.999
55.981
O
O
OH
HO
O
O
43
210
200
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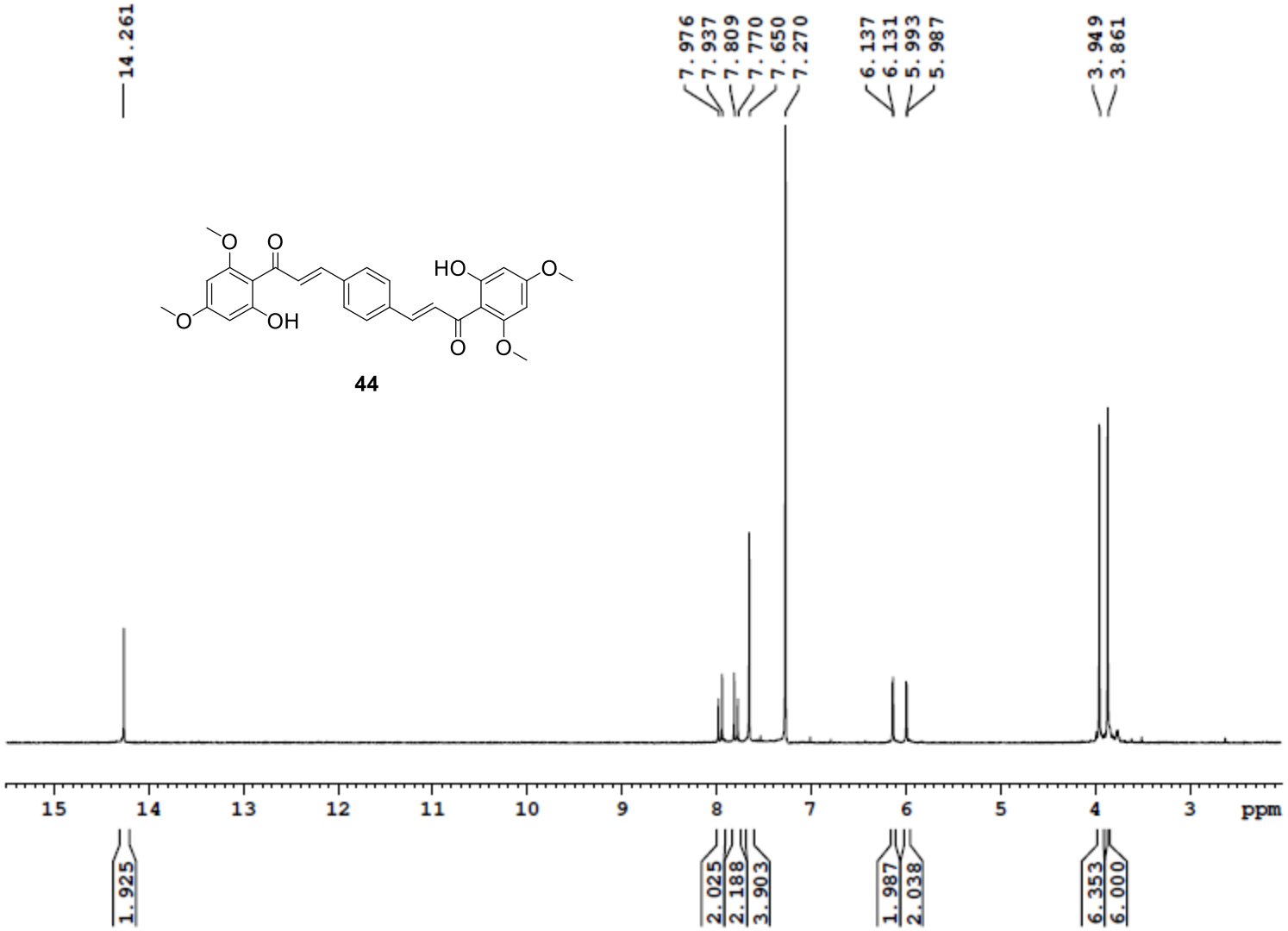
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.937
7.809
7.770
7.650
7.270
6.137
6.131
5.993
5.987
3.949
3.861
HO
O
OH
15
14
13
12
11
10
9
8
7
6
5
4
3
ppm
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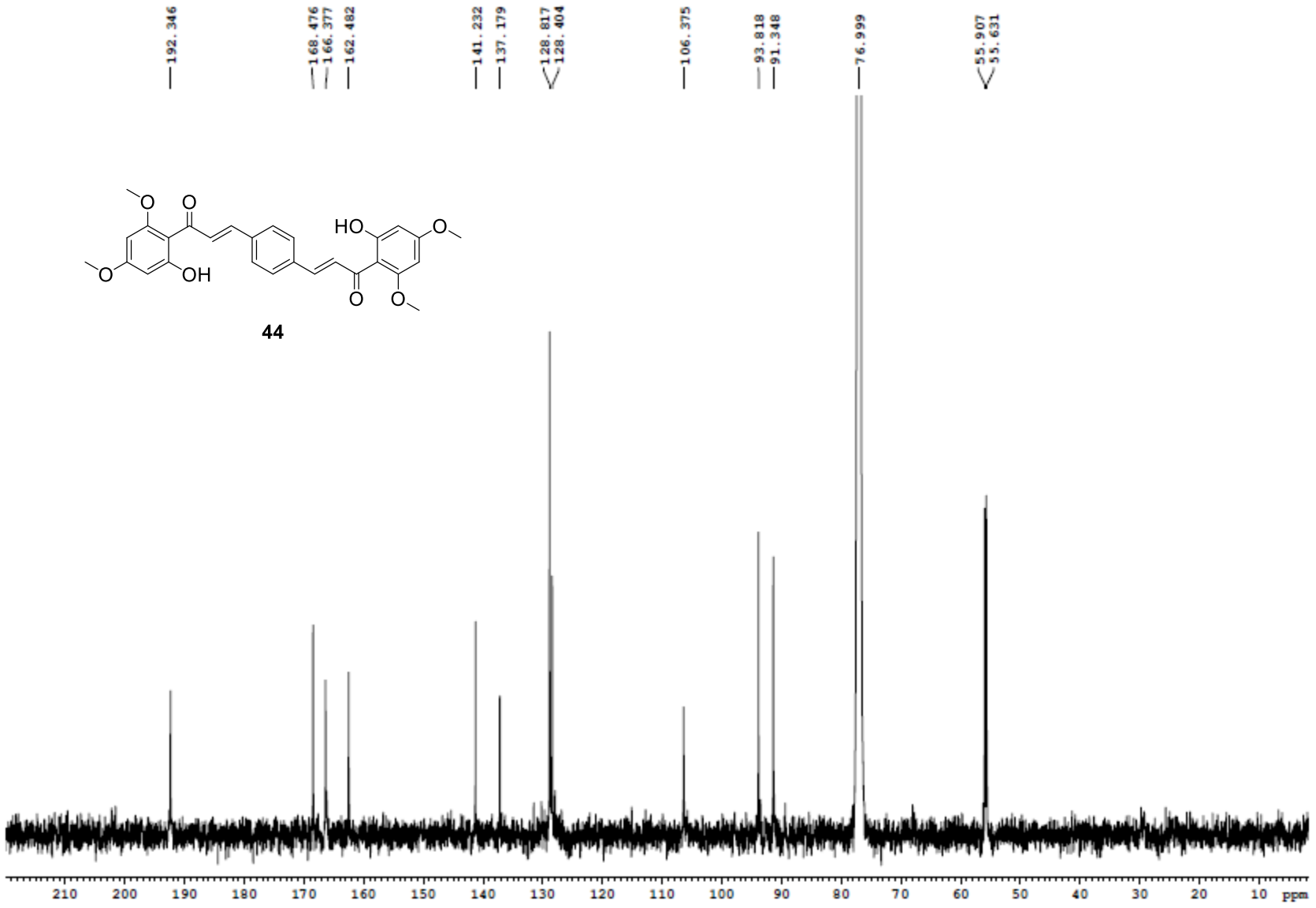
2.025
2.188
3.903
1.987
2.038
6.353
6.000

44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128.404
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91.348
76.999
55.907
55.631
HO
O
OH
210
200
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180
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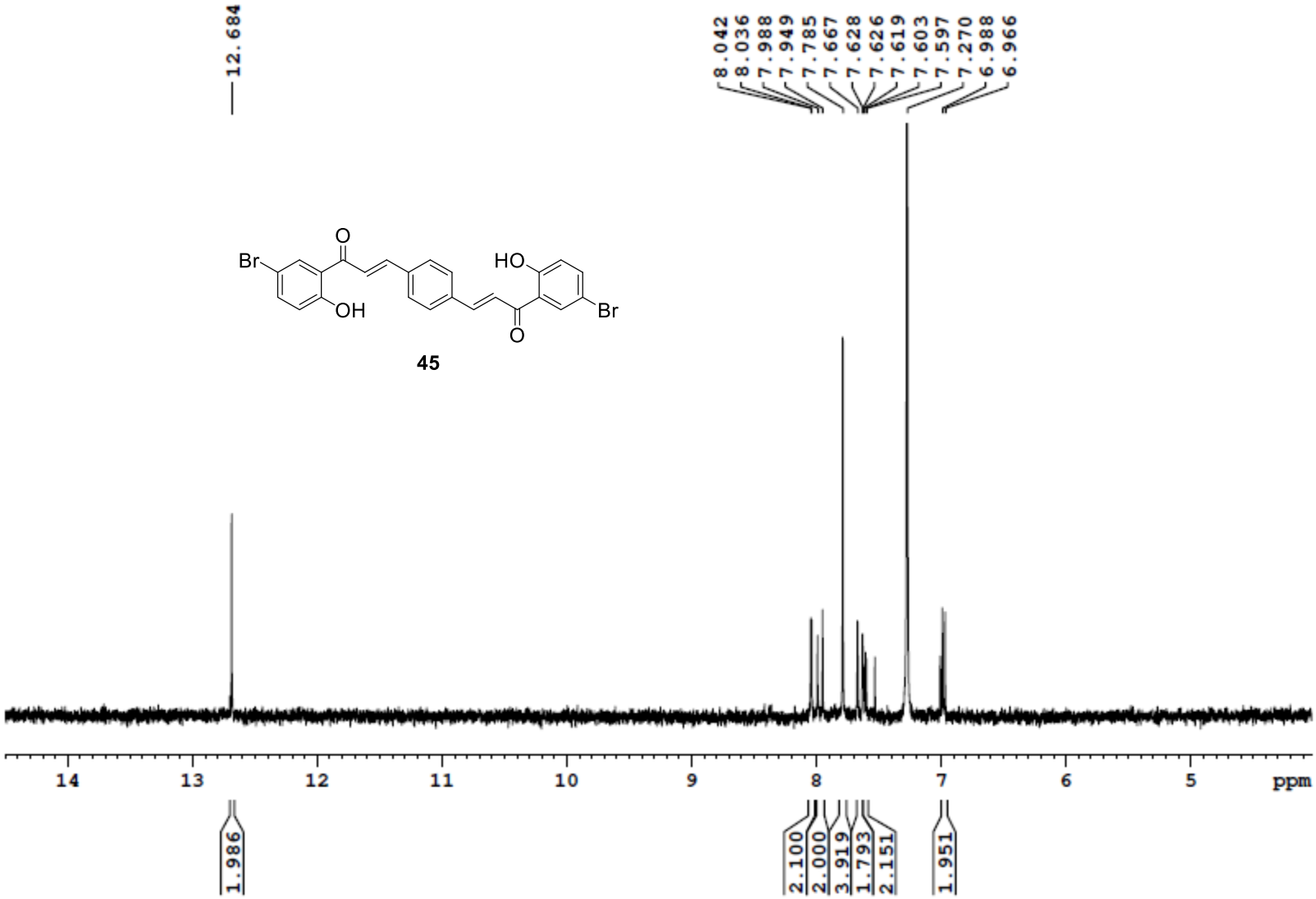
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

44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7.785
7.667
7.628
7.626
7.619
7.603
7.597
7.270
6.988
6.966
Br
O
OH
HO
Br
O
45
14
13
12
11
10
9
8
7
6
5
ppm
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2.000
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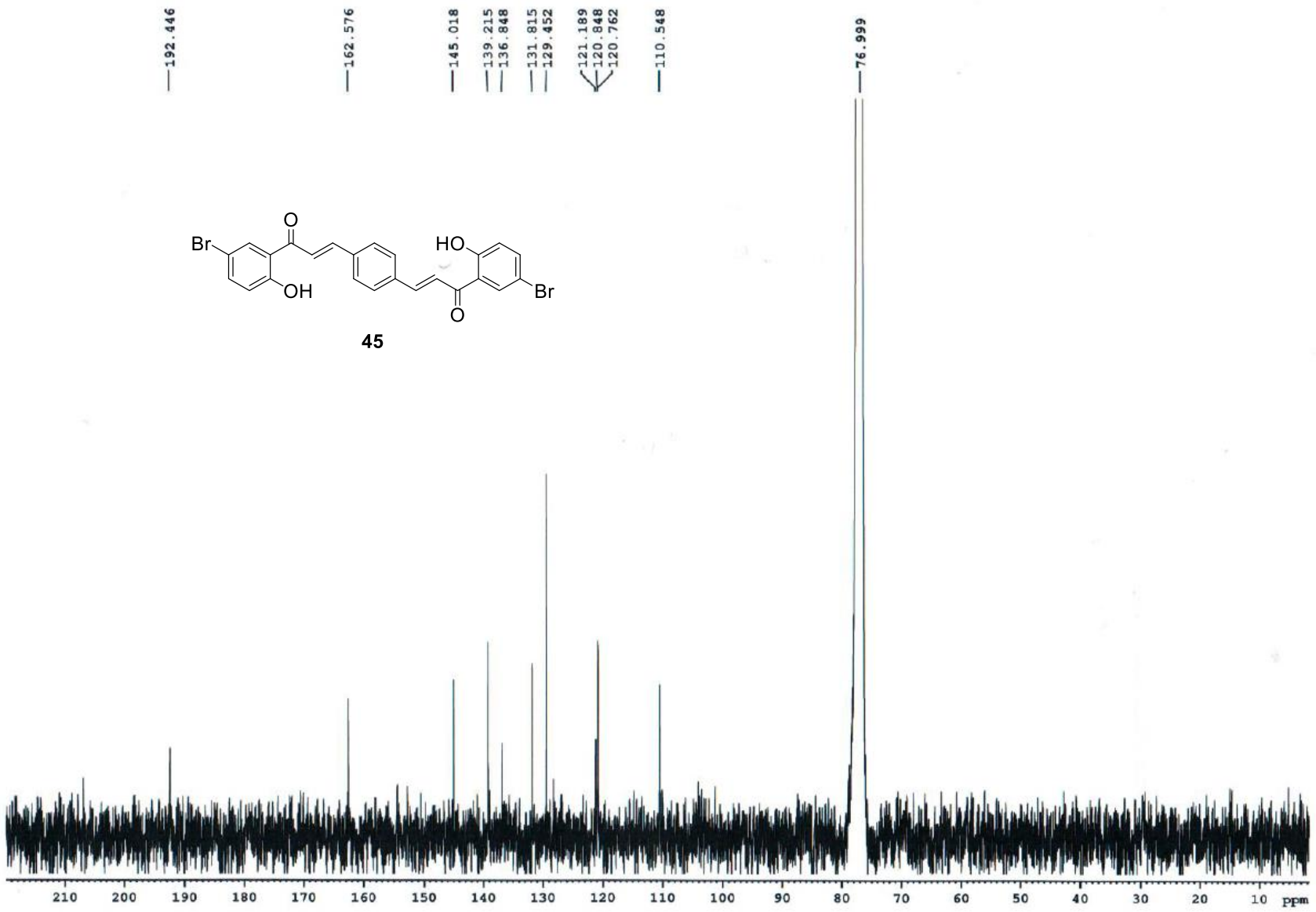
1.793
2.151
1.951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139.215
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131.815
129.452
121.189
120.848
120.762
110.548
76.999
Br
OH
O
HO
Br
O
45
210
200
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150
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130
120
110
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90
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70
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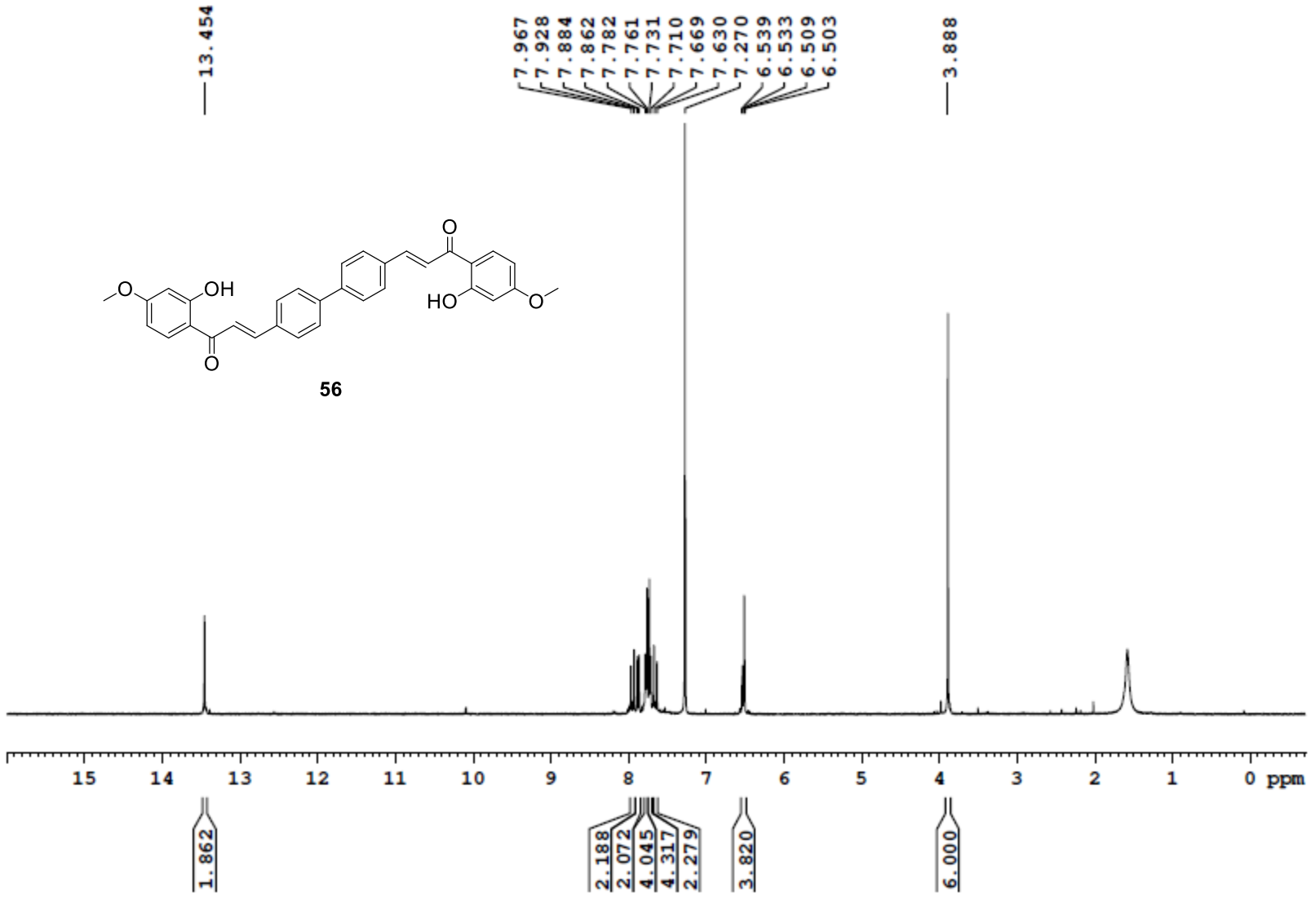
30
20
10
ppm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7.731
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7.630
7.270
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6.533
6.509
6.503
3.888
O
OH
HO
O
O
O
56
15
14
13
12
11
10
9
8
7
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5
4
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0 ppm
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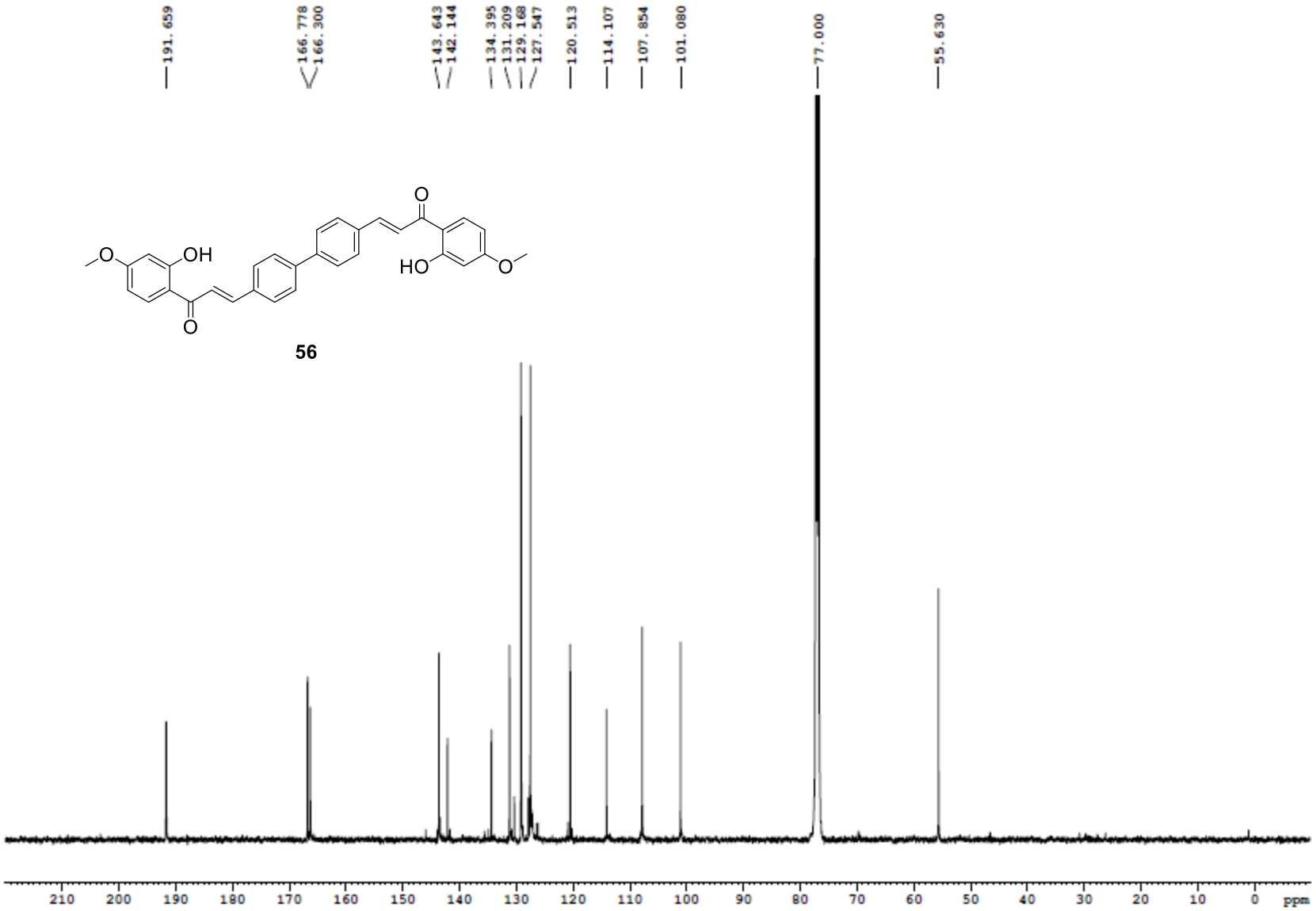
6.000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129.168
127.547
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114.107
107.854
101.080
77.000
55.630
O
OH
HO
O
O
O
56
210
200
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180
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140
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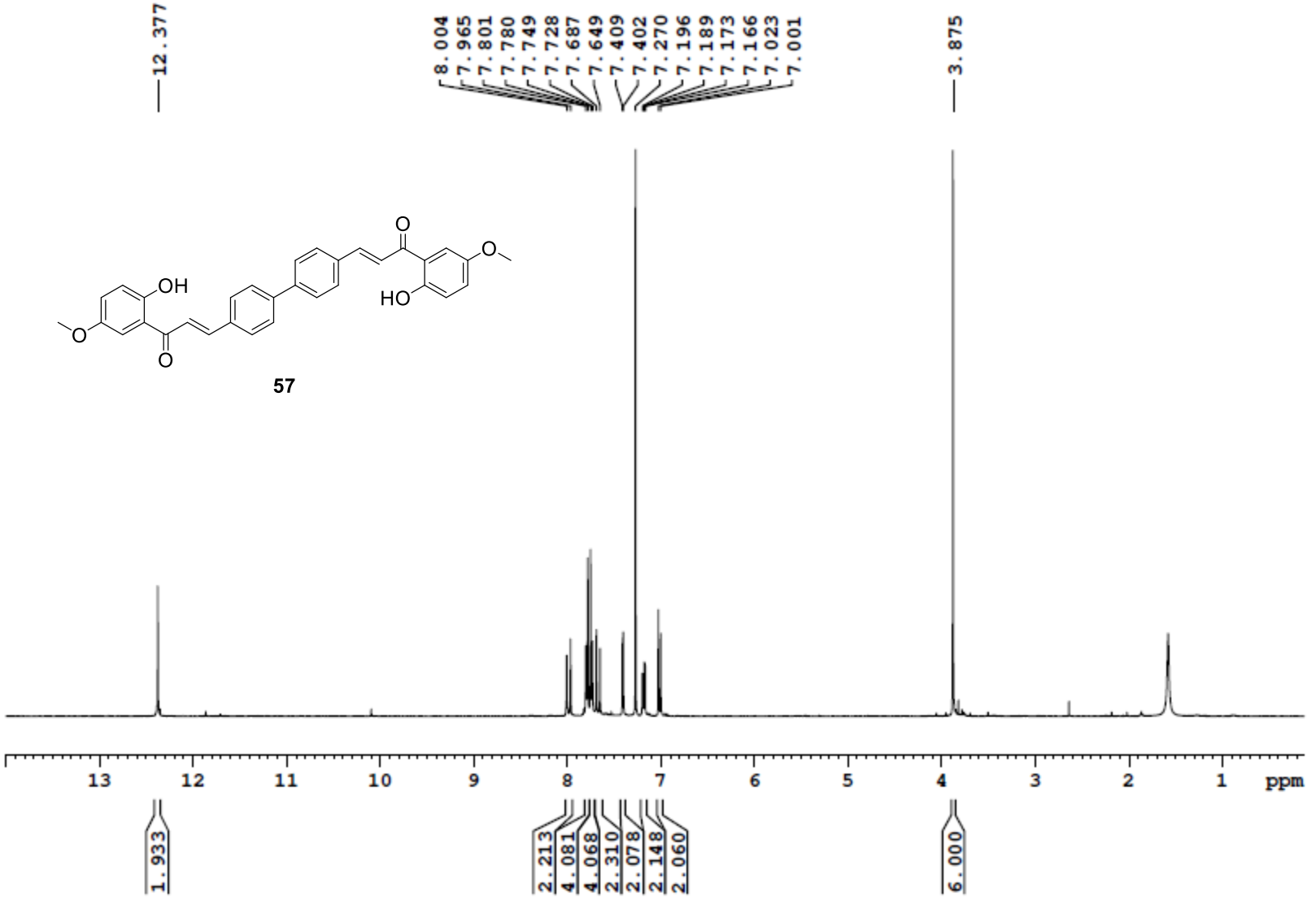
ppm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7.749
7.728
7.687
7.649
7.409
7.402
7.270
7.196
7.189
7.173
7.166
7.023
7.001
3.875
OH
O
O
HO
O
13
12
11
10
9
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7
6
5
4
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2.060
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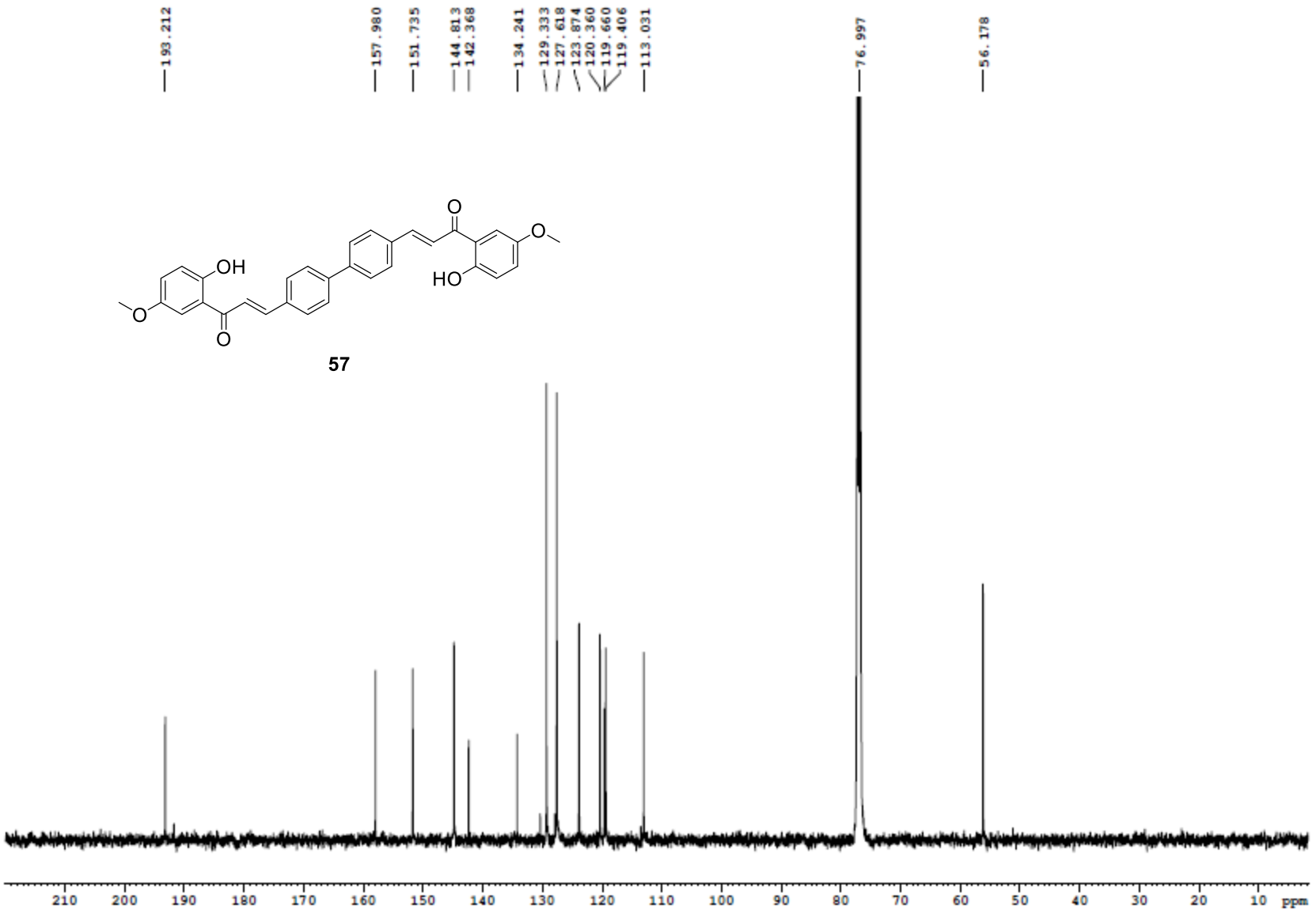
57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134.241
129.333
127.618
123.874
120.360
119.660
119.406
113.031
76.997
56.178
OH
O
O
HO
O
210
200
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60
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40
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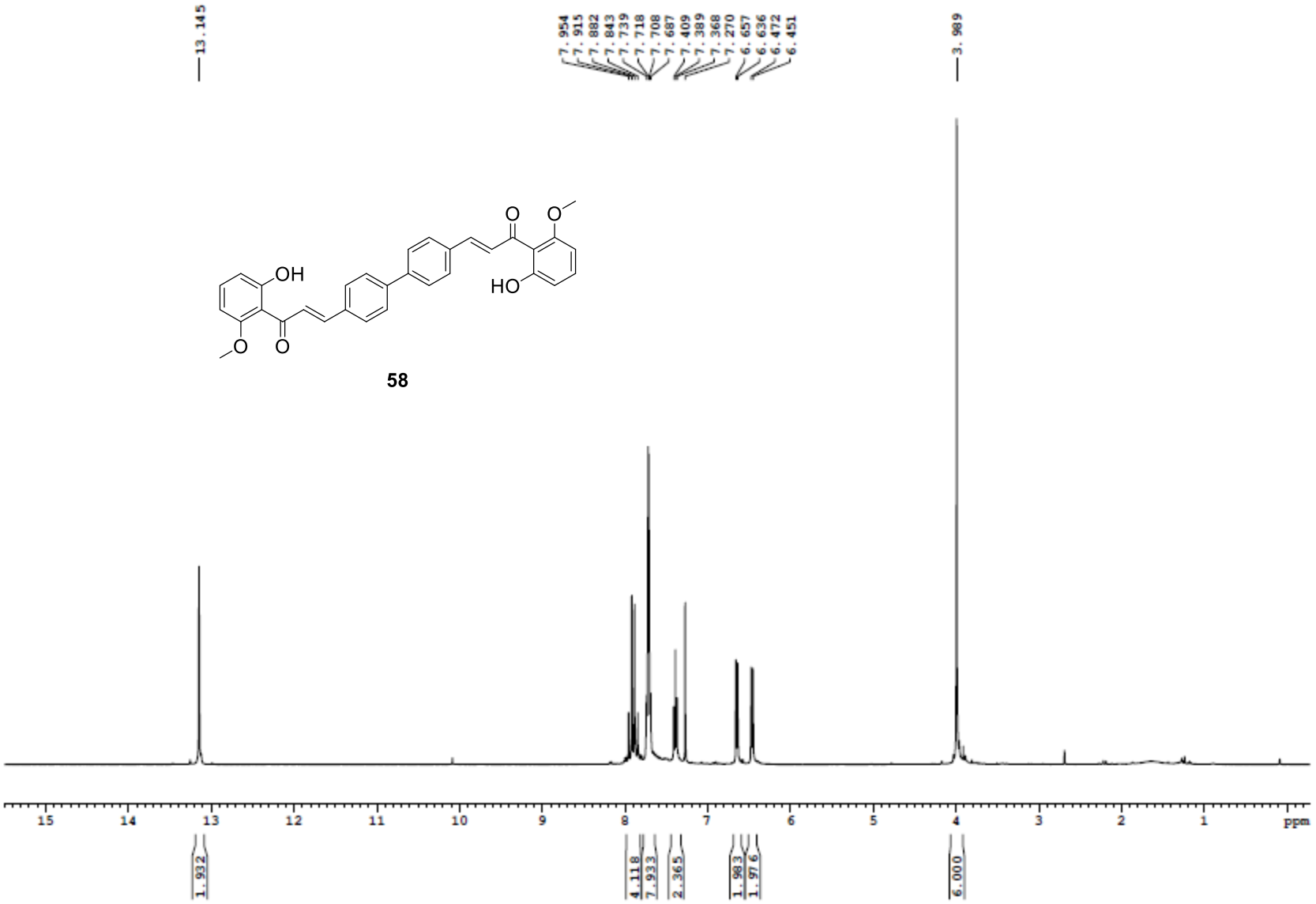
20
10
ppm

57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7.708
7.687
7.409
7.389
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6.636
6.472
6.451
3.989
OH
HO
O
O
O
O
15
14
13
12
11
10
9
8
7
6
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1
ppm
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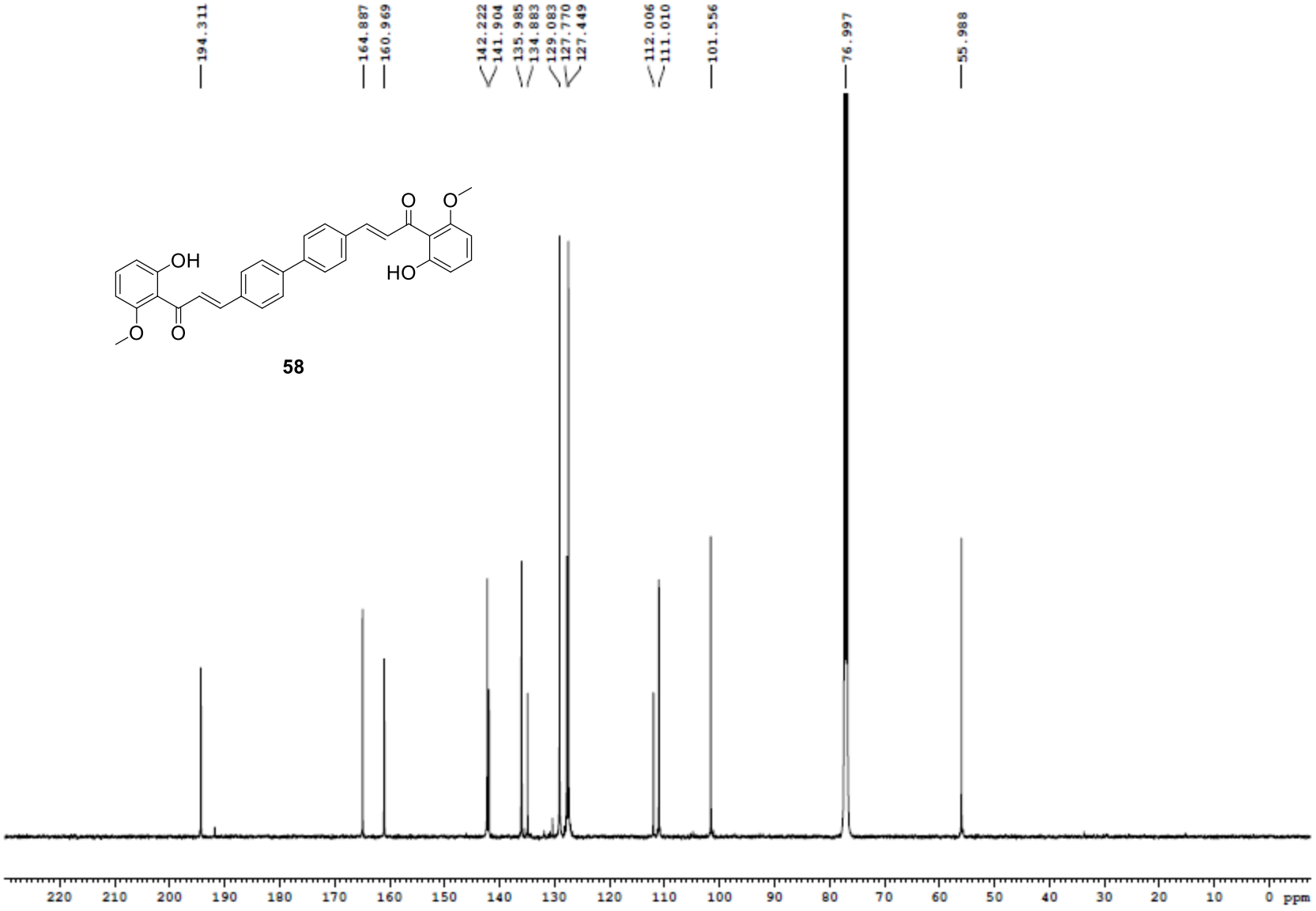
6.000

58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135.985
134.883
129.083
127.770
127.449
112.006
111.010
101.556
76.997
55.988
OH
HO
O
O
O
O
220
210
200
190
180
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160
150
140
130
120
110
100
90
80
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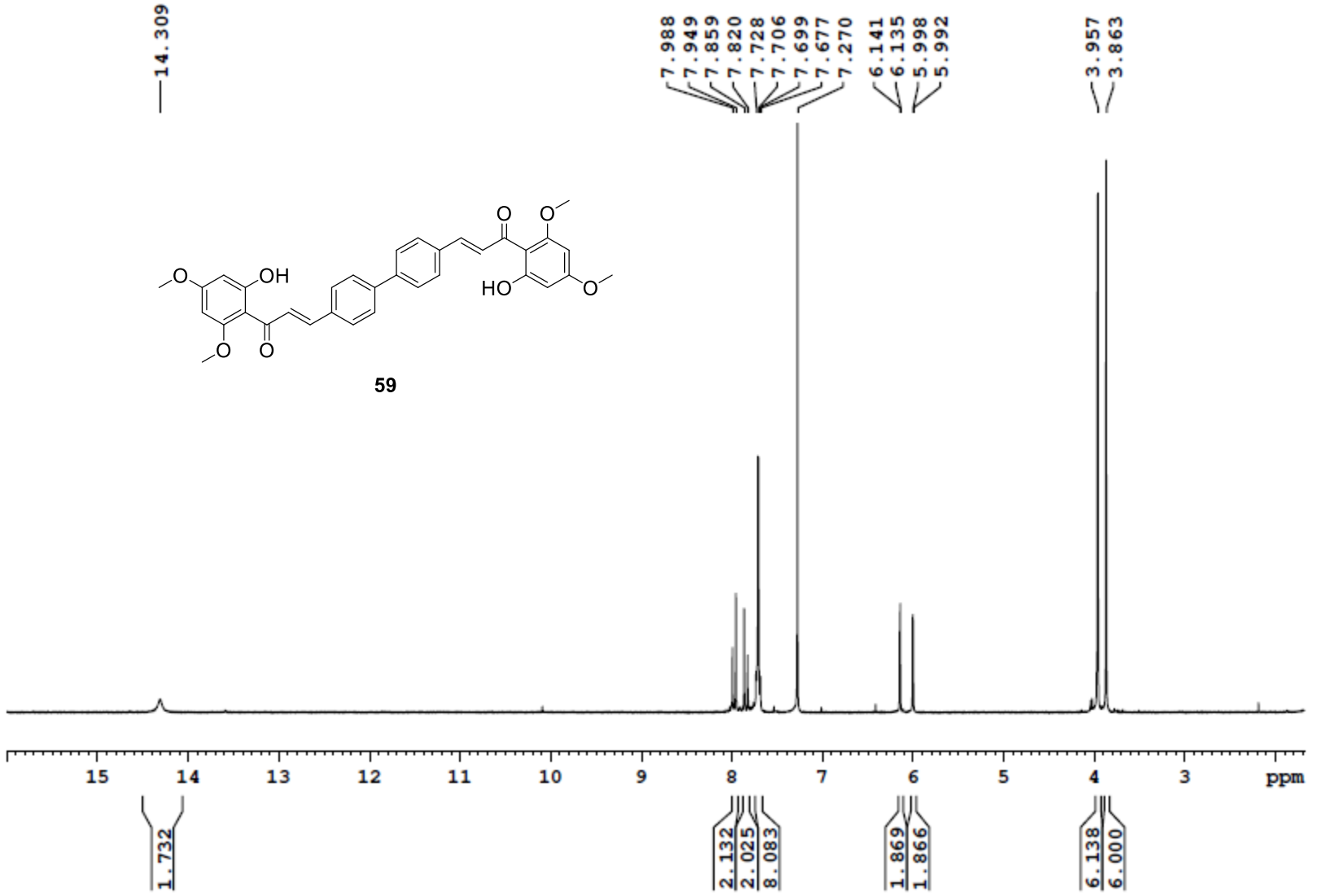
60
50
40
30
20
10
0 ppm

58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7.728
7.706
7.699
7.677
7.270
6.141
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5.998
5.992
3.957
3.863
OH
HO
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O
O
O
O
O
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13
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10
9
8
7
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5
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3
ppm
1.732
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1.866
6.138
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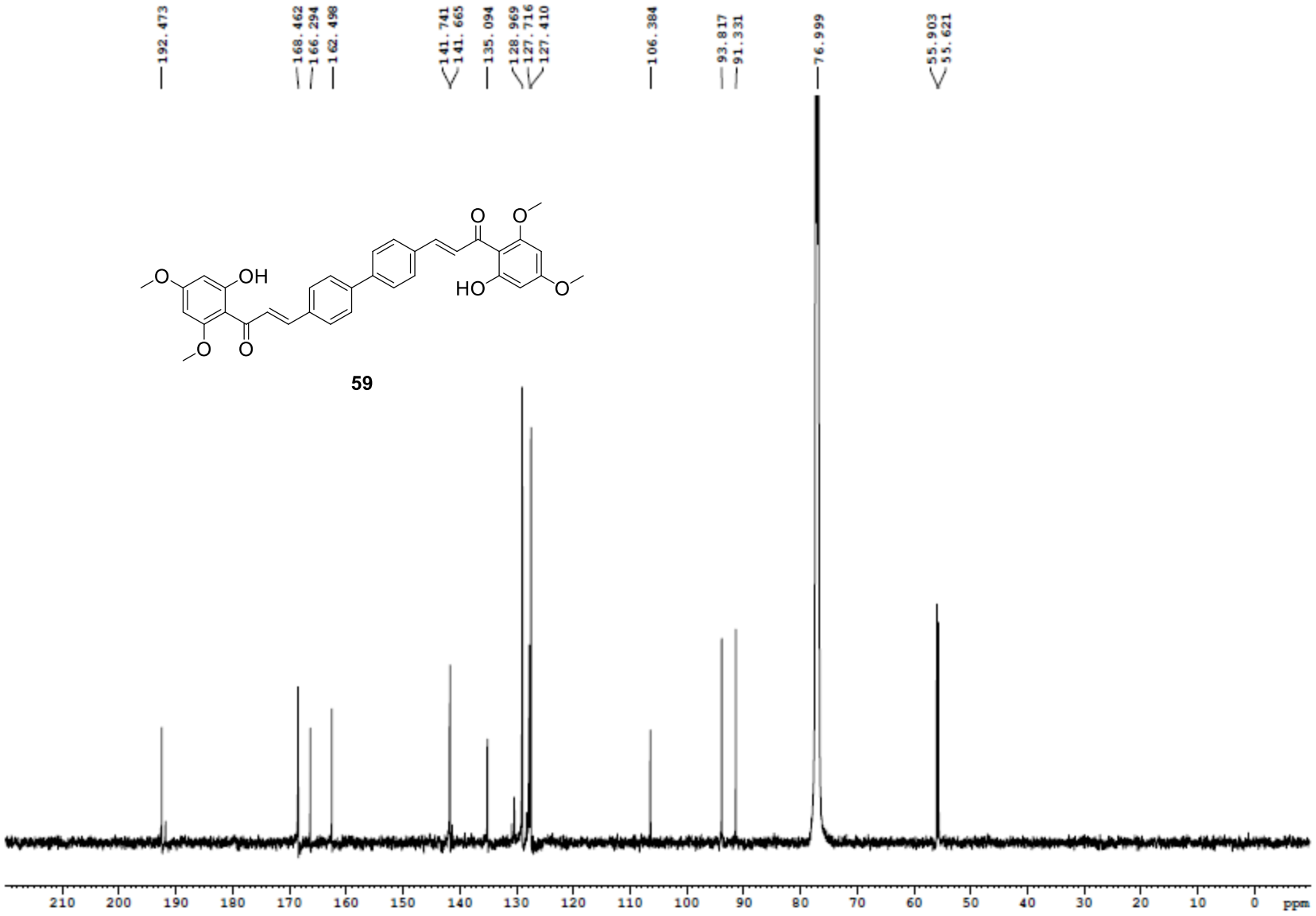
59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135.094
128.969
127.716
127.410
106.384
93.817
91.331
76.999
55.903
55.621
OH
HO
O
O
O
O
O
O
210
200
190
180
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130
120
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90
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50
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10
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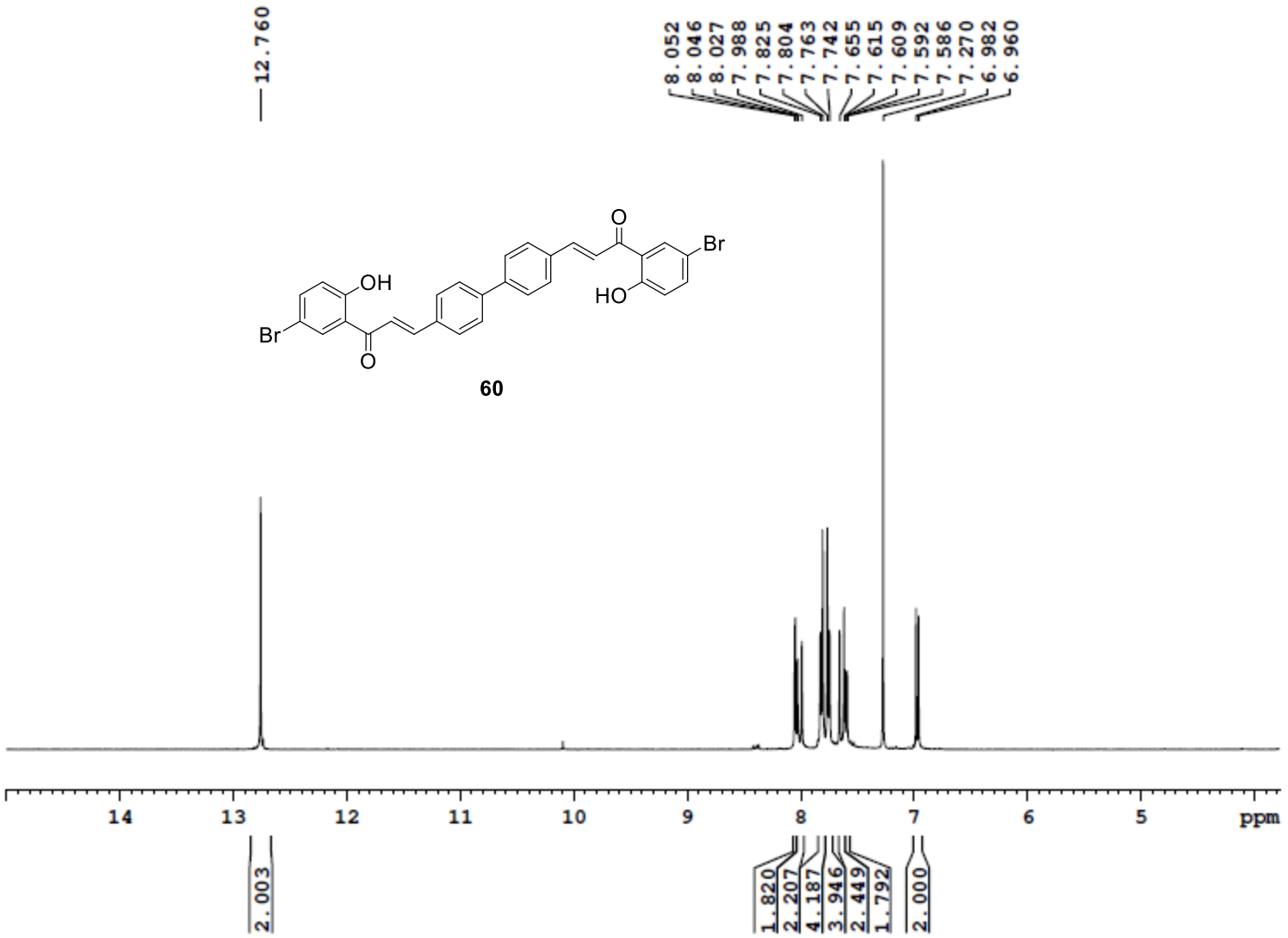
ppm

59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8.027
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7.825
7.804
7.763
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7.655
7.615
7.609
7.592
7.586
7.270
6.982
6.960
OH
Br
O
HO
Br
O
60
14
13
12
11
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8
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5
ppm
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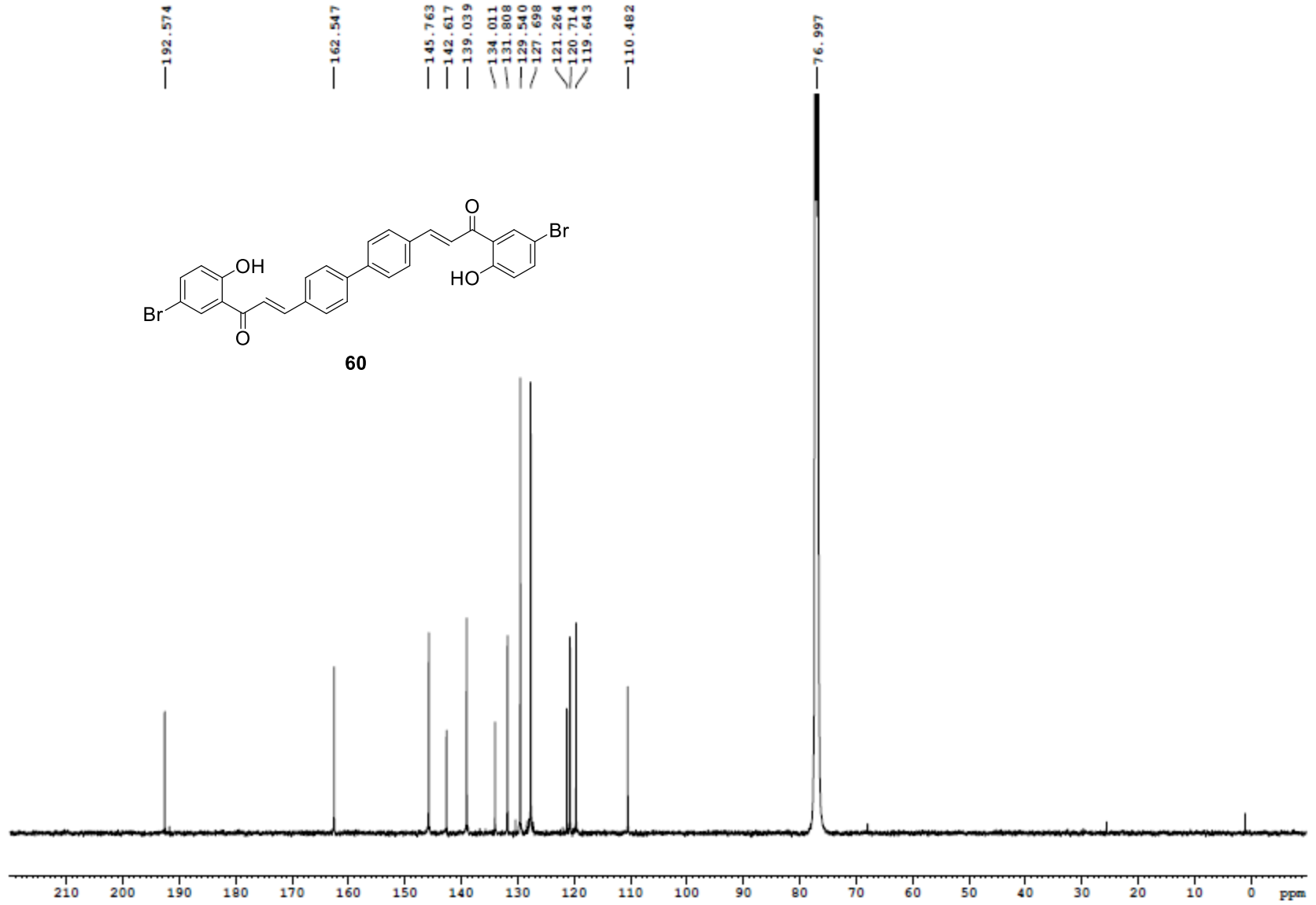
2.000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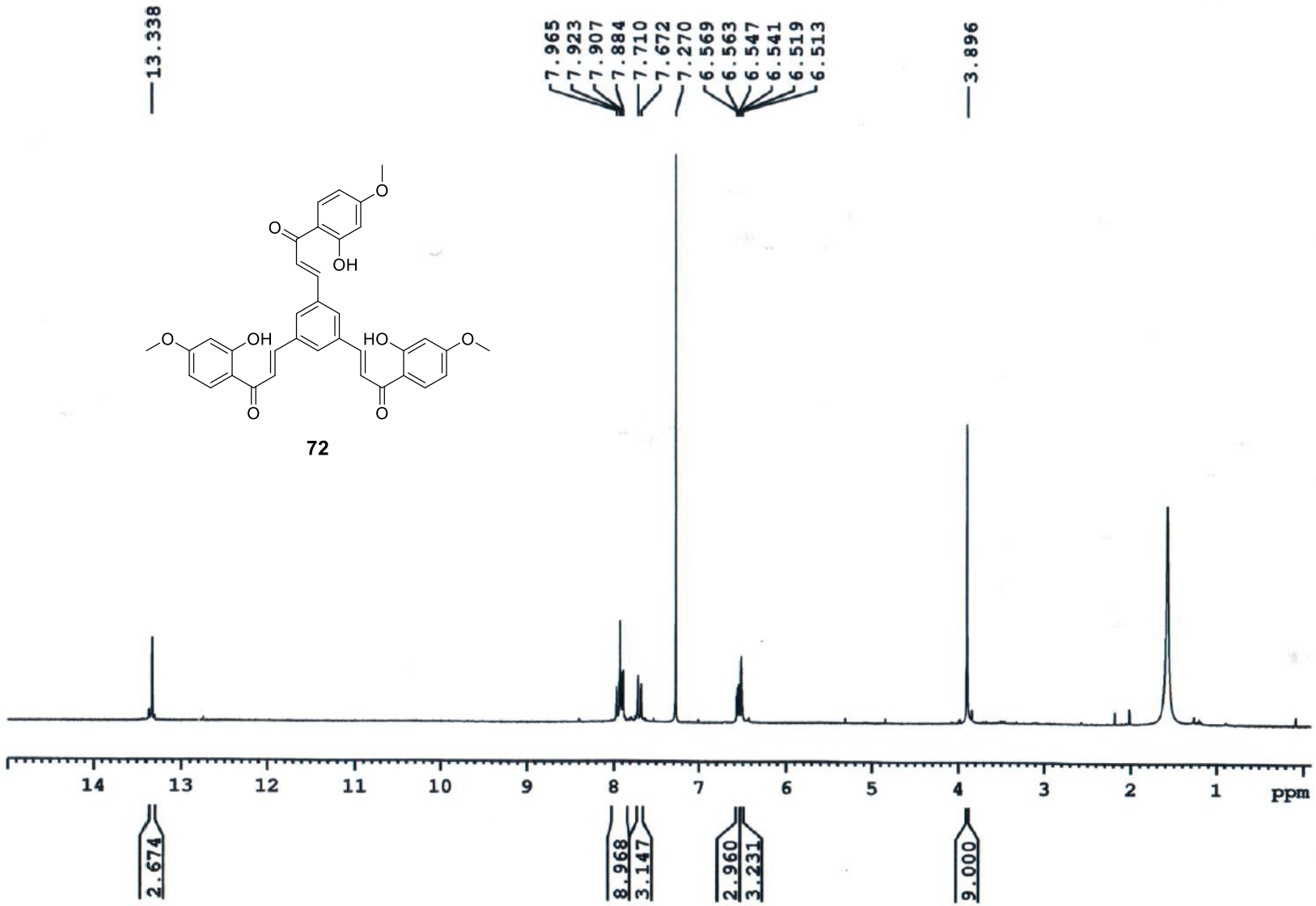
120.714
119.643
110.482
76.997
OH
Br
O
O
HO
Br
60
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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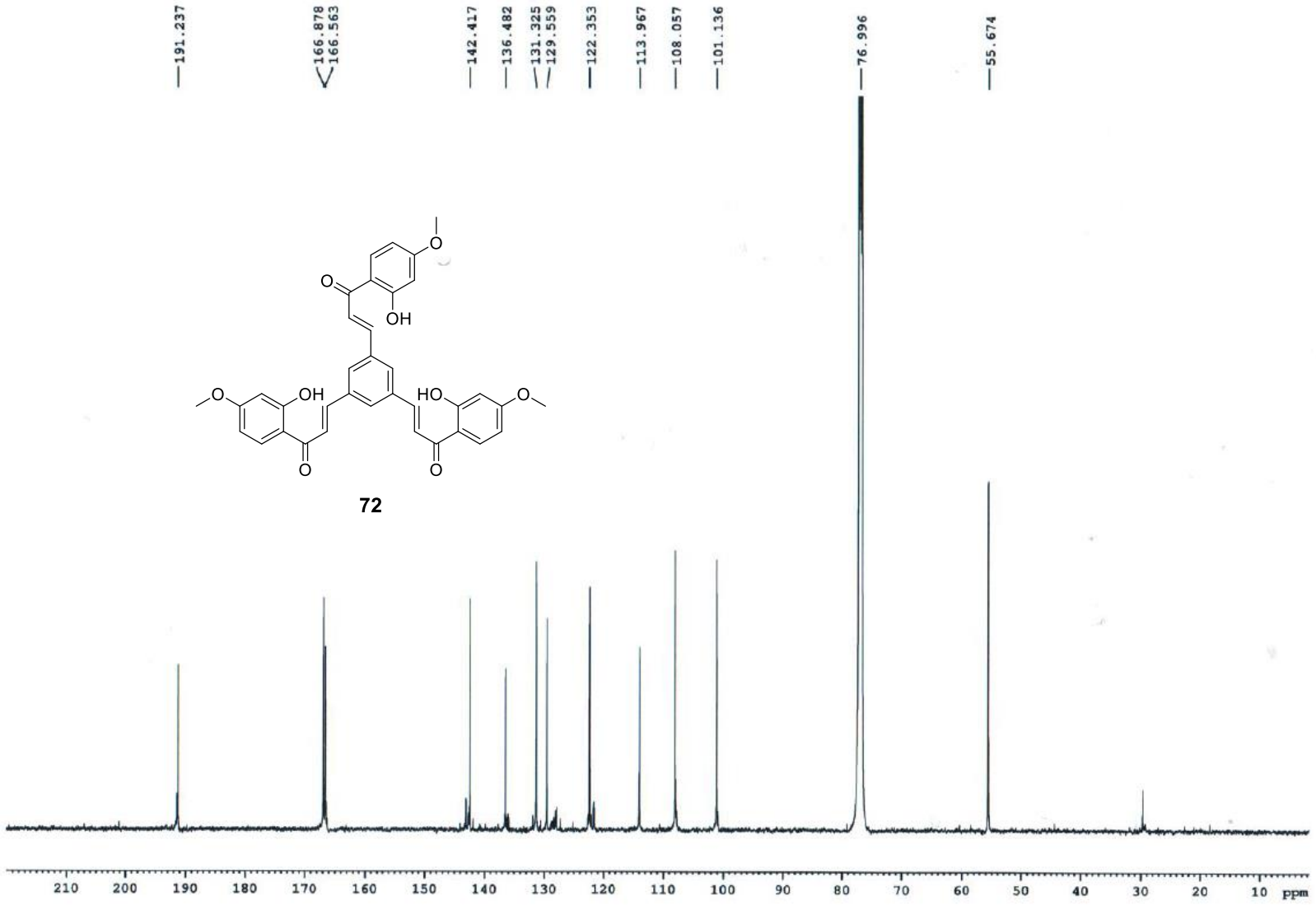
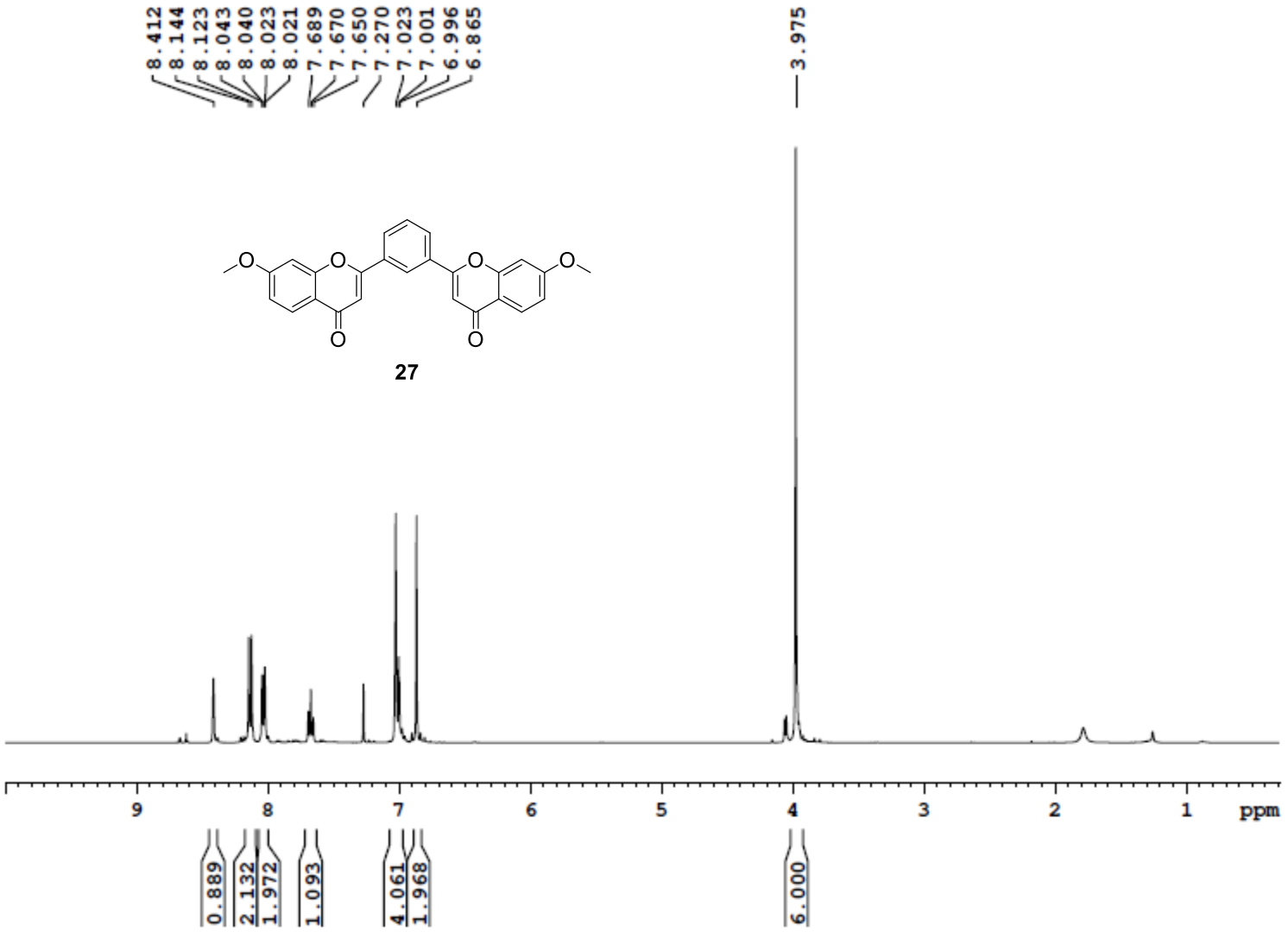
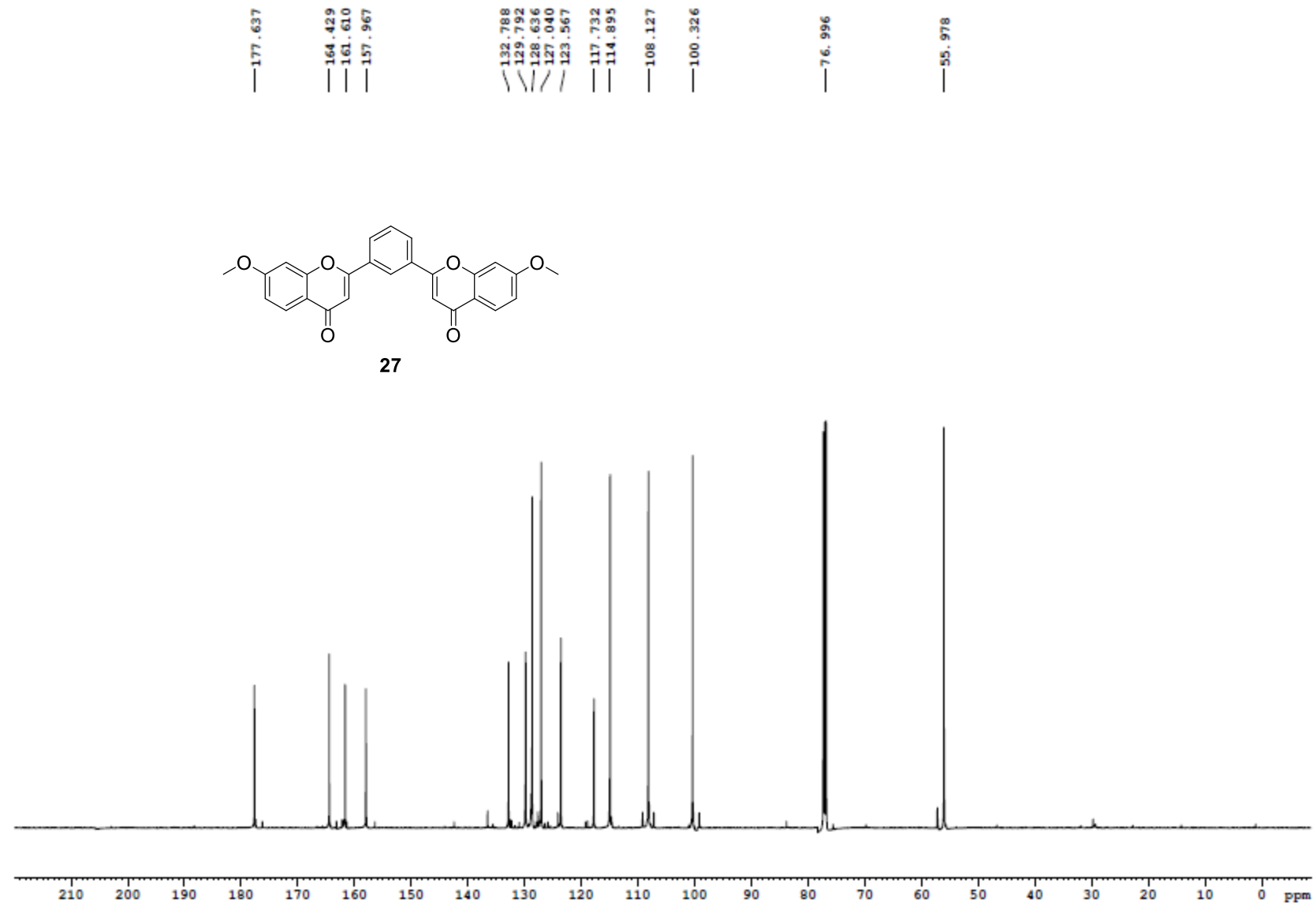
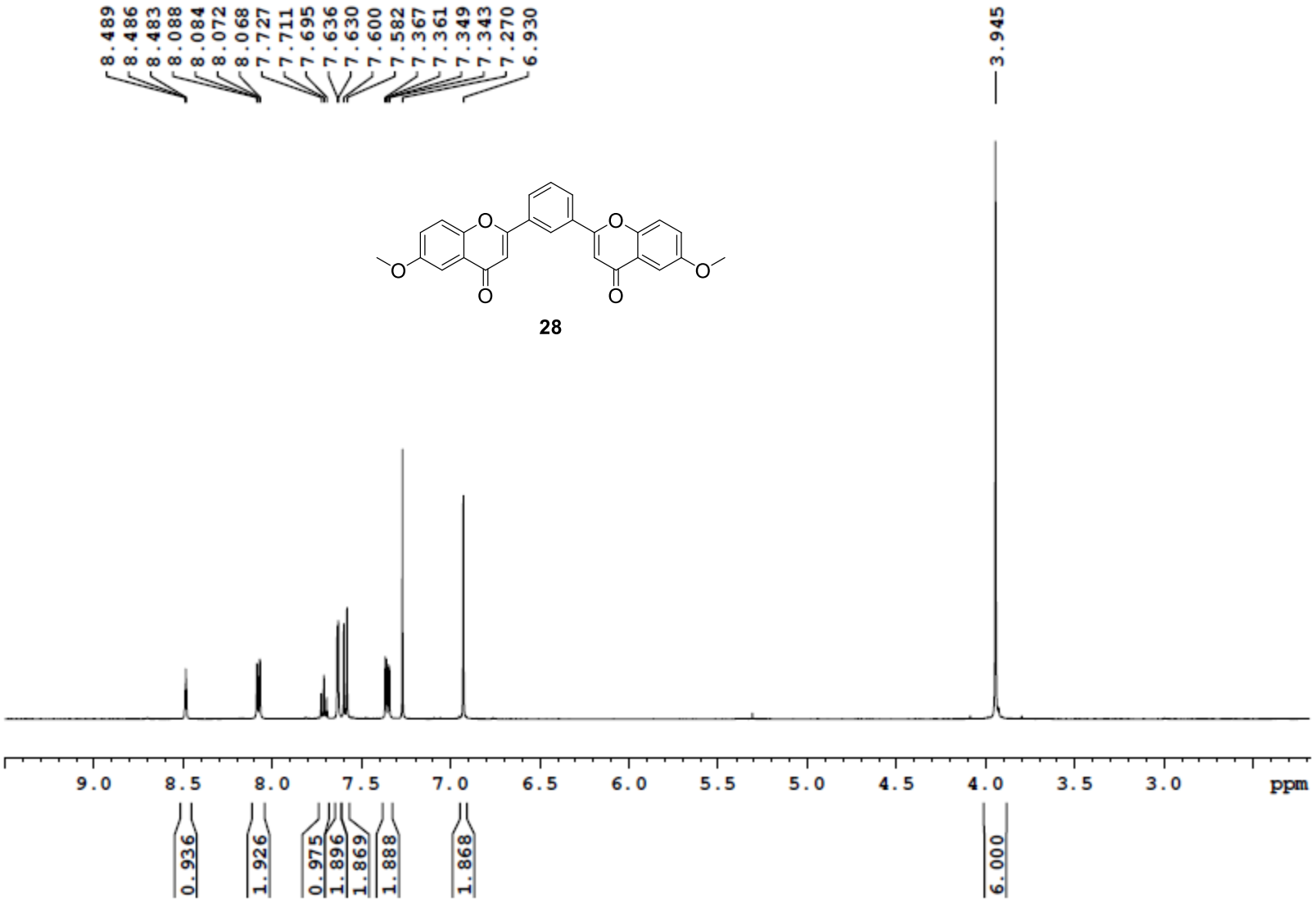
7.965
7.923
7.907
7.884
7.710
7.672
7.270
6.569
6.563
6.547
6.541
6.519
6.513
3.896
O
O
OH
O
OH
HO
O
O
O
72
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
2.674
8.968
3.147
2.960
3.231
9.000


191.237
166.878
166.563
142.417
136.482
131.325
129.559
122.353
113.967
108.057
101.136
76.996
55.674
O
OH
O
OH
HO
O
O
O
72
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

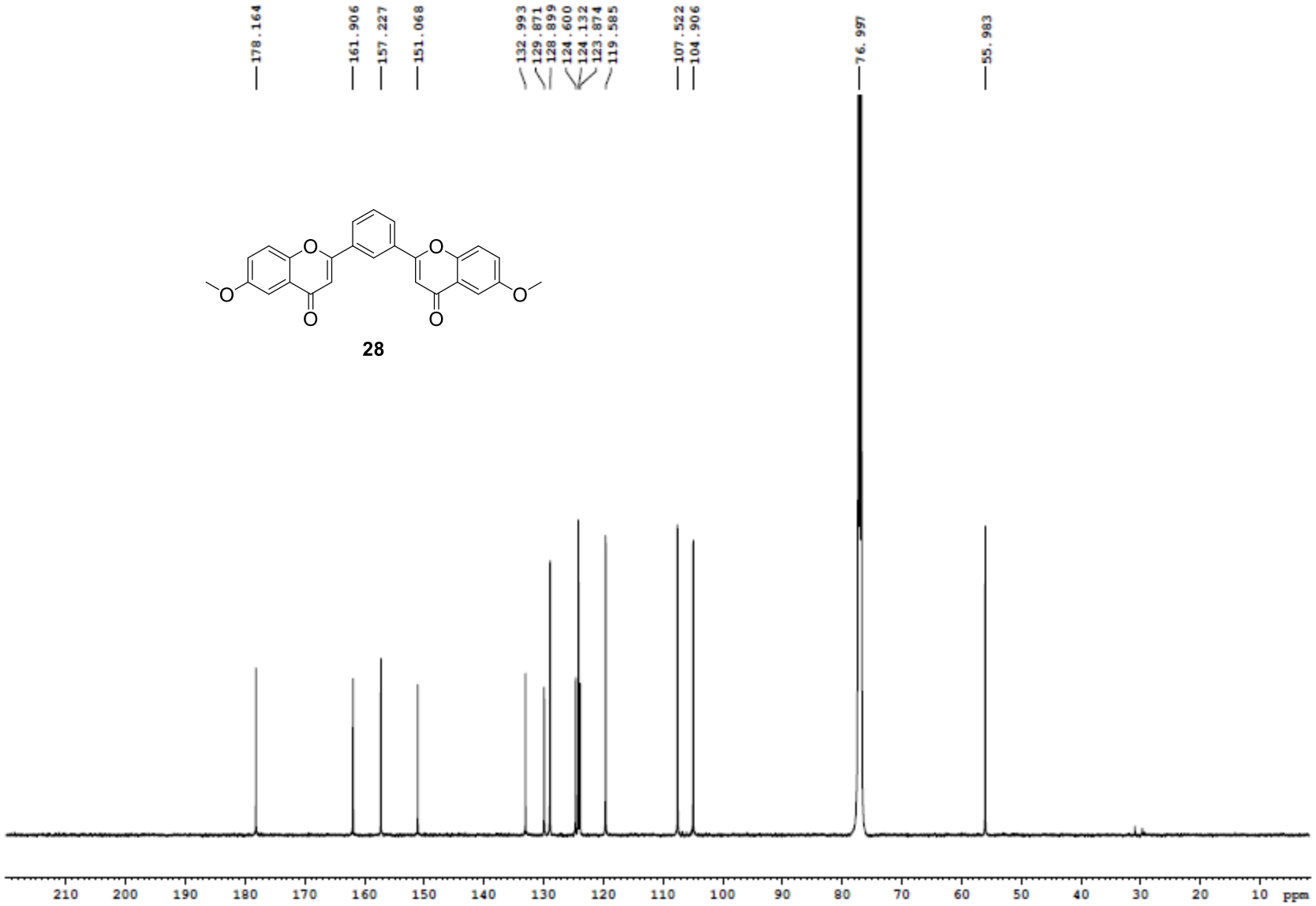

8.412
8.144
8.123
8.043
8.040
8.023
8.021
7.689
7.670
7.650
7.270
7.023
7.001
6.996
6.865
3.975
O
O
O
O
O
O
27
9
8
7
6
5
4
3
2
1
ppm
0.889
2.132
1.972
1.093
4.061
1.968
6.000


177.637
164.429
161.610
157.967
132.788
129.792
128.636
127.040
123.567
117.732
114.895
108.127
100.326
76.996
55.978
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

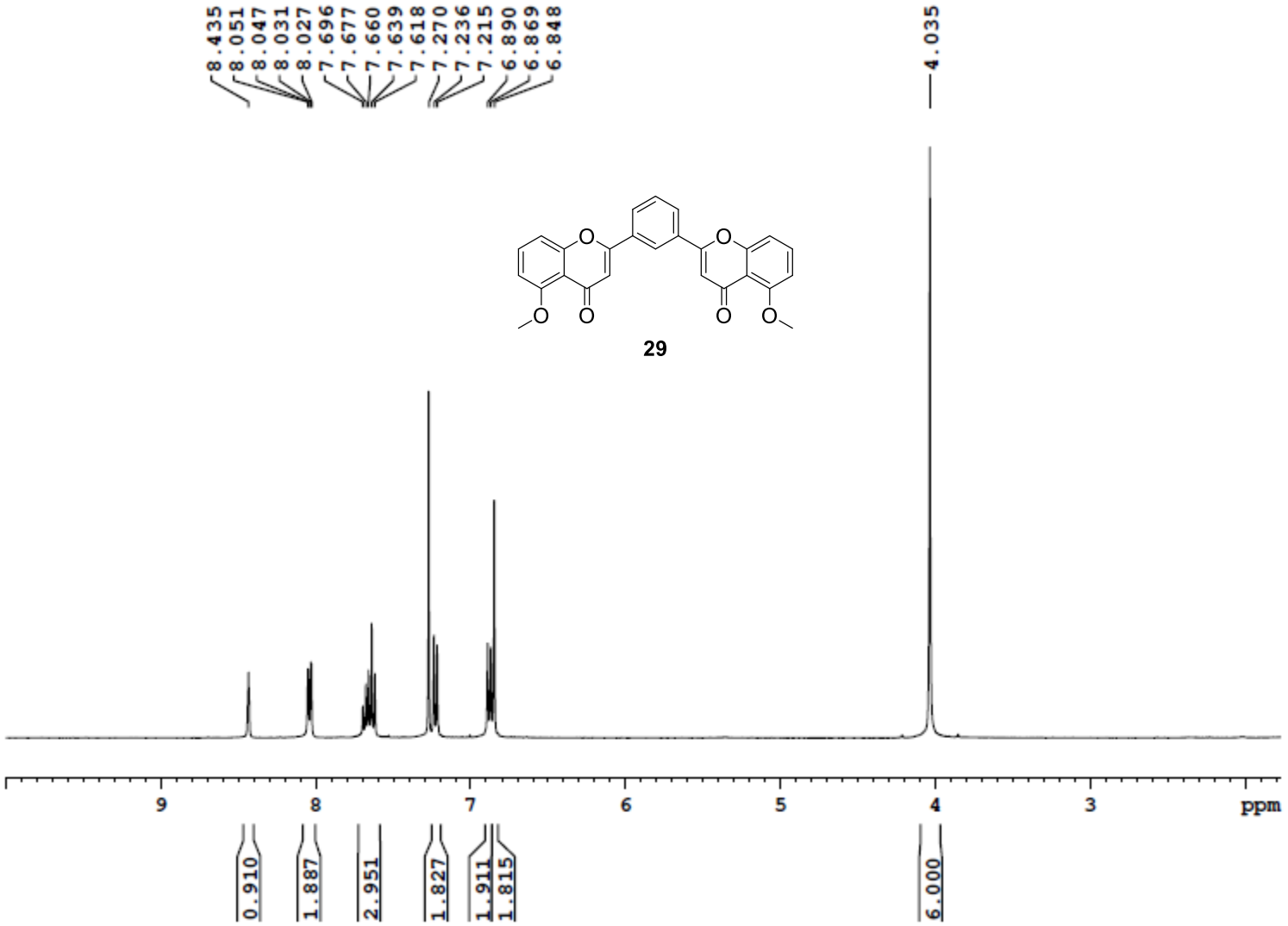
27


8.489
8.486
8.483
8.088
8.084
8.072
8.068
7.727
7.711
7.695
7.636
7.630
7.600
7.582
7.367
7.361
7.349
7.343
7.270
6.930
3.945
O
O
O
O
O
O
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
0.936
1.926
0.975
1.896
1.869
1.888
1.868
6.000

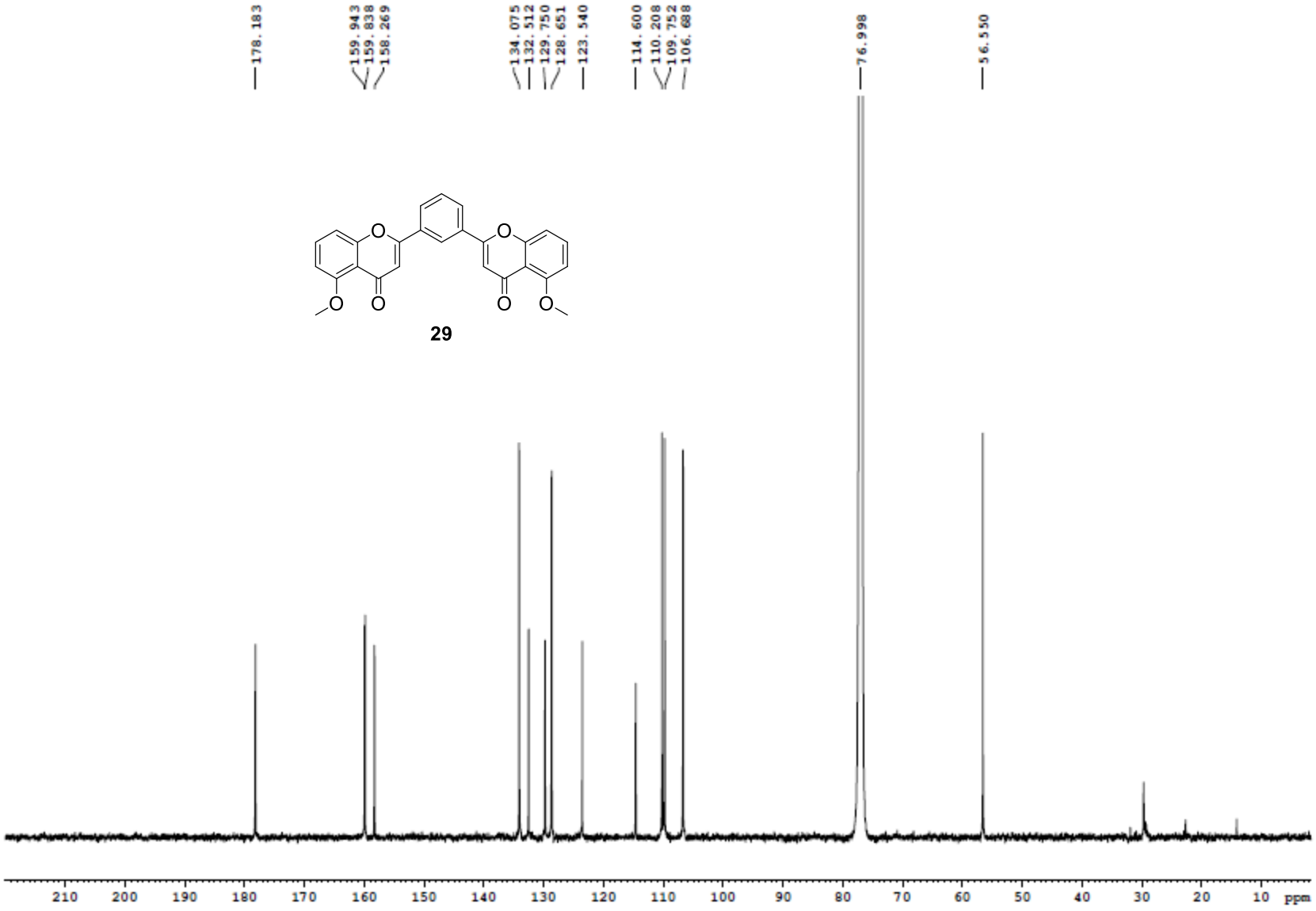
28


178.164
161.906
157.227
151.068
132.993
129.871
128.899
124.600
124.132
123.874
119.585
107.522
104.906
76.997
55.983
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

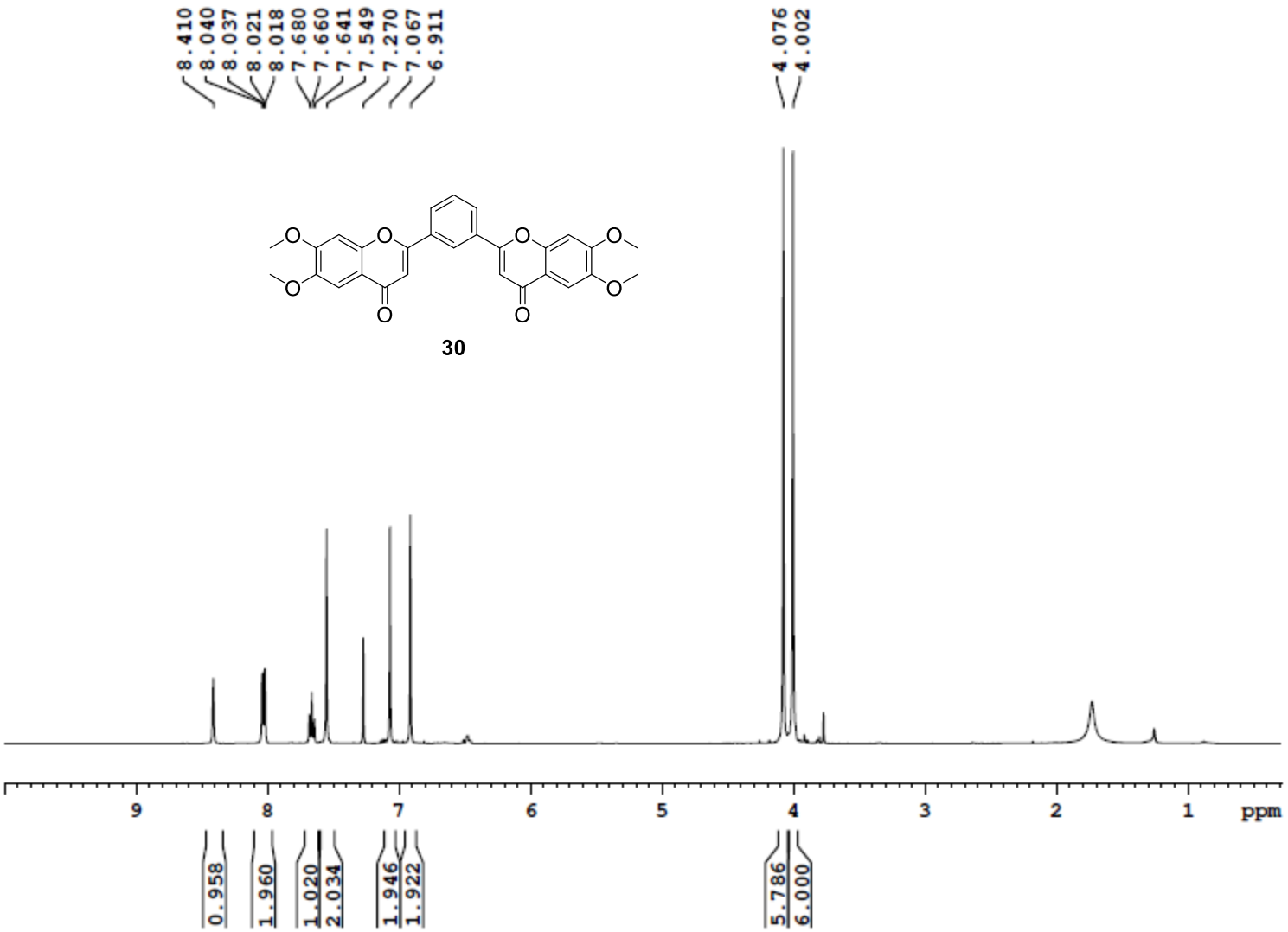
28

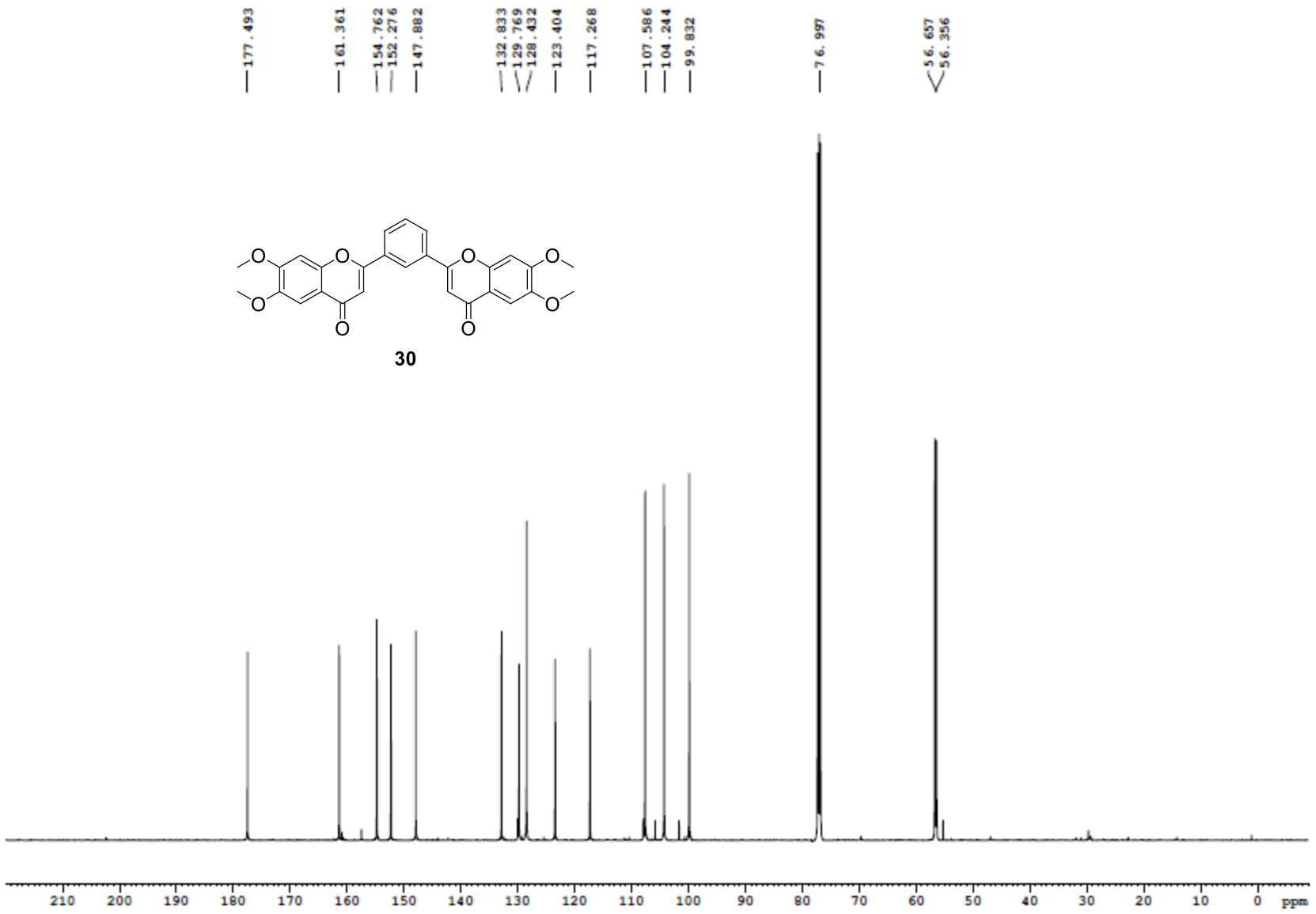

8.435
8.051
8.047
8.031
8.027
7.696
7.677
7.660
7.639
7.618
7.270
7.236
7.215
6.890
6.869
6.848
4.035
O
O
O
O
O
O
9
8
7
6
5
4
3
ppm
0.910
1.887
2.951
1.827
1.911
1.815
6.000

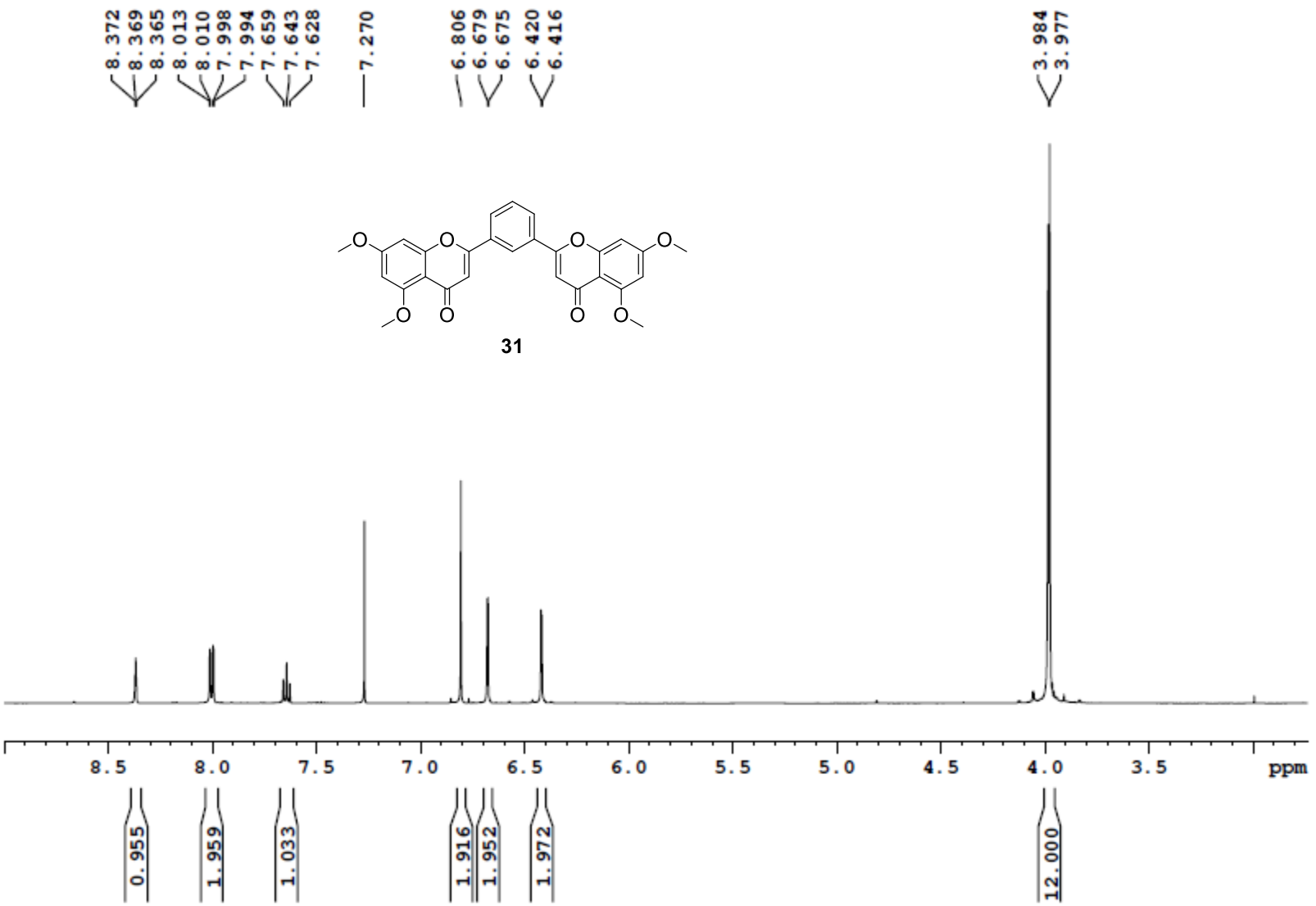
29

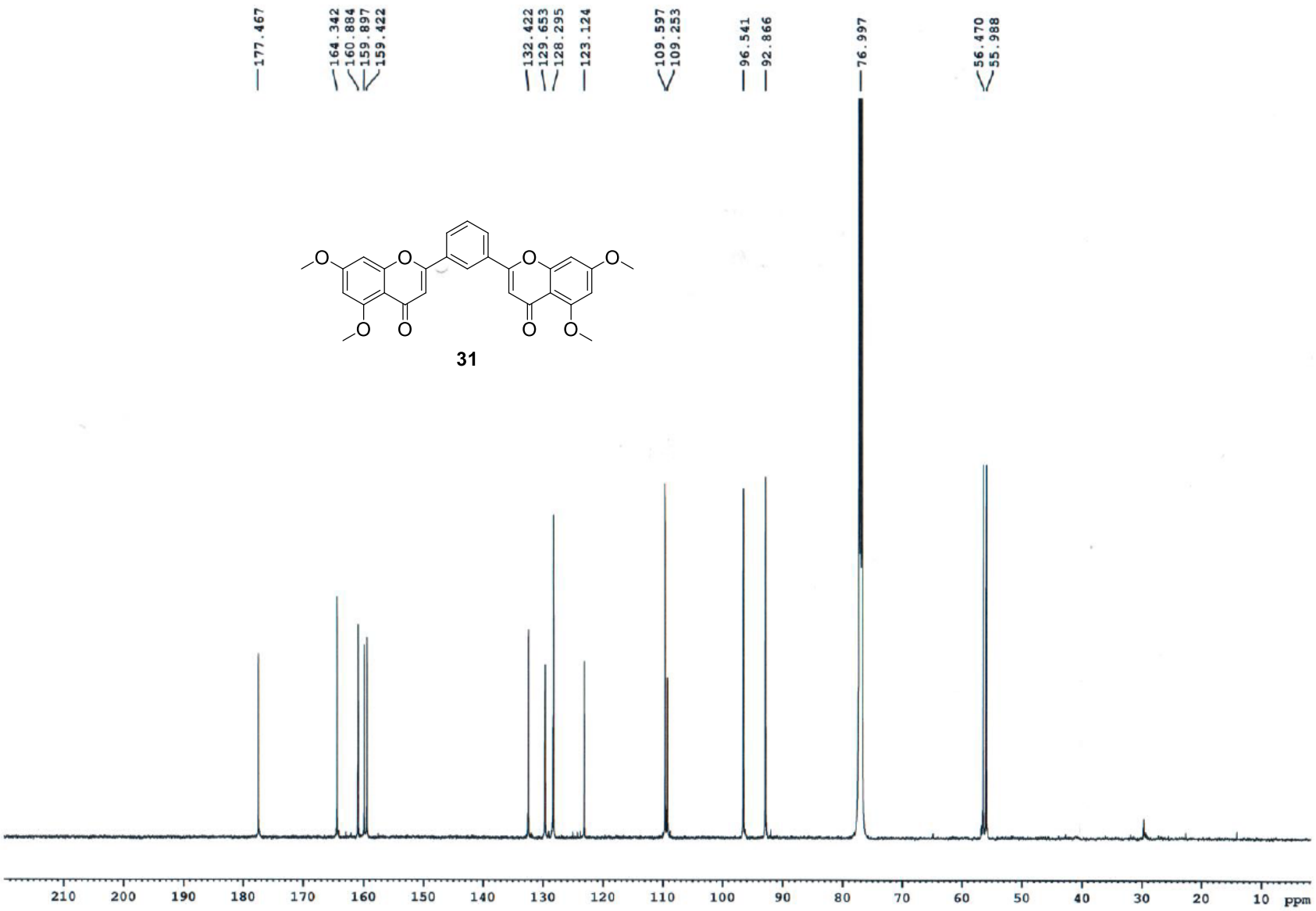

178.183
159.943
159.838
158.269
134.075
132.512
129.750
128.651
123.540
114.600
110.208
109.752
106.688
76.998
56.550
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

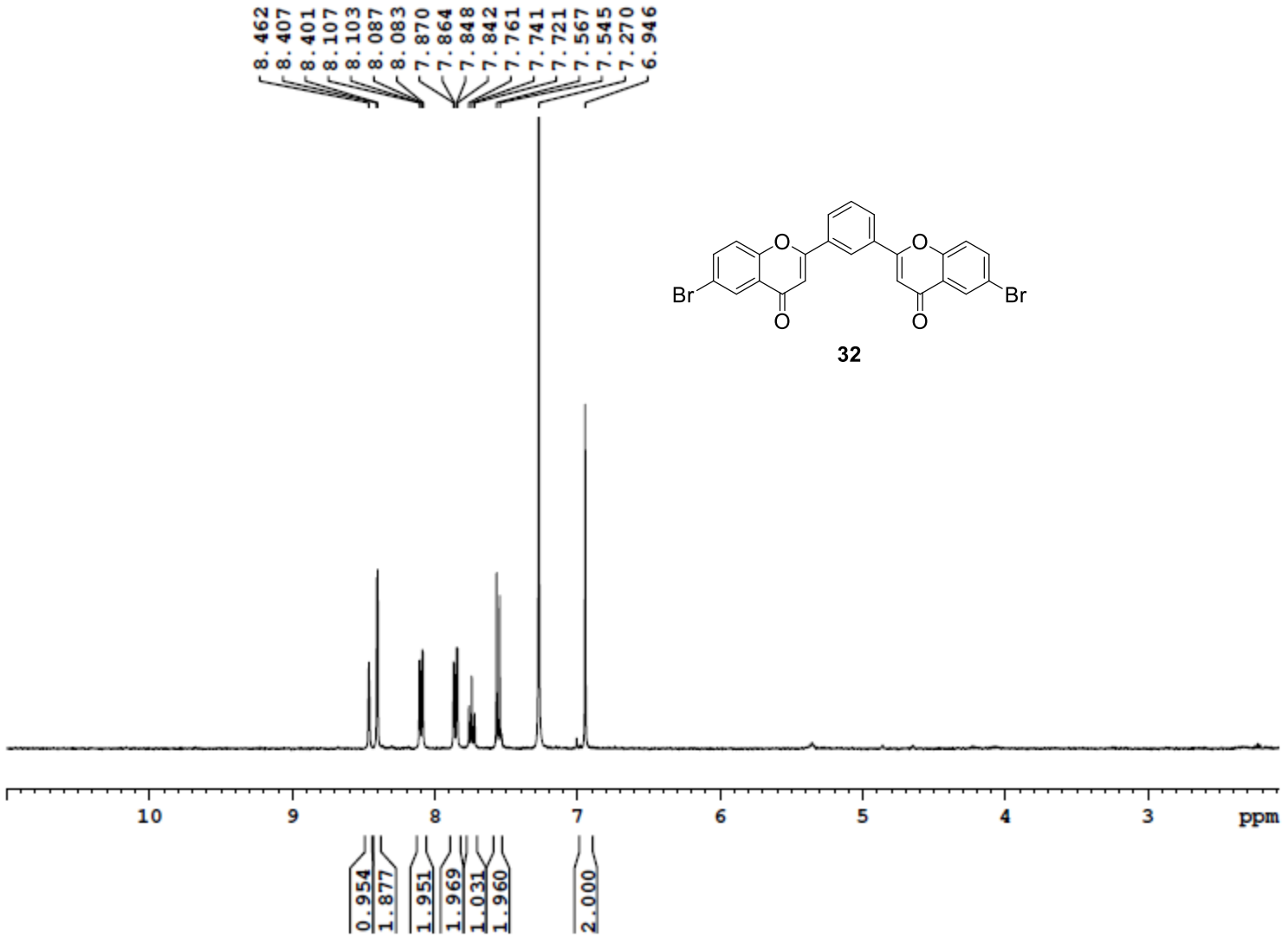
29

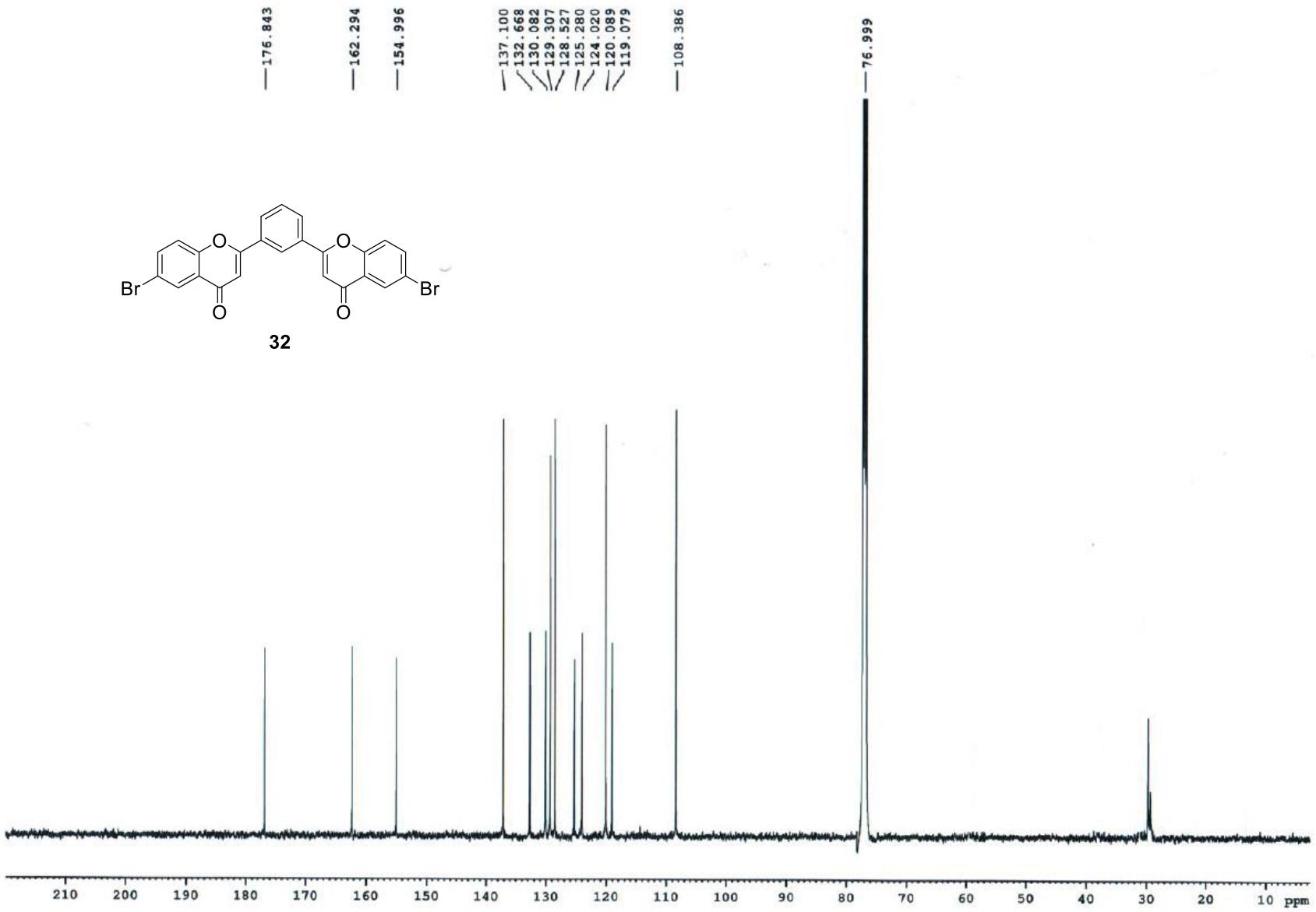

8.410
8.040
8.037
8.021
8.018
7.680
7.660
7.641
7.549
7.270
7.067
6.911
4.076
4.002
30
9
8
7
6
5
4
3
2
1
ppm
0.958
1.960
1.020
2.034
1.946
1.922
5.786
6.000


177.493
161.361
154.762
152.276
147.882
132.833
129.769
128.432
123.404
117.268
107.586
104.244
99.832
76.997
56.657
56.356
O
O
O
O
O
O
O
O
30
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

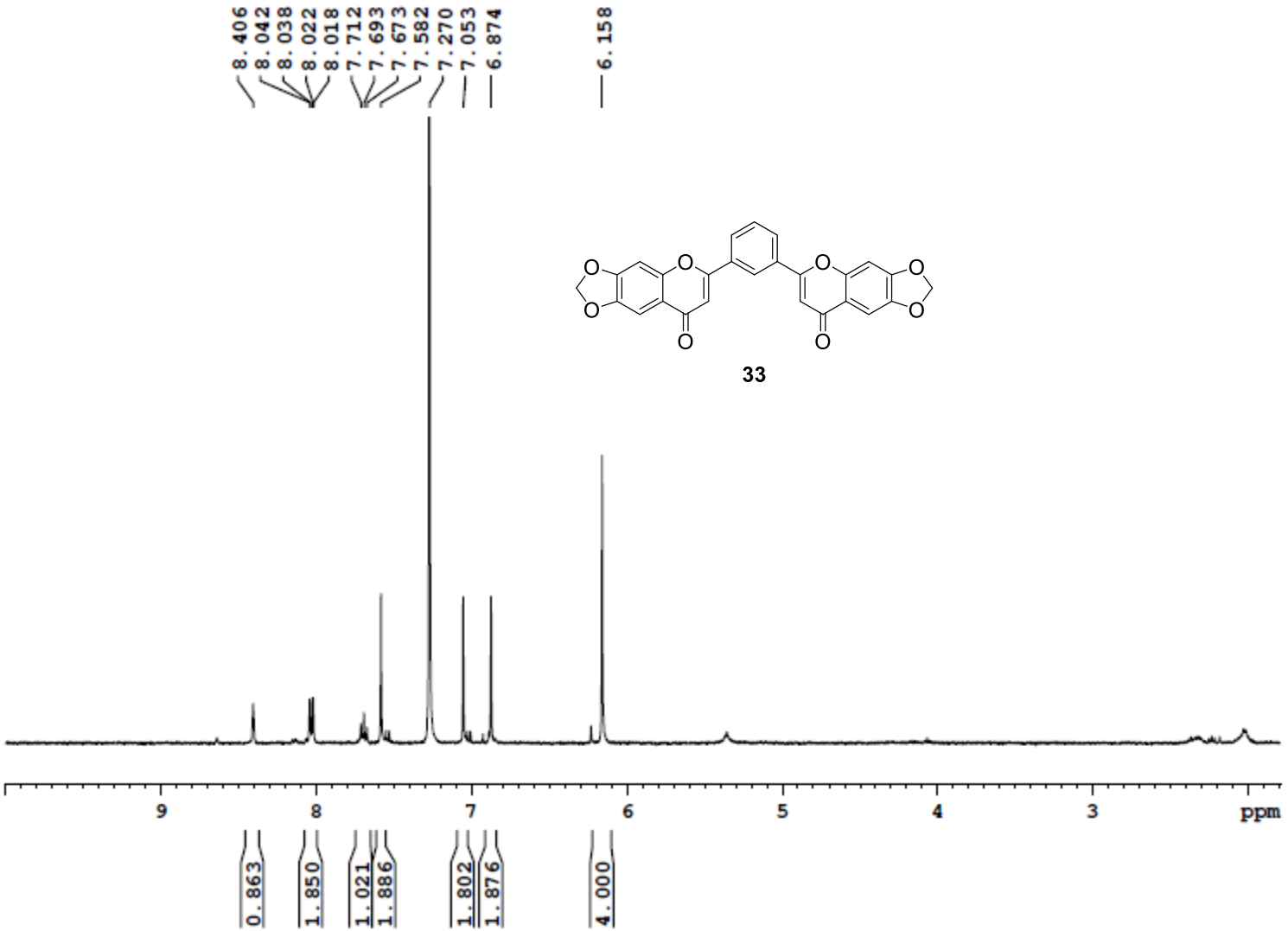

8.372
8.369
8.365
8.013
8.010
7.998
7.994
7.659
7.643
7.628
7.270
6.806
6.679
6.675
6.420
6.416
3.984
3.977
31
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm
0.955
1.959
1.033
1.916
1.952
1.972
12.000


177.467
164.342
160.884
159.897
159.422
132.422
129.653
128.295
123.124
109.597
109.253
96.541
92.866
76.997
56.470
55.988
31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

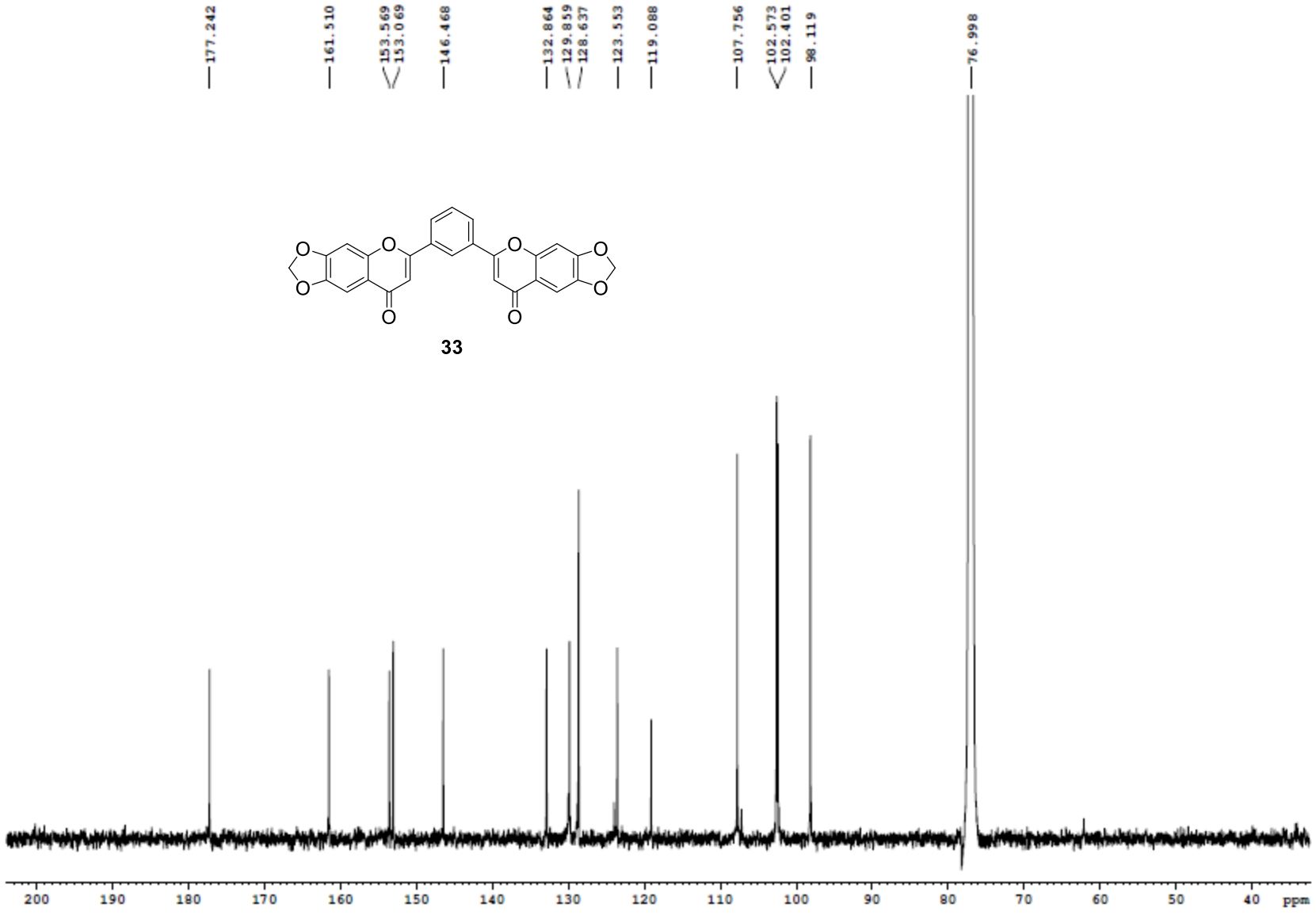

8.462
8.407
8.401
8.107
8.103
8.087
8.083
7.870
7.864
7.848
7.842
7.761
7.741
7.721
7.567
7.545
7.270
6.946
Br
Br
O
O
O
O
32
10
9
8
7
6
5
4
3
ppm
0.954
1.877
1.951
1.969
1.031
1.960
2.000


176.843
162.294
154.996
137.100
132.668
130.082
129.307
128.527
125.280
124.020
120.089
119.079
108.386
76.999
Br
Br
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

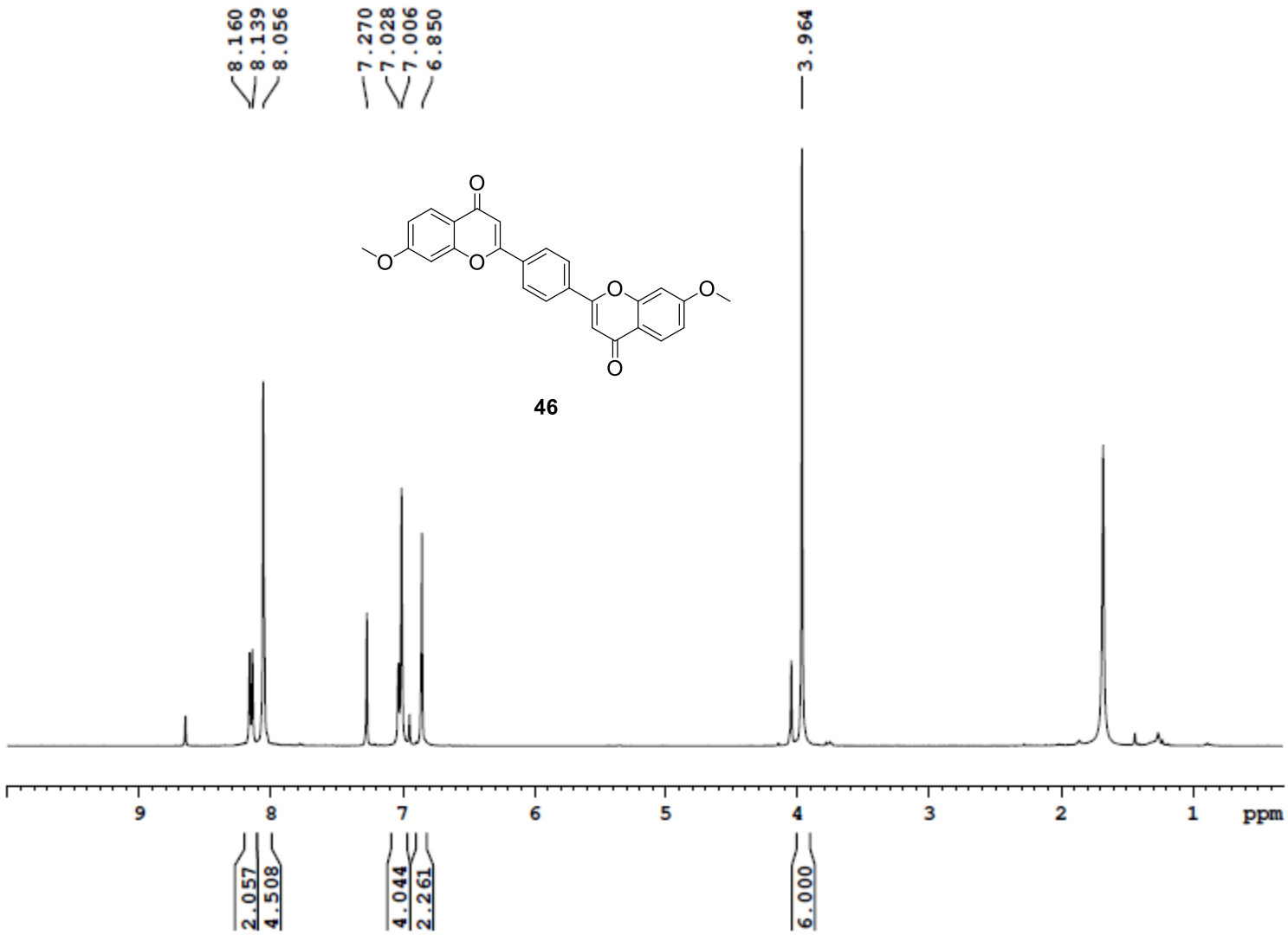
32


8.406
8.042
8.038
8.022
8.018
7.712
7.693
7.673
7.582
7.270
7.053
6.874
6.158
9
8
7
6
5
4
3
ppm
0.863
1.850
1.021
1.886
1.802
1.876
4.000

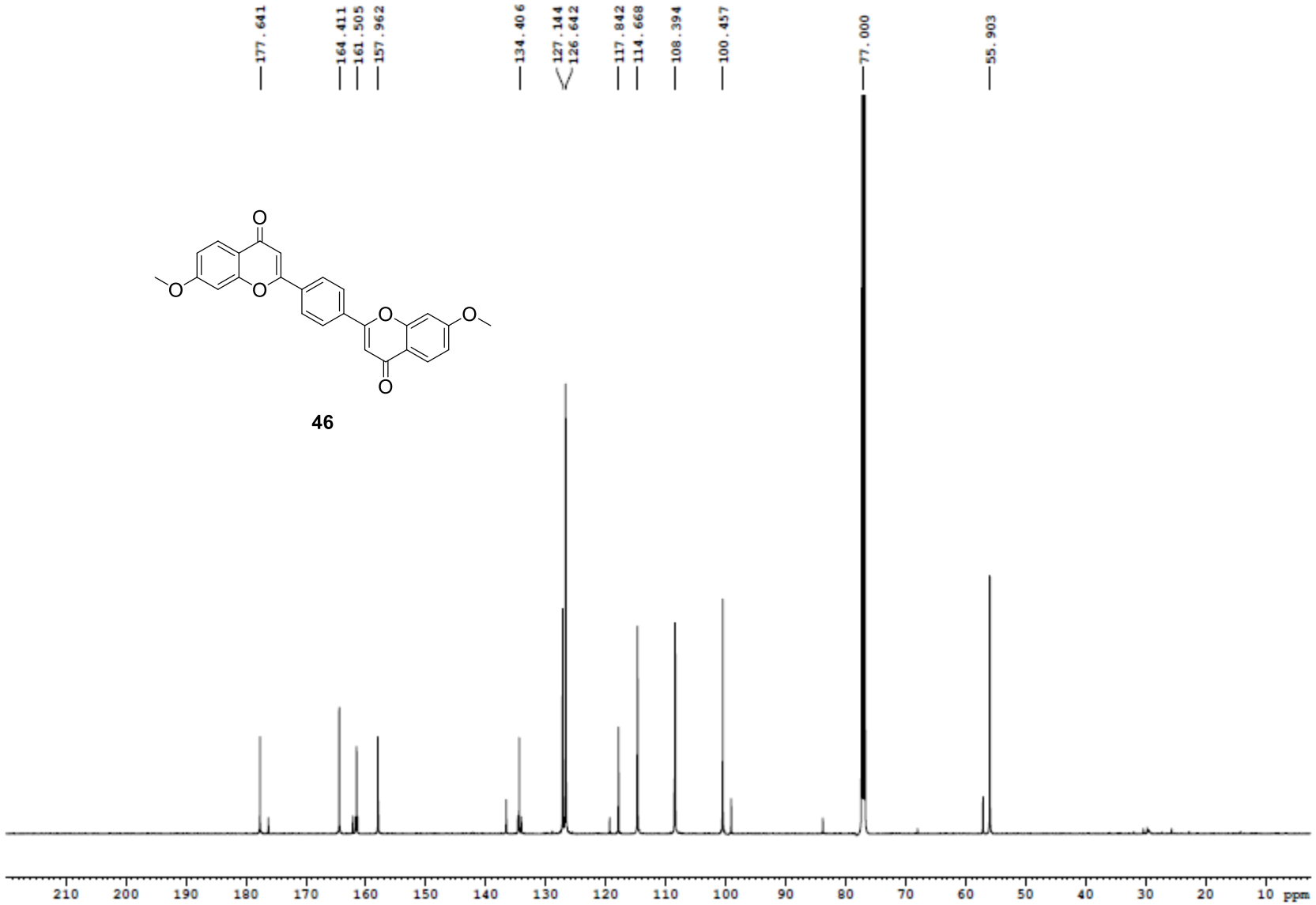
33


177.242
161.510
153.569
153.069
146.468
132.864
129.859
128.637
123.553
119.088
107.756
102.573
102.401
98.119
76.998
O
O
O
O
O
O
O
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
ppm

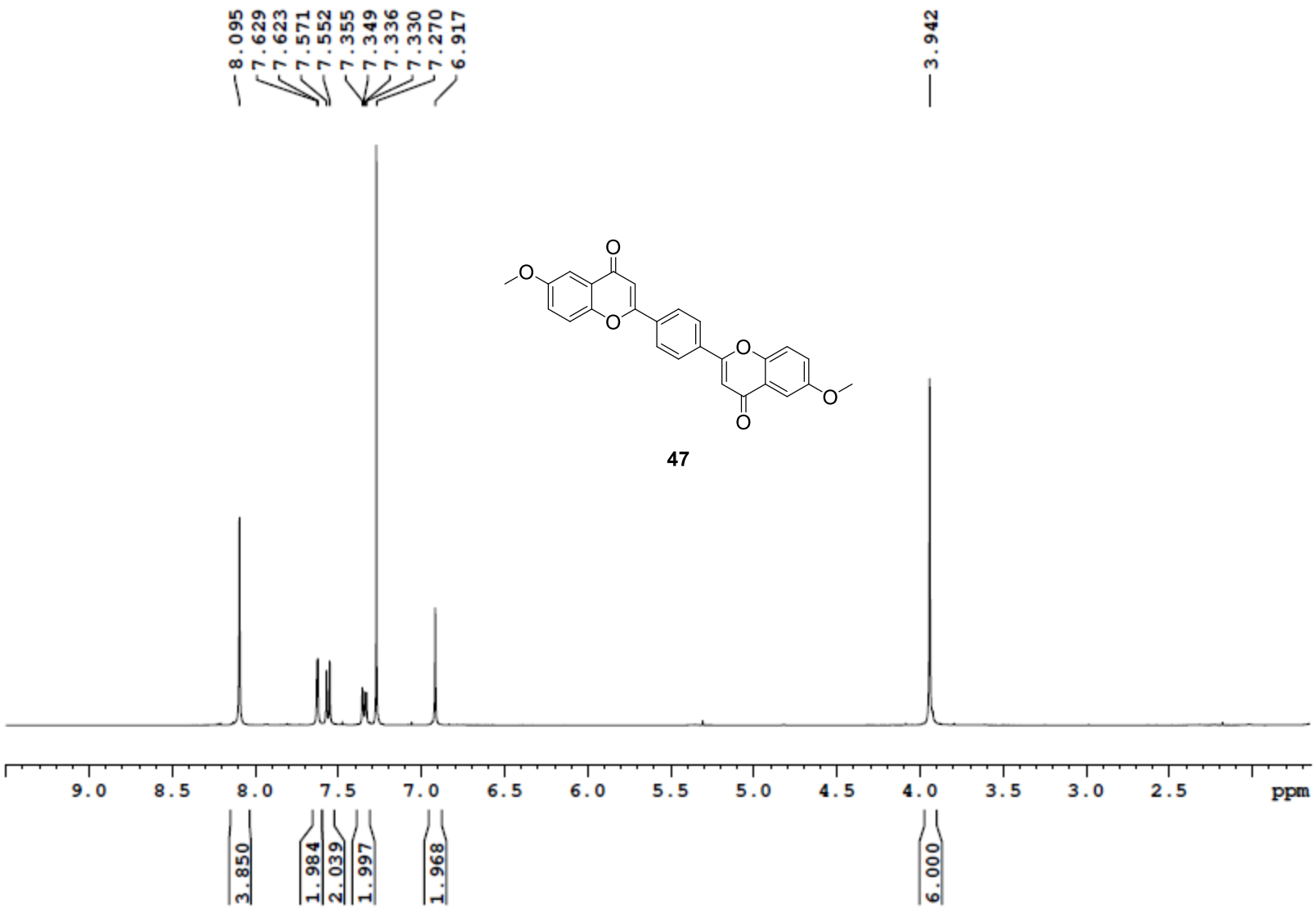
33


8.160
8.139
8.056
7.270
7.028
7.006
6.850
3.964
O
O
O
O
O
O
9
8
7
6
5
4
3
2
1
ppm
2.057
4.508
4.044
2.261
6.000

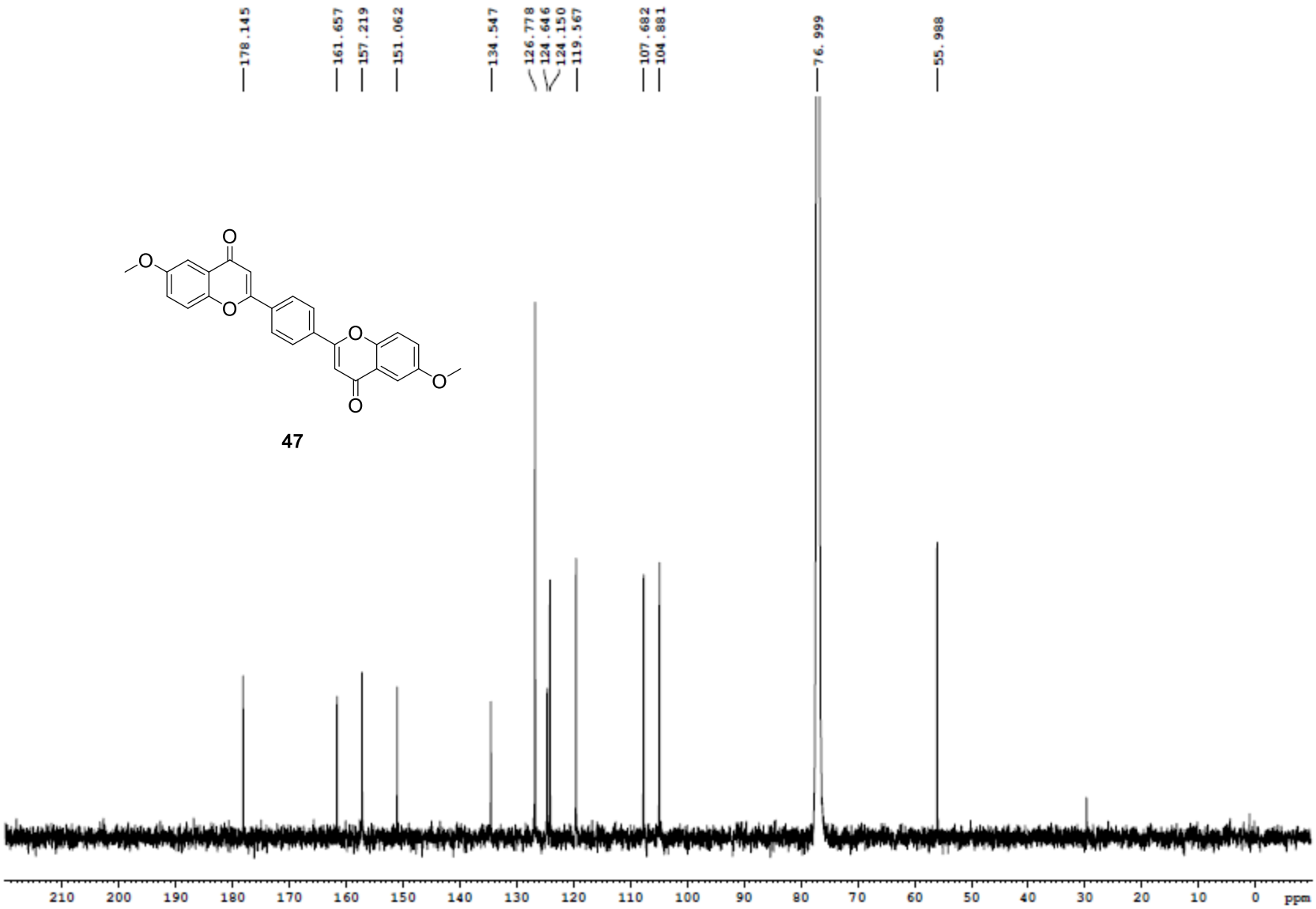
46

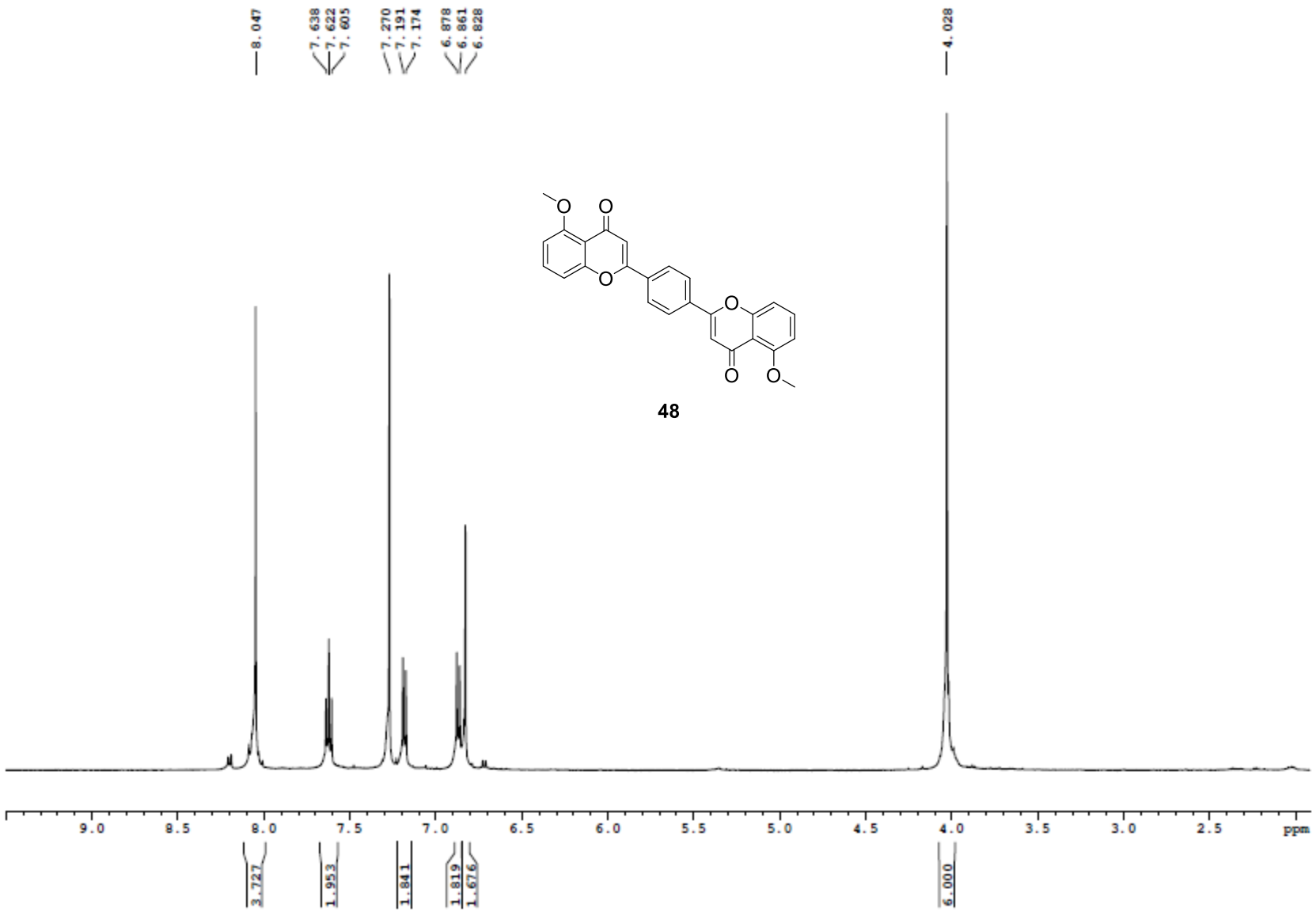

177.641
164.411
161.505
157.962
134.406
127.144
126.642
117.842
114.668
108.394
100.457
77.000
55.903
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

46

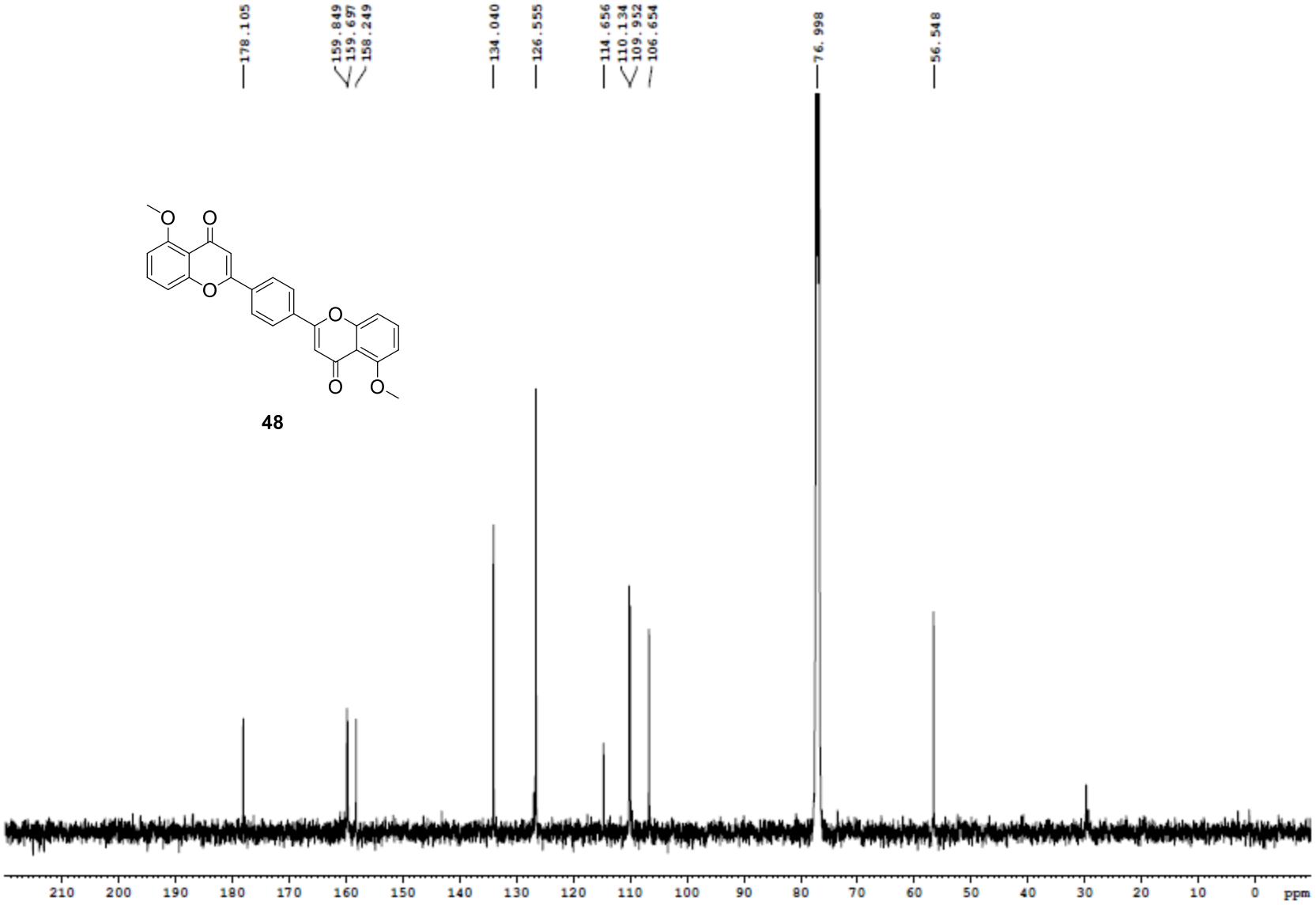

8.095
7.629
7.623
7.571
7.552
7.355
7.349
7.336
7.330
7.270
6.917
3.942
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.850
1.984
2.039
1.997
1.968
6.000

47

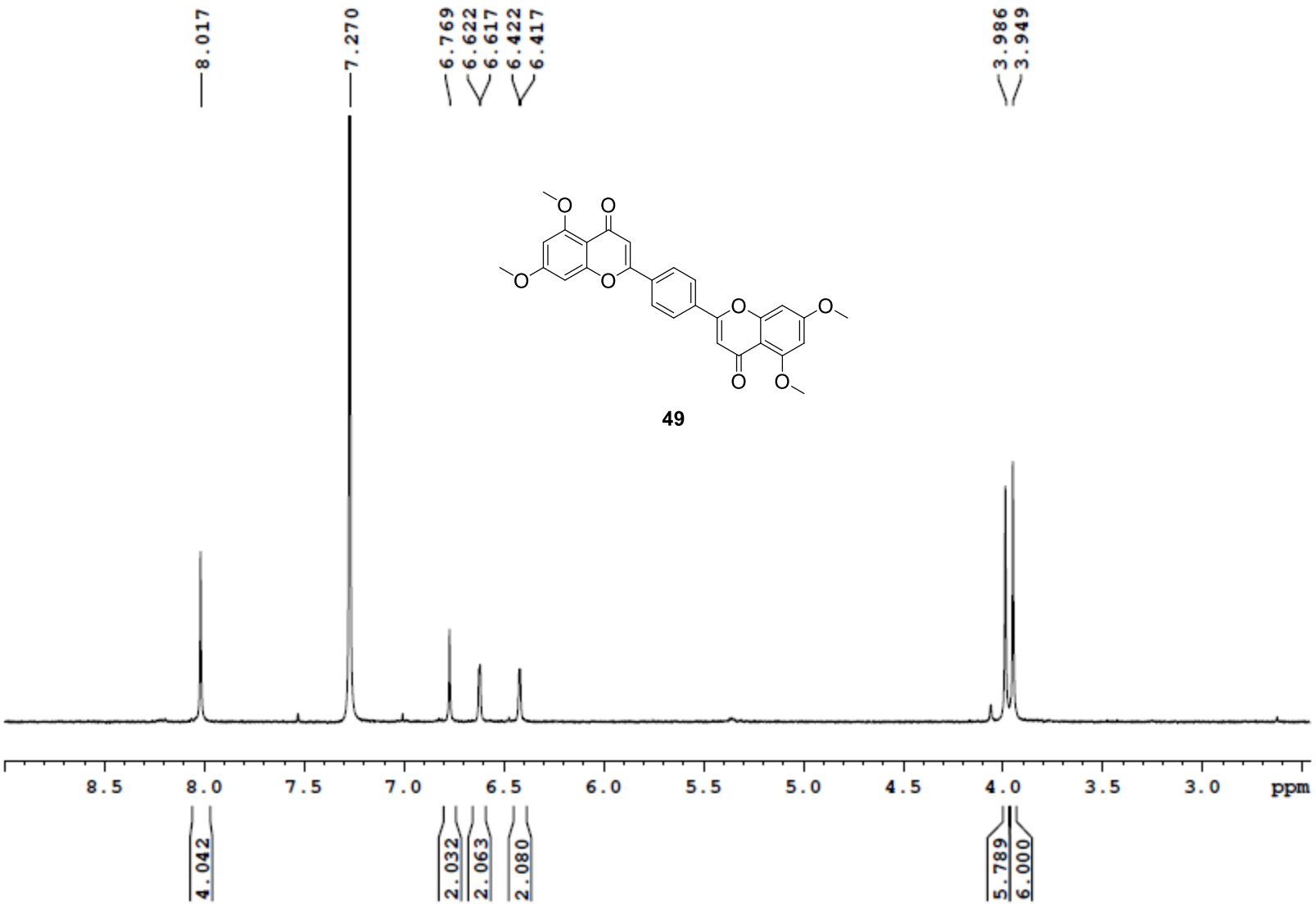

178.145
161.657
157.219
151.062
134.547
126.778
124.646
124.150
119.567
107.682
104.881
76.999
55.988
O
O
O
O
O
O
47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.047
7.638
7.622
7.605
7.270
7.191
7.174
6.878
6.861
6.828
4.028
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
3.727
1.953
1.841
1.819
1.676
6.000

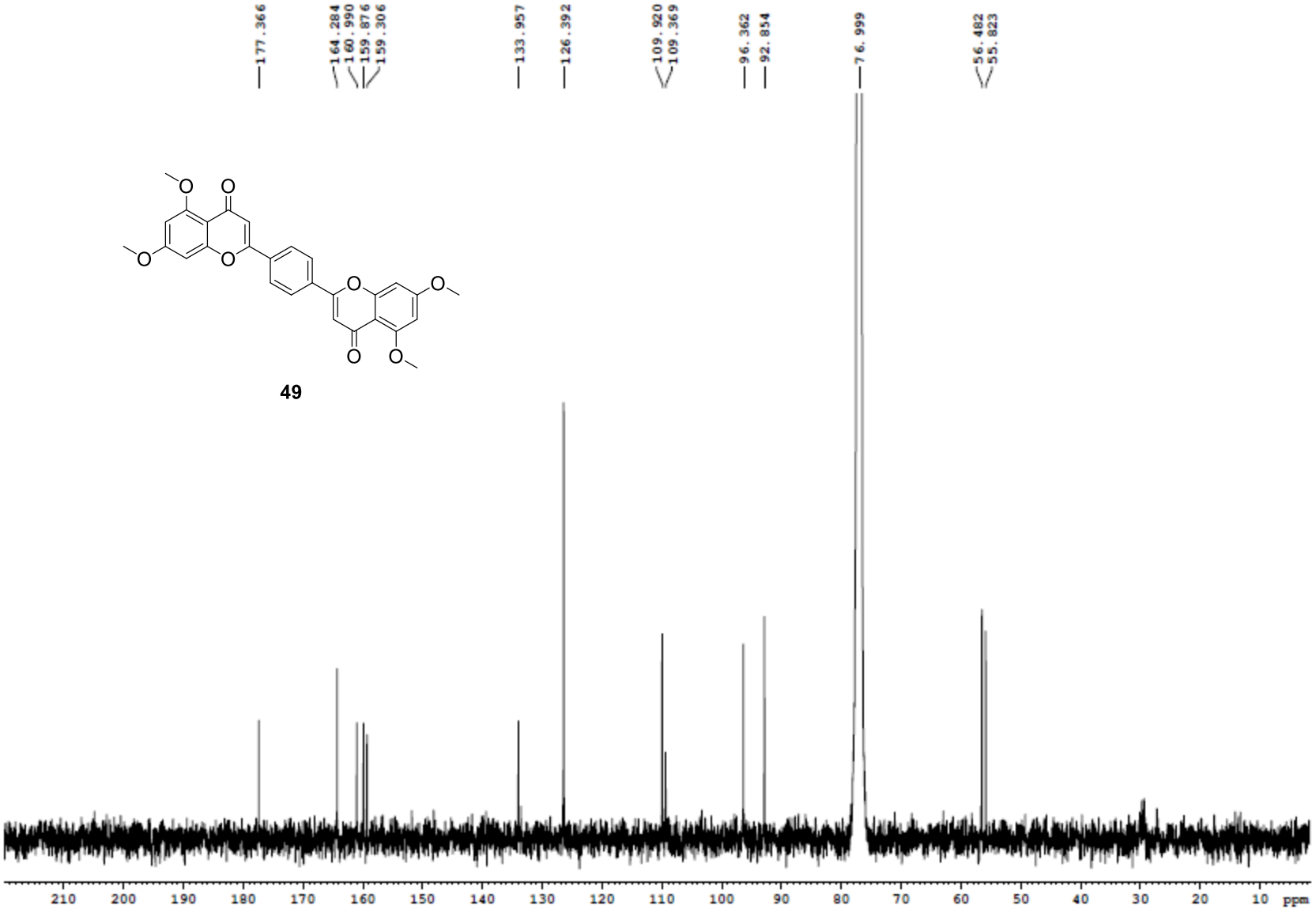
48

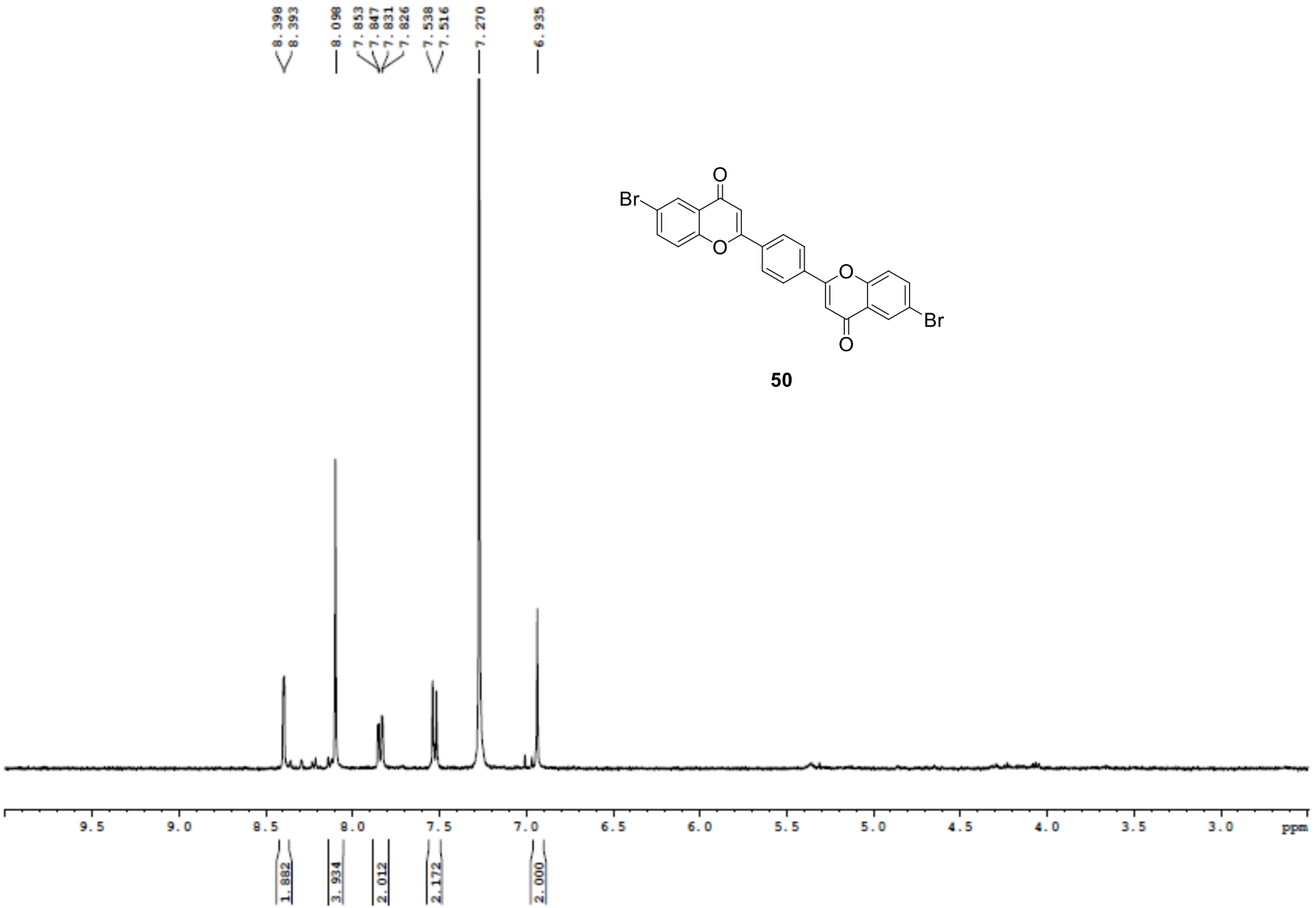

178.105
159.849
159.697
158.249
134.040
126.555
114.656
110.134
109.952
106.654
76.998
56.548
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

48

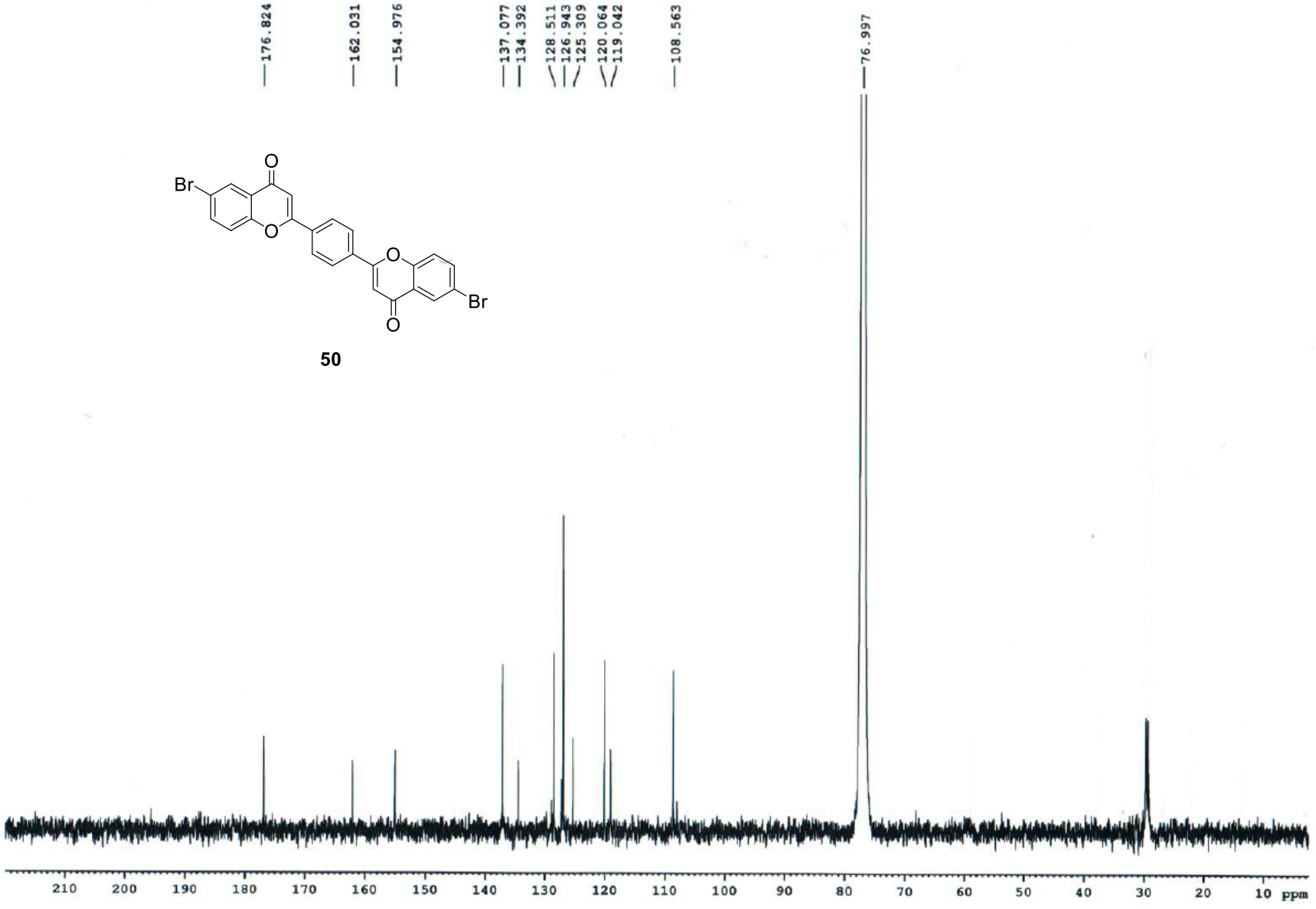

8.017
7.270
6.769
6.622
6.617
6.422
6.417
3.986
3.949
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm
4.042
2.032
2.063
2.080
5.789
6.000

49

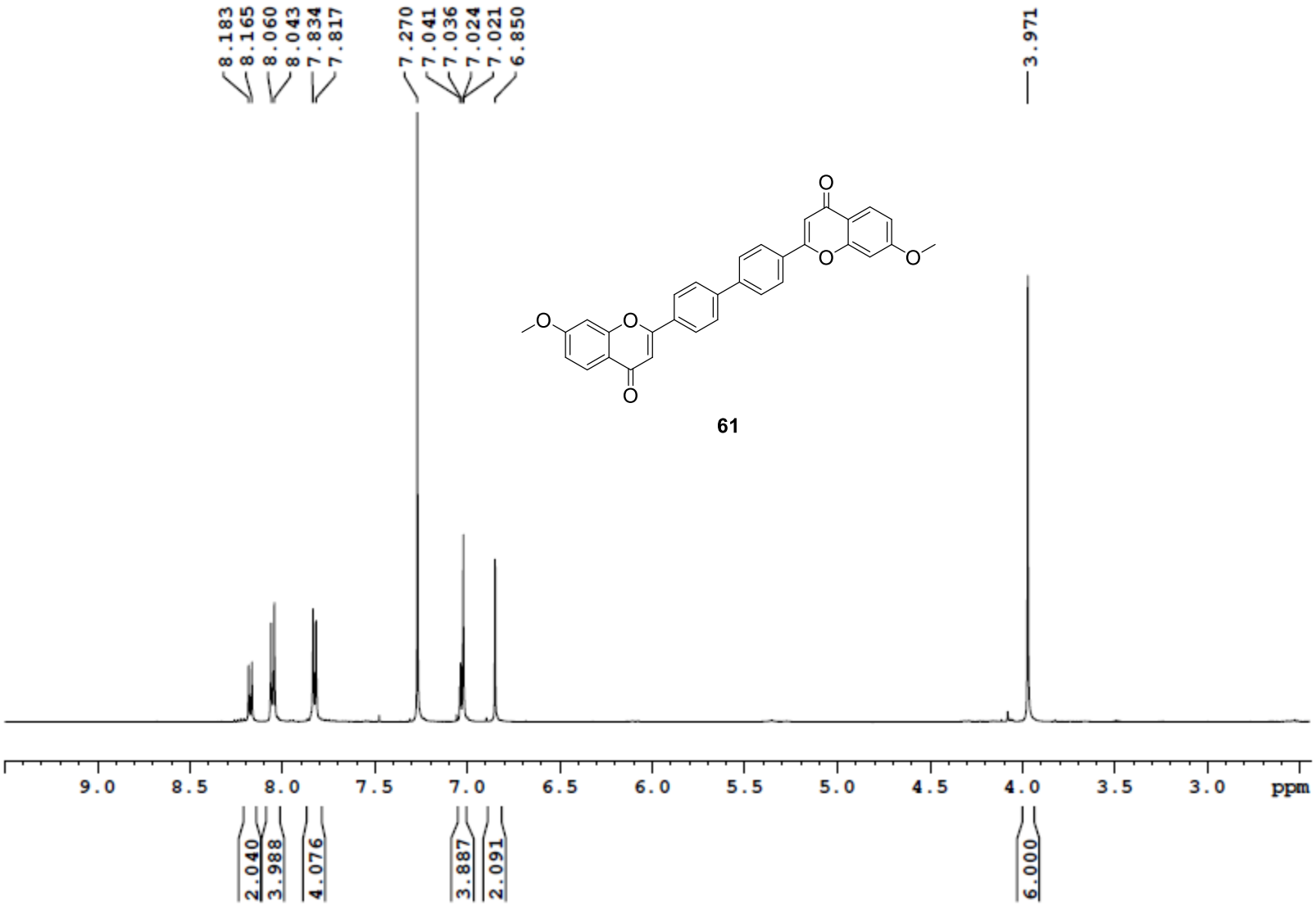

177.366
164.284
160.990
159.876
159.306
133.957
126.392
109.920
109.369
96.362
92.854
76.999
56.482
55.823
49
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.398
8.393
8.098
7.853
7.847
7.831
7.826
7.538
7.516
7.270
6.935
Br
O
O
O
O
Br
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
1.882
3.934
2.012
2.172
2.000

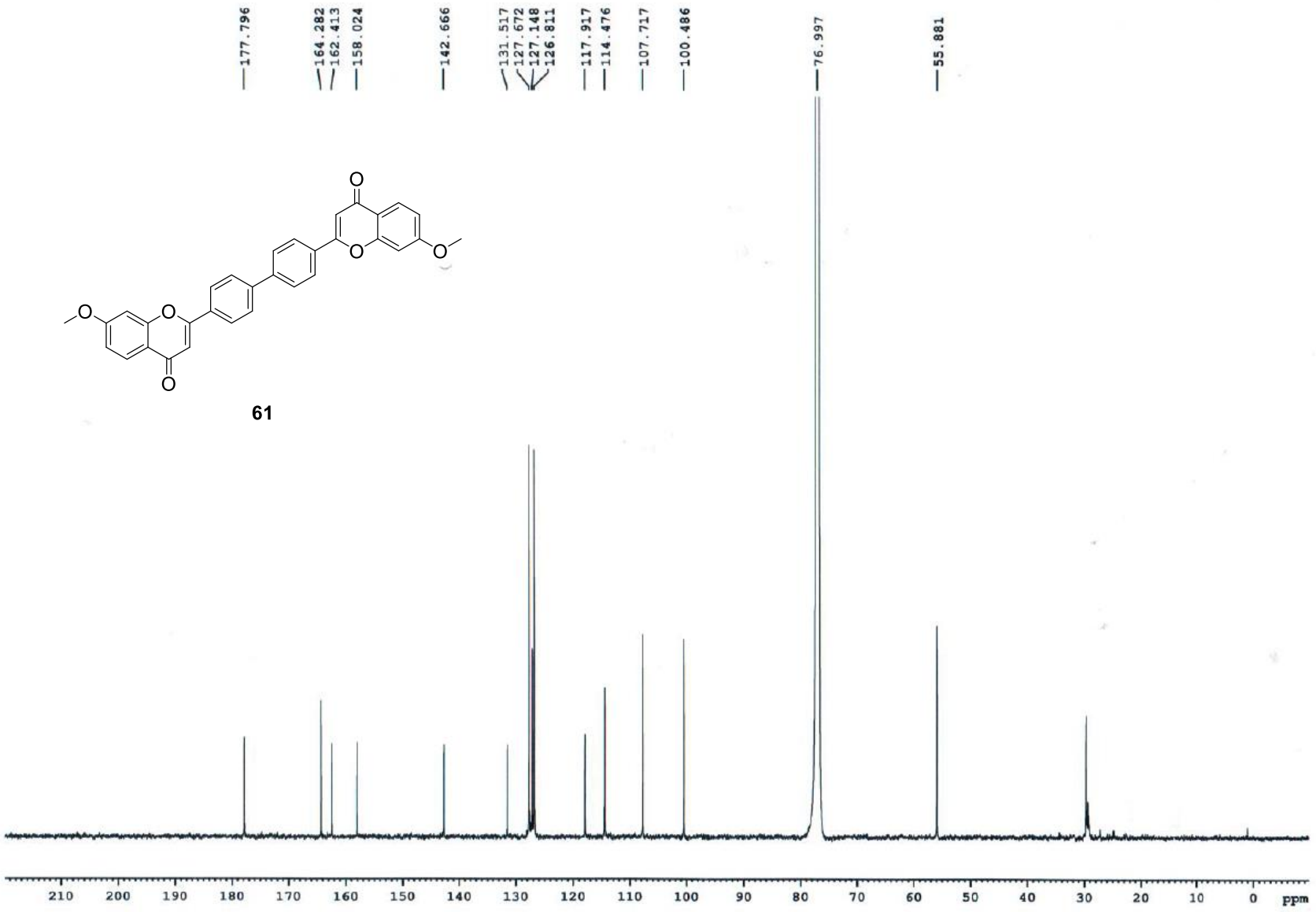
50

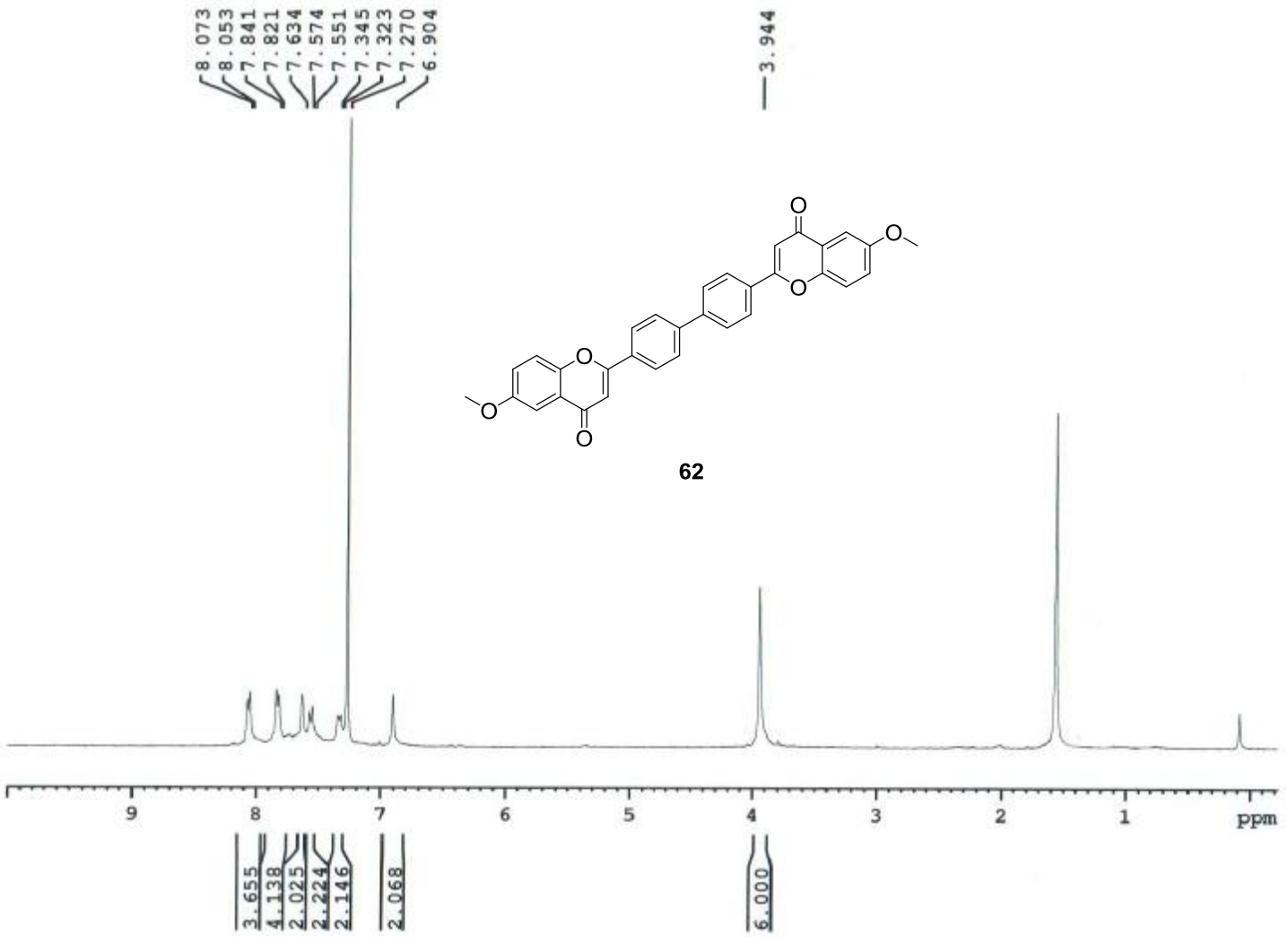

176.824
162.031
154.976
137.077
134.392
128.511
126.943
125.309
120.064
119.042
108.563
76.997
Br
O
O
O
O
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

50

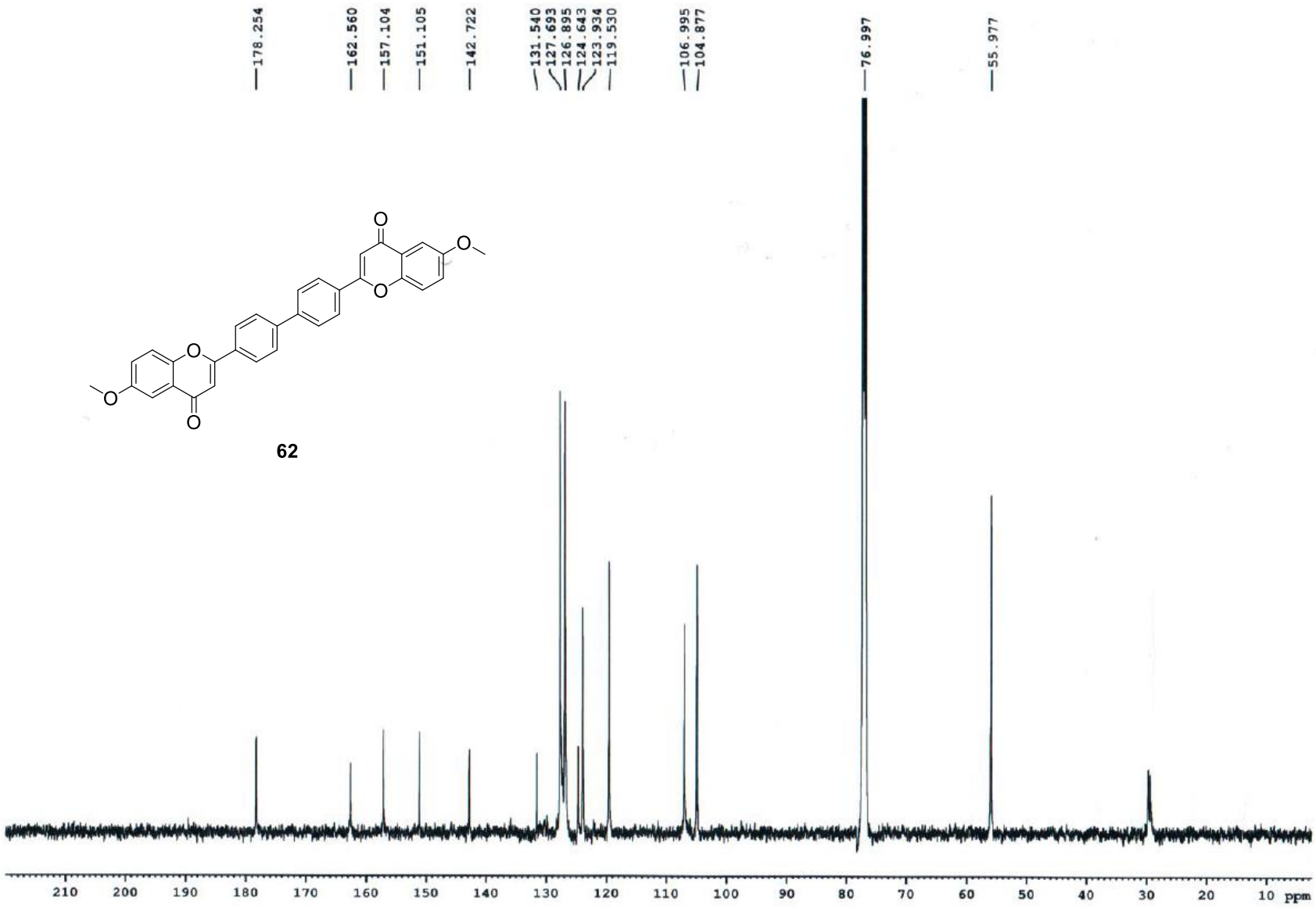

8.183
8.165
8.060
8.043
7.834
7.817
7.270
7.041
7.036
7.024
7.021
6.850
3.971
O
O
O
O
O
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
ppm
2.040
3.988
4.076
3.887
2.091
6.000

61

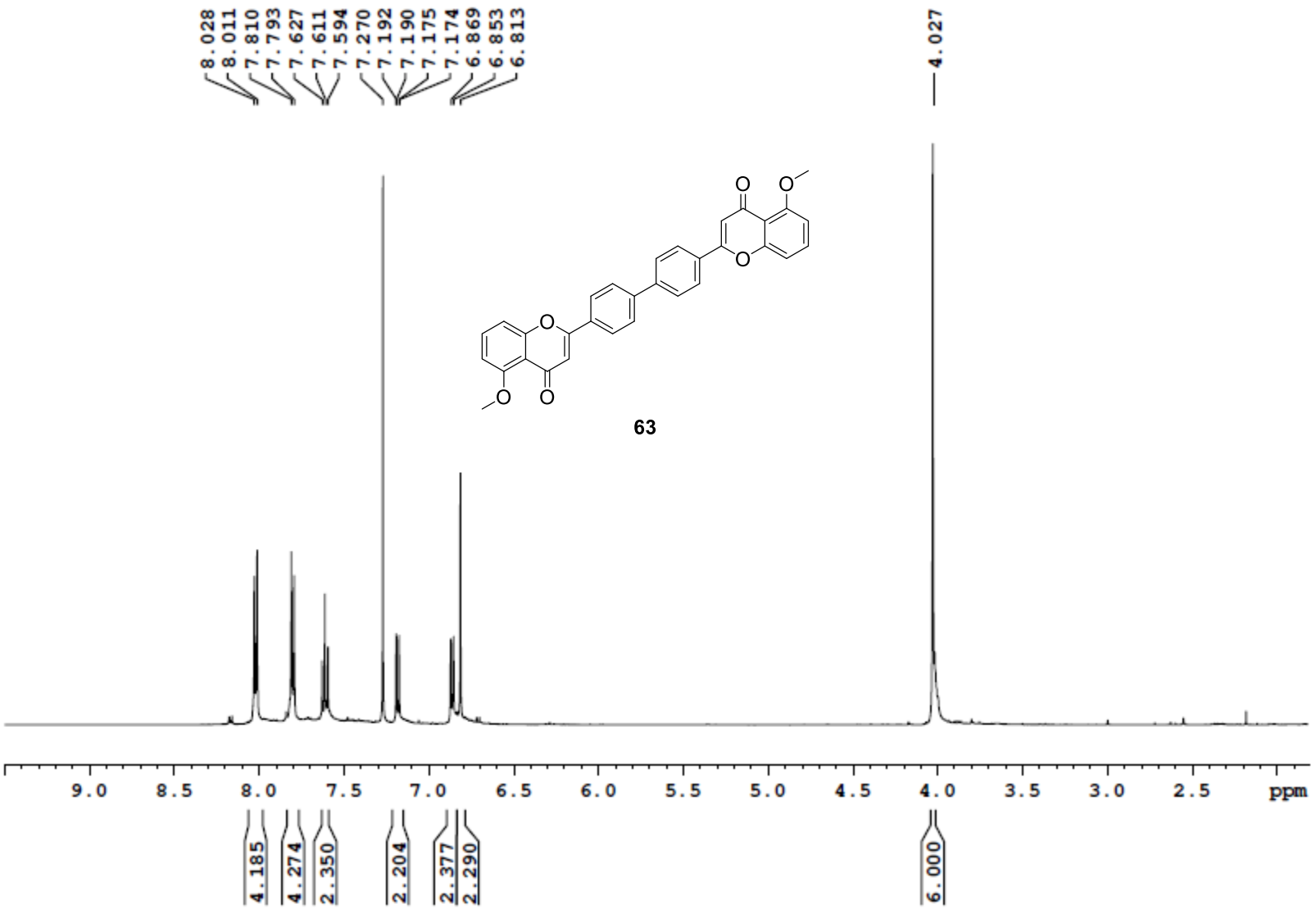

177.796
164.282
162.413
158.024
142.666
131.517
127.672
127.148
126.811
117.917
114.476
107.717
100.486
76.997
55.881
O
O
O
O
O
O
61
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.073
8.053
7.841
7.821
7.634
7.574
7.551
7.345
7.323
7.270
6.904
3.944
O
O
O
O
O
O
9
8
7
6
5
4
3
2
1
ppm
3.655
4.138
2.025
2.224
2.146
2.068
6.000

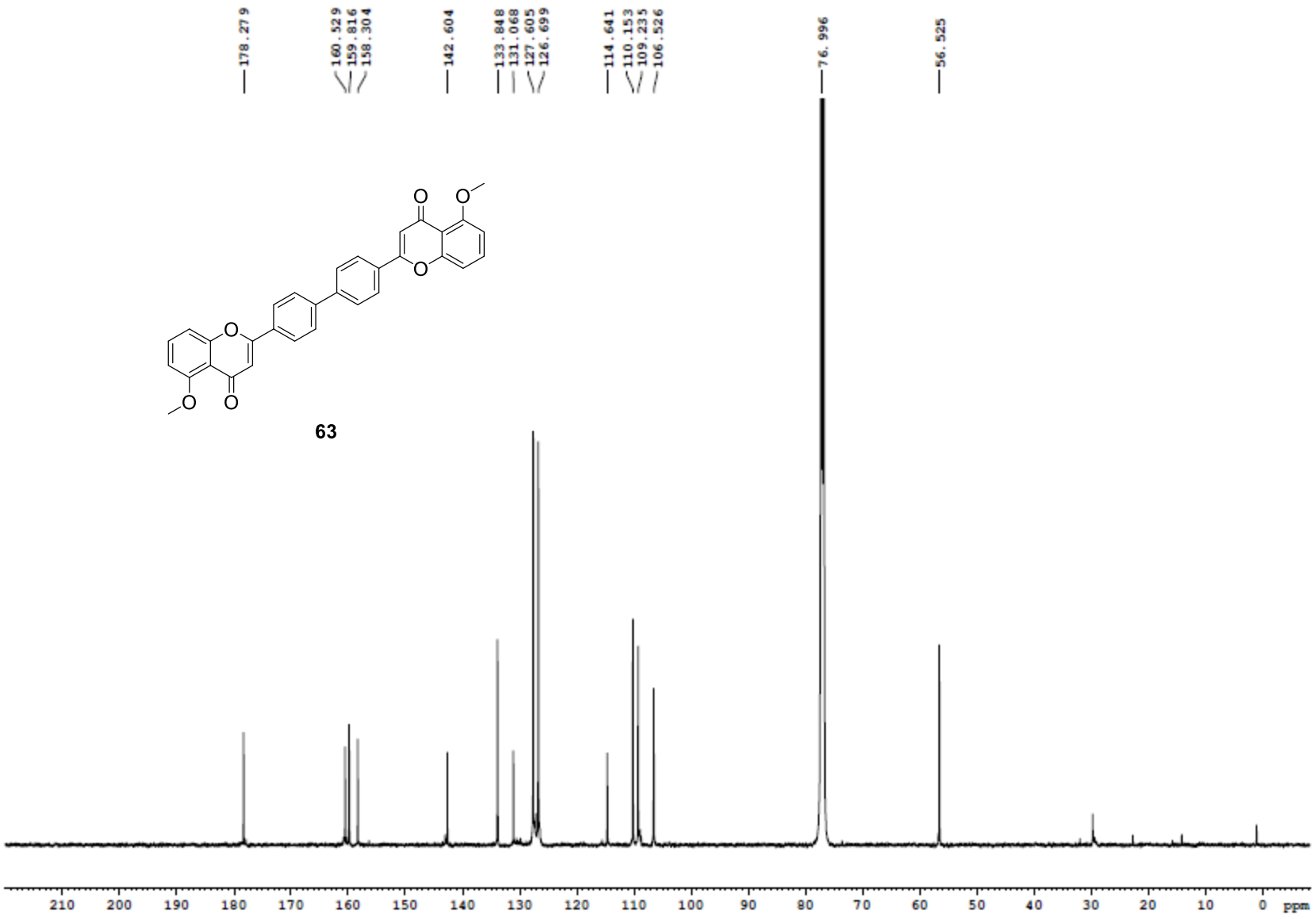
62

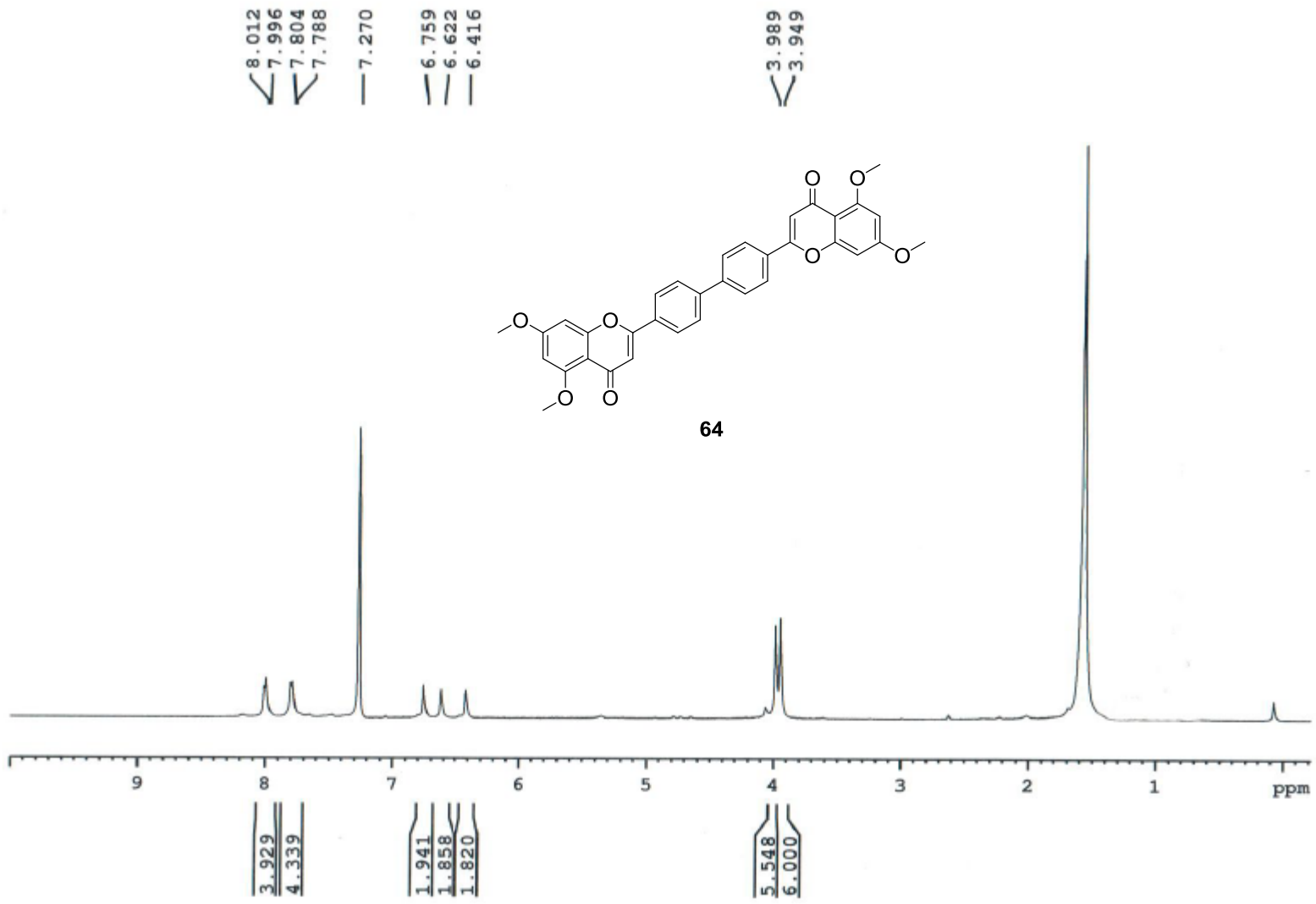

178.254
162.560
157.104
151.105
142.722
131.540
127.693
126.895
124.643
123.934
119.530
106.995
104.877
76.997
55.977
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

62

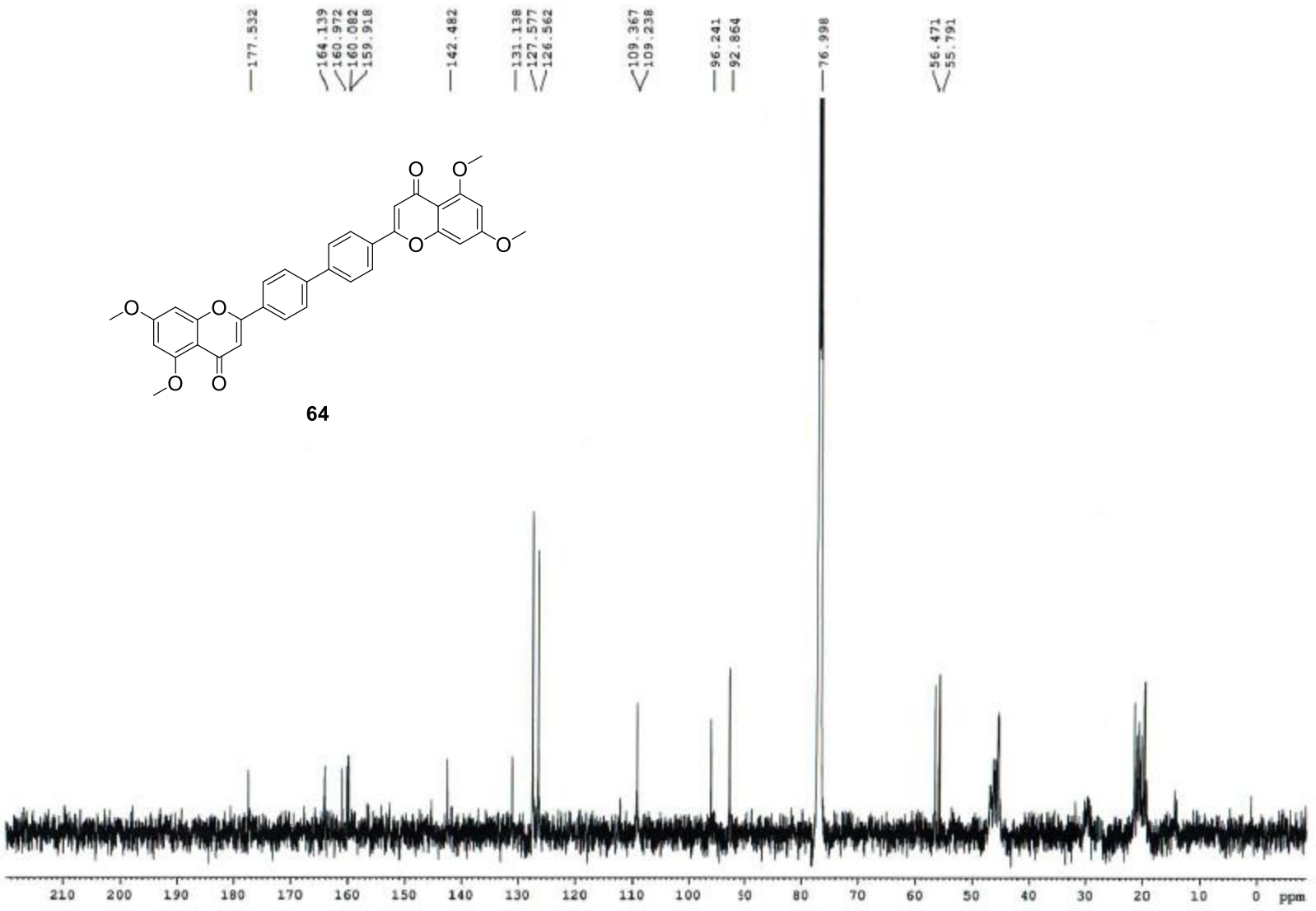

8.028
8.011
7.810
7.793
7.627
7.611
7.594
7.270
7.192
7.190
7.175
7.174
6.869
6.853
6.813
4.027
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
4.185
4.274
2.350
2.204
2.377
2.290
6.000

63

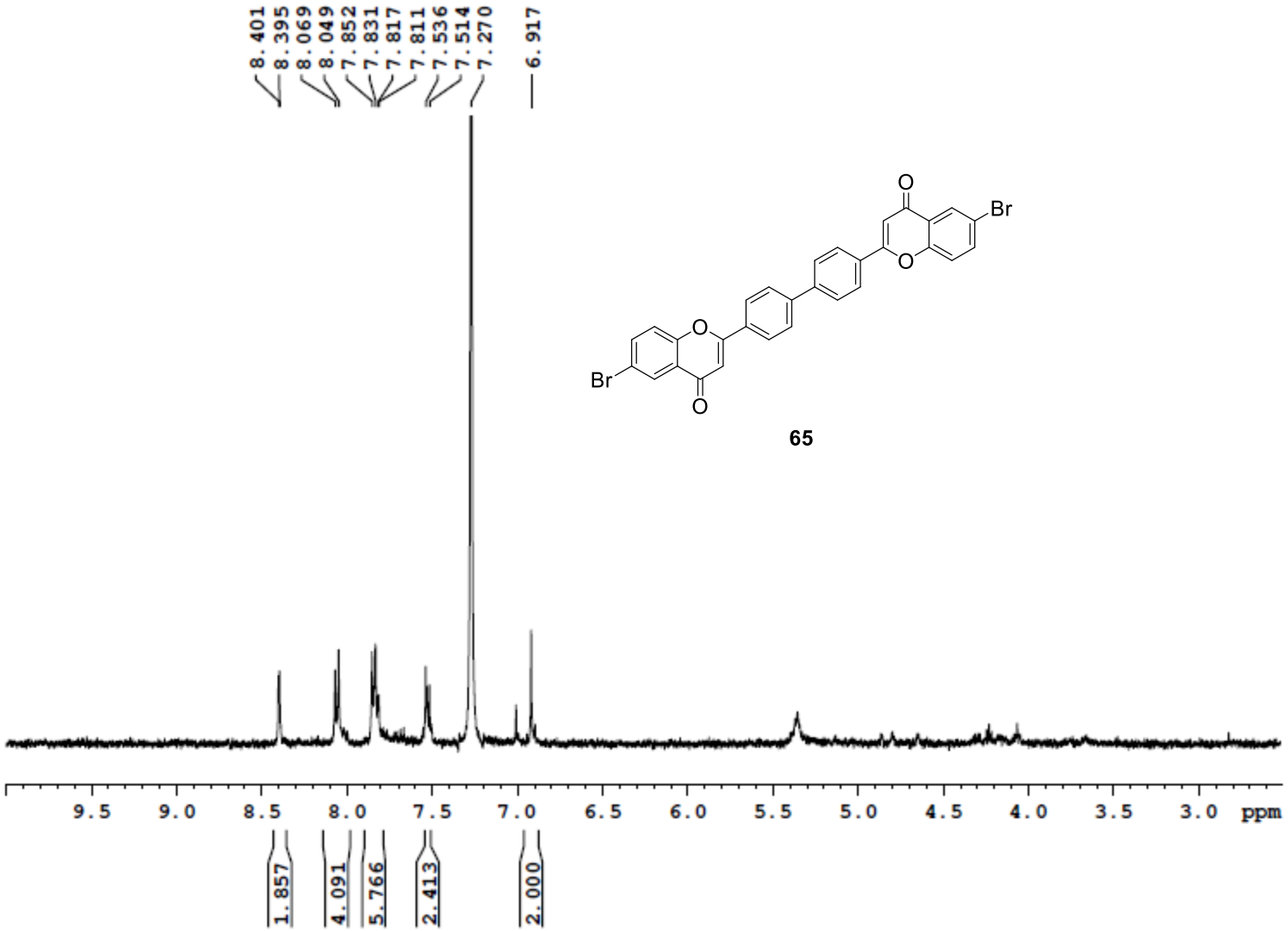

178.279
160.529
159.816
158.304
142.604
133.848
131.068
127.605
126.699
114.641
110.153
109.235
106.526
76.996
56.525
63
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.012
7.996
7.804
7.788
7.270
6.759
6.622
6.416
3.989
3.949
9
8
7
6
5
4
3
2
1
ppm
3.929
4.339
1.941
1.858
1.820
5.548
6.000

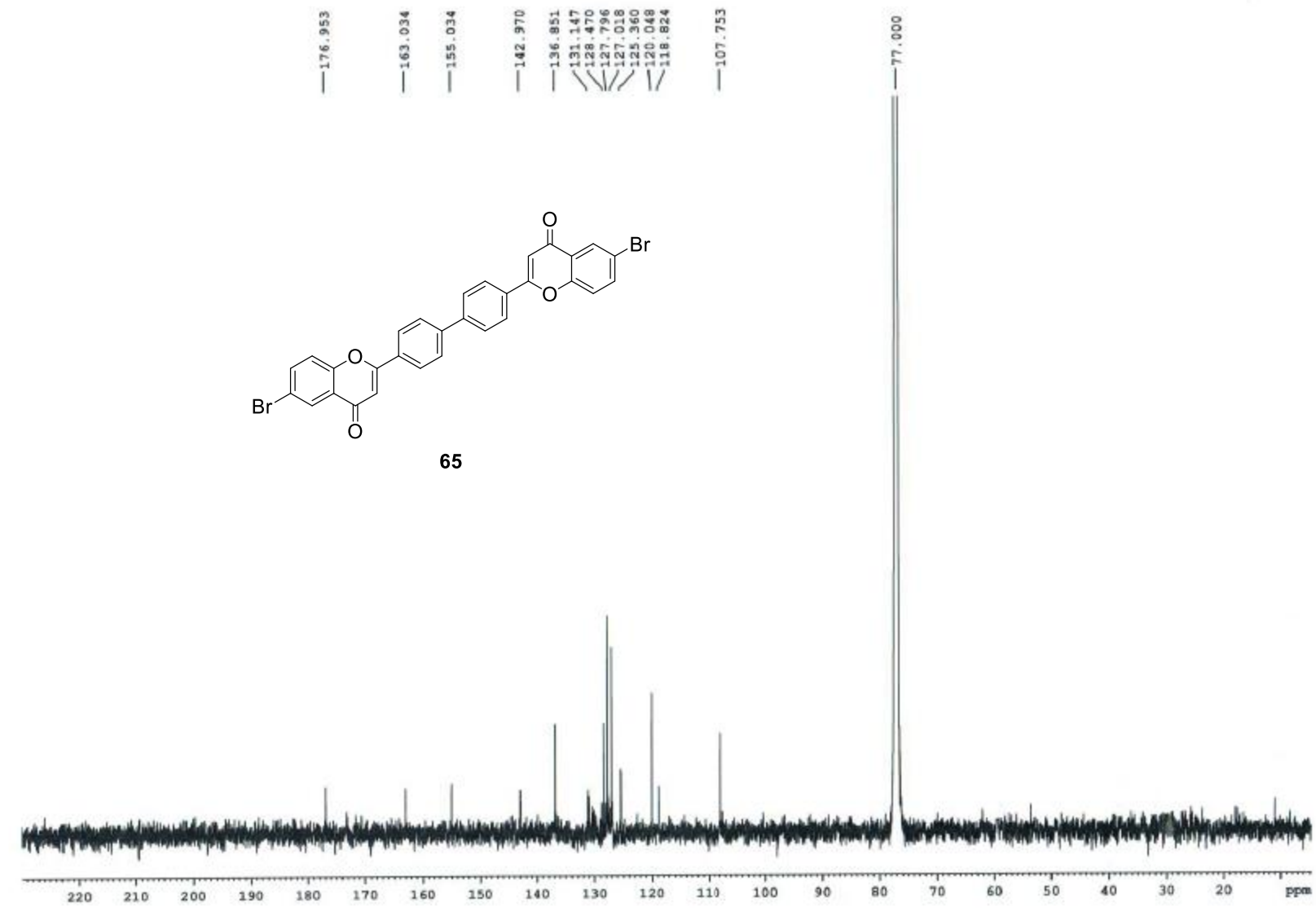
64


177.532
164.139
160.972
160.082
159.918
142.482
131.138
127.577
126.562
109.367
109.238
96.241
92.864
76.998
56.471
55.791
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

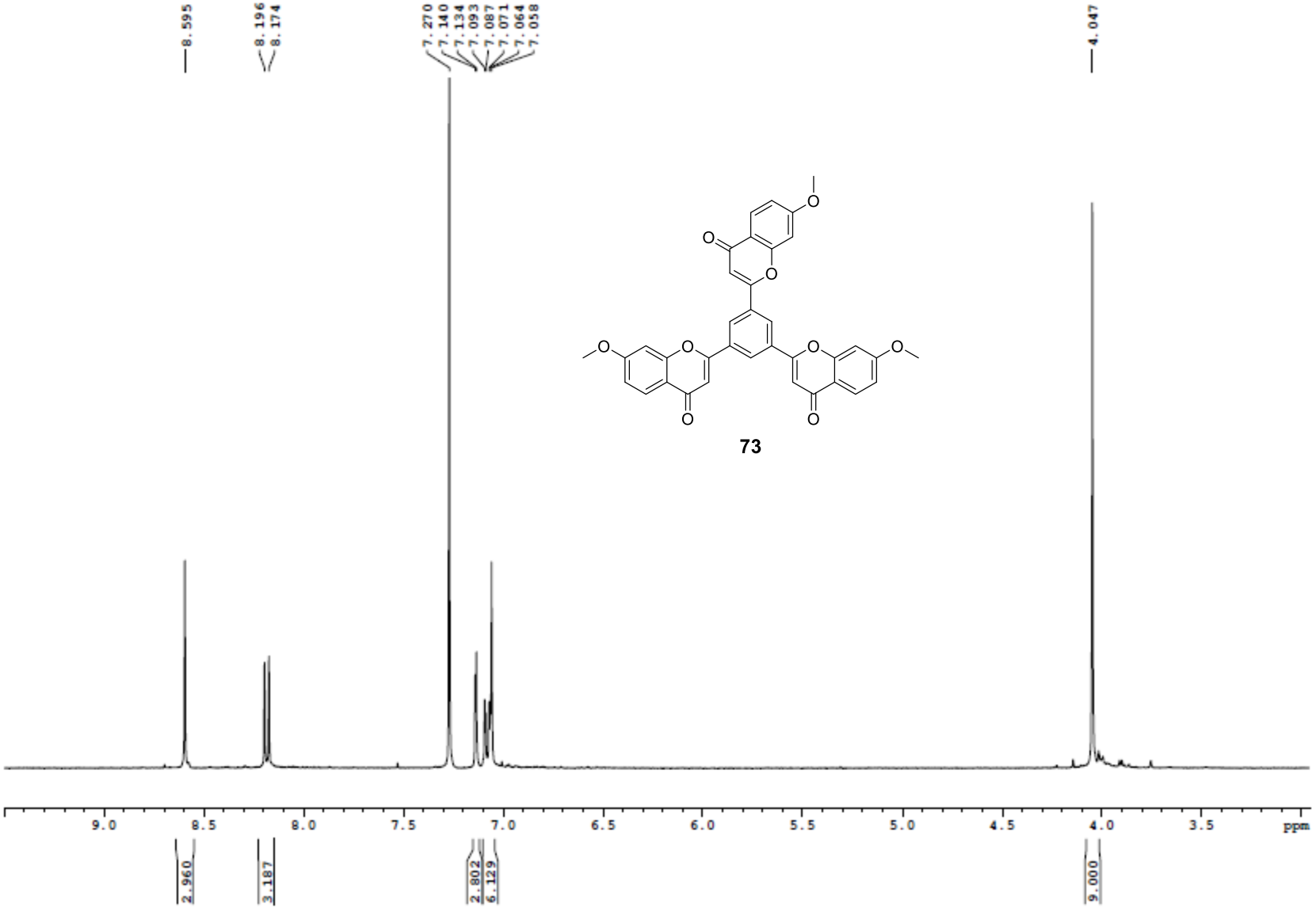
64


8.401
8.395
8.069
8.049
7.852
7.831
7.817
7.811
7.536
7.514
7.270
6.917
Br
O
O
Br
O
O
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
1.857
4.091
5.766
2.413
2.000

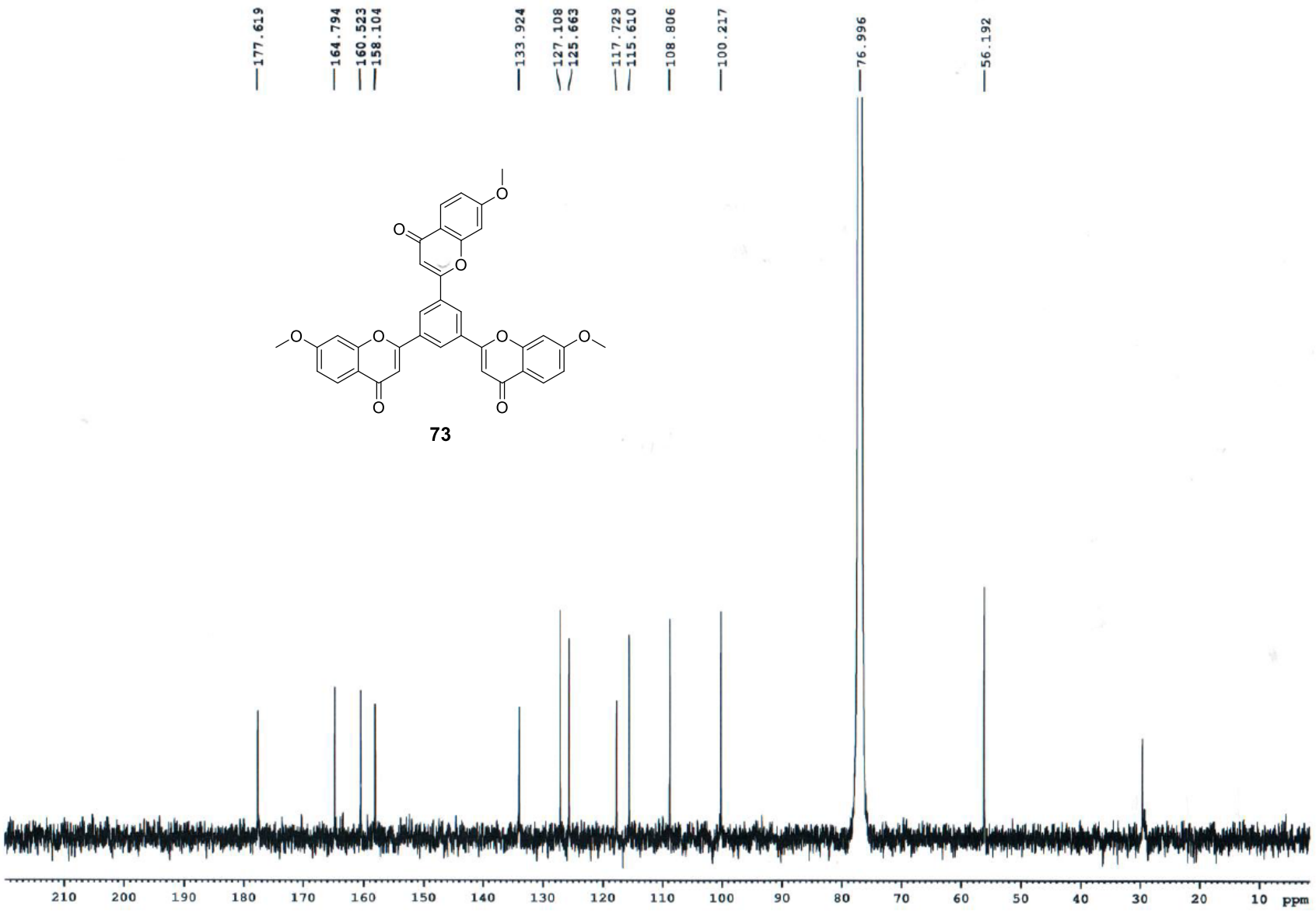
65


176.953
163.034
155.034
142.970
136.851
131.147
128.470
127.796
127.018
125.360
120.048
118.824
107.753
77.000
O
Br
O
O
Br
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

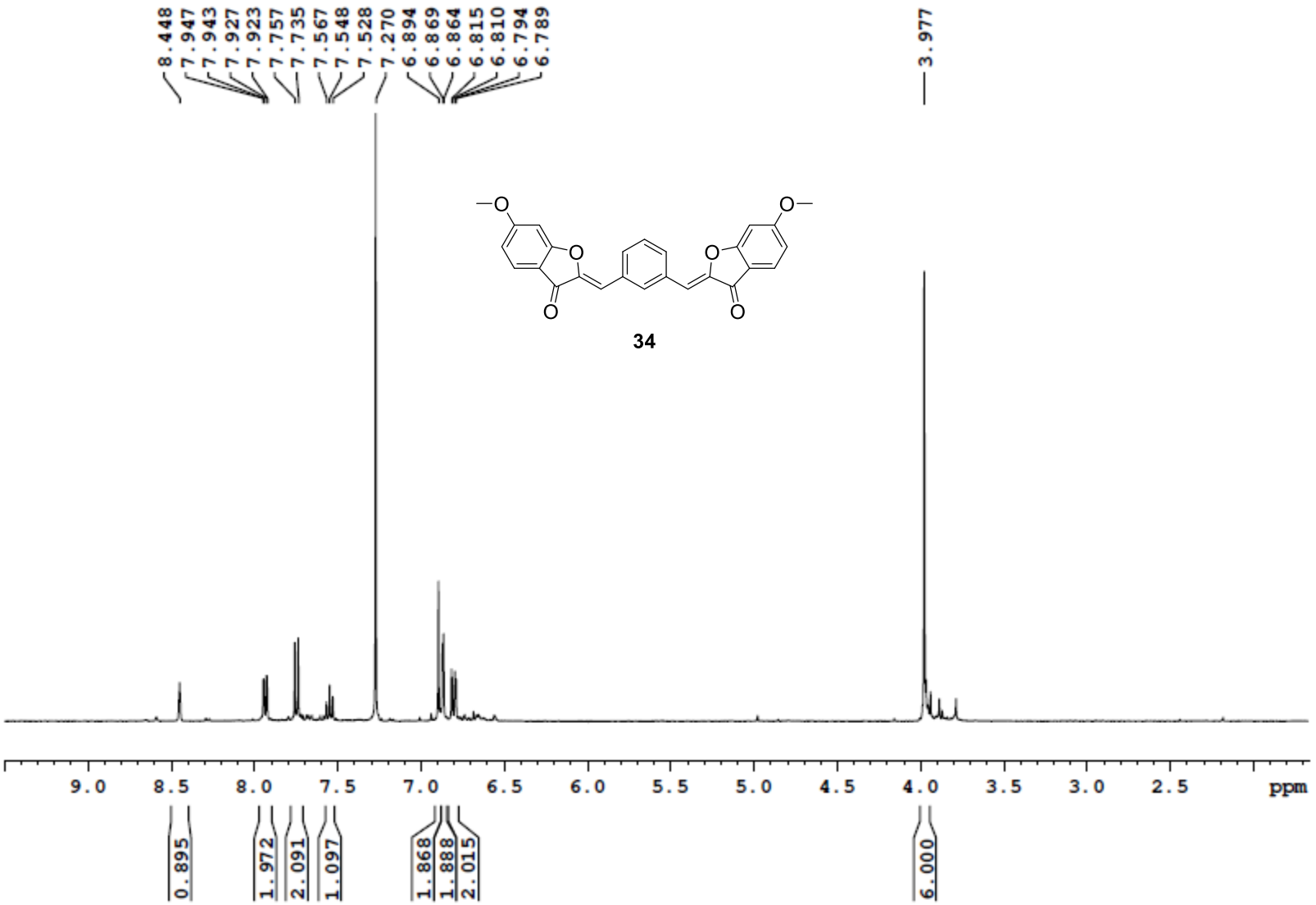
65


8.595
8.196
8.174
7.270
7.140
7.134
7.093
7.087
7.071
7.064
7.058
4.047
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
2.960
3.187
2.802
6.129
9.000

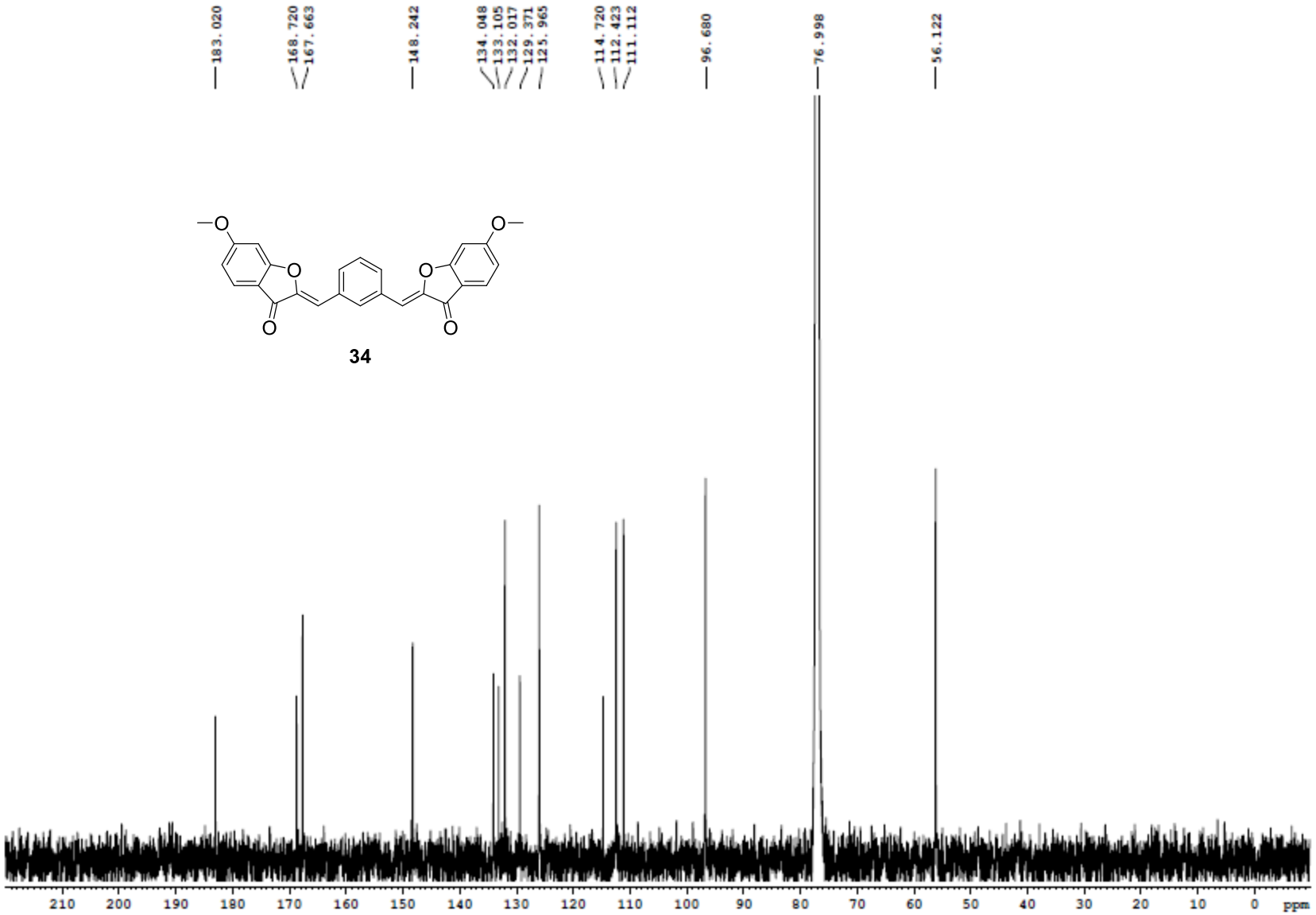
73

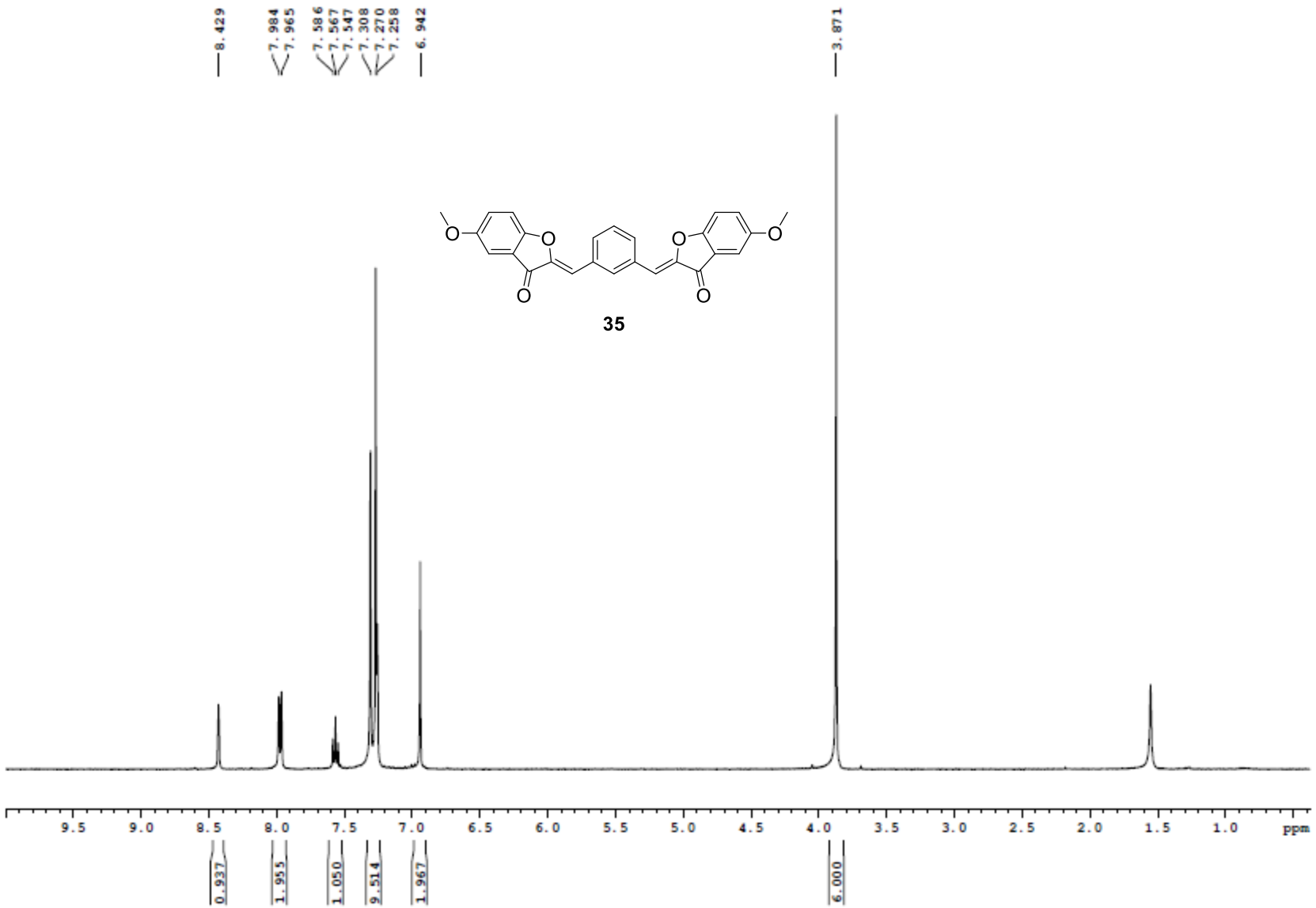

177.619
164.794
160.523
158.104
133.924
127.108
125.663
117.729
115.610
108.806
100.217
76.996
56.192
O
O
O
O
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

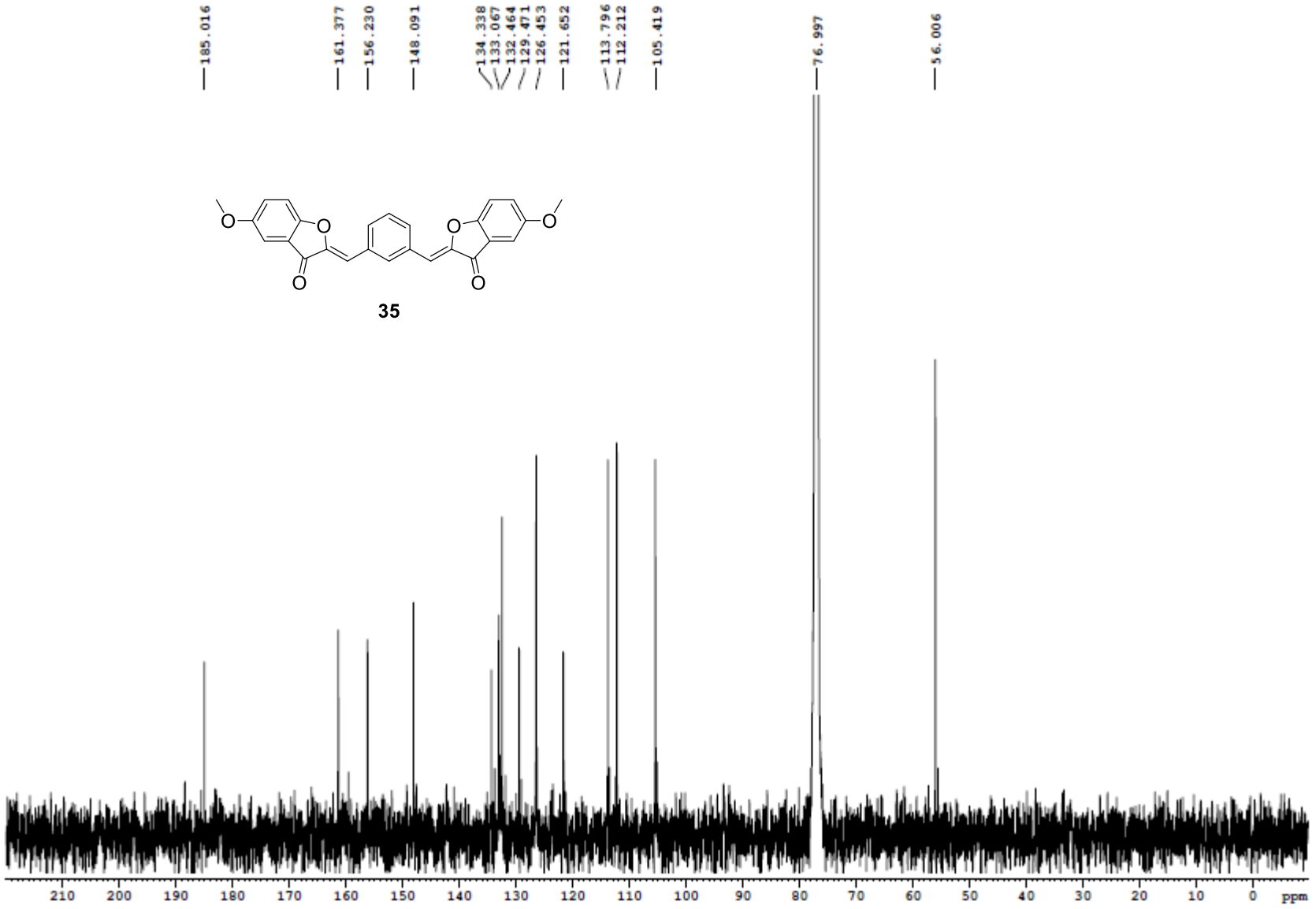
73

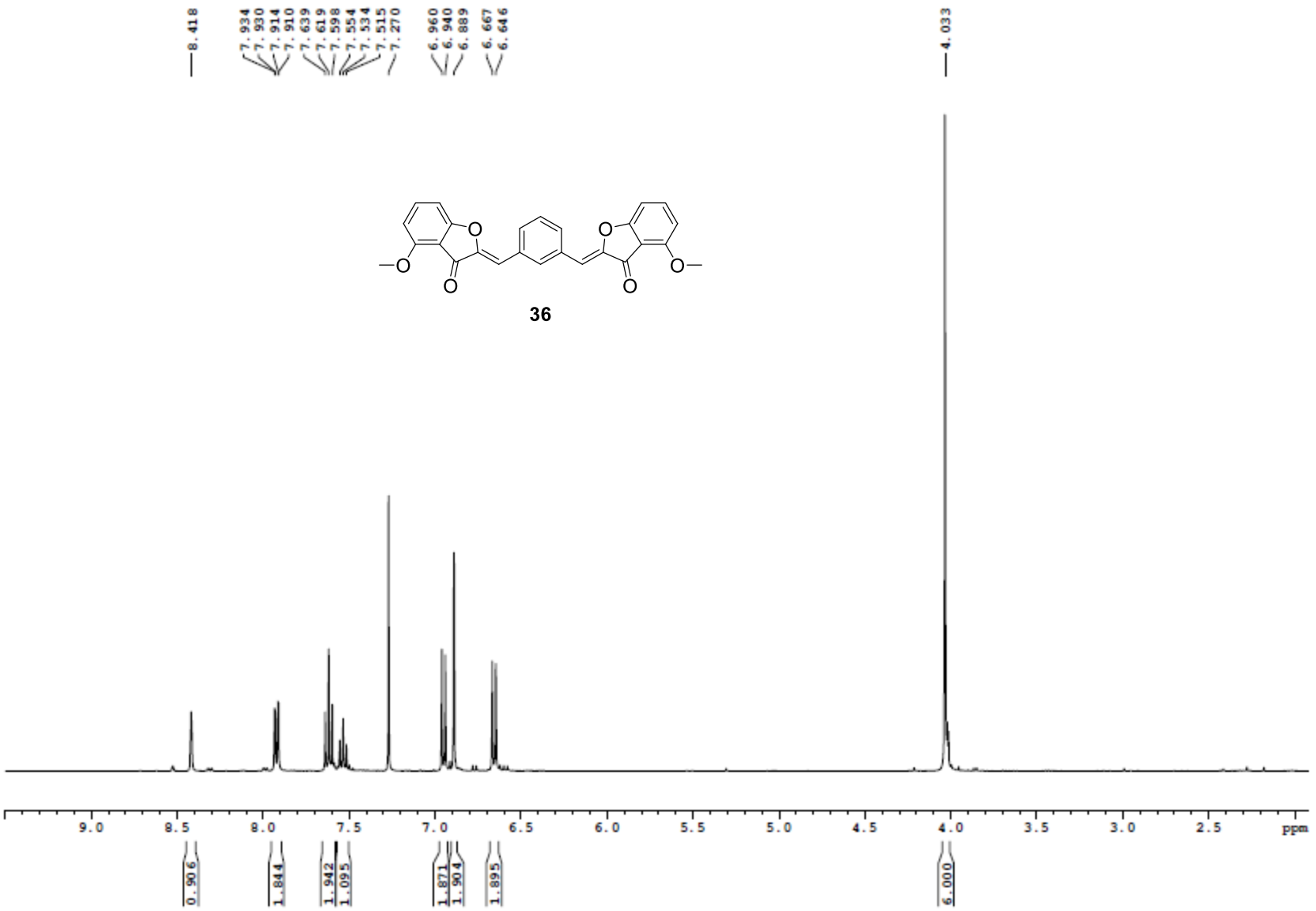

8.448
7.947
7.943
7.927
7.923
7.757
7.735
7.567
7.548
7.528
7.270
6.894
6.869
6.864
6.815
6.810
6.794
6.789
3.977
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.895
1.972
2.091
1.097
1.868
1.888
2.015
6.000

34

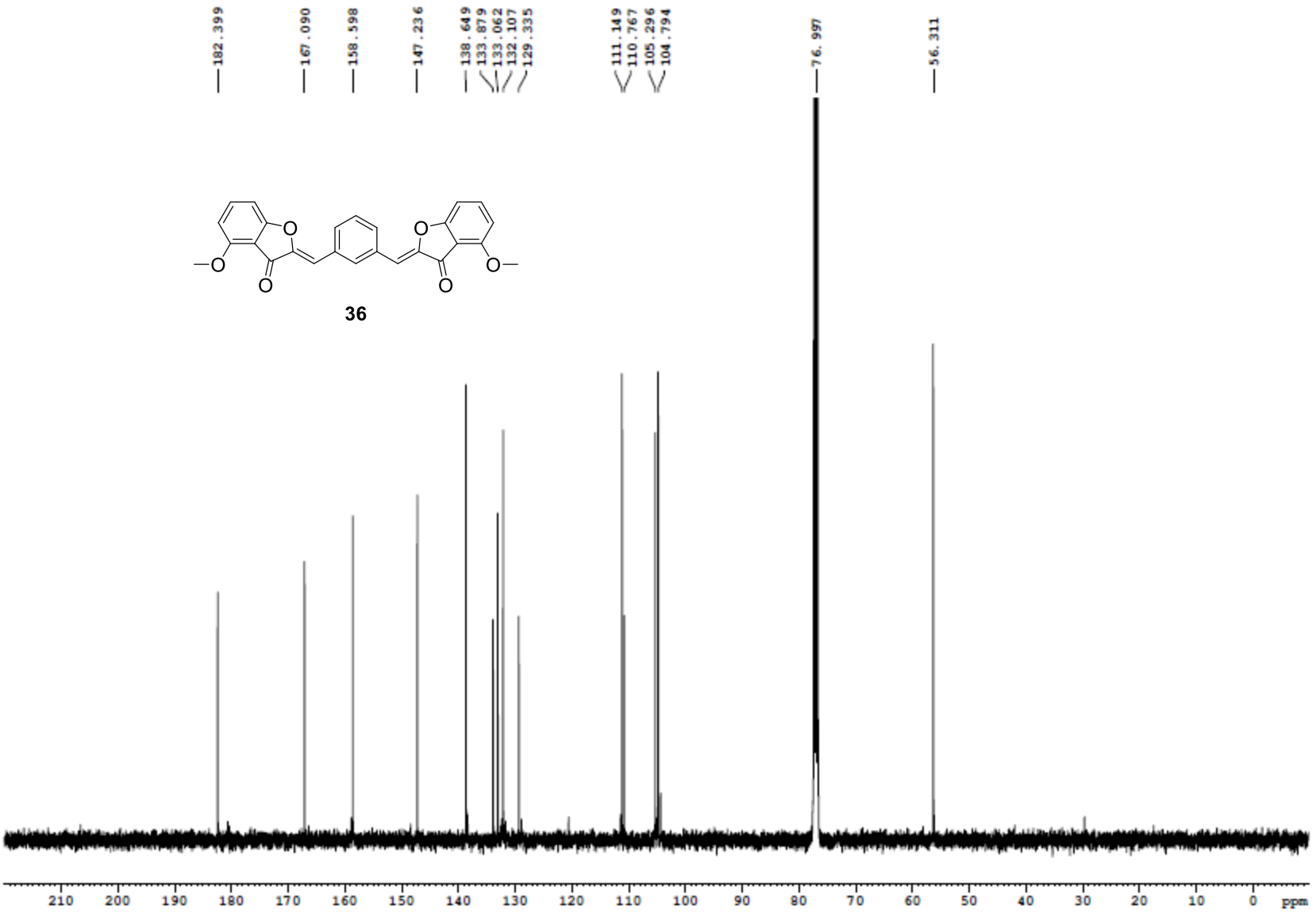

183.020
168.720
167.663
148.242
134.048
133.105
132.017
129.371
125.965
114.720
112.423
111.112
96.680
76.998
56.122
O
O
O
O
O
O
34
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

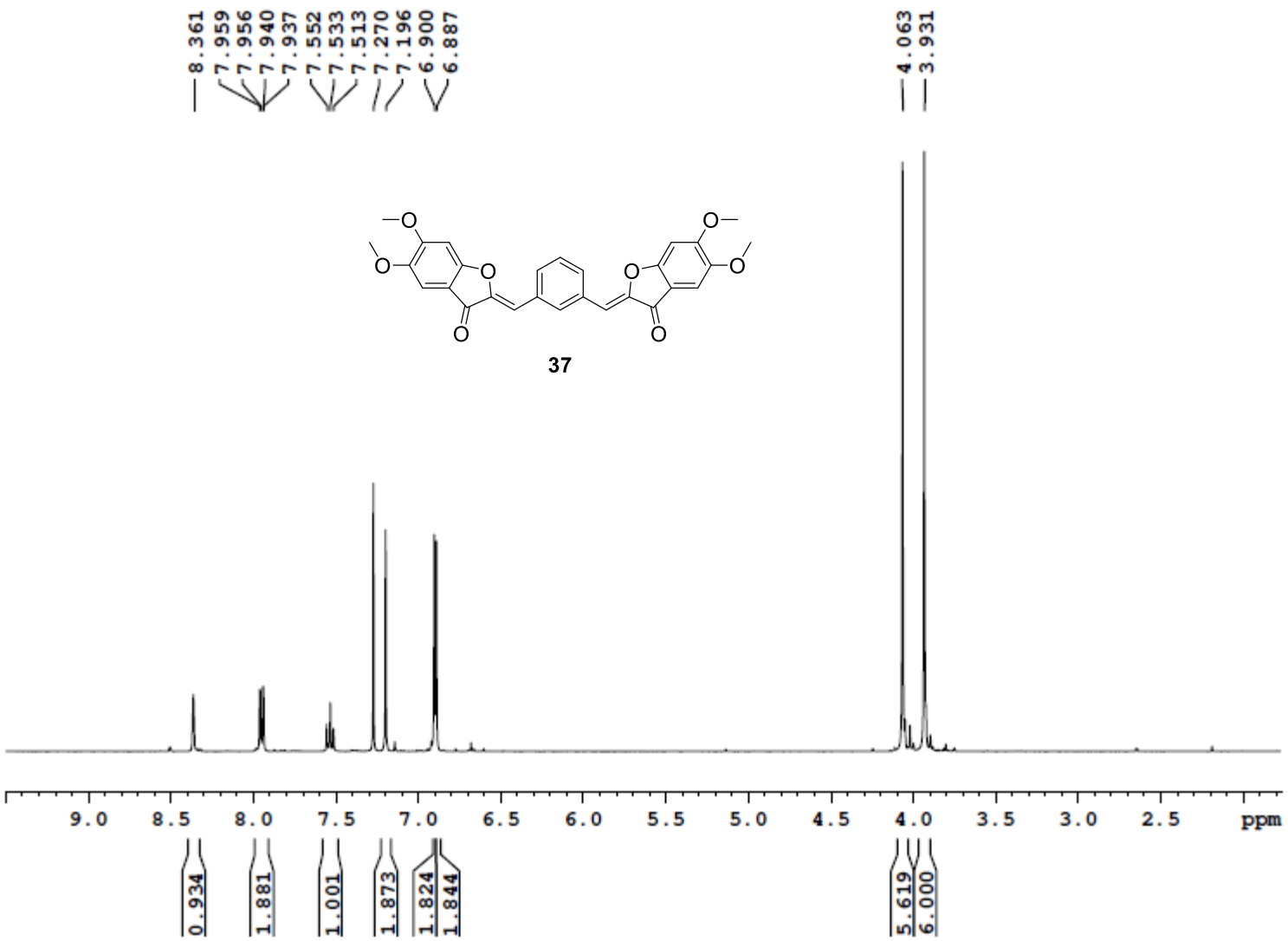

8.429
7.984
7.965
7.586
7.567
7.547
7.308
7.270
7.258
6.942
3.871
O
O
O
O
O
O
35
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.937
1.955
1.050
9.514
1.967
6.000

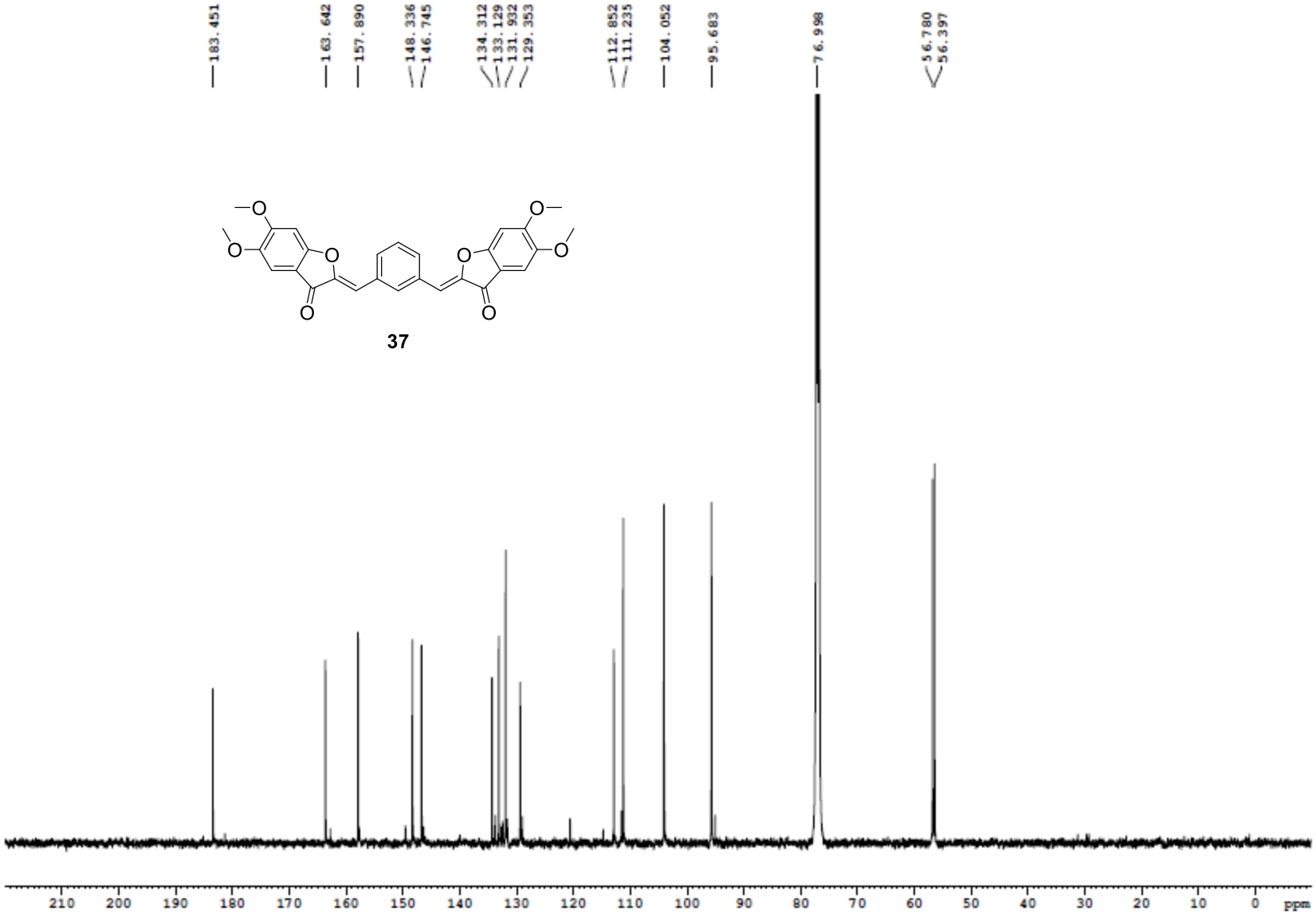

185.016
161.377
156.230
148.091
134.338
133.067
132.464
129.471
126.453
121.652
113.796
112.212
105.419
76.997
56.006
O
O
O
O
O
O
35
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

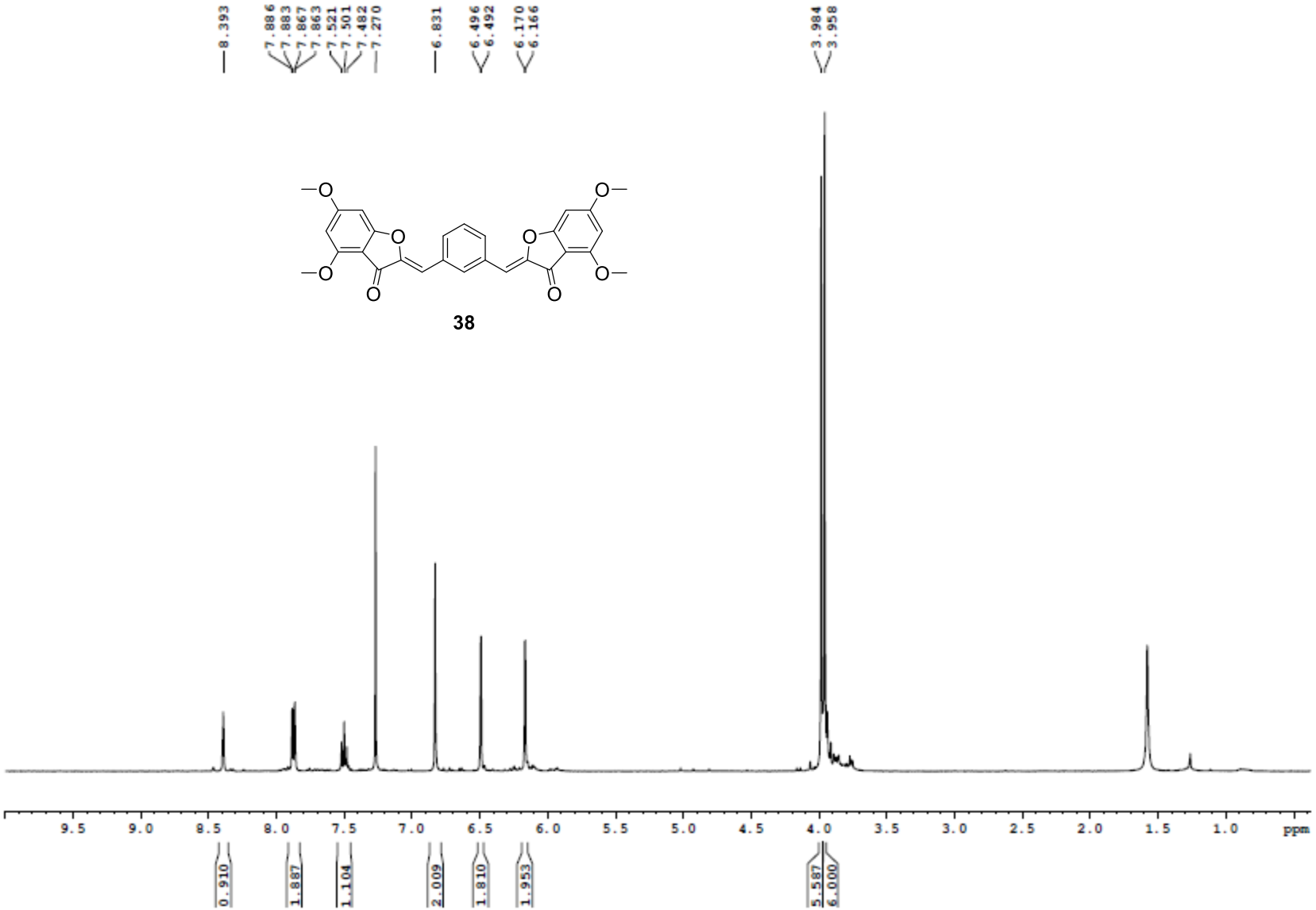

8.418
7.934
7.930
7.914
7.910
7.639
7.619
7.598
7.554
7.534
7.515
7.270
6.960
6.940
6.889
6.667
6.646
4.033
O
O
O
O
O
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.906
1.844
1.942
1.095
1.871
1.904
1.895
6.000

36

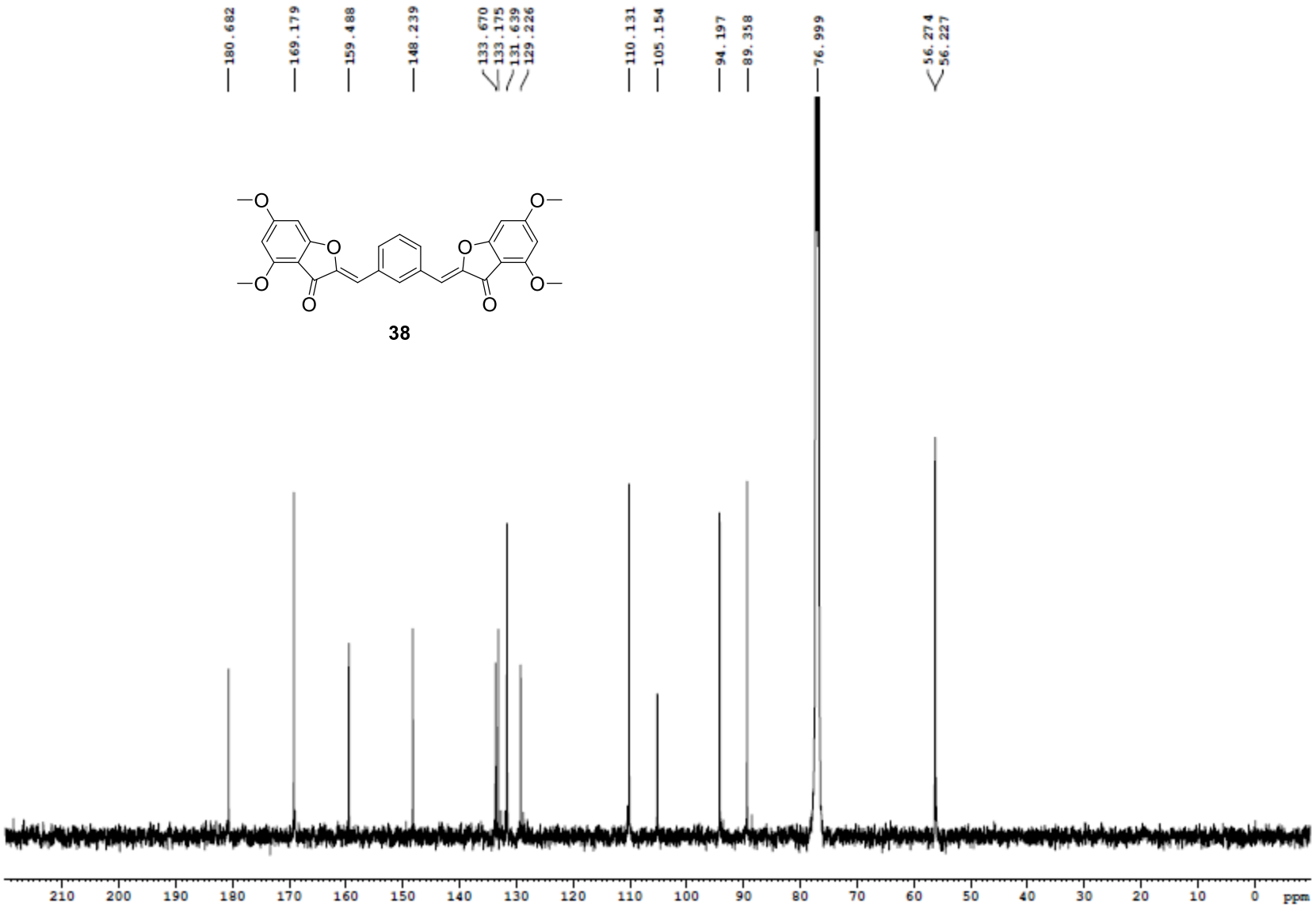

182.399
167.090
158.598
147.236
138.649
133.879
133.062
132.107
129.335
111.149
110.767
105.296
104.794
76.997
56.311
O
O
O
O
O
O
36
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

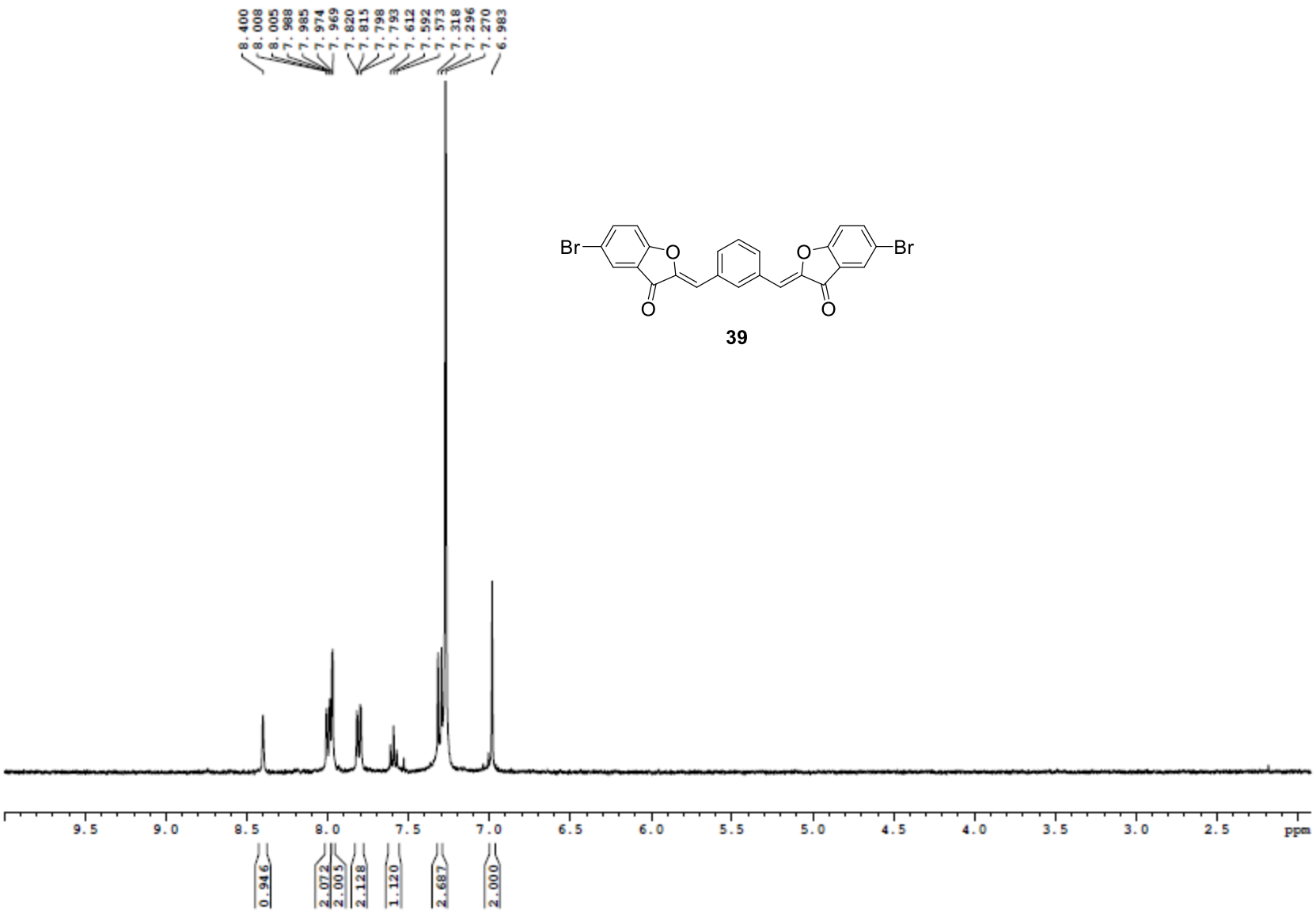

8.361
7.959
7.956
7.940
7.937
7.552
7.533
7.513
7.270
7.196
6.900
6.887
4.063
3.931
37
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.934
1.881
1.001
1.873
1.824
1.844
5.619
6.000


183.451
163.642
157.890
148.336
146.745
134.312
133.129
131.932
129.353
112.852
111.235
104.052
95.683
76.998
56.780
56.397
37
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

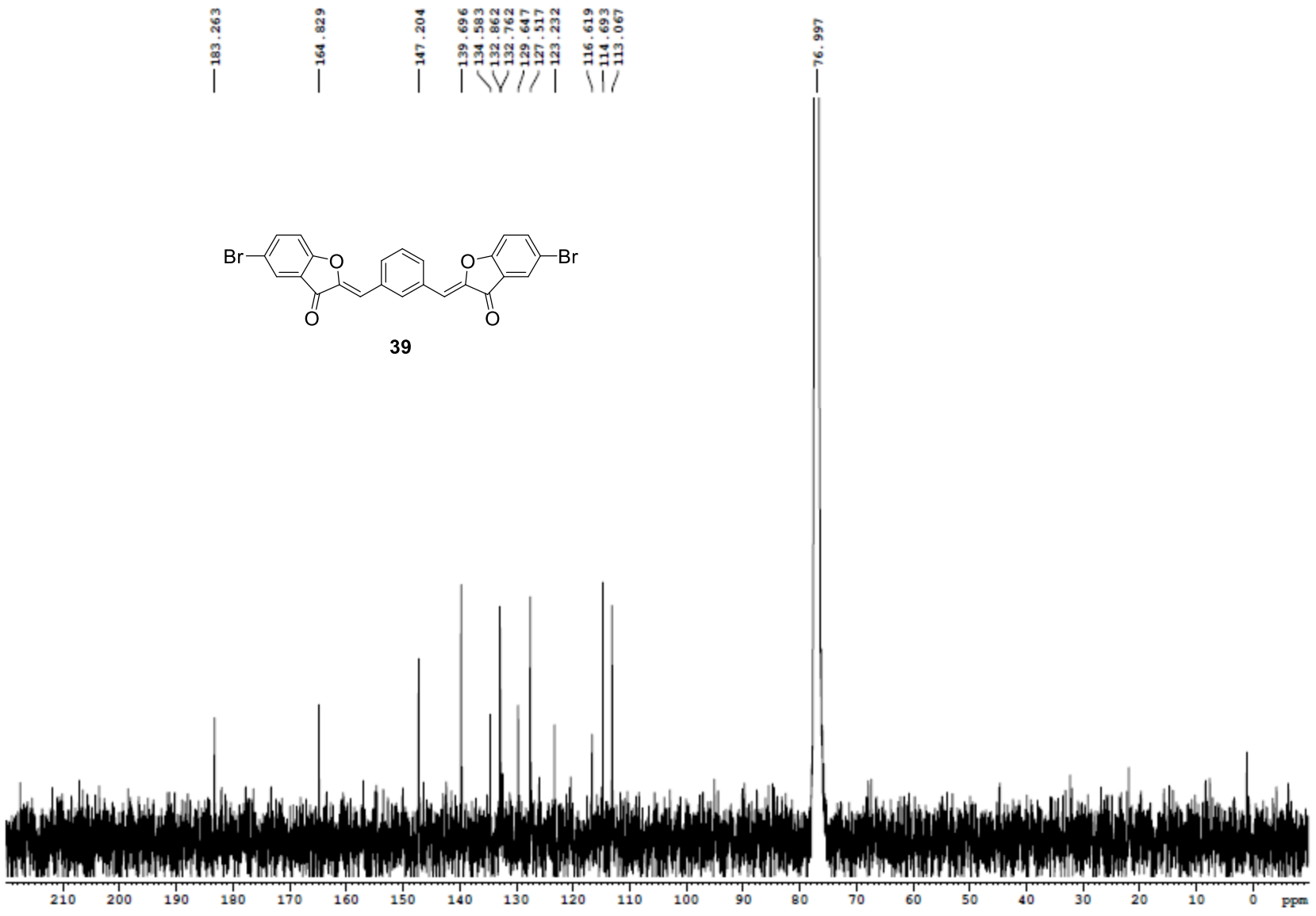

8.393
7.886
7.883
7.867
7.863
7.521
7.501
7.482
7.270
6.831
6.496
6.492
6.170
6.166
3.984
3.958
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.910
1.887
1.104
2.009
1.810
1.953
5.587
6.000

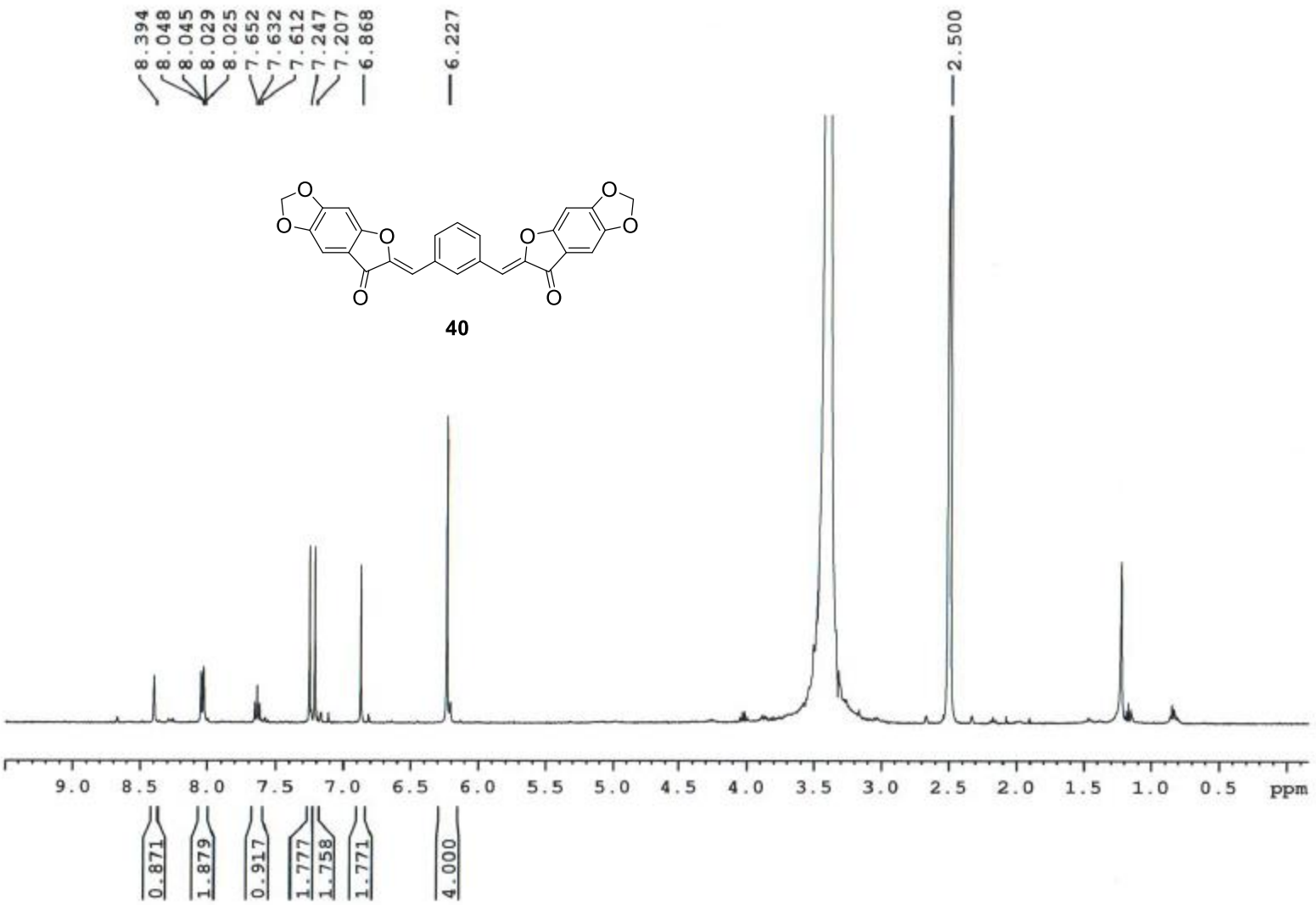
38


180.682
169.179
159.488
148.239
133.670
133.175
131.639
129.226
110.131
105.154
94.197
89.358
76.999
56.274
56.227
38
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

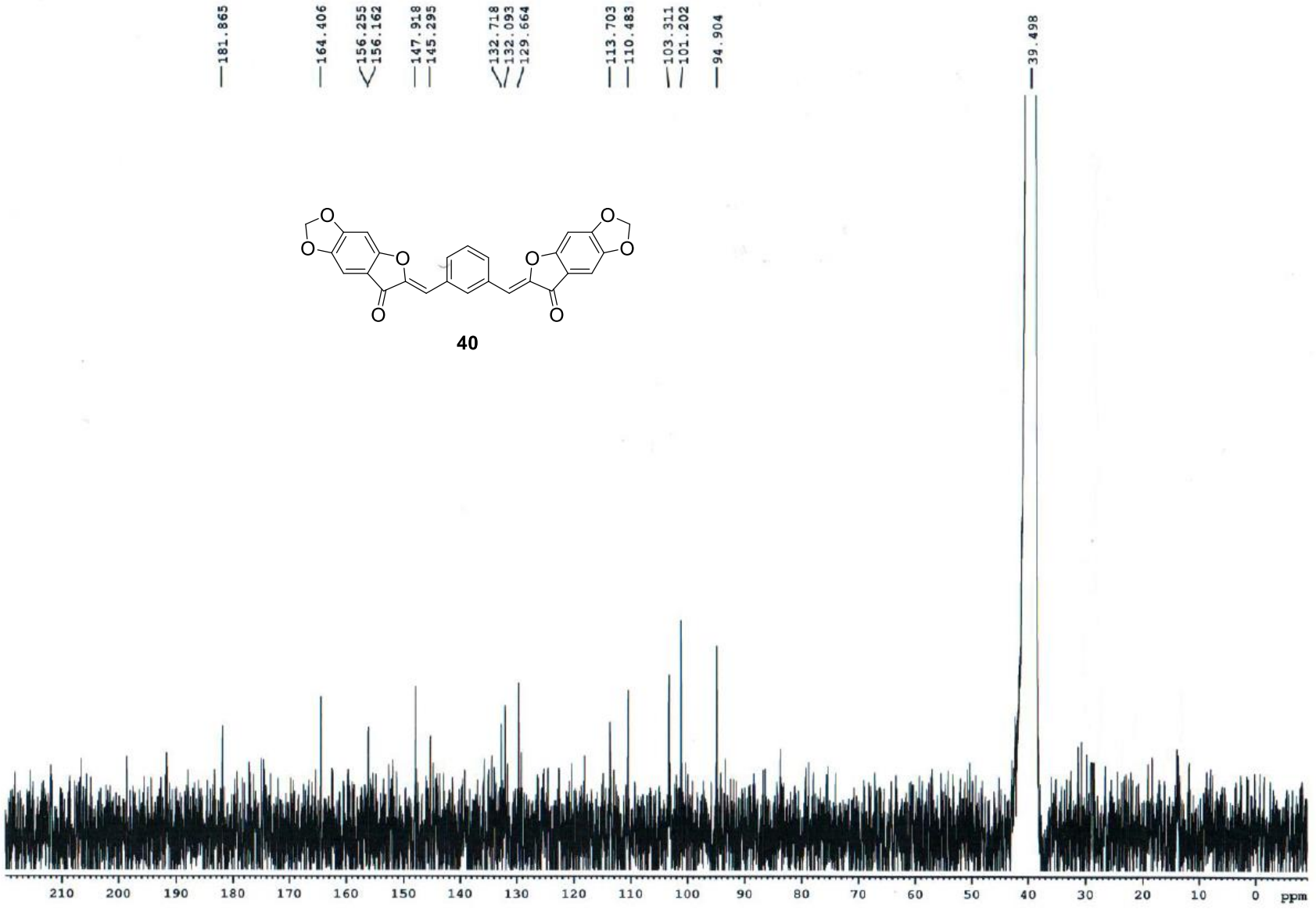

8.400
8.008
8.005
7.988
7.985
7.974
7.969
7.820
7.815
7.798
7.793
7.612
7.592
7.573
7.318
7.296
7.270
6.983
Br
O
O
O
O
Br
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
0.946
2.072
2.005
2.128
1.120
2.687
2.000

39

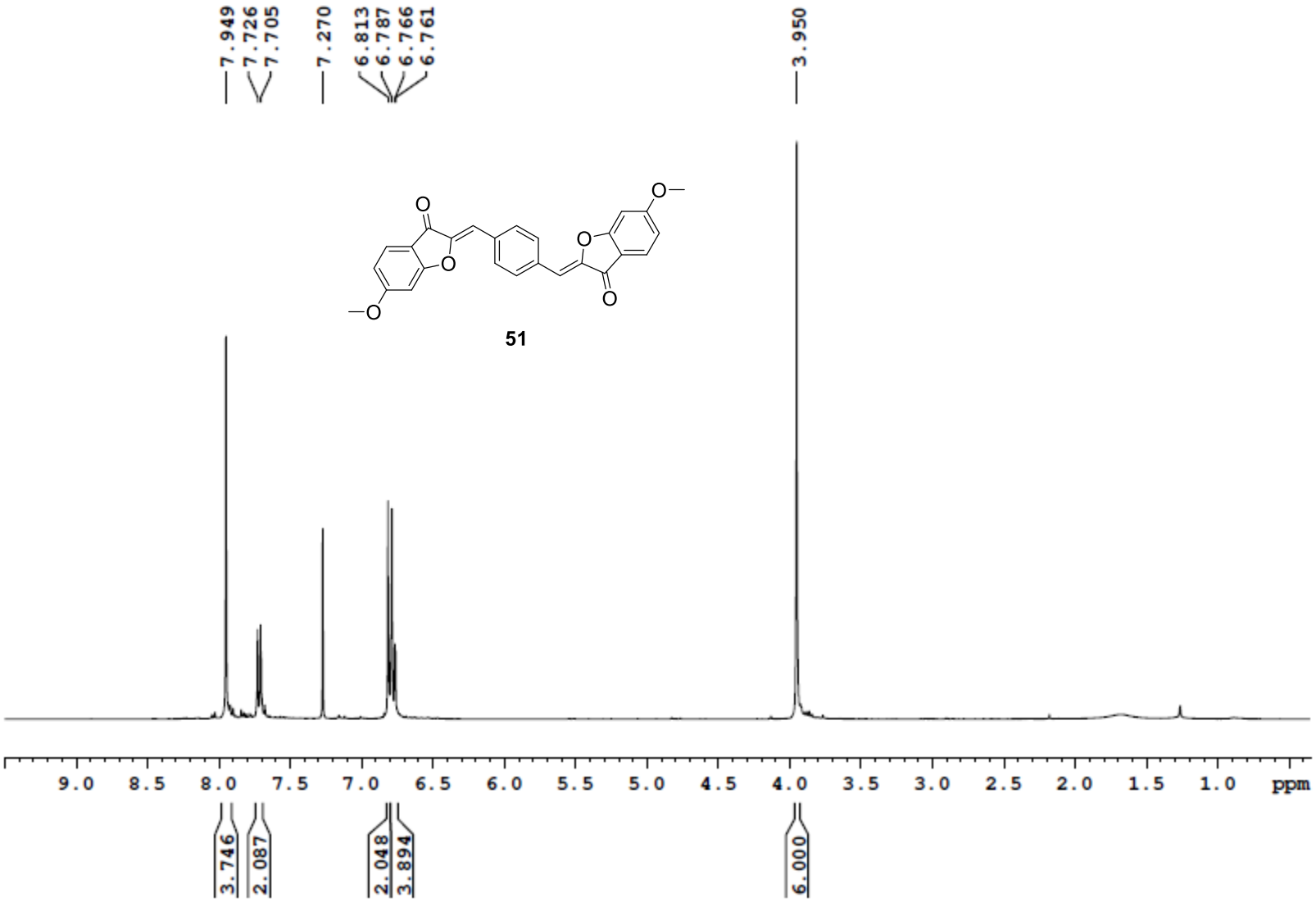

183.263
164.829
147.204
139.696
134.583
132.862
132.762
129.647
127.517
123.232
116.619
114.693
113.067
76.997
Br
O
O
O
O
Br
39
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.394
8.048
8.045
8.029
8.025
7.652
7.632
7.612
7.247
7.207
6.868
6.227
2.500
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
0.871
1.879
0.917
1.777
1.758
1.771
4.000

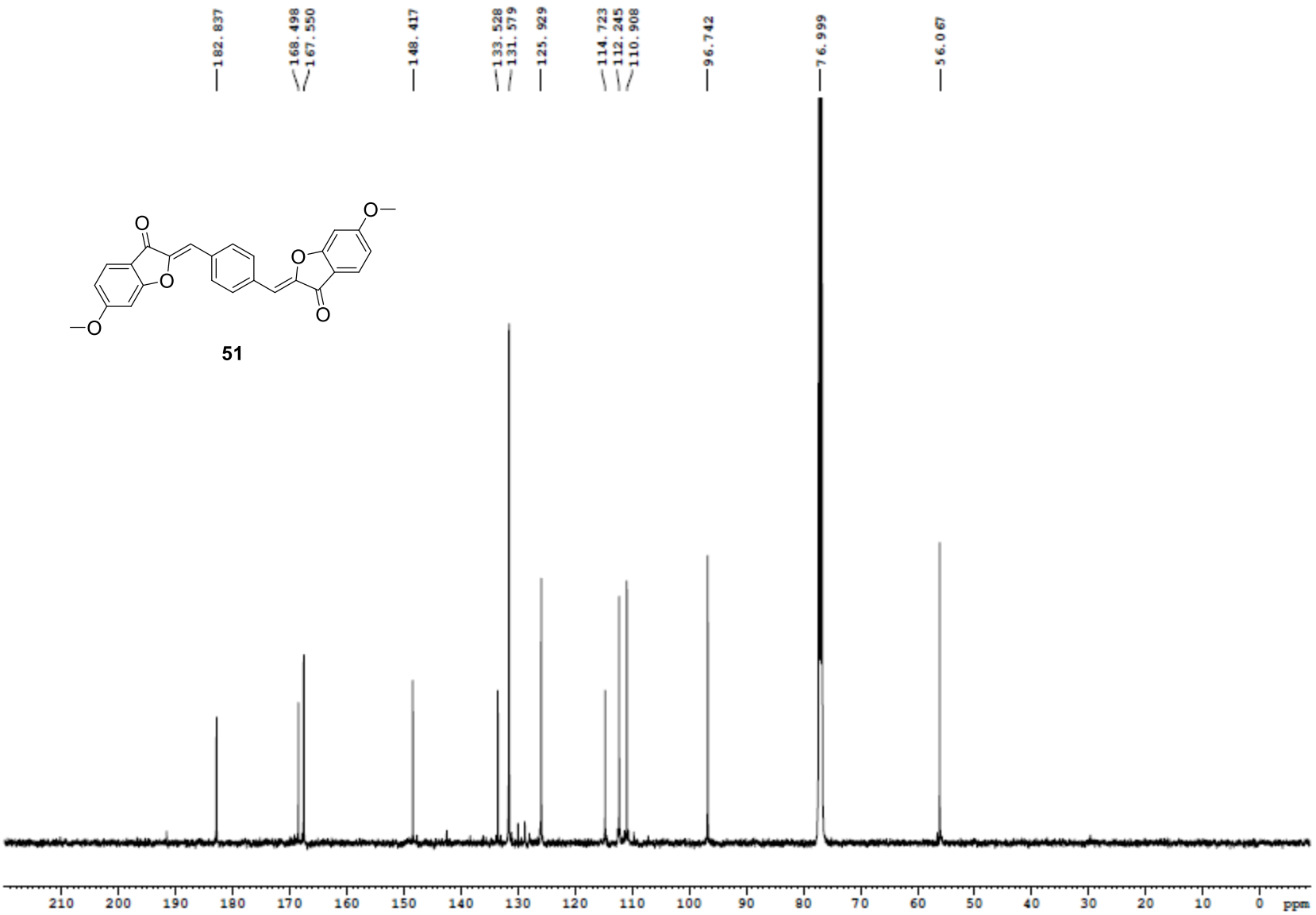
40

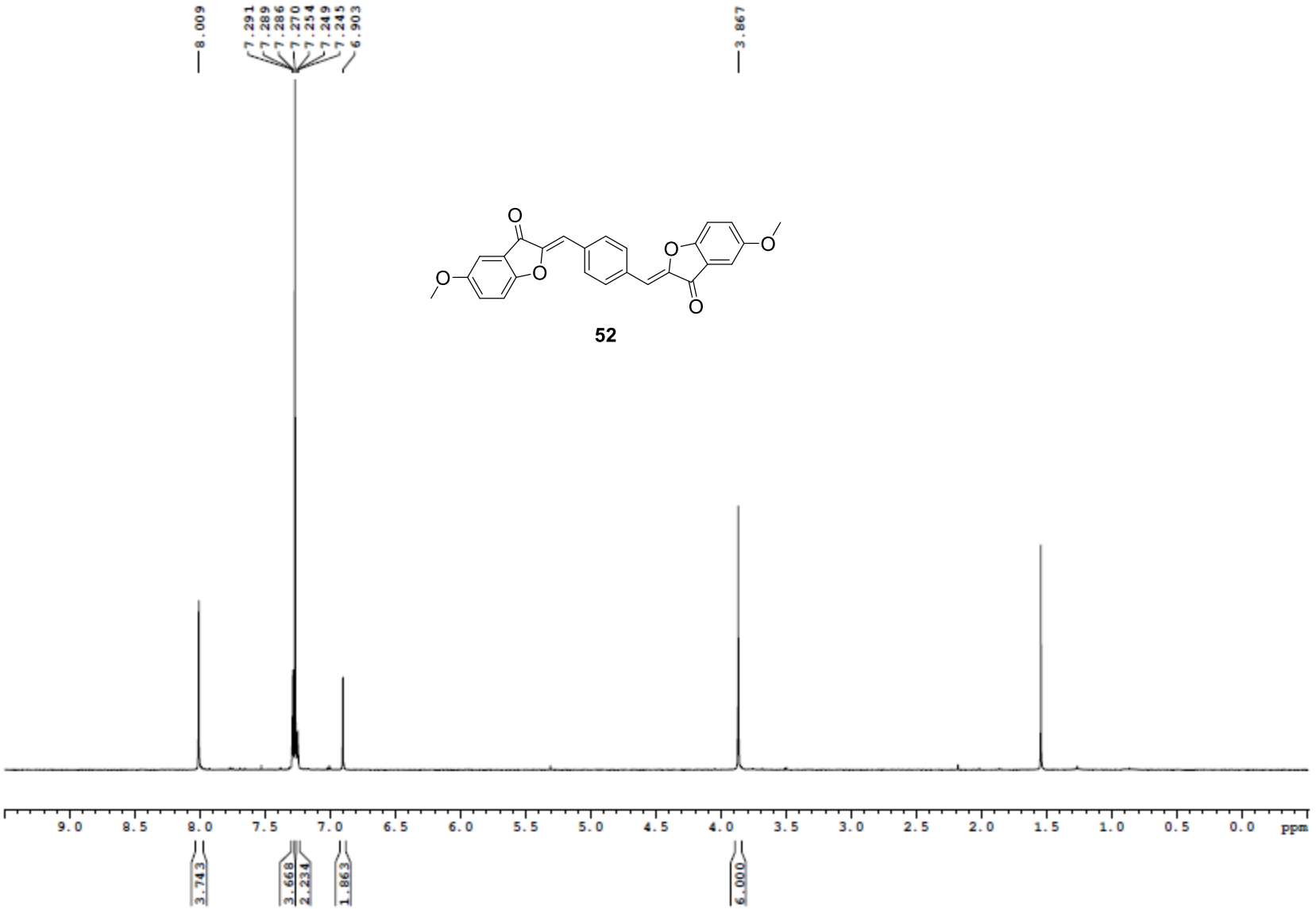

181.865
164.406
156.255
156.162
147.918
145.295
132.718
132.093
129.664
113.703
110.483
103.311
101.202
94.904
39.498
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

40

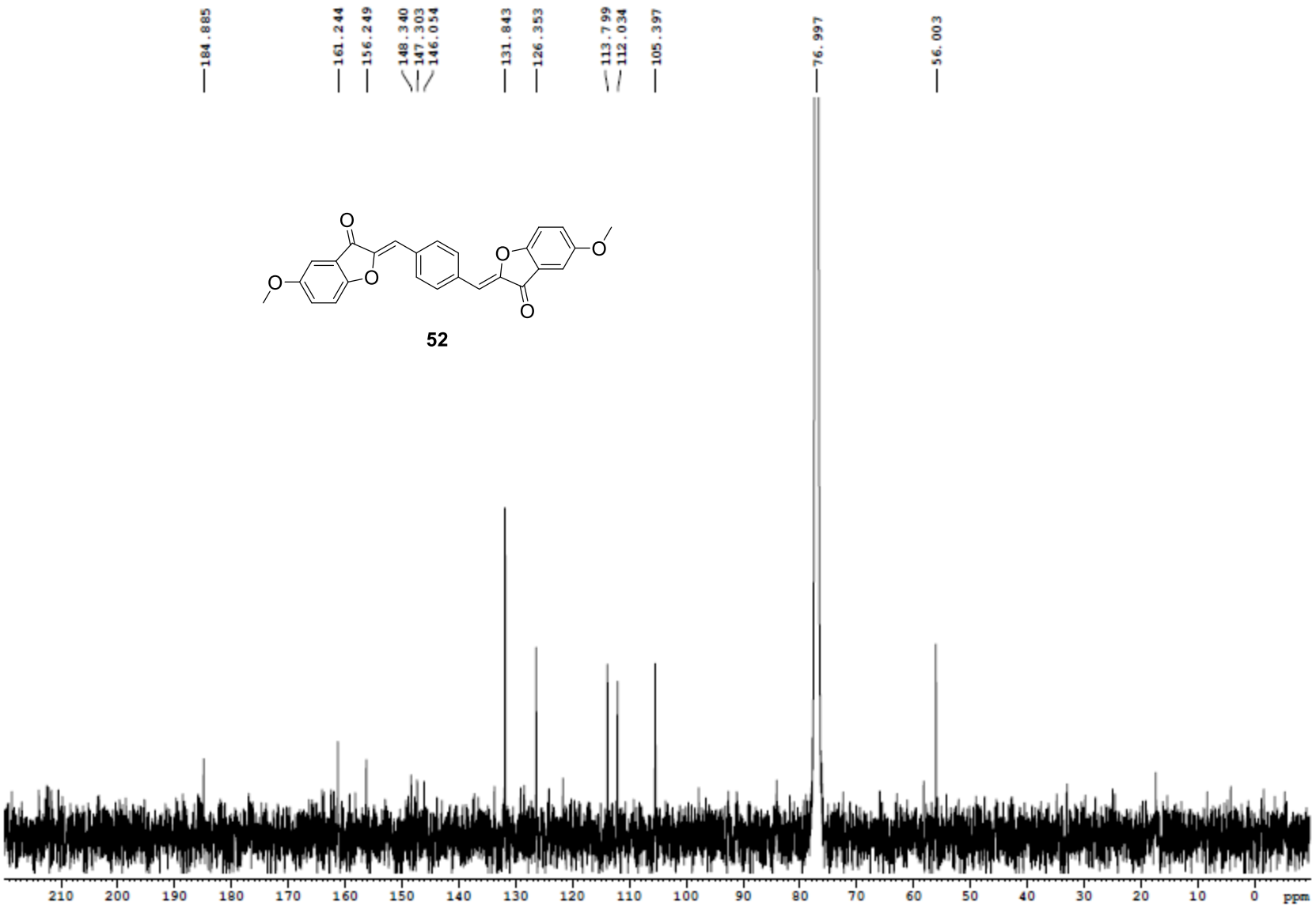

7.949
7.726
7.705
7.270
6.813
6.787
6.766
6.761
3.950
O
O
O
O
O
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.746
2.087
2.048
3.894
6.000

51


182.837
168.498
167.550
148.417
133.528
131.579
125.929
114.723
112.245
110.908
96.742
76.999
56.067
O
O
O
O
O
O
51
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.009
7.291
7.289
7.286
7.270
7.254
7.249
7.245
6.903
3.867
O
O
O
O
O
O
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
3.743
3.668
2.234
1.863
6.000

52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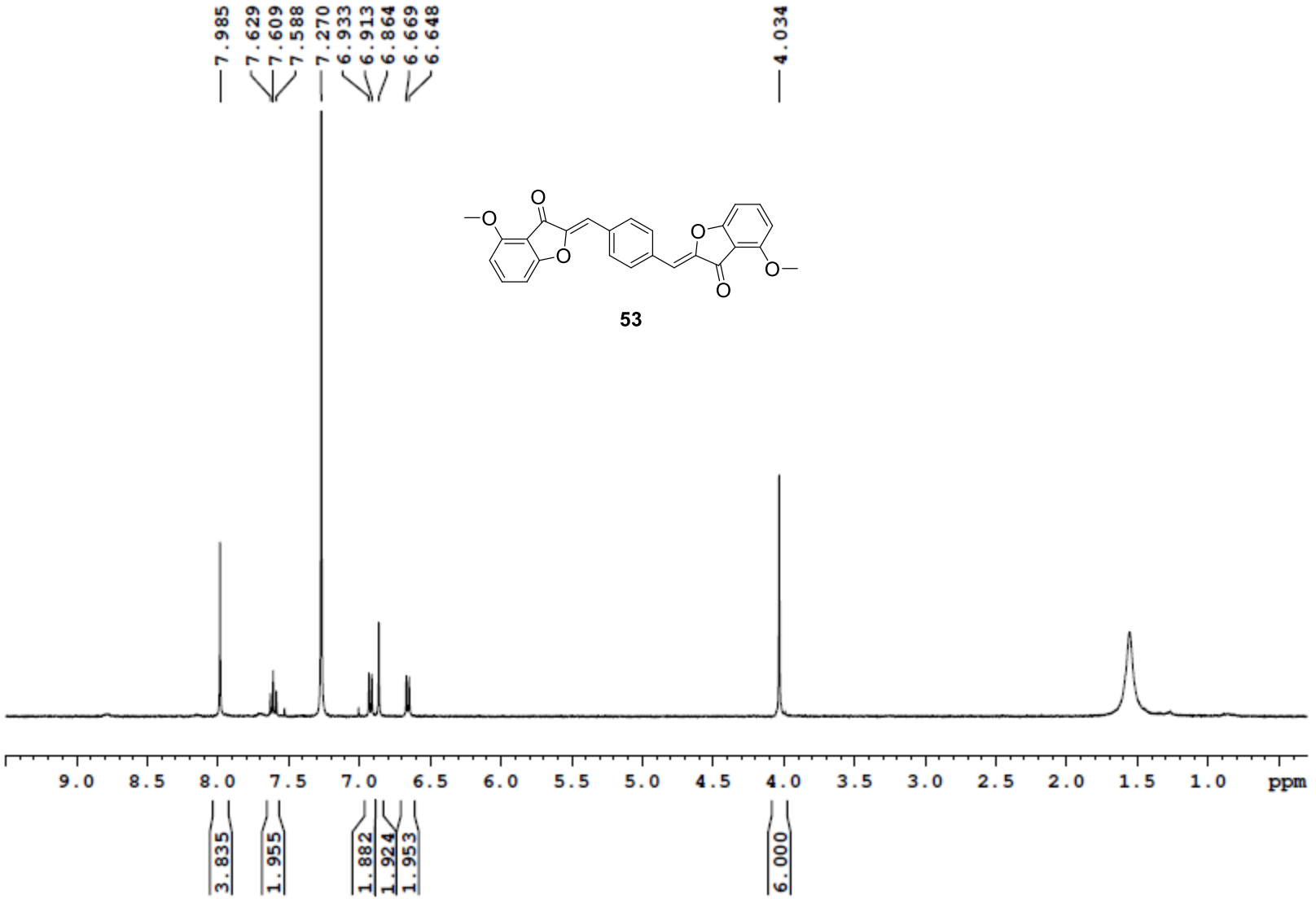
161.244
156.249
148.340
147.303
146.054
131.843
126.353
113.799
112.034
105.397
76.997
56.003
O
O
O
O
O
O
52
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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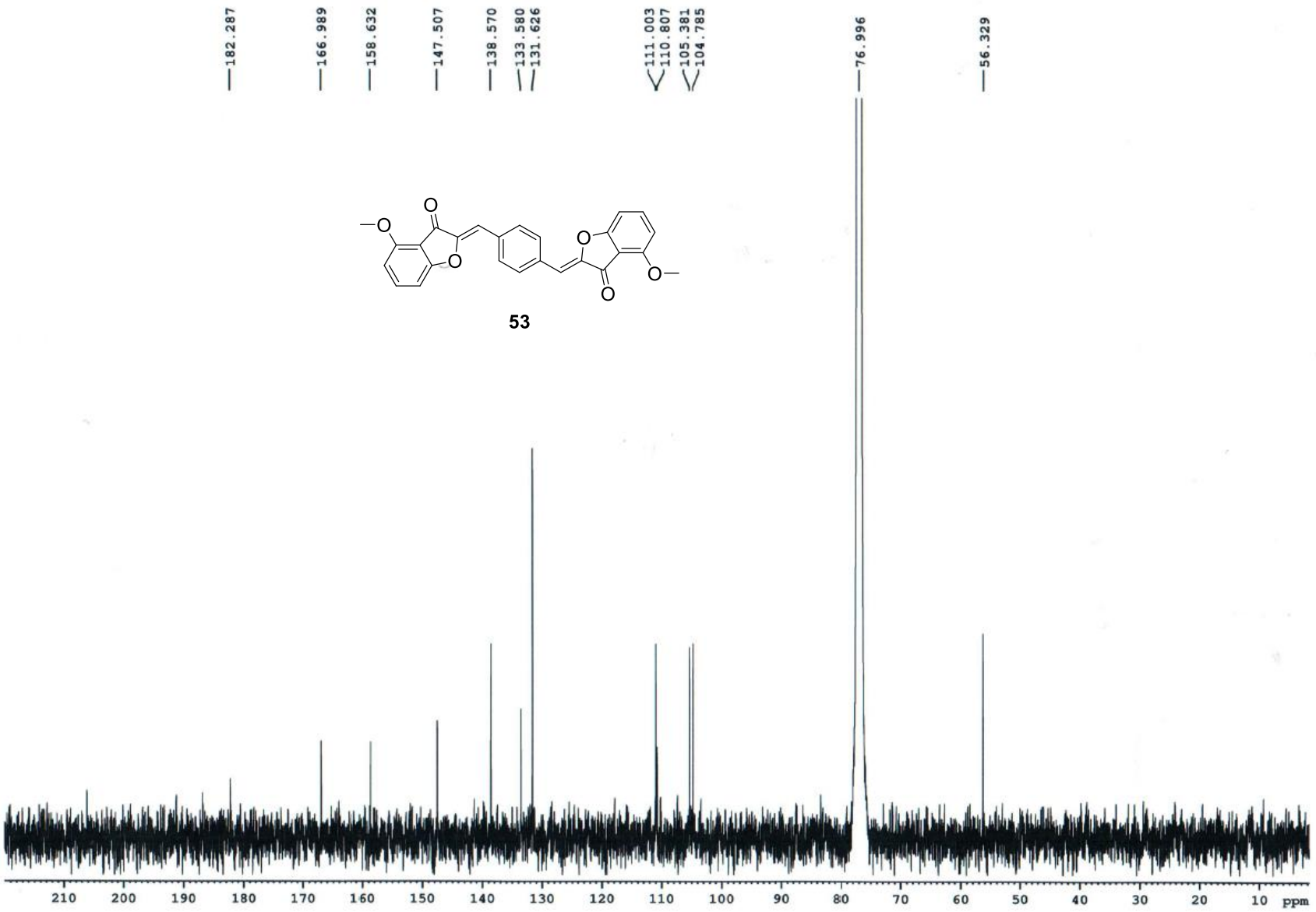
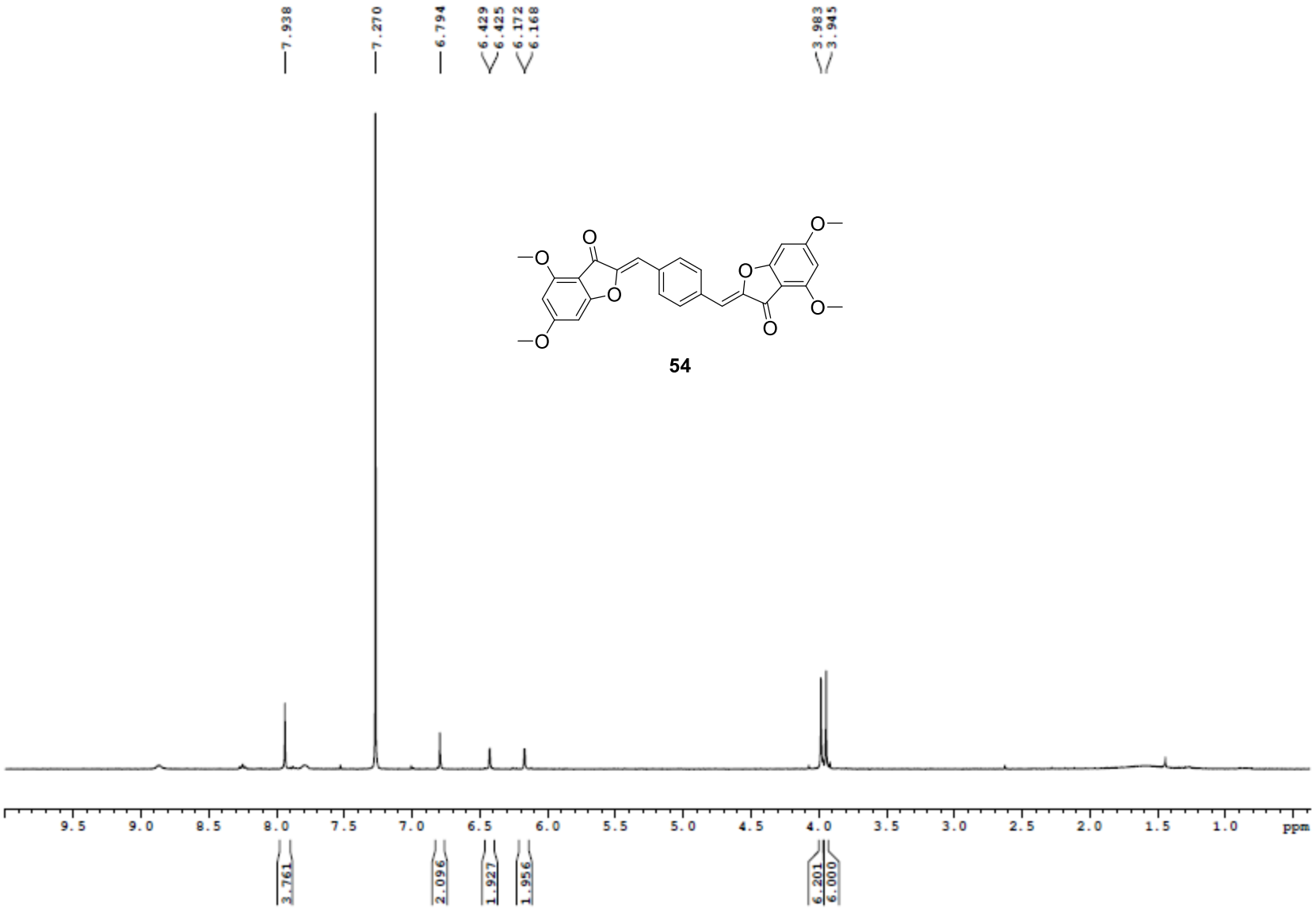
7.629
7.609
7.588
7.270
6.933
6.913
6.864
6.669
6.648
4.034
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
3.835
1.955
1.882
1.924
1.953
6.000

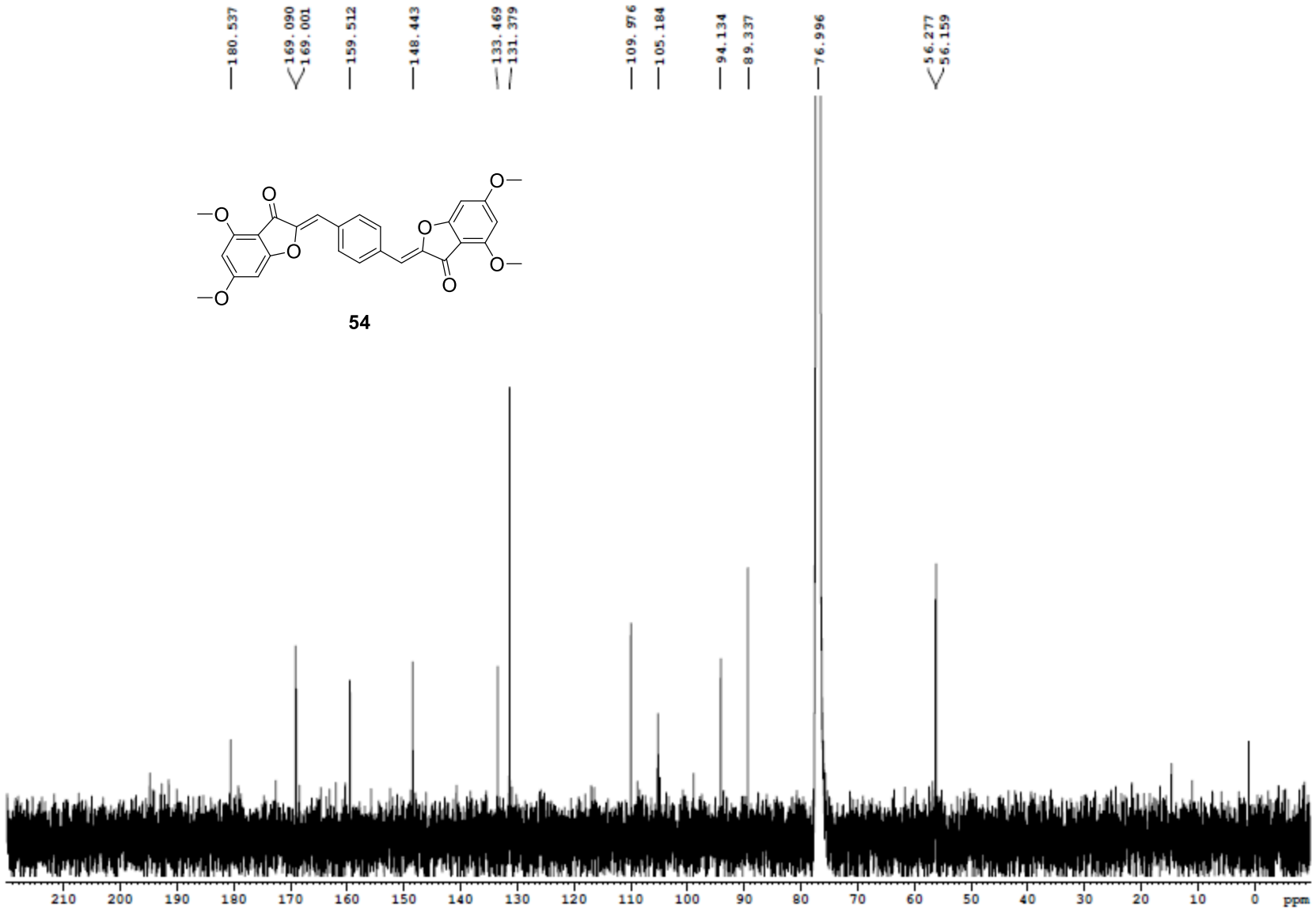
53

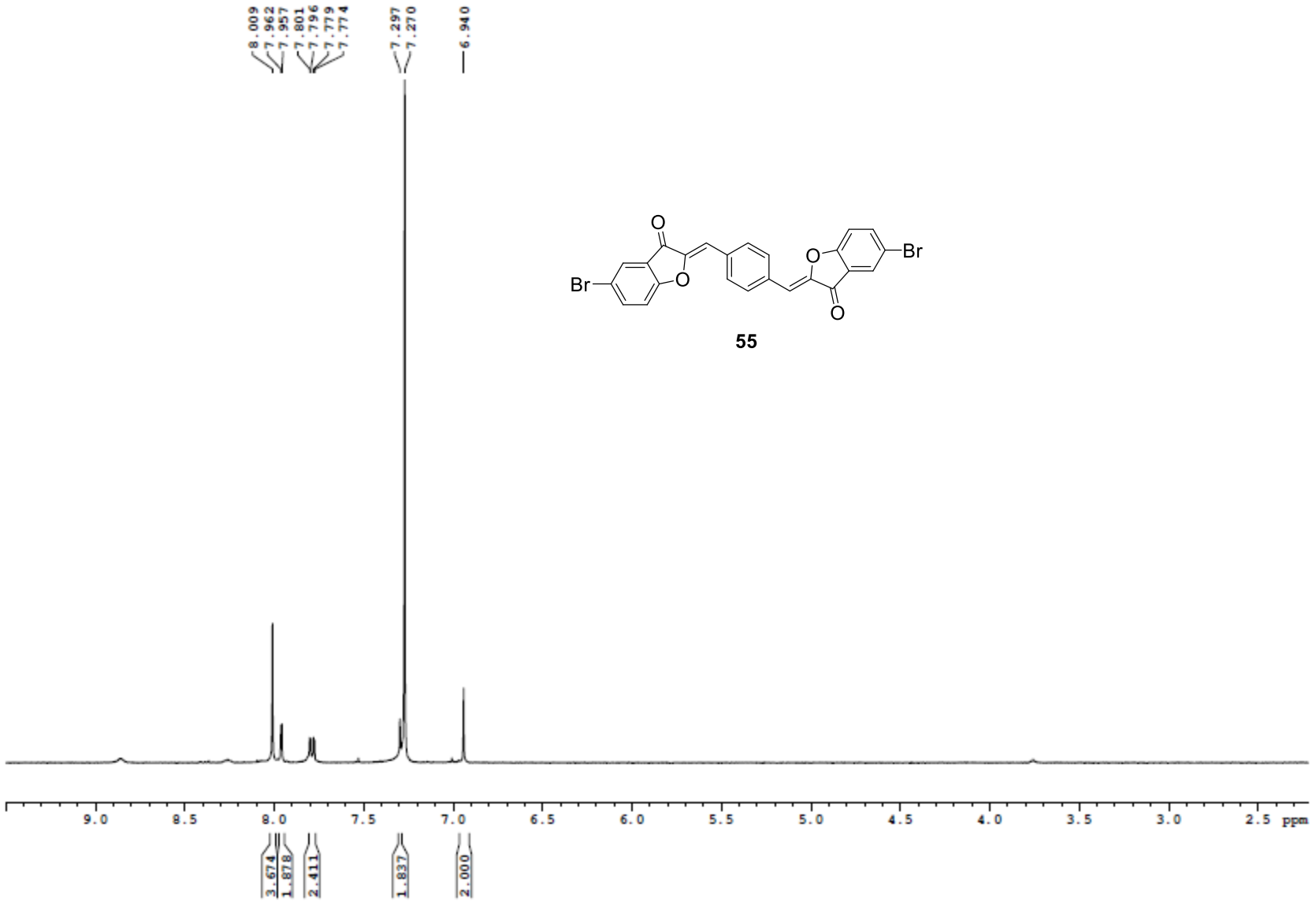

182.287
166.989
158.632
147.507
138.570
133.580
131.626
111.003
110.807
105.381
104.785
76.996
56.329
O
O
O
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

53


7.938
7.270
6.794
6.429
6.425
6.172
6.168
3.983
3.945
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
ppm
3.761
2.096
1.927
1.956
6.201
6.000

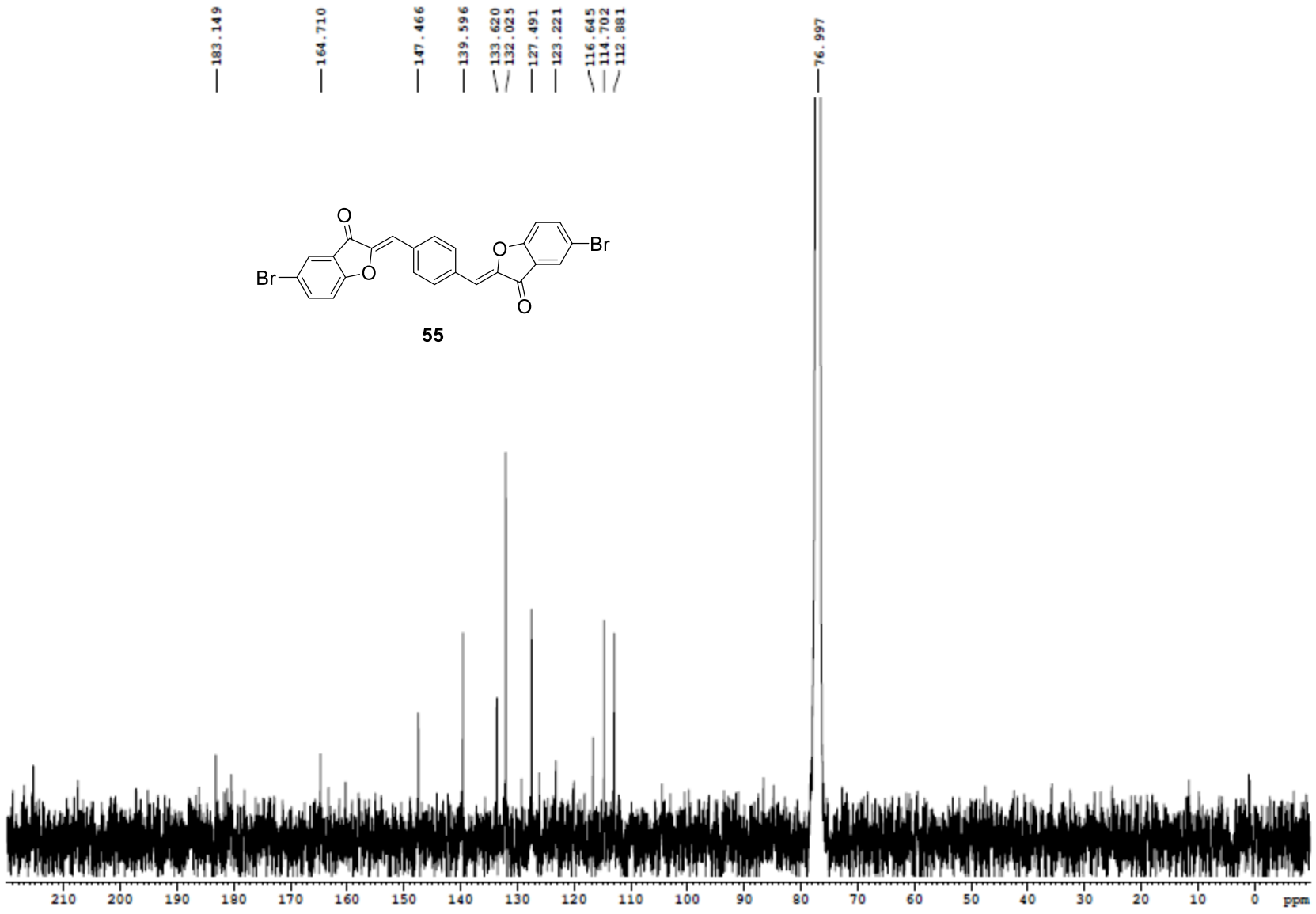
54


180.537
169.090
169.001
159.512
148.443
133.469
131.379
109.976
105.184
94.134
89.337
76.996
56.277
56.159
54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

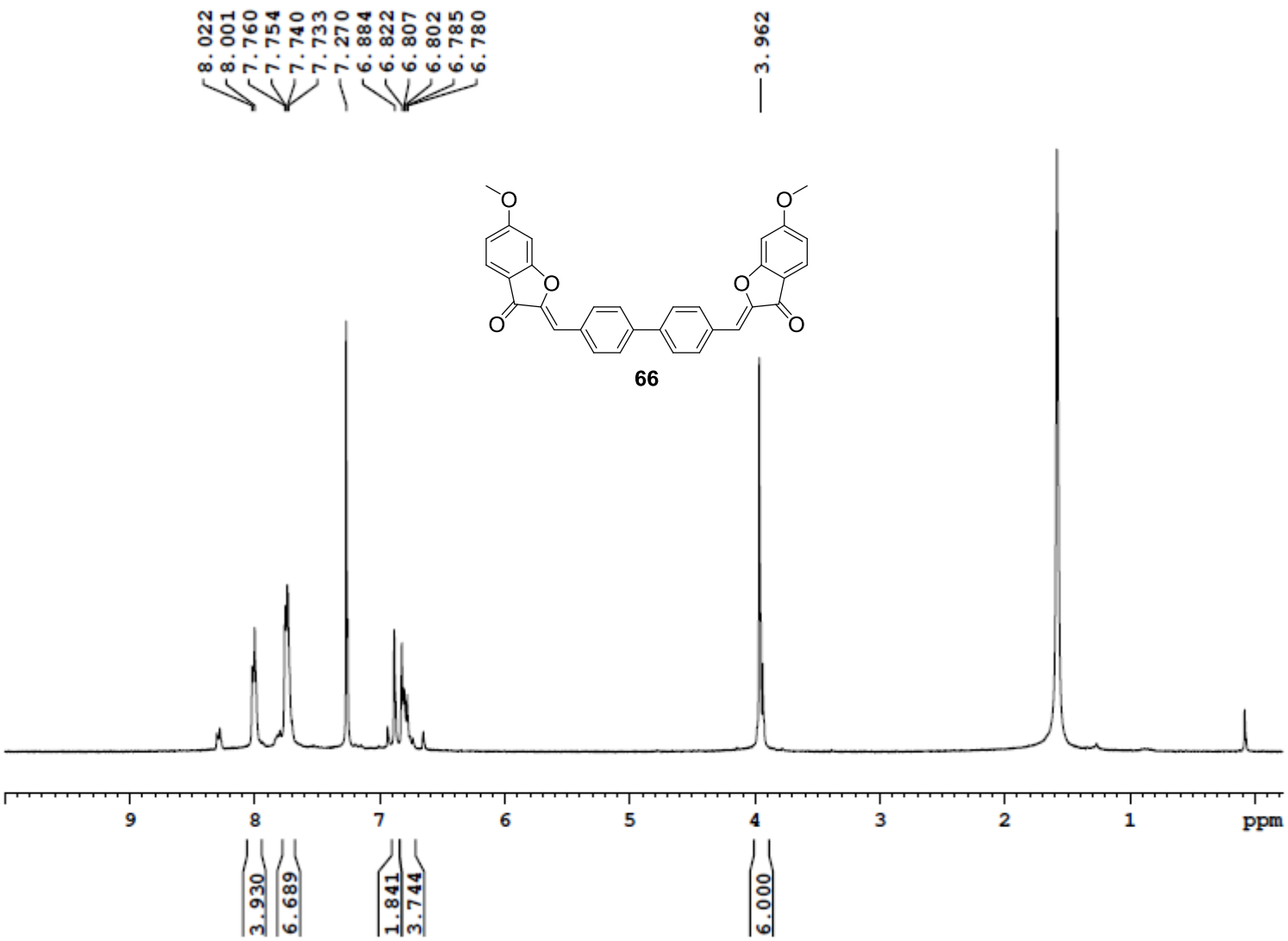

8.009
7.962
7.957
7.801
7.796
7.779
7.774
7.297
7.270
6.940
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.674
1.878
2.411
1.837
2.000

O
Br
O
O
O
Br

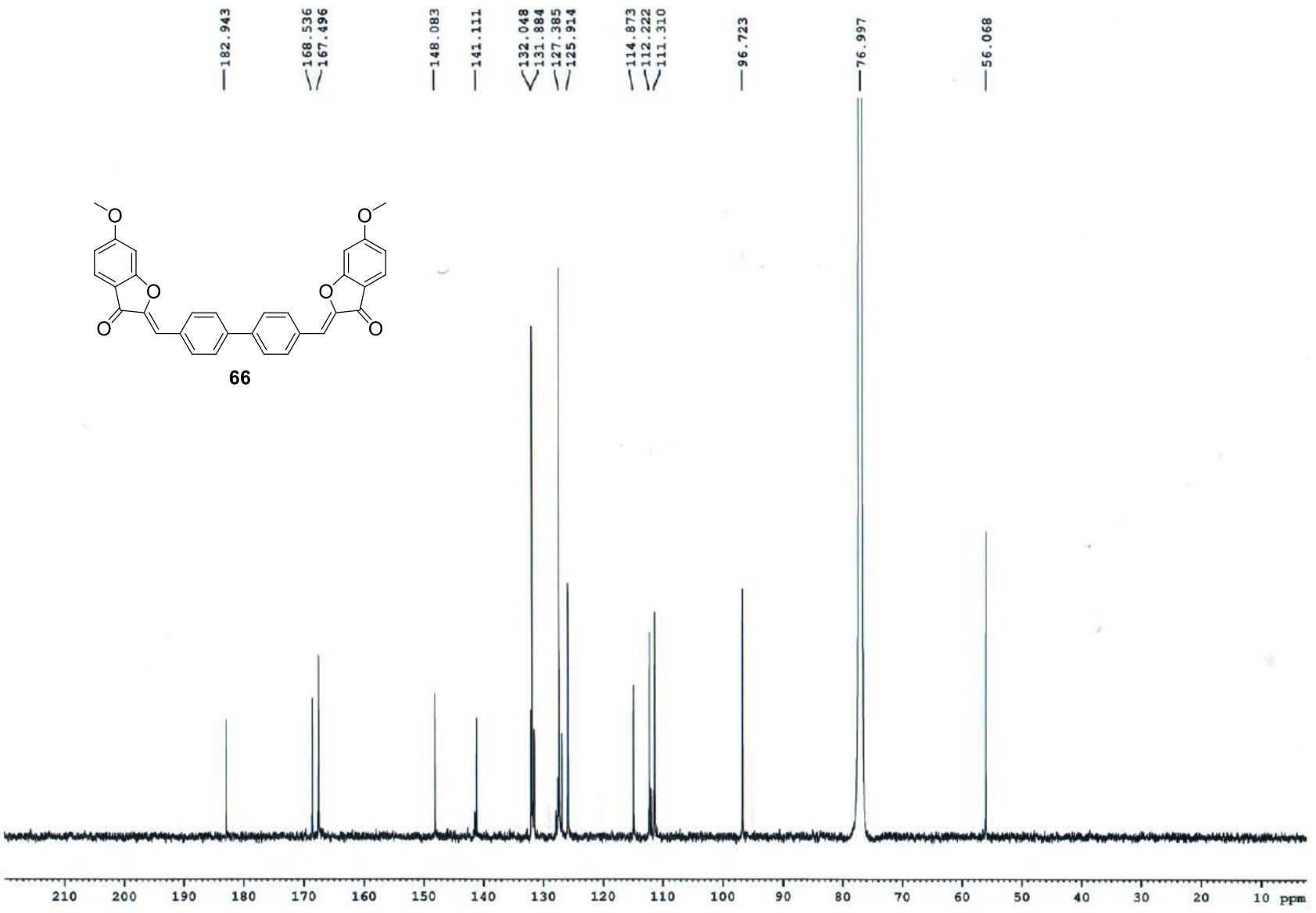
55

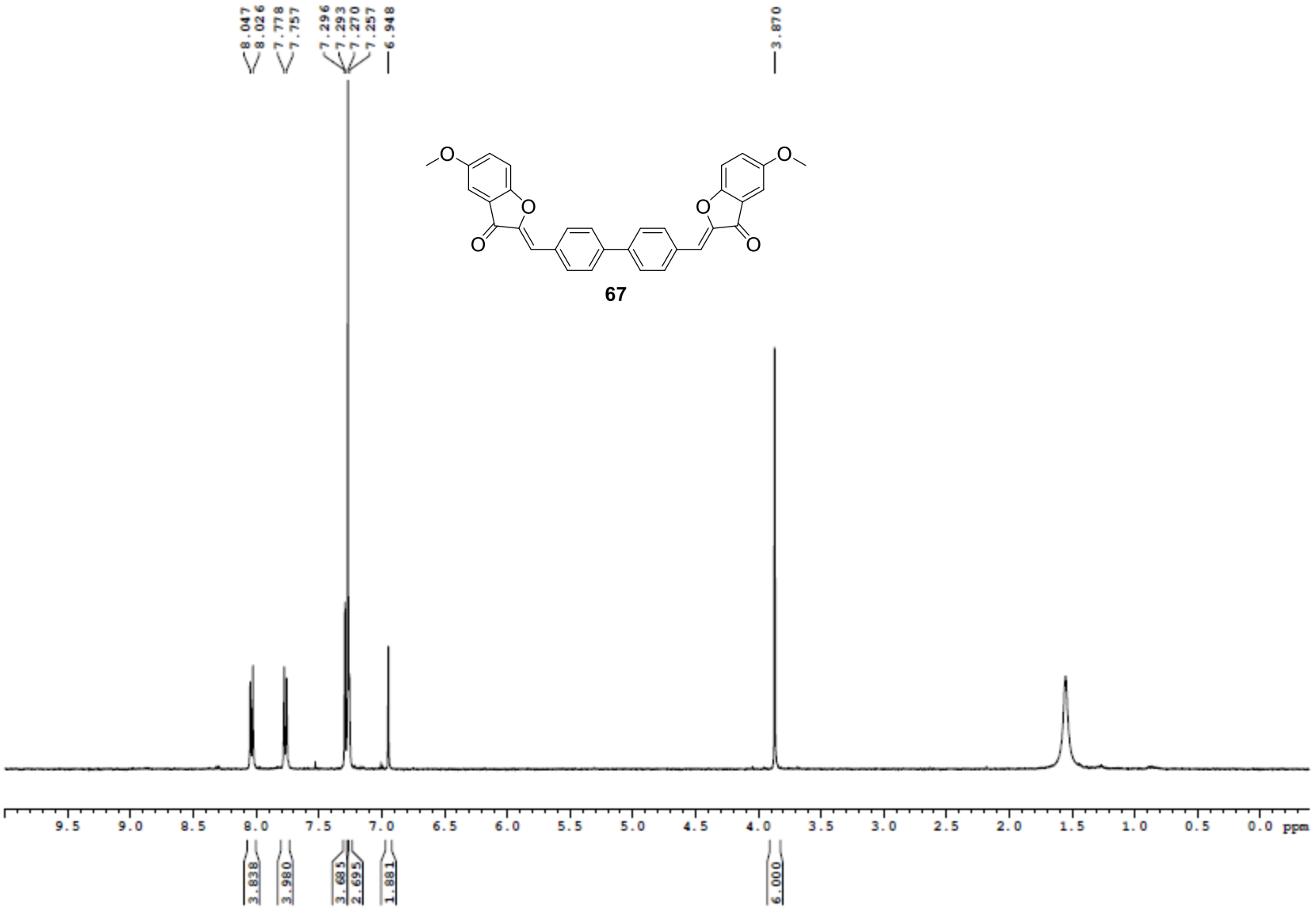

183.149
164.710
147.466
139.596
133.620
132.025
127.491
123.221
116.645
114.702
112.881
76.997
O
O
Br
O
Br
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

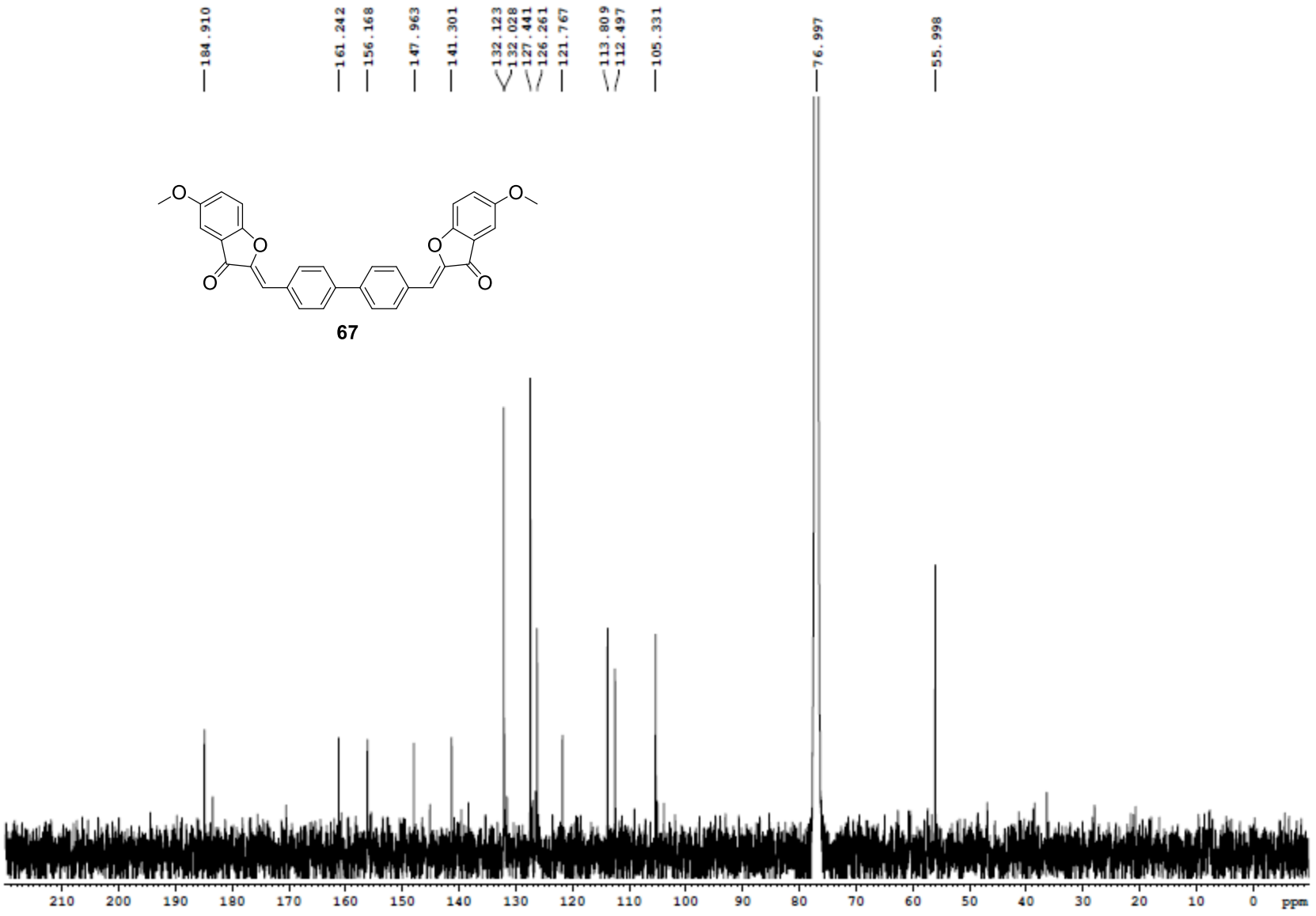
55

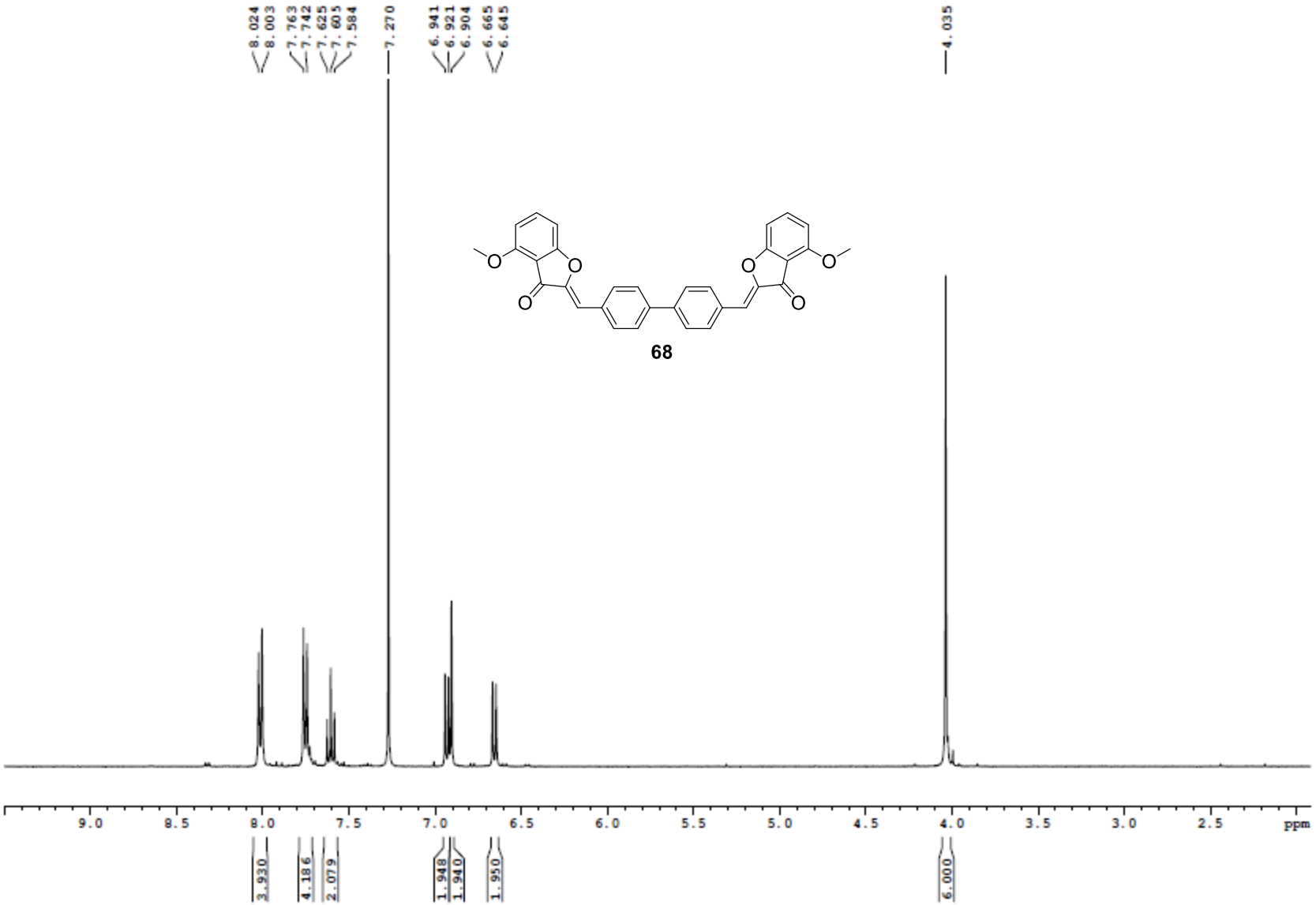

8.022
8.001
7.760
7.754
7.740
7.733
7.270
6.884
6.822
6.807
6.802
6.785
6.780
3.962
9
8
7
6
5
4
3
2
1
ppm
3.930
6.689
1.841
3.744
6.000

66

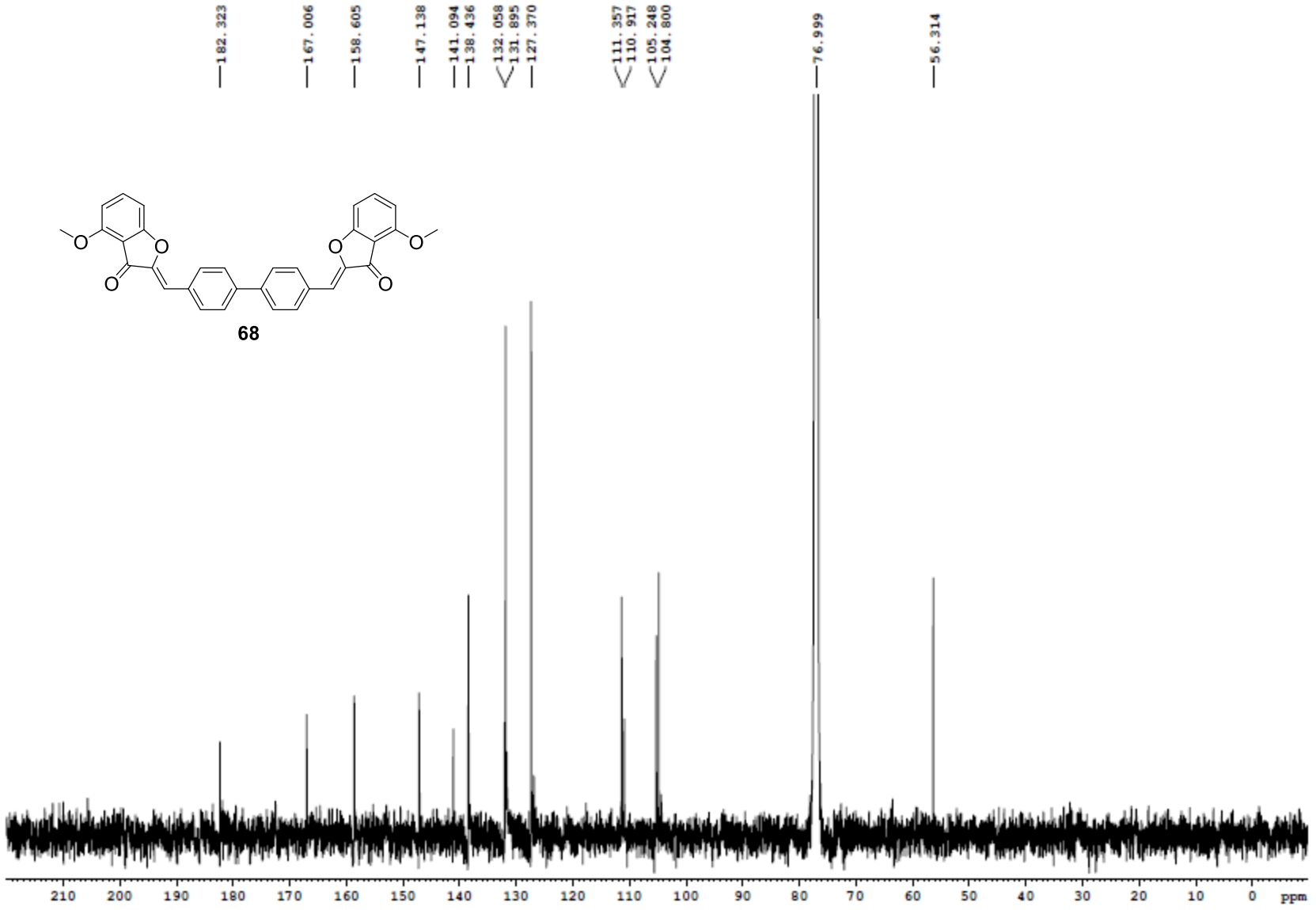

182.943
168.536
167.496
148.083
141.111
132.048
131.884
127.385
125.914
114.873
112.222
111.310
96.723
76.997
56.068
O
O
O
O
O
O
66
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

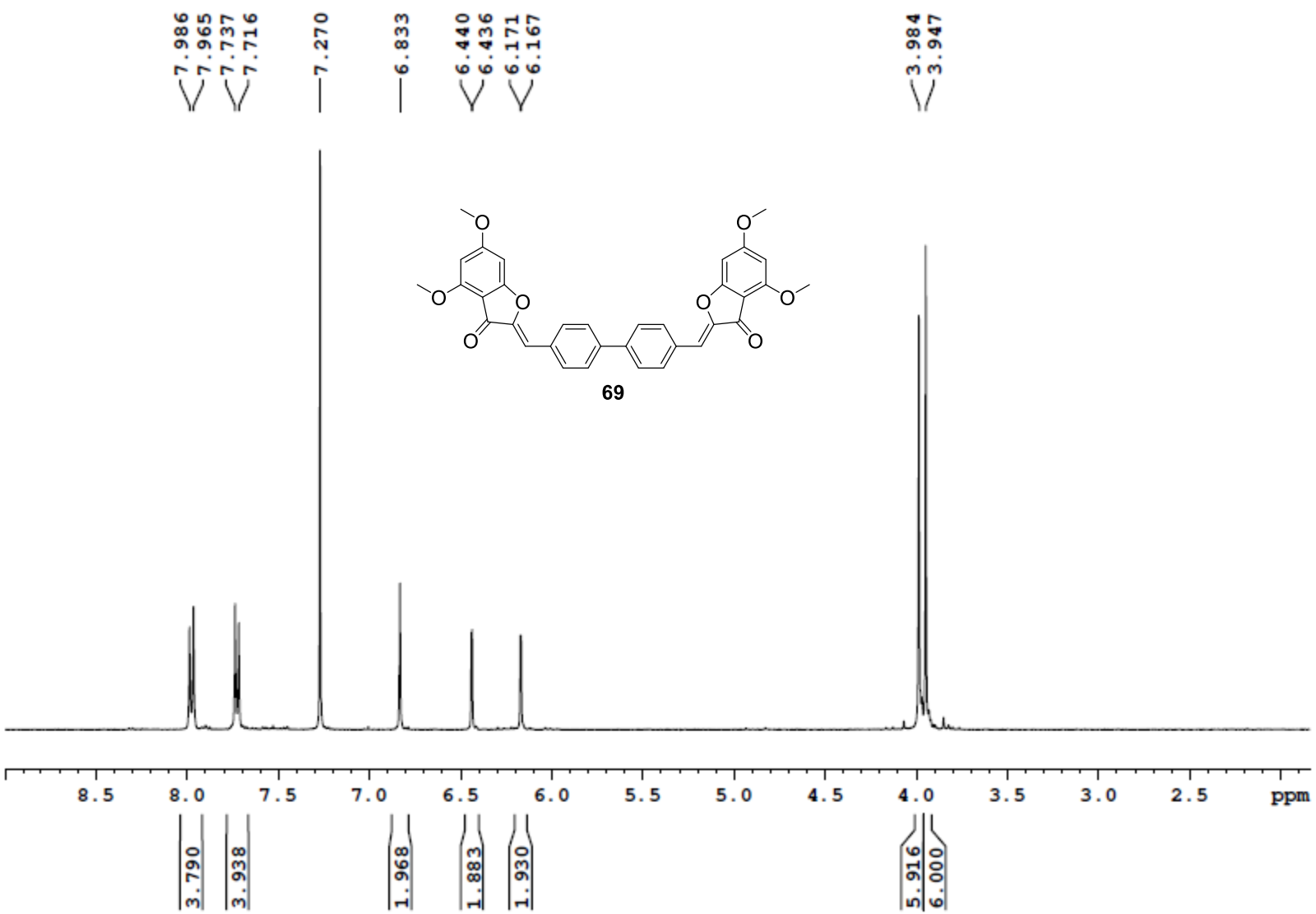

8.047
8.026
7.778
7.757
7.296
7.293
7.270
7.257
6.948
3.870
O
O
O
O
O
O
67
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
3.838
3.980
3.685
2.695
1.881
6.000


184.910
161.242
156.168
147.963
141.301
132.123
132.028
127.441
126.261
121.767
113.809
112.497
105.331
76.997
55.998
O
O
O
O
O
O
67
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

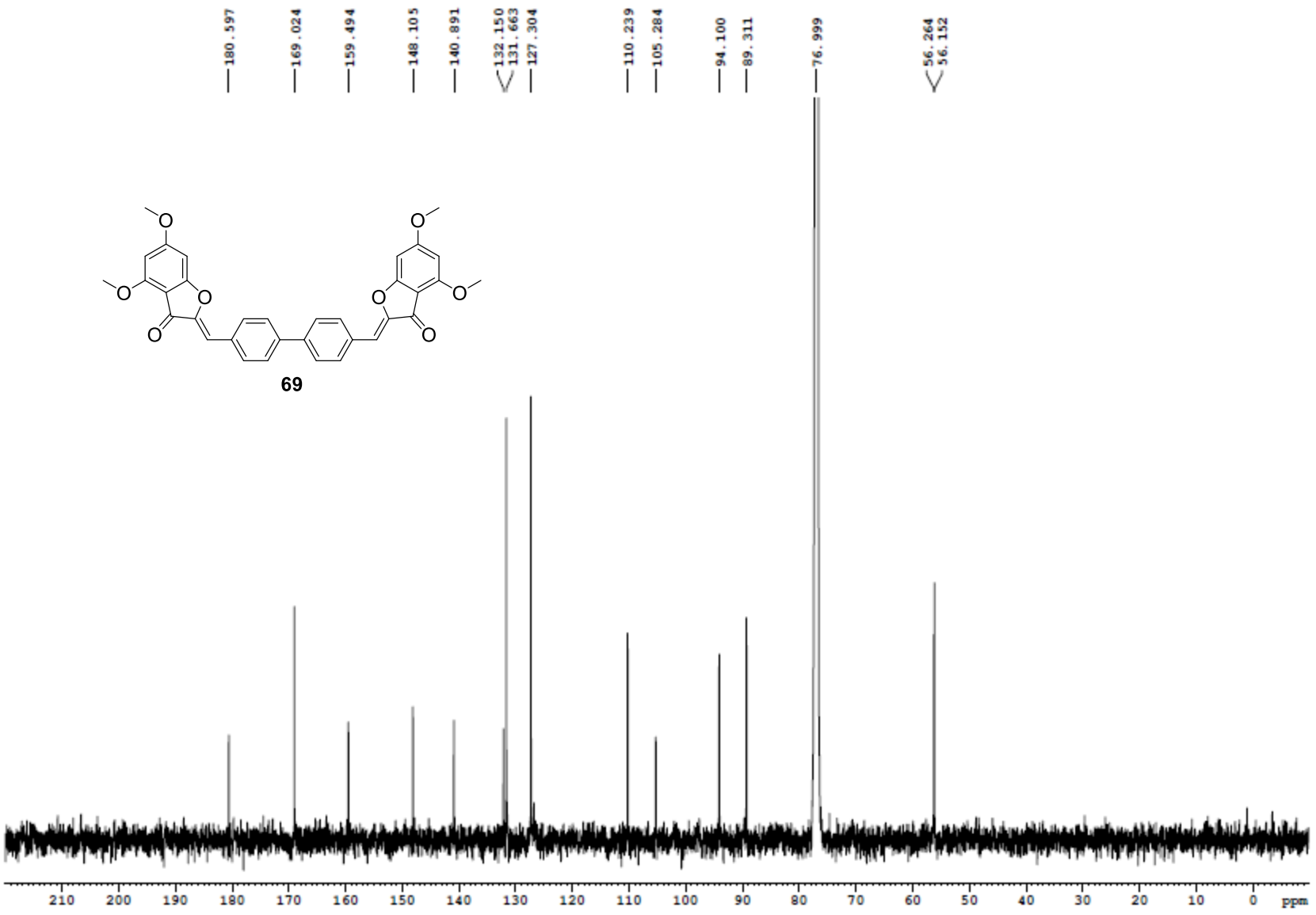

8.024
8.003
7.763
7.742
7.625
7.605
7.584
7.270
6.941
6.921
6.904
6.665
6.645
4.035
O
O
O
O
O
O
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.930
4.186
2.079
1.948
1.940
1.950
6.000

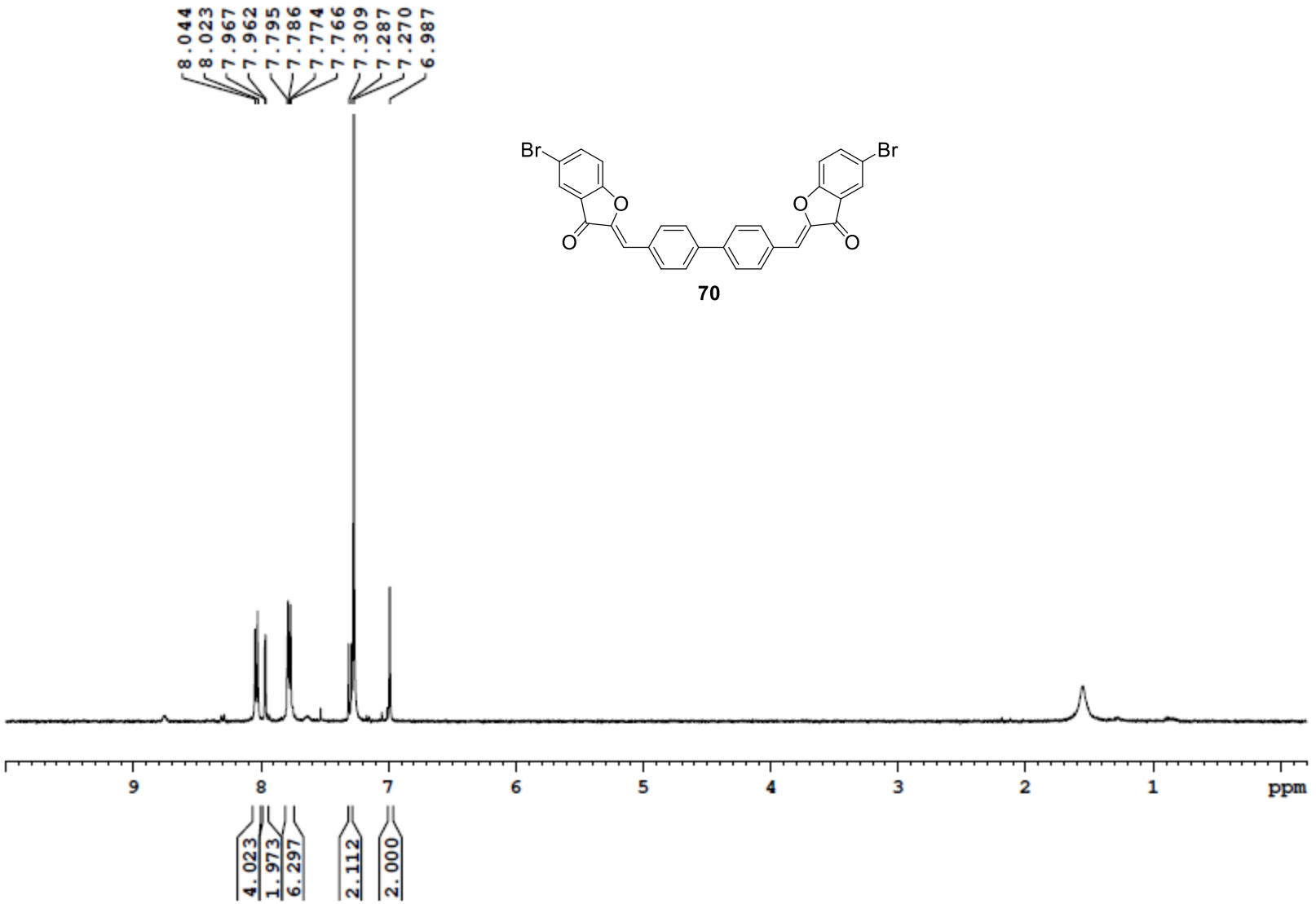
68


182.323
167.006
158.605
147.138
141.094
138.436
132.058
131.895
127.370
111.357
110.917
105.248
104.800
76.999
56.314
68
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

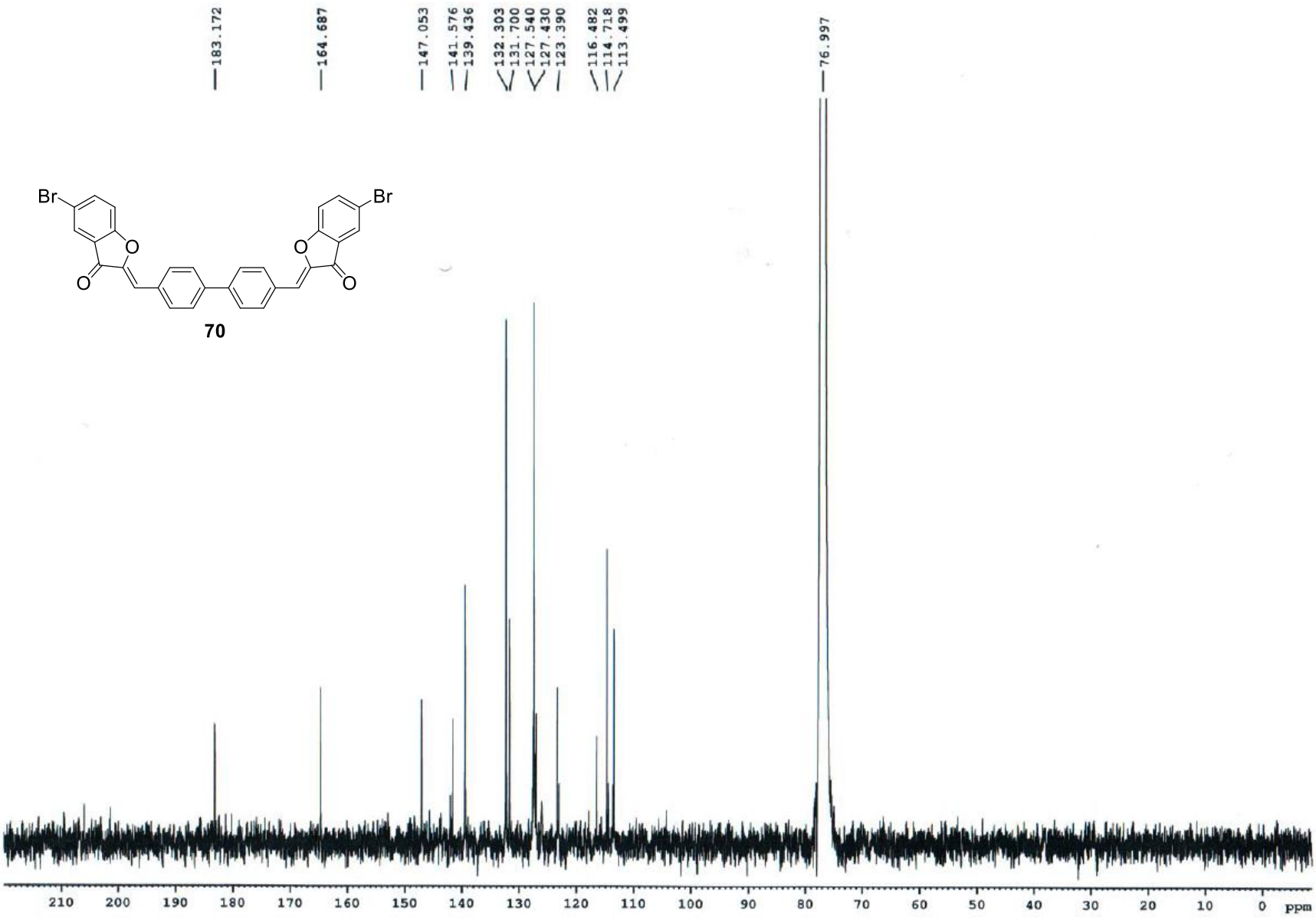

7.986
7.965
7.737
7.716
7.270
6.833
6.440
6.436
6.171
6.167
3.984
3.947
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.790
3.938
1.968
1.883
1.930
5.916
6.000

69


180.597
169.024
159.494
148.105
140.891
132.150
131.663
127.304
110.239
105.284
94.100
89.311
76.999
56.264
56.152
O
O
O
O
O
O
O
O
69
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.044
8.023
7.967
7.962
7.795
7.786
7.774
7.766
7.309
7.287
7.270
6.987
Br
Br
O
O
O
O
9
8
7
6
5
4
3
2
1
ppm
4.023
1.973
6.297
2.112
2.000

70


183.172
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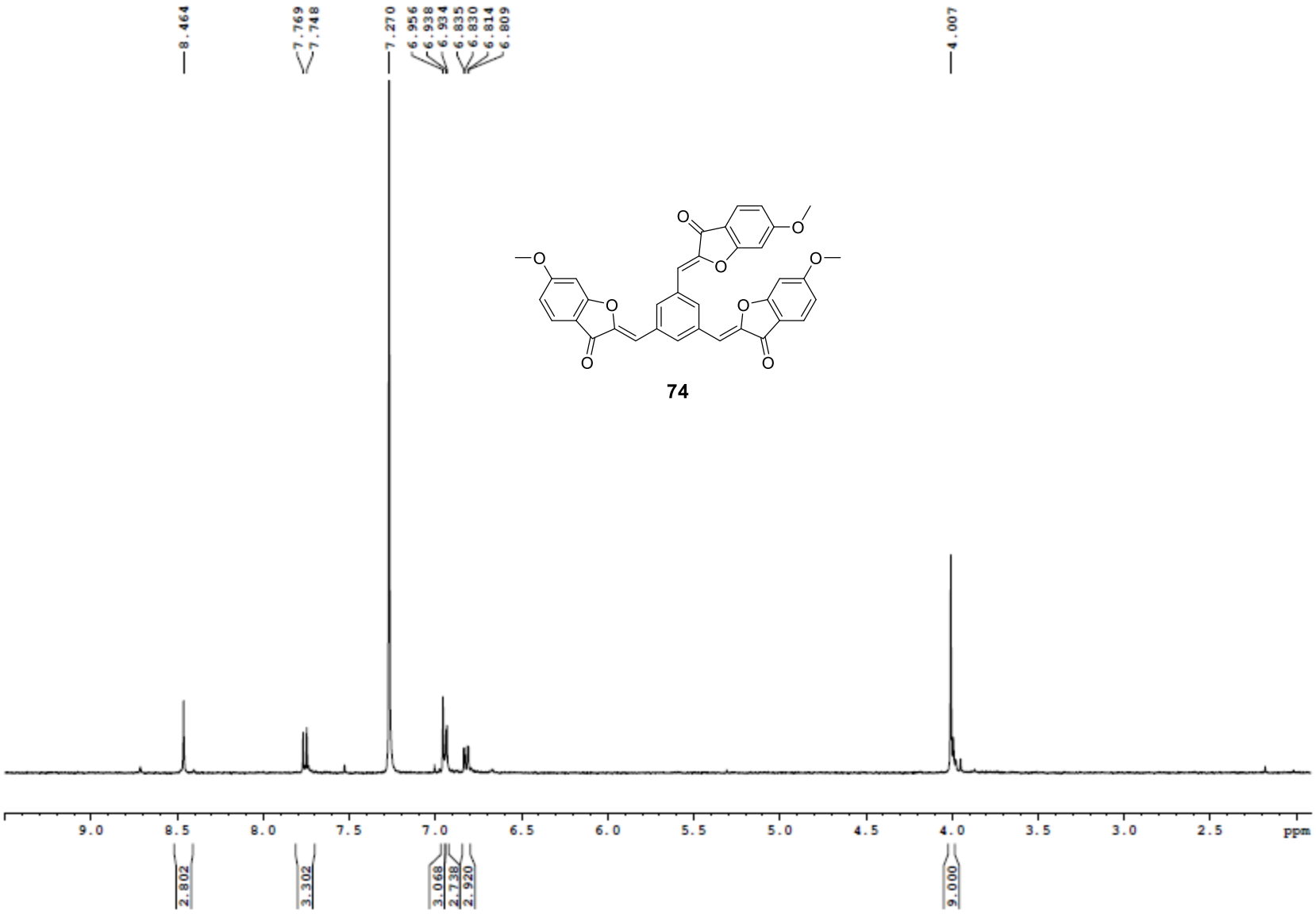
141.576
139.436
132.303
131.700
127.540
127.430
123.390
116.482
114.718
113.499
76.997
Br
Br
O
O
O
O
70
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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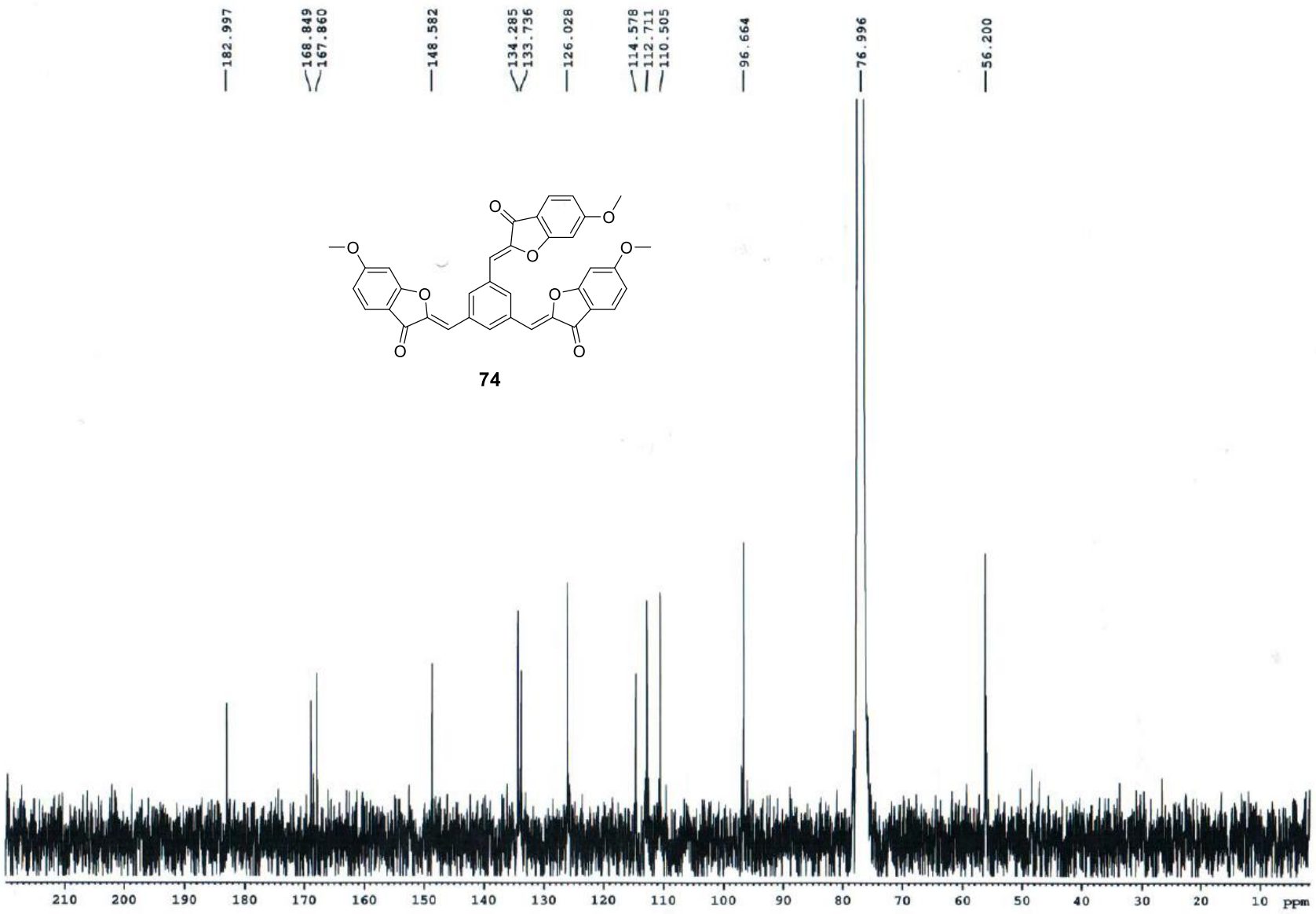
7.769
7.748
7.270
6.956
6.938
6.934
6.835
6.830
6.814
6.809
4.007
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
2.802
3.302
3.068
2.738
2.920
9.000

74


182.997
168.849
167.860
148.582
134.285
133.736
126.028
114.578
112.711
110.505
96.664
76.996
56.200
74
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm