Supporting Information

Iodine-Mediated Sulfenylation of 4-hydroxycoumarins with Sulfonyl Hydrazides under Aqueous Conditions

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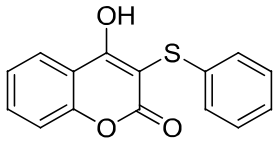
Experimental:

^{1}H and ^{13}CNMR spectra were recorded in DMSO-D_6 and $CDCl_3$ on a Bruker AV-400 spectrometer. Chemical shifts for ^{1}H NMR spectra are reported in ppm relative to residual DMSO-D_6 as internal reference (δ 2.50 ppm for ^{1}H) and $CDCl_3$ as internal reference (δ 7.26 ppm for ^{1}H) downfield from TMS, chemical shifts for ^{13}C NMR spectra are reported in ppm relative to internal DMSO-D6 (δ 39.5 ppm for ^{13}C) and $CDCl_3$ (δ 77.16 ppm for ^{13}C). Coupling constants (J) are given in Hertz (Hz). The terms m, s, d, t, q refer to multiplet, singlet, doublet, triplet, quartlet respectively; br refers to a broad signal.Reagents and solvents used were mostly AR grade. Silica gel coated plates were used for TLC.

Typical Procedure.

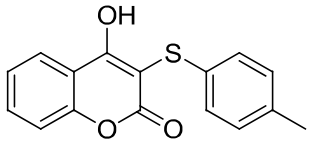
The mixture of 4-hydroxyquinolinone (0.2 mmol), sulfonyl hydrazides (0.24 mmol), I_2 (50 mol%), H_2O (2 ml) was stirred at 100 °C for 12 h until the reaction was complete (TLC). After cooling to r.t., the reaction mixture was diluted with EtOAc (20 mL), and washed with H_2O (20 mL). The obtained top organic layer was dried with anhydrous Na_2SO_4. The mixture was concentrated in vacuo and the residue was purified by column chromatography on silica gel (EA/n-Hexane=20%) to afford pure product.

Characteristic Data.



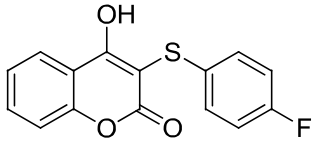
4-hydroxy-3-(phenylthio)-2*H*-chromen-2-one (3a)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 (dd, J = 7.9, 1.6 Hz, 1H), 7.76 – 7.71 (m, 1H), 7.48 – 7.40 (m, 2H), 7.34 – 7.27 (m, 2H), 7.26 – 7.13 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.89, 161.34, 153.49, 136.31, 134.19, 129.58, 126.63, 126.02, 124.82, 124.76, 116.97, 116.06, 94.80. MS (EI): 269 (M^+)



4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (3b)

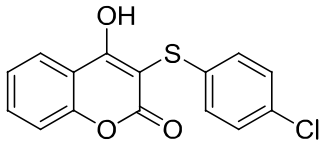
Whitle solid.^{1}H NMR (400 MHz, DMSO-d_6) δ 7.96 (d, J = 7.9 Hz, 1H), 7.70 (t, J = 8.0 Hz, 1H), 7.40 (t, J = 9.4 Hz, 2H), 7.13 (t, J = 7.3 Hz, 4H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.44, 161.29, 153.41, 135.66, 134.04, 132.64, 130.16, 127.42, 124.77, 124.71, 116.92, 116.08, 95.72, 20.94.



3-((4-fluorophenyl)thio)-4-hydroxy-2H-chromen-2-one (3c)

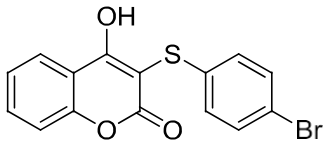
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (dd, J = 8.0, 1.6 Hz, 1H), 7.73 (t, J = 7.9 Hz, 1H), 7.50 – 7.38 (m, 2H), 7.31 (dd, J = 8.5, 5.3 Hz, 2H), 7.21 – 7.05 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.67, 162.39, 161.35, 159.98, 153.46, 134.13, 131.77 (d, J = 3.0 Hz), 129.52 (d, J = 4.2 Hz), 124.83, 124.72,

116.79(d, *J* = 30 Hz), 116.29 (d, *J* = 26 Hz), 95.57.



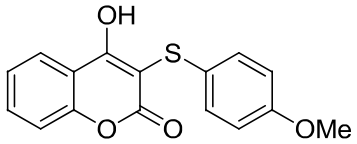
3-((4-chlorophenyl)thio)-4-hydroxy-2H-chromen-2-one (3d)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.98 (d, *J* = 7.9 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.42 (dd, *J* = 13.1, 7.7 Hz, 2H), 7.37 – 7.31 (m, 2H), 7.23 (dd, *J* = 8.8, 2.1 Hz, 2H).^{13}C NMR (101 MHz, DMSO-d_6) δ 169.13, 161.32, 153.53, 135.67, 134.19, 130.59, 129.40, 128.47, 124.87, 124.72, 116.97, 116.27, 94.43.



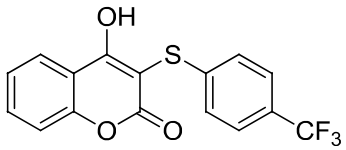
3-((4-bromophenyl)thio)-4-hydroxy-2H-chromen-2-one (3e)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.02 – 7.86 (m, 1H), 7.68 (d, *J* = 8.9 Hz, 1H), 7.48 – 7.33 (m, 4H), 7.20 – 7.10 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 169.08, 161.26, 153.50, 136.19, 134.18, 132.25, 128.73, 124.84, 124.70, 118.79, 116.95, 116.17, 94.38.



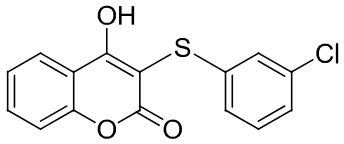
4-hydroxy-3-((4-methoxyphenyl)thio)-2H-chromen-2-one (3f)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.82 (dd, *J* = 7.8 Hz, 1.6 Hz, 1H), 7.44 – 7.40 (m, 1H), 7.13 (t, *J* = 7.9 Hz, 2 H), 6.96 – 6.93 (m, 2H), 6.76 – 6.72 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.83, 161.38, 158.71, 153.27, 133.90, 130.51, 128.16, 126.33, 124.66, 123.63, 115.21, 114.44, 97.18, 55.62.



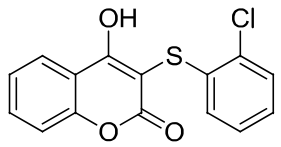
4-hydroxy-3-((4-(trifluoromethyl)phenyl)thio)-2H-chromen-2-one (3g)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.00 (d, *J* = 7.7 Hz, 1H), 7.75 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.55 – 7.27 (m, 4H).^{13}C NMR (101 MHz, DMSO-d_6) δ 169.67, 161.32, 153.63, 142.73, 134.31, 127.08, 126.24 (q, *J* = 3.4 Hz), 125.94, 124.91, 124.74, 123.40, 117.02, 116.34, 93.11.



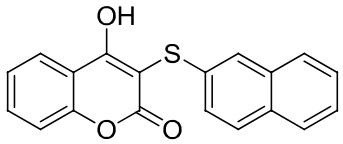
3-((3-chlorophenyl)thio)-4-hydroxy-2H-chromen-2-one (3h)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.97 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.71 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.46 – 7.36 (m, 2H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.26 – 7.11 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 169.31, 161.34, 153.58, 139.21, 134.22, 134.17, 131.12, 125.92, 125.83, 125.24, 124.88, 124.69, 116.98, 116.24, 93.95.



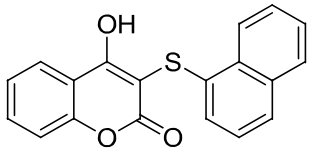
3-((2-chlorophenyl)thio)-4-hydroxy-2H-chromen-2-one (3i)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.99 (d, J = 8.0 Hz, 1H), 7.74 (q, J = 8.0, 7.6 Hz, 1H), 7.69 – 7.30 (m, 4H), 7.26 – 7.13 (m, 1H), 6.97 (d, J = 7.8 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 169.94, 161.20, 153.68, 135.58, 134.31, 133.49, 131.68, 130.48, 130.23, 129.98, 129.52, 128.85, 128.20, 128.08, 126.81, 126.28, 124.87, 124.71, 117.01, 116.32, 92.64.



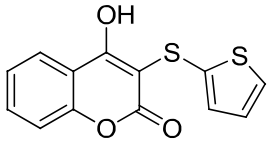
4-hydroxy-3-(naphthalen-2-ylthio)-2H-chromen-2-one (3k)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 – 7.97 (m, 1H), 7.85 (dq, J = 10.8, 7.8, 5.6 Hz, 3H), 7.73 (d, J = 10.3 Hz, 2H), 7.45 (p, J = 7.6 Hz, 4H), 7.40 – 7.27 (m, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.99, 161.38, 153.59, 134.14, 134.02, 133.86, 131.61, 129.52, 129.02, 128.07, 127.37, 127.13, 126.19, 125.99, 125.38, 124.89, 124.73, 124.28, 117.02, 116.30, 94.77.



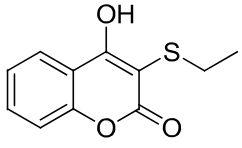
4-hydroxy-3-(naphthalen-1-ylthio)-2H-chromen-2-one (3l)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.32 (d, J = 8.0 Hz, 2H), 8.02 - 7.96 (m, 2H), 7.46 (d, d, J = 9.6 Hz, 2H), 7.67 – 7.58 (m, 2H), 7.47 – 7.36 (m, 2H), 7.20 (d, d, J = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 168.67, 160.51, 153.14, 133.62, 133.48, 132.81, 130.51, 128.41, 126.29, 126.25, 125.98, 125.58, 124.30, 124.21, 123.64, 123.01, 116.28, 115.69, 93.20.



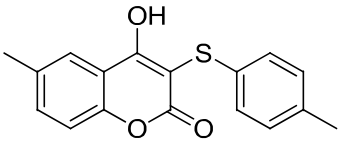
4-hydroxy-3-(thiophen-2-ylthio)-2H-chromen-2-one (3m)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.95 (dd, J = 8.0, 1.6 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.52 (dd, J = 5.6, 1.2 Hz, 1H), 7.39 – 7.36 (m, 2H), 7.28 (dd, J = 3.6, 1.2 Hz, 1H), 7.00 – 6.98 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 166.96, 160.67, 152.85, 133.56, 133.45, 131.75, 129.01, 127.55, 124.41, 124.16, 116.36, 115.80, 97.49.



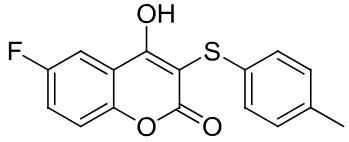
3-(ethylthio)-4-hydroxy-2H-chromen-2-one (3n)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dd, J = 7.9, 1.7 Hz, 1H), 7.61 (ddd, J = 8.7, 7.2, 1.6 Hz, 1H), 7.39 – 7.30 (m, 2H), 2.86 (q, J = 7.4 Hz, 2H), 1.27 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.47, 163.04, 152.95, 129.41, 123.81, 120.97, 119.04, 114.36, 86.58, 25.72, 13.51.



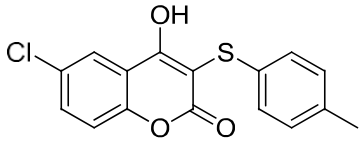
4-hydroxy-6-methyl-3-(p-tolylthio)-2H-chromen-2-one (3o)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 (s, 1H), 7.51 (dd, *J* = 9.6, 2.0 Hz, 1H), 7.31 (d, 8.0 Hz, 1H), 7.09 (s, 4H), 2.40 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 168.15, 161.03, 151.28, 135.09, 134.35, 133.66, 132.10, 129.56, 126.65, 123.89, 116.19, 115.18, 94.99, 20.22, 20.10.



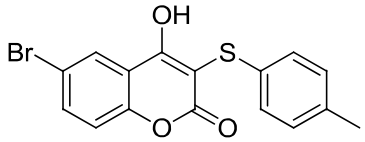
6-fluoro-4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (3p)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.69 (dd, *J* = 9.2, 3.4 Hz, 1H), 7.61 – 7.56 (m, 1H), 7.50 – 7.46 (m, 1H), 7.14 – 7.09 (m, 4H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 167.08, 160.79, 158.31 (d, *J* = 245.2 Hz), 149.11, 135.07, 131.90, 129.56, 126.94, 120.86 (d, *J* = 29.6 Hz), 118.56 (d, *J* = 9.9 Hz), 116.76 (d, *J* = 9.6 Hz), 109.57 (d, *J* = 27 Hz), 95.89, 19.86.



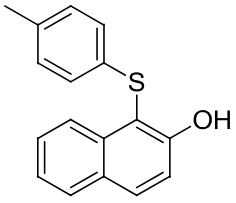
6-chloro-4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (3q)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.77 (d, *J* = 2.4 Hz, 1H), 7.47 (dd, *J* = 8.8, 2.8 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.88 (d, *J* = 8.0 Hz, 2H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 173.11, 163.33, 152.27, 137.51, 132.00, 130.19, 128.88, 126.00, 124.60, 124.26, 124.05, 117.82, 85.08, 20.79.



6-bromo-4-hydroxy-3-(p-tolylthio)-2H-chromen-2-one (3r)

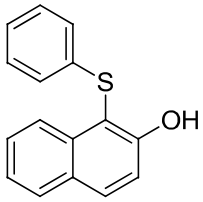
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.87 (d, *J* = 2.8 Hz, 1H), 7.57 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.13 (d, *J* = 8.8 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 172.80, 163.17, 152.16, 137.52, 133.03, 131.67, 128.52, 127.21, 124.62, 124.58, 118.09, 113.63, 85.00, 20.60.



1-(p-tolylthio)naphthalen-2-ol (3u)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.5 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.48 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.40 – 7.29 (m, 2H), 7.21 (s, 1H), 7.05 – 6.89 (m, 4H), 2.23 (s,

3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.88, 135.90, 135.45, 132.66, 131.76, 129.97, 129.49, 128.56, 127.90, 126.70, 124.76, 123.82, 116.85, 108.71, 20.92.



1-(phenylthio)naphthalen-2-ol (3v)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 8.9 Hz, 1H), 7.79 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.47 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.41 – 7.29 (m, 2H), 7.20 – 7.11 (m, 3H), 7.11 – 7.05 (m, 1H), 7.05 – 6.97 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.04, 135.48, 132.89, 129.52, 129.23, 128.62, 128.01, 126.40, 125.93, 124.74, 123.92, 116.92, 108.06.

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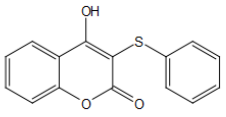

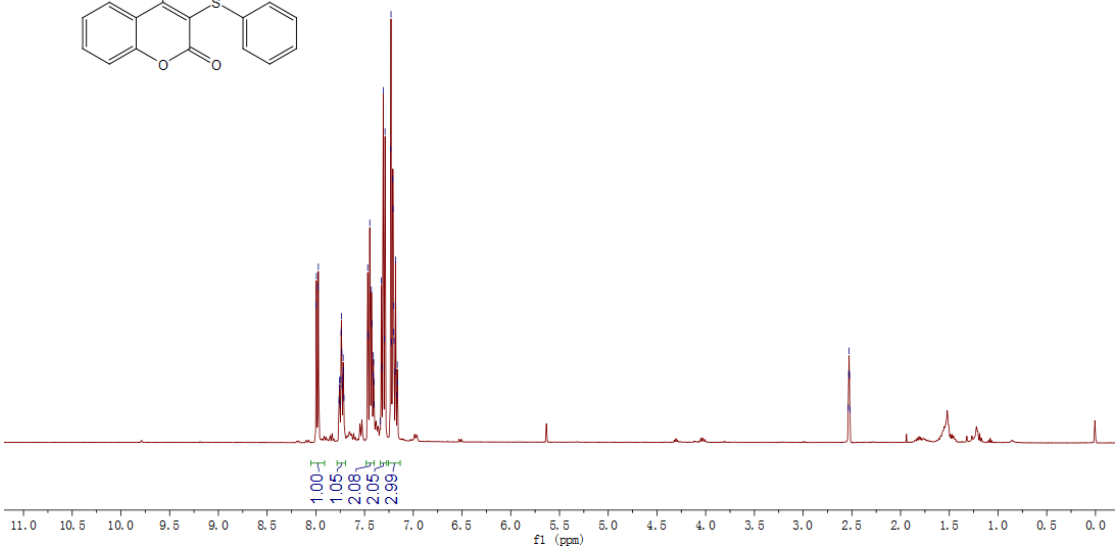

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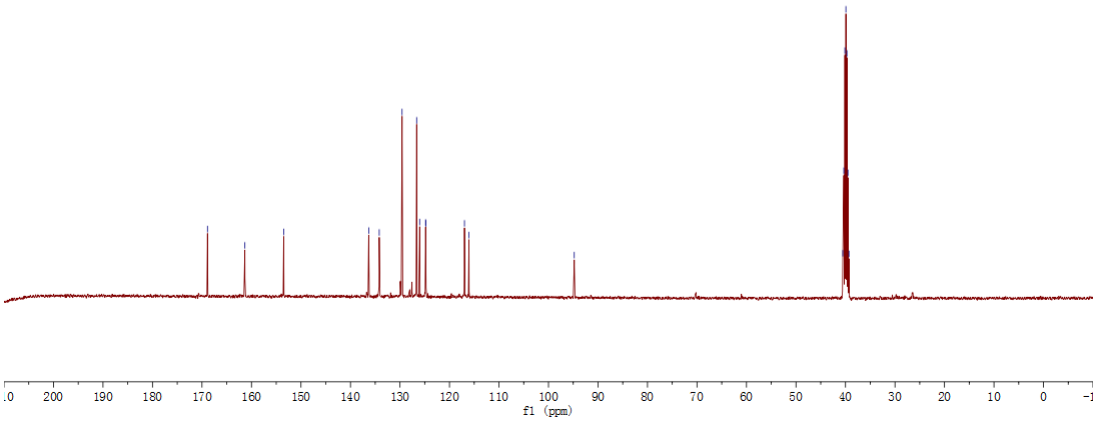

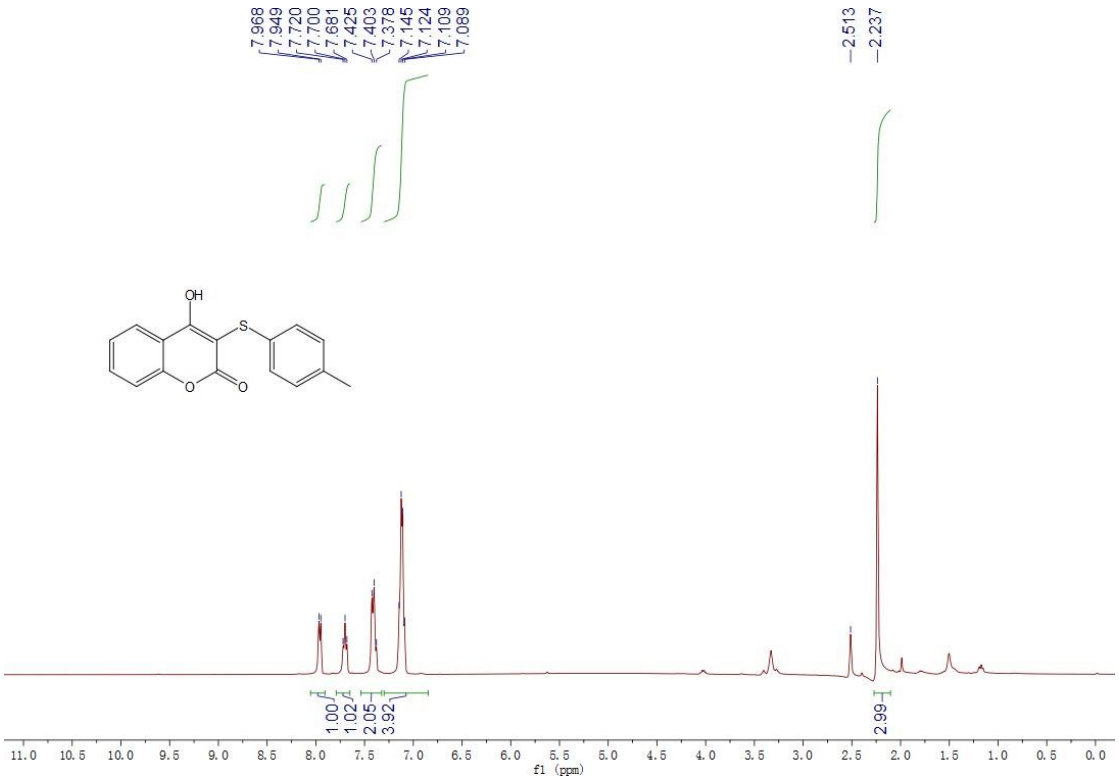
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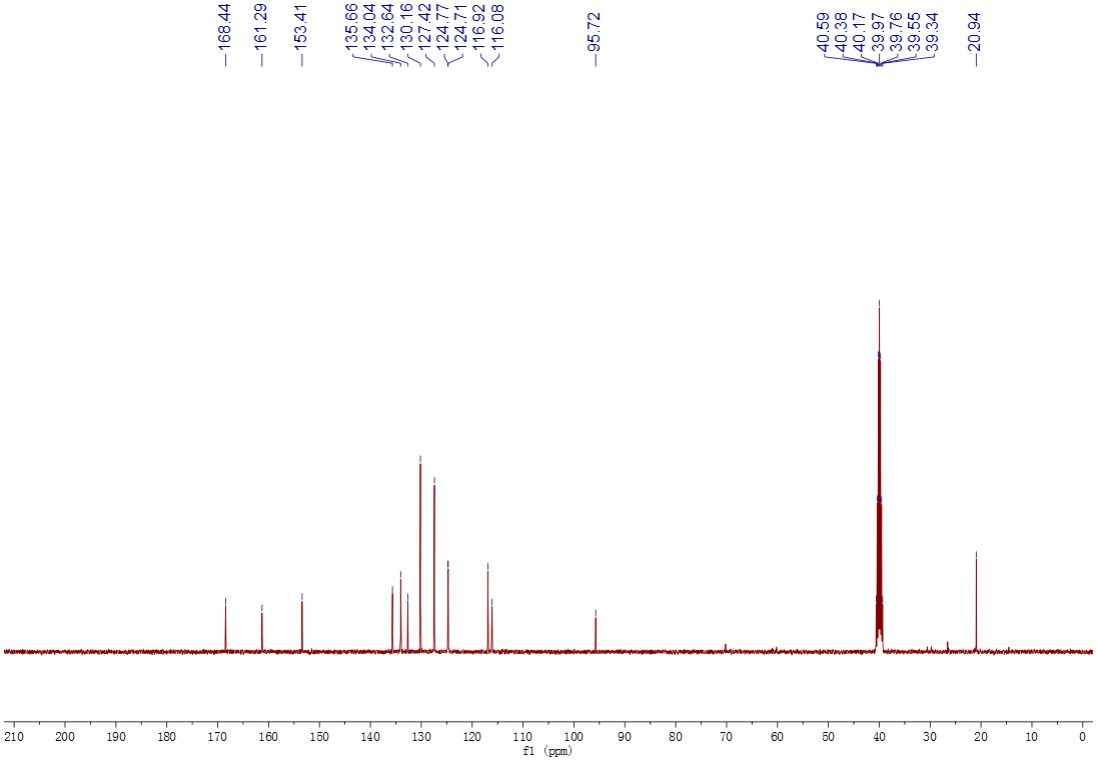
2.99
f1 (ppm)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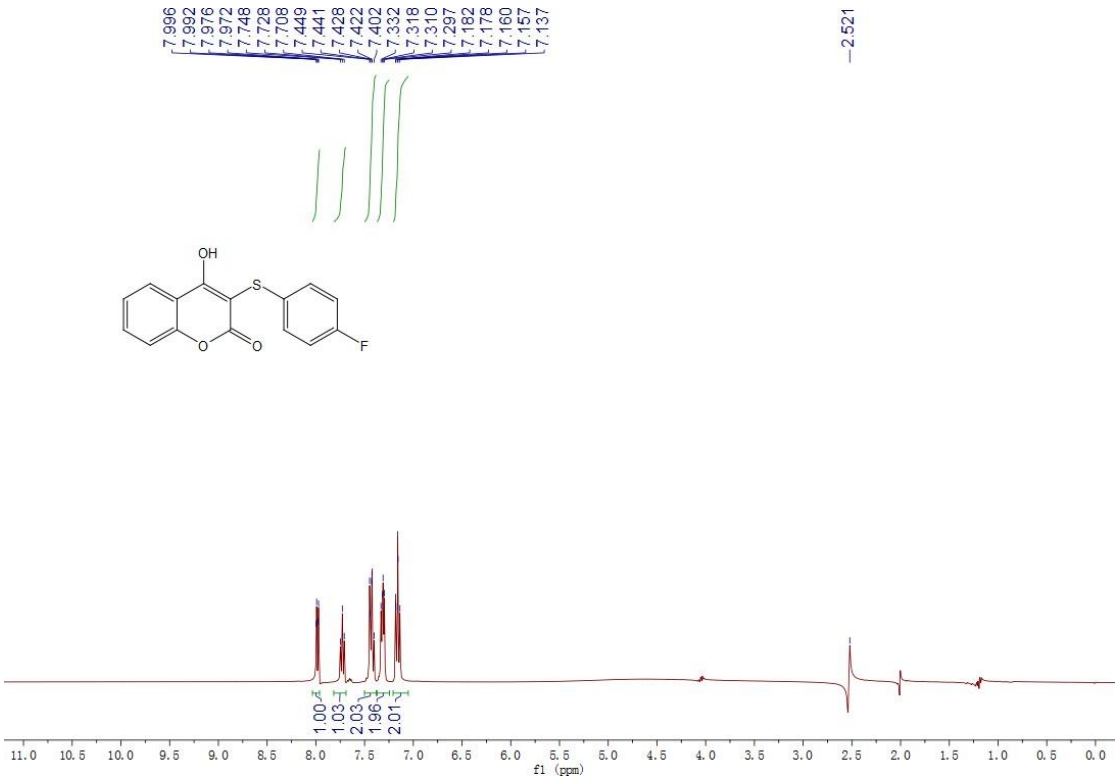
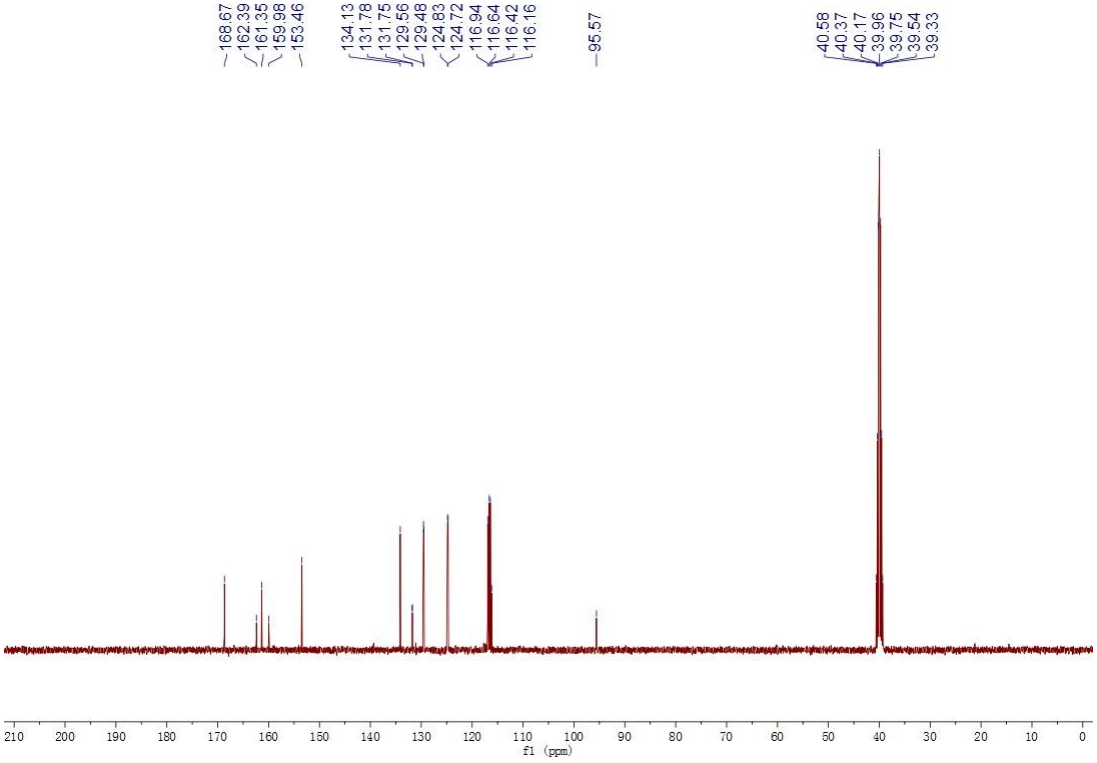
161.29
153.41
135.66
134.04
132.64
130.16
127.42
124.77
124.71
116.92
116.08
95.72
40.59
40.38
40.17
39.97
39.76
39.55
39.34
20.94
f1 (ppm)


7.996
7.992
7.976
7.972
7.748
7.728
7.708
7.449
7.441
7.428
7.422
7.402
7.332
7.318
7.310
7.297
7.182
7.178
7.160
7.157
7.137
2.521
OH
S
O
O
F
1.00
1.03
2.03
1.96
2.01
f1 (ppm)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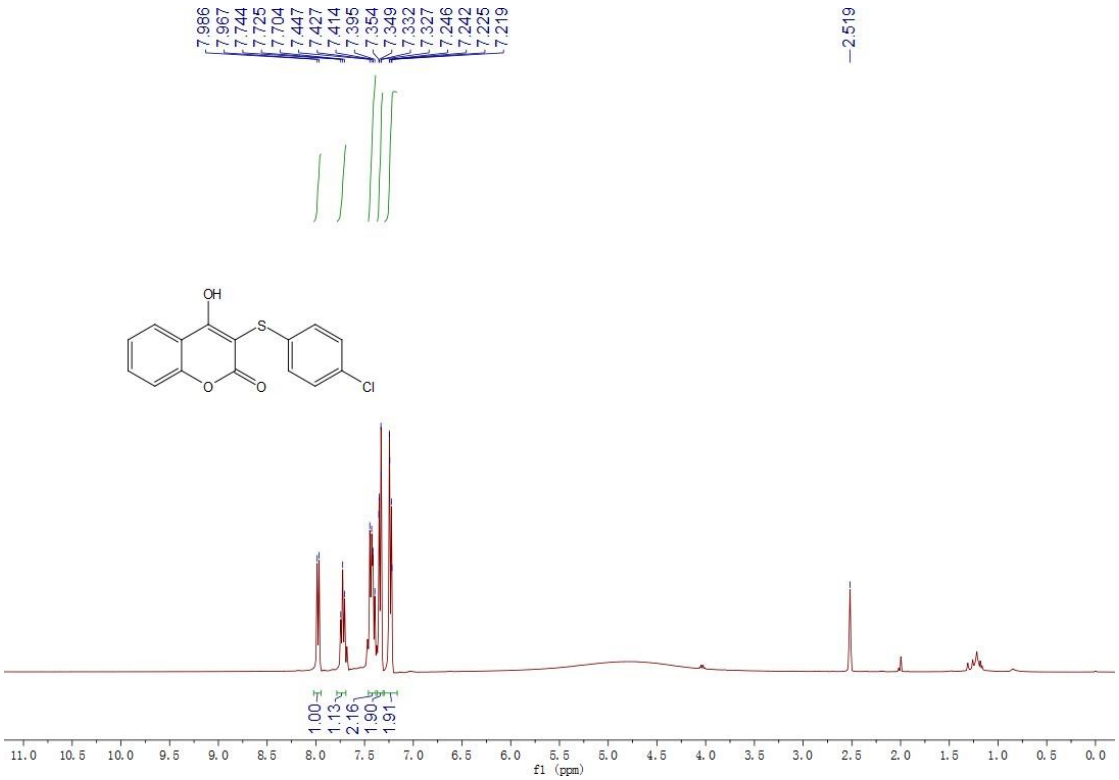
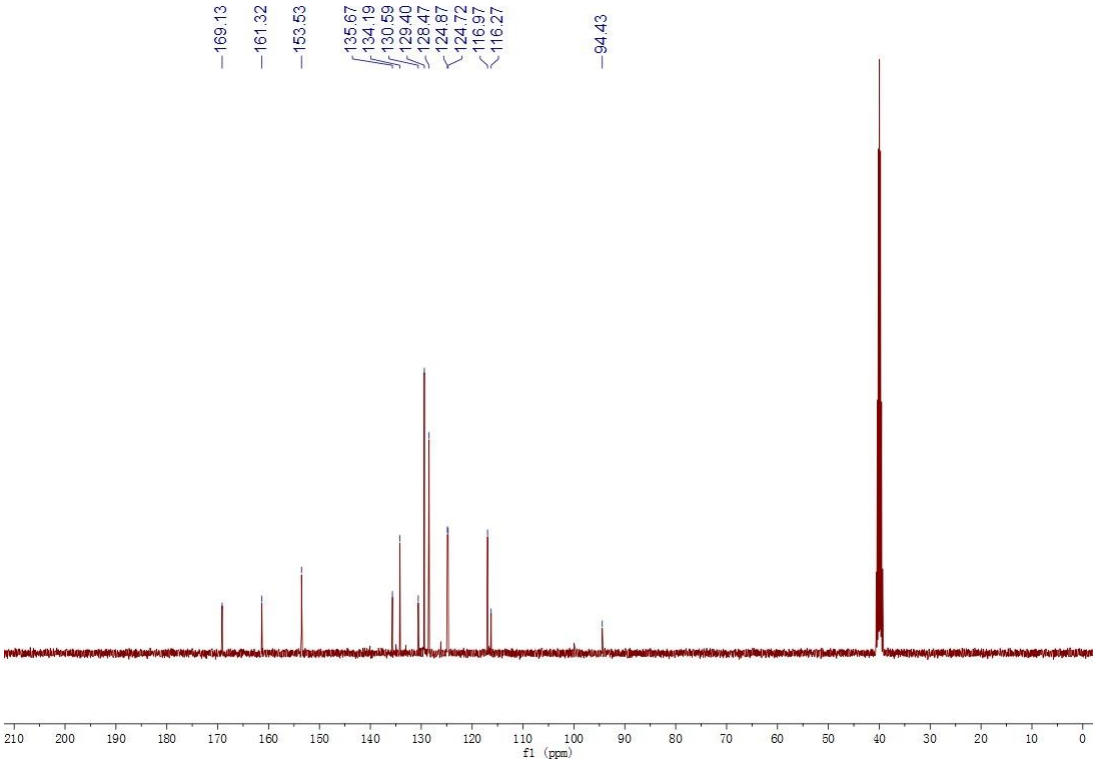
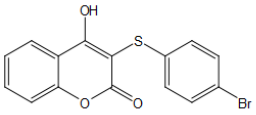
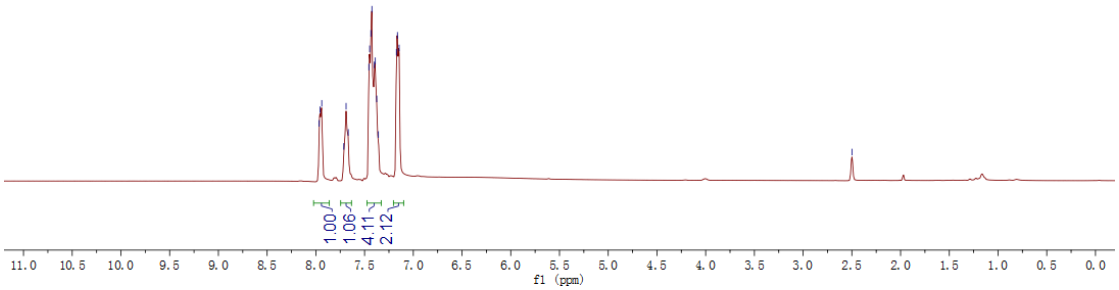
162.39
161.35
159.98
153.46
134.13
131.78
131.75
129.56
129.48
124.83
124.72
116.94
116.64
116.42
116.16
95.57
40.58
40.37
40.17
39.96
39.75
39.54
39.33
f1 (ppm)


7.986
7.967
7.744
7.725
7.704
7.447
7.427
7.414
7.395
7.354
7.349
7.332
7.327
7.246
7.242
7.225
7.219
2.519
OH
S
O
O
Cl
1.00
1.13
2.16
1.90
1.91
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

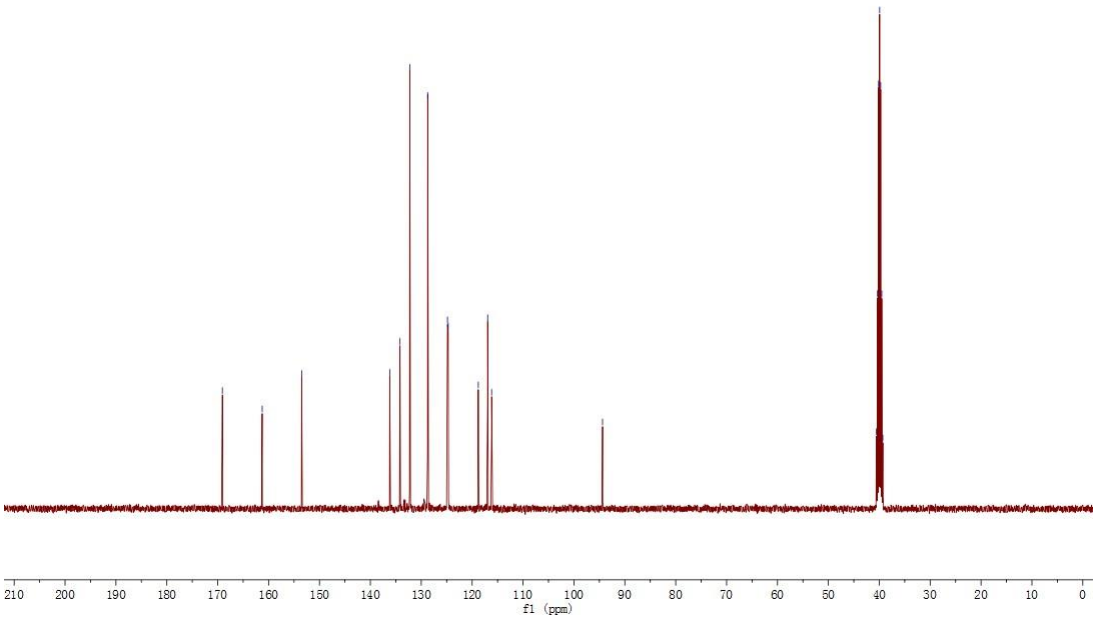

169.13
161.32
153.53
135.67
134.19
130.59
129.40
128.47
124.87
124.72
116.97
116.27
94.43
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

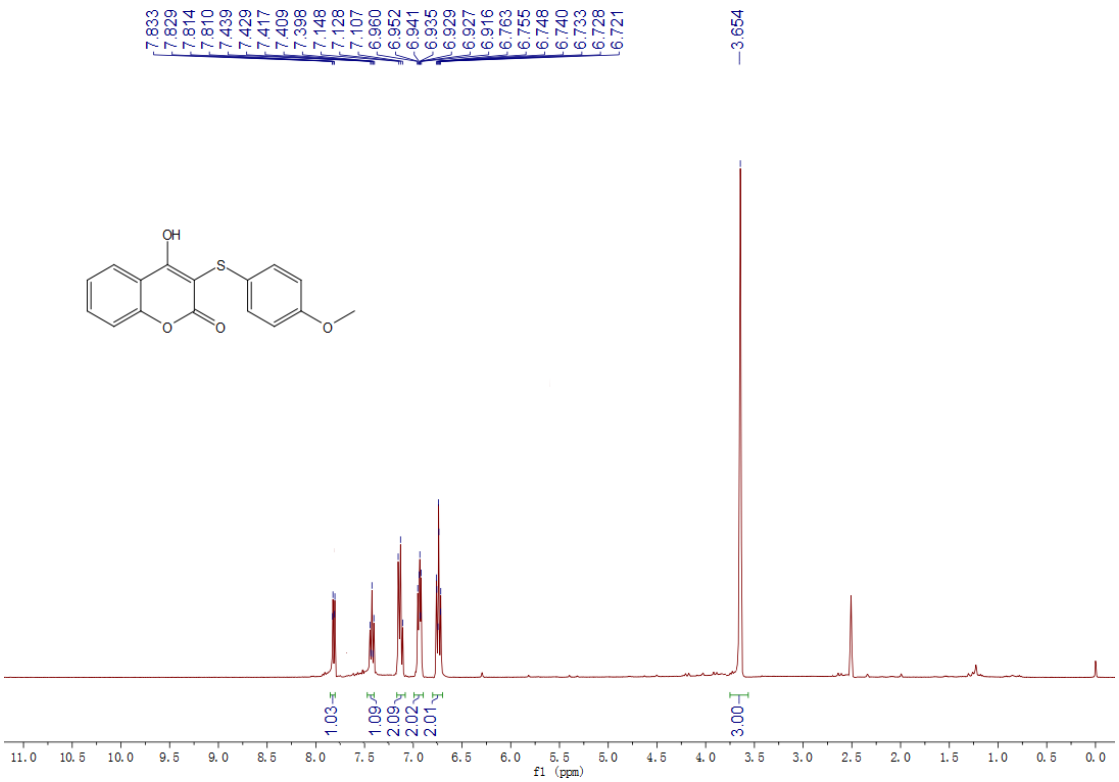

7.967
7.956
7.939
7.713
7.690
7.667
7.456
7.448
7.436
7.425
7.399
7.390
7.375
7.358
7.174
7.163
7.145
2.499

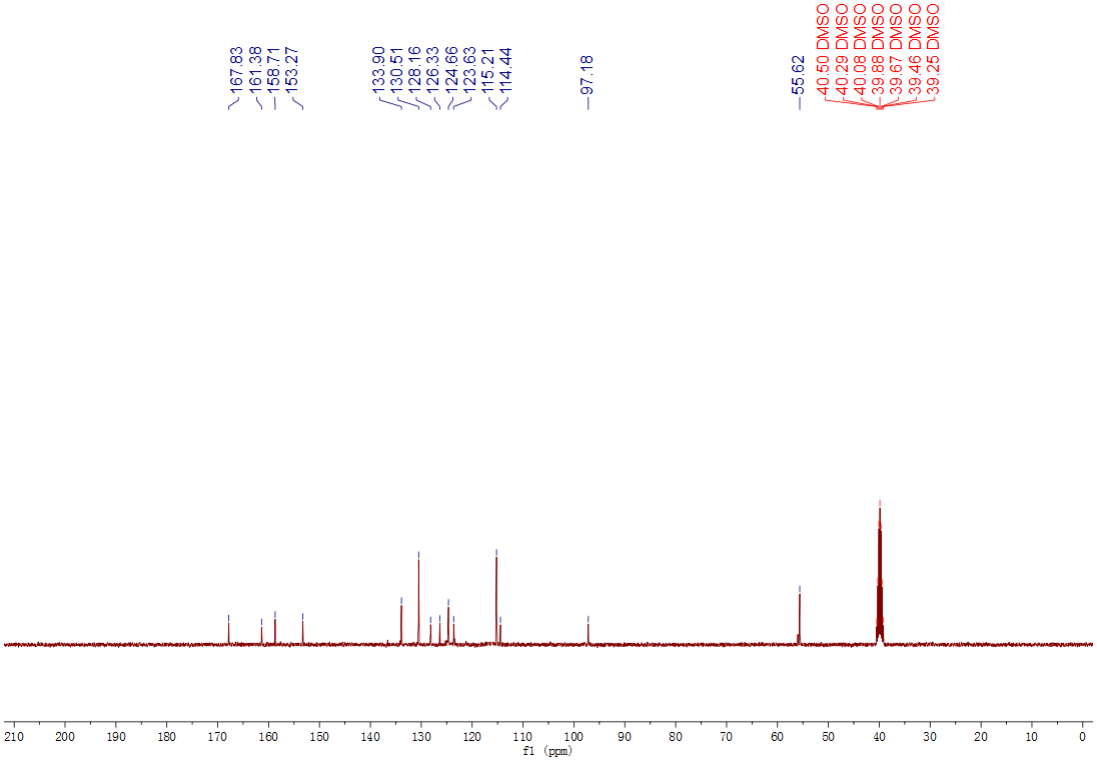

OH
S
O
O
Br


1.00
1.06
4.11
2.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

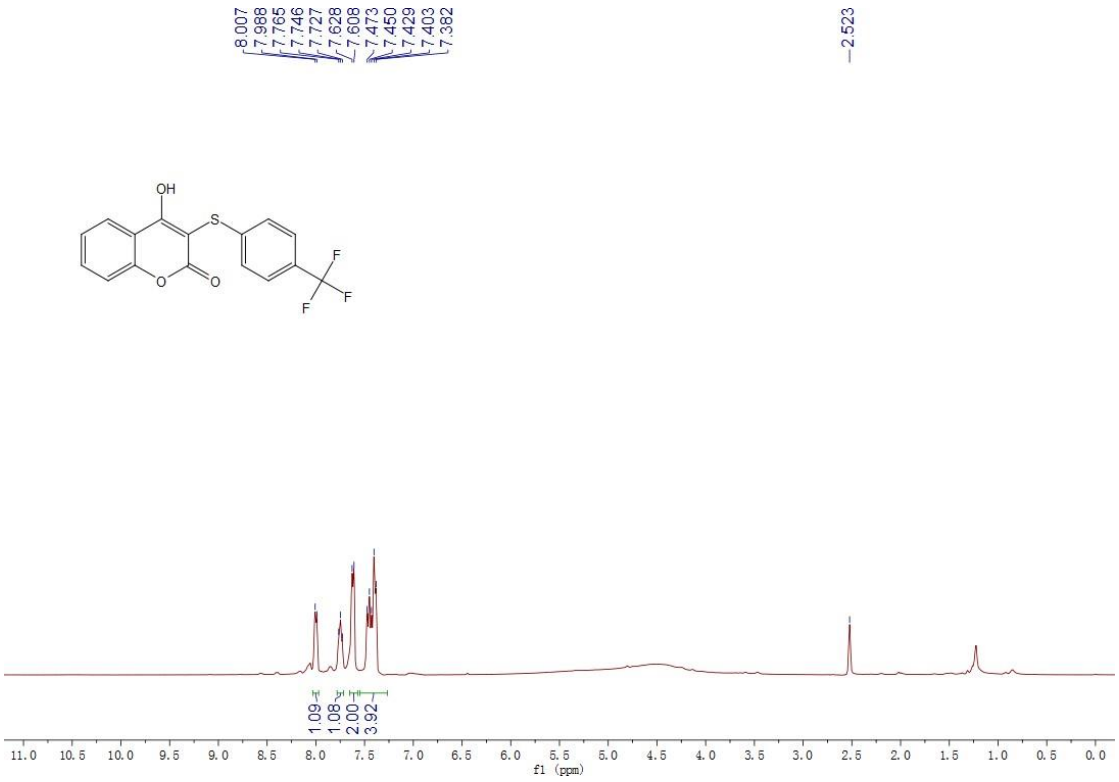

169.08
161.26
153.50
136.19
134.18
132.25
128.73
124.84
124.70
118.79
116.95
116.17
94.38
40.55
40.34
40.14
39.93
39.72
39.51
39.30

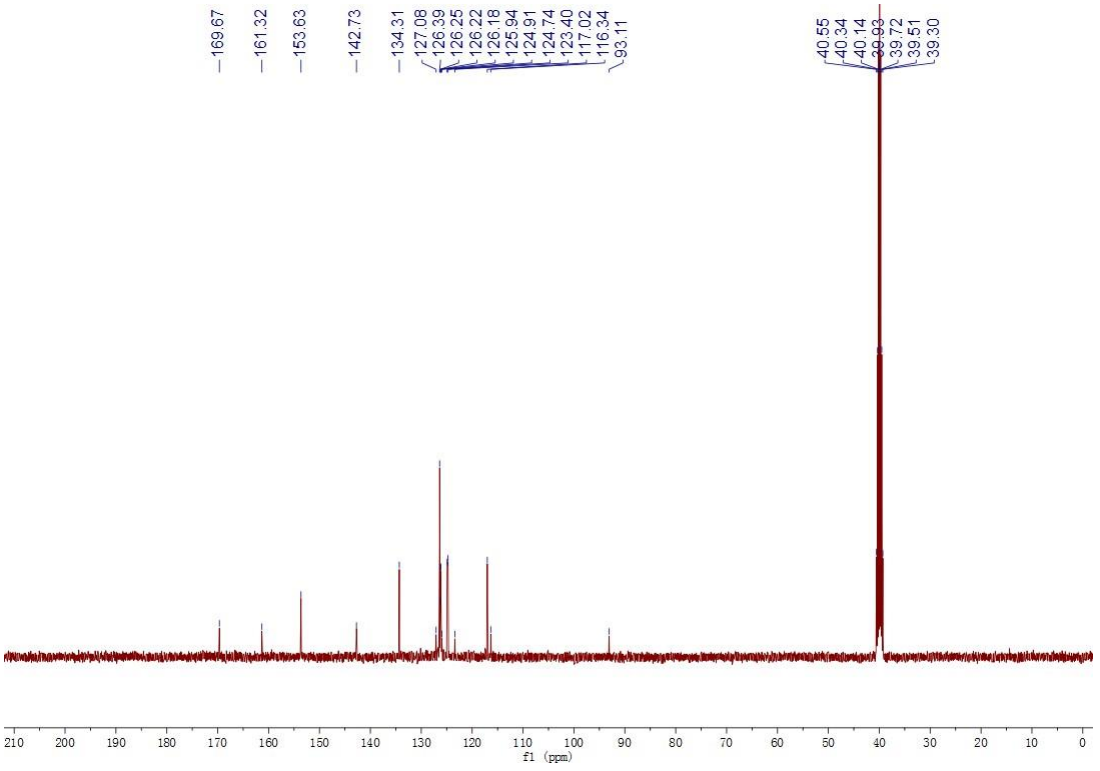

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

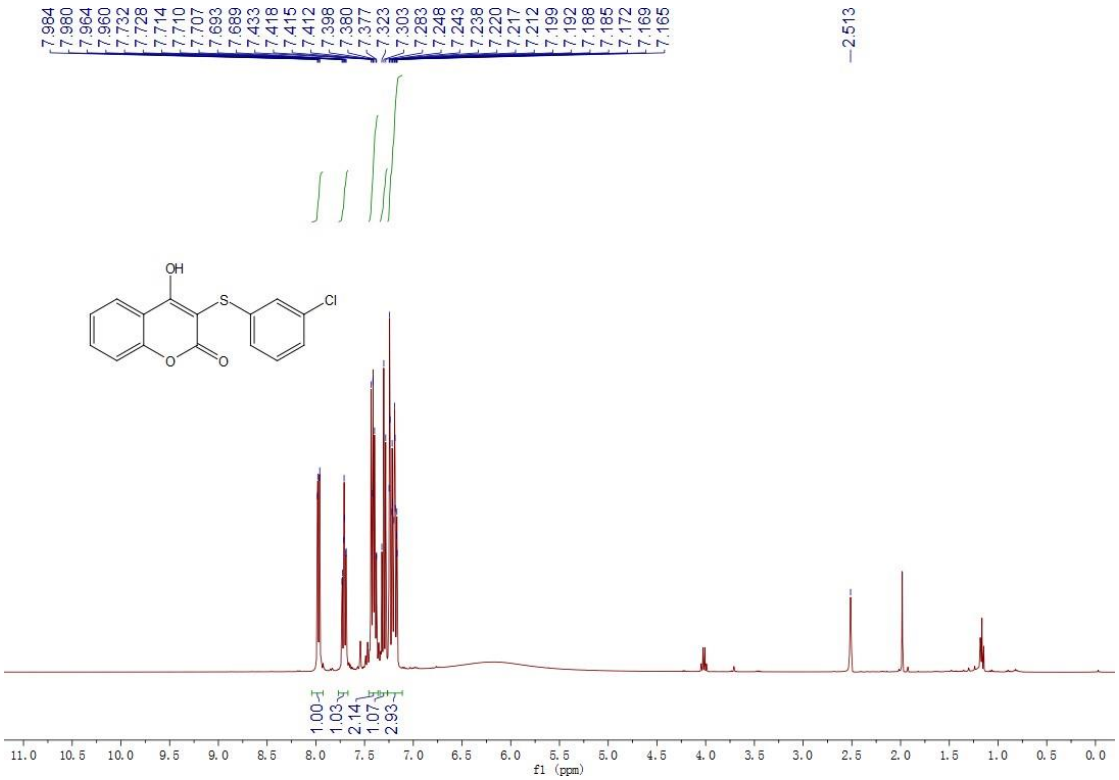

7.833
7.829
7.814
7.810
7.439
7.429
7.417
7.409
7.398
7.148
7.128
7.107
6.960
6.952
6.941
6.935
6.929
6.927
6.916
6.763
6.755
6.748
6.740
6.733
6.728
6.721
3.654
OH
S
O
O
O
1.03
1.09
2.09
2.02
2.01
3.00
f1 (ppm)

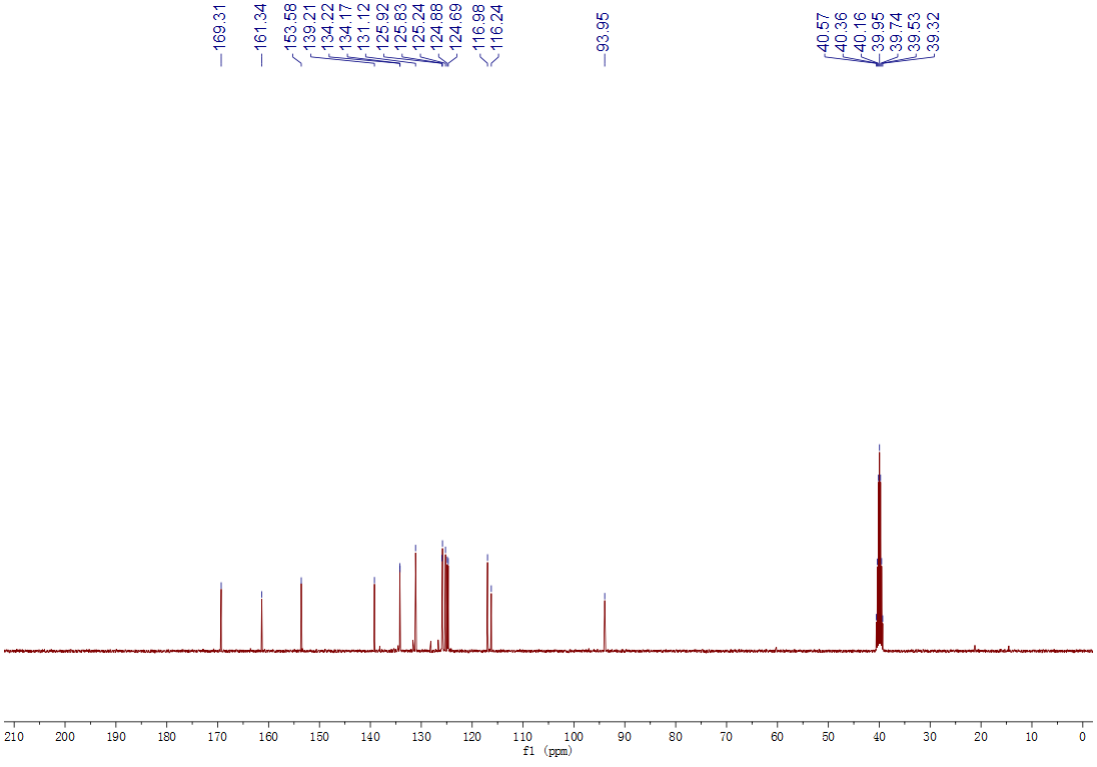

167.83
161.38
158.71
153.27
133.90
130.51
128.16
126.33
124.66
123.63
115.21
114.44
97.18
55.62
40.50 DMSO
40.29 DMSO
40.08 DMSO
39.88 DMSO
39.67 DMSO
39.46 DMSO
39.25 DMSO
f1 (ppm)

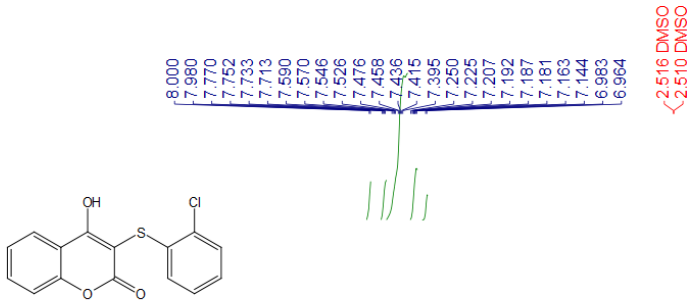
OH
S
F
F
F
O
O

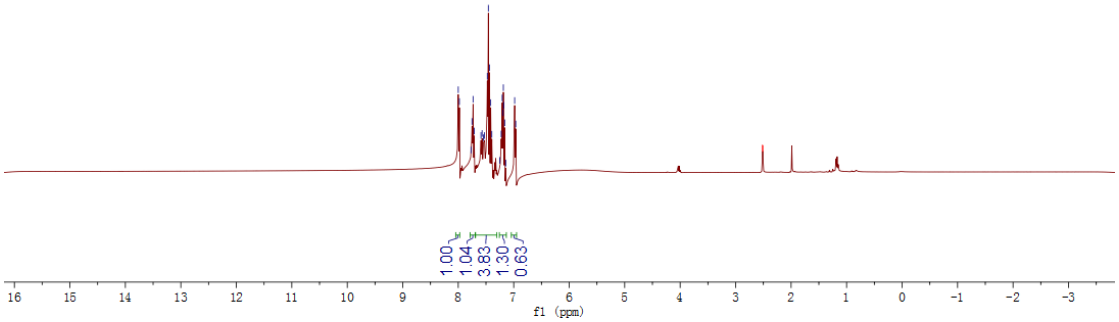

8.007
7.988
7.765
7.746
7.727
7.628
7.608
7.473
7.450
7.429
7.403
7.382
2.523
1.09
1.08
2.00
3.92
f1 (ppm)


169.67
161.32
153.63
142.73
134.31
127.08
126.39
126.25
126.22
126.18
125.94
124.91
124.74
123.40
117.02
116.34
93.11
40.55
40.34
40.14
39.93
39.72
39.51
39.30
f1 (ppm)

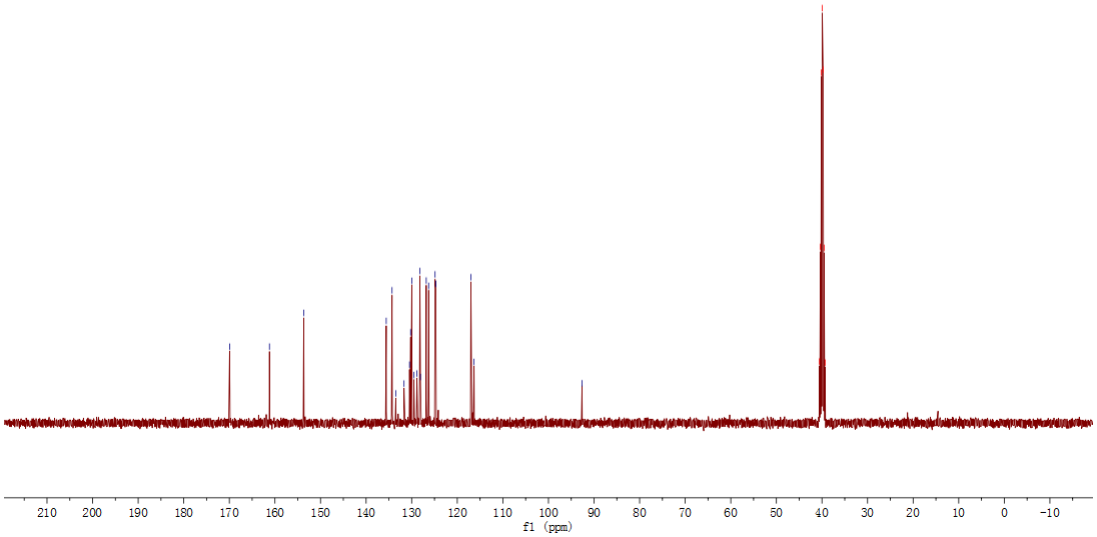

7.984
7.980
7.964
7.960
7.732
7.728
7.714
7.710
7.707
7.693
7.689
7.433
7.418
7.415
7.412
7.398
7.380
7.377
7.323
7.303
7.283
7.248
7.243
7.238
7.220
7.217
7.212
7.199
7.192
7.188
7.185
7.172
7.169
7.165
2.513
OH
S
Cl
O
O
1.00
1.03
2.14
1.07
2.93
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

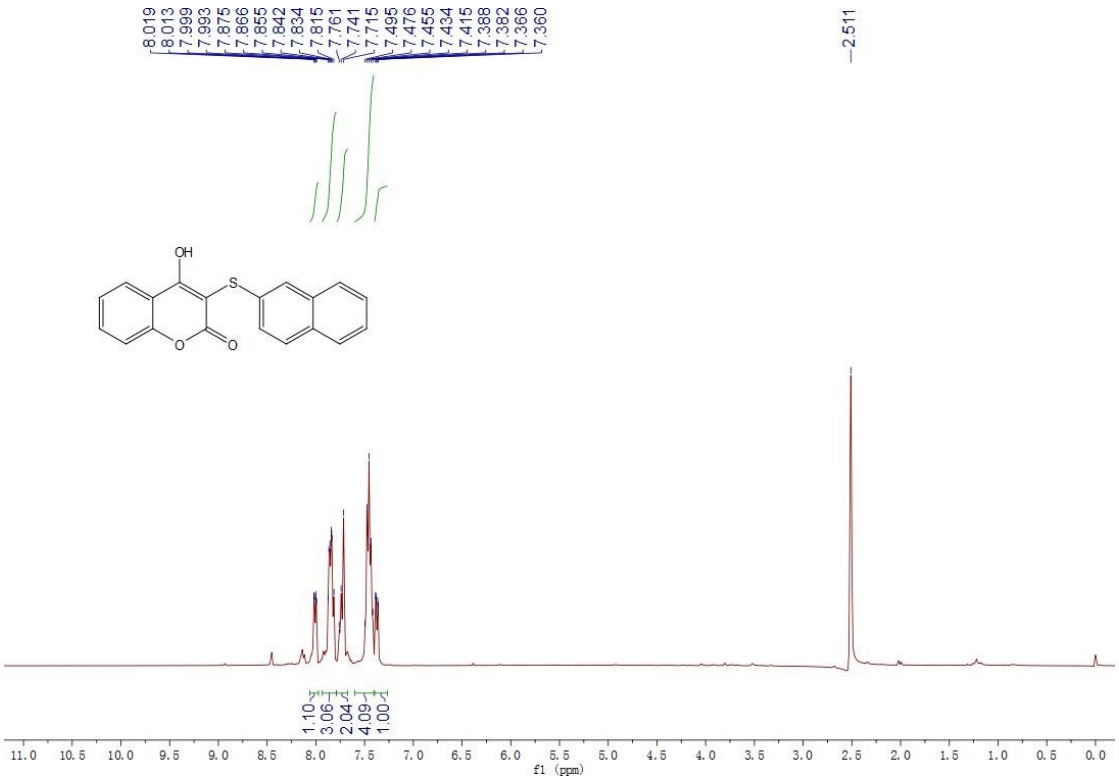

169.31
161.34
153.58
139.21
134.22
134.17
131.12
125.92
125.83
125.24
124.88
124.69
116.98
116.24
93.95
40.57
40.36
40.16
39.95
39.74
39.53
39.32
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

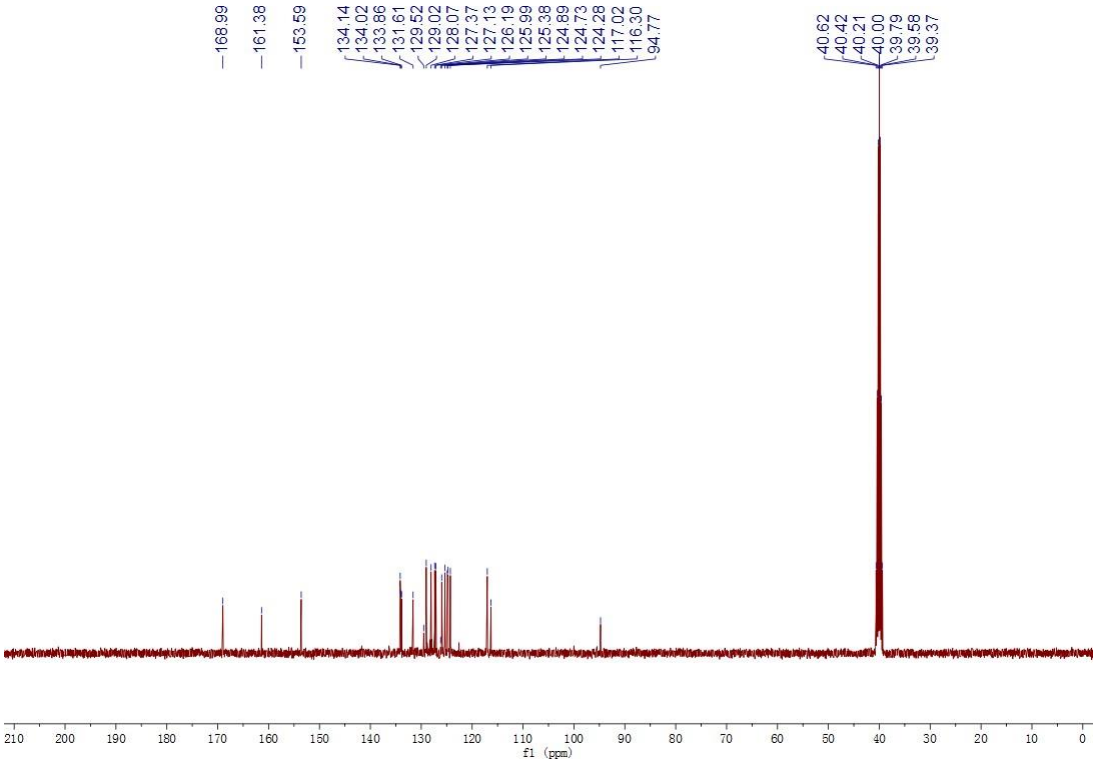

8.000
7.980
7.770
7.752
7.733
7.713
7.590
7.570
7.546
7.526
7.476
7.458
7.436
7.415
7.395
7.250
7.225
7.207
7.192
7.187
7.181
7.163
7.144
6.983
6.964
2.516 DMSO
2.510 DMSO
OH
Cl
S
O
O


1.00
1.04
3.83
1.30
0.63
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


169.94
161.20
153.68
135.58
134.31
133.49
131.68
130.48
130.23
129.98
129.52
128.85
128.20
128.08
126.81
126.28
124.87
124.71
117.01
116.32
92.64
40.56 DMSO
40.35 DMSO
40.14 DMSO
39.93 DMSO
39.73 DMSO
39.52 DMSO
39.31 DMSO


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.019
8.013
7.999
7.993
7.875
7.866
7.855
7.842
7.834
7.815
7.761
7.741
7.715
7.495
7.476
7.455
7.434
7.415
7.388
7.382
7.366
7.360
2.511
OH
S
O
O
1.10
3.06
2.04
4.09
1.00
f1 (ppm)


168.99
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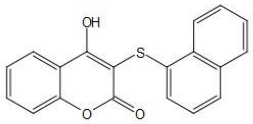
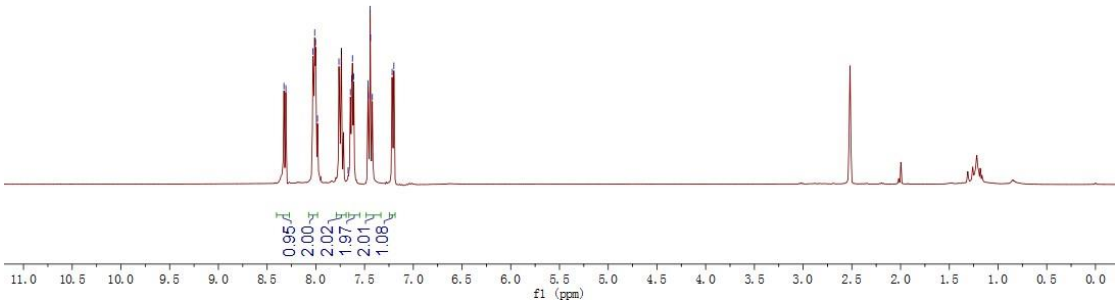
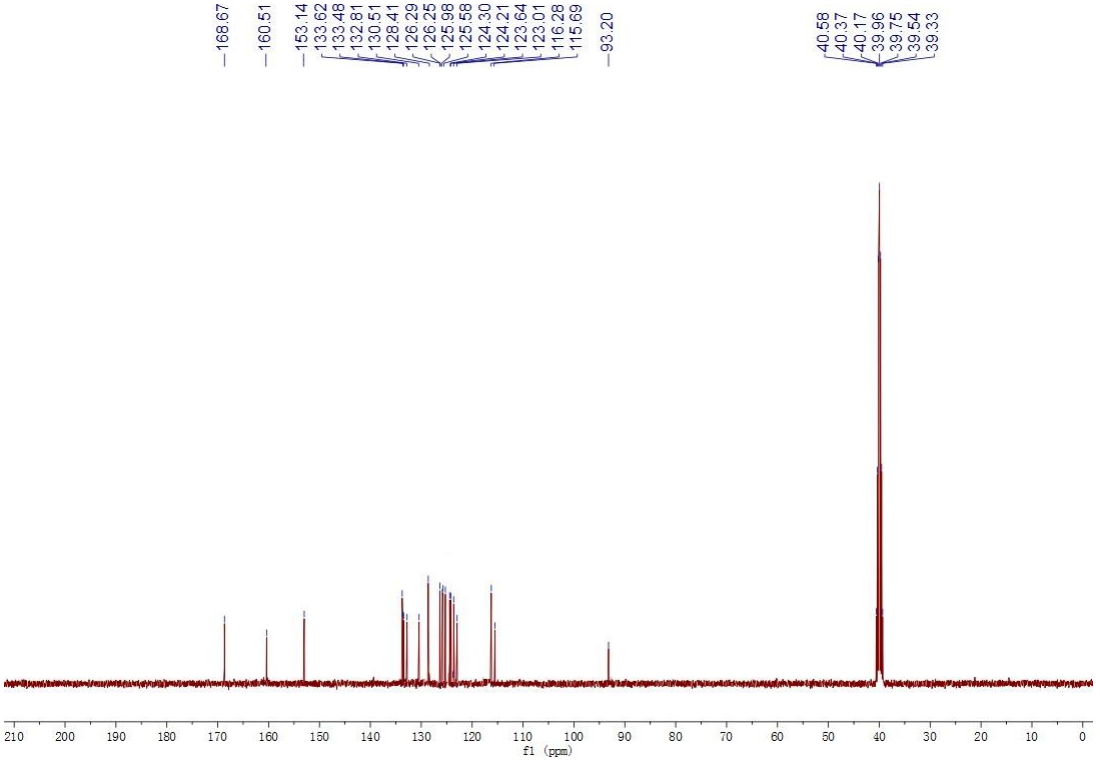
153.59
134.14
134.02
133.86
131.61
129.52
129.02
128.07
127.37
127.13
126.19
125.99
125.38
124.89
124.73
124.28
117.02
116.30
94.77
40.62
40.42
40.21
40.00
39.79
39.58
39.37
f1 (ppm)

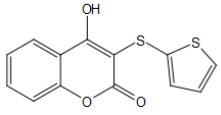

8.328
8.308
8.020
8.000
7.980
7.960
7.758
7.734
7.675
7.655
7.635
7.618
7.601
7.580
7.466
7.446
7.428
7.404
7.382
7.361
7.208
7.189

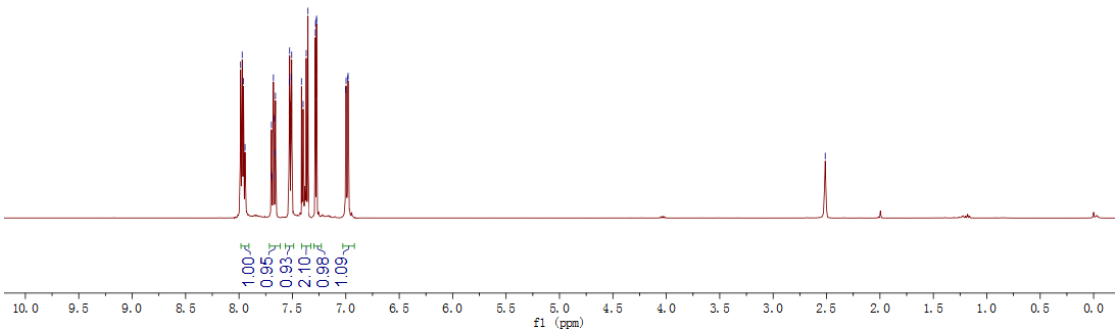

OH
S
O
O

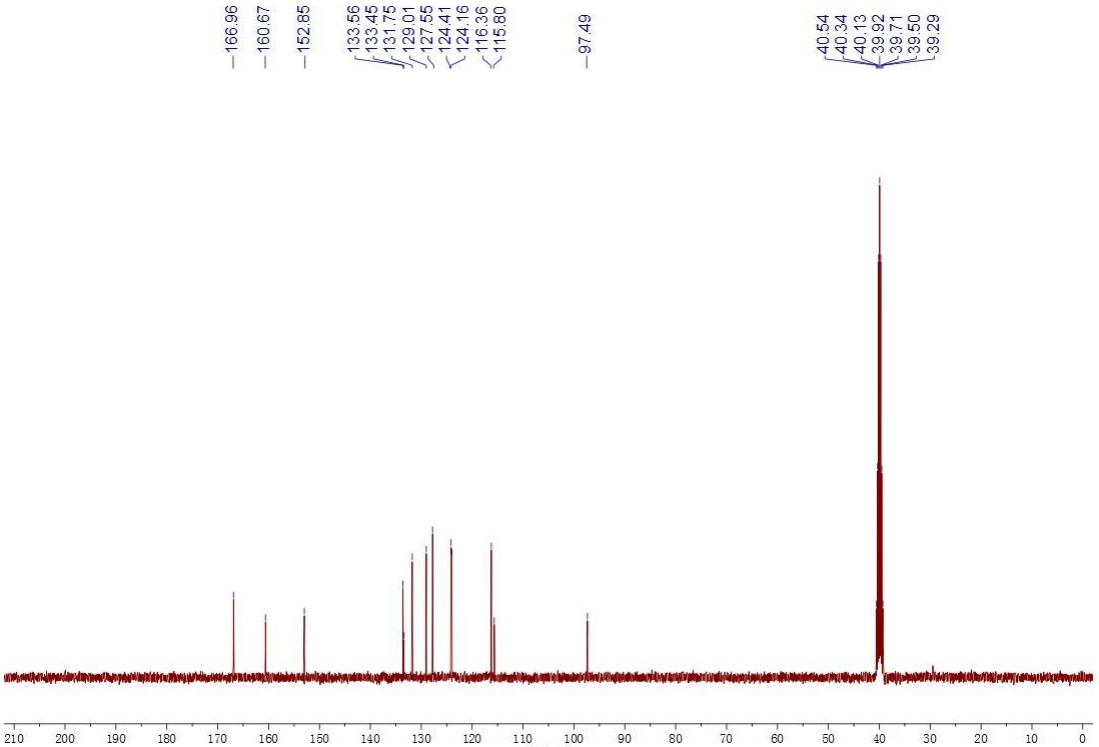

0.95
2.00
2.02
1.97
2.01
1.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

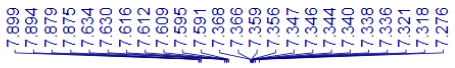

168.67
160.51
153.14
133.62
133.48
132.81
130.51
128.41
126.29
126.25
125.98
125.58
124.30
124.21
123.64
123.01
116.28
115.69
93.20
40.58
40.37
40.17
39.96
39.75
39.54
39.33
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.961
7.957
7.940
7.937
7.694
7.676
7.674
7.659
7.655
7.530
7.527
7.517
7.514
7.393
7.390
7.388
7.375
7.369
7.357
7.284
7.281
7.275
7.272
6.998
6.989
6.985
6.976
2.512


OH
S
S
O
O


1.00
0.95
0.93
2.10
0.98
1.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.96
160.67
152.85
133.56
133.45
131.75
129.01
127.55
124.41
124.16
116.36
115.80
97.49
40.54
40.34
40.13
39.92
39.71
39.50
39.29
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.899
7.894
7.879
7.875
7.634
7.630
7.616
7.612
7.609
7.595
7.591
7.368
7.366
7.359
7.356
7.347
7.346
7.344
7.340
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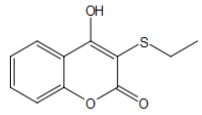
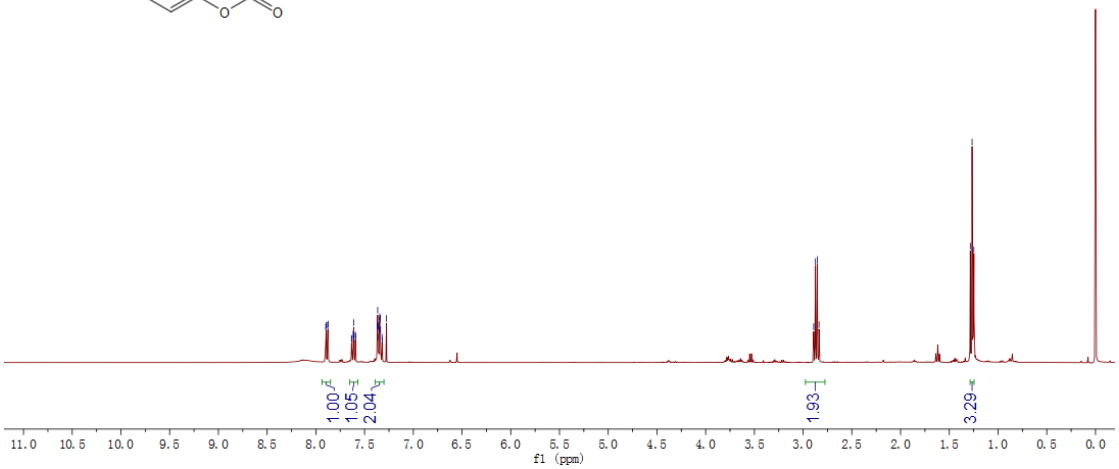
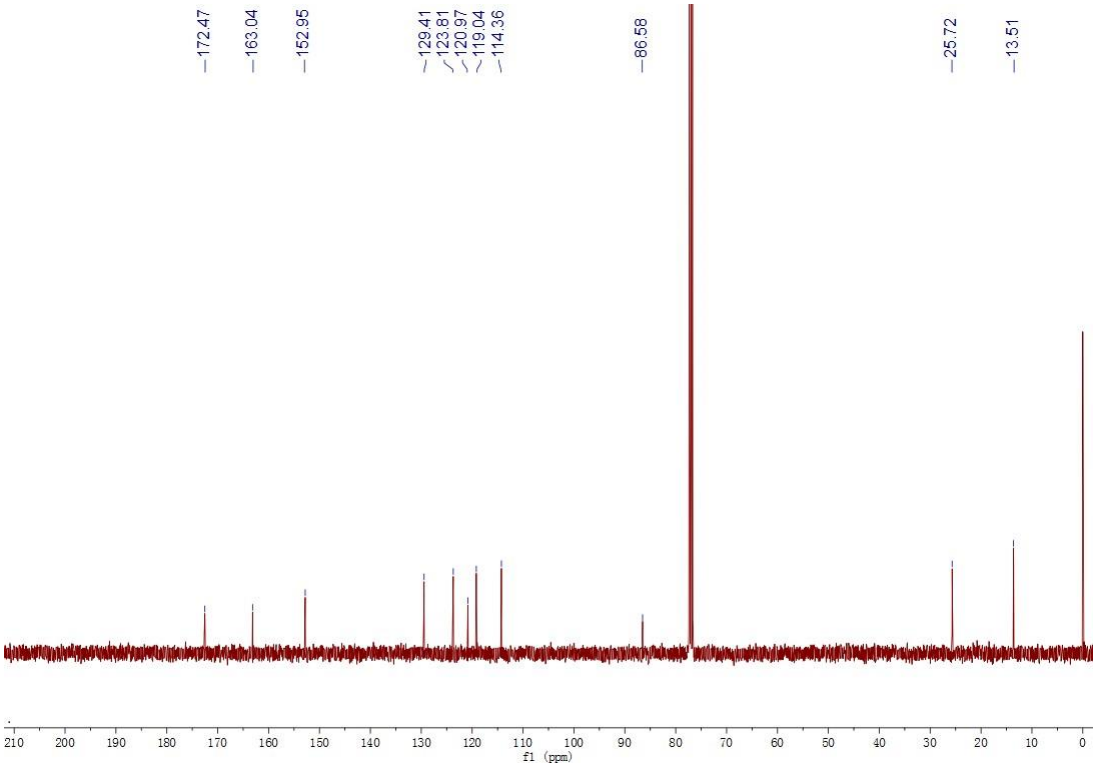
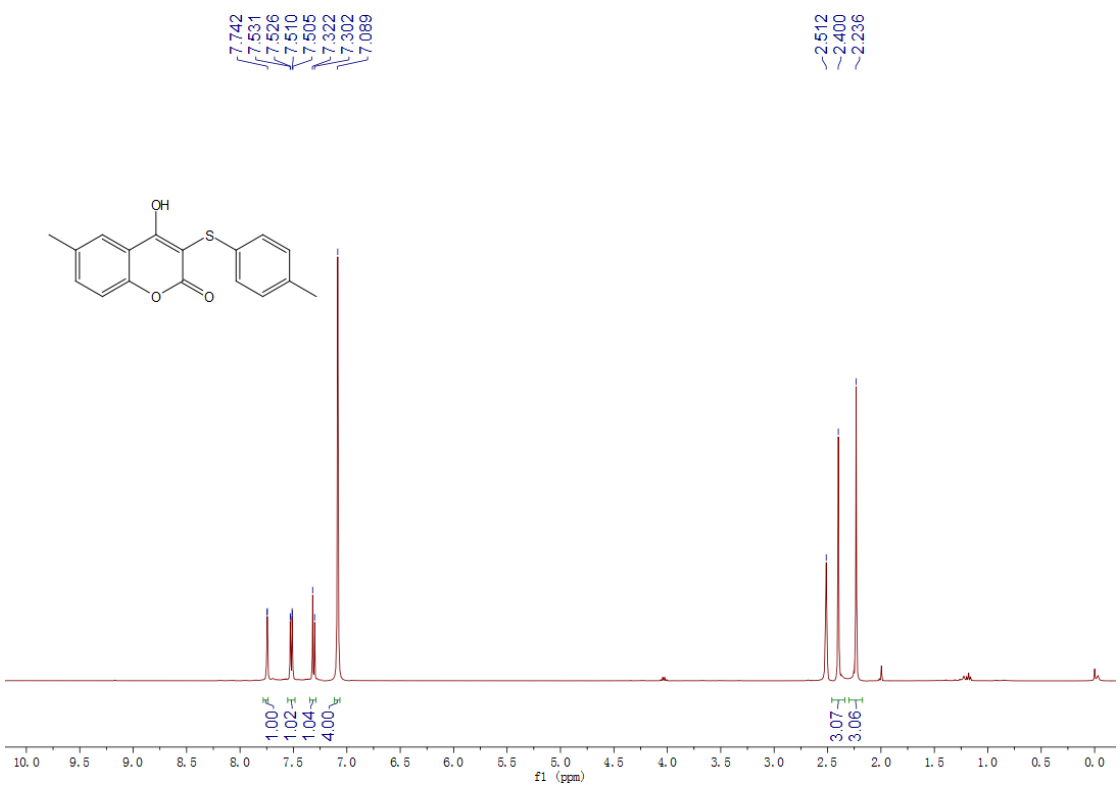
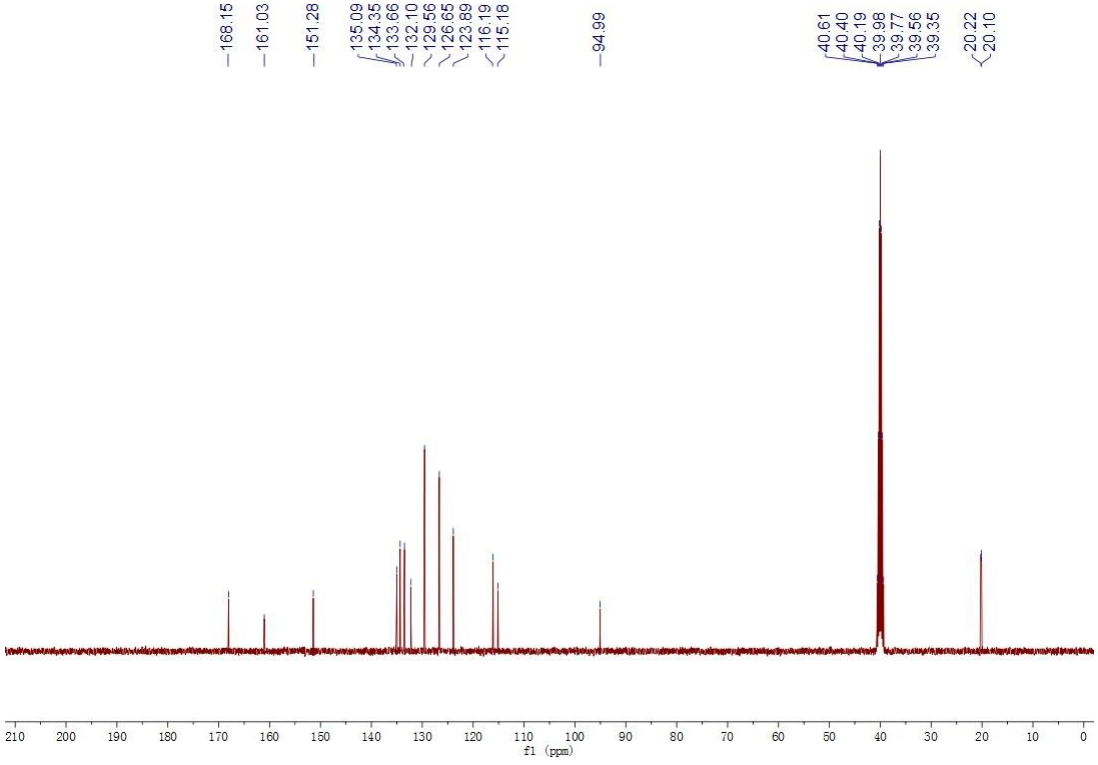
1.285
1.266
1.248


OH
S
O
O


1.00
1.05
2.04
1.93
3.29
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.47
163.04
152.95
129.41
123.81
120.97
119.04
114.36
86.58
25.72
13.51
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.742
7.531
7.526
7.510
7.505
7.322
7.302
7.089
2.512
2.400
2.236
OH
S
O
O
1.00
1.02
1.04
4.00
3.07
3.06
f1 (ppm)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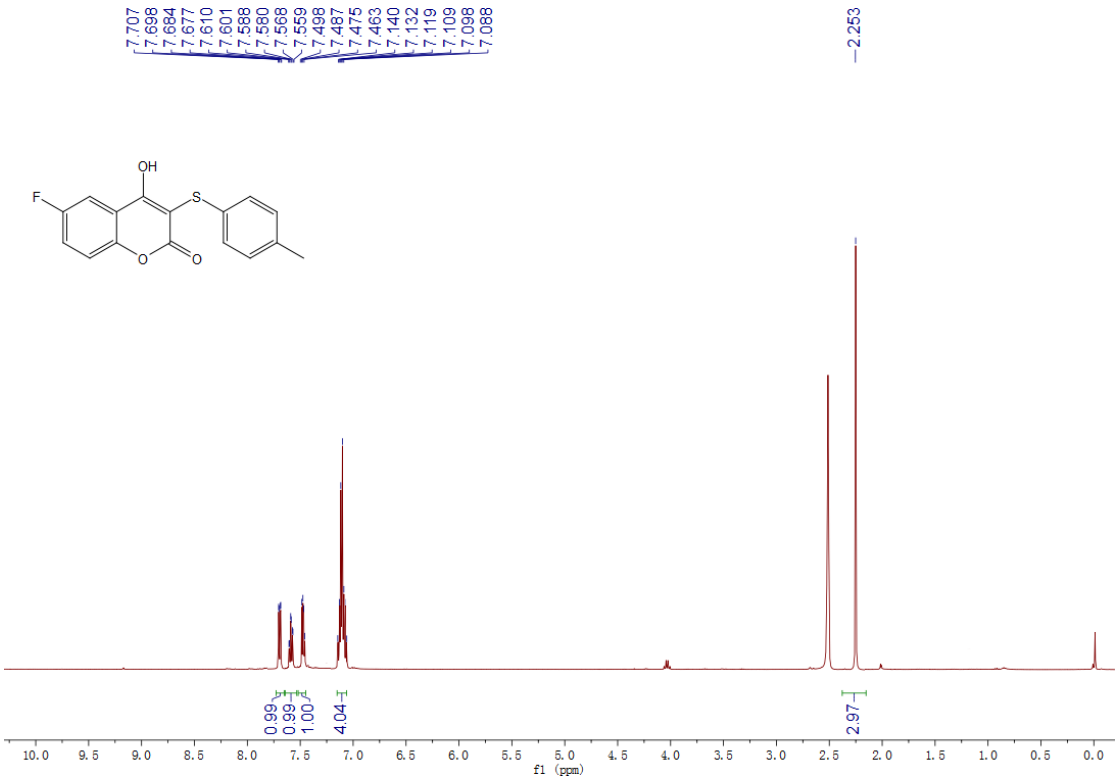
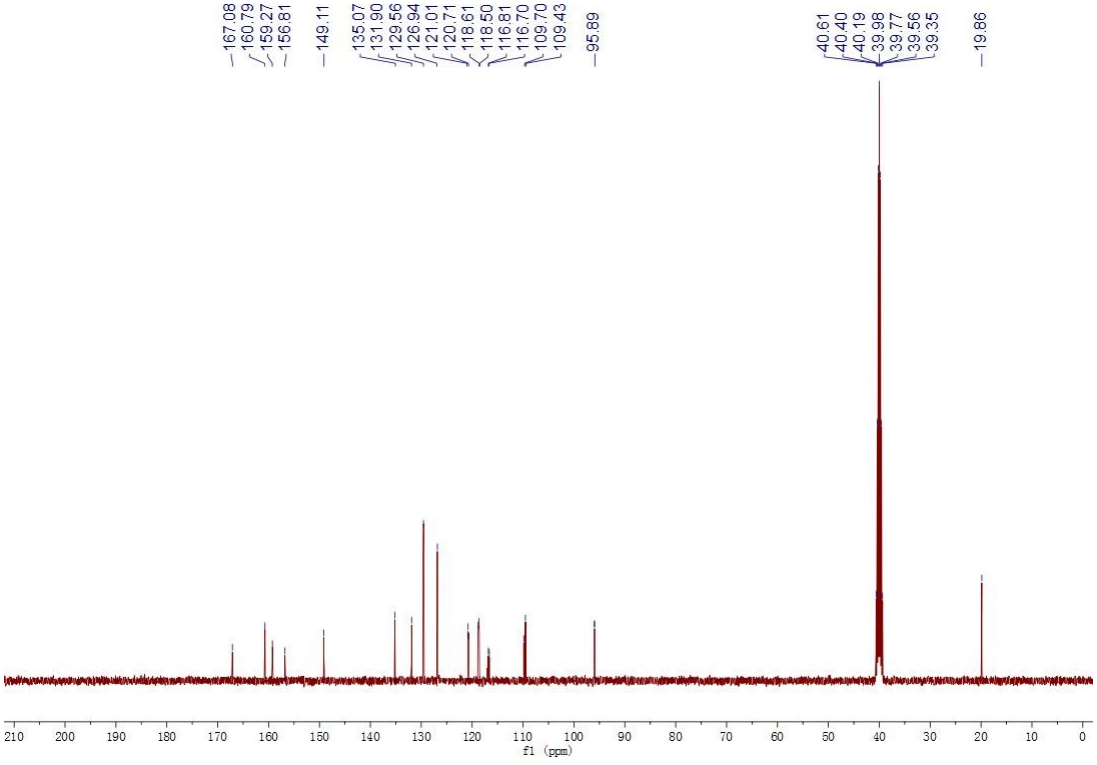
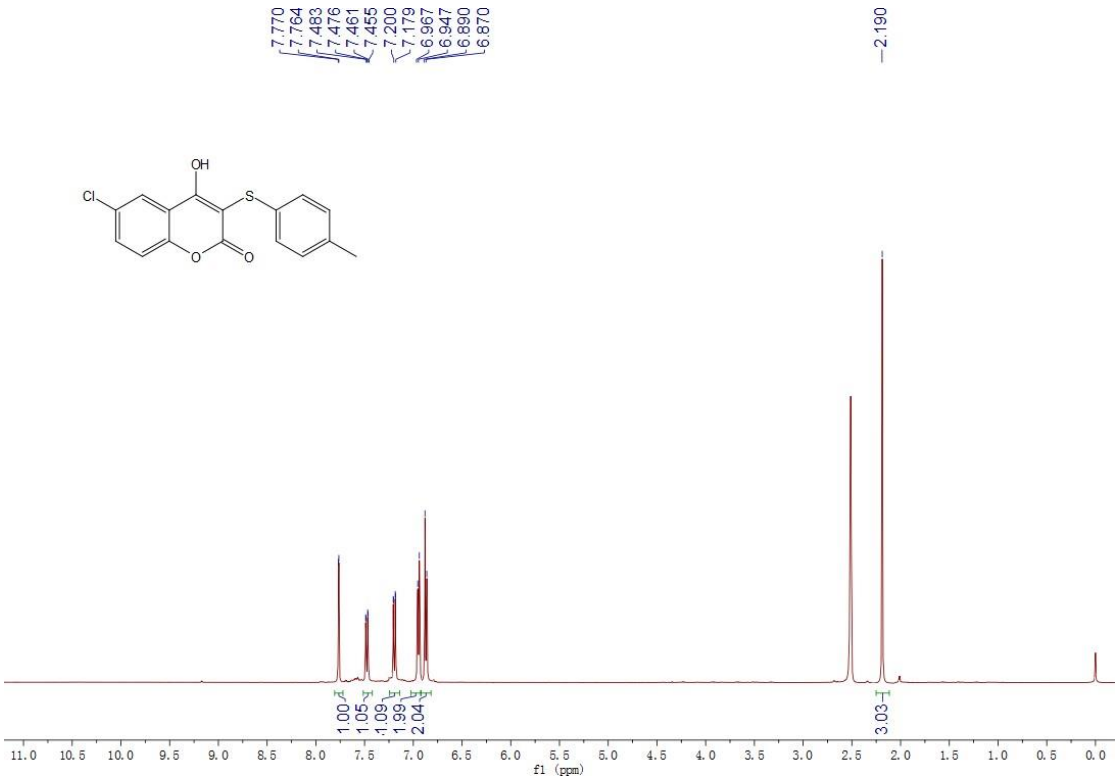
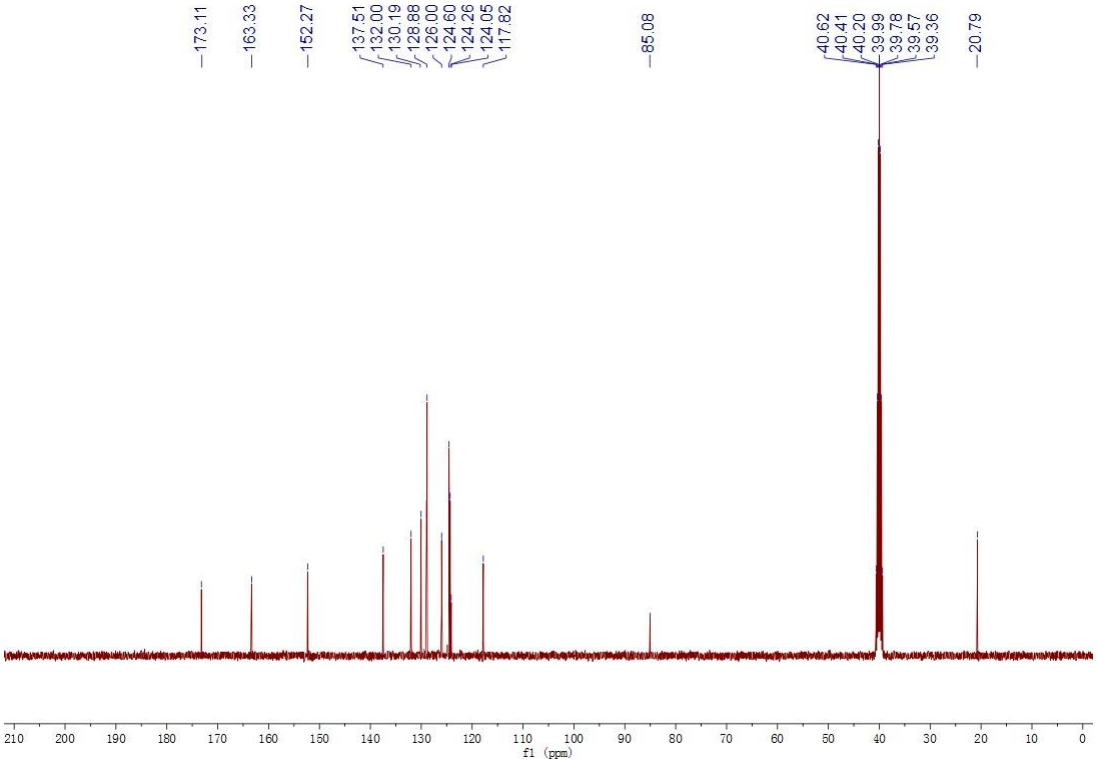
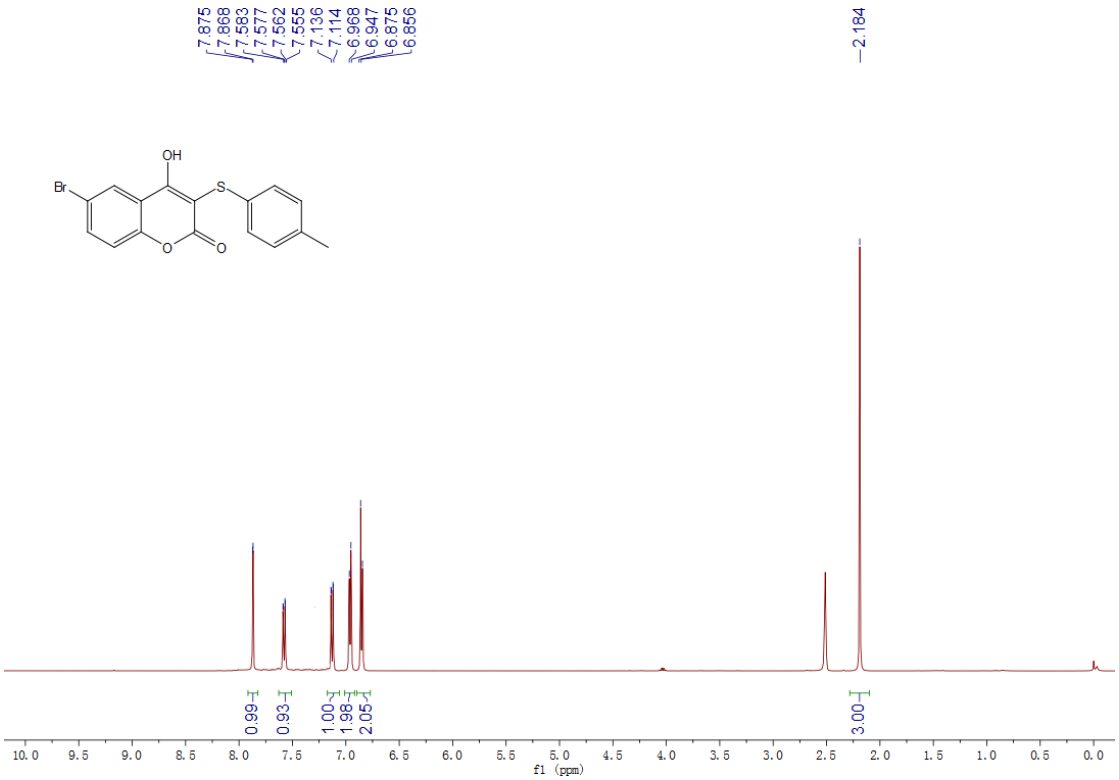
161.03
151.28
135.09
134.35
133.66
132.10
129.56
126.65
123.89
116.19
115.18
94.99
40.61
40.40
40.19
39.98
39.77
39.56
39.35
20.22
20.10
f1 (ppm)

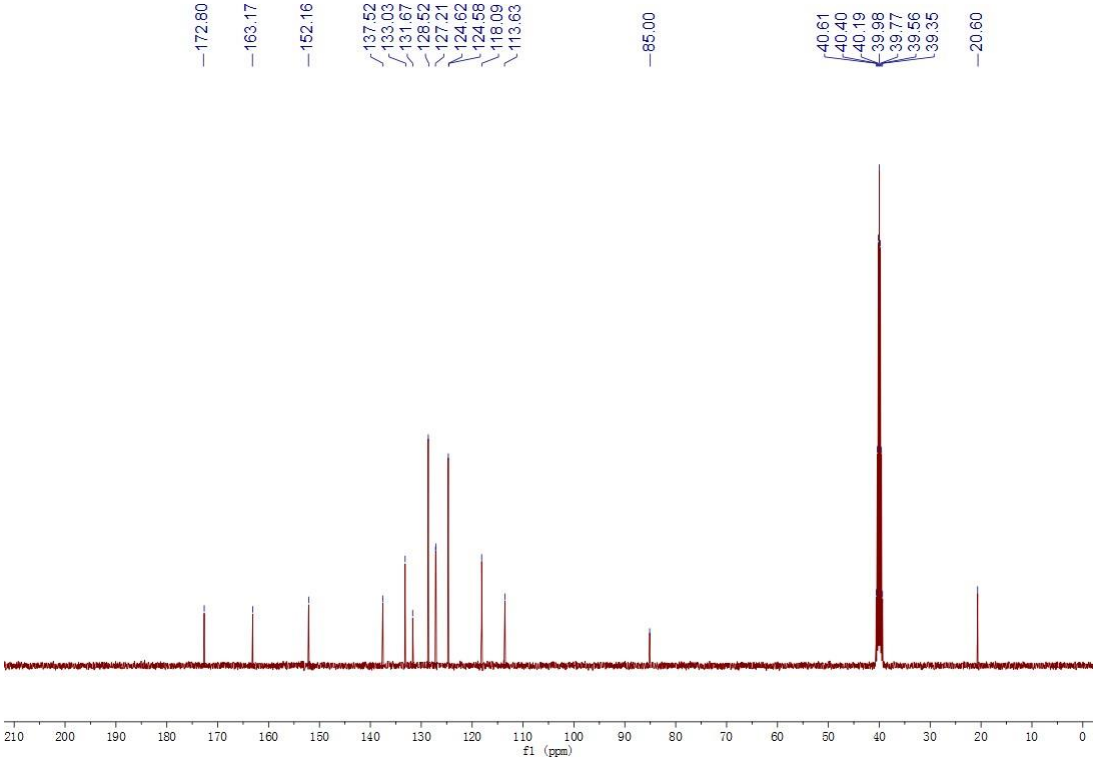

7.707
7.698
7.684
7.677
7.610
7.601
7.588
7.580
7.568
7.559
7.498
7.487
7.475
7.463
7.140
7.132
7.119
7.109
7.098
7.088
2.253
OH
F
S
O
O
0.99
0.99
1.00
4.04
2.97
f1 (ppm)

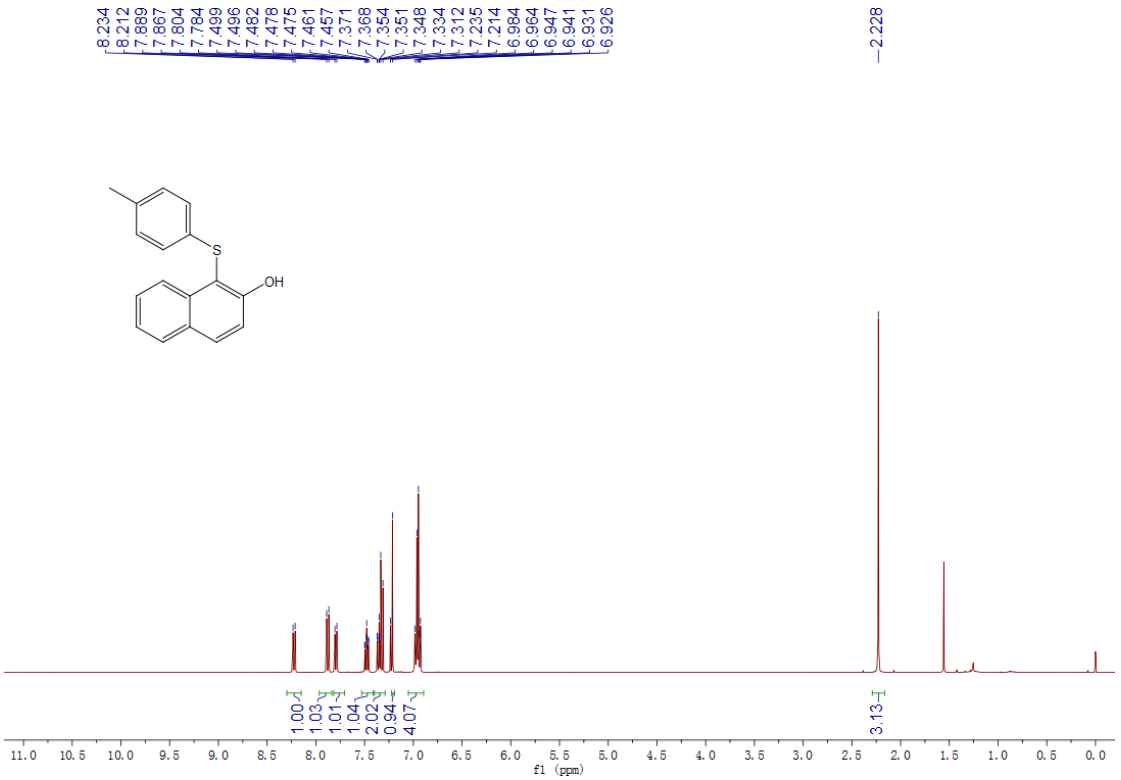

167.08
160.79
159.27
156.81
149.11
135.07
131.90
129.56
126.94
121.01
120.71
118.61
118.50
116.81
116.70
109.70
109.43
95.89
40.61
40.40
40.19
39.98
39.77
39.56
39.35
19.86
f1 (ppm)

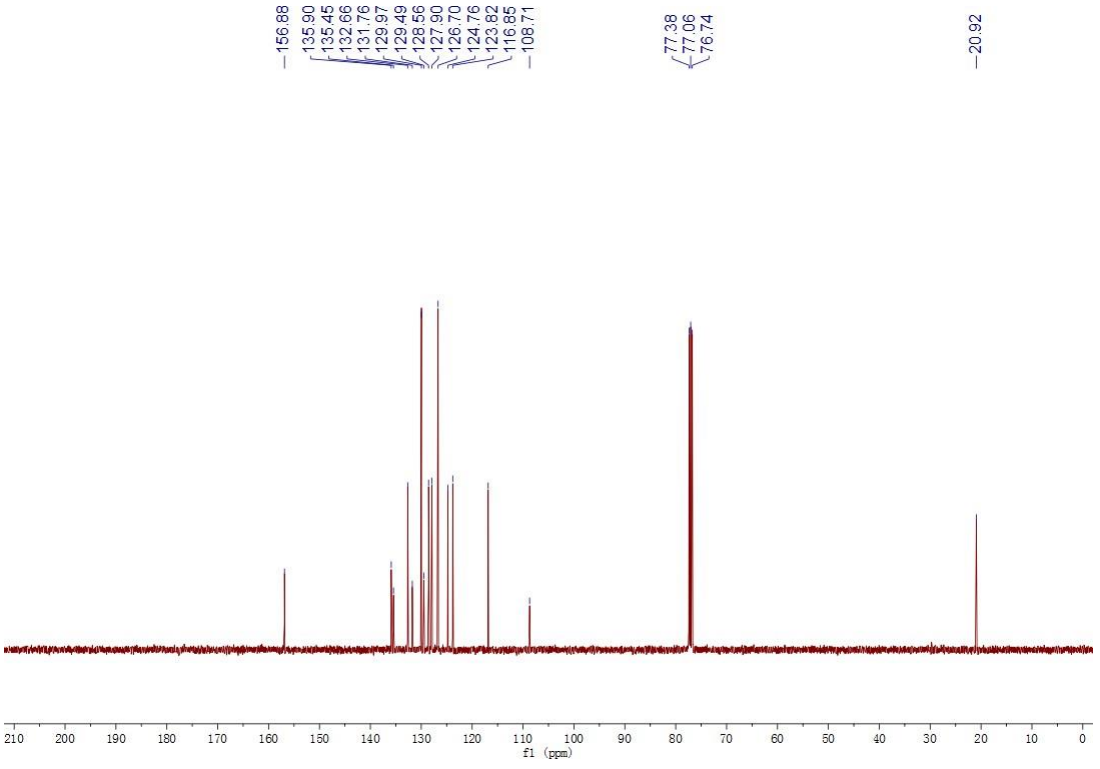

7.770
7.764
7.483
7.476
7.461
7.455
7.200
7.179
6.967
6.947
6.890
6.870
2.190
OH
Cl
S
O
O
1.00
1.05
1.09
1.99
2.04
3.03
f1 (ppm)

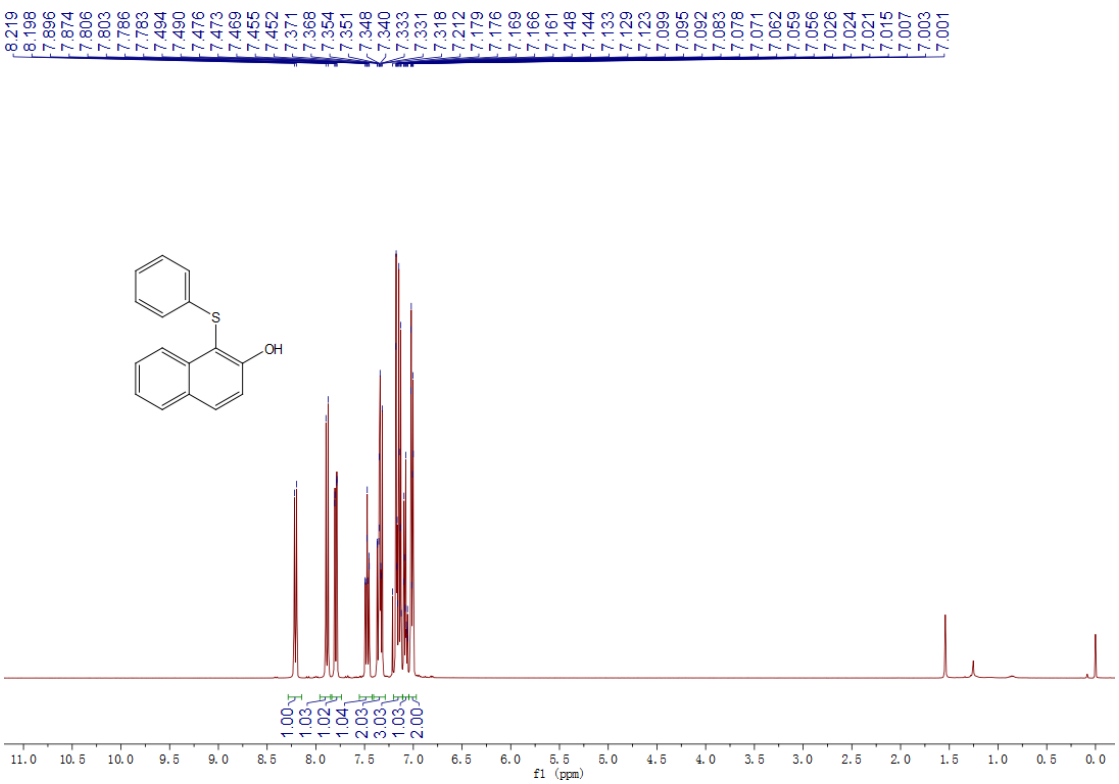

173.11
163.33
152.27
137.51
132.00
130.19
128.88
126.00
124.60
124.26
124.05
117.82
85.08
40.62
40.41
40.20
39.99
39.78
39.57
39.36
20.79
f1 (ppm)

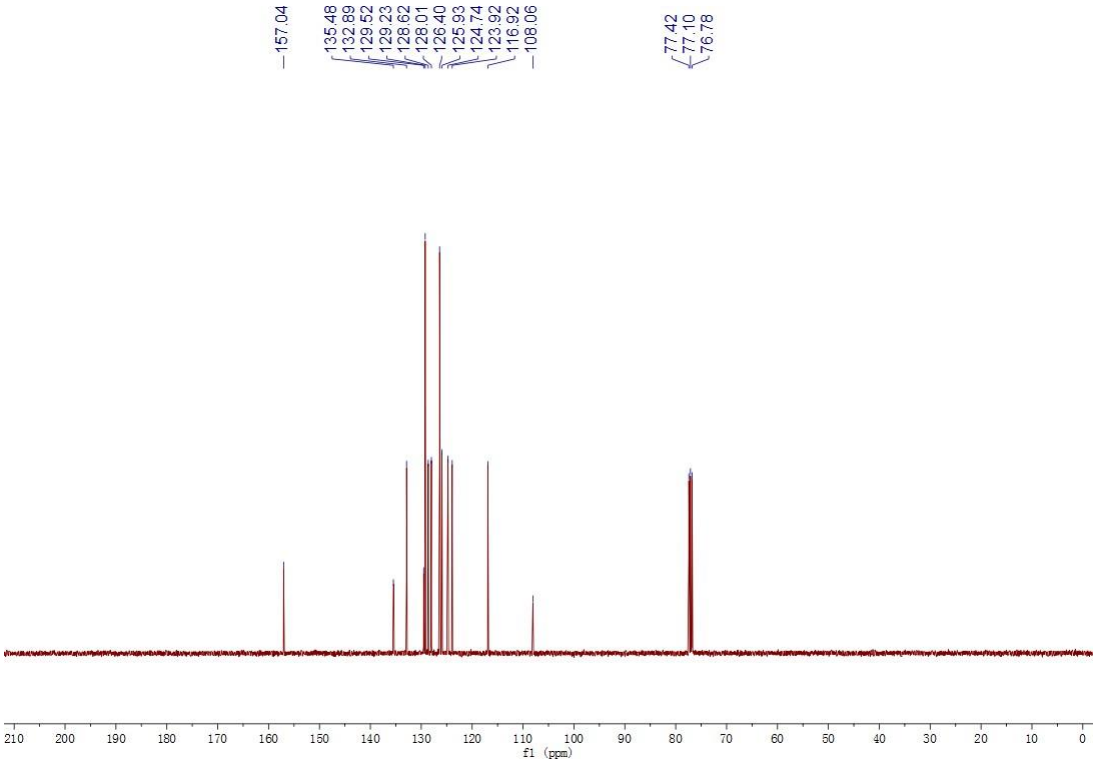

7.875
7.868
7.583
7.577
7.562
7.555
7.136
7.114
6.968
6.947
6.875
6.856
2.184
OH
Br
S
O
O
0.99
0.93
1.00
1.98
2.05
3.00
f1 (ppm)


172.80
163.17
152.16
137.52
133.03
131.67
128.52
127.21
124.62
124.58
118.09
113.63
85.00
40.61
40.40
40.19
39.98
39.77
39.56
39.35
20.60
f1 (ppm)


8.234
8.212
7.889
7.867
7.804
7.784
7.499
7.496
7.482
7.478
7.475
7.461
7.457
7.371
7.368
7.354
7.351
7.348
7.334
7.312
7.235
7.214
6.984
6.964
6.947
6.941
6.931
6.926
2.228
S
OH
1.00
1.03
1.01
1.04
2.02
0.94
4.07
3.13
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


156.88
135.90
135.45
132.66
131.76
129.97
129.49
128.56
127.90
126.70
124.76
123.82
116.85
108.71
77.38
77.06
76.74
20.92
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.219
8.198
7.896
7.874
7.806
7.803
7.786
7.783
7.494
7.490
7.476
7.473
7.469
7.455
7.452
7.371
7.368
7.354
7.351
7.348
7.340
7.333
7.331
7.318
7.212
7.179
7.176
7.169
7.166
7.161
7.148
7.144
7.133
7.129
7.123
7.099
7.095
7.092
7.083
7.078
7.071
7.062
7.059
7.056
7.026
7.024
7.021
7.015
7.007
7.003
7.001
S
OH
1.00
1.03
1.02
1.04
2.03
3.03
1.03
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.04
135.48
132.89
129.52
129.23
128.62
128.01
126.40
125.93
124.74
123.92
116.92
108.06
77.42
77.10
76.78
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)