Supporting Information

Generation of ArS-substituted Flavone Derivatives via Using Aryl Thiols as Sulfenylating Agents

Wannian Zhao,[a] Ping Xie,[b] Zhaogang Bian,[a] Aihua Zhou,[a*] Haibo Ge,[c*] Ben Niu,[a] and Yingcai Ding,[a]

[a]*Pharmacy School, Jiangsu University, Xuefu Road 301, Zhenjiang City, Jiangsu, China, 212013,*

[b]*Scientific Information Research Institute, Jiangsu University (Library)*

[c]*Department of Chemistry and Chemical Biology, Indiana University Purdue University Indianapolis, Indianapolis IN 46202 (USA)*

ahz@ujs.edu.cn

Table of contents

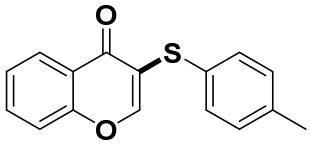
General experimental procedures

All reactions were carried out in sealed tubes; stirring was achieved with an oven-dried magnetic stirring bar. Solvents were purified by standard methods unless otherwise noted. Commercially available reagents were purchased from Aladdin Company in China and used throughout without further purification other than those detailed below. Flash column chromatography was performed on silica gel (200-300 mesh). All reactions were monitored by TLC analysis. Deuterated solvents were purchased from Cambridge Isotope laboratories. ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz respectively. HRMS spectrometry (LC-HRMS) was recorded on a LXQ Spectrometer (Thermo Scientific) operating on ESI-TOF (MeOH as a solvent). Flavones derivatives were synthesized according to the literature.

General procedure for the syntheses of compounds 3a-q

Flavone **1a** (0.5 mmol, 1.0 equiv.) was added to a dried sealed tube with DMF (0.5 mL), followed by the addition of NH_4I (2.0 equiv.) and aryl thiol (1.2 equiv.). The mixture was stirred at 135 ^{o}C. After 15 h, the reaction was cooled down to room temperature, diluted with ethyl acetate, washed with brine, dried over anhydrous Na_2SO_4 and concentrated under vacuum. The residue was purified by flash chromatography (Petroleum ether: EtOAc =15:1) on silica gel to give the desired product **3a** as a colorless oil in an 86% yield. The same procedure was applied to the production of other compounds **3b-q**.

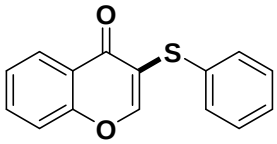
3-(*p*-Tolylthio)-4H-chromen-4-one (3a)



FTIR : 3075, 2923, 2359, 1647, 1464, 1114, 758 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz):

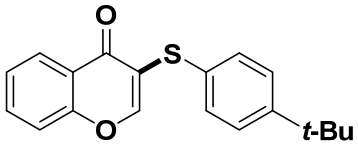
δ 8.26 (dd, *J*=8.0, 1.6 Hz, 1H), 8.07 (s, 1H), 7.72-7.68 (m, 1H), 7.49-7.42 (m, 2H), 7.37 (d, *J*=8.0 Hz, 2H), 7.13 (d, *J*=8.0 Hz, 2H), 2.33 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 156.3, 156.2, 137.6, 133.9, 131.0, 130.1, 129.8, 126.4, 125.4, 123.6, 121.1, 118.1, 21.1; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{12}NaO_2S^+$ 291.0450 $(M+Na)^+$, found 291.0447.

3-(Phenylthio)-4H-chromen-4-one (3b)



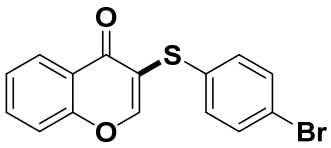
FTIR : 3058, 2925，1653, 1612, 1464, 1309, 1113, 760 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.28 (dd, *J*=8.0, 1.6 Hz, 1H), 8.18 (s, 1H), 7.74-7.70 (m, 1H), 7.51-7.40 (m, 4H), 7.33-7.22 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 157.4, 156.4, 134.0, 129.9, 129.2, 127.1, 126.5, 125.8, 123.7, 120.0, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_{10}NaO_2S^+$ 277.0294 $(M+Na)^+$, found 277.0296.

3-((4-(*tert*-Butyl)phenyl)thio)-4*H*-chromen-4-one (3c)



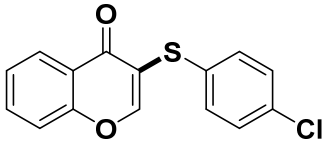
FTIR : 3070, 2963, 1649, 1611, 1560, 1462, 1115, 846, 764 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.27 (dd, *J*=8.0, 1.2 Hz, 1H), 8.09 (s, 1H), 7.73-7.68 (s, 1H), 7.49-7.43 (m, 2H), 7.40-7.33 (m, 4H), 1.30 (s, 9H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.2, 156.6, 156.3, 150.7, 133.9, 130.5, 130.0, 126.7, 126.4, 126.3, 125.7, 123.6, 118.1, 34.6, 31.2; **HRMS (**ESI-TOF) m/z calculated for $C_{19}H_{18}NaO_2S^+$ 333. 0920 $(M+Na)^+$, found 333. 0917.

3-((4-Bromophenyl)thio)-4H-chromen-4-one (3d)



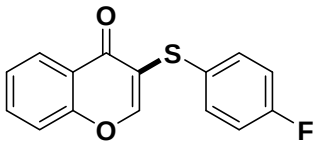
FTIR : 3061, 2925, 1641, 1463, 1086, 901, 798 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.26(dd, *J*=7.2, 4.8 Hz, 2H), 7.76-7.71 (m, 1H), 7.52-7.45 (m, 2H), 7.41 (dd, *J*=6.8, 2.0 Hz, 2H), 7.26 (dd, *J*=8.8, 6.8 Hz, 2H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.9, 158.1, 156.4, 134.2, 133.6, 132.2, 131.0, 126.5, 126.0, 123.7, 121.0, 119.0, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9BrNaO_2S^+$ 354.9399 $(M+Na)^+$, found 354.9394.

3-((4-Chlorophenyl)thio)-4H-chromen-4-one (3e)



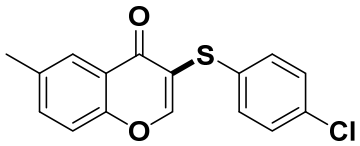
FTIR : 3051, 1648, 1478，1465, 1313, 1091, 827, 758 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.25 (m, 2H), 7.75-7.71 (m, 1H), 7.52-7.45 (m, 2H), 7.35-7.25 (m, 4H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.0, 157.9, 156.4, 134.2, 133.1, 132.8, 130.9, 129.3, 126.5, 125.9, 123.7, 119.2, 118.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9ClNaO_2S^+$ 310.9904 $(M+Na)^+$, found 310.9894.

3-((4-Fluorophenyl)thio)-4H-chromen-4-one (3f)



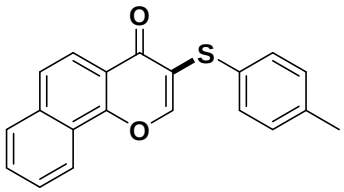
FTIR : 3053, 2361, 1645, 1491, 1465, 1222, 829, 758 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.24 (dd, *J*=8.0, 1.2 Hz, 1H), 8.16 (s, 1H), 7.73-7.69 (m, 1H), 7.49-7.43 (m, 4H), 7.01 (t, *J*=8.8 Hz, 2H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 163.6, 161.1, 156.9, 156.3, 134.1, 132.9, 132.8, 128.8, 126.4, 125.8, 123.7, 120.5, 118.2, 116.5, 116.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9FNaO_2S^+$ 295.0199 $(M+Na)^+$, found 295.0205.

3-((4-Chlorophenyl)thio)-6-methyl-4H-chromen-4-one (3g)



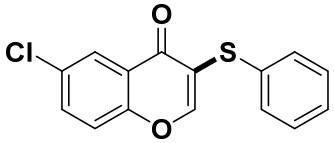
FTIR : 3053, 2922, 1639, 1478, 1311, 1091, 812, 789 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.24 (s, 1H), 8.03 (d, *J*=1.2 Hz, 1H), 7.53 (dd, *J*=8.4, 2.0 Hz, 1H), 7.40 (d, *J*=8.8 Hz, 1H), 7.33-7.22 (m, 4H), 2.47 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.1, 158.1, 154.7, 136.1, 135.4, 133.1, 132.9, 130.7, 129.2, 125.7, 123.4, 118.8, 118.0, 21.0; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}ClNaO_2S^+$ 325.0060 $(M+Na)^+$, found 325.0049.

3-(*p*-Tolylthio)-4H-benzo[h]chromen-4-one (3h)



FTIR : 3057, 2920, 2361, 1650, 1633, 1384, 1113, 886, 765 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.40 (d, *J*=8.0 Hz, 1H), 8.16 (d, *J*=8.8 Hz, 1H), 8.08 (s, 1H), 7.91 (d, *J*=7.6 Hz, 1H), 7.77-7.64 (m, 3H), 7.43 (d, *J*=8.0 Hz, 2H), 7.16 (d, *J*=8.0 Hz, 2H), 2.35 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.8, 154.3, 153.7, 138.0, 135.8, 131.7, 130.2, 129.5, 129.1, 128.1, 127.3, 125.7, 123.8, 123.4, 122.2, 121.0, 119.6, 21.2; **HRMS (**ESI-TOF) m/z calculated for $C_{20}H_{14}NaO_2S^+$ 341.0607 $(M+Na)^+$, found 341.0603.

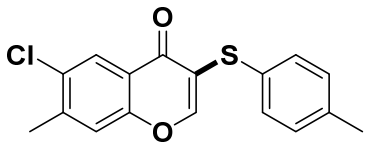
6-Chloro-3-(phenylthio)-4H-chromen-4-one (3i)



FTIR : 3068, 2925, 2360, 1653, 1466, 1303, 1122, 918, 821, 755 cm^{-1}; **^{1}H-NMR** (CDCl3, 400 MHz): δ 8.22 (d, *J* = 2.6 Hz, 1H), 8.12 (s, 1H), 7.65 (dd, *J*=9.2, 2.8 Hz, 1H), 7.47-7.40 (m, 3H), 7.34-7.25 (m, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.0,

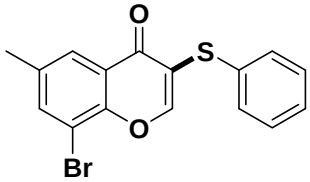
157.0, 154.7, 134.2, 133.4, 131.7, 130.3, 129.3, 127.5, 125.7, 124.5, 120.5, 120.0; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9ClNaO_2S^+$ 310.9904 $(M+Na)^+$, found 310.9914.

6-Chloro-7-methyl-3-(*p*-tolylthio)-4H-chromen-4-one (3j)



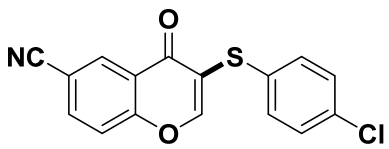
FTIR : 3060, 2924, 1651，1412, 1097, 899, 786 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.19 (s, 1H), 7.98 (s, 1H), 7.35 (d, *J*=8.0 Hz, 3H), 7.13 (d, *J*=8.0 Hz, 2H), 2.51 (s, 3H), 2.33 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.0, 155.9, 154.6, 143.3, 137.8, 132.3, 131.2, 130.1, 129.5, 122.5, 121.2, 119.9, 21.1, 20.9; **HRMS (**ESI-TOF) m/z calculated for $C_{17}H_{13}ClNaO_2S^+$ 339.0217 $(M+Na)^+$, found 339.0213.

8-Bromo-6-methyl-3-(phenylthio)-4H-chromen-4-one (3k)



FTIR : 3054, 2925, 2360, 1660, 1463, 1299, 1090, 785, 691 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.11 (s, 1H), 7.98 (d, *J*=1.2 Hz, 1H), 7.75 (d, *J*=2.0 Hz, 1H), 7.43 (dd, *J*=3.6, 1.6 Hz, 2H), 7.34-7.24 (m, 3H), 2.45 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 174.5, 156.4, 151.2, 138.5, 136.8, 133.2, 130.5, 129.3, 127.5, 125.3, 124.3, 120.8, 111.2, 20.8; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}BrNaO_2S^+$ 368.9555 $(M+Na)^+$, found 368. 9553.

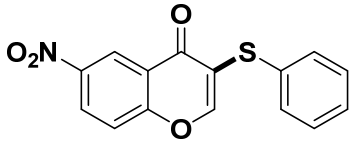
3-((4-Chlorophenyl)thio)-4-oxo-4H-chromene-6-carbonitrile (3l)



FTIR : 3054, 2924, 2361, 1654, 1475, 1313, 815, 670 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400

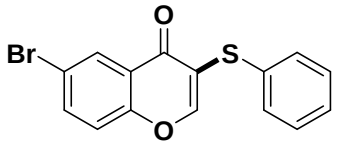
MHz): δ 8.58 (d, *J*=2.0 Hz, 1H), 8.16 (s, 1H), 7.94 (dd, *J*=8.8, 2.0 Hz, 1H), 7.62 (d, *J*=8.4 Hz, 1H), 7.40 (d, *J*=8.4 Hz, 2H), 7.30 (d, *J*=8.4 Hz, 2H); ^{13}**C-NMR** ($CDCl_3$, 100 MHz): δ 173.2, 158.0, 156.7, 136.3, 134.1, 132.2, 132.1, 131.1, 129.6, 123.9, 121.7, 120.0, 117.2, 110.2; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_8ClNNaO_2S^+$ 335.9856 $(M+Na)^+$, found 335.9853.

6-Nitro-3-(phenylthio)-4H-chromen-4-one (3m)



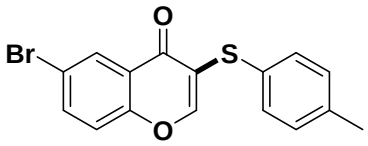
FTIR : 3061, 2342, 1655, 1524, 1346, 1105, 835, 738 cm^{-1}; ^{1}**H-NMR** ($CDCl_3$, 400 MHz): δ 9.11 (d, *J*=2.8 Hz, 1H), 8.52 (dd, *J*=9.2, 2.8 Hz,1H), 8.04 (s, 1H), 7.60 (d, *J*=9.2 Hz, 1H), 7.48 (dd, *J*=8.0, 1.6 Hz, 2H), 7.38-7.32 (m, 3H); ^{13}**C-NMR** ($CDCl_3$, 100 MHz): δ 173.6, 159.0, 155.7, 145.0, 132.1, 131.4, 129.5, 128.2, 128.1, 123.4, 123.2, 122.7, 120.0; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9NNaO_4S^+$ 322.0144 $(M+Na)^+$, found 322.0143.

6-Bromo-3-(phenylthio)-4H-chromen-4-one (3n)



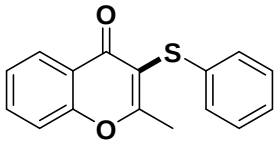
FTIR : 3058, 2923, 1652, 1548, 1462, 1121, 908, 818, 735 cm^{-1}; ^{1}**H-NMR** ($CDCl_3$, 400 MHz): δ 8.38 (d, *J*=2.4 Hz, 1H), 8.12 (s, 1H), 7.78 (q, *J*=2.4, 1H), 7.43-7.38 (m, 3H), 7.34-7.24 (m, 3H); ^{13}**C-NMR** ($CDCl_3$, 100 MHz): δ 173.8, 157.0, 155.1, 137.0, 133.4, 130.3, 129.3, 129.0, 127.5, 124.8, 120.6, 120.2, 119.2; **HRMS (**ESI-TOF) m/z calculated for $C_{15}H_9BrNaO_3S^+$ 354.9399 $(M+Na)^+$, found 354.9394.

6-Bromo-3-(*p*-tolylthio)-4H-chromen-4-one (3o)



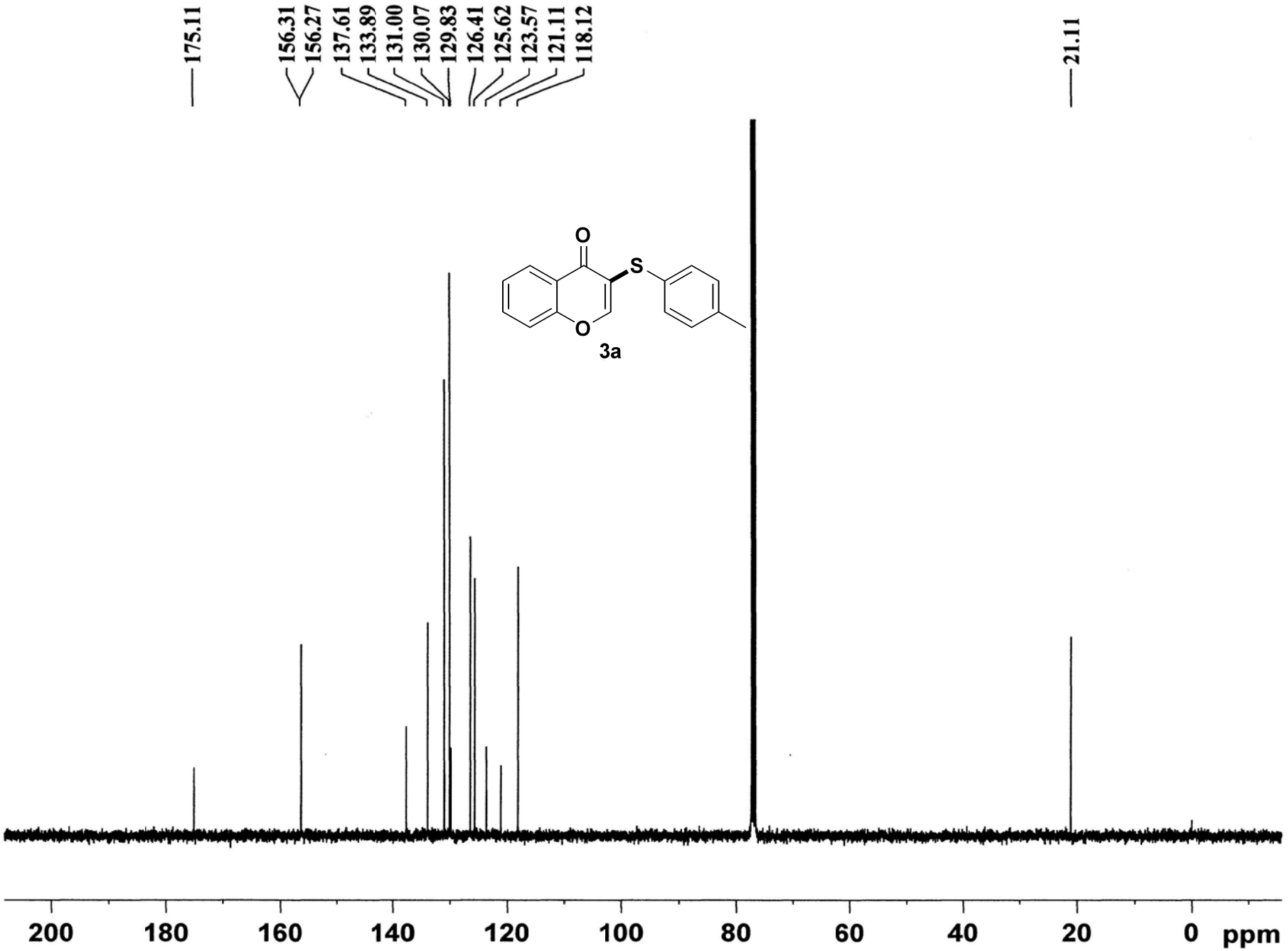
FTIR : 3052, 2913, 1657, 1548, 1465, 1122, 908, 818, 735 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.37 (d, *J*=2.4 Hz, 1H), 8.00 (s, 1H), 7.76 (dd, *J*=8.8, 2.4 Hz, 1H), 7.37 (d, *J*=8.4 Hz, 3H), 7.14 (m, *J*=8.0 Hz, 3H), 2.34 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 173.8, 155.8, 155.1, 138.0, 136.9, 131.5, 130.2, 129.1, 128.9, 124.7, 121.9, 120.1, 119.0, 119, 21.1; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{11}BrNaO_2S^+$ 368.9555 $(M+Na)^+$, found 368. 9531.

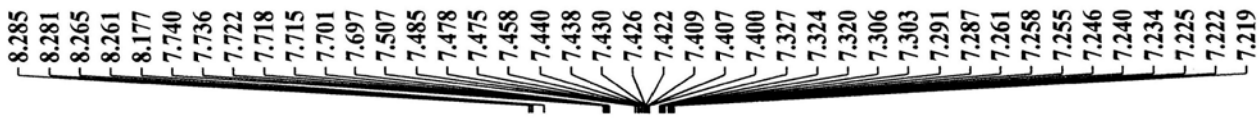
2-Methyl-3-(phenylthio)-4H-chromen-4-one (3q)

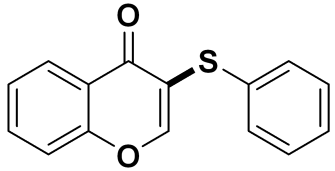


FTIR : 3050, 2924, 1647, 1465, 1120, 982, 764, 691 cm^{-1}; **^{1}H-NMR** ($CDCl_3$, 400 MHz): δ 8.23 (dd, *J*=8.0, 1.6 Hz, 1H), 7.71-7.67 (m, 1H), 7.47-7.40 (m, 2H), 7.28-7.22 (m, 4H), 7.17-7.12 (m, 1H), 2.74 (s, 3H); **^{13}C-NMR** ($CDCl_3$, 100 MHz): δ 175.3, 171.5, 155.6, 135.7, 133.8, 129.3, 129.0, 127.5, 126.6, 126.0, 125.5, 122.9, 117.7, 115.3, 20.8; **HRMS (**ESI-TOF) m/z calculated for $C_{16}H_{12}NaO_2S^+$ 291.0450 $(M+Na)^+$, found 291.0451.

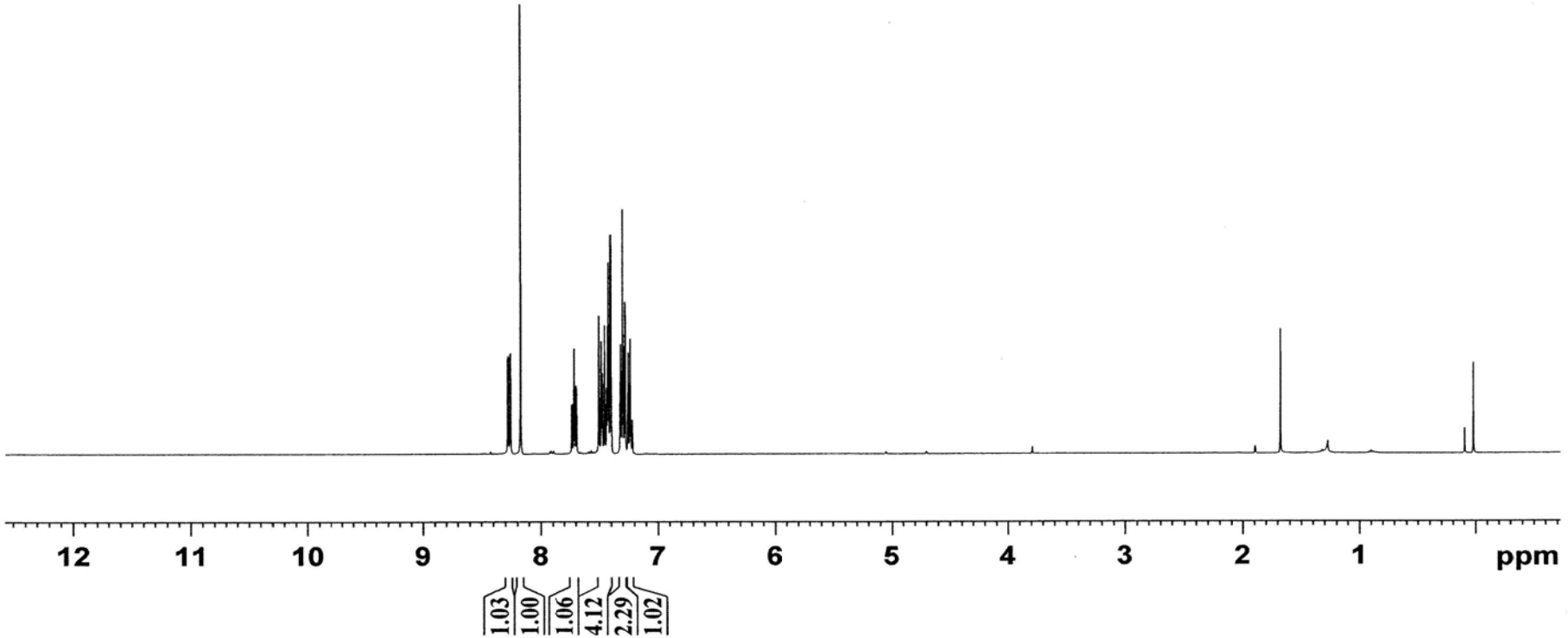
8.274
8.271
8.254
8.251
8.067
7.723
7.719
7.705
7.701
7.698
7.684
7.680
7.485
7.463
7.442
7.424
7.422
7.380
7.359
7.144
7.124
2.332
S
O
O
3a
ppm
0
1
2
3
4
5
6
7
8
9
3.00
1.91
1.89
1.94
1.00
0.95
0.97

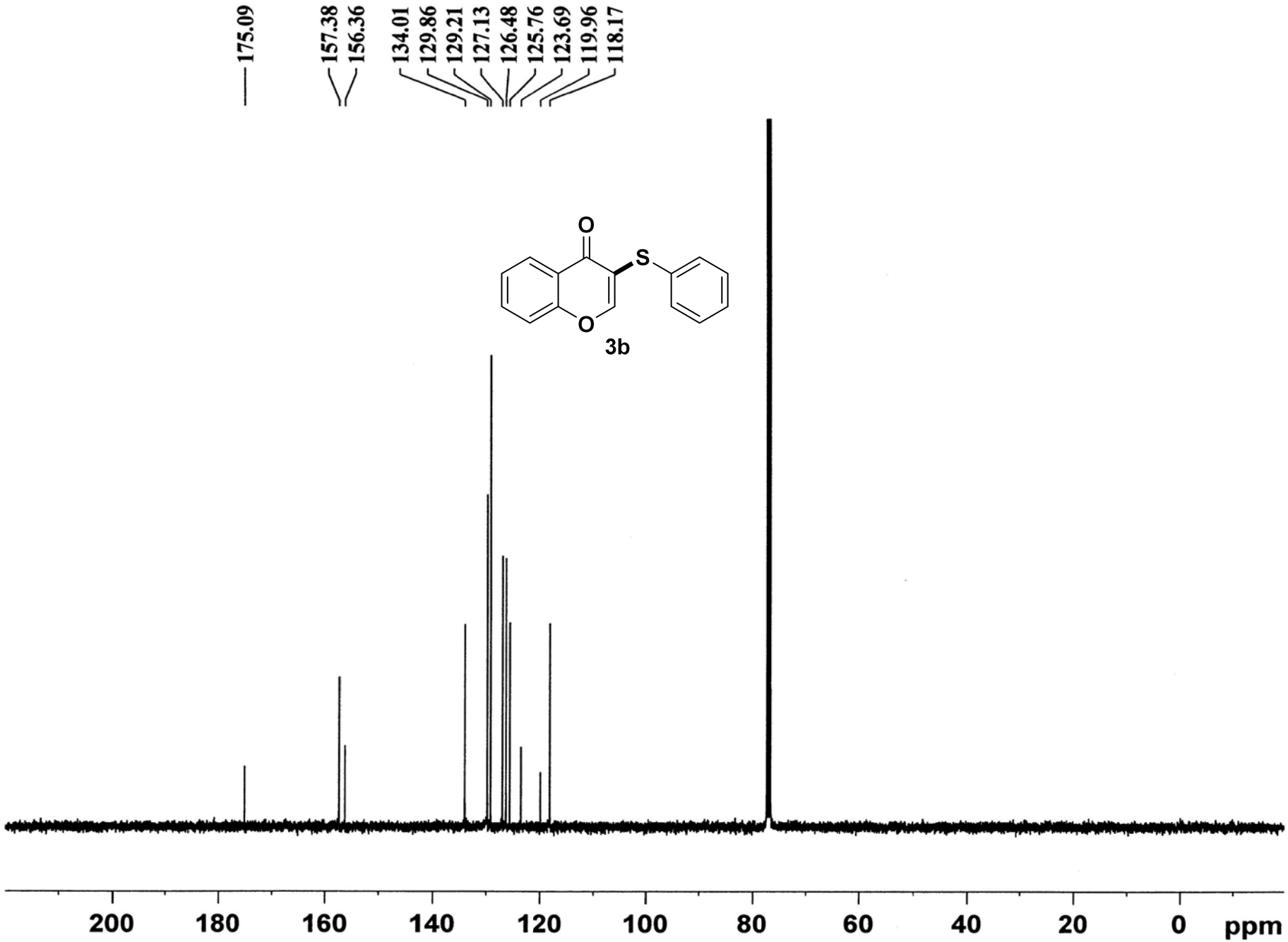

175.11
156.31
156.27
137.61
133.89
131.00
130.07
129.83
126.41
125.62
123.57
121.11
118.12
21.11
O
S
O
3a
200
180
160
140
120
100
80
60
40
20
0
ppm

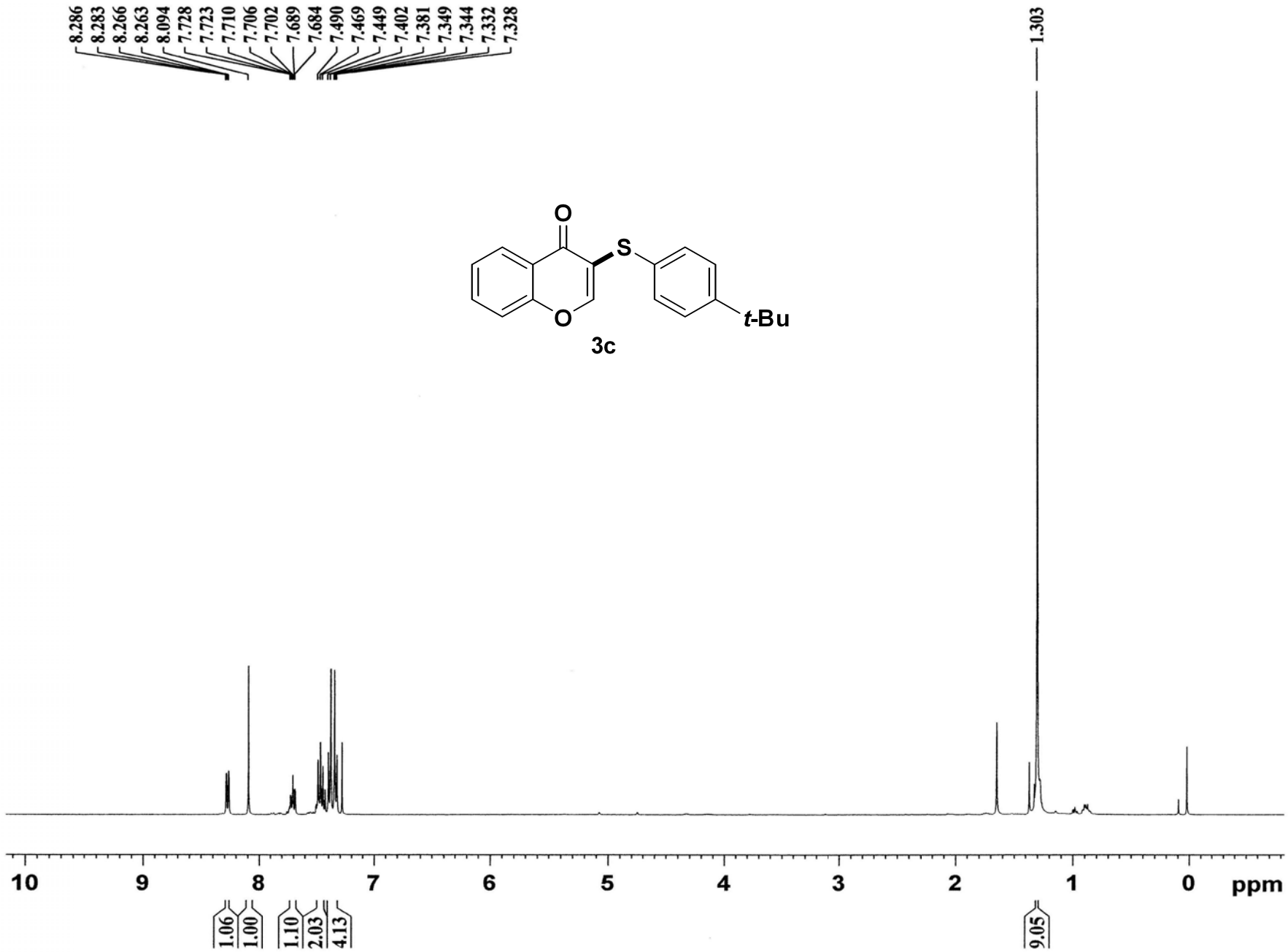

8.285
8.281
8.265
8.261
8.177
7.740
7.736
7.722
7.718
7.715
7.701
7.697
7.507
7.485
7.478
7.475
7.458
7.440
7.438
7.430
7.426
7.422
7.409
7.407
7.400
7.327
7.324
7.320
7.306
7.303
7.291
7.287
7.261
7.258
7.255
7.246
7.240
7.234
7.225
7.222
7.219

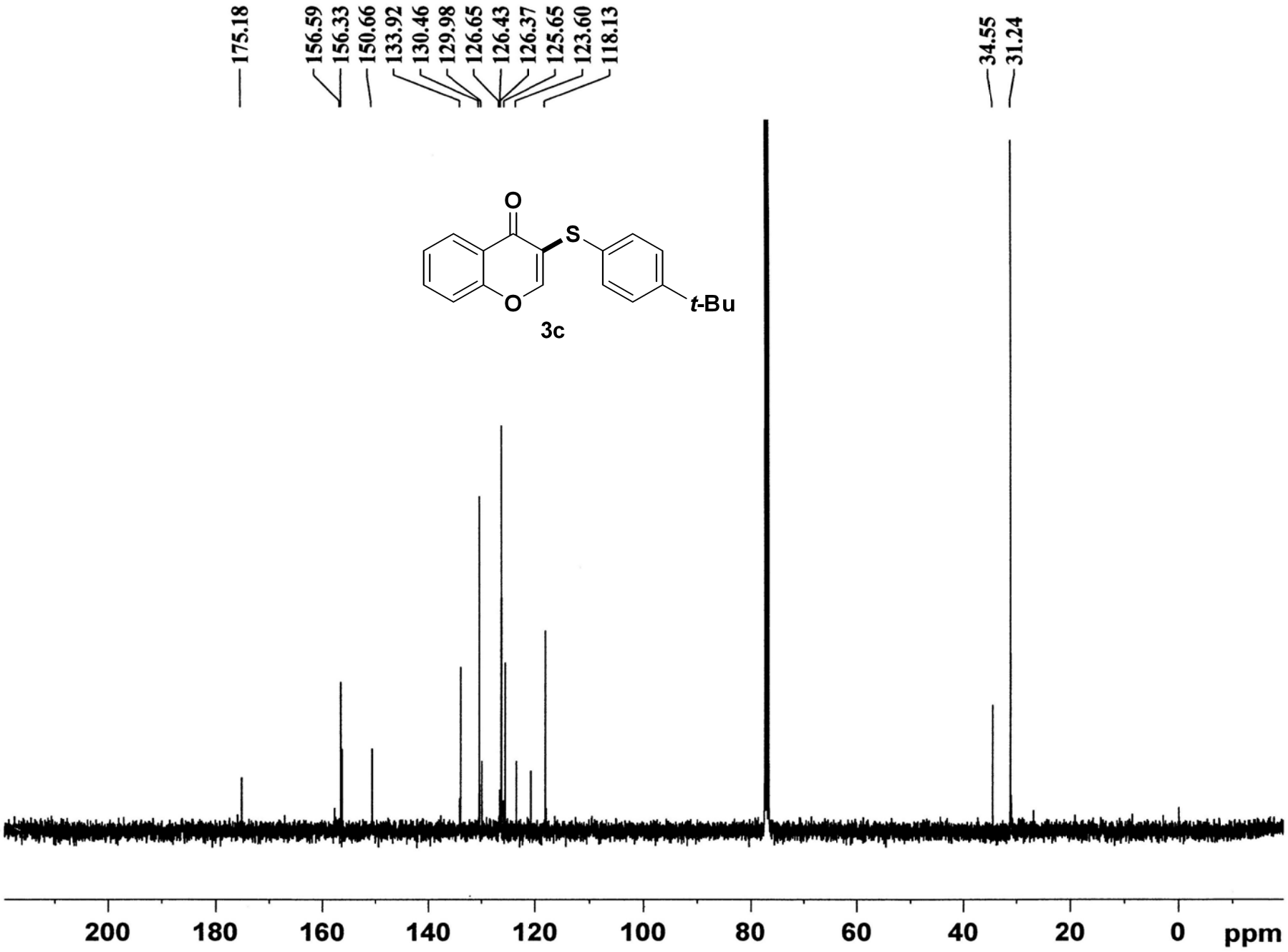

O
S
O

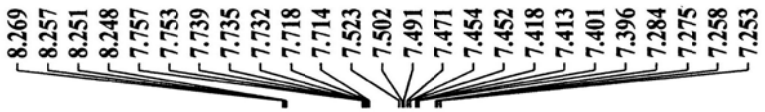
3b

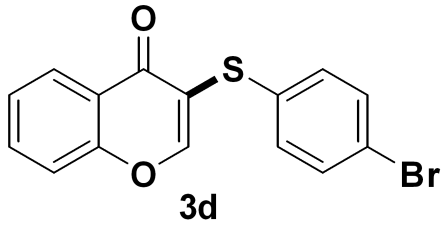

12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.00
1.06
4.12
2.29
1.02


175.09
157.38
156.36
134.01
129.86
129.21
127.13
126.48
125.76
123.69
119.96
118.17
O
S
O
3b
200
180
160
140
120
100
80
60
40
20
0
ppm

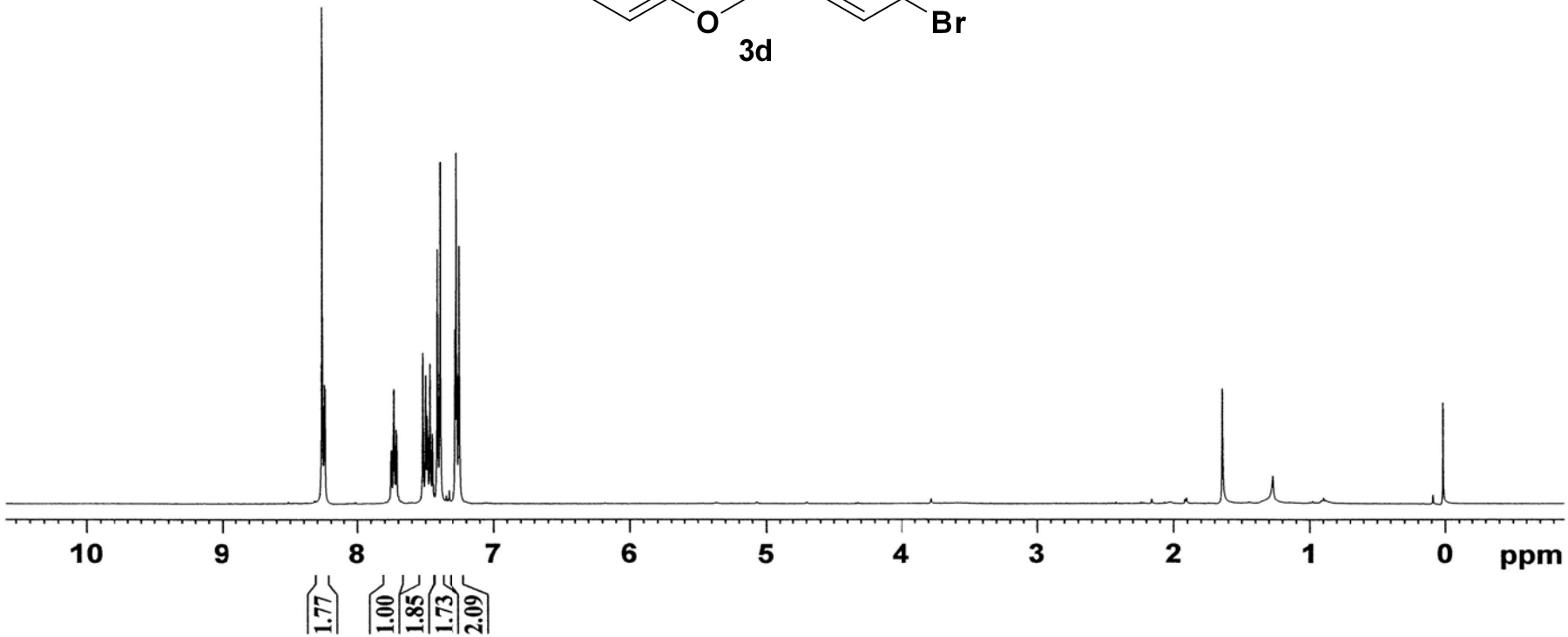

8.286
8.283
8.266
8.263
8.094
7.728
7.723
7.710
7.706
7.702
7.689
7.684
7.490
7.469
7.449
7.402
7.381
7.349
7.344
7.332
7.328
1.303
O
S
O
t-Bu
3c
10
9
8
7
6
5
4
3
2
1
0
ppm
1.06
1.00
1.10
2.03
4.13
9.05

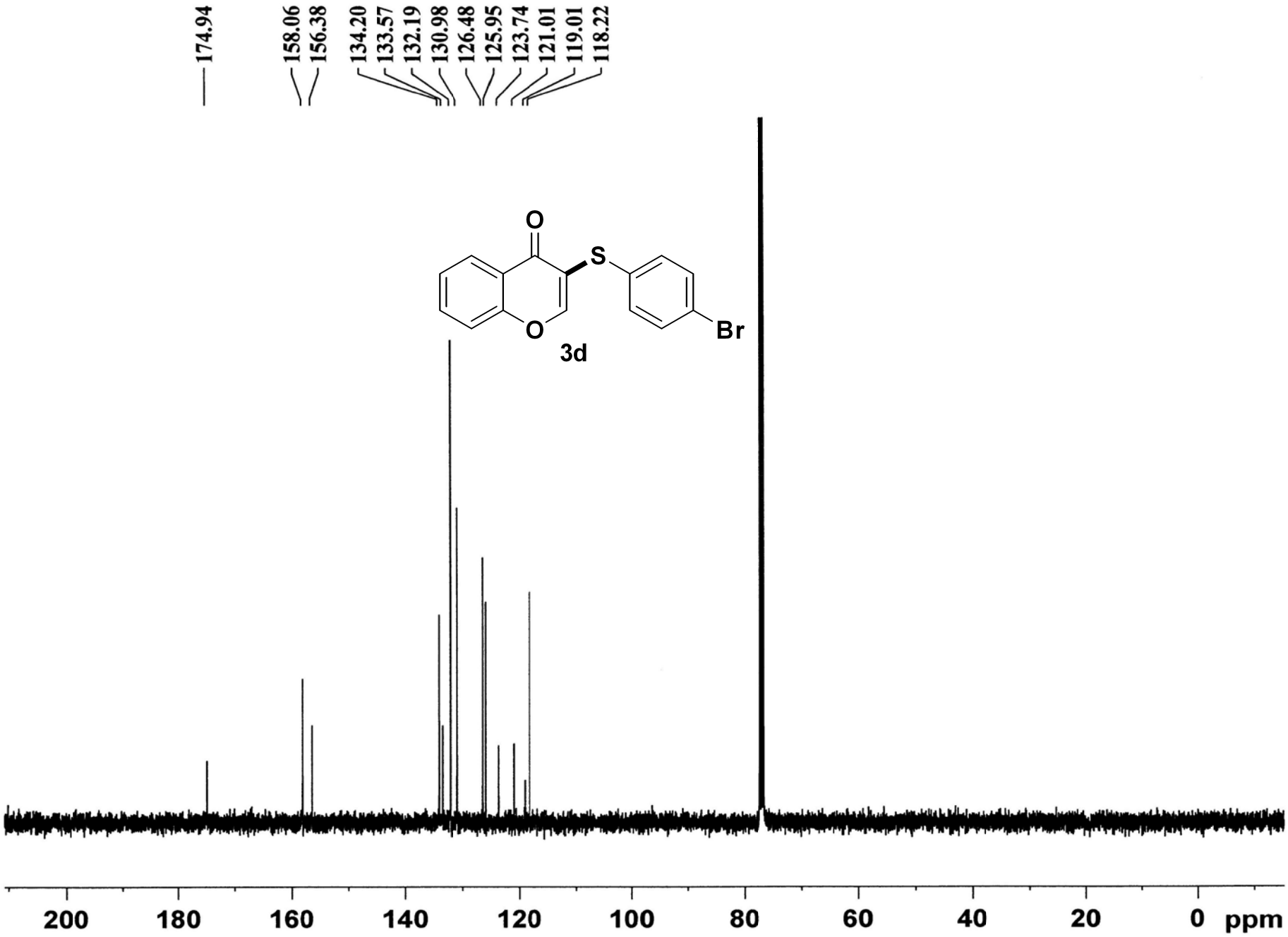

175.18
156.59
156.33
150.66
133.92
130.46
129.98
126.65
126.43
126.37
125.65
123.60
118.13
34.55
31.24
O
S
O
t-Bu
3c
200
180
160
140
120
100
80
60
40
20
0
ppm

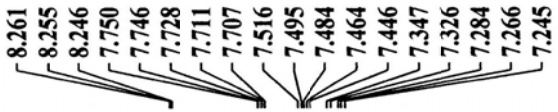

8.269
8.257
8.251
8.248
7.757
7.753
7.739
7.735
7.732
7.718
7.714
7.523
7.502
7.491
7.471
7.454
7.452
7.418
7.413
7.401
7.396
7.284
7.275
7.258
7.253

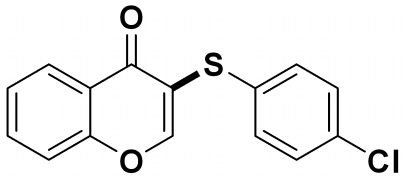

O
S
O
Br

3d

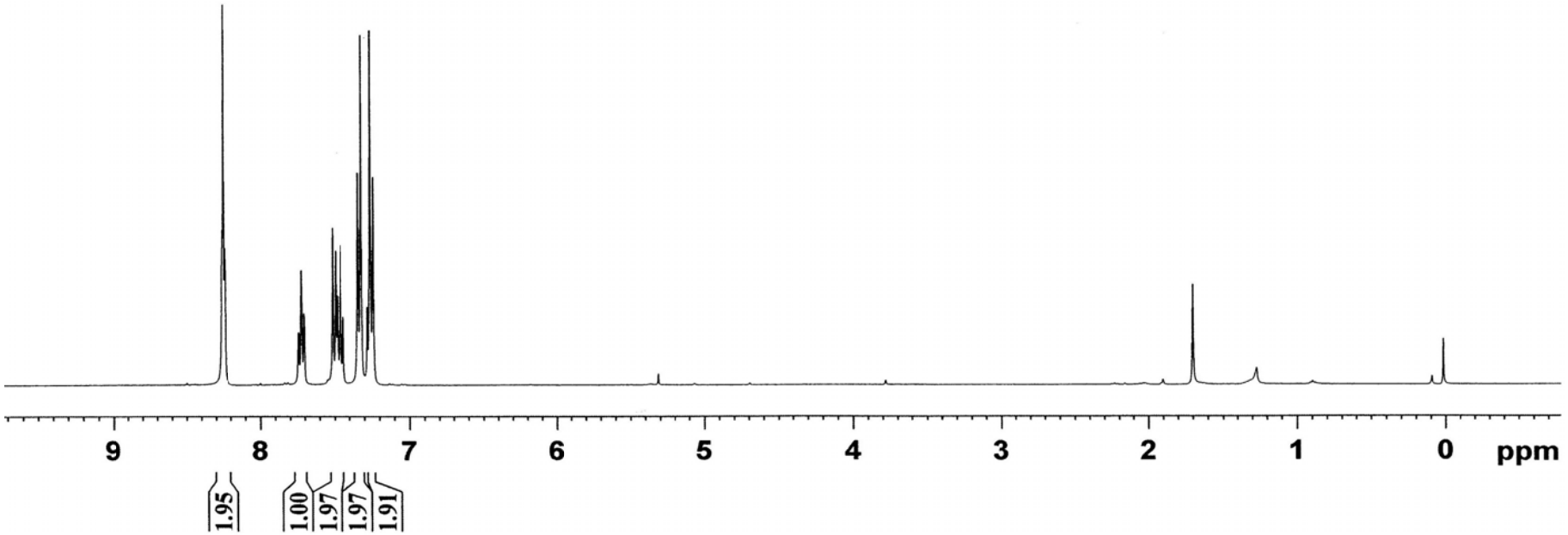

10
9
8
7
6
5
4
3
2
1
0
ppm
1.77
1.00
1.85
1.73
2.09

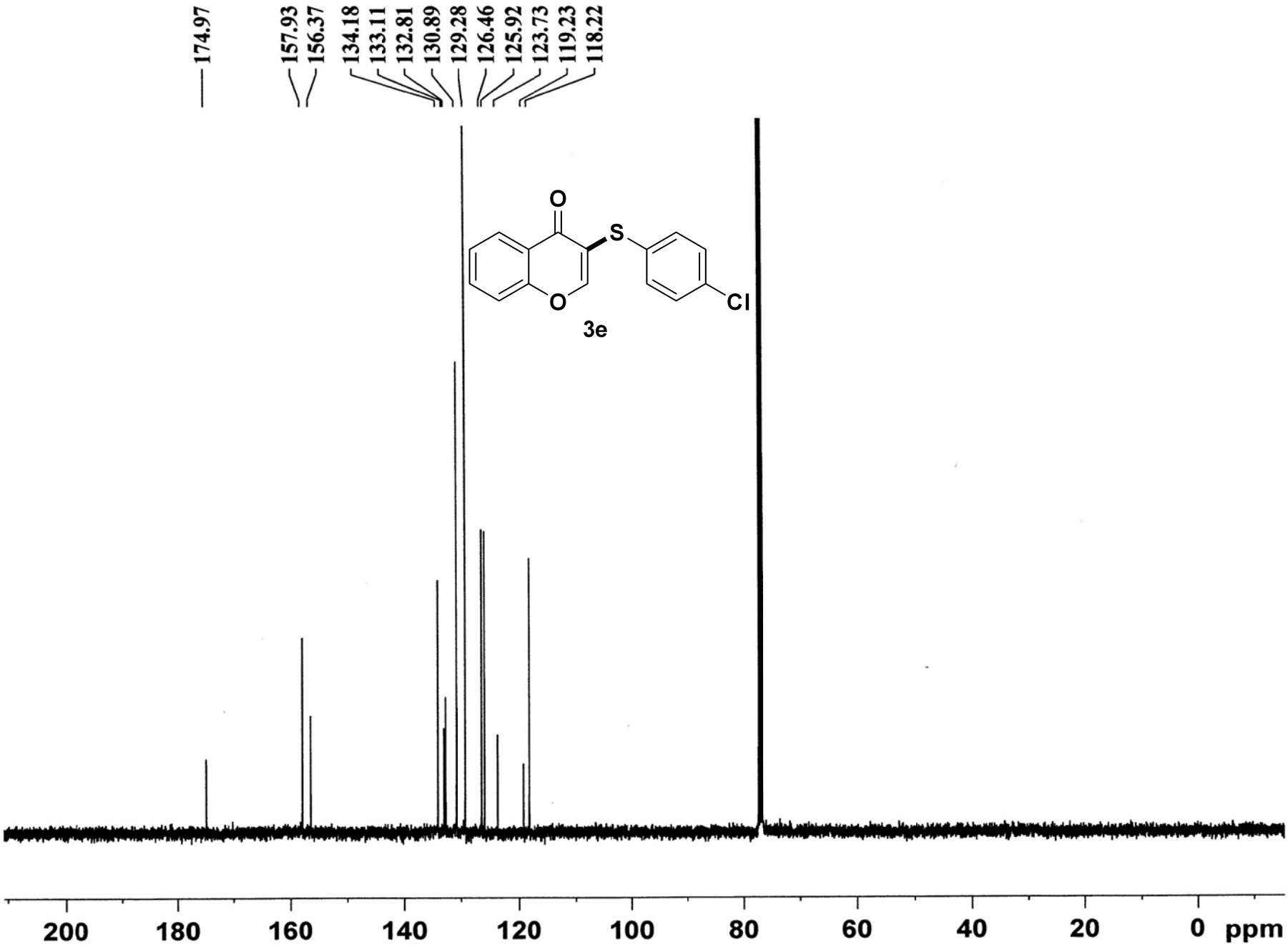

174.94
158.06
156.38
134.20
133.57
132.19
130.98
126.48
125.95
123.74
121.01
119.01
118.22
O
S
O
Br
3d
200
180
160
140
120
100
80
60
40
20
0
ppm


8.261
8.255
8.246
7.750
7.746
7.728
7.711
7.707
7.516
7.495
7.484
7.464
7.446
7.347
7.326
7.284
7.266
7.245

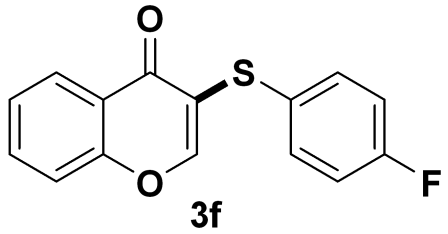

O
S
O
Cl

3e

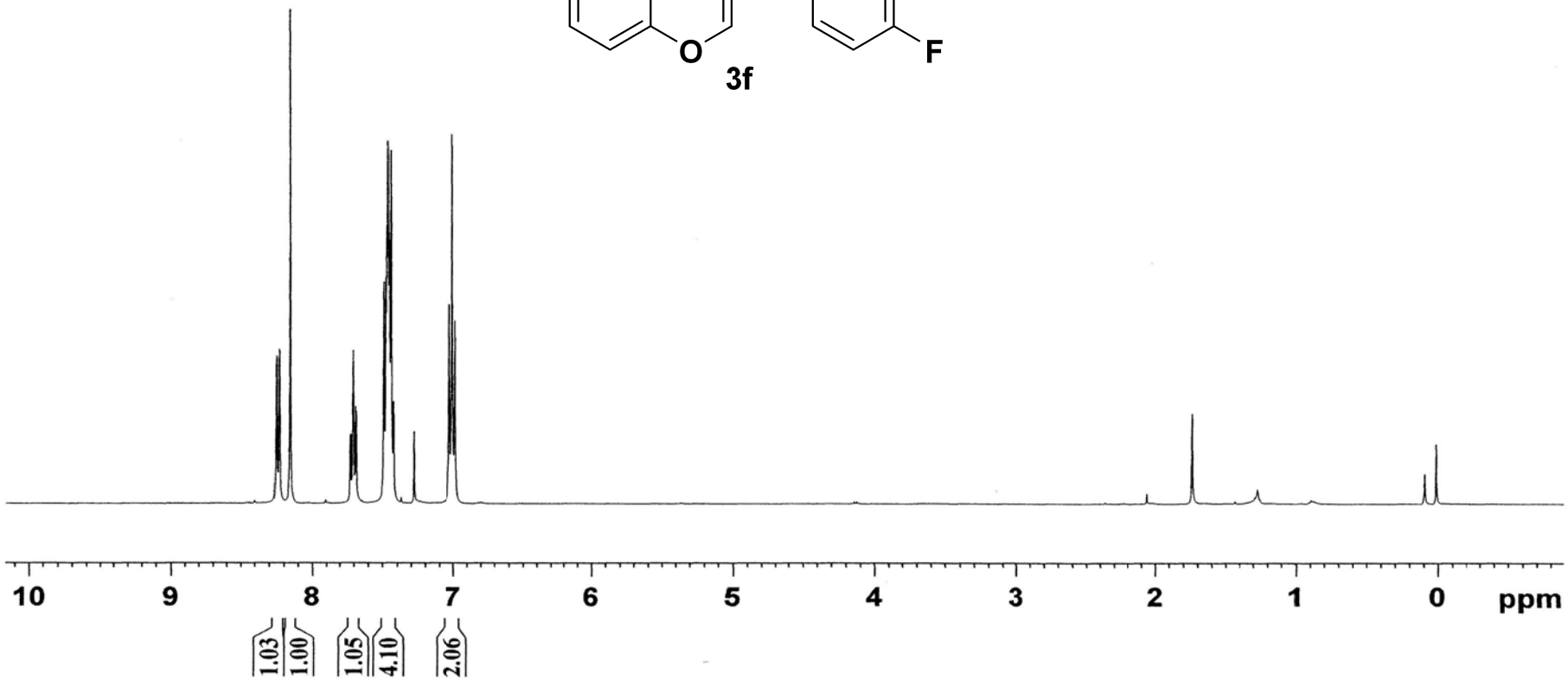

9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.00
1.97
1.97
1.91

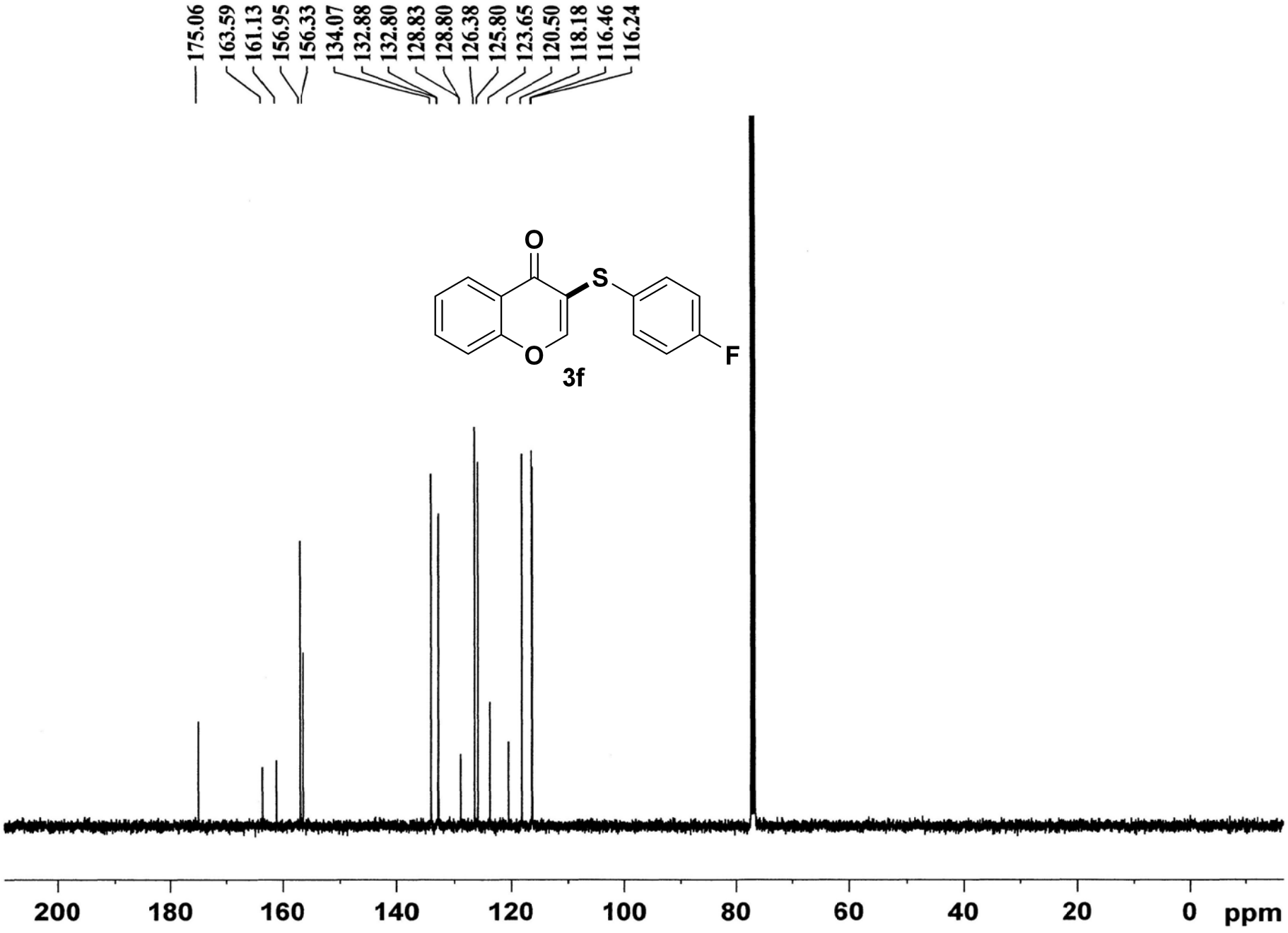

174.97
157.93
156.37
134.18
133.11
132.81
130.89
129.28
126.46
125.92
123.73
119.23
118.22
O
S
O
Cl
3e
200
180
160
140
120
100
80
60
40
20
0
ppm

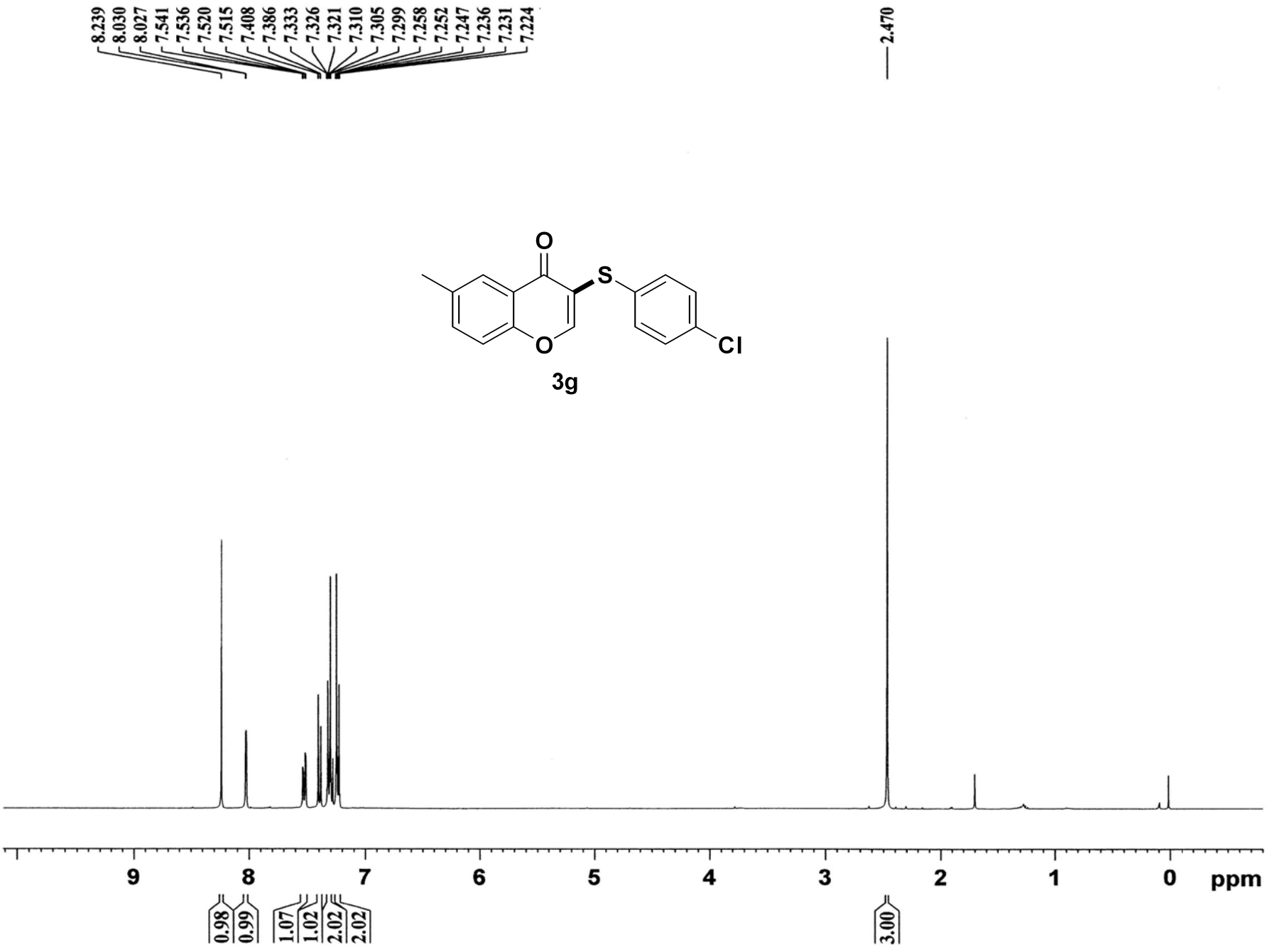

8.258
8.255
8.238
8.235
8.160
7.731
7.727
7.709
7.692
7.688
7.493
7.479
7.473
7.467
7.458
7.446
7.429
7.032
7.010
6.989

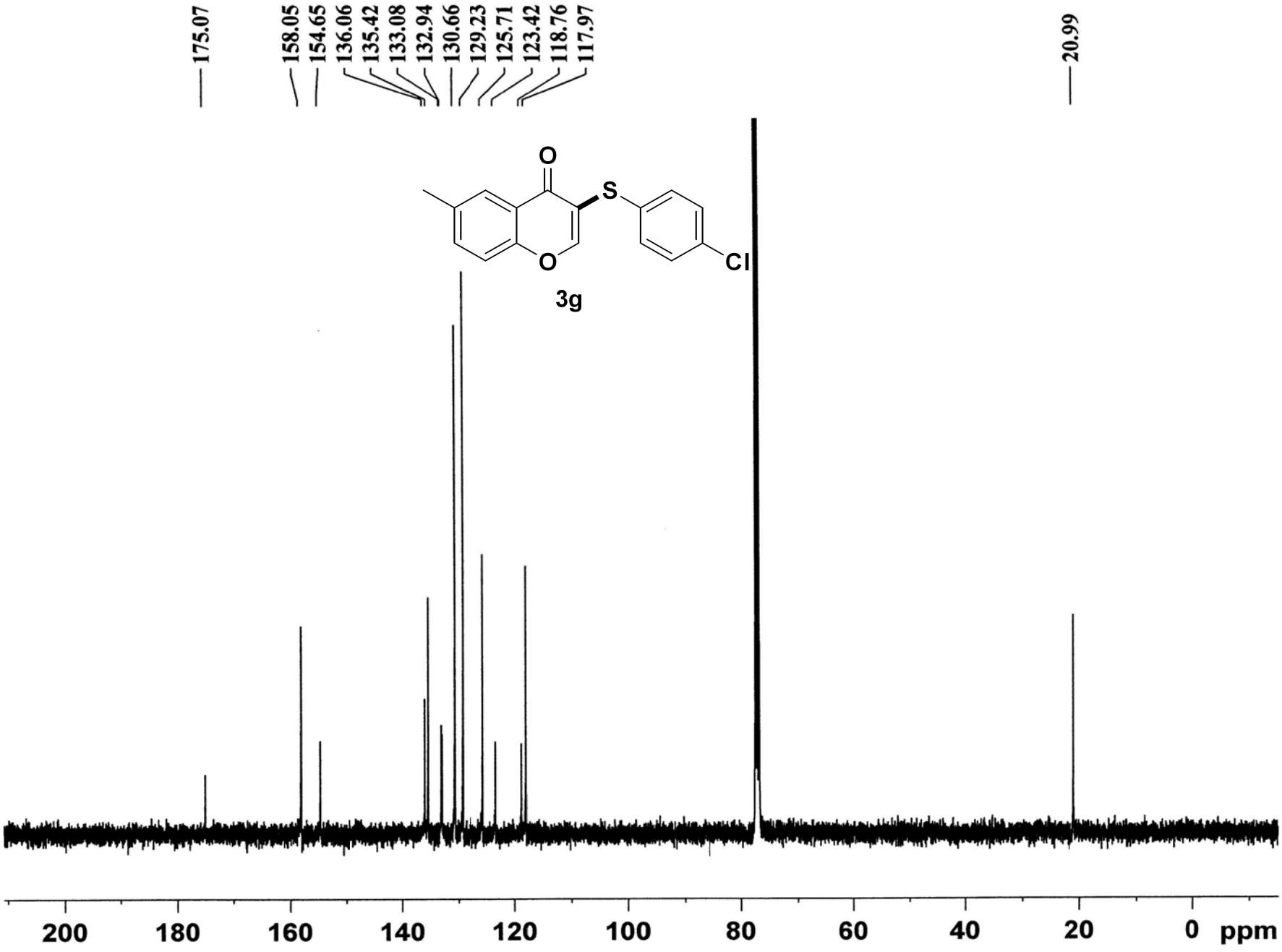

O
S
O
F

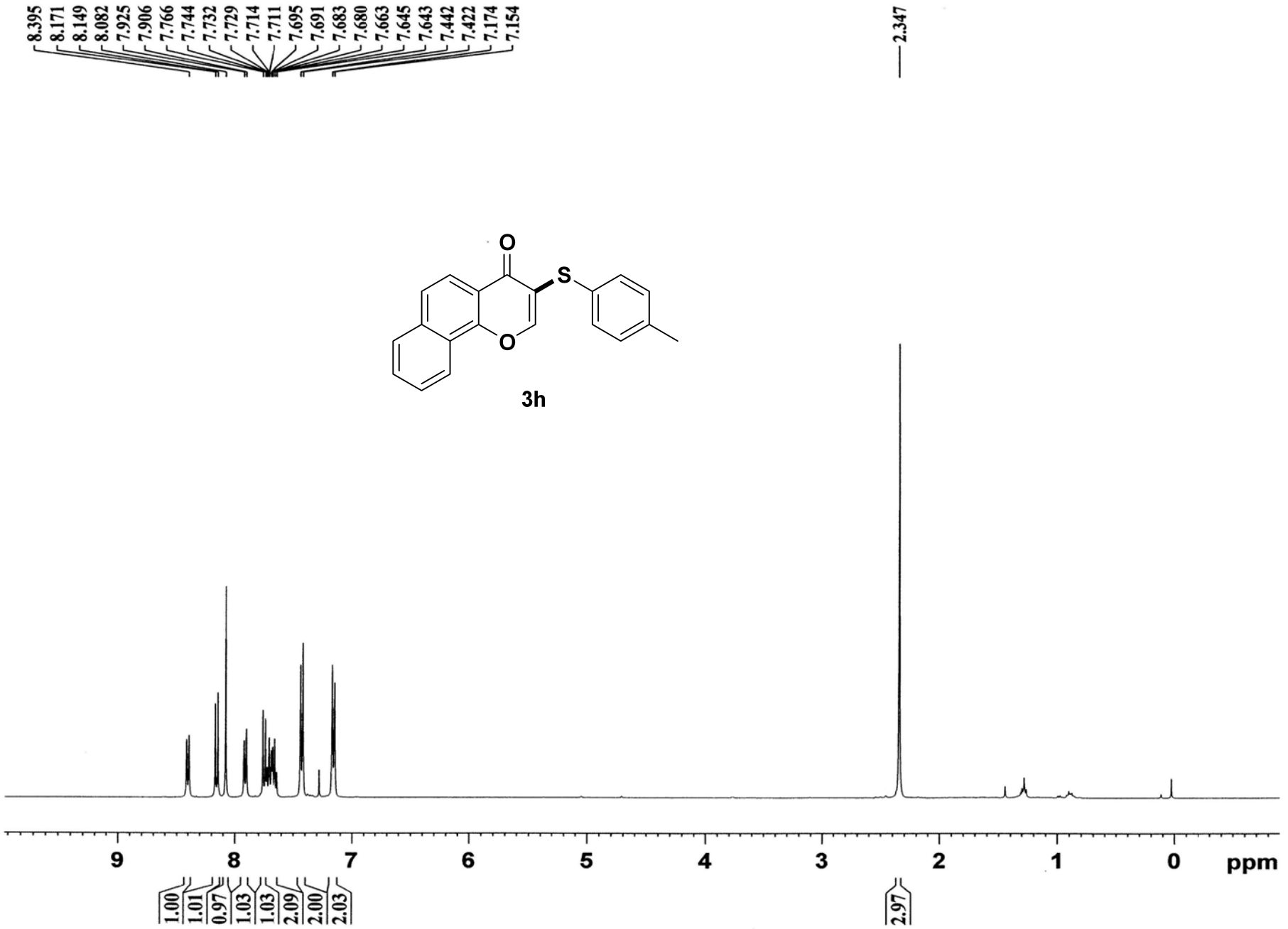
3f

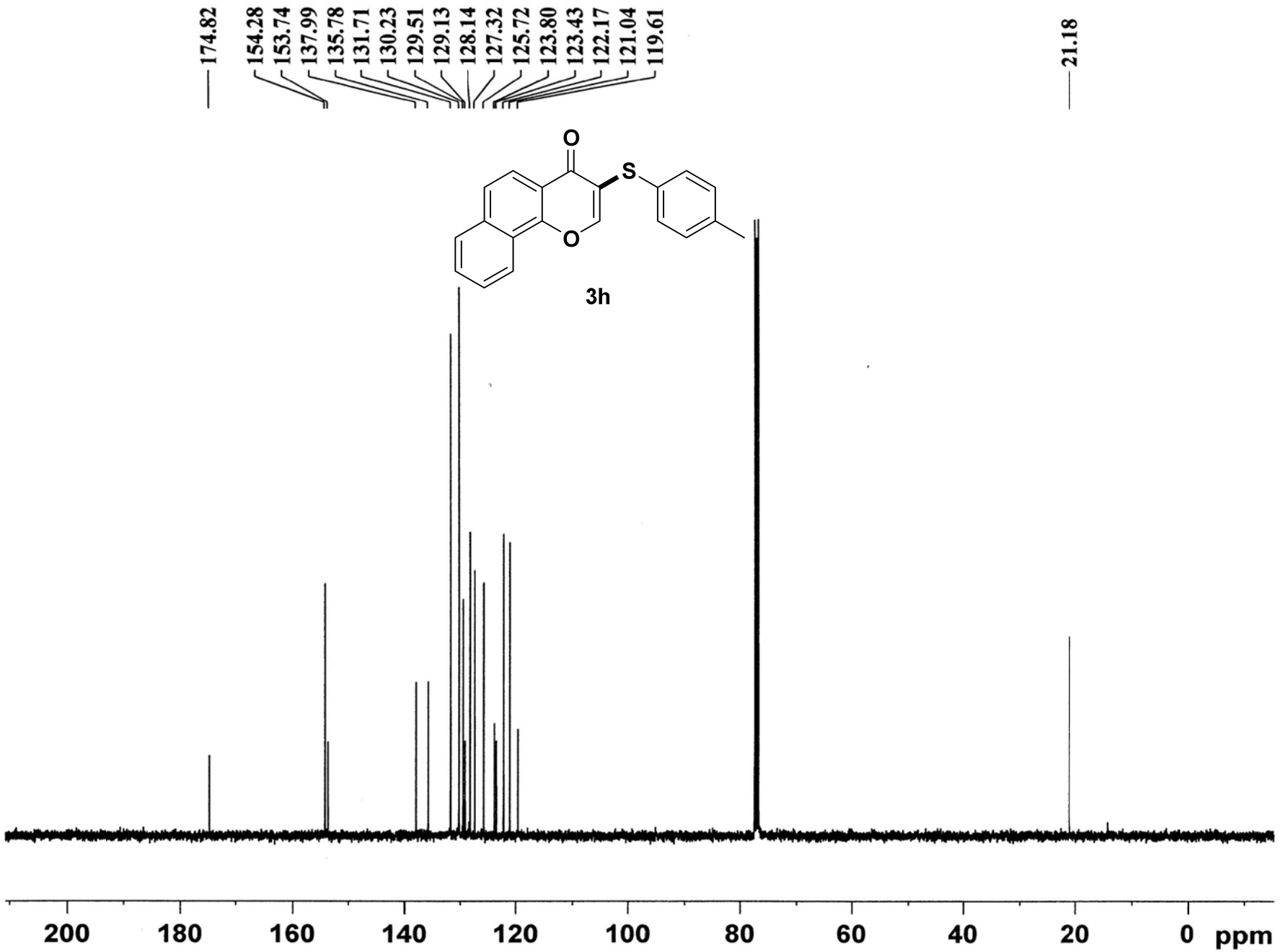

10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.00
1.05
4.10
2.06


175.06
163.59
161.13
156.95
156.33
134.07
132.88
132.80
128.83
128.80
126.38
125.80
123.65
120.50
118.18
116.46
116.24
O
S
O
F
3f
200
180
160
140
120
100
80
60
40
20
0
ppm


8.239
8.030
8.027
7.541
7.536
7.520
7.515
7.408
7.386
7.333
7.326
7.321
7.310
7.305
7.299
7.258
7.252
7.247
7.236
7.231
7.224
2.470
O
S
O
Cl
3g
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.99
1.07
1.02
2.02
2.02
3.00

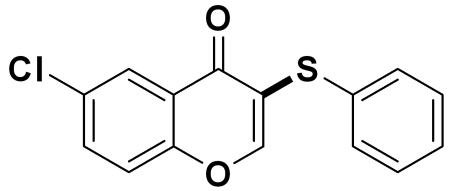

175.07
158.05
154.65
136.06
135.42
133.08
132.94
130.66
129.23
125.71
123.42
118.76
117.97
20.99
O
S
O
Cl
3g
200
180
160
140
120
100
80
60
40
20
0
ppm


8.395
8.171
8.149
8.082
7.925
7.906
7.766
7.744
7.732
7.729
7.714
7.711
7.695
7.691
7.683
7.680
7.663
7.645
7.643
7.442
7.422
7.174
7.154
2.347
O
S
O
3h
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
0.97
1.03
1.03
2.09
2.00
2.03
2.97

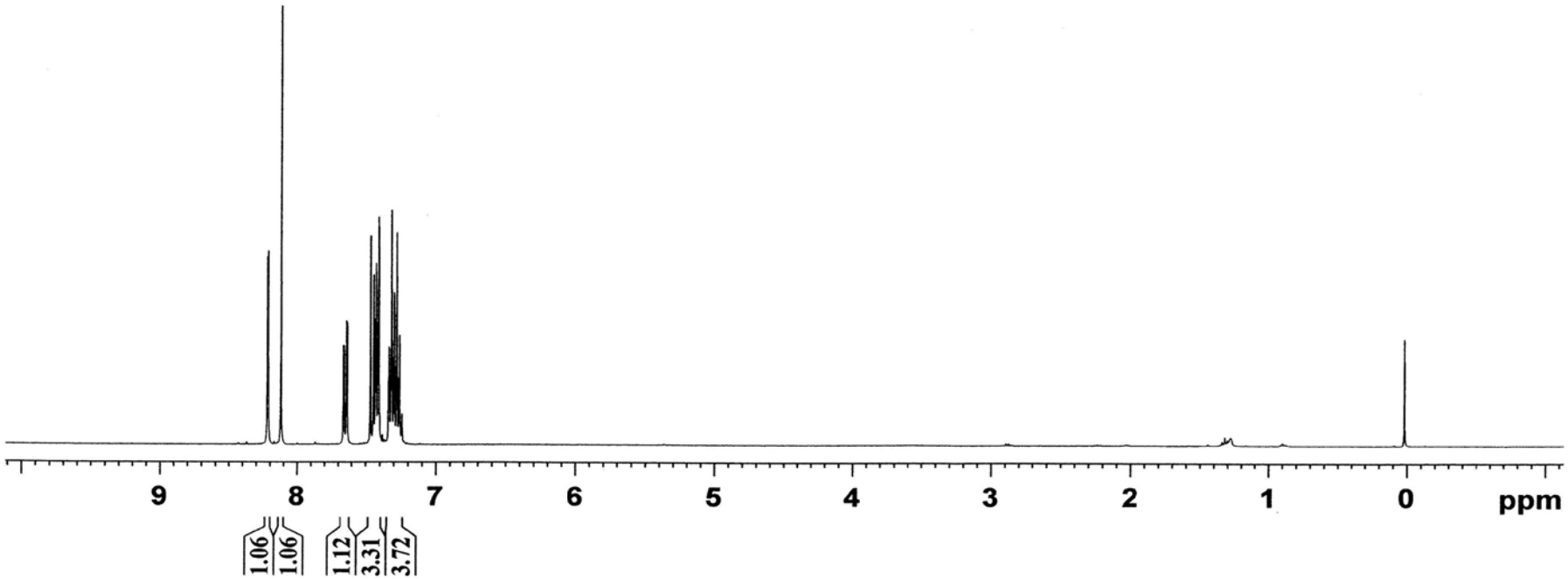

174.82
154.28
153.74
137.99
135.78
131.71
130.23
129.51
129.13
128.14
127.32
125.72
123.80
123.43
122.17
121.04
119.61
21.18
O
S
O
3h
200
180
160
140
120
100
80
60
40
20
0
ppm

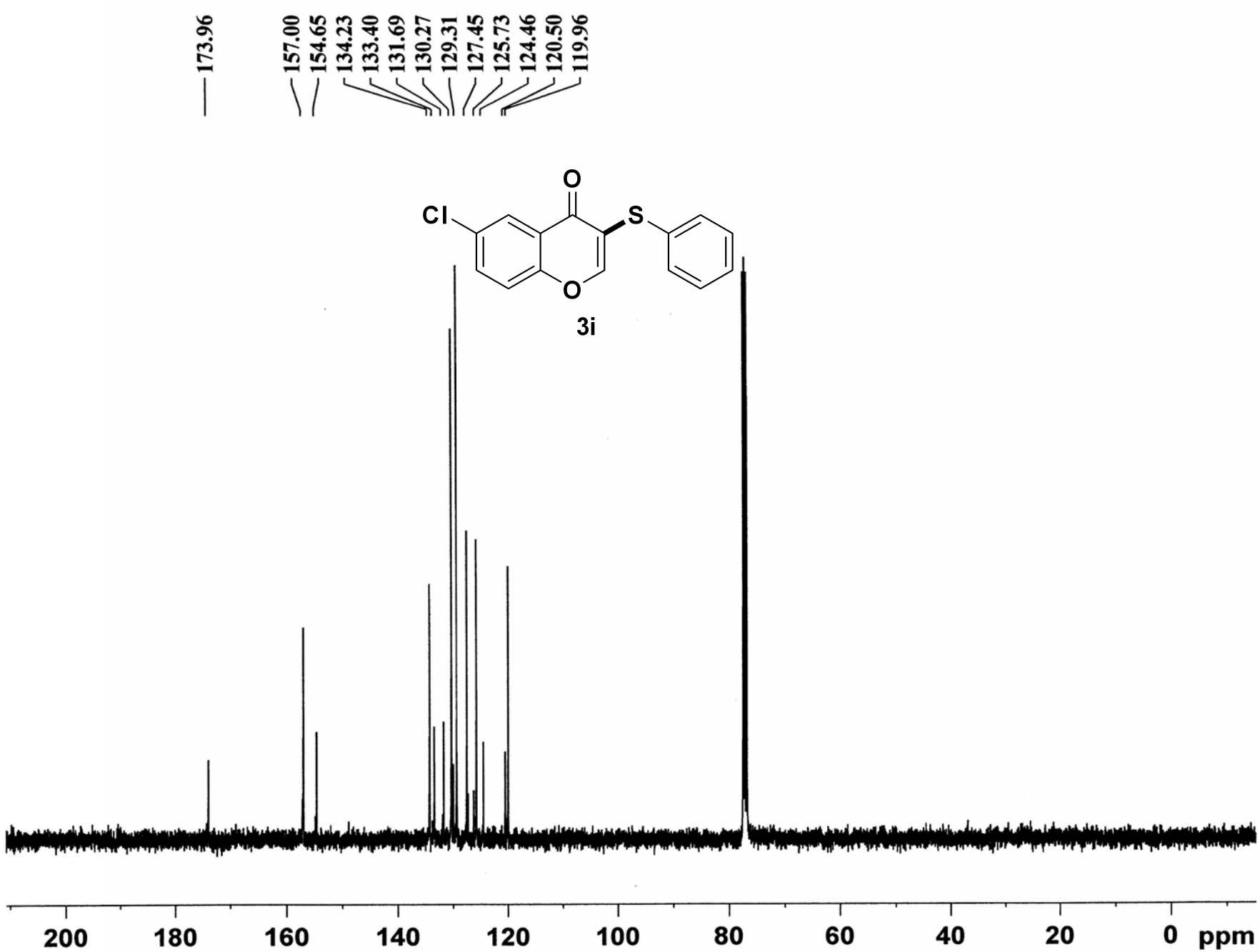
8.217
8.124
7.665
7.659
7.643
7.636
7.469
7.447
7.434
7.430
7.425
7.412
7.410
7.404
7.341
7.337
7.333
7.320
7.316
7.304
7.301
7.295
7.284
7.278
7.270
7.264
7.245

1.648

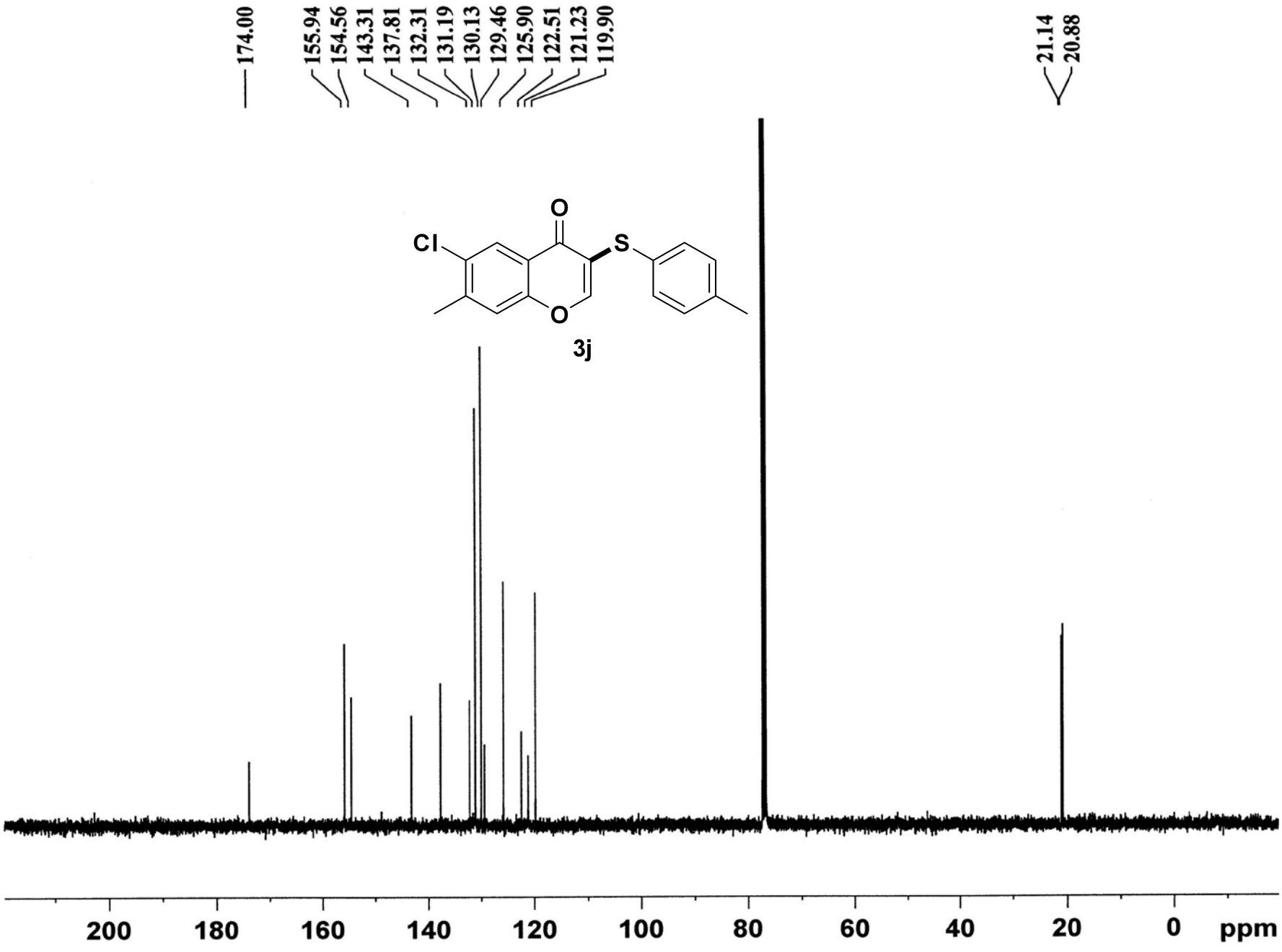


3i

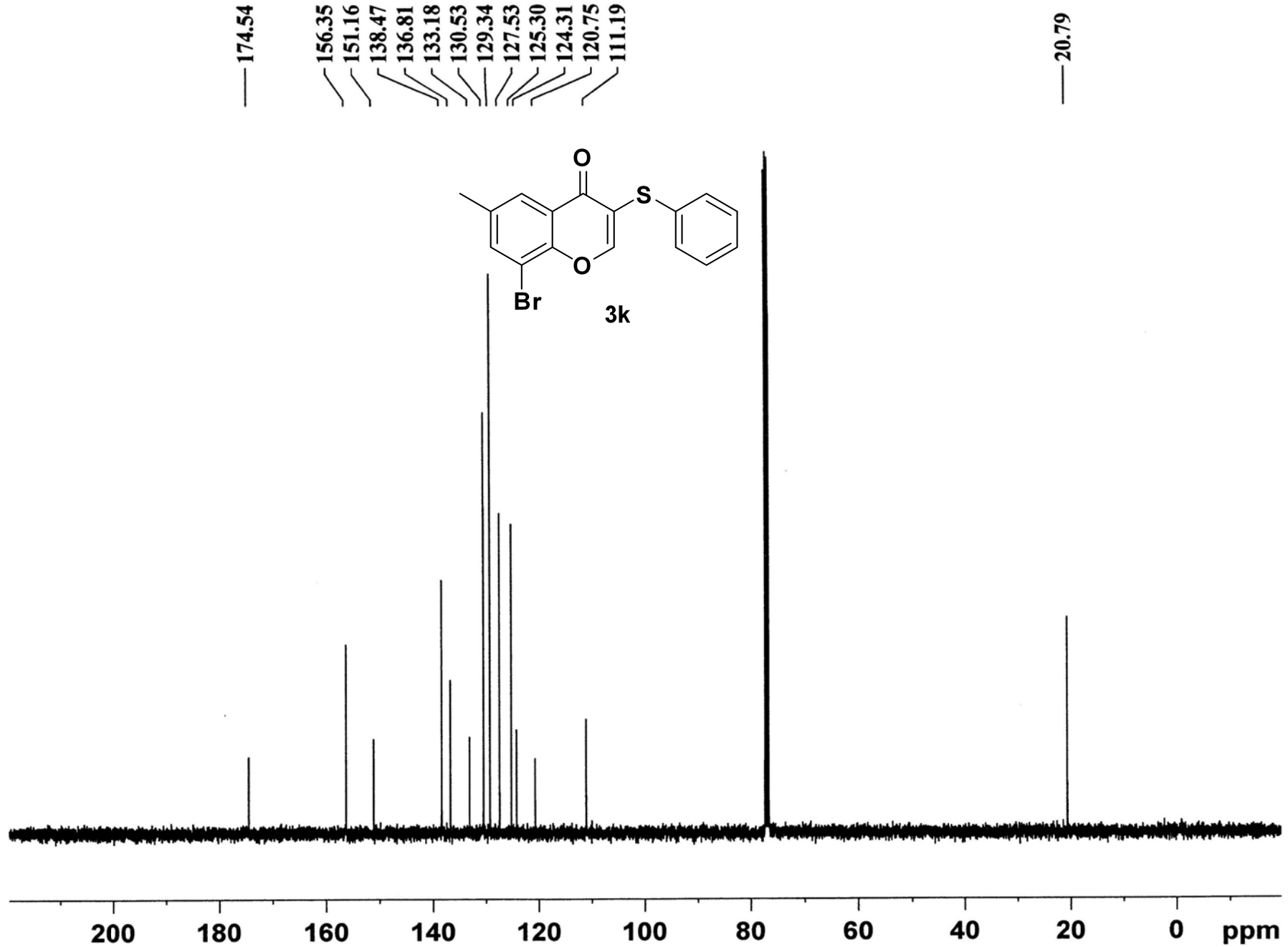


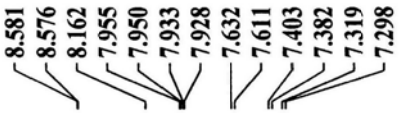

173.96
157.00
154.65
134.23
133.40
131.69
130.27
129.31
127.45
125.73
124.46
120.50
119.96
O
Cl
S
O
3i
200
180
160
140
120
100
80
60
40
20
0
ppm

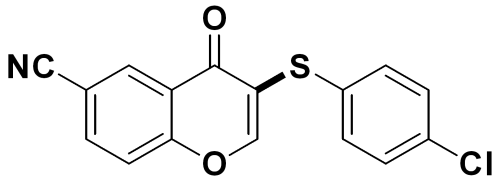
2.332
2.505
8.185
7.981
7.366
7.346
7.142
7.122
3j
0.98
0.99
3.03
1.98
3.00
3.00
ppm


174.00
155.94
154.56
143.31
137.81
132.31
131.19
130.13
129.46
125.90
122.51
121.23
119.90
21.14
20.88
O
Cl
S
O
3j
200
180
160
140
120
100
80
60
40
20
0
ppm

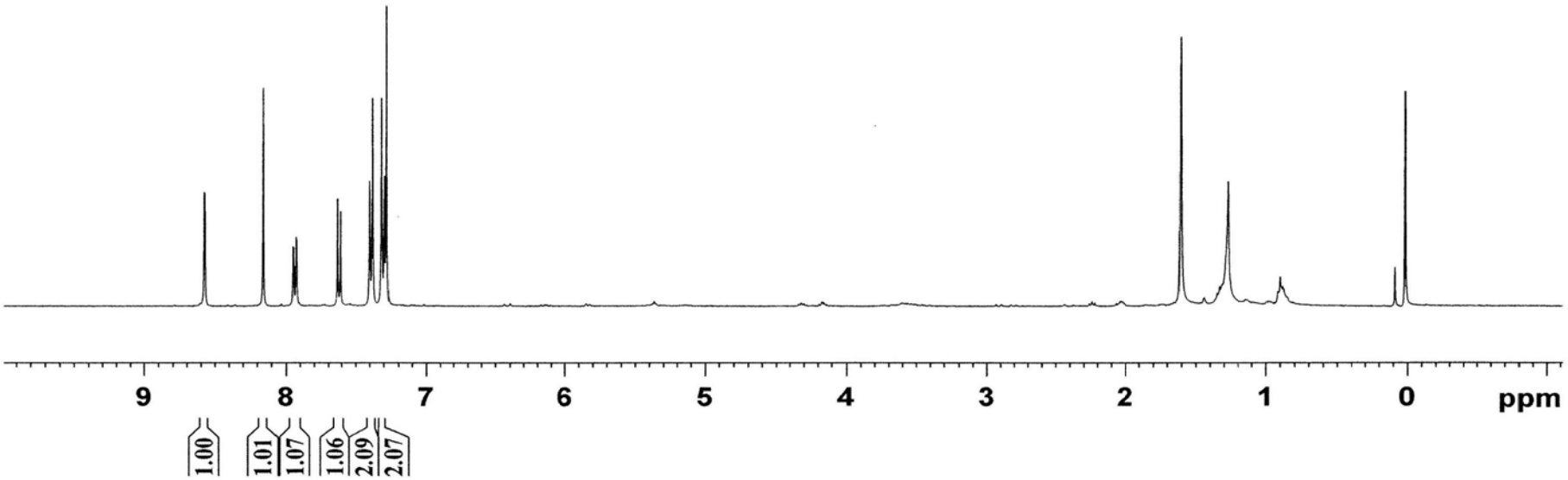
8.113
7.981
7.978
7.752
7.747
7.442
7.439
7.434
7.421
7.337
7.334
7.329
7.316
7.312
7.297
7.283
7.278
7.275
7.266
7.260
7.253
7.244
7.242
2.448
S
O
O
Br
3k
3.00
0.97
0.99
0.98
2.01
3.19
9
8
7
6
5
4
3
2
1
0 ppm

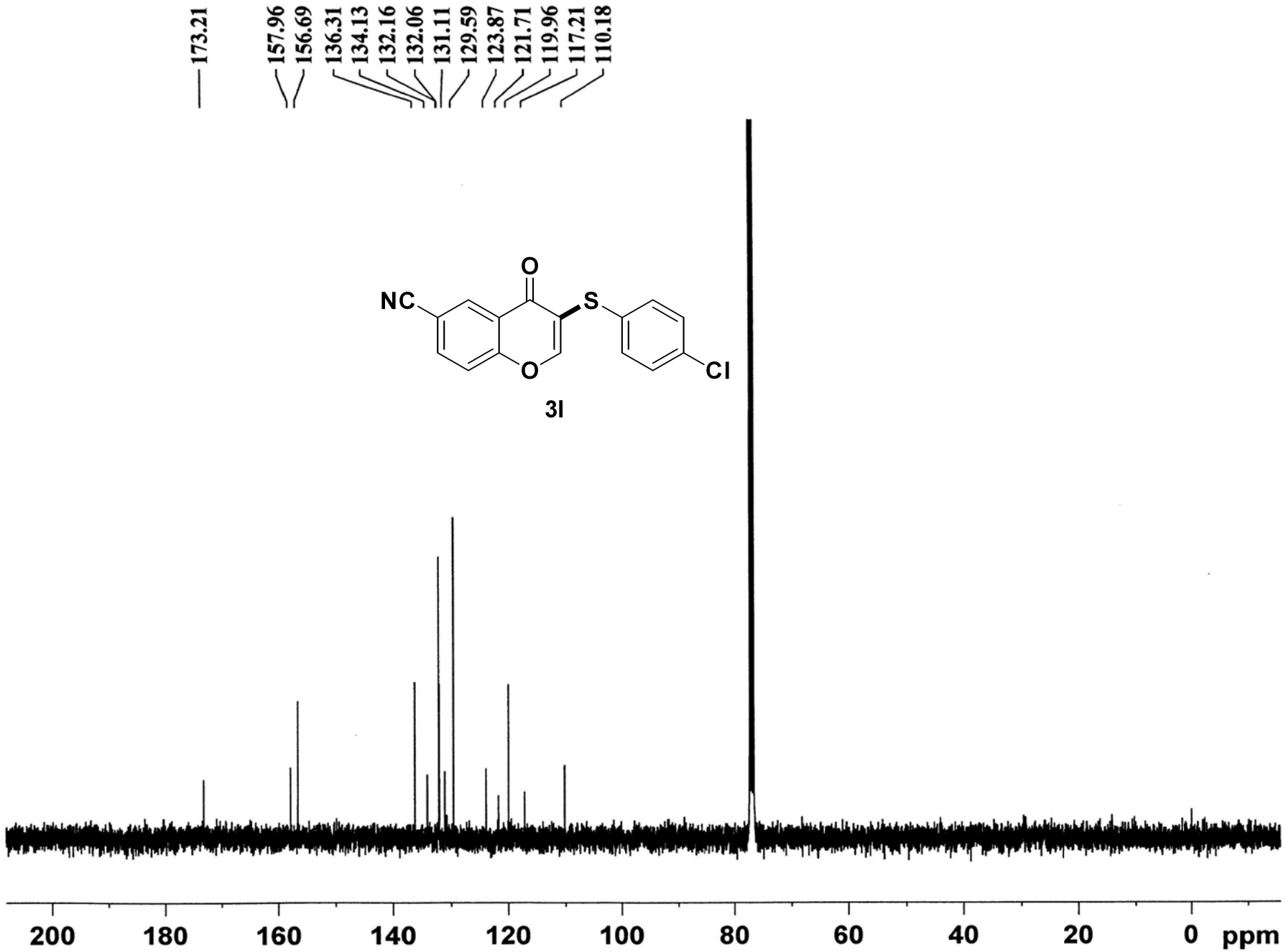

174.54
156.35
151.16
138.47
136.81
133.18
130.53
129.34
127.53
125.30
124.31
120.75
111.19
20.79
O
S
O
Br
3k
200
180
160
140
120
100
80
60
40
20
0
ppm


8.581
8.576
8.162
7.955
7.950
7.933
7.928
7.632
7.611
7.403
7.382
7.319
7.298

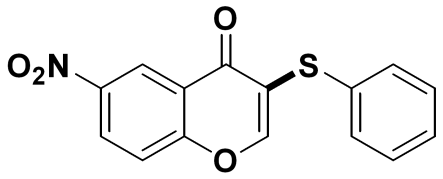

O
NC
S
O
Cl

3l

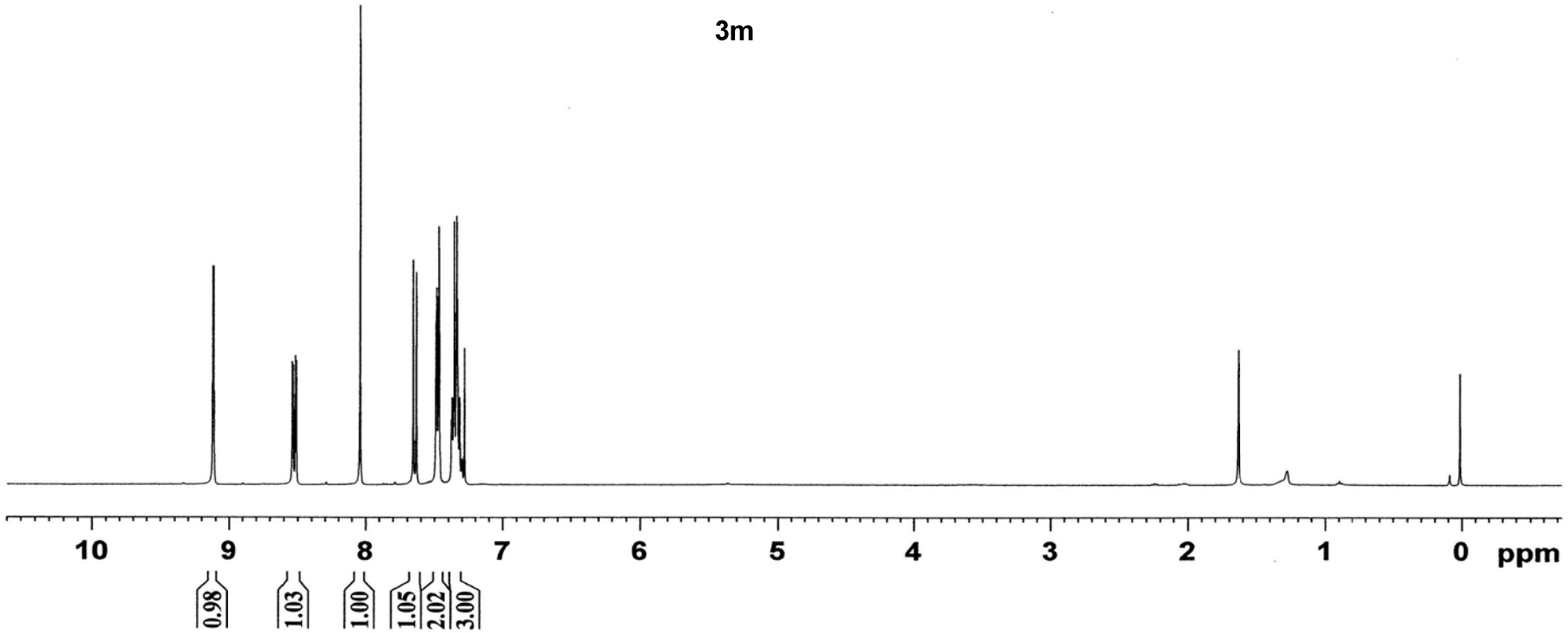

9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.07
1.06
2.09
2.07

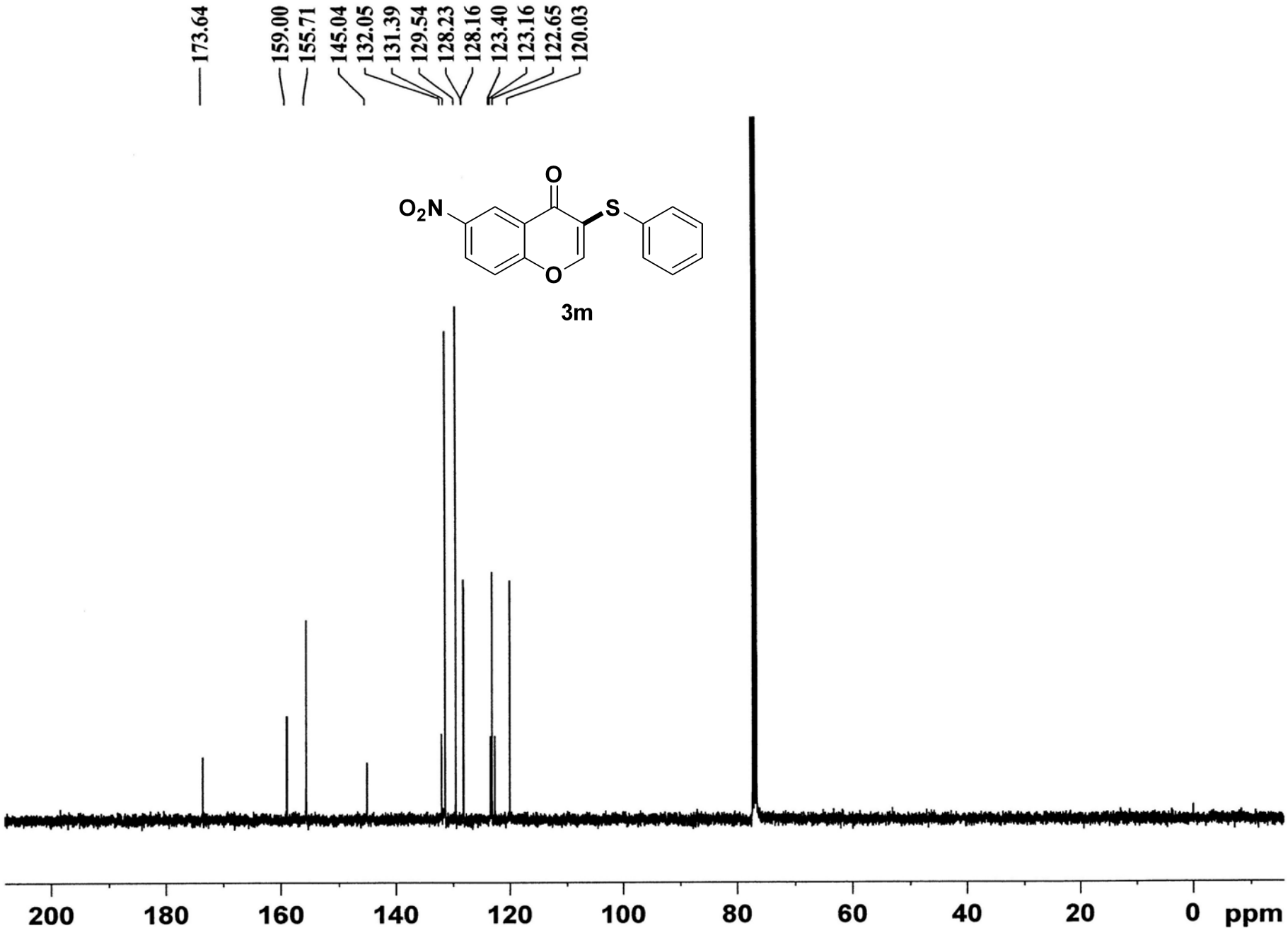

173.21
157.96
156.69
136.31
134.13
132.16
132.06
131.11
129.59
123.87
121.71
119.96
117.21
110.18
O
NC
S
Cl
O
3l
200
180
160
140
120
100
80
60
40
20
0
ppm


9.124
9.117
8.544
8.537
8.521
8.514
8.044
7.660
7.637
7.493
7.489
7.473
7.470
7.382
7.376
7.372
7.360
7.341
7.336
7.327
7.320

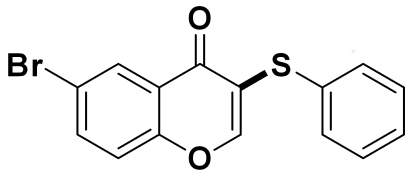

O
O2N
S
O

3m

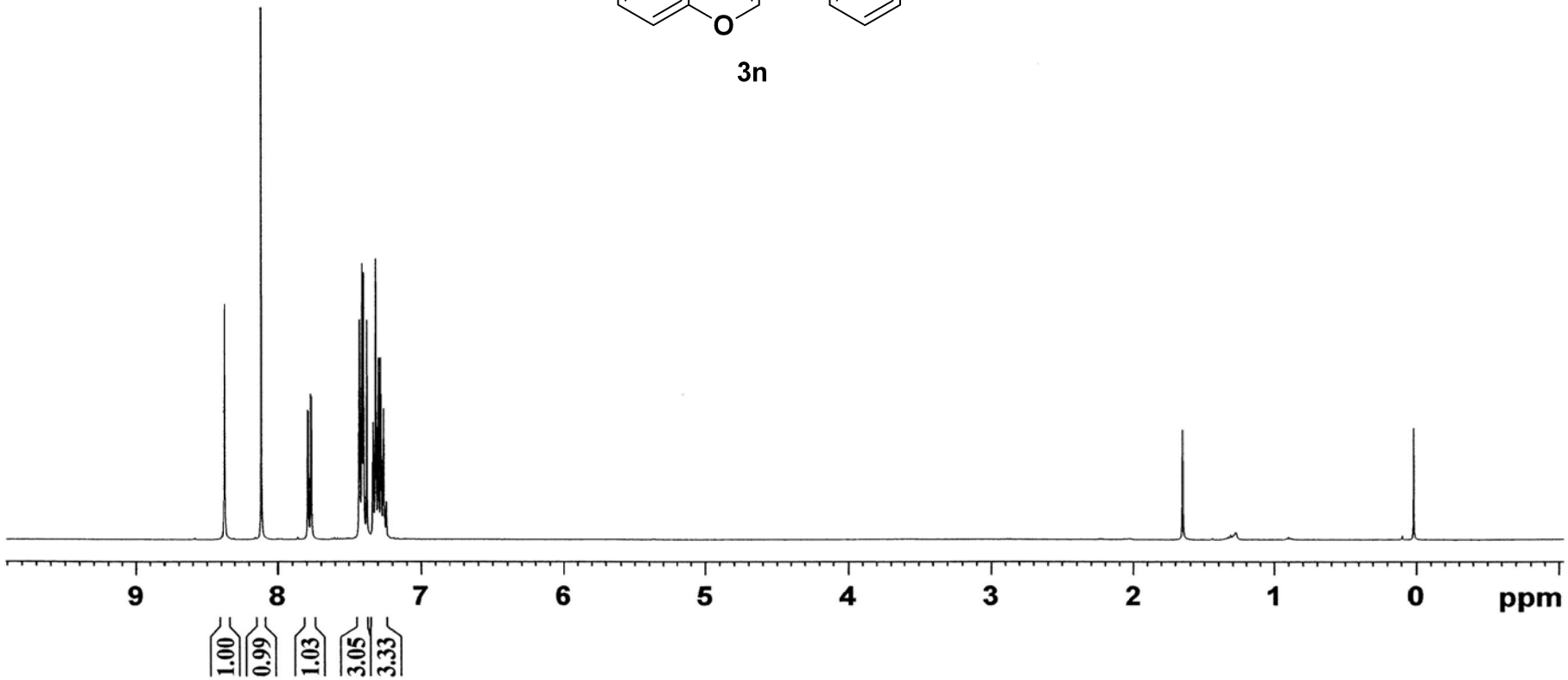

10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.03
1.00
1.05
2.02
3.00

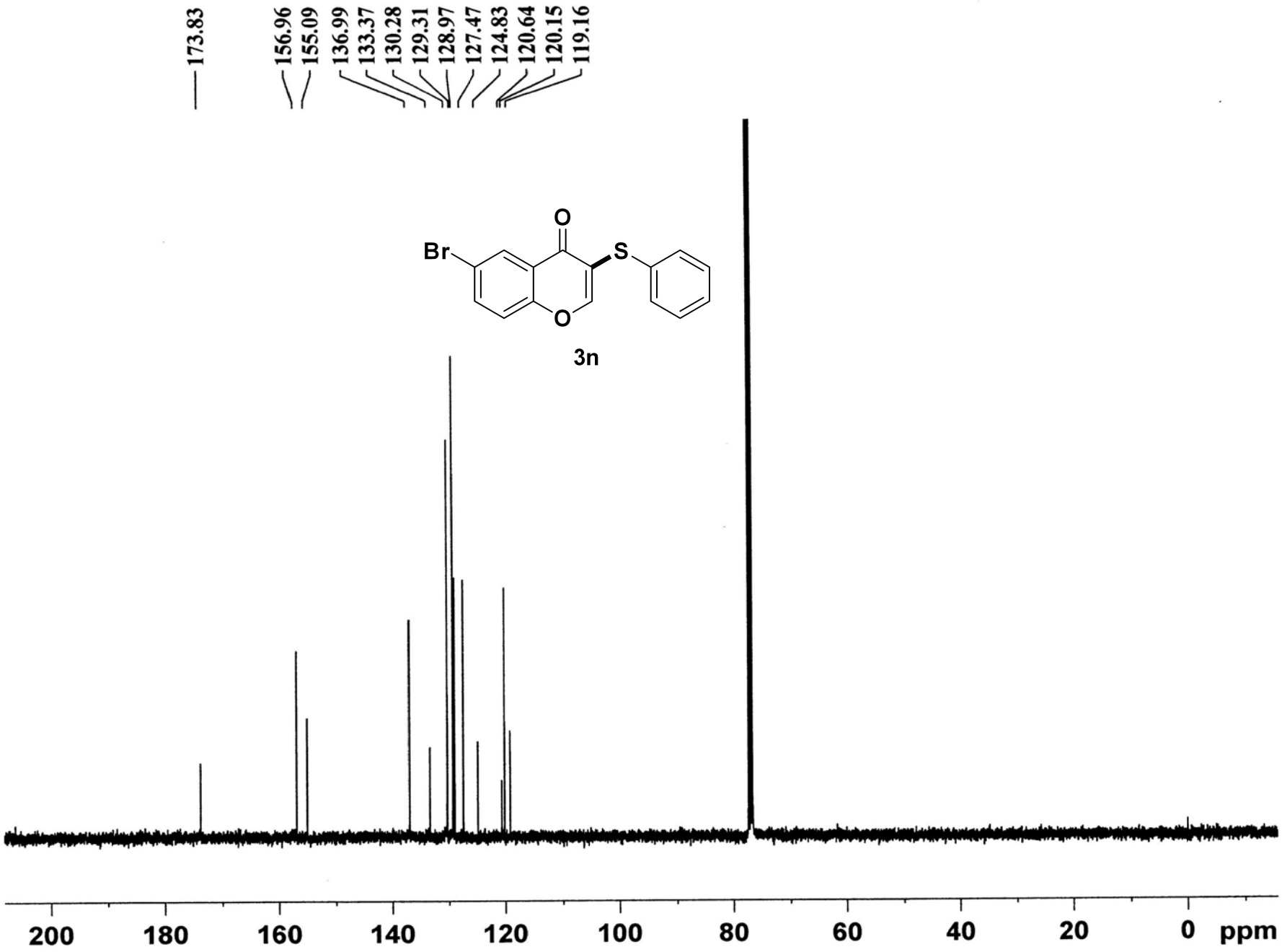

173.64
159.00
155.71
145.04
132.05
131.39
129.54
128.23
128.16
123.40
123.16
122.65
120.03
O
O2N
S
O
3m
200
180
160
140
120
100
80
60
40
20
0
ppm

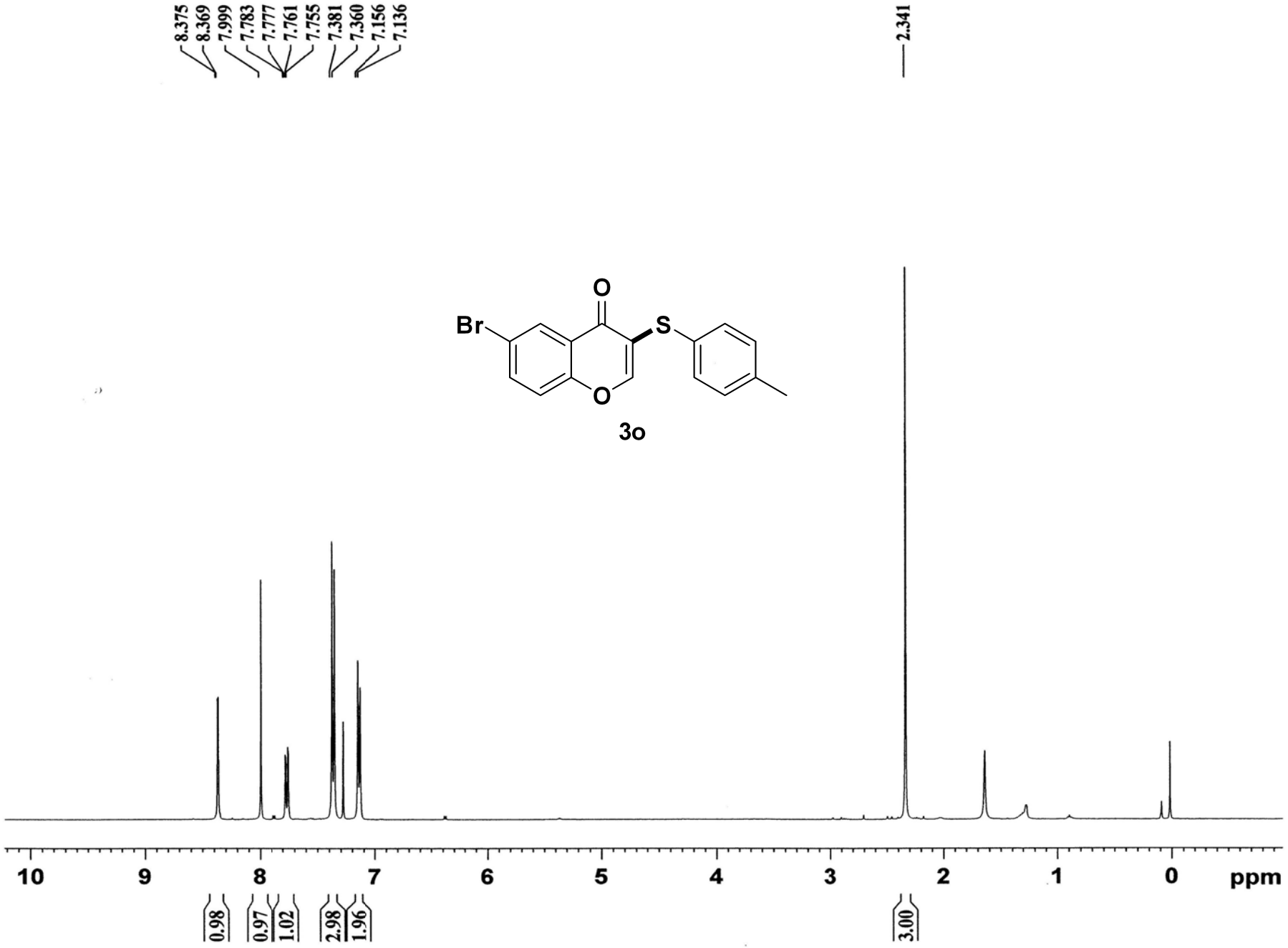

7.797
7.791
7.775
7.769
7.432
7.428
7.423
7.411
7.408
7.400
7.378
7.338
7.335
7.330
7.317
7.313
7.302
7.298
7.292
7.283
7.279
7.276
7.268
7.261
7.254
7.246
7.243
7.240

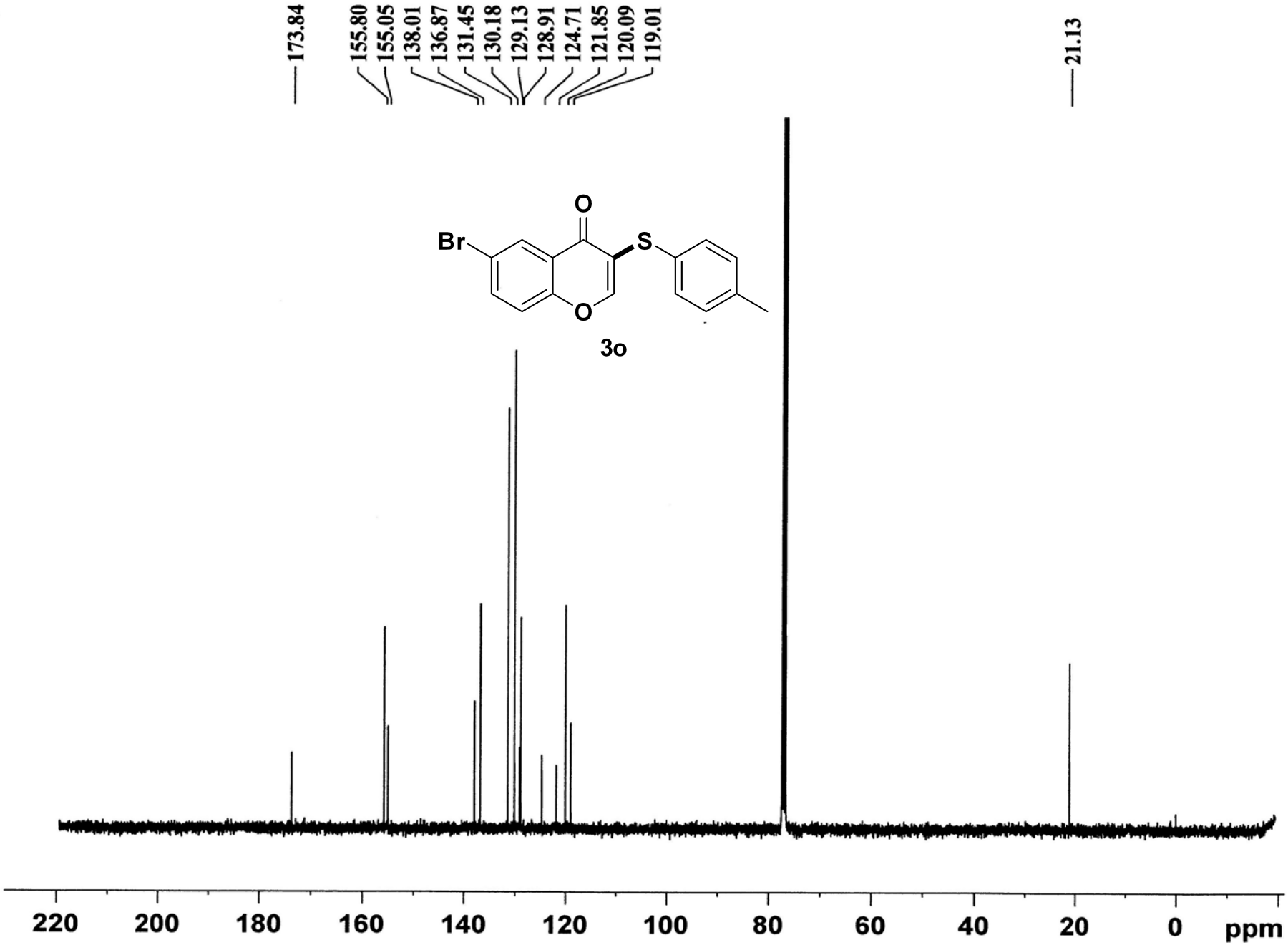

O
Br
S
O

3n

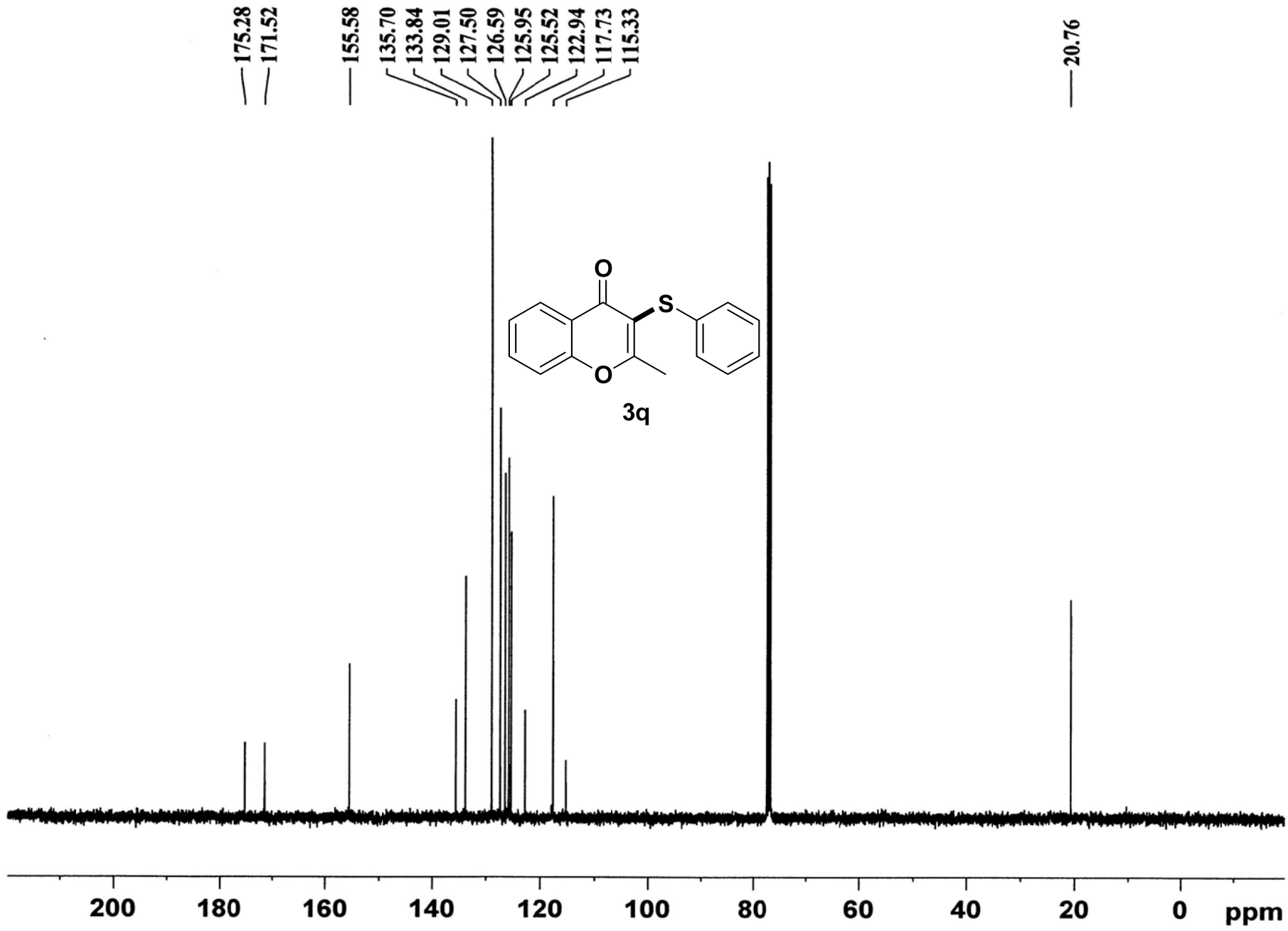

9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.99
1.03
3.05
3.33


173.83
156.96
155.09
136.99
133.37
130.28
129.31
128.97
127.47
124.83
120.64
120.15
119.16
O
Br
S
O
3n
200
180
160
140
120
100
80
60
40
20
0
ppm


8.375
8.369
7.999
7.783
7.777
7.761
7.755
7.381
7.360
7.156
7.136
2.341
O
Br
S
O
3o
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.97
1.02
2.98
1.96
3.00


173.84
155.80
155.05
138.01
136.87
131.45
130.18
129.13
128.91
124.71
121.85
120.09
119.01
21.13
O
Br
S
O
3o
220
200
180
160
140
120
100
80
60
40
20
0
ppm

7.687
7.673
7.669
7.474
7.453
7.453
7.441
7.439
7.421
7.404
7.401
7.284
7.277
7.272
7.267
7.256
7.253
7.236
7.231
7.220
7.216
7.165
7.160
7.154
7.149
7.143
7.137
7.132
7.127
7.122
2.744
S
O
O
3q
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.01
2.06
4.11
0.98
3.00


175.28
171.52
155.58
135.70
133.84
129.01
127.50
126.59
125.95
125.52
122.94
117.73
115.33
20.76
O
S
O
3q
200
180
160
140
120
100
80
60
40
20
0
ppm