Supporting Information to

Copper-Catalyzed Decarboxylative Methylthiolation of Aromatic Carboxylate Salts with DMSO

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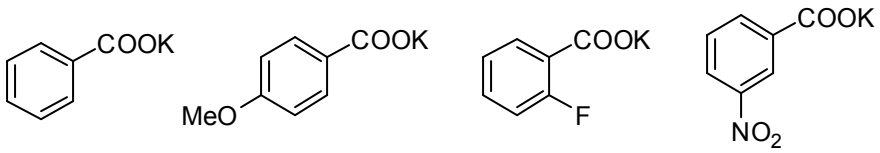
General information

^{1}H NMR, ^{13}C NMR and ^{19}F NMR were recorded in $CDCl_3$ at room temperature on the Varian INOVA-400 spectrometer (400 MHz, ^{1}H). The ^{1}H NMR chemical-shifts scale is based on internal TMS. The peak patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; qui, quintet; sxt, sextet. The coupling constants, *J* are reported in Hertz (Hz). High-resolution mass spectral (HRMS) analyses were carried out using a TOF MS instrument with an ESI source. Melting points were measured by a melting point instrument and were uncorrected.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. Anhydrous CuBr was purchased from Alfa Aesar. All solvents were purified and dried according to standard methods prior to use. Products were purified by flash column chromatography on 300-400 mesh silica gel, SiO_2.

Ineffective substrates



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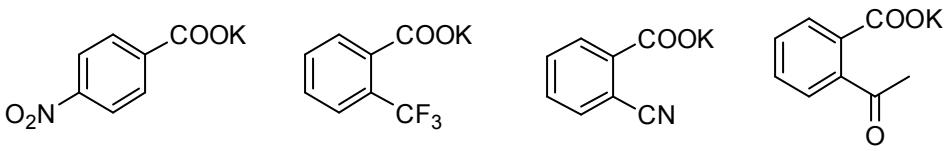

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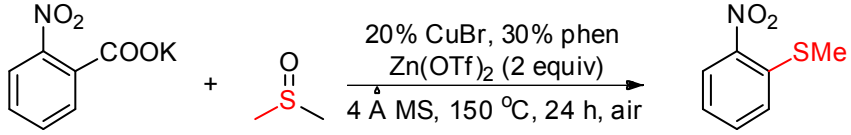
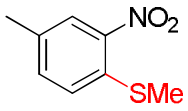
General procedure for copper-catalyzed decarboxylative methylthiolation of aromatic carboxylate salts:



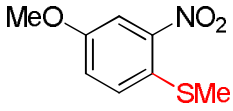
1a **2** **3a**

*Compound **3a***. To a mixture of aromatic carboxylate salt **1a** (61.5 mg, 0.3 mmol), CuBr (8.6 mg, 0.06 mmol), Phen. (17.8 mg, 0.09 mmol), $Zn(OTf)_2$ (218.0 mg, 0.6 mmol) and 4 Å MS (50 mg) was added dimethyl sulfoxide **2** (2 ml) under an air atmosphere. After stirring at 150℃ for 24 h, the reaction mixture was quenched with H_2O (20 ml), extracted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4, and concentrated. Column chromatography on silica gel (EtOAc/petroleum ether = 1:50) gave **3a** as a yellow solid (43.1 mg, 85% yield); *Methyl(2-nitrophenyl)sulfane (**3a**)*. 85% yield (43.1 mg); yellow soild, mp: 55–57 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.3 Hz, 1H), 7.59 (t, J = 7.7 Hz, 1H), 7.38 (d, J = 8.2 Hz, 1H), 7.26 (t, J = 7.7 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 139.3, 133.6, 126.1, 125.6, 124.1, 15.9; HRMS (ESI) calcd for $C_7H_7NNaO_2S$ $(M + Na)^+$ 192.0095, found 192.0087.



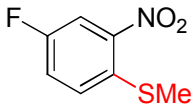
3b

Methyl(4-methyl-2-nitrophenyl)sulfane (***3b***). 81% yield (44.4 mg); yellow soild, mp: 63–65 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.40 (d, J = 8.2 Hz, 1H), 7.26 (d, J = 8.0 Hz, 1H), 2.48 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 135.7, 134.7, 134.6, 126.3, 125.6, 20.4, 16.0; HRMS (ESI) calcd for $C_8H_9NNaO_2S$ $(M + Na)^+$ 206.0252, found 206.0240.



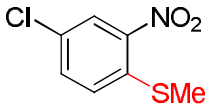
3c

(4-methoxy-2-nitrophenyl)(methyl)sulfane (***3c***). 80% yield (47.8 mg); yellow soild, mp: 71–73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 2.7 Hz, 1H), 7.30–7.27 (m, 1H), 7.20 (dd, J = 8.9, 2.7 Hz, 1H), 3.87 (s, 3H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 146.1, 130.1, 127.0, 121.9, 109.6, 55.9, 16.2; HRMS (ESI) calcd for $C_8H_9NNaO_3S$ $(M + Na)^+$ 222.0201, found 222.0185.



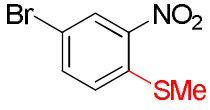
3d

(4-fluoro-2-nitrophenyl)(methyl)sulfane (***3d***). 78% yield (43.8 mg); yellow soild, mp: 66–68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.4 Hz, 1H), 7.37–7.35 (m, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0 (d, J = 246.6 Hz), 134.7 (d, J = 3.3 Hz), 127.2 (d, J = 7.3 Hz), 121.6 (d, J = 21.8 Hz), 113.4, 113.1, 16.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116. 8; HRMS (ESI) calcd for $C_7H_6FNNaO_2S$ $(M + Na)^+$ 210.0001, found 210.0007.



3e

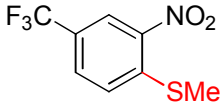
(4-chloro-2-nitrophenyl)(methyl)sulfane (***3e***). 71% yield (43.2 mg); yellow soild, mp: 82–84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.56 (d, J = 8.7 Hz, 1H), 7.31 (d, J = 8.7 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 138.0, 133.7, 130.0, 126.8, 126.0, 16.0; HRMS (ESI) calcd for $C_7H_6ClNNaO_2S$ $(M + Na)^+$ 225.9705, found 225.9697.



3f

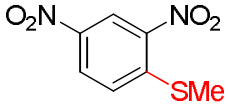
(4-chloro-2-nitrophenyl)(methyl)sulfane (***3f***). 67% yield (49.6 mg); yellow soild, mp: 95–97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.68 (d, J = 8.7 Hz, 1H), 7.27–7.23 (m, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.7, 138.6, 136.5,

128.8, 127.0, 117.0, 16.0; HRMS (ESI) calcd for $C_7H_6BrNNaO_2S$ $(M + Na)^+$ 269.9200, found 269.9189.



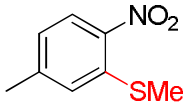
3g

Methyl(2-nitro-4-(trifluoromethyl)phenyl)sulfane ***(3g)***. 73% yield (51.9 mg); yellow soild, mp: 88–90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.81 (d, J = 8.5 Hz, 1H), 7.51 (d, J = 8.5 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 144.3, 129.7 (q, J = 3.3 Hz), 126.7 (q, J = 18.1 Hz), 126.3, 123.5 (q, J = 4.0 Hz), 123.0 (q, J = 270.4 Hz), 16.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.6; HRMS (ESI) calcd for $C_8H_6F_3NNaO_2S$ $(M + Na)^+$ 259.9969, found 259.9973.



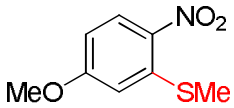
3h

(2,4-dinitrophenyl)(methyl)sulfane ***(3h)***. 41% yield (26.3 mg); yellow soild, mp: 112–114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.41 (d, J = 9.0 Hz, 1H), 7.56 (d, J = 9.0 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 144.5, 143.7, 127.2, 126.3, 121.6, 16.3; HRMS (ESI) calcd for $C_7H_6N_2NaO_4S$ $(M + Na)^+$ 236.9946, found 236.9951.



3i

Methyl(5-methyl-2-nitrophenyl)sulfane ***(3i)***. 71% yield (39.0 mg); yellow soild, mp: 70–72 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 8.4 Hz, 1H), 7.13 (s, 1H), 7.04 (d, J = 8.5 Hz, 1H), 2.49 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 143.6, 139.3, 126.3, 125.8, 125.1, 21.8, 15.9; HRMS (ESI) calcd for $C_8H_9NNaO_2S$ $(M + Na)^+$ 206.0252, found 206.0236.



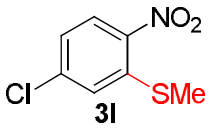
3j

(5-methoxy-2-nitrophenyl)(methyl)sulfane ***(3j)***. 67% yield (40.0 mg); yellow soild, mp: 77–79 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 9.1 Hz, 1H), 6.76 (s, 1H), 6.73 (d, J = 9.3 Hz, 1H), 3.92 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 142.3, 138.9, 128.8, 110.6, 109.1, 55.9, 16.0; HRMS (ESI) calcd for $C_8H_9NNaO_3S$ $(M + Na)^+$ 222.0201, found 222.0186.

3k

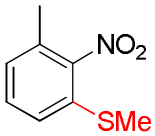
(5-fluoro-2-nitrophenyl)(methyl)sulfane ***(3k)***. 72% yield (40.4 mg); yellow soild, mp:

71–73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35–8.32 (m, 1H), 7.04 (d, J = 9.7 Hz, 1H), 6.96–6.92 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4 (d, J = 256.8 Hz), 143.4 (d, J = 9.6 Hz), 129.0 (d, J = 10.7 Hz), 124.4 (d, J = 110.0 Hz), 112.4 (d, J = 26.8 Hz), 111.5 (d, J = 23.6 Hz), 16.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.4; HRMS (ESI) calcd for $C_7H_6FNNaO_2S$ $(M + Na)^+$ 210.0001, found 210.0007.



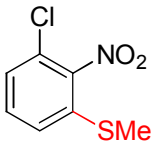
3l

*(5-chloro-2-nitrophenyl)(methyl)sulfane (**3l**)*. 75% yield (45.5 mg); yellow soild, mp: 87–89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 8.8 Hz, 1H), 7.31 (s, 1H), 7.21 (d, J = 8.8 Hz, 1H), 2.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 141.6, 140.7, 127.4, 125.3, 124.3, 16.1; HRMS (ESI) calcd for $C_7H_6ClNNaO_2S$ $(M + Na)^+$ 225.9705, found 225.9705.



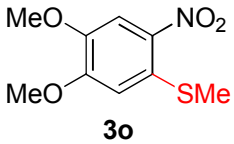
3m

*Methyl(3-methyl-2-nitrophenyl)sulfane (**3m**)*. 61% yield (33.5 mg); yellow soild, mp: 73–75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (t, J = 7.7 Hz, 1H), 7.27 (d, J = 6.6 Hz, 1H), 7.11 (d, J = 7.4 Hz, 1H), 2.48 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 131.8, 131.0, 130.4, 128.6, 126.7, 17.9, 17.3; HRMS (ESI) calcd for $C_8H_9NNaO_2S$ $(M + Na)^+$ 206.0252, found 206.0240.



3n

*(3-chloro-2-nitrophenyl)(methyl)sulfane (**3n**)*. 54% yield (32.9 mg); yellow soild, mp: 87–89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.37 (m, 1H), 7.34–7.30 (m, 2H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 133.6, 130.9, 127.5, 127.3, 125.8, 17.1; HRMS (ESI) calcd for $C_7H_6ClNNaO_2S$ $(M + Na)^+$ 225.9705, found 225.9687.

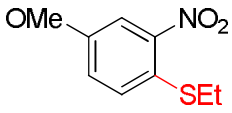


3o

*(4,5-dimethoxy-2-nitrophenyl)(methyl)sulfane (**3o**)*. 83% yield (57.0 mg); yellow soild, mp: 123–125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (s, 1H), 6.73 (s, 1H), 4.01 (s, 3H), 3.94 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 145.9, 138.0, 134.1, 108.7, 106.6, 56.4, 56.3, 16.2; HRMS (ESI) calcd for $C_9H_{11}NNaO_4S$ $(M + Na)^+$ 252.0306, found 252.0290.

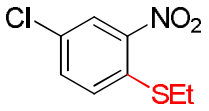
3p

Ethyl(2-nitrophenyl)sulfane (***3p***). 67% yield (36.8 mg); yellow soild, mp: 89–91 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.3 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.42 (d, J = 8.1 Hz, 1H), 7.24 (t, J = 7.7 Hz, 1H), 3.00 (q, J = 7.3 Hz, 2H), 1.41 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 138.0, 133.4, 126.4, 126.1, 124.3, 26.3, 12.8; HRMS (ESI) calcd for $C_8H_9NNaO_2S$ $(M + Na)^+$ 206.0252, found 206.0239.



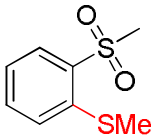
3q

Ethyl(4-methoxy-2-nitrophenyl)sulfane (***3q***). 65% yield (41.5 mg); yellow soild, mp: 105–107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 2.0 Hz, 1H), 7.34 (d, J = 8.9 Hz, 1H), 7.15 (dd, J = 8.9, 2.2 Hz, 1H), 3.86 (s, 3H), 2.96 (q, J = 7.3 Hz, 2H), 1.36 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 147.1, 128.5, 128.0, 121.3, 109.5, 55.8, 26.8, 13.1; HRMS (ESI) calcd for $C_9H_{11}NNaO_3S$ $(M + Na)^+$ 236.0357, found 236.0339.



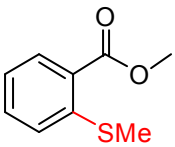
3r

(4-chloro-2-nitrophenyl)(ethyl)sulfane (***3r***). 60% yield (39.1 mg); yellow soild, mp: 101–103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.52 (d, J = 8.7 Hz, 1H), 7.35 (d, J = 8.7 Hz, 1H), 2.99 (q, J = 7.3 Hz, 2H), 1.41 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.0, 136.7, 133.5, 130.1, 127.6, 125.9, 26.4, 12.7; HRMS (ESI) calcd for $C_8H_8ClNaO_2S$ $(M + Na)^+$ 239.9862, found 239.9851.



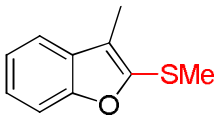
3t

Methyl(2-(methylsulfonyl)phenyl)sulfane (***3t***). 45% yield (27.3 mg); yellow soild, mp: 70–72 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.8 Hz, 1H), 7.69–7.65 (m, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.33–7.29 (m, 1H), 3.24 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 137.0, 133.7, 129.9, 126.5, 124.8, 41.5, 16.0; HRMS (ESI) calcd for $C_8H_{10}NaO_2S_2$ $(M + Na)^+$ 225.0020, found 225.0011.



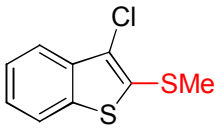
3u

methyl 2-(methylthio)benzoate (3u). 67% yield (36.6 mg); colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.8 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 7.29–7.26 (m, 1H), 7.15 (t, J = 7.5 Hz, 1H), 3.92 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 143.3, 132.5, 131.3, 126.8, 124.3, 123.4, 52.0, 15.6; HRMS (ESI) calcd for $C_9H_{10}NaO_2S$ $(M + Na)^+$ 205.0299, found 205.0291.



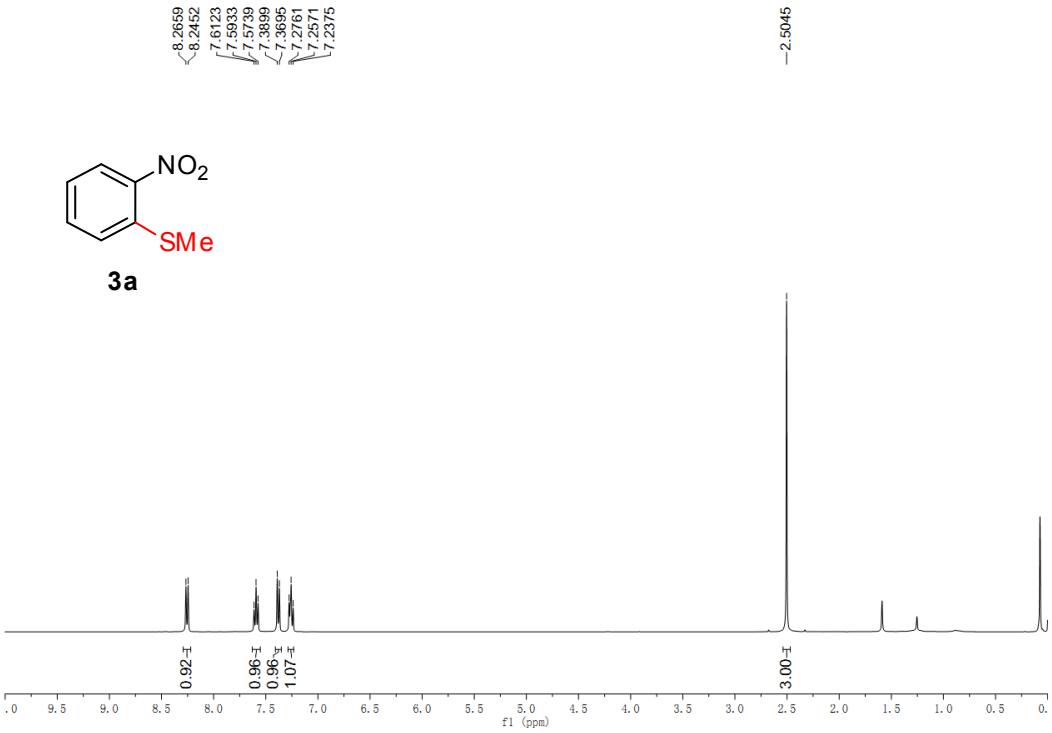
3v

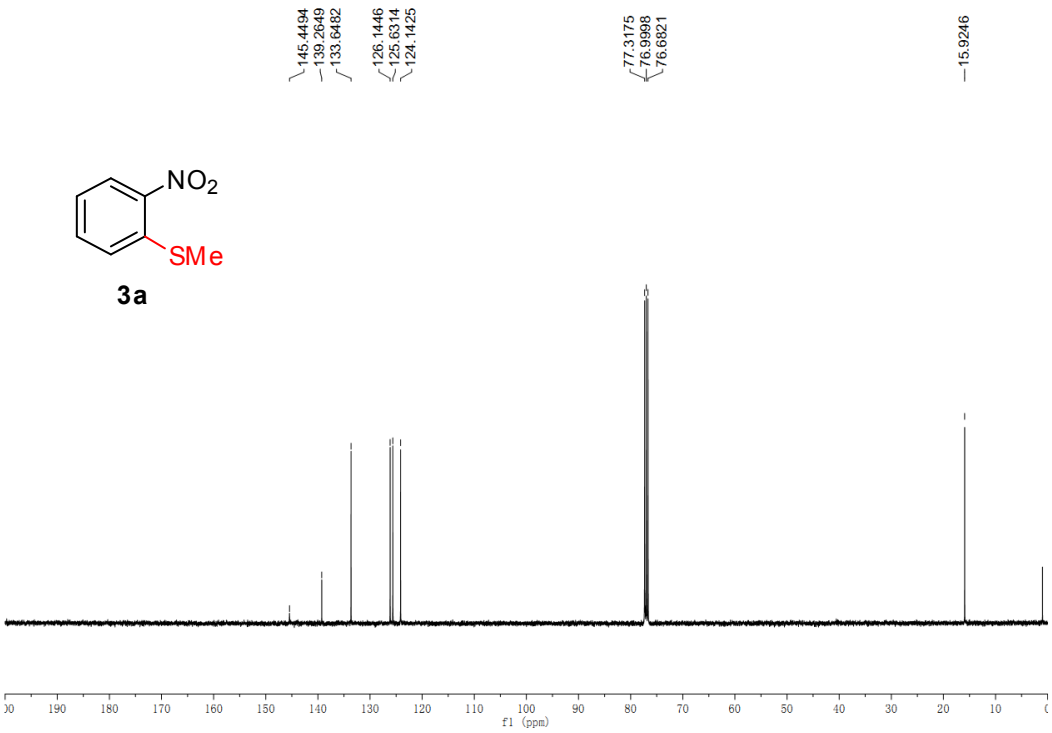
*3-methyl-2-(methylthio)benzofuran (**3v**)*. 54% yield (28.8 mg); colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.40 (m, 2H), 7.30–7.20 (m, 2H), 2.46 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 146.9, 129.6, 124.6, 122.4, 119.3, 119.2, 110.8, 17.9, 9.0; HRMS (ESI) calcd for $C_{10}H_{10}NaOS$ $(M + Na)^+$ 201.0350, found 201.0339.

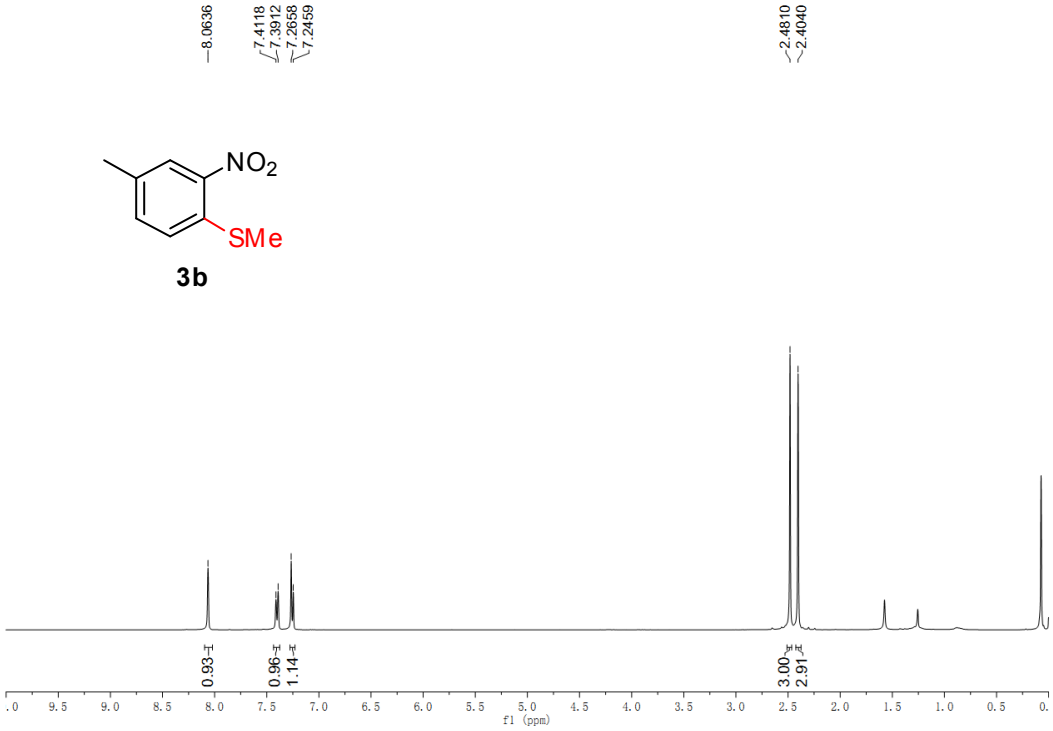


3w

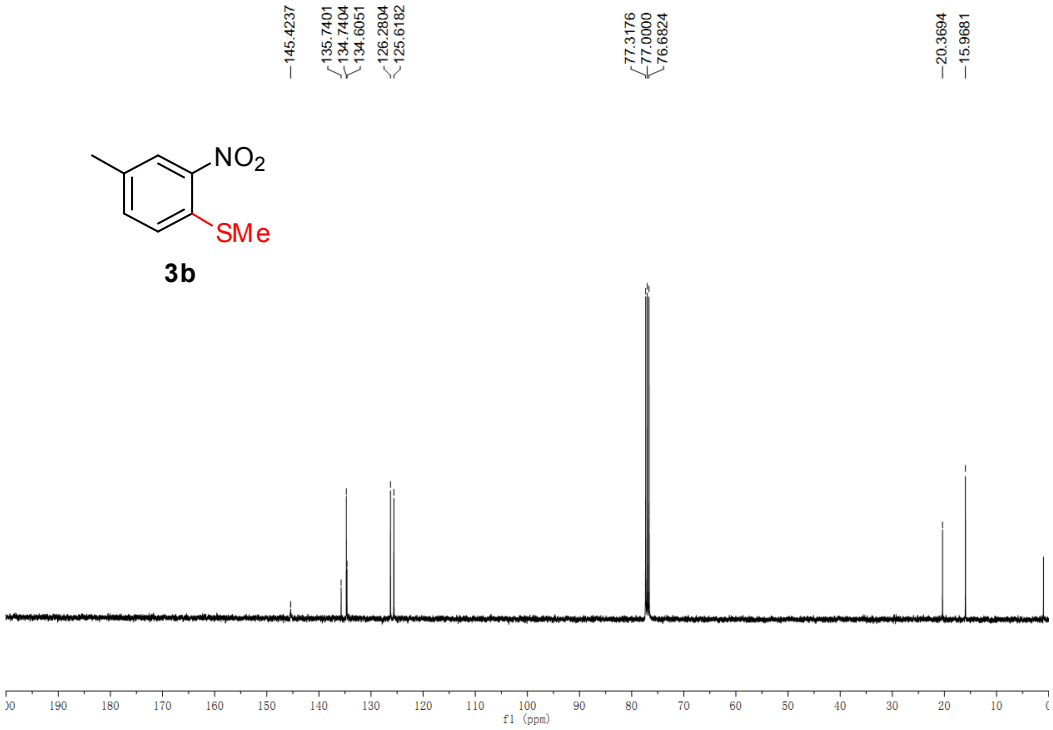
*3-chloro-2-(methylthio)benzothiophene (**3w**)*. 51% yield (32.7 mg); colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74–7.70 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.35 (t, J = 7.5 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 136.9, 132.7, 125.2, 125.1, 122.0, 121.9, 121.5, 19.0; HRMS (ESI) calcd for $C_9H_7NaClS_2$ $(M + Na)^+$ 236.9575, found 236.9582.


8.2659
8.2452
7.6123
7.5933
7.5739
7.3899
7.3695
7.2761
7.2571
7.2375
2.5045
NO2
SMe
3a
0.92
0.96
0.96
1.07
3.00
f1 (ppm)

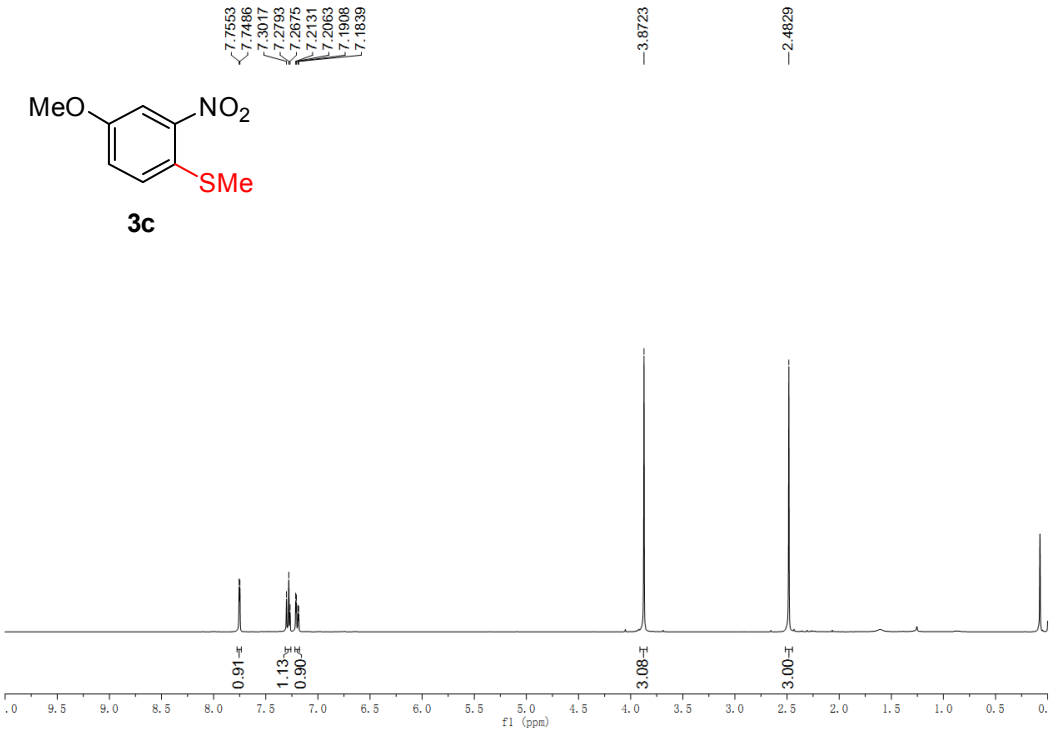

145.4494
139.2649
133.6482
126.1446
125.6314
124.1425
77.3175
76.9998
76.6821
15.9246
NO2
SMe
3a
f1 (ppm)


8.0636
7.4118
7.3912
7.2658
7.2459
2.4810
2.4040
NO2
SMe
0.93
0.96
1.14
3.00
2.91
f1 (ppm)

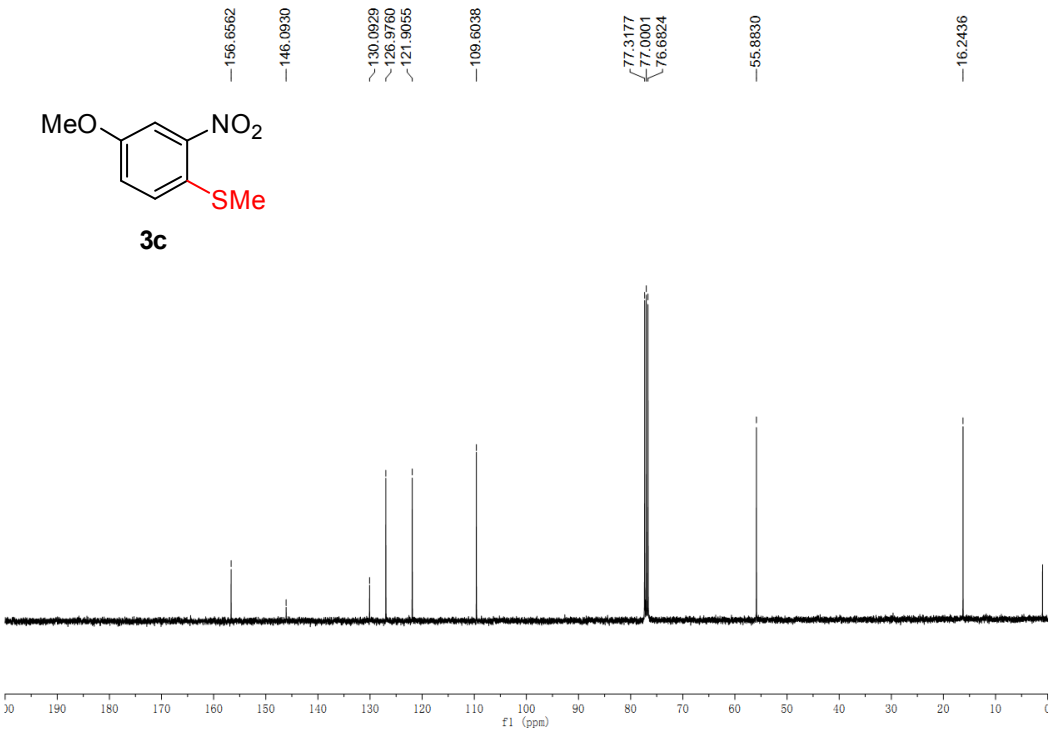
3b


145.4237
135.7401
134.7404
134.6051
126.2804
125.6182
77.3176
77.0000
76.6824
20.3694
15.9681
NO2
SMe
f1 (ppm)

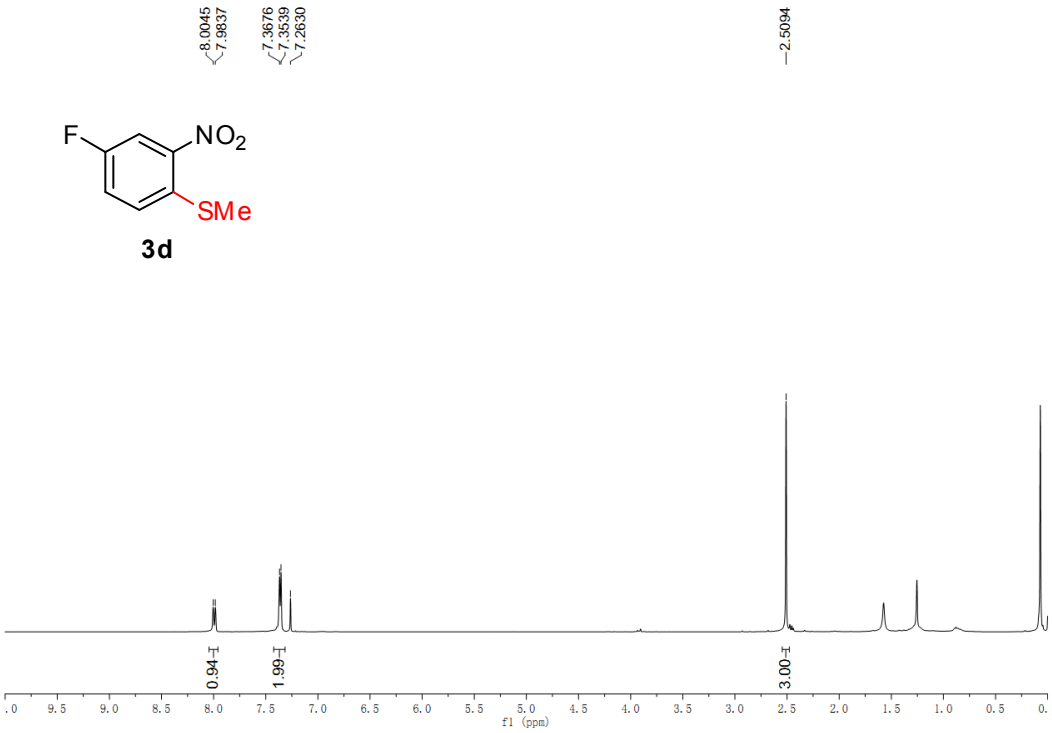
3b

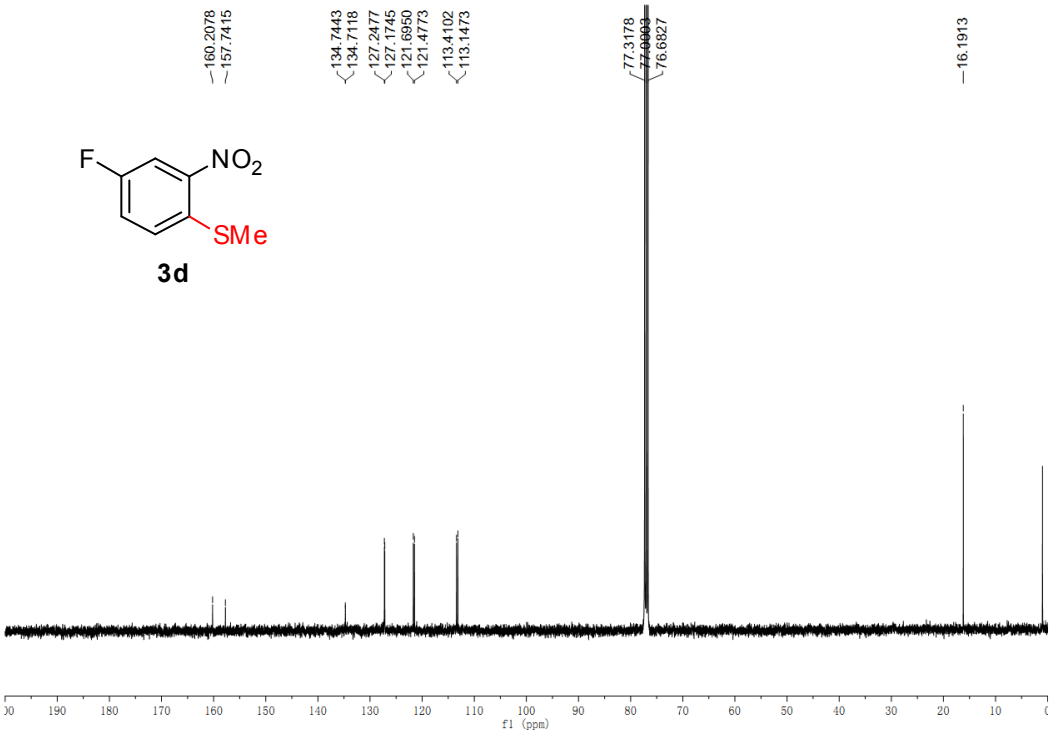

7.7553
7.7486
7.3017
7.2793
7.2675
7.2131
7.2063
7.1908
7.1839
3.8723
2.4829
MeO
NO2
SMe
0.91
1.13
0.90
3.08
3.00
f1 (ppm)

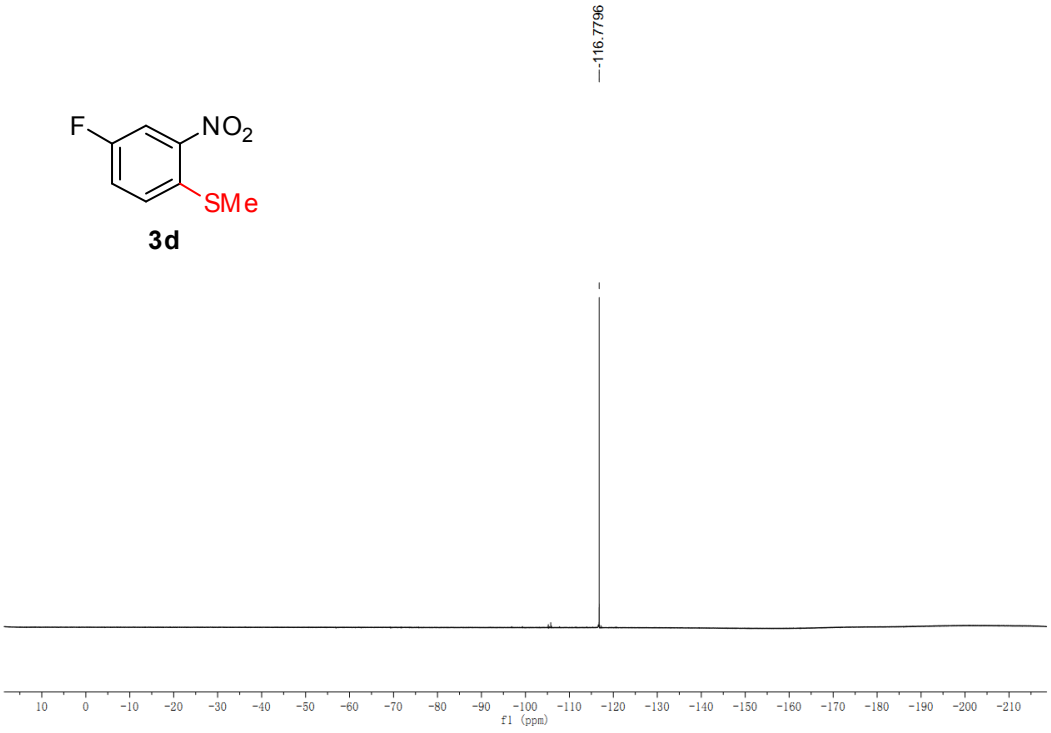
3c


156.6562
146.0930
130.0929
126.9760
121.9055
109.6038
77.3177
77.0001
76.6824
55.8830
16.2436
MeO
NO2
SMe
f1 (ppm)

3c


8.0045
7.9837
7.3676
7.3539
7.2630
2.5094
F
NO2
SMe
3d
0.94
1.99
3.00
f1 (ppm)


160.2078
157.7415
134.7443
134.7118
127.2477
127.1745
121.6950
121.4773
113.4102
113.1473
77.3178
77.0003
76.6827
16.1913
F
NO2
SMe
3d
f1 (ppm)


F
NO2
SMe
3d
-116.7796
10
0
-10
-20
-30
-40
-50
-60
-70
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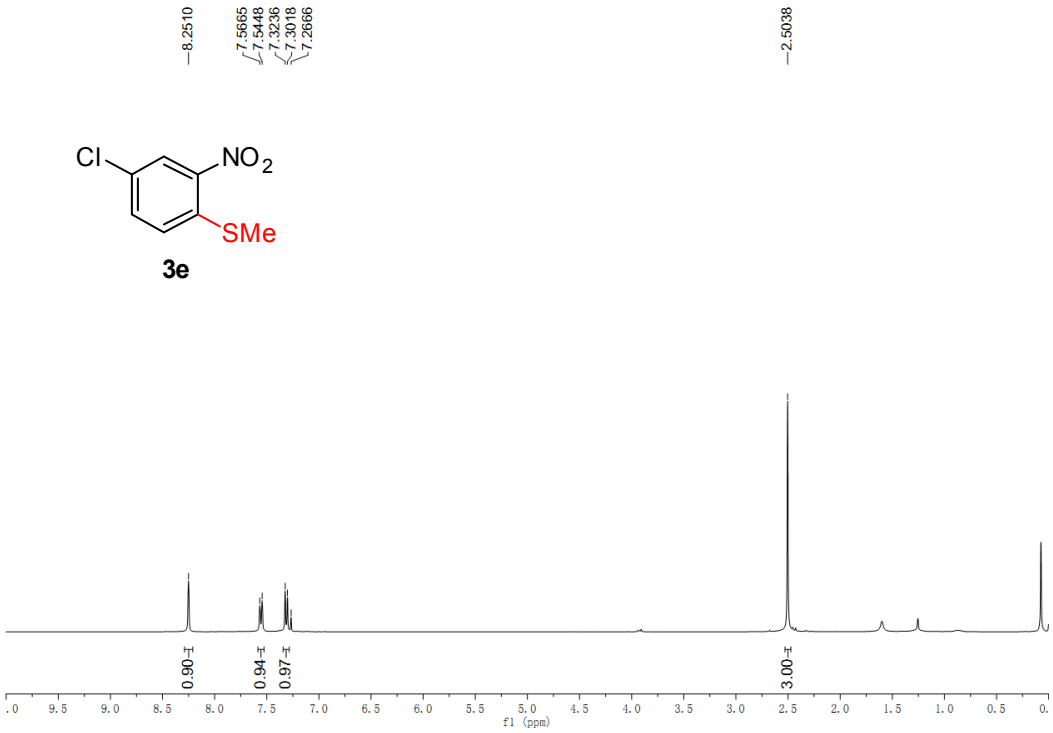
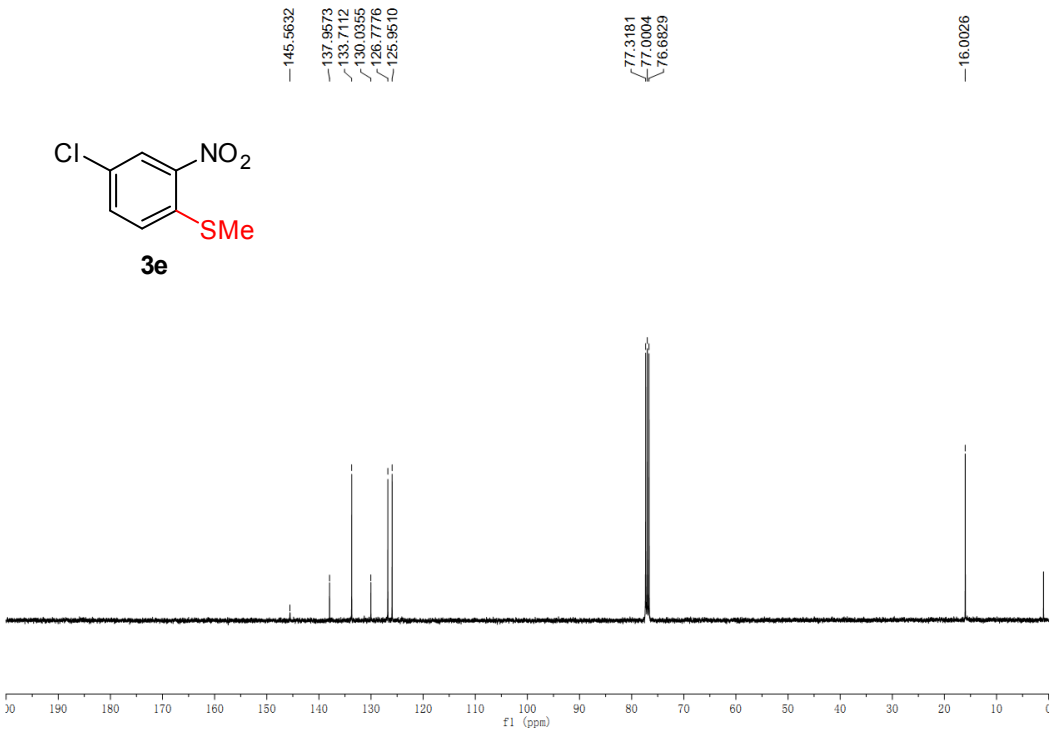
-170
-180
-190
-200
-210
f1 (ppm)


8.2510
7.5665
7.5448
7.3236
7.3018
7.2666
2.5038
Cl
NO2
SMe
0.90
0.94
0.97
3.00
f1 (ppm)

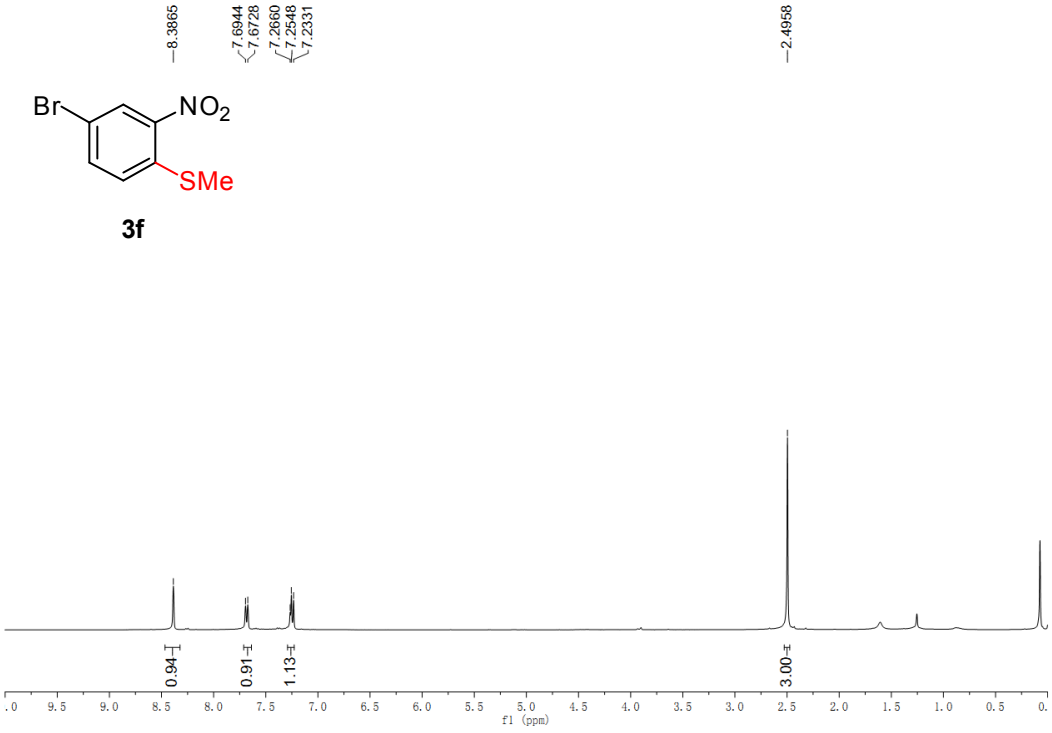
3e


145.5632
137.9573
133.7112
130.0355
126.7776
125.9510
77.3181
77.0004
76.6829
16.0026
Cl
NO2
SMe
f1 (ppm)

3e

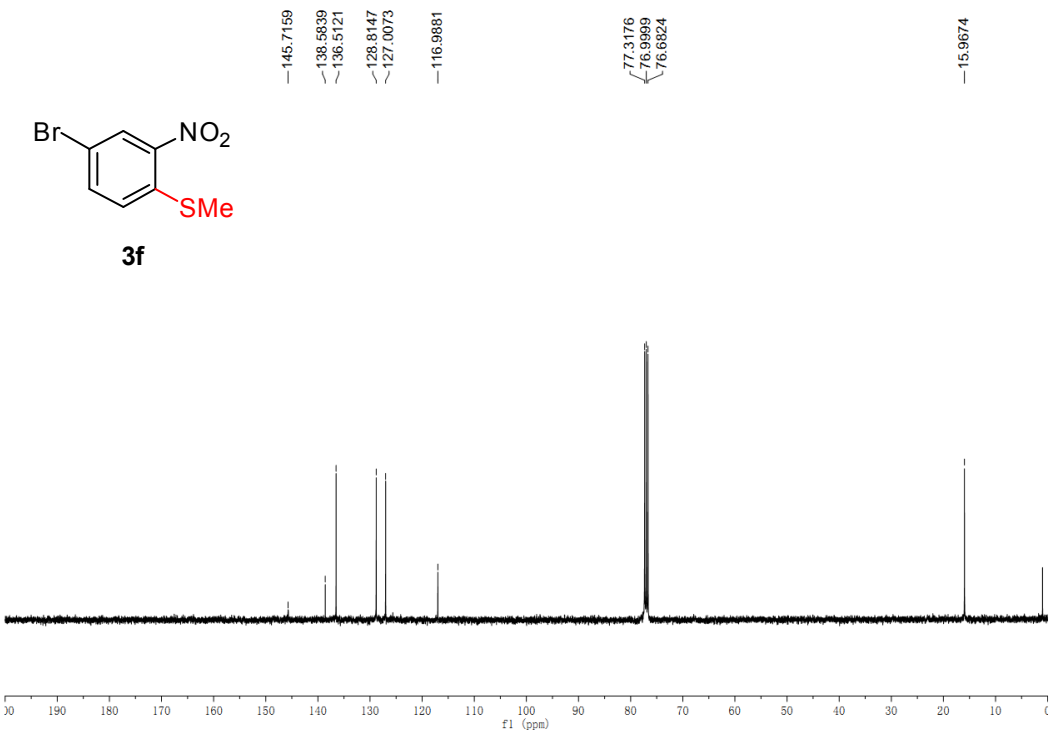
Br
NO2
SMe

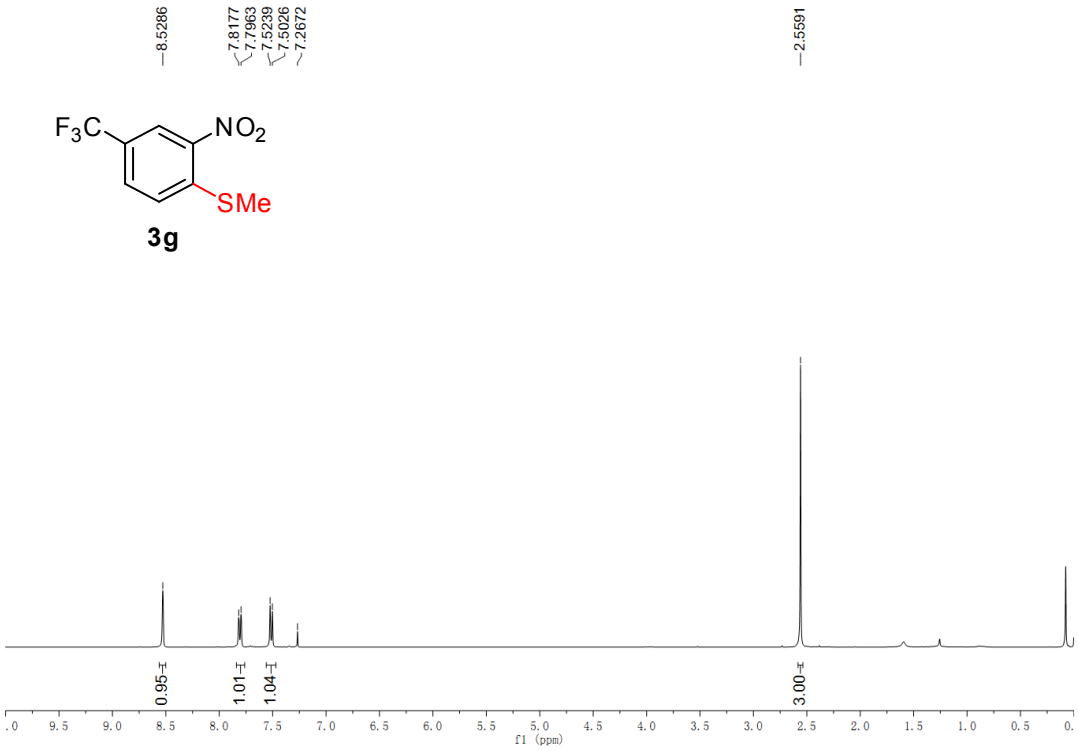
3f

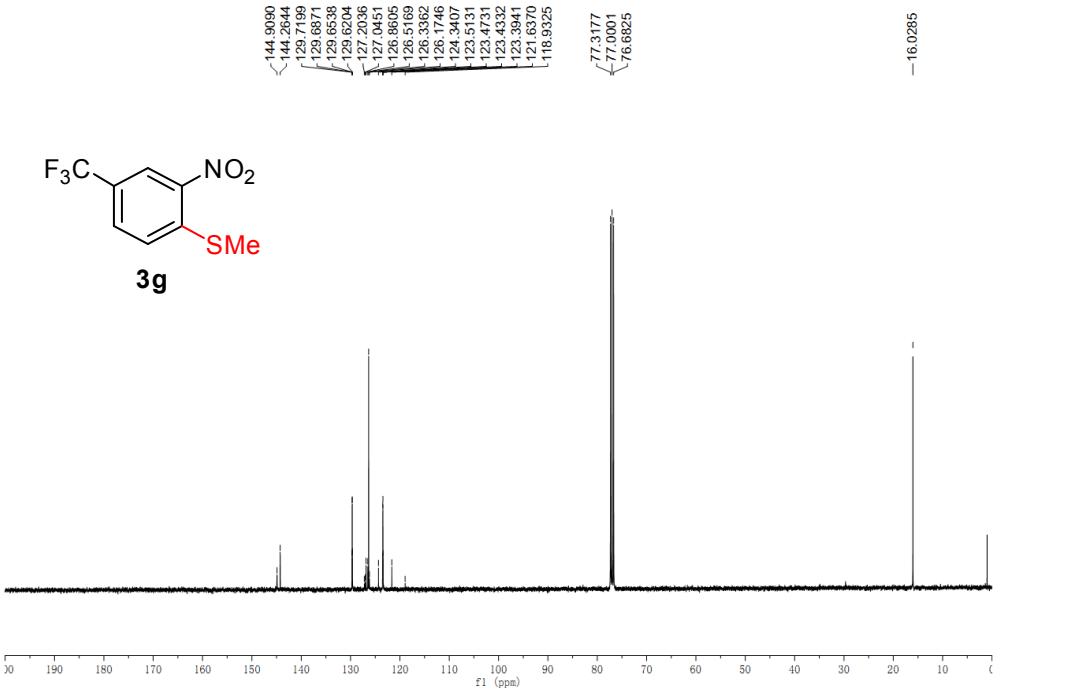

8.3865
7.6944
7.6728
7.2660
7.2548
7.2331
2.4958
0.94
0.91
1.13
3.00
f1 (ppm)

Br
NO2
SMe

3f


145.7159
138.5839
136.5121
128.8147
127.0073
116.9881
77.3176
76.9999
76.6824
15.9674
f1 (ppm)


8.5286
7.8177
7.7963
7.5239
7.5026
7.2672
2.5591
F3C
NO2
SMe
3g
0.95
1.01
1.04
3.00
f1 (ppm)


144.9090
144.2644
129.7199
129.6871
129.6538
129.6204
127.2036
127.0451
126.8605
126.5169
126.3362
126.1746
124.3407
123.5131
123.4731
123.4332
123.3941
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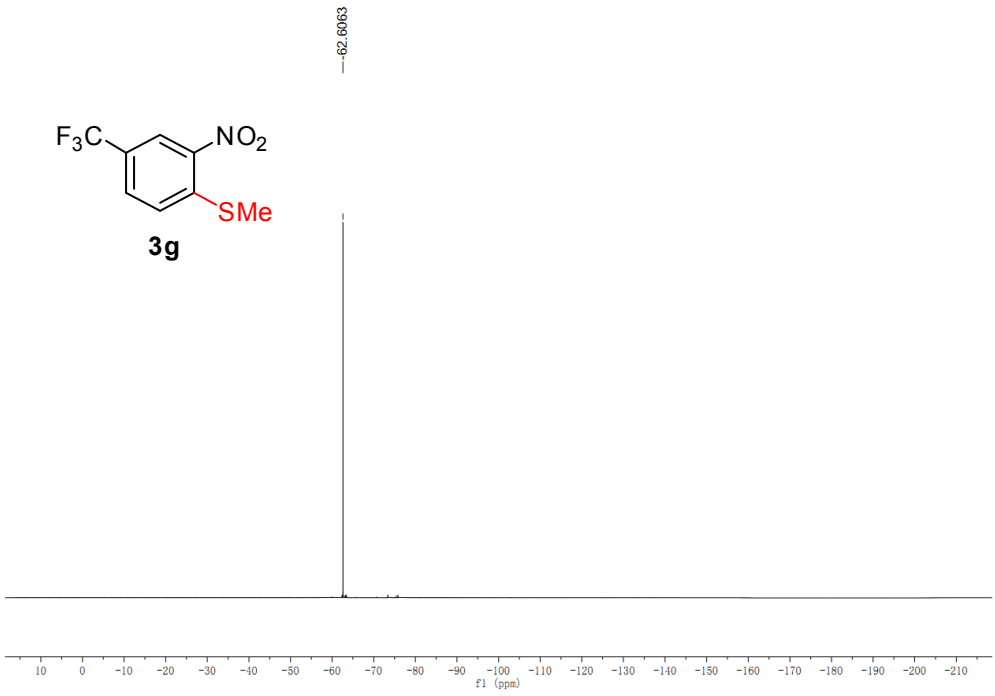
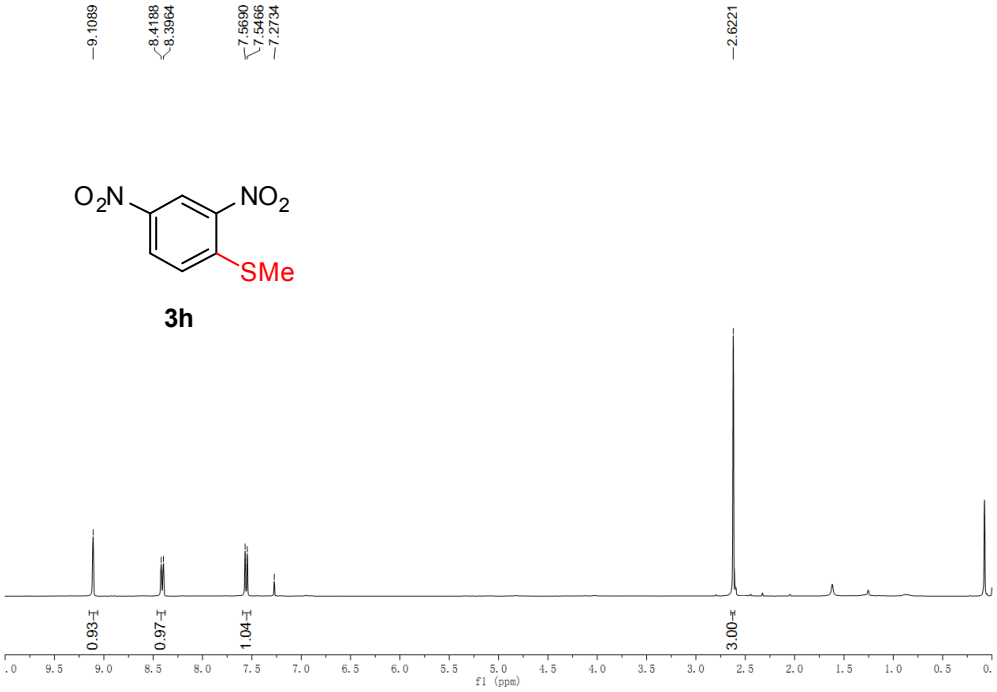
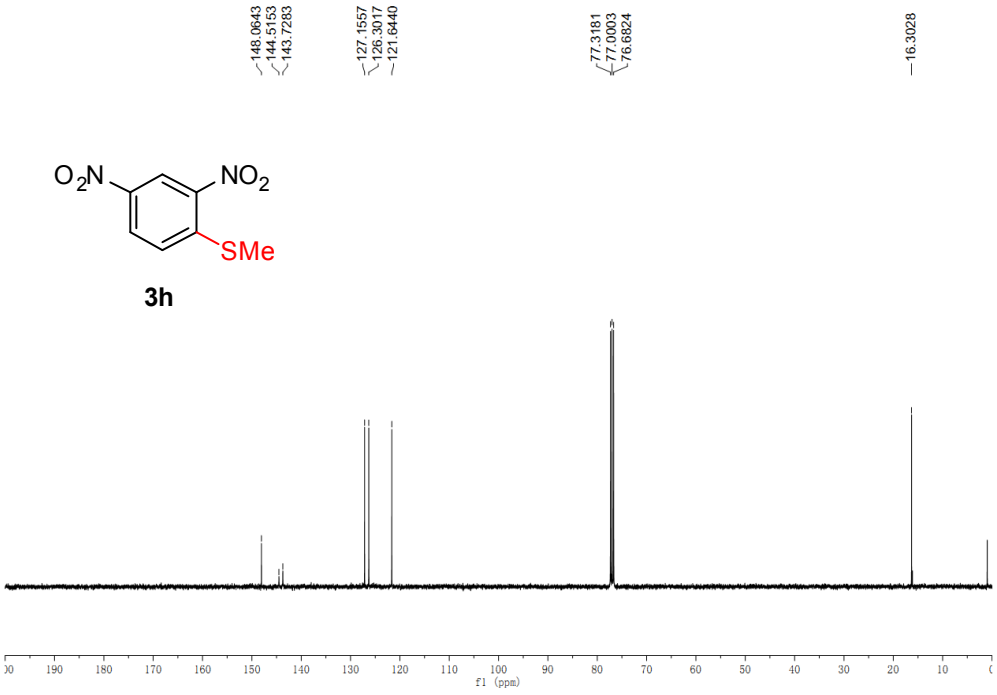
118.9325
77.3177
77.0001
76.6825
16.0285
F3C
NO2
SMe
3g
f1 (ppm)

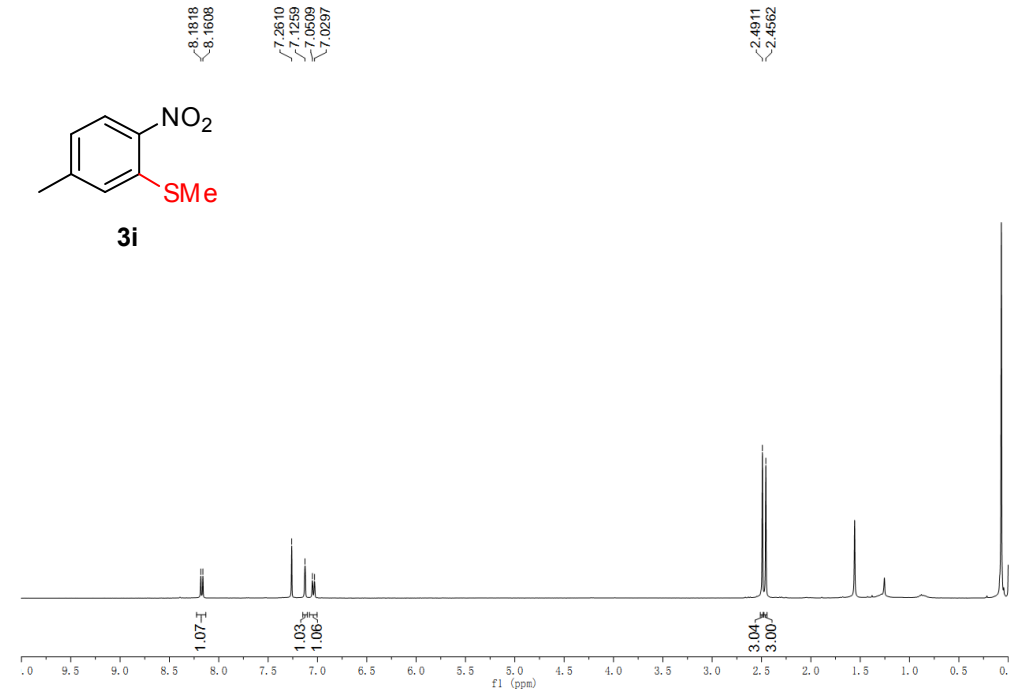

-62.6063
F3C
NO2
SMe
3g
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

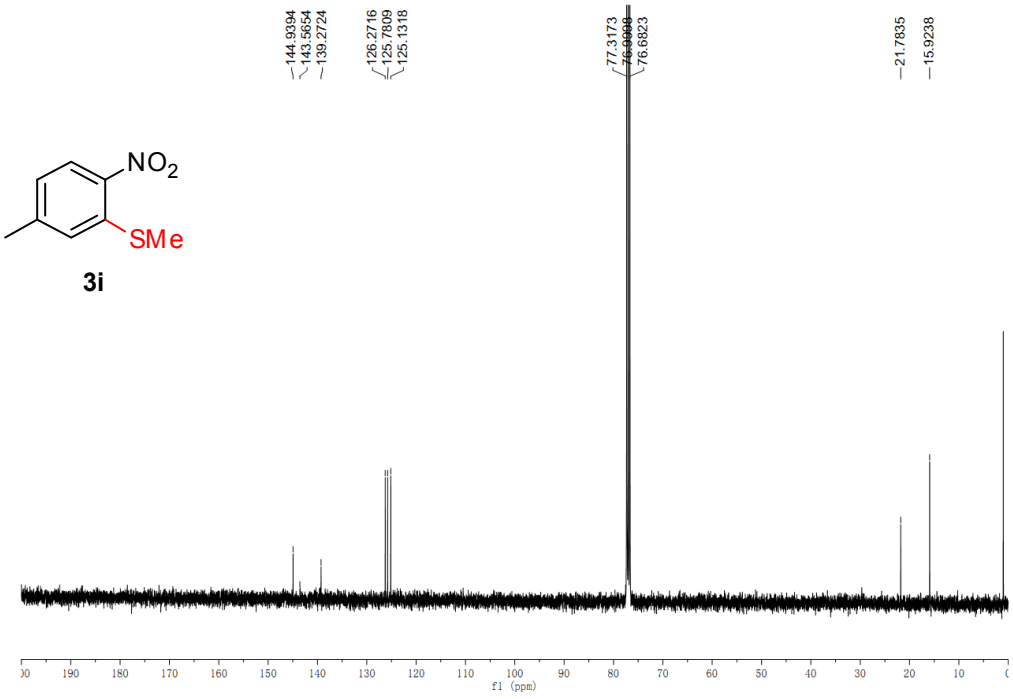

9.1089
8.4188
8.3964
7.5690
7.5466
7.2734
2.6221
O2N
NO2
SMe
0.93
0.97
1.04
3.00
f1 (ppm)

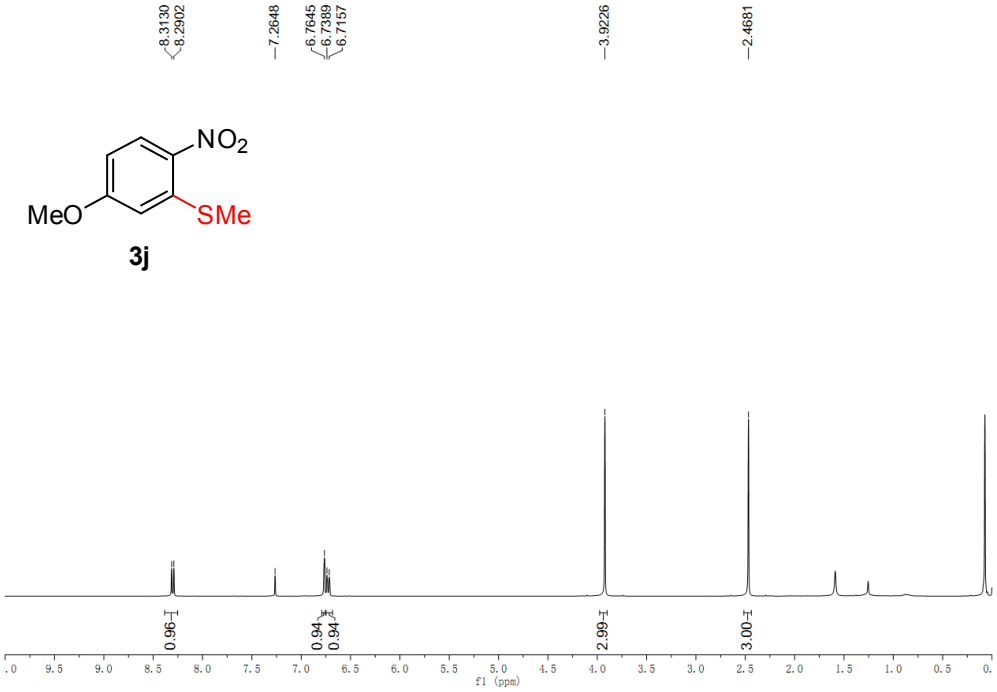
3h

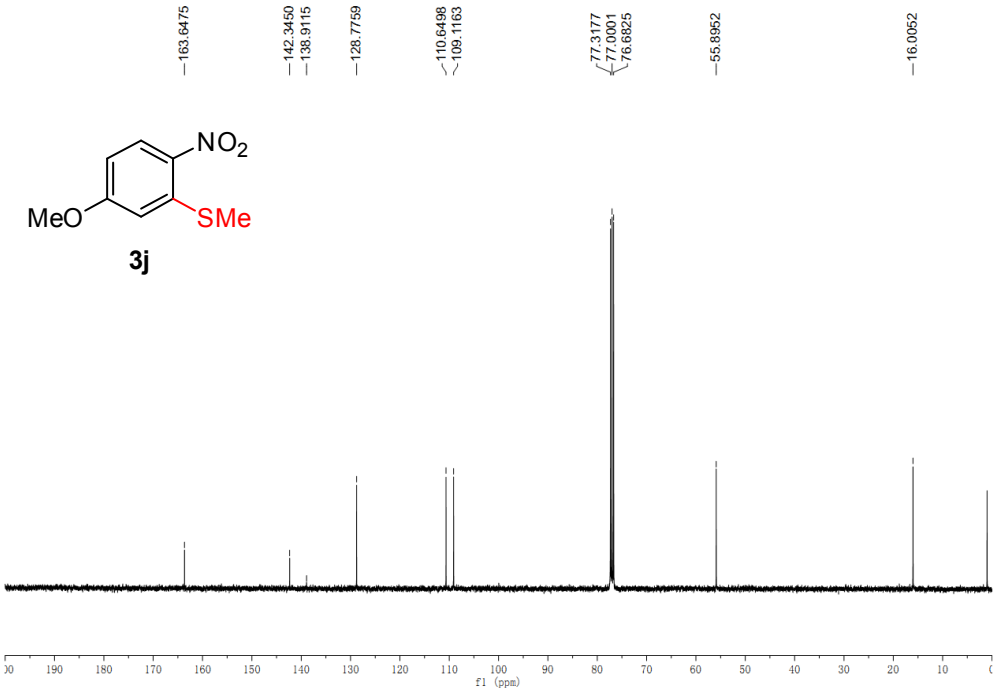

148.0643
144.5153
143.7283
127.1557
126.3017
121.6440
77.3181
77.0003
76.6824
16.3028
O2N
NO2
SMe
f1 (ppm)

3h


8.1818
8.1608
7.2610
7.1259
7.0509
7.0297
2.4911
2.4562
NO2
SMe
3i
1.07
1.03
1.06
3.04
3.00
f1 (ppm)


144.9394
143.5654
139.2724
126.2716
125.7809
125.1318
77.3173
76.8998
76.6823
21.7835
15.9238
NO2
SMe
3i
f1 (ppm)


8.3130
8.2902
7.2648
6.7645
6.7389
6.7157
3.9226
2.4681
NO2
MeO
SMe
3j
0.96
0.94
0.94
2.99
3.00
f1 (ppm)


163.6475
142.3450
138.9115
128.7759
110.6498
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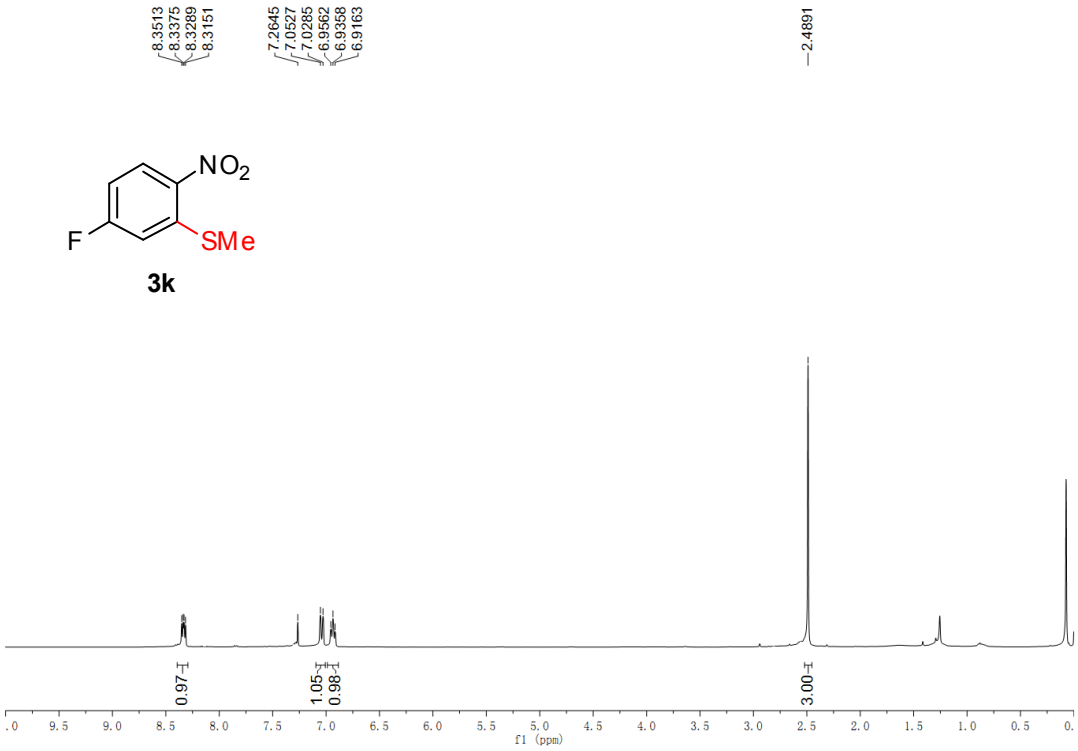
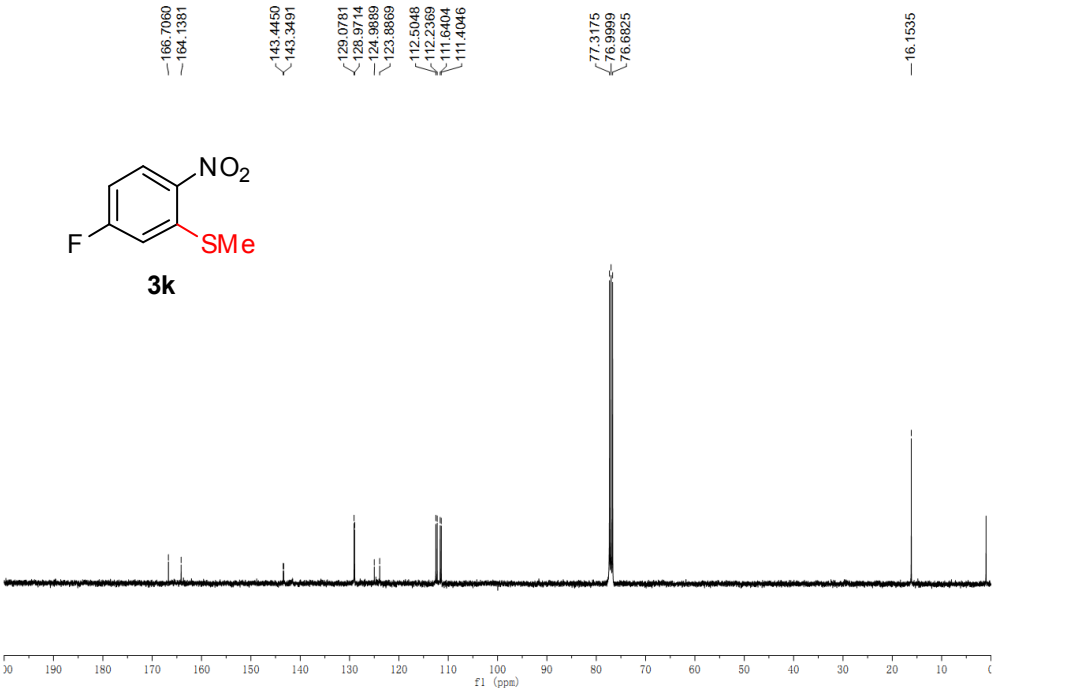
77.3177
77.0001
76.6825
55.8952
16.0052
NO2
MeO
SMe
3j
f1 (ppm)


8.3513
8.3375
8.3289
8.3151
7.2645
7.0527
7.0285
6.9562
6.9358
6.9163
2.4891
NO2
F
SMe
0.97
1.05
0.98
3.00
f1 (ppm)

3k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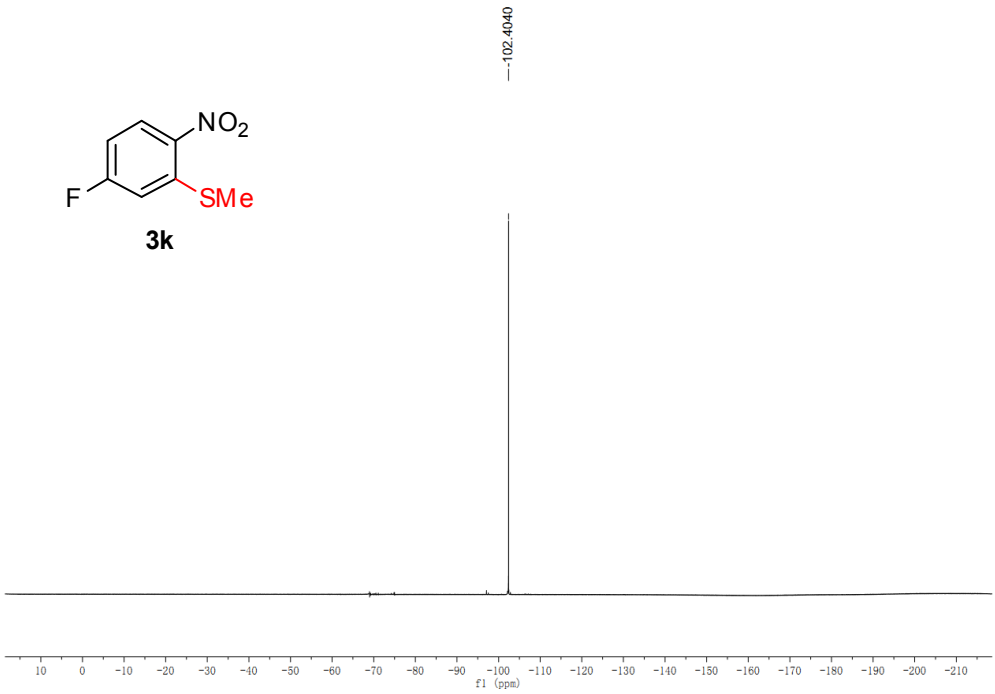
164.1381
143.4450
143.3491
129.0781
128.9714
124.9889
123.8869
112.5048
112.2369
111.6404
111.4046
77.3175
76.9999
76.6825
16.1535
NO2
F
SMe
f1 (ppm)

3k

NO2
F
SMe

3k


-102.4040
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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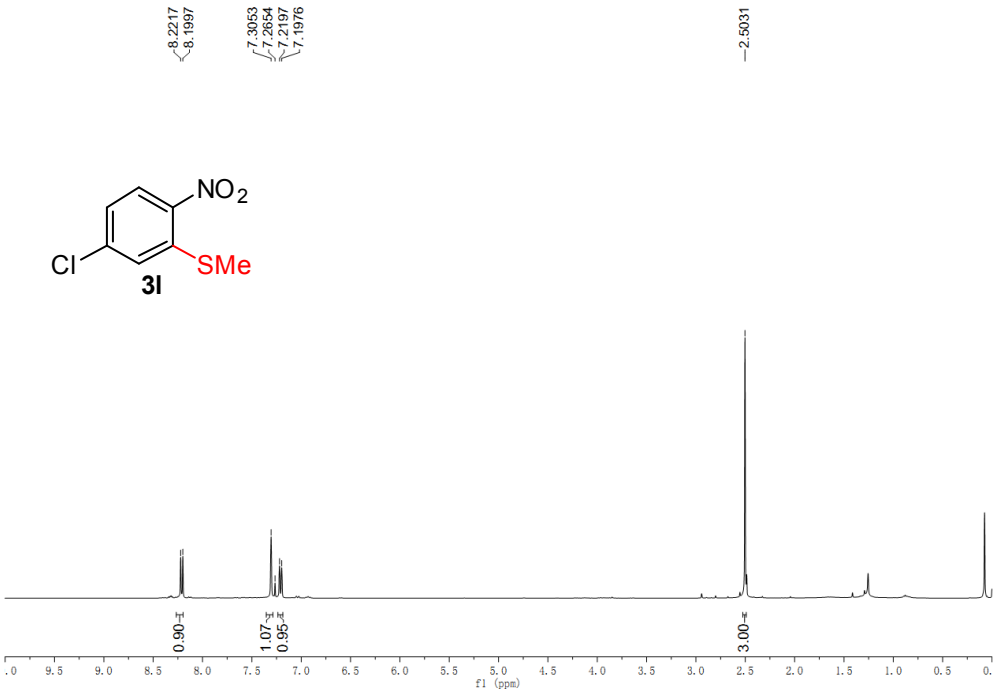
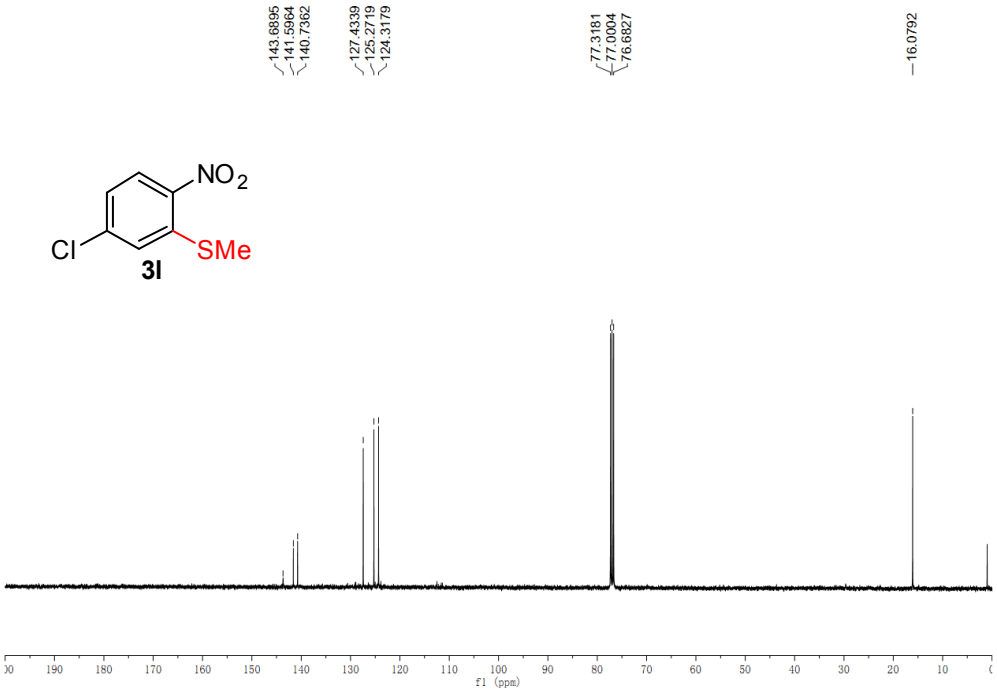
-200
-210
f1 (ppm)


8.2217
8.1997
7.3053
7.2654
7.2197
7.1976
2.5031
NO2
Cl
SMe
3l
0.90
1.07
0.95
3.00
f1 (ppm)


143.6895
141.5964
140.7362
127.4339
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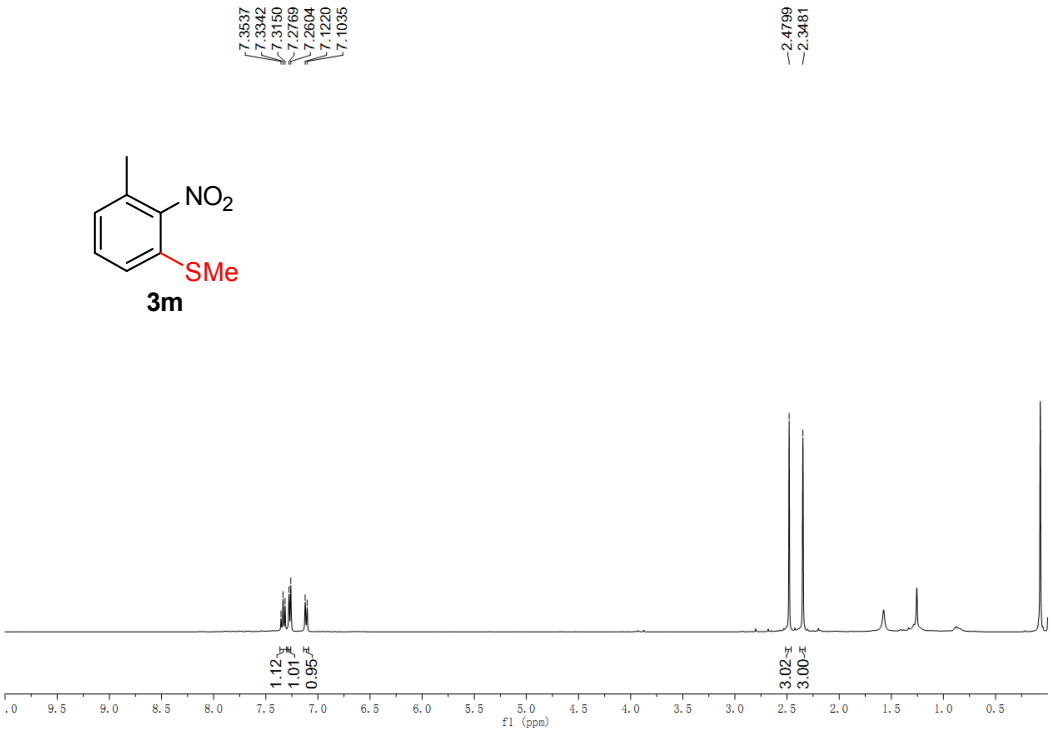
NO2
Cl
SMe
3l
f1 (ppm)


7.3537
7.3342
7.3150
7.2769
7.2604
7.1220
7.1035
2.4799
2.3481
NO2
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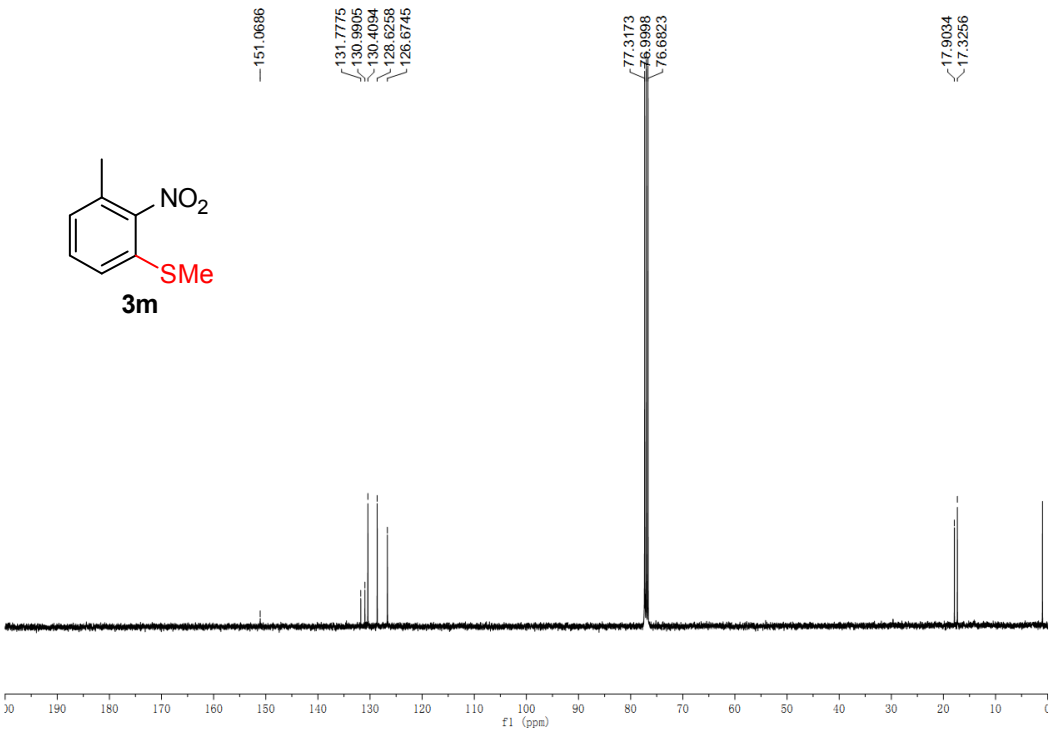
3m
1.12
1.01
0.95
3.02
3.00
f1 (ppm)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17.9034
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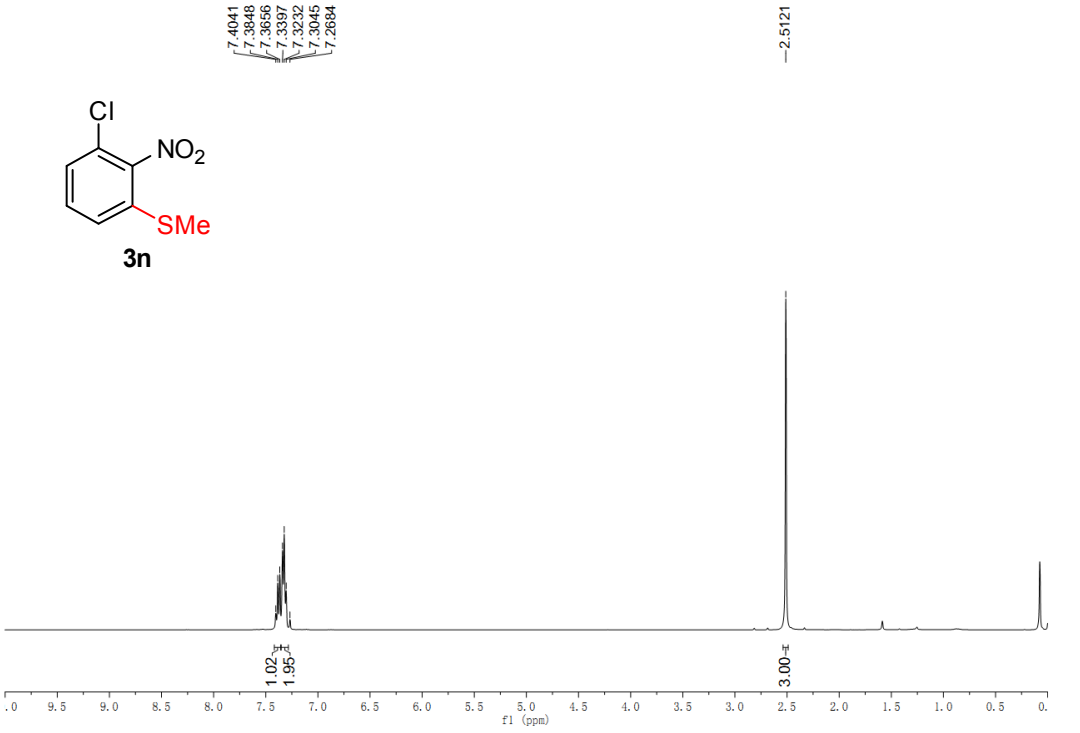
SMe
3m
f1 (ppm)


7.4041
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7.3656
7.3397
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7.3045
7.2684
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NO2
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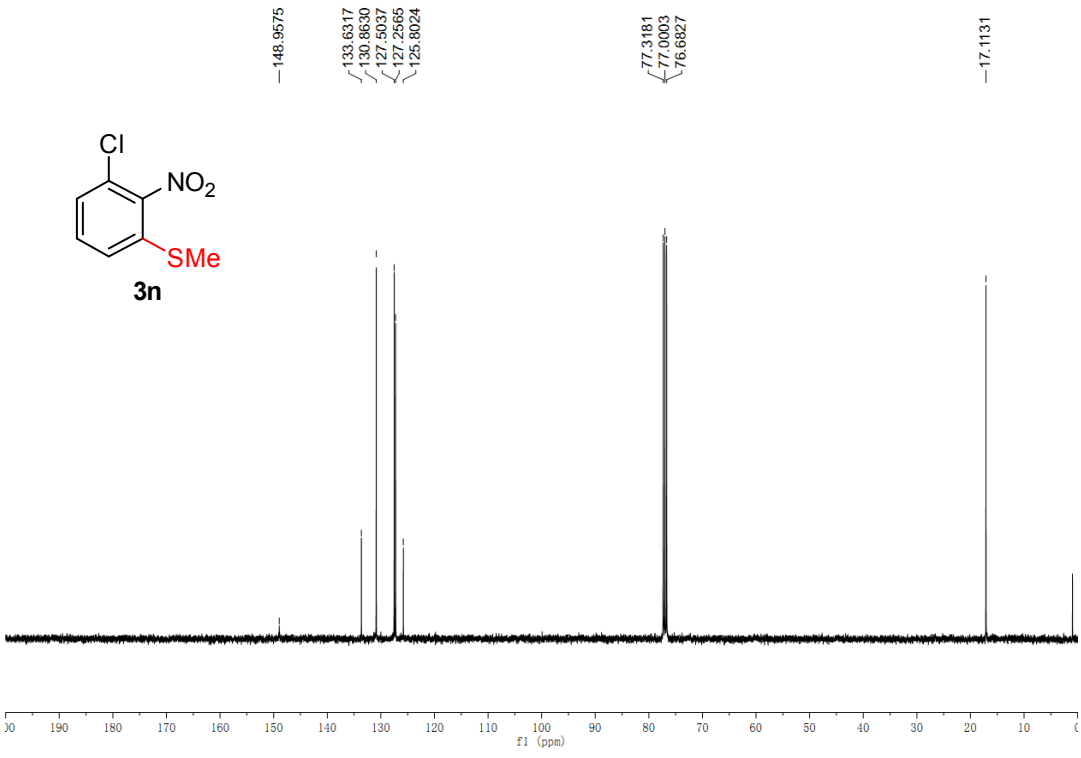
1.95
3.00
f1 (ppm)


148.9575
133.6317
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127.5037
127.2565
125.8024
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77.0003
76.6827
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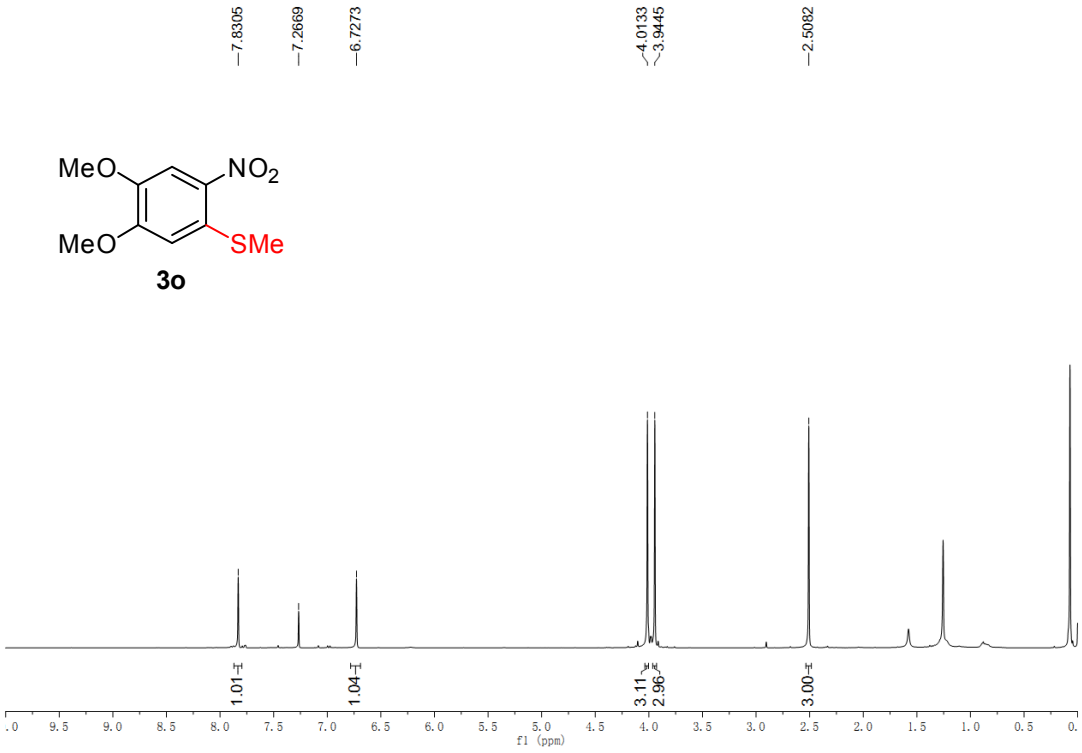
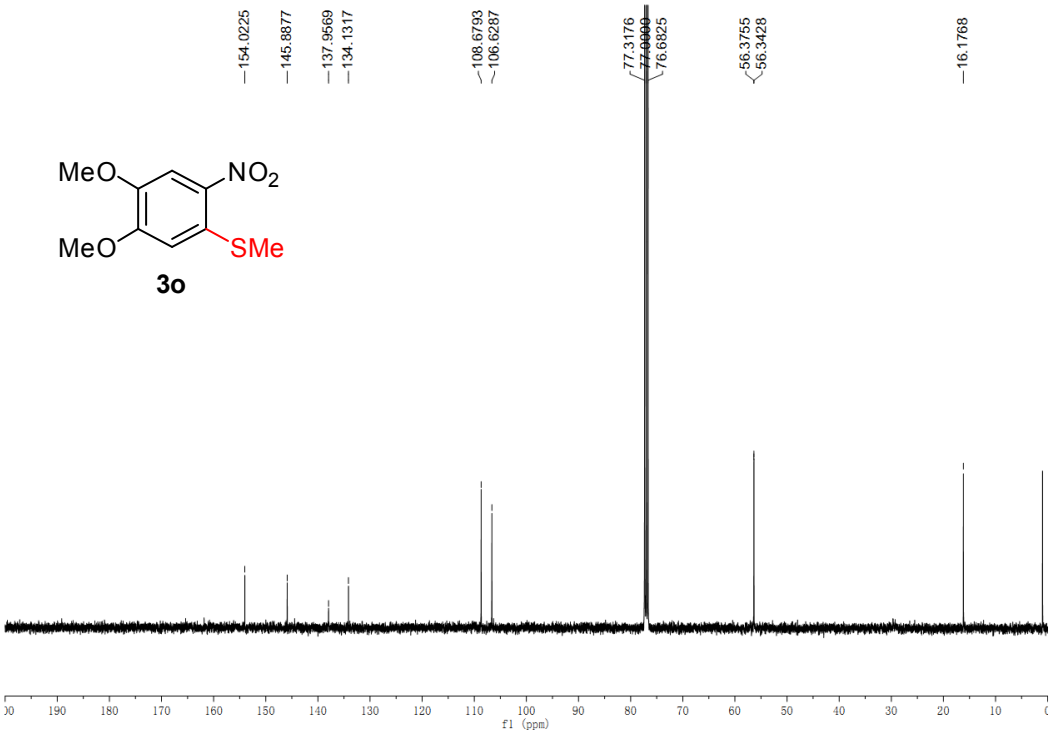
Cl
NO2
SMe
3n
f1 (ppm)


7.8305
7.2669
6.7273
4.0133
3.9445
2.5082
MeO
NO2
MeO
SMe
3o
1.01
1.04
3.11
2.96
3.00
f1 (ppm)


154.0225
145.8877
137.9569
134.1317
108.6793
106.6287
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77.0000
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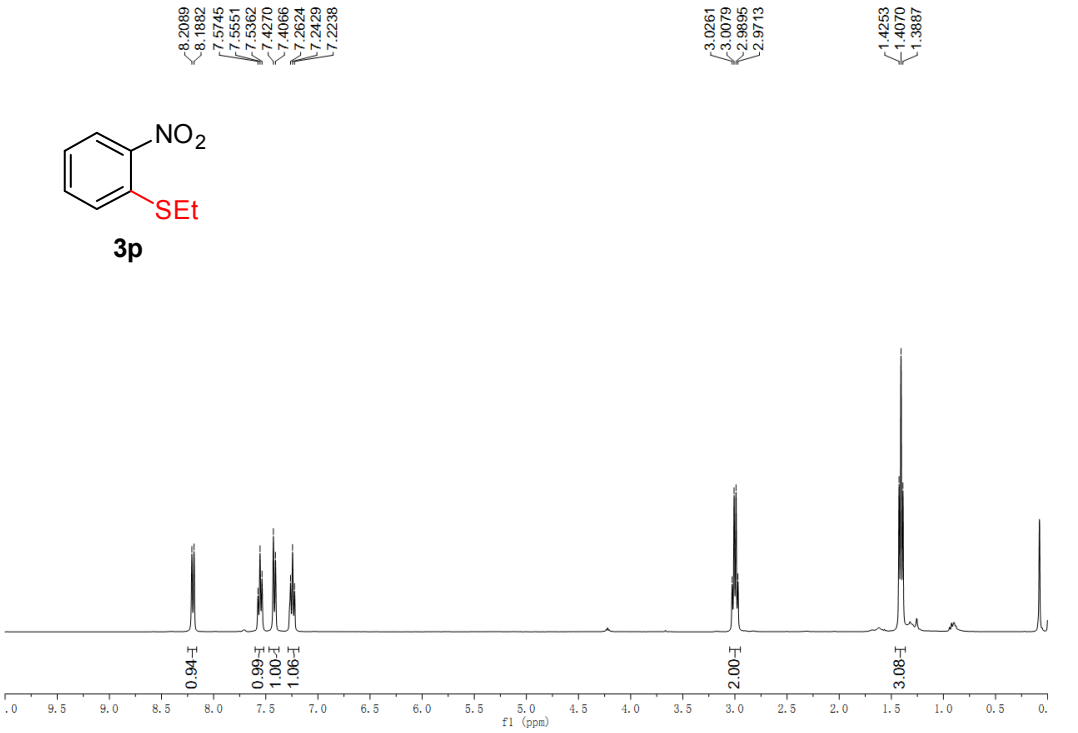
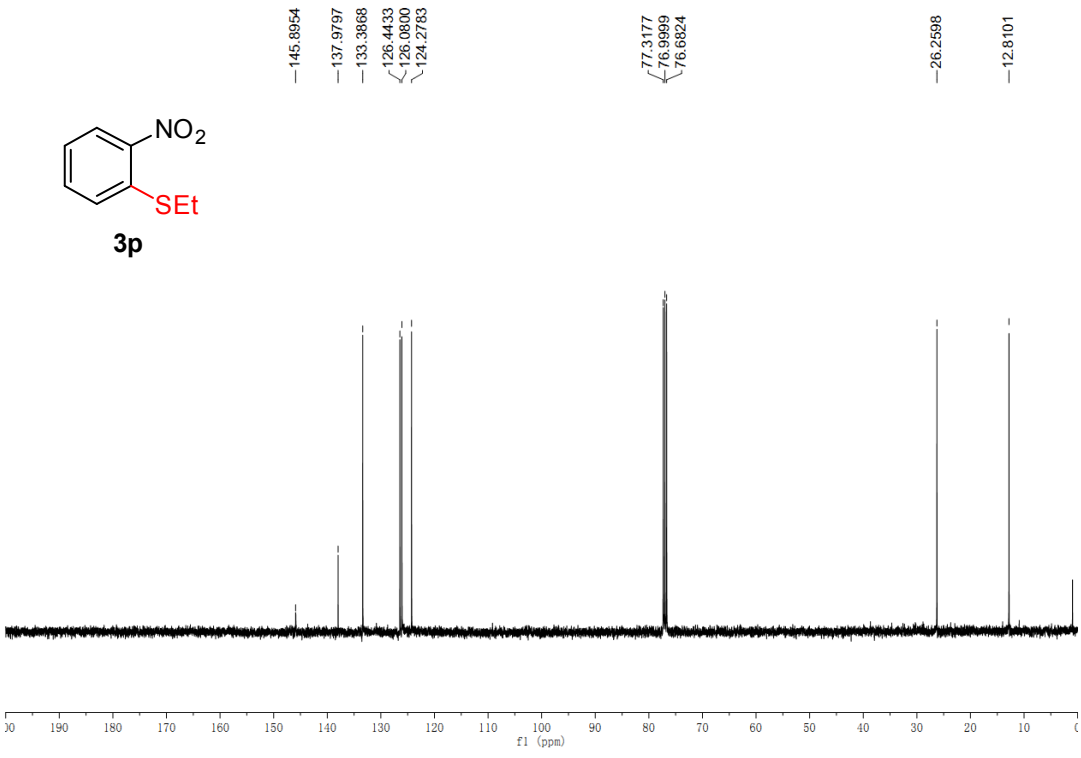
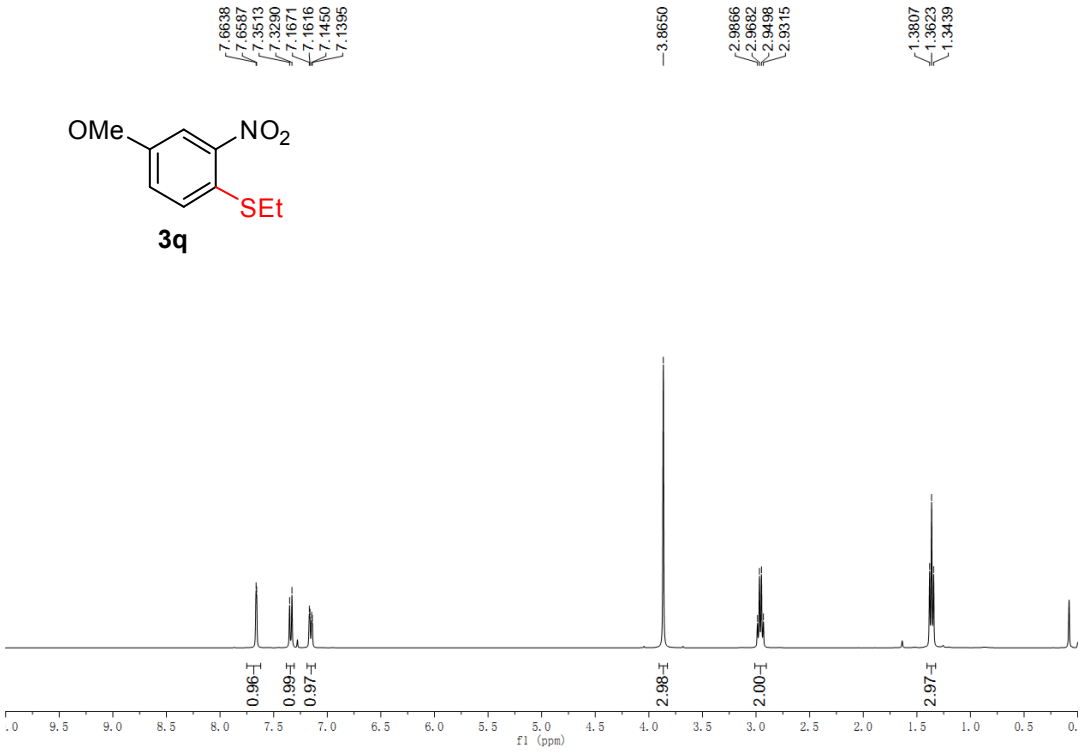
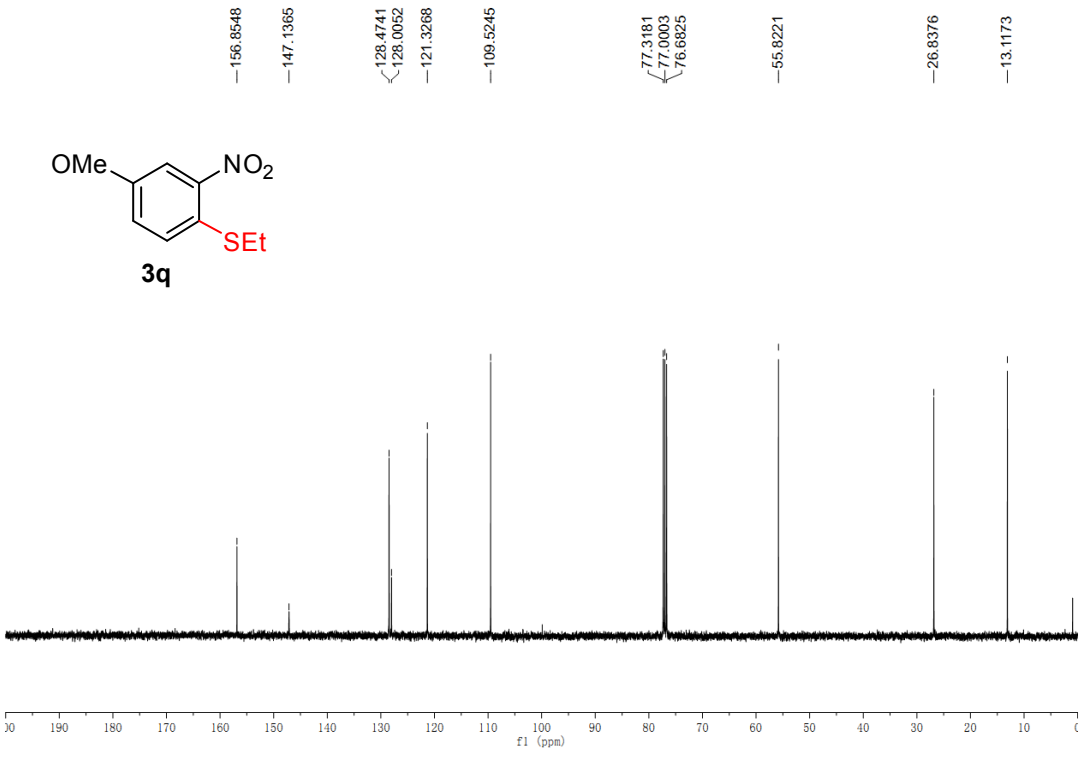
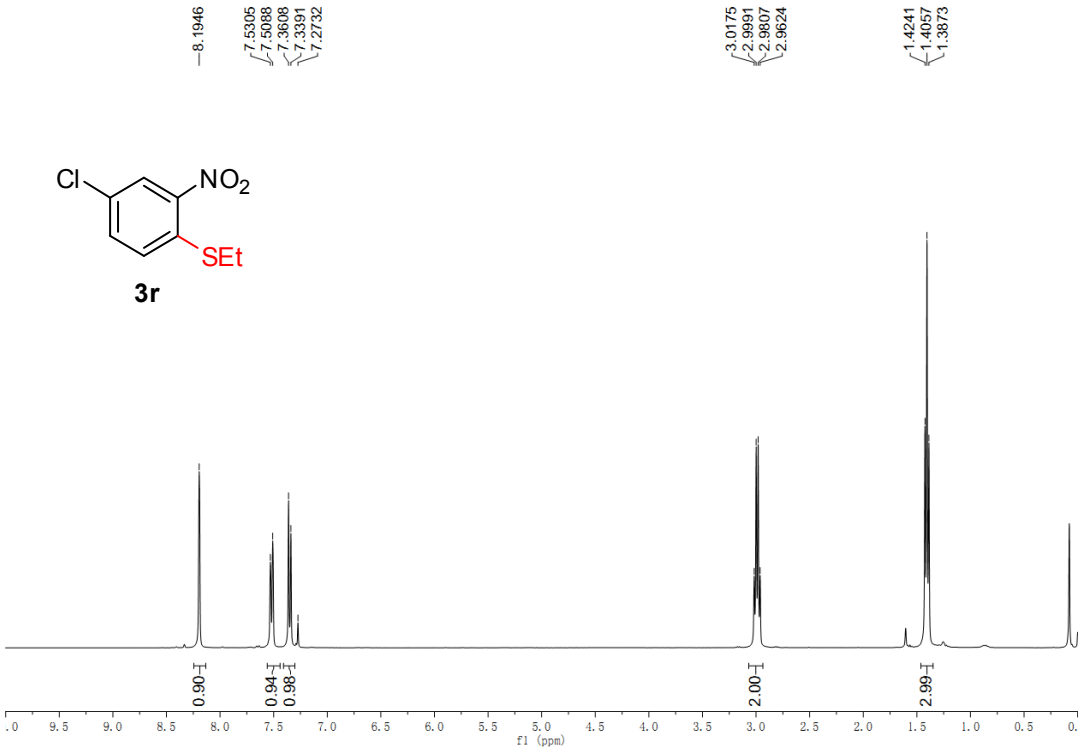
56.3428
16.1768
MeO
NO2
MeO
SMe
3o
f1 (ppm)

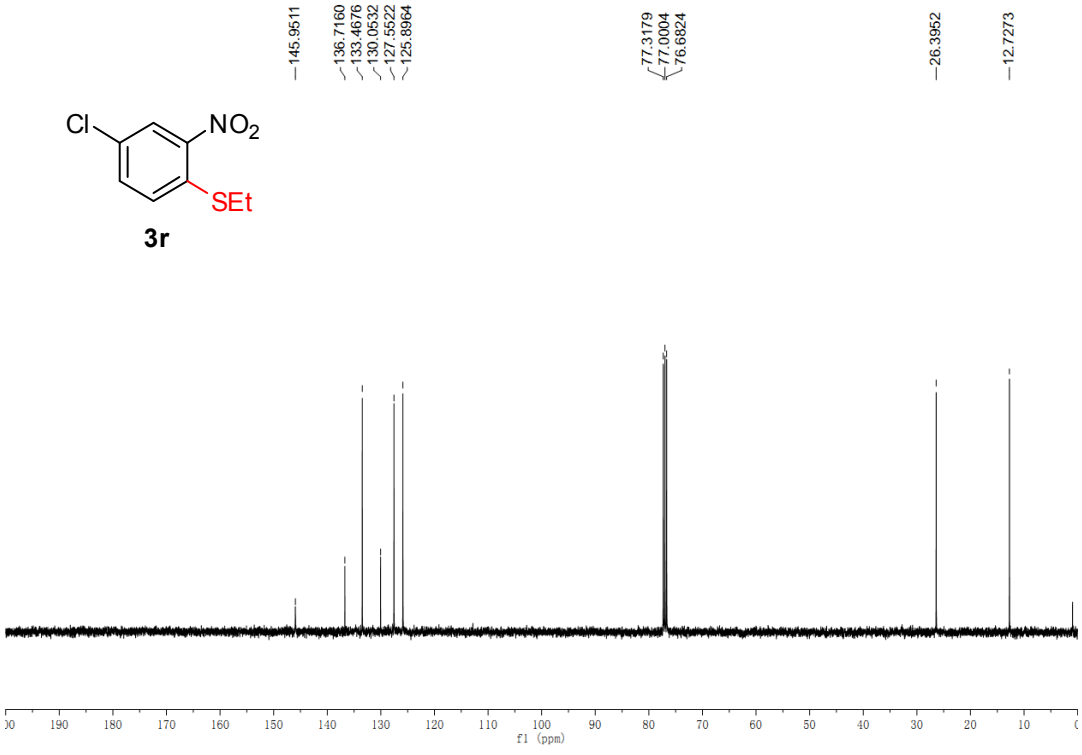

8.2089
8.1882
7.5745
7.5551
7.5362
7.4270
7.4066
7.2624
7.2429
7.2238
3.0261
3.0079
2.9895
2.9713
1.4253
1.4070
1.3887
NO2
SEt
3p
0.94
0.99
1.00
1.06
2.00
3.08
f1 (ppm)

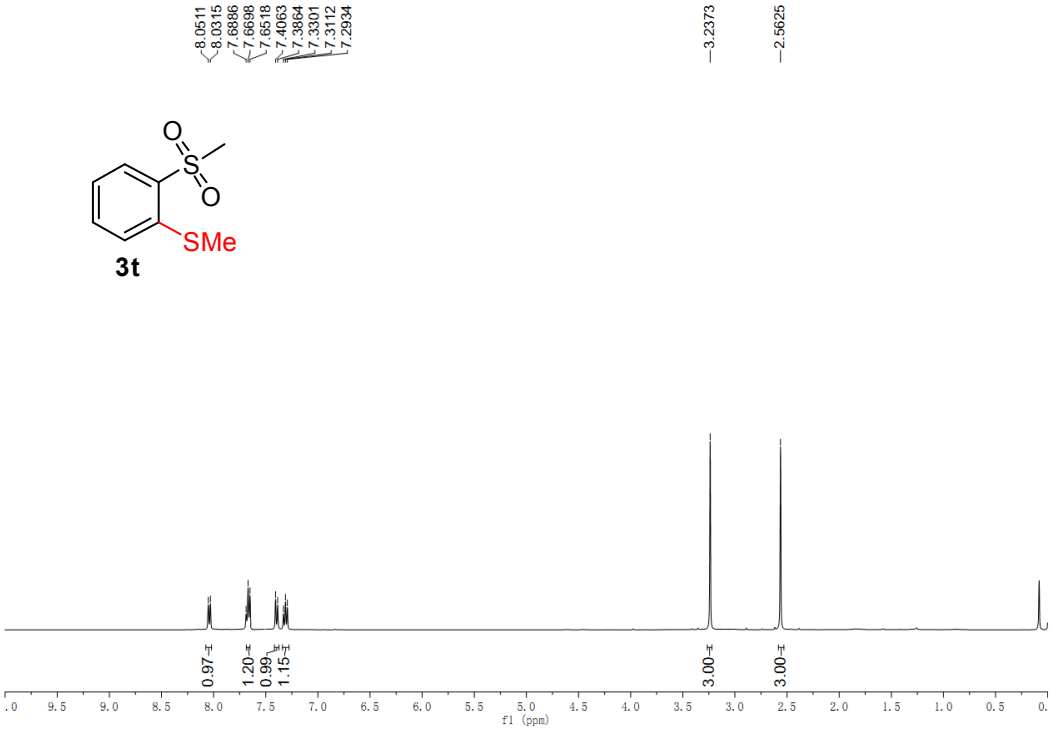

145.8954
137.9797
133.3868
126.4433
126.0800
124.2783
77.3177
76.9999
76.6824
26.2598
12.8101
NO2
SEt
3p
f1 (ppm)

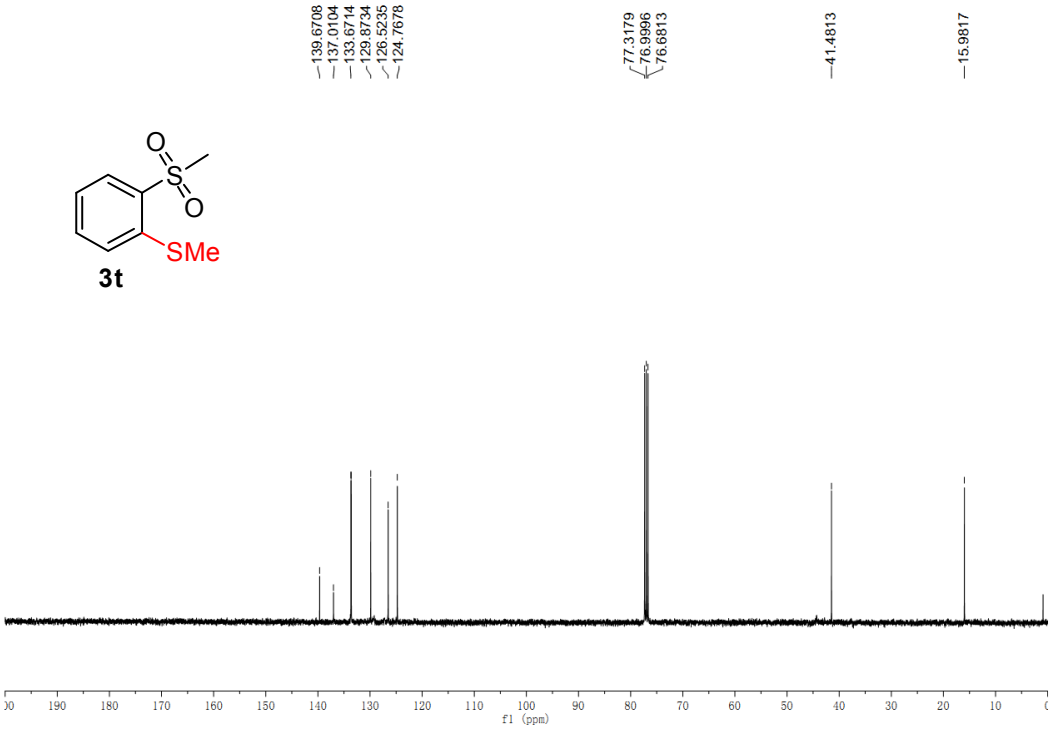

7.6638
7.6587
7.3513
7.3290
7.1671
7.1616
7.1450
7.1395
3.8650
2.9866
2.9682
2.9498
2.9315
1.3807
1.3623
1.3439
OMe
NO2
SEt
3q
0.96
0.99
0.97
2.98
2.00
2.97
f1 (ppm)

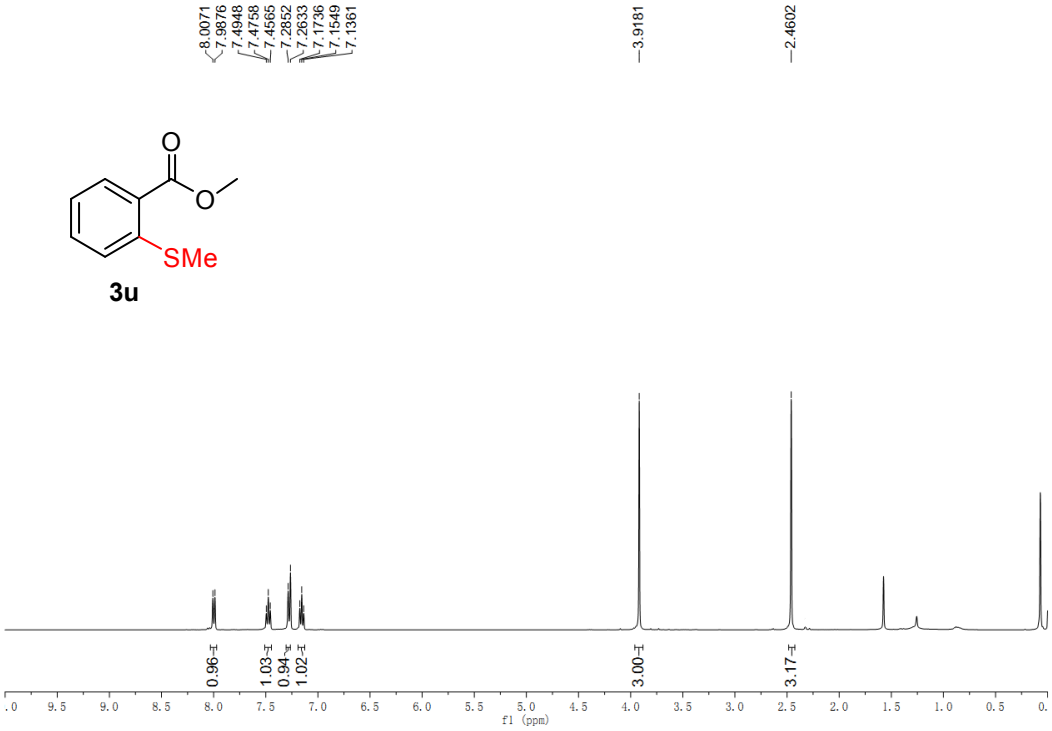

156.8548
147.1365
128.4741
128.0052
121.3268
109.5245
77.3181
77.0003
76.6825
55.8221
26.8376
13.1173
OMe
NO2
SEt
3q
f1 (ppm)


8.1946
7.5305
7.5088
7.3608
7.3391
7.2732
3.0175
2.9991
2.9807
2.9624
1.4241
1.4057
1.3873
Cl
NO2
SEt
3r
0.90
0.94
0.98
2.00
2.99
f1 (ppm)

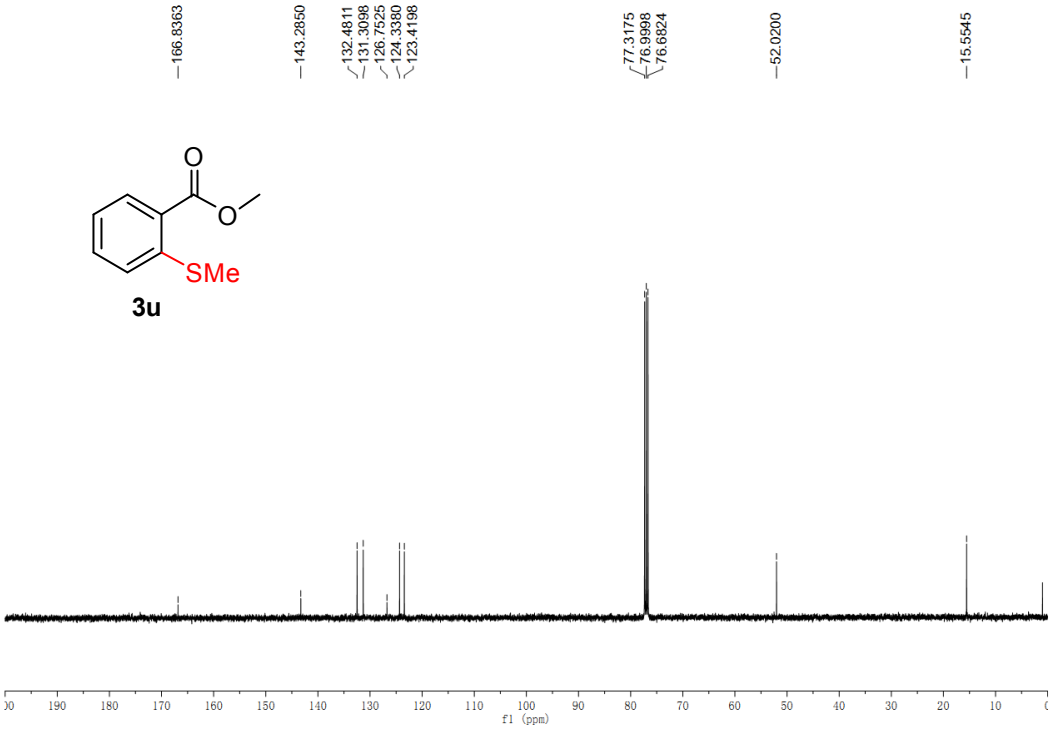

145.9511
136.7160
133.4676
130.0532
127.5522
125.8964
77.3179
77.0004
76.6824
26.3952
12.7273
Cl
NO2
SEt
3r
f1 (ppm)


8.0511
8.0315
7.6886
7.6698
7.6518
7.4063
7.3864
7.3301
7.3112
7.2934
3.2373
2.5625
SMe
3t
0.97
1.20
0.99
1.15
3.00
3.00
f1 (ppm)

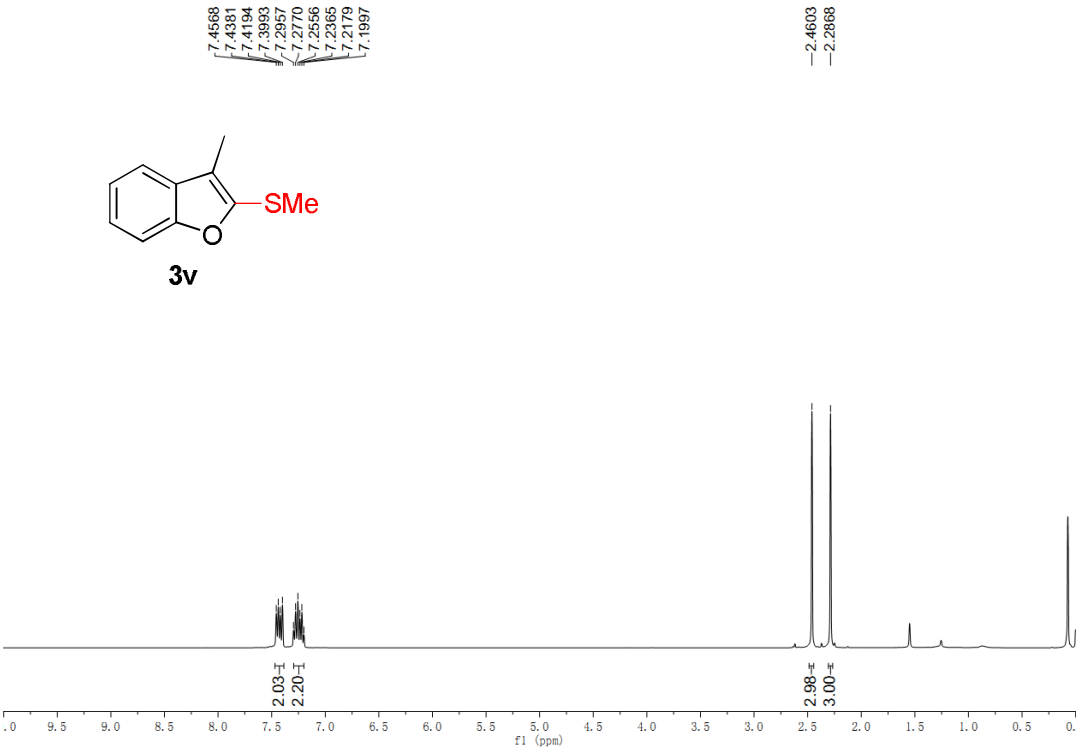

139.6708
137.0104
133.6714
129.8734
126.5235
124.7678
77.3179
76.9996
76.6813
41.4813
15.9817
SMe
3t
f1 (ppm)

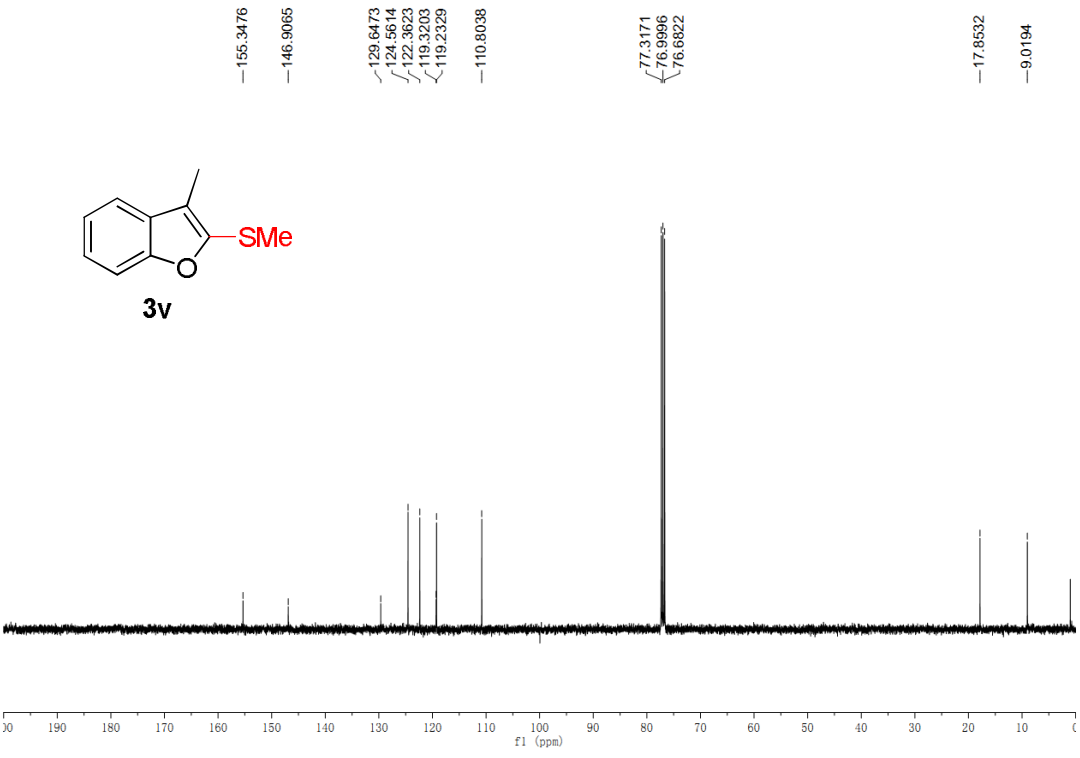

8.0071
7.9876
7.4948
7.4758
7.4565
7.2852
7.2633
7.1736
7.1549
7.1361
3.9181
2.4602
O
O
SMe
0.96
1.03
0.94
1.02
3.00
3.17
f1 (ppm)

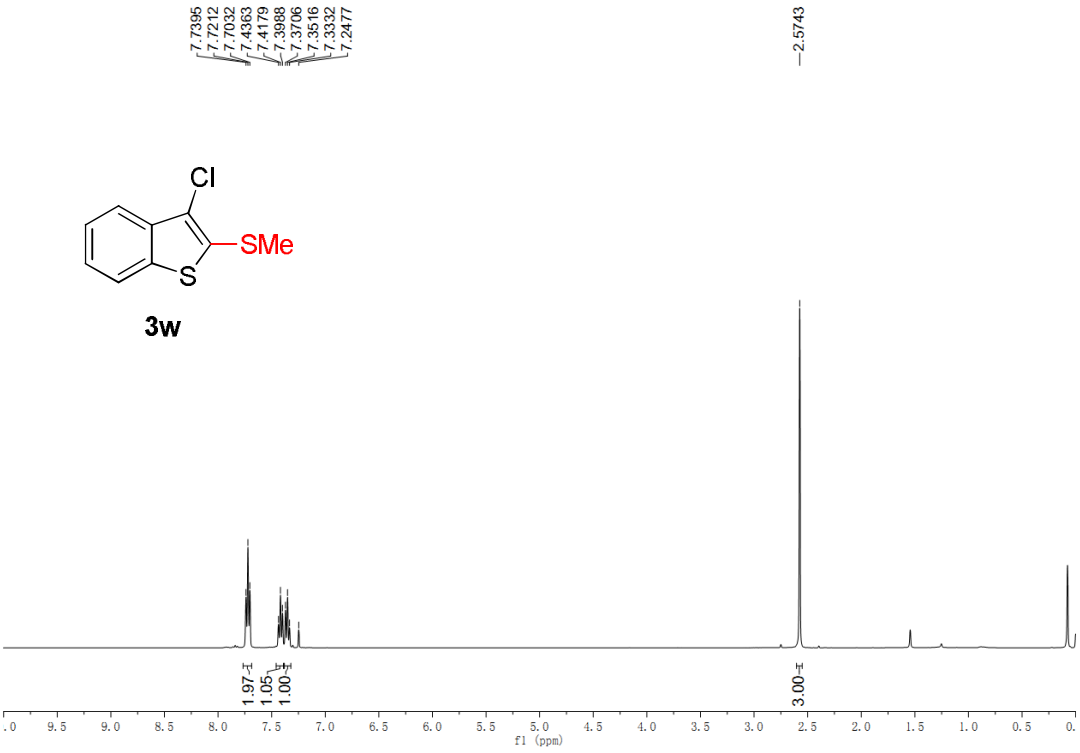
3u

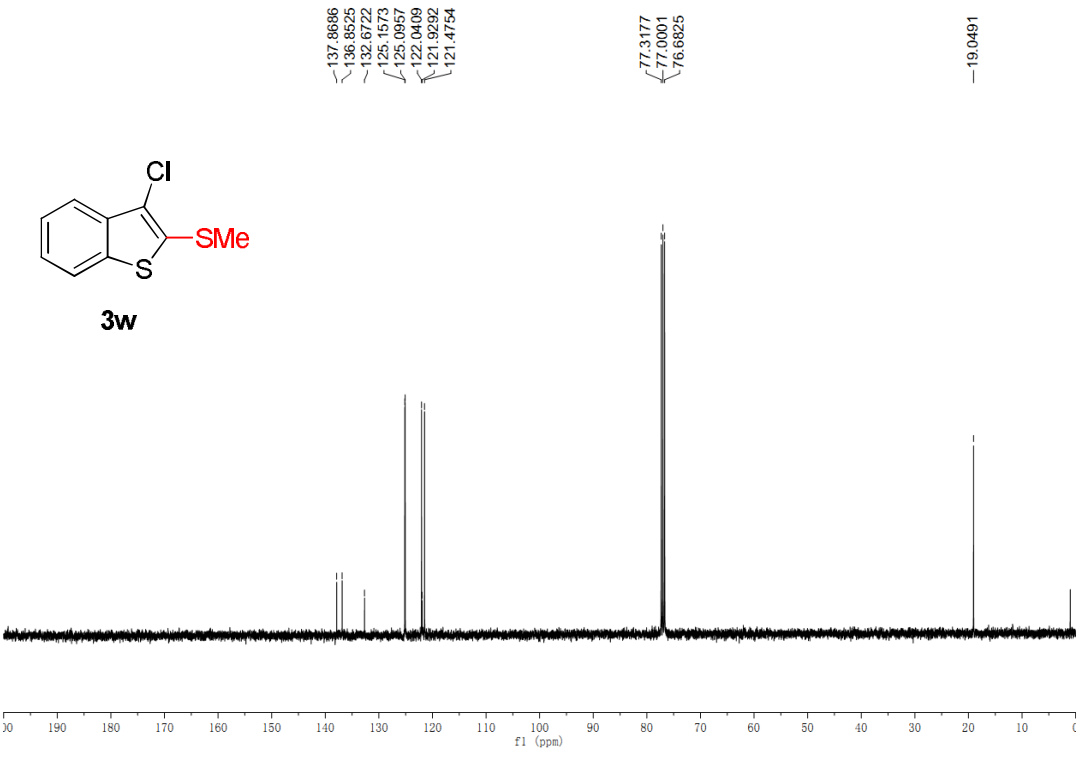

166.8363
143.2850
132.4811
131.3098
126.7525
124.3380
123.4198
77.3175
76.9998
76.6824
52.0200
15.5545
O
O
SMe
f1 (ppm)

3u


7.4568
7.4381
7.4194
7.3993
7.2957
7.2770
7.2556
7.2365
7.2179
7.1997
2.4603
2.2868
SMe
3v
2.03
2.20
2.98
3.00
f1 (ppm)


155.3476
146.9065
129.6473
124.5614
122.3623
119.3203
119.2329
110.8038
77.3171
76.9996
76.6822
17.8532
9.0194
SMe
3v
f1 (ppm)


7.7395
7.7212
7.7032
7.4363
7.4179
7.3988
7.3706
7.3516
7.3332
7.2477
2.5743
Cl
SMe
S
3w
1.97
1.05
1.00
3.00
f1 (ppm)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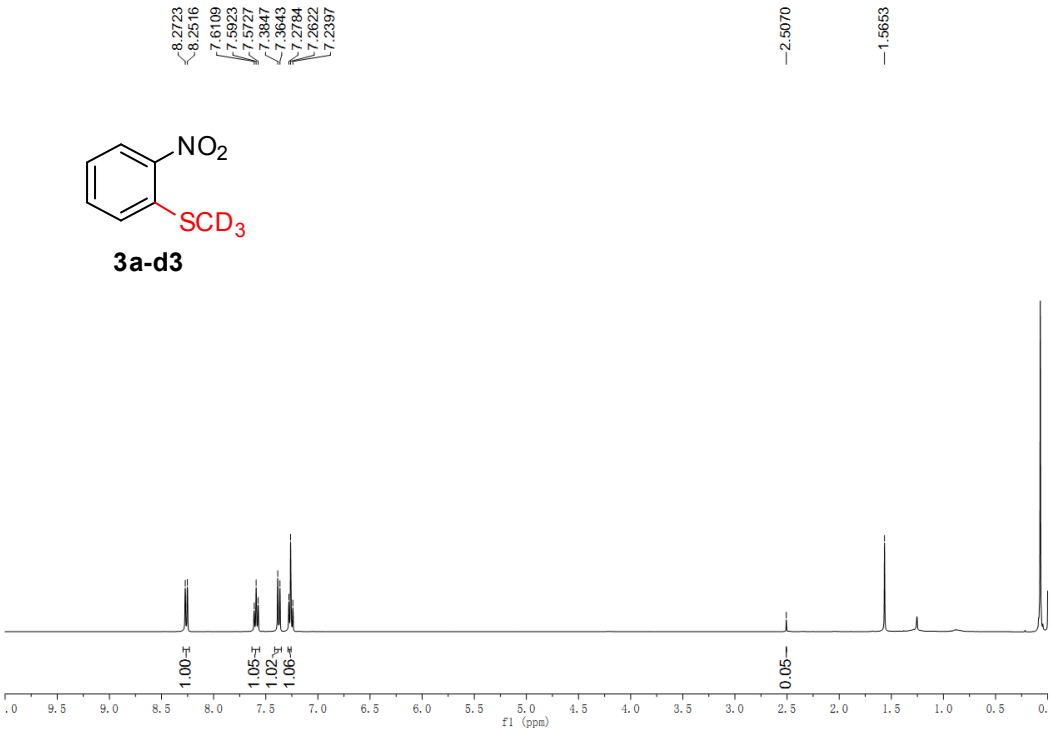
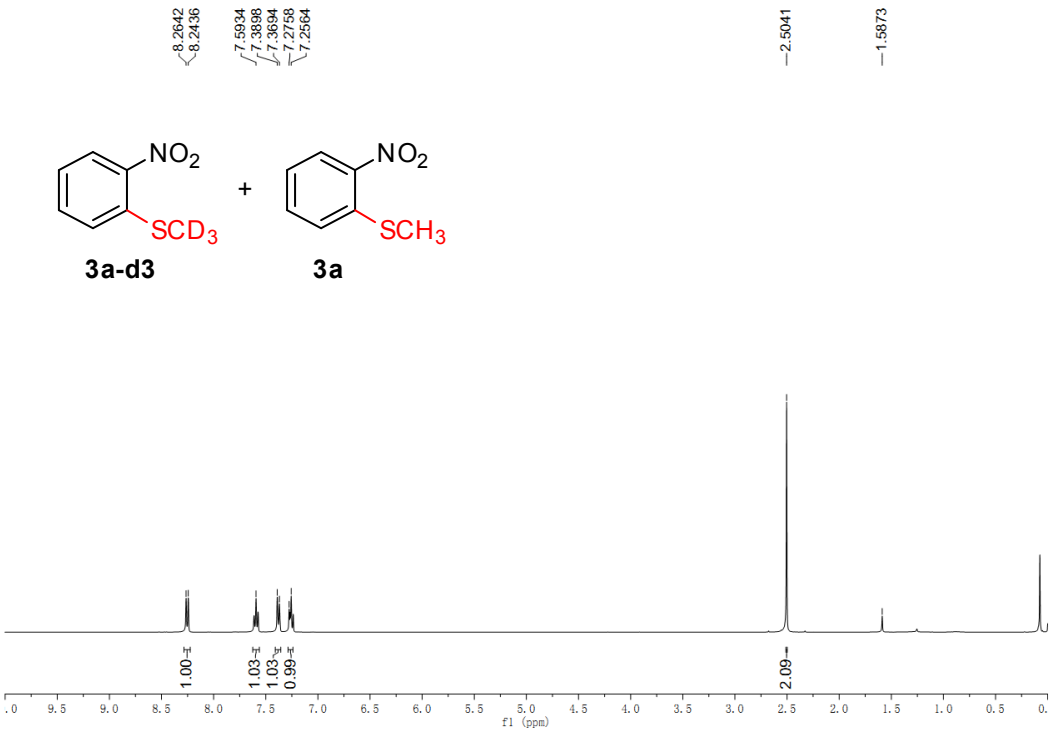
136.8525
132.6722
125.1573
125.0957
122.0409
121.9292
121.4754
77.3177
77.0001
76.6825
19.0491
Cl
SMe
S
3w
f1 (ppm)


8.2723
8.2516
7.6109
7.5923
7.5727
7.3847
7.3643
7.2784
7.2622
7.2397
2.5070
1.5653
NO2
SCD3
1.00
1.05
1.02
1.06
0.05
f1 (ppm)

3a-d3


8.2642
8.2436
7.5934
7.3898
7.3694
7.2758
7.2564
2.5041
1.5873
NO2
SCD3
NO2
SCH3
1.00
1.03
1.03
0.99
2.09
f1 (ppm)

3a-d3 + **3a**