Supporting Information

A Radical Coupling Reaction of DMSO with Sodium Arylsulfinates in Air: Mild Utilization of DMSO as C_1 Resource for the synthesis of arylsulfonyl dibromomethane

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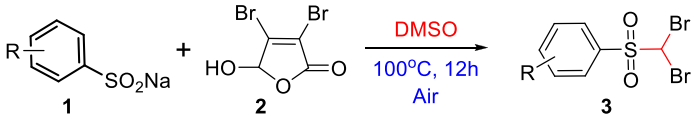
General Information

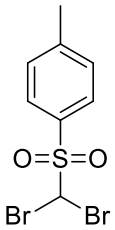
^{1}H and ^{13}C NMR spectra were recorded on BRUKER DRX-400 spectrometer using $CDCl_3$ as solvent and TMS as an internal standard. Gas chromatograph mass spectra (GC-MS) were performed on a SHIMADZU model GCMS-QP5000 spectrometer. High-resolution mass spectra (ESI) were tested on a LCMS-IT-TOF mass spectrometer. Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and used without further purification. 3,4-Dibromo-5-hydroxy-2(5*H*)-furanone was synthesized according to the literature procedure.[1]

Experimental Procedure for Compounds 3



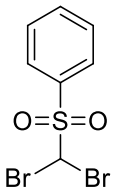
The mixture of sodium arylsulfinates **1** (0.55 mmol) and 3,4-dibromo-2(5*H*)-furanone **2** (0.50 mmol) in DMSO (3 mL) was stirred at 100 ℃ under air for 12 h. At room temperature, the reaction mixture was diluted with H_2O (15 mL) and extracted with EtOAc (3 × 15 mL). The combined organic extracts were dried over $MgSO_4$. After filtration and evaporation of the solvents under reduced pressure, the crude product was purified by column chromatography on silica gel to afford desired product.

Characterization Data for All Products 3



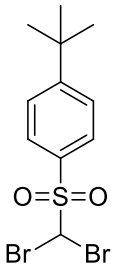
1-(Dibromomethylsulfonyl)-4-methylbenzene (3a)

Yellow liquid (138 mg, 84%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 8.0 Hz, 2H), 7.42 (d, J = 8.0 Hz, 2H), 6.23 (s, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.9, 131.2, 129.9, 129.1, 50.8, 21.9. IR (film), v, cm^{-1}: 3040, 2974, 1592, 1495, 1331, 1150, 814, 643, 544. ESI-MS, m/z (%): Calcd for $C_8H_7Br_2O_2S^-$ ([M-H]$^-$): 326.85 (100.0), Found: 326.96 (30.0). Anal. Calcd for $C_8H_8Br_2O_2S$: C 29.29, H 2.46, O 9.76, Found: C 29.17, H 2.56, O 9.67.



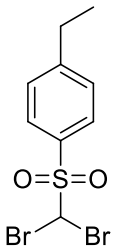
(Dibromomethylsulfonyl)benzene (3b)

Yellow liquid (129 mg, 82%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.99 (d, J = 8.0 Hz, 2H), 7.70 (t, J = 8.0 Hz, 1H), 7.59-7.53 (m, 2H), 6.18 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.4, 132.2, 131.2, 129.2, 50.5. IR (film), v, cm^{-1}: 3066, 2917, 2854, 1581, 1504, 1450, 1342, 1163, 824, 684, 556. ESI-MS, m/z (%): Calcd for $C_7H_5Br_2O_2S^-$ ([M-H]$^-$): 312.84 (100.0), Found: 313.09 (52.7). Anal. Calcd for $C_7H_6Br_2O_2S$: C 26.78, H 1.93, O 10.19, Found: C 26.87, H 1.86, O 10.26.



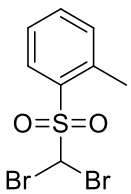
1-*Tert*-butyl-4-(dibromomethylsulfonyl)benzene (3c)

Yellow solid (148 mg, 79%). m.p. 72.9-74.5 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.97 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 6.23 (s, 1H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.72, 131.1, 129.0, 126.3, 50.8, 35.51, 31.0. IR (film), v, cm^{-1}: 3063, 2961, 2866, 1597, 1503, 1338, 1161, 832, 608, 514. ESI-MS, m/z (%): Calcd for $C_{11}H_{13}Br_2O_2S^-$ ([M-H]$^-$): 368.90 (100.0), Found: 368.83 (68.3). Anal. Calcd for $C_{11}H_{14}Br_2O_2S$: C 35.70, H 3.81, O 8.65, Found: C 35.78, H 3.93, O 8.79.



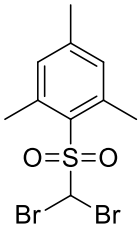
1-(Dibromomethylsulfonyl)-4-ethylbenzene (3d)

Yellow liquid (138 mg, 72%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.98 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 6.26 (s, 1H), 2.84-2.78 (q, J = 8.0 Hz, 2H), 1.32 (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.9, 131.3, 129.2, 128.7, 50.8, 29.0, 14.9. IR (film), v, cm^{-1}: 3052, 2958, 2870, 1600, 1502, 1451, 1331, 1155, 825, 648, 547. ESI-MS, m/z (%): Calcd for $C_9H_9Br_2O_2S^-$ ([M-H]$^-$): 340.87 (100.0), Found: 340.86 (45.3). Anal. Calcd for $C_9H_{10}Br_2O_2S$: C 31.60, H 2.95, O 3.96, Found: C 31.78, H 2.83, O 3.89.



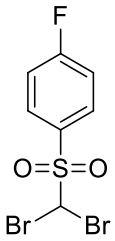
1-(Dibromomethylsulfonyl)-2-methylbenzene (3e)

Yellow liquid (128 mg, 78%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87-7.83 (m, 2H), 7.57-7.48 (m, 2H), 6.24 (s, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.7, 136.2, 132.0, 131.2, 129.1, 128.3, 50.7, 21.4. IR (film), v, cm^{-1}: 3065, 2921, 2849, 1600, 1503, 1477, 1451, 1330, 1155, 855, 682, 572. ESI-MS, m/z (%): Calcd for $C_8H_8Br_2O_2S^-$ ([M-H]$^-$): 326.85 (100.0), Found: 327.07 (77.2). Anal. Calcd for $C_8H_8Br_2O_2S$: C 29.29, H 2.46, O 9.76, Found: C 29.18, H 2.53, O 9.89.



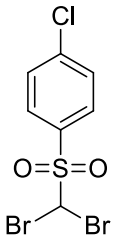
2-(Dibromomethylsulfonyl)-1,3,5-trimethylbenzene (3f)

Yellow solid (132 mg, 74%). m.p. 115.6-117.6 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.05 (s, 2H), 6.37 (s, 1H), 2.73 (s, 6H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.1, 141.0, 131.6, 51.3 (C-1), 22.3, 20.1. IR (film), v, cm^{-1}: 3034, 2920, 2848, 1600, 1502, 1455, 1331, 1155, 803, 642, 516. ESI-MS, m/z (%): Calcd for $C_{10}H_{11}Br_2O_2S^-$ ([M-H]$^-$): 354.88 (100.0), Found: 355.24 (40.3). Anal. Calcd for $C_{10}H_{12}Br_2O_2S$: C 33.73, H 3.40, O 8.99, Found: C 33.68, H 3.53, O 8.89.



1-(Dibromomethylsulfonyl)-4-fluorobenzene (3g)

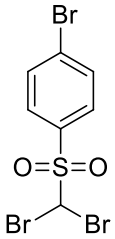
Yellow liquid (130 mg, 78%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11-8.08 (m, 2H), 7.33-7.29 (m, 2H), 6.27 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.0 (d, J = 258.0 Hz), 133.3 (d, J = 10.0 Hz), 127.0 (d, J = 3.0 Hz), 115.7 (d, J = 23.0 Hz), 49.4. IR (film), v, cm^{-1}: 3102, 2920, 2853, 1583, 1493, 1455, 1339, 1244, 1155, 834, 622, 548. ESI-MS, m/z (%): Calcd for $C_7H_4Br_2FO_2S^-$ ([M-H]$^-$): 330.83 (100.0), Found: 331.26 (100.0). Anal. Calcd for $C_7H_5Br_2FO_2S$: C 25.32, H 1.52, O 9.64, Found: C 25.48, H 1.43, O 9.79.



1-Chloro-4-(dibromomethylsulfonyl)benzene (3h)

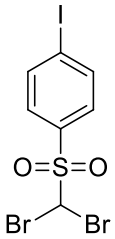
Yellow solid (133 mg, 76%). m.p. 127.8-129.2 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 6.19 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.6, 132.6, 130.5, 129.6, 50.2. IR (film), v, cm^{-1}: 3091, 2959, 2858, 1579, 1507, 1457, 1339, 1187, 826, 710, 649, 556. ESI-MS, m/z (%): Calcd for $C_7H_4Br_2ClO_2S^-$ ([M-H]$^-$): 346.80 (100.0), Found: 346.98 (100.0). Anal. Calcd for $C_7H_5Br_2ClO_2S$:

C 24.13, H 1.45, O 9.18, Found: C 24.28, H 1.33, O 9.29.



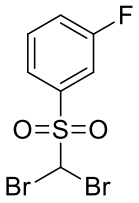
1-Bromo-4-(dibromomethylsulfonyl)benzene (3i)

White solid (142 mg, 72%). m.p. 130.1-131.3 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (d, J = 8.0 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 6.25 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 132.62, 132.61, 131.3, 131.0, 50.2. IR (film), v, cm^{-1}: 3095, 2916, 2849, 1574, 1502, 1451, 1339, 1155, 826, 635, 579. ESI-MS, m/z (%): Calcd for $C_7H_4Br_3O_2S^-$ ([M-H]$^-$): 392.74 (100.0), Found: 393.15 (98.7). Anal. Calcd for $C_7H_5Br_3O_2S$: C 21.40, H 1.28, O 8.14, Found: C 21.48, H 1.43, O 8.29.



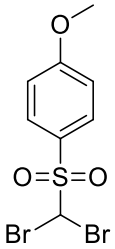
1-(Dibromomethylsulfonyl)-4-iodobenzene (3j)

Yellow solid (152 mg, 69%). m.p. 124.8-126.3 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.00 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H), 6.23 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.6, 132.3, 131.8, 104.3, 50.1. IR (film), v, cm^{-1}: 3086, 2920, 2844, 1571, 1455, 1339, 1155, 821, 636, 579, 527. ESI-MS, m/z (%): Calcd for $C_7H_4Br_2IO_2S^-$ ([M-H]$^-$): 438.73 (100.0), Found: 439.11 (67.7). Anal. Calcd for $C_7H_5Br_2IO_2S$: C 19.11, H 1.15, O 7.29, Found: C 19.28, H 1.23, O 7.17.



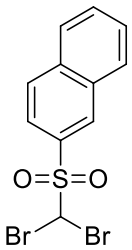
1-(Dibromomethylsulfonyl)-3-fluorobenzene (3k)

Yellow liquid (118 mg, 71%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.66-7.60 (m, 1H), 7.50-7.46 (m, 1H), 6.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.2 (d, J = 252.0 Hz), 134.1 (d, J = 7.0 Hz), 131.0 (d, J = 8.0 Hz), 127.1 (d, J = 4.0 Hz), 122.8 (d, J = 21.0 Hz), 118.5 (d, J = 24.0 Hz), 50.0. IR (film), v, cm^{-1}: 3077, 2985, 2853, 1601, 1498, 1440, 1339, 1224, 1154, 801, 673, 547. ESI-MS, m/z (%): Calcd for $C_7H_5Br_2FO_2S^-$ ([M-H]$^-$): 330.83 (100.0), Found: 331.09 (100.0). Anal. Calcd for $C_7H_5Br_2FO_2S$: C 25.32, H 1.52, O 9.64, Found: C 25.38, H 1.34, O 9.79.



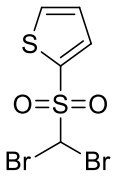
1-(Dibromomethylsulfonyl)-4-methoxybenzene (3l)

Gray solid (154 mg, 90%). m.p. 90.0-91.3 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90 (d, J = 8.0 Hz, 2H), 7.00 (d, J = 8.0 Hz, 2H), 6.16 (s, 1H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.2, 133.5, 123.0, 114.5, 55.9, 51.1. IR (film), v, cm^{-1}: 3086, 2980, 2840, 1587, 1498, 1457, 1339, 1264, 1155, 821, 651, 555. ESI-MS, m/z (%): Calcd for $C_8H_7Br_2O_3S^-$ ([M-H]$^-$): 342.85 (100.0), Found: 343.05 (30.7). Anal. Calcd for $C_8H_8Br_2O_3S$: C 27.93, H 2.34, O 13.95, Found: C 27.98, H 2.45, O 13.89.



2-(Dibromomethylsulfonyl)naphthalene (3m)

Yellow solid (153 mg, 84%). m.p. 126.9-128.7 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.65 (s, 1H), 8.05-7.96 (m, 4H), 7.76-7.66 (m, 2H), 6.33 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.1, 133.8, 131.9, 130.3, 129.7, 129.4, 129.1, 128.1, 128.0, 124.8, 50.8. IR (film), v, cm^{-1}: 3053, 2981, 1592, 1507, 1453, 1331, 1155, 813, 753, 653, 549. ESI-MS, m/z (%): Calcd for $C_{11}H_7Br_2O_3S^-$ ([M-H]$^-$): 362.85 (100.0), Found: 362.59 (65.7). Anal. Calcd for $C_{11}H_8Br_2O_2S$: C 36.29, H 2.21, O 8.79, Found: C 36.18, H 2.33, O 8.89.



2-(Dibromomethylsulfonyl)thiophene (3n)

Gray solid (168 mg, 77%). m.p. 120.9-122.8 ℃. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88-7.83 (m, 2H), 7.21-7.18 (m, 1H), 6.27 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.0, 137.4, 131.4, 128.2, 51.0. IR (film), v, cm^{-1}: 3095, 2923, 1503, 1457, 1339, 1155, 744, 627, 577. ESI-MS, m/z (%): Calcd for $C_5H_3Br_2O_2S_2^-$ ([M-H]$^-$): 318.79 (100.0), Found: 319.36 (64.7). Anal. Calcd for $C_5H_4Br_2O_2S_2$: C 18.77, H 1.26, O 10.00, Found: C 18.88, H 1.37, O 10.26.

References

1. (a) Y.-H. Tan, J.-X. Li, F.-L. Xue, J. Qi, Z.-Y. Wang, *Tetrahedron* **2012**, *68*. 2827. (b) F.-L. Xue, J.-X.

Li, Z.-Y. Wang, J.-F. Xiong. *Res. Chem. Intermed.* **2013**, *39*, 1153. (c) J.-P. Huo, P. Peng, G.-H. Deng, W. Wu, J.-F. Xiong, M.-L. Zhong, Z.-Y. Wang, *Macromol. Rapid Commun*. **2013**, *34*, 1779. (d) J.-P. Huo, J.-C. Luo, W. Wu, J.-F. Xiong, G.-Z. Mo, Z.-Y. Wang, *Ind. Eng. Chem. Res*. **2013**, *52*, 11850.

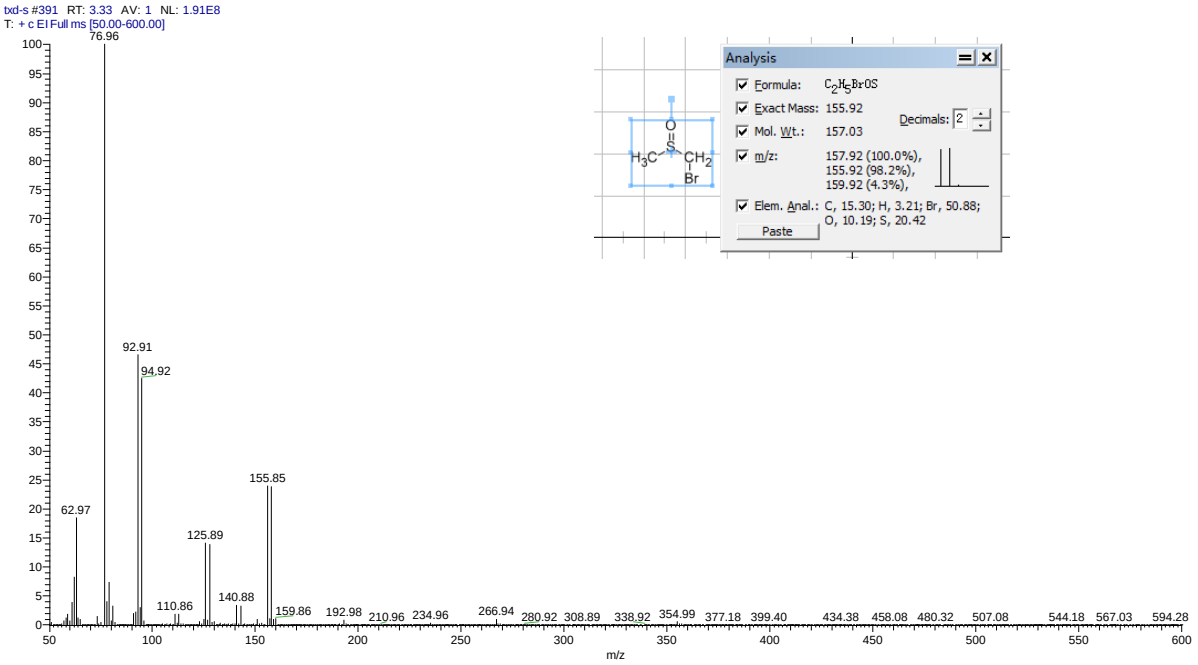
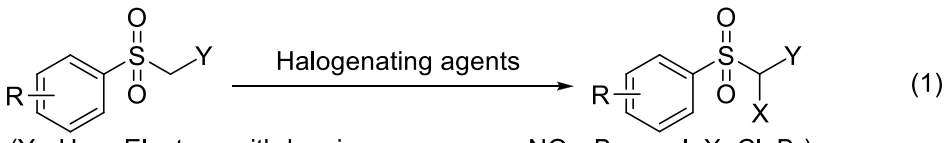


Figure S1. MS spectrum of intermediate **I** in **Schemes 3** and **4** detected by GC-MS

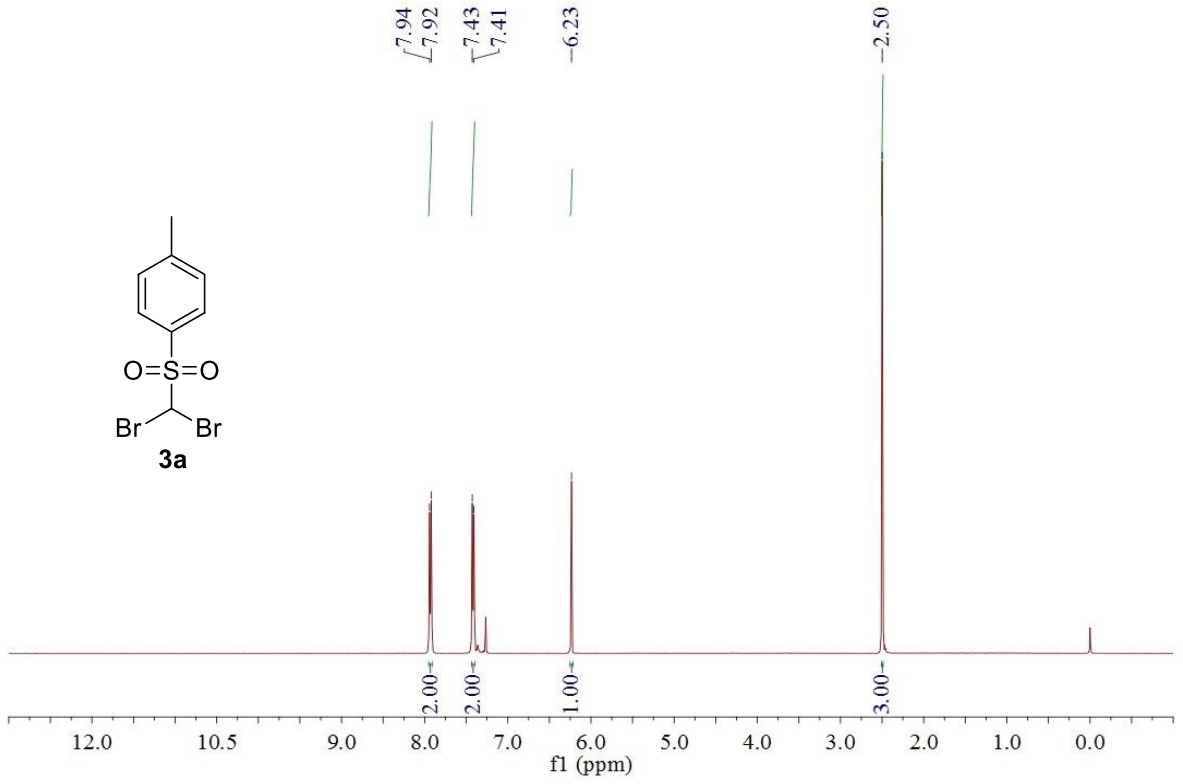


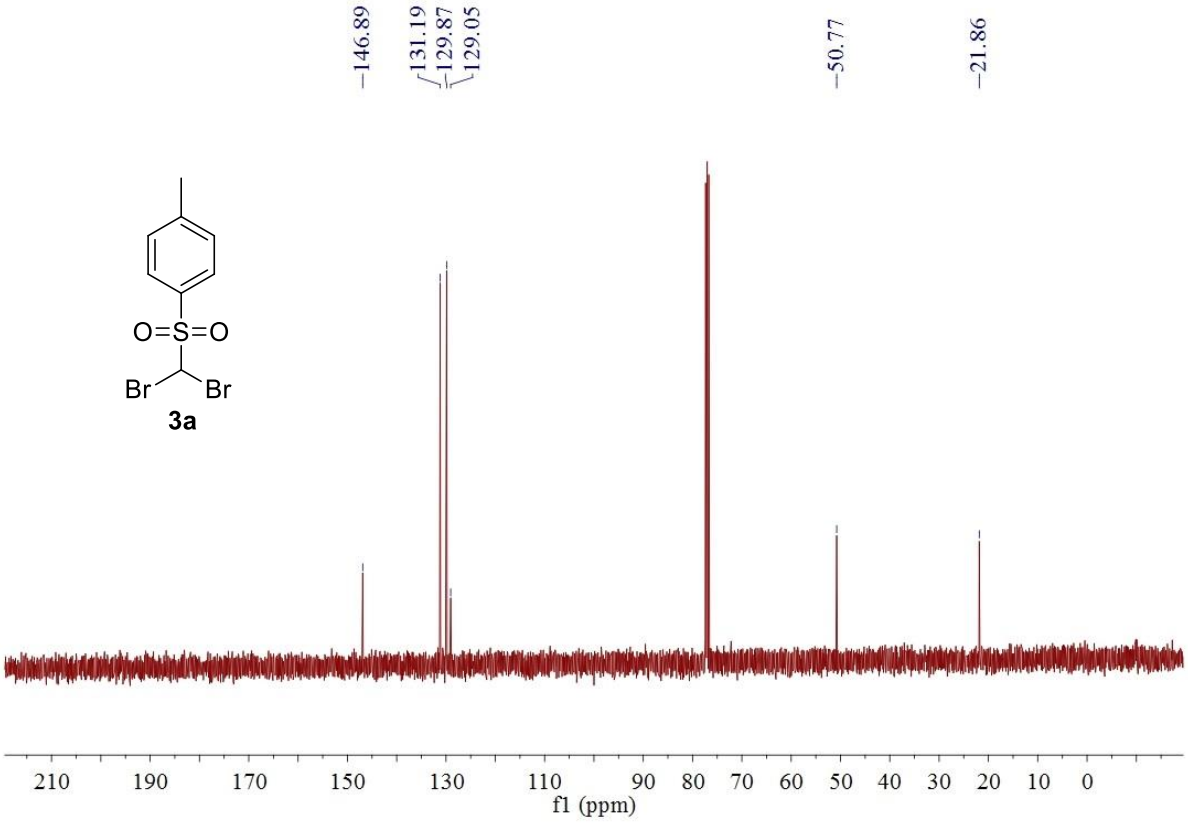
$$RSO_2Na + CHX_3 \xrightarrow{KOH} RSO_2CHX_2 + NaX \quad (2)$$

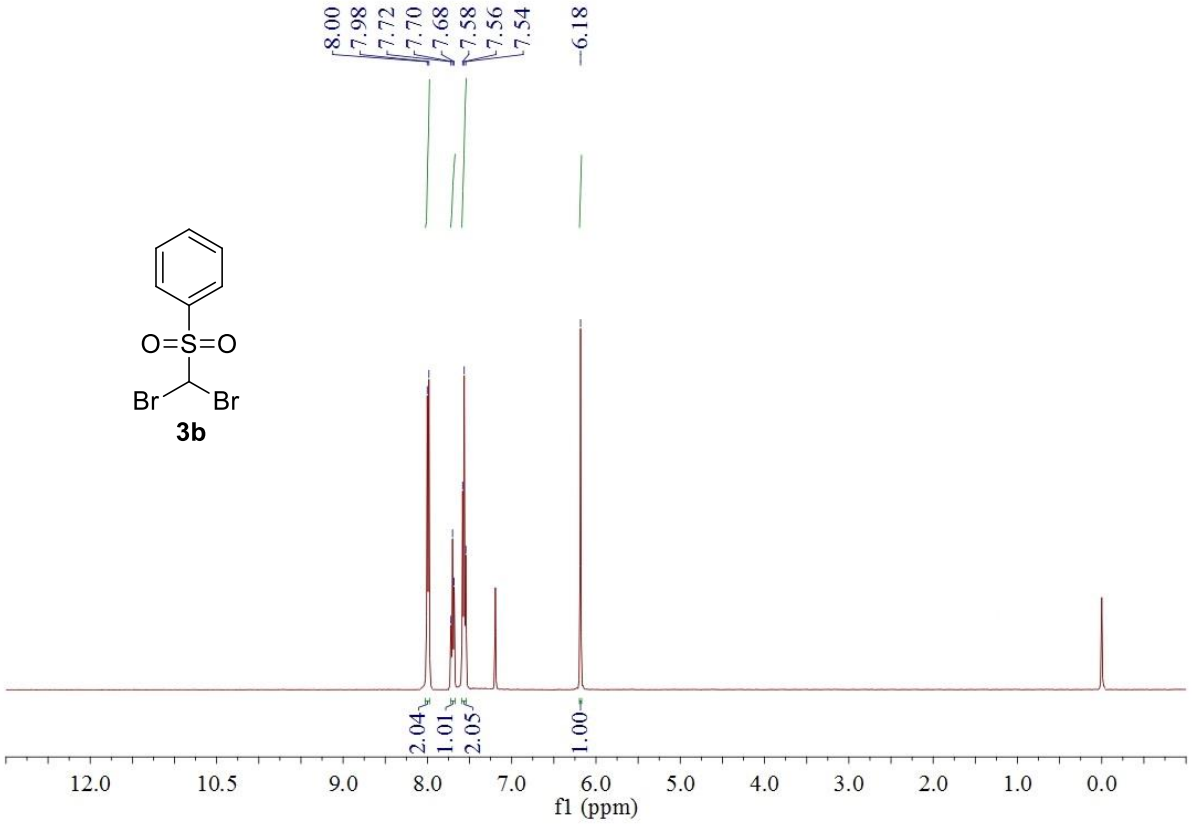
(X=Cl, Br)

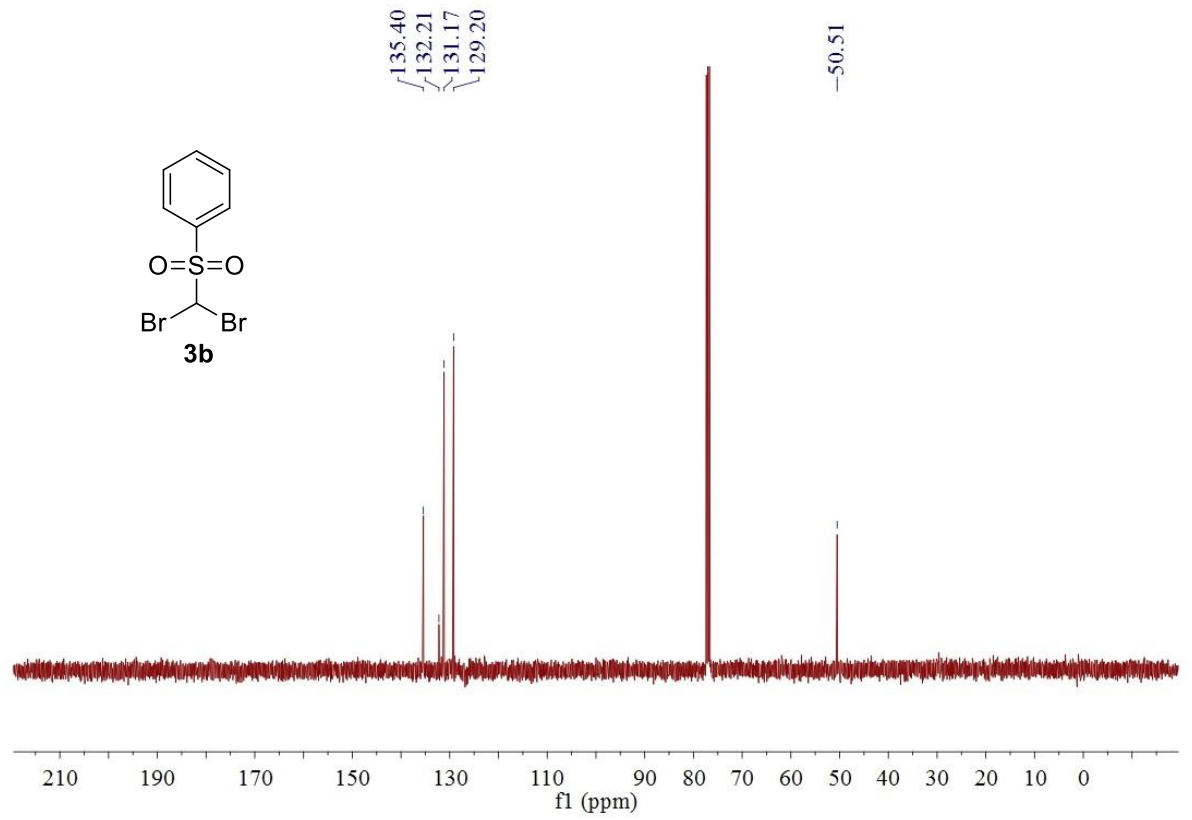
Scheme S1. The reported synthetic methods of arylsulfonyl dibromomethanes

NMR Spectra for All Compounds 3






8.00
7.98
7.72
7.70
7.68
7.58
7.56
7.54
6.18
O=S=O
Br
Br
3b
2.04
1.01
2.05
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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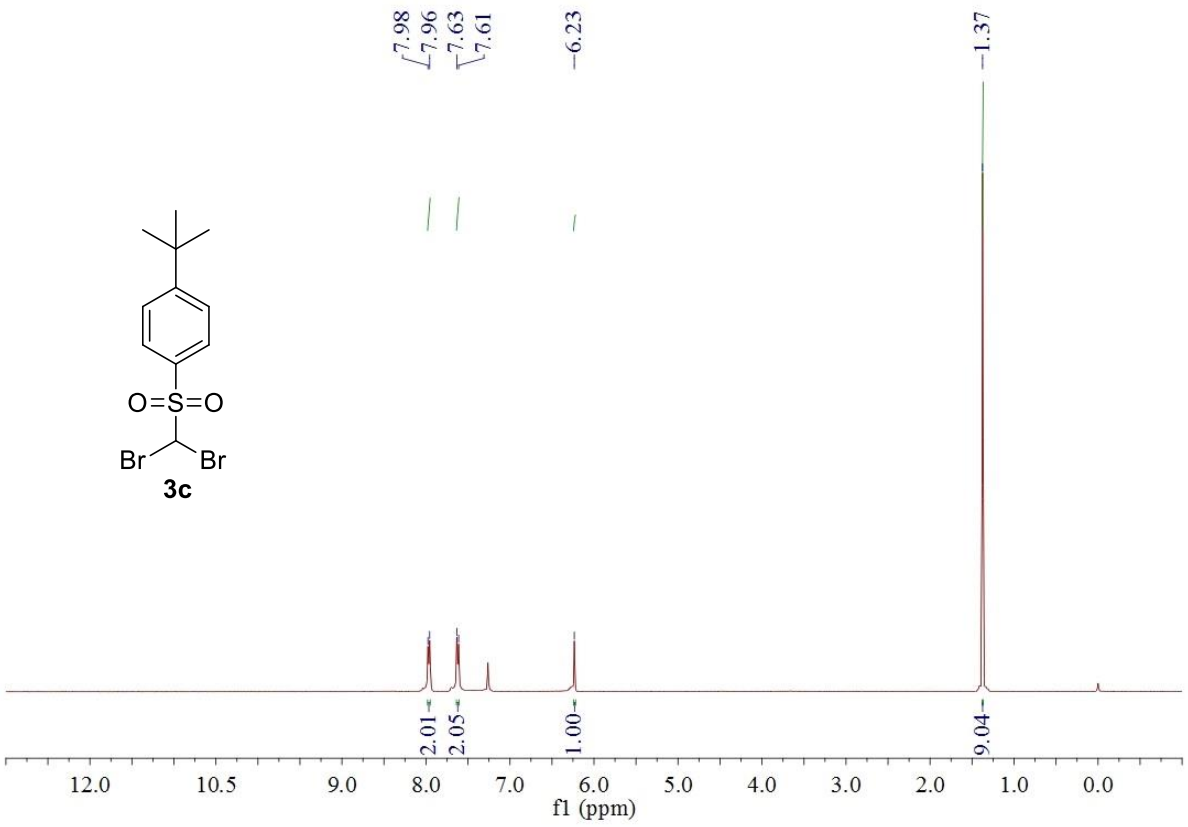
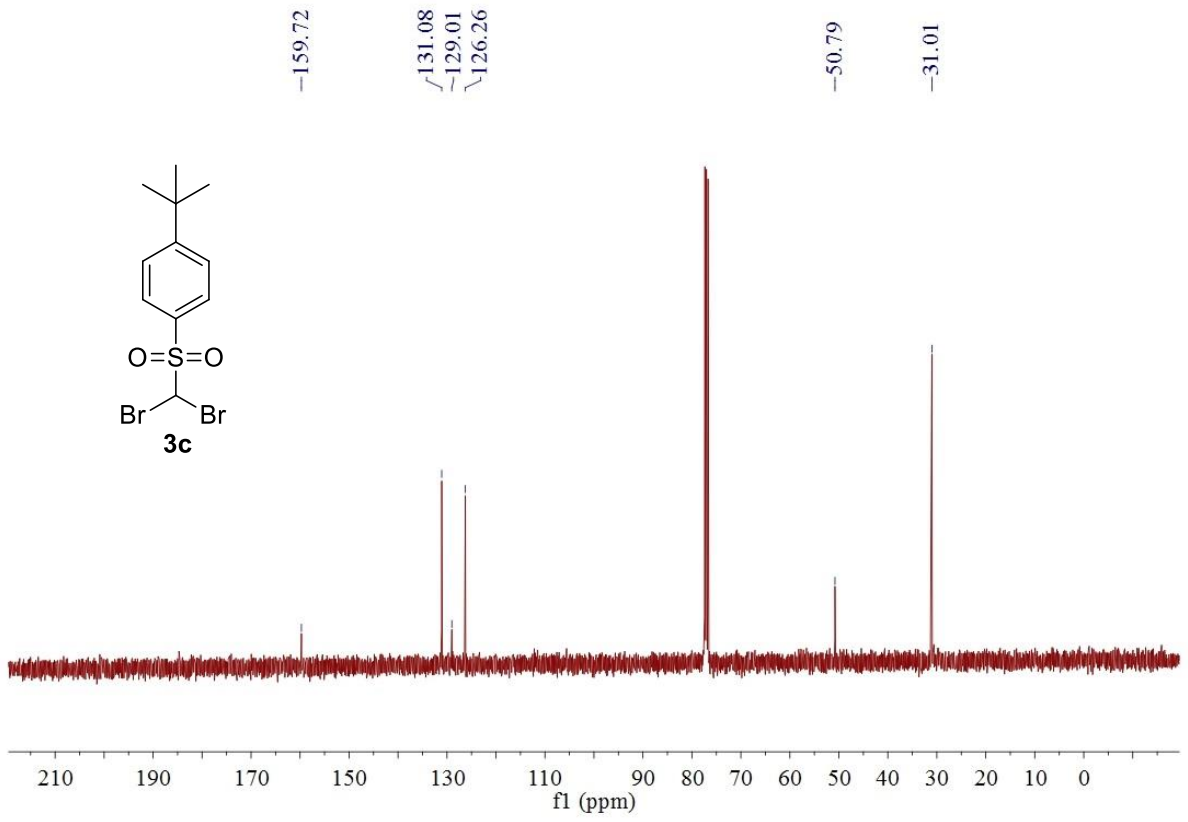
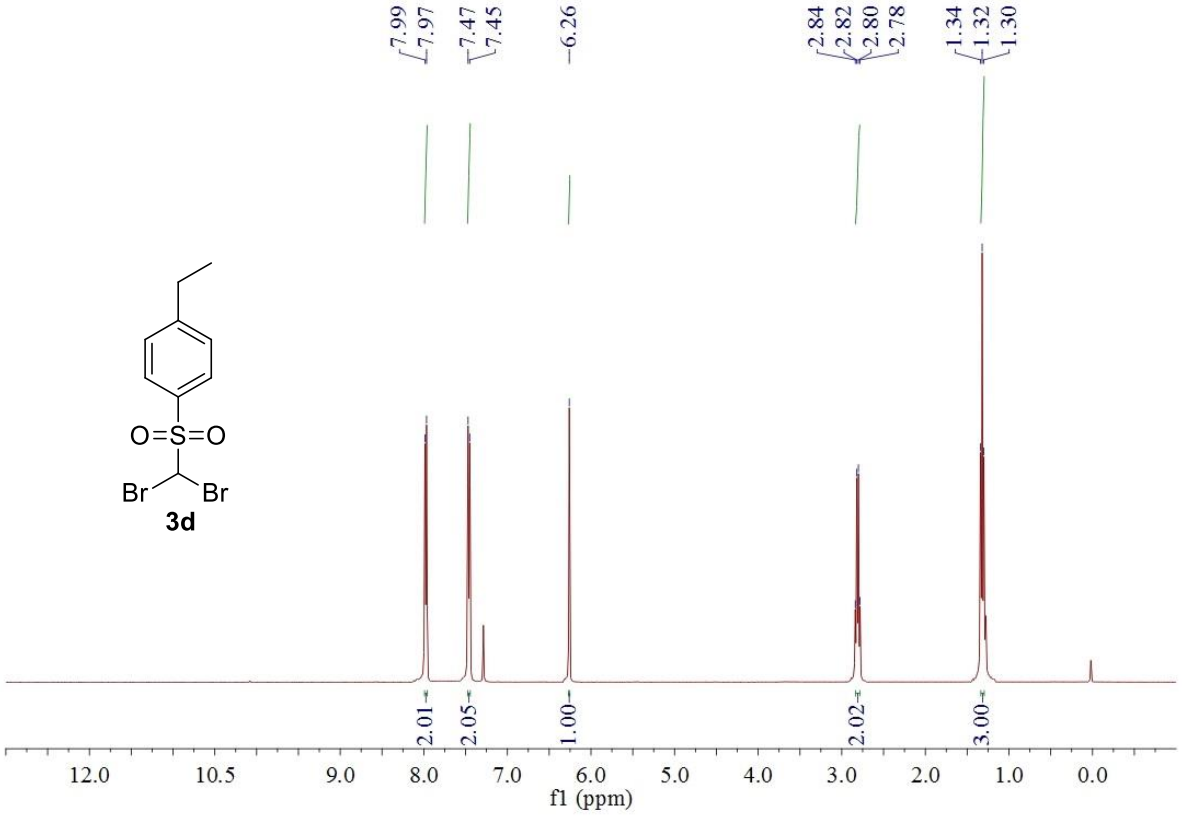
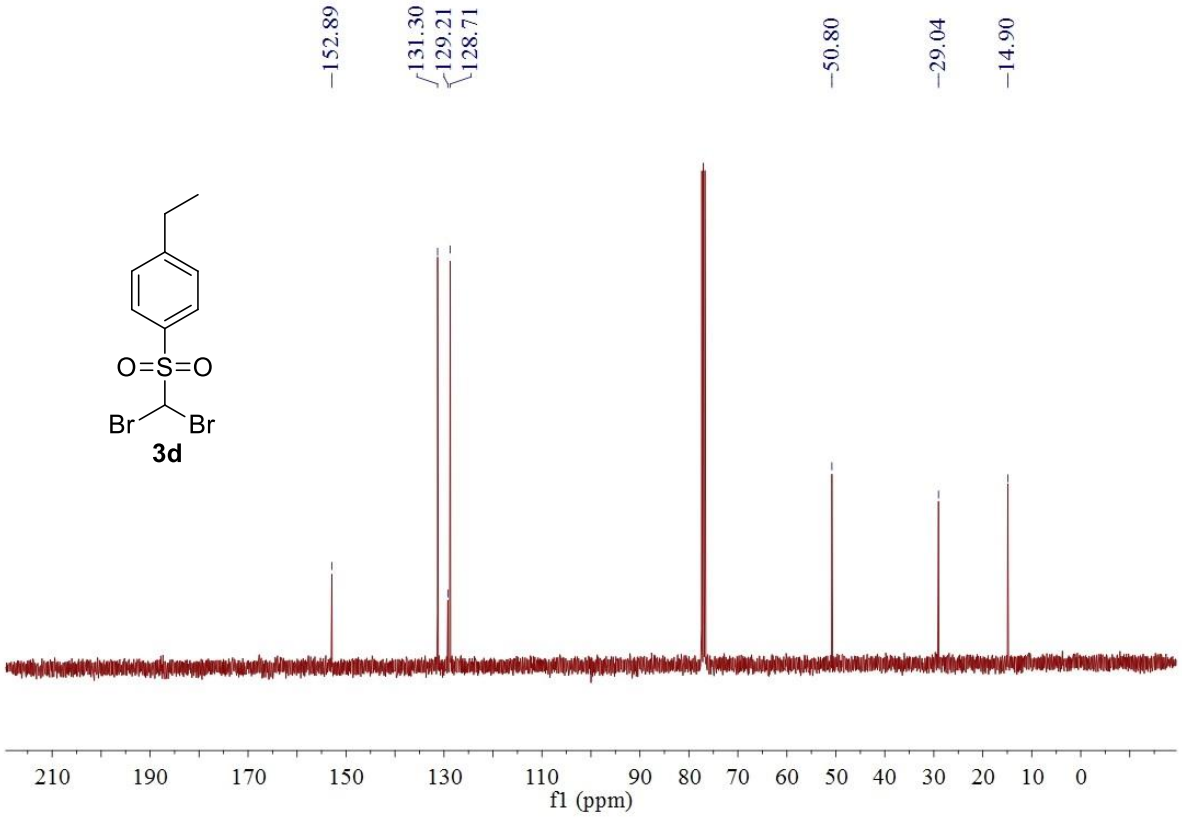
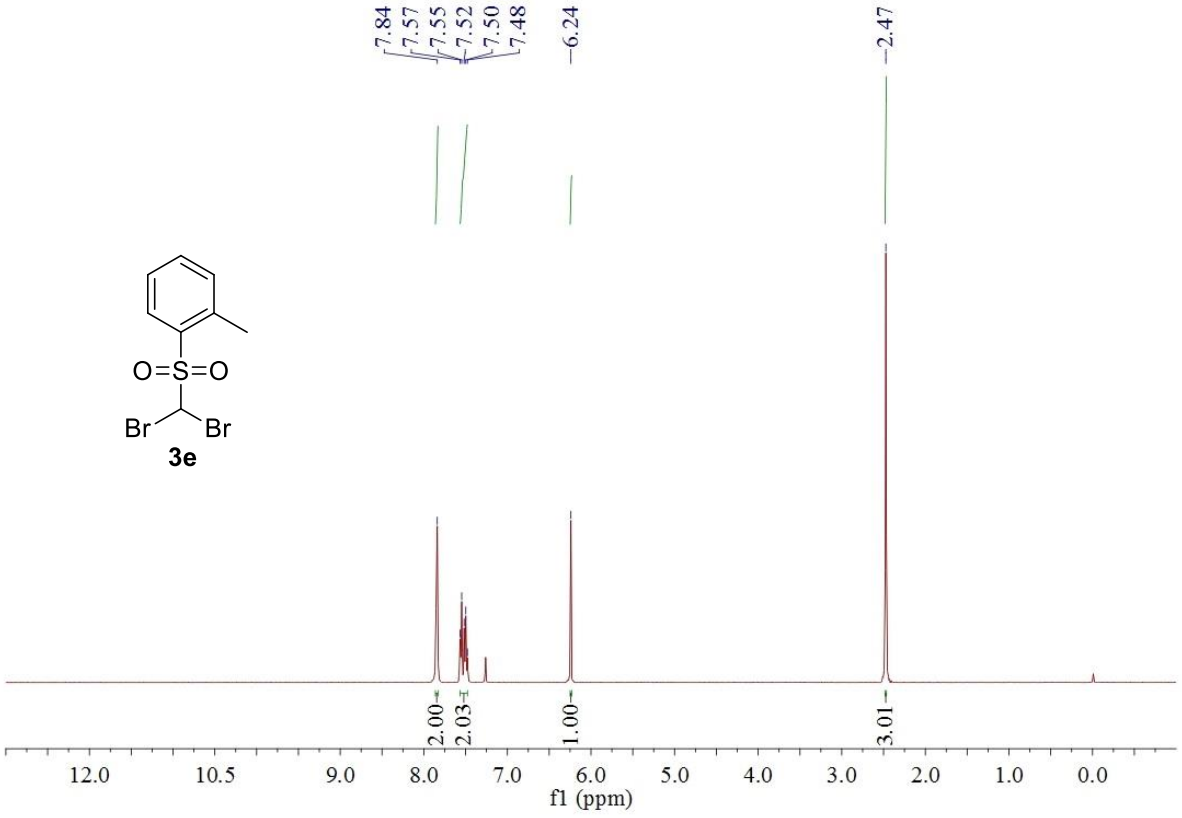
132.21
131.17
129.20
50.51
O=S=O
Br
Br
3b
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

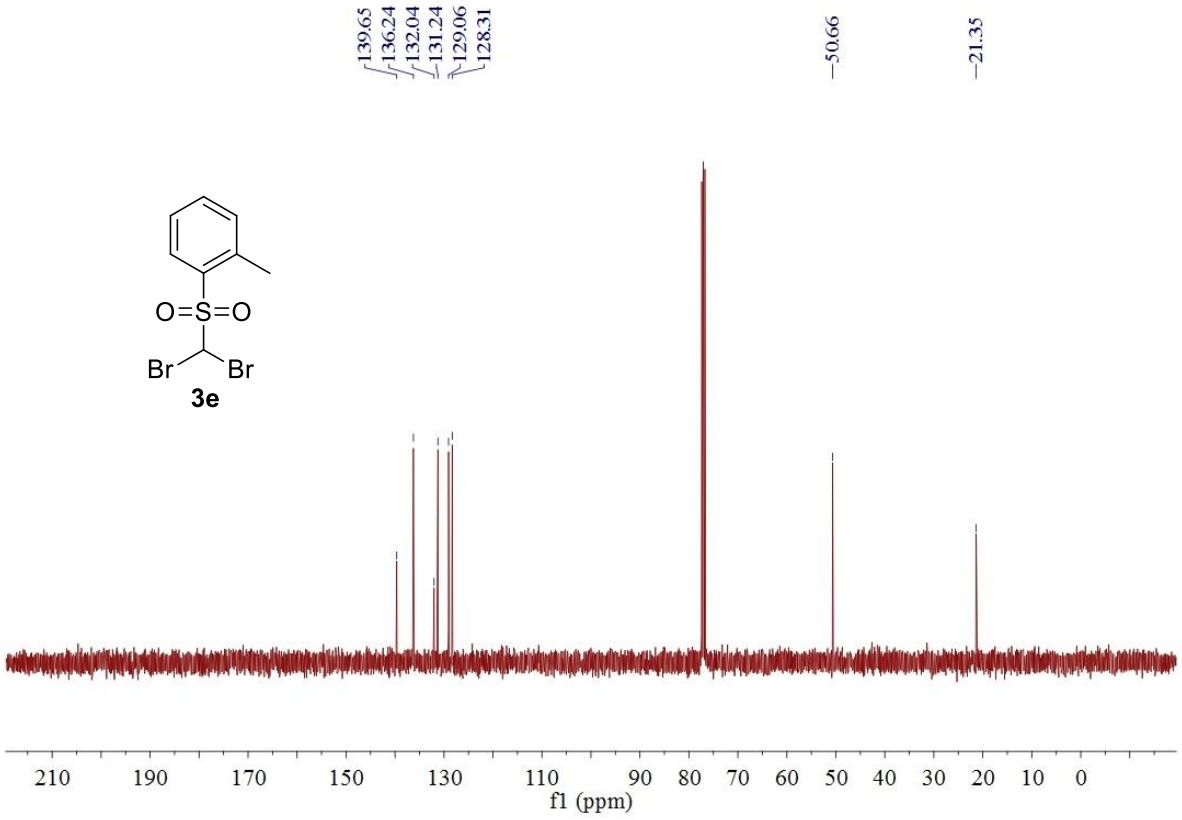

7.98
7.96
7.63
7.61
6.23
1.37
O=S=O
Br
Br
3c
2.01
2.05
1.00
9.04
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

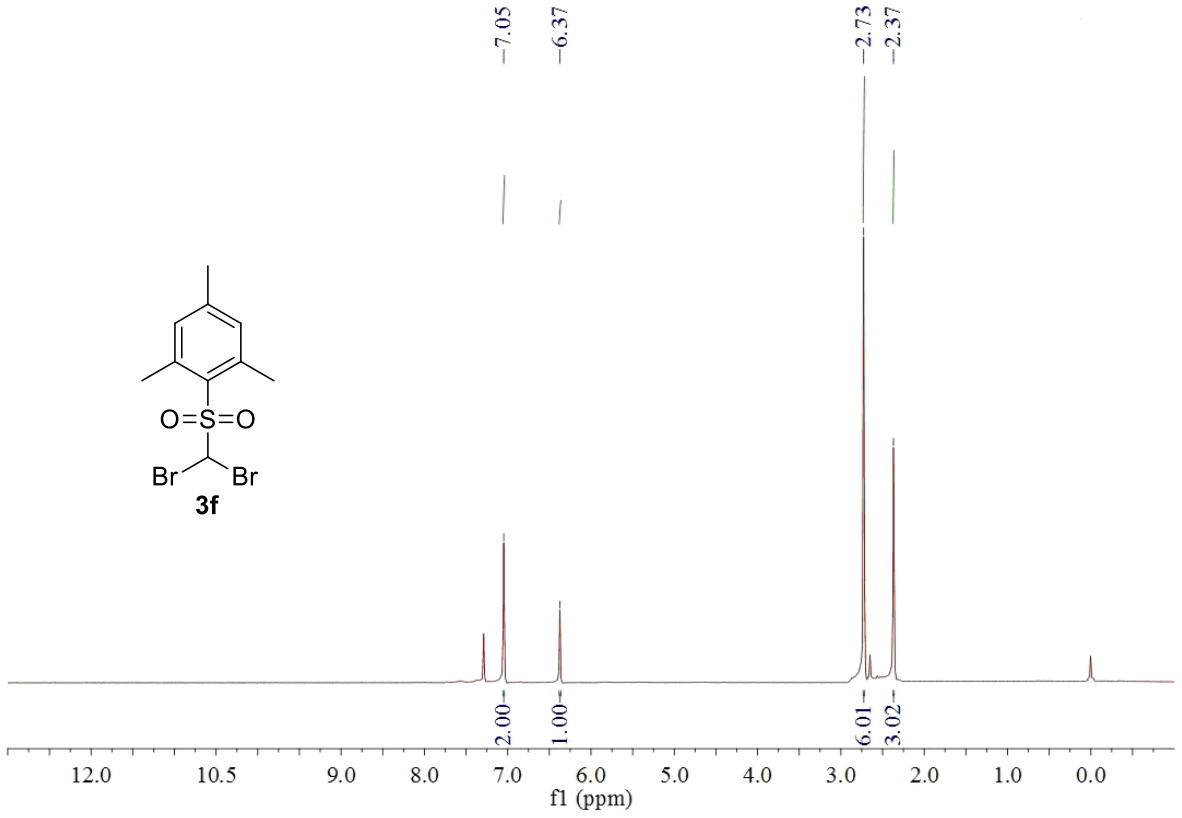

159.72
131.08
129.01
126.26
50.79
31.01
O=S=O
Br
Br
3c
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

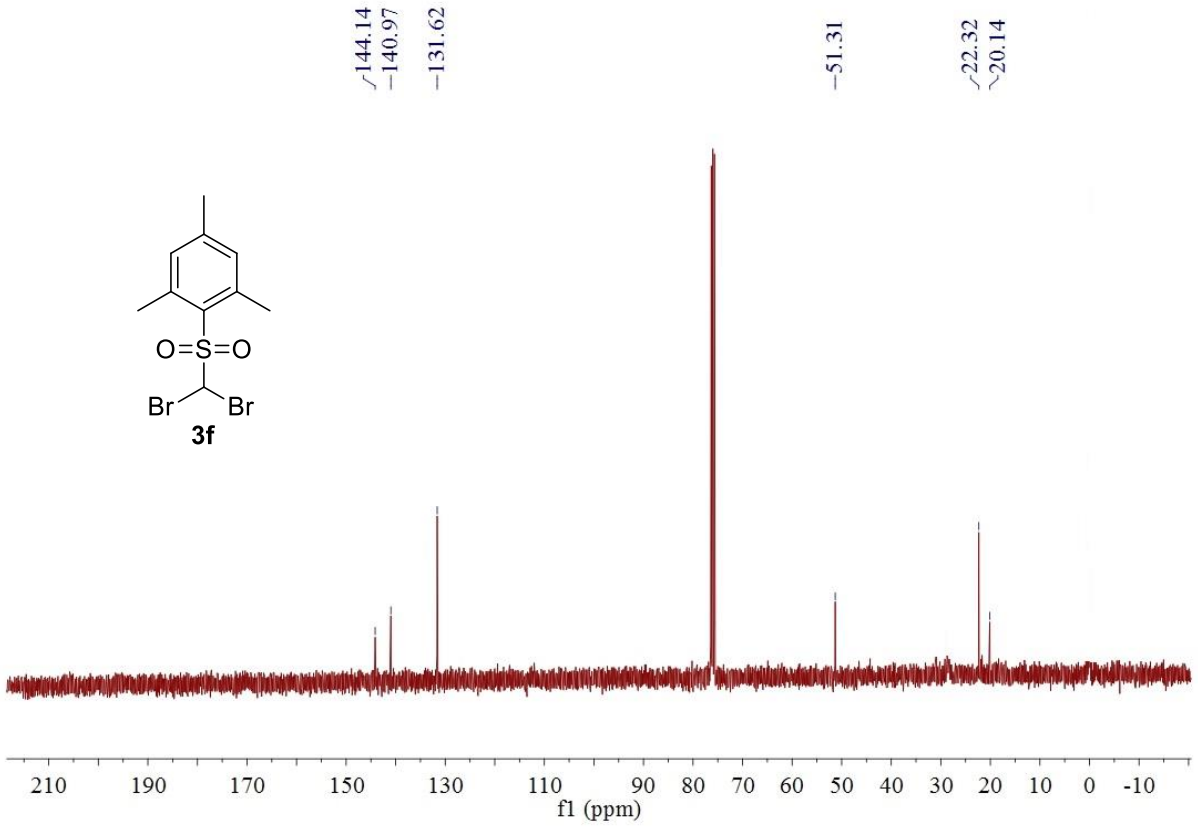

7.99
7.97
7.47
7.45
6.26
2.84
2.82
2.80
2.78
1.34
1.32
1.30
O=S=O
Br
Br
3d
2.01
2.05
1.00
2.02
3.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

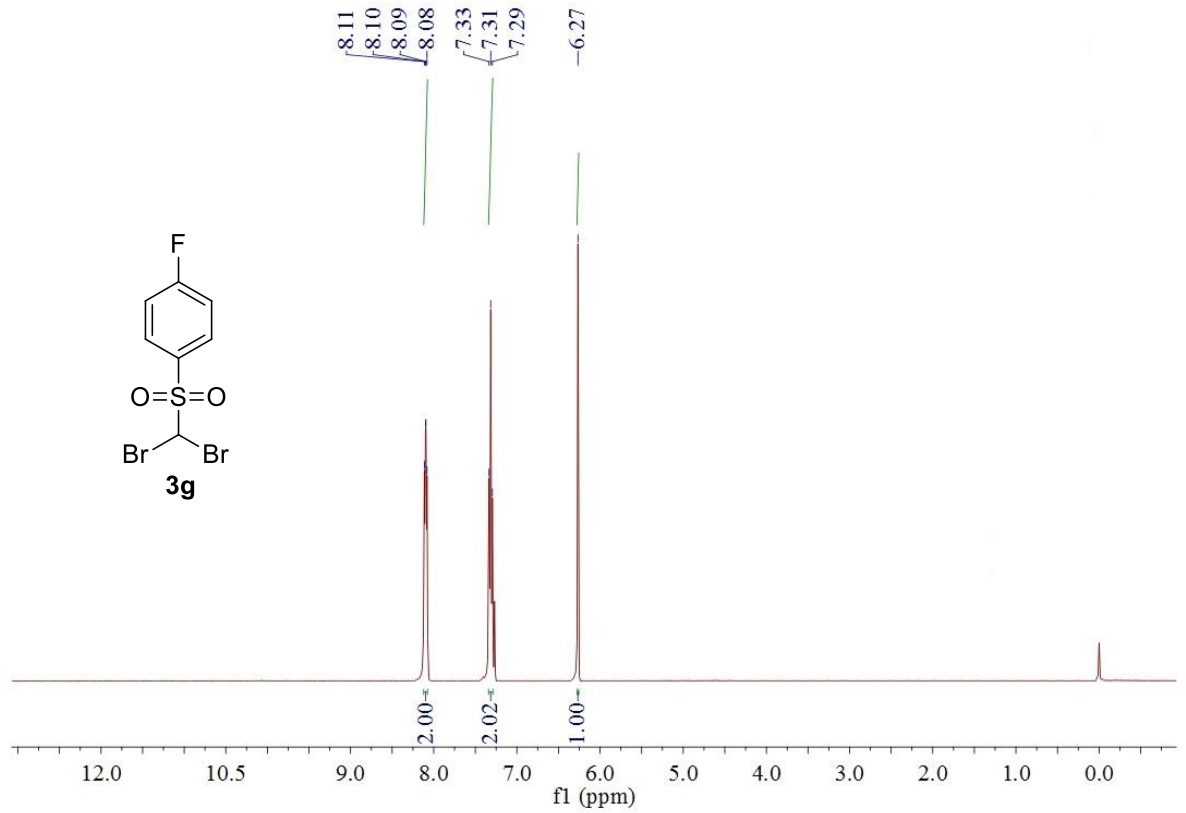

152.89
131.30
129.21
128.71
50.80
29.04
14.90
O=S=O
Br
Br
3d
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

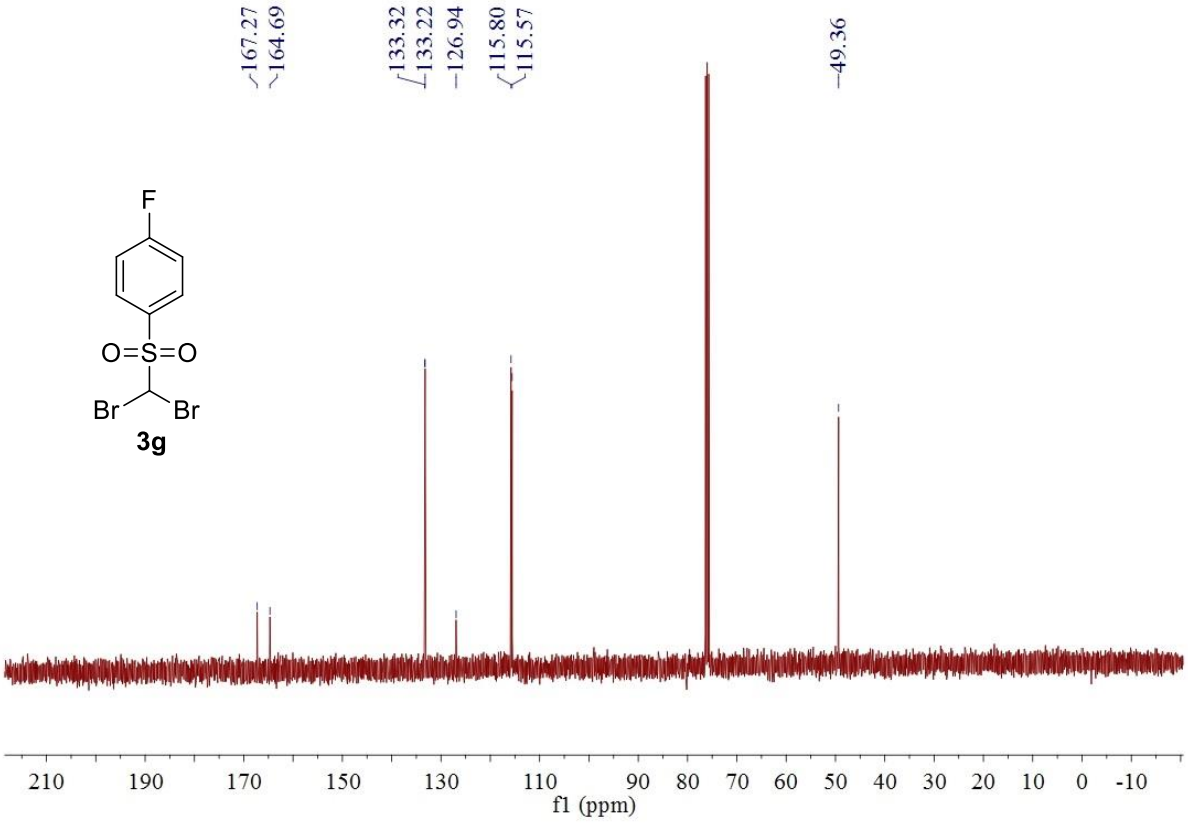

7.84
7.57
7.55
7.52
7.50
7.48
6.24
2.47
O=S=O
Br
Br
3e
2.00
2.03
1.00
3.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

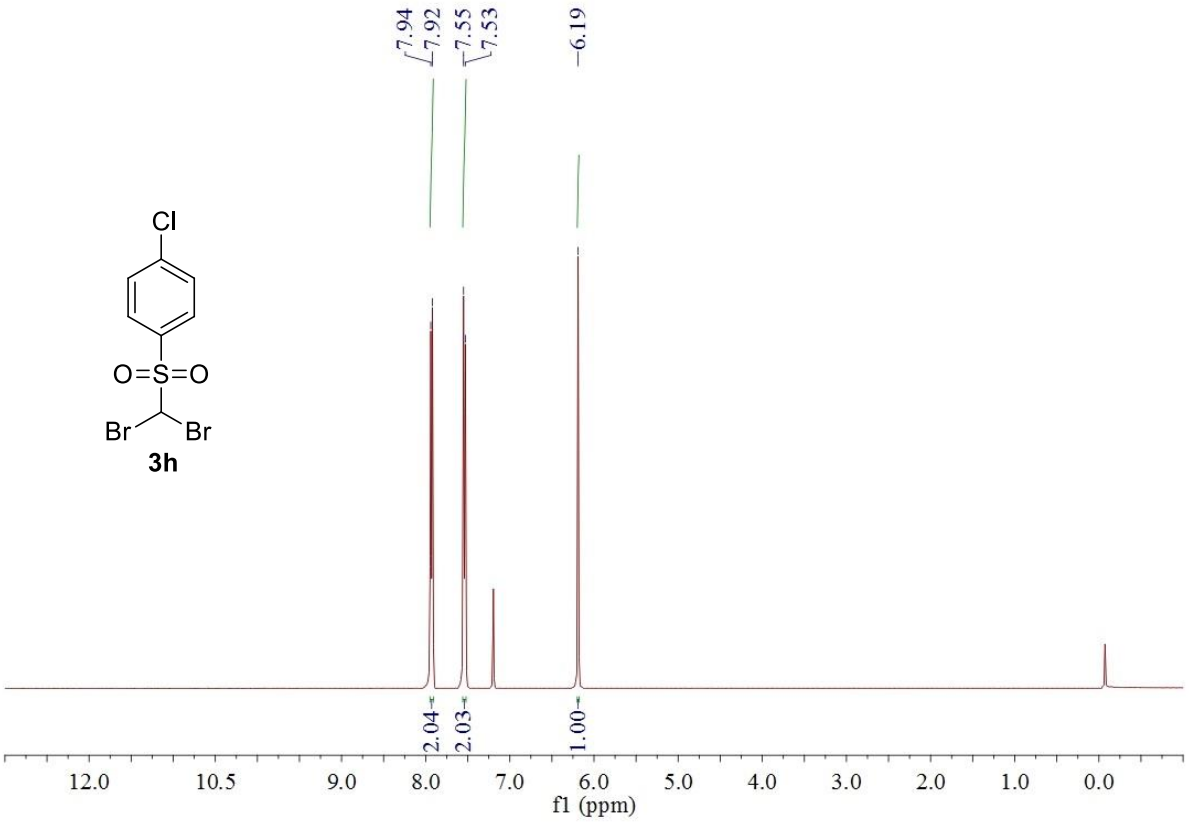

139.65
136.24
132.04
131.24
129.06
128.31
50.66
21.35
O=S=O
Br
Br
3e
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

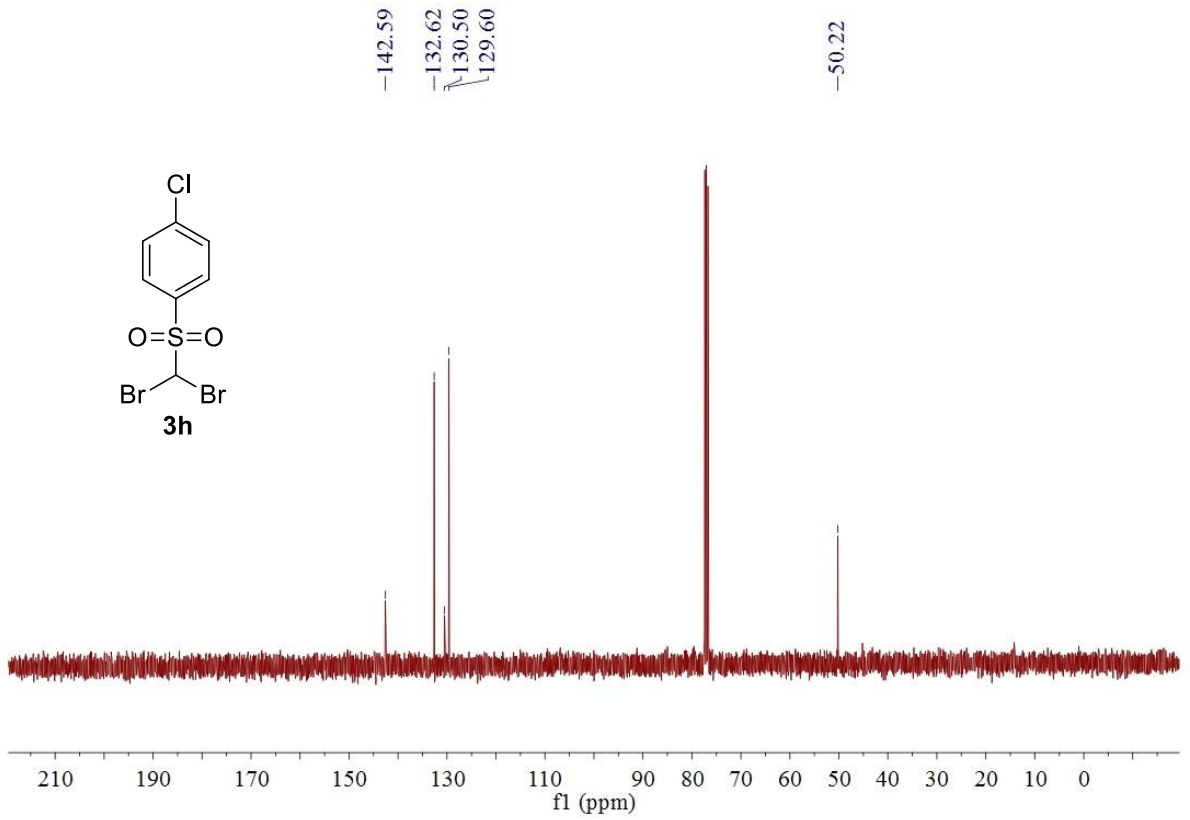

7.05
6.37
2.73
2.37
O=S=O
Br
Br
3f
2.00
1.00
6.01
3.02
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

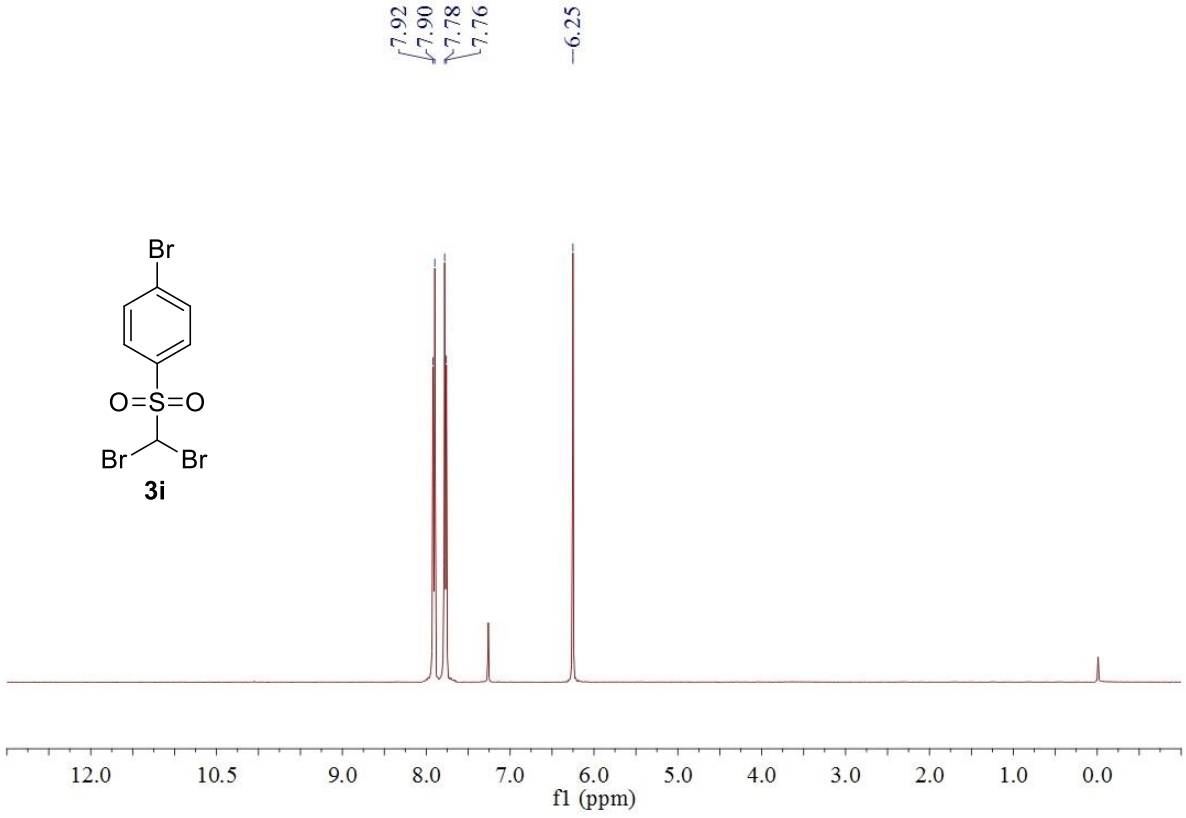

144.14
140.97
131.62
51.31
22.32
20.14
O=S=O
Br
Br
3f
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

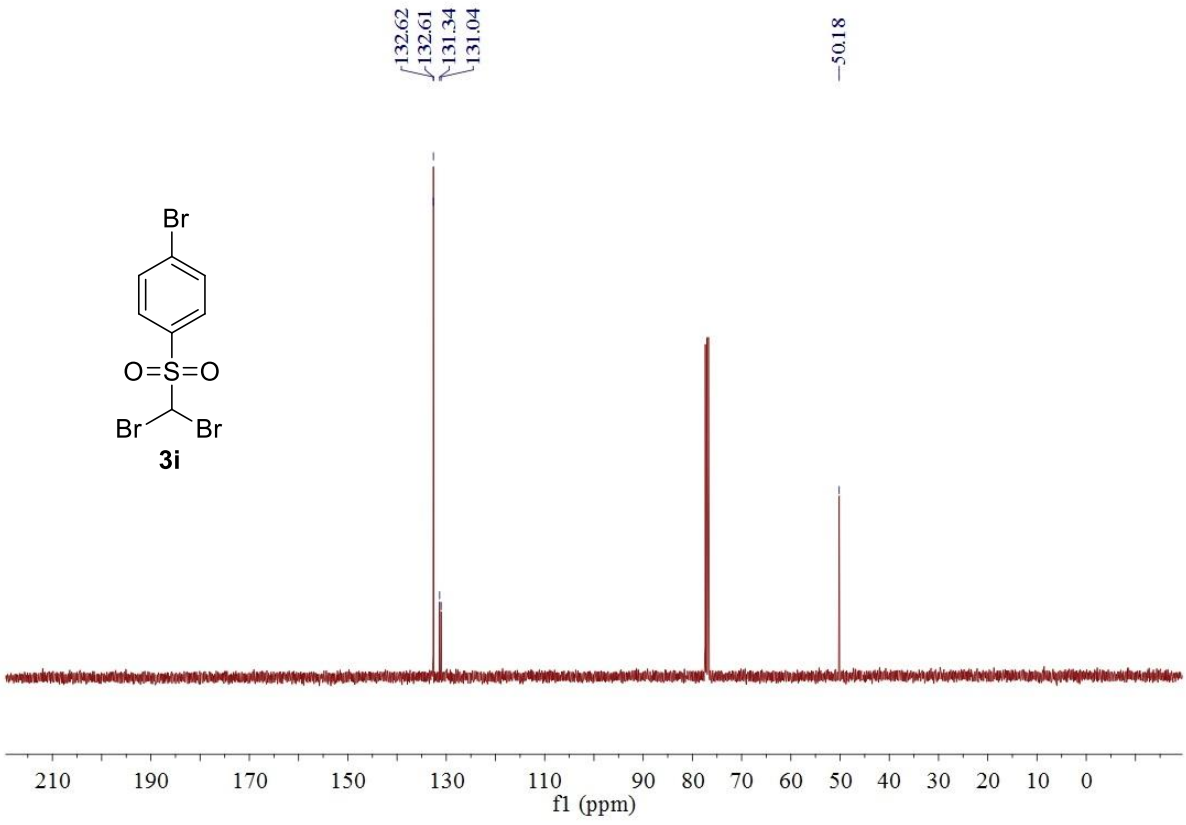

8.11
8.10
8.09
8.08
7.33
7.31
7.29
6.27
F
O=S=O
Br
Br
3g
2.00
2.02
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

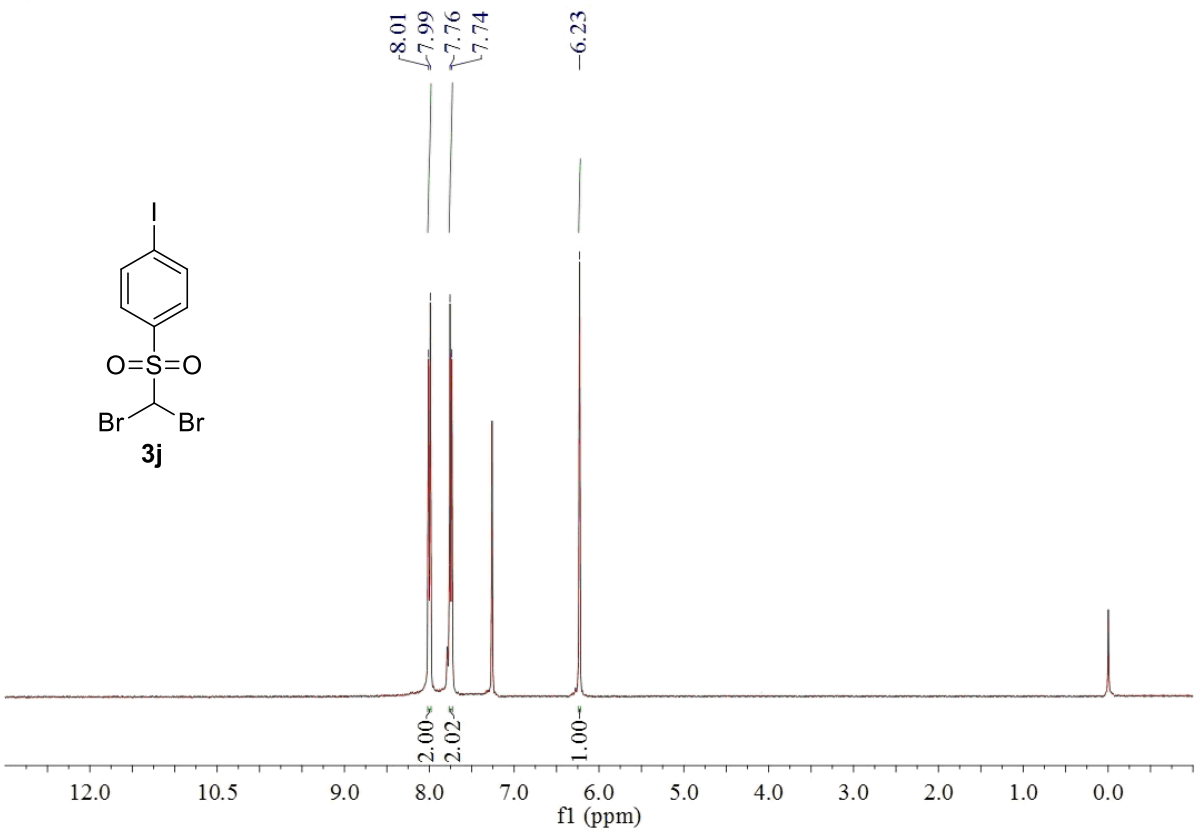

167.27
164.69
133.32
133.22
126.94
115.80
115.57
49.36
F
O=S=O
Br
Br
3g
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

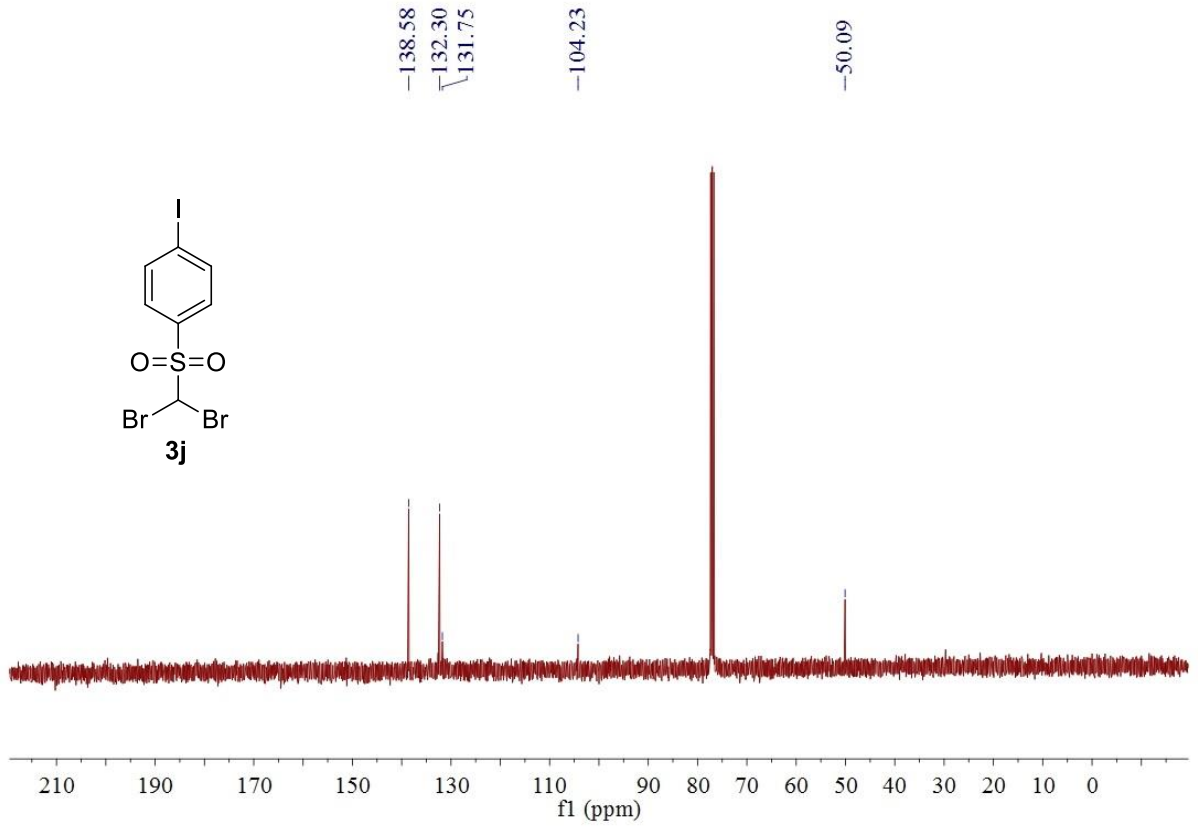

7.94
7.92
7.55
7.53
6.19
Cl
O=S=O
Br
Br
3h
2.04
2.03
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

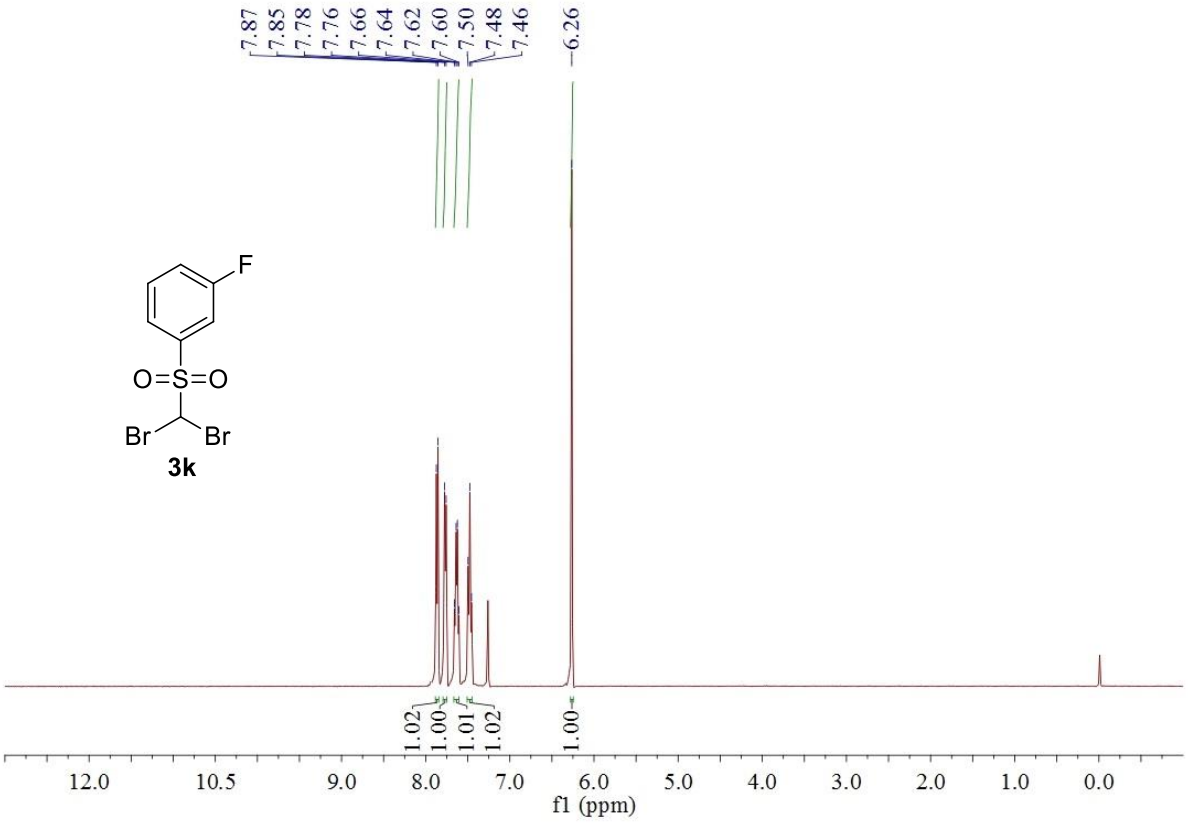

142.59
132.62
130.50
129.60
50.22
Cl
O=S=O
Br
Br
3h
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

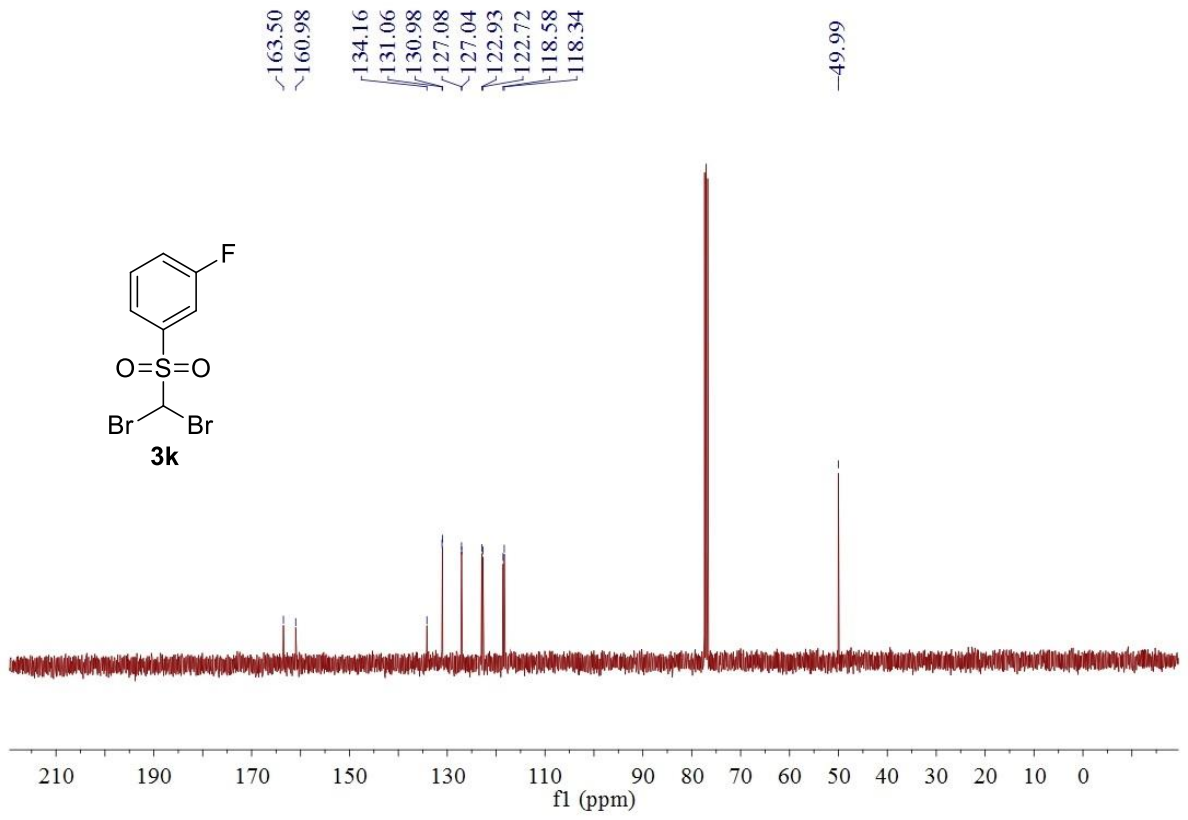

7.92
7.90
7.78
7.76
6.25
Br
O=S=O
Br
Br
3i
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

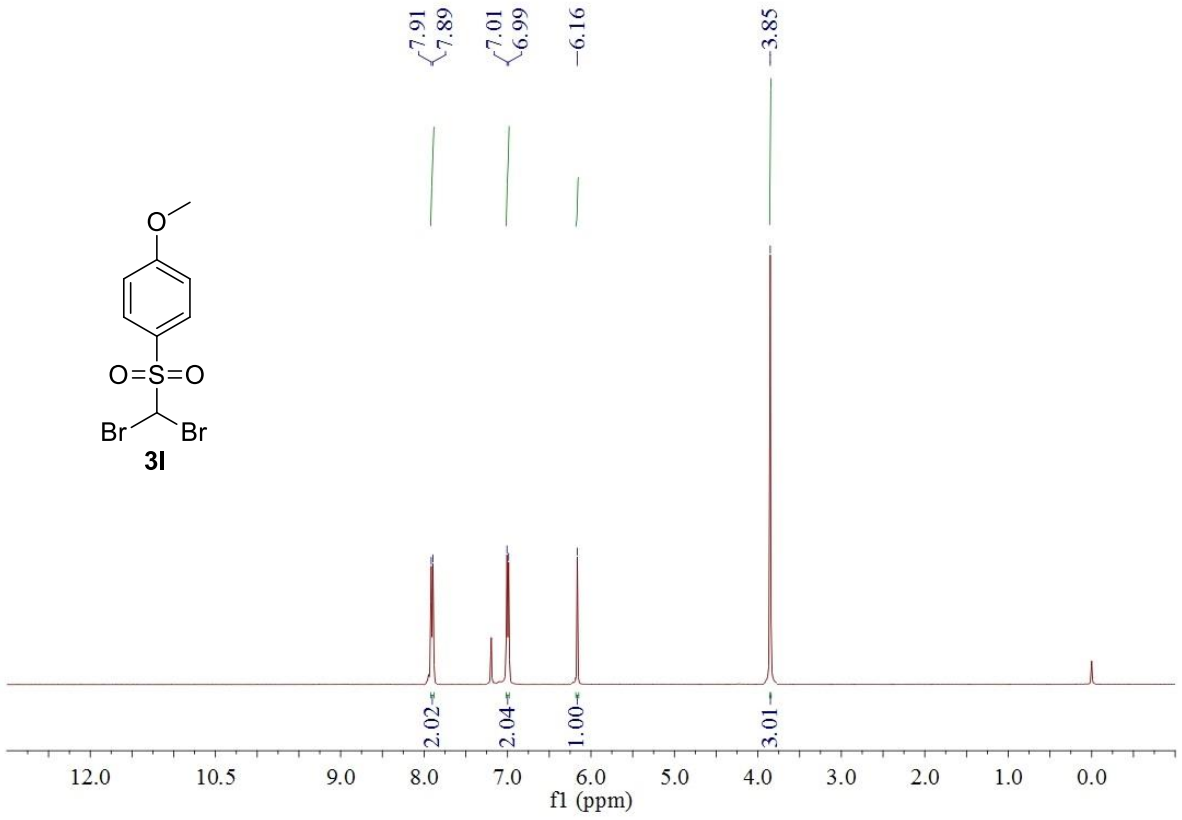

132.62
132.61
131.34
131.04
50.18
Br
O=S=O
Br
Br
3i
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

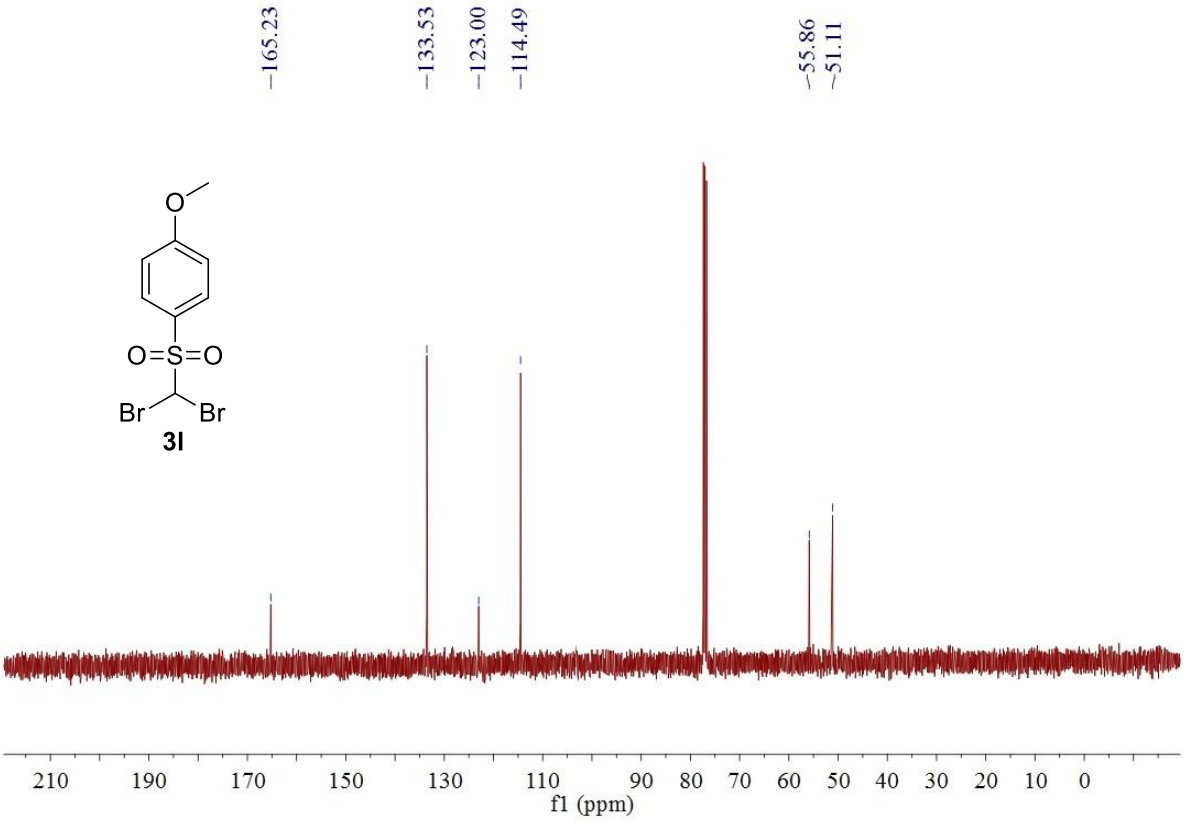

8.01
7.99
7.76
7.74
6.23
I
O=S=O
Br
Br
3j
2.00
2.02
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

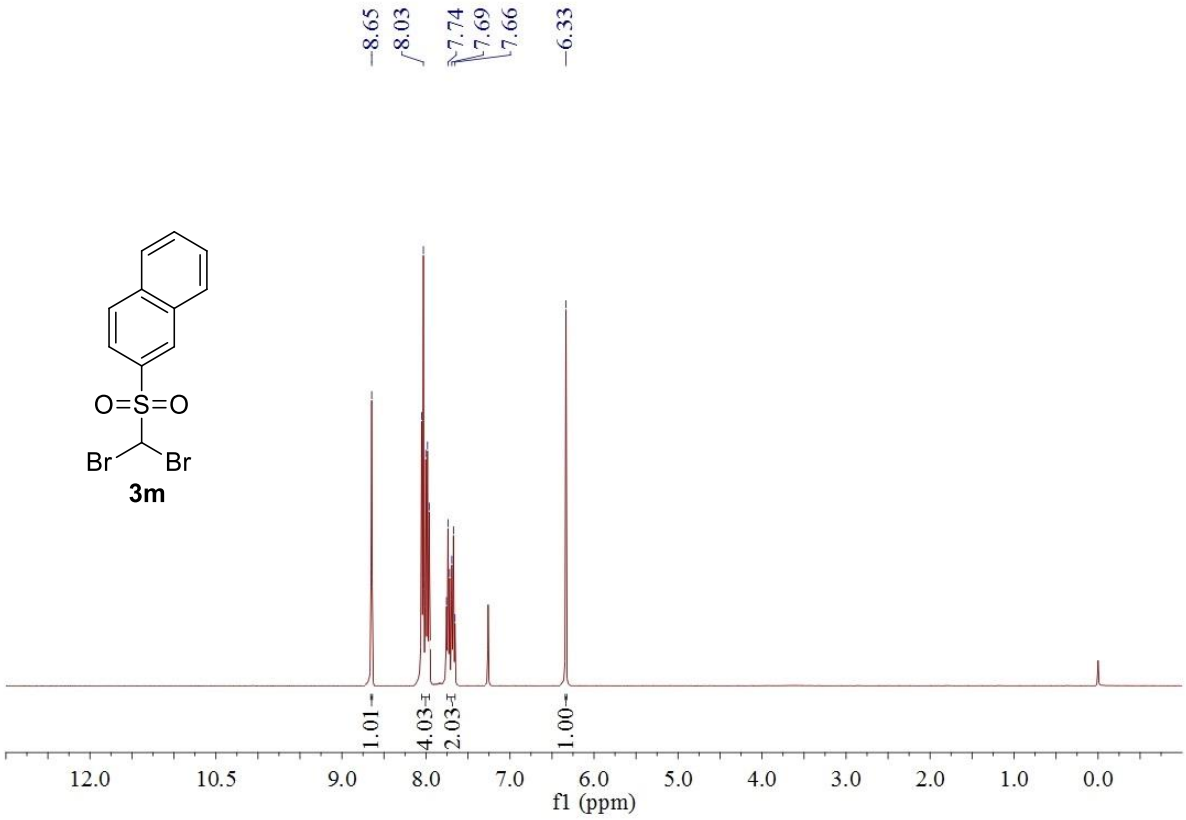

138.58
132.30
131.75
104.23
50.09
I
O=S=O
Br
Br
3j
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

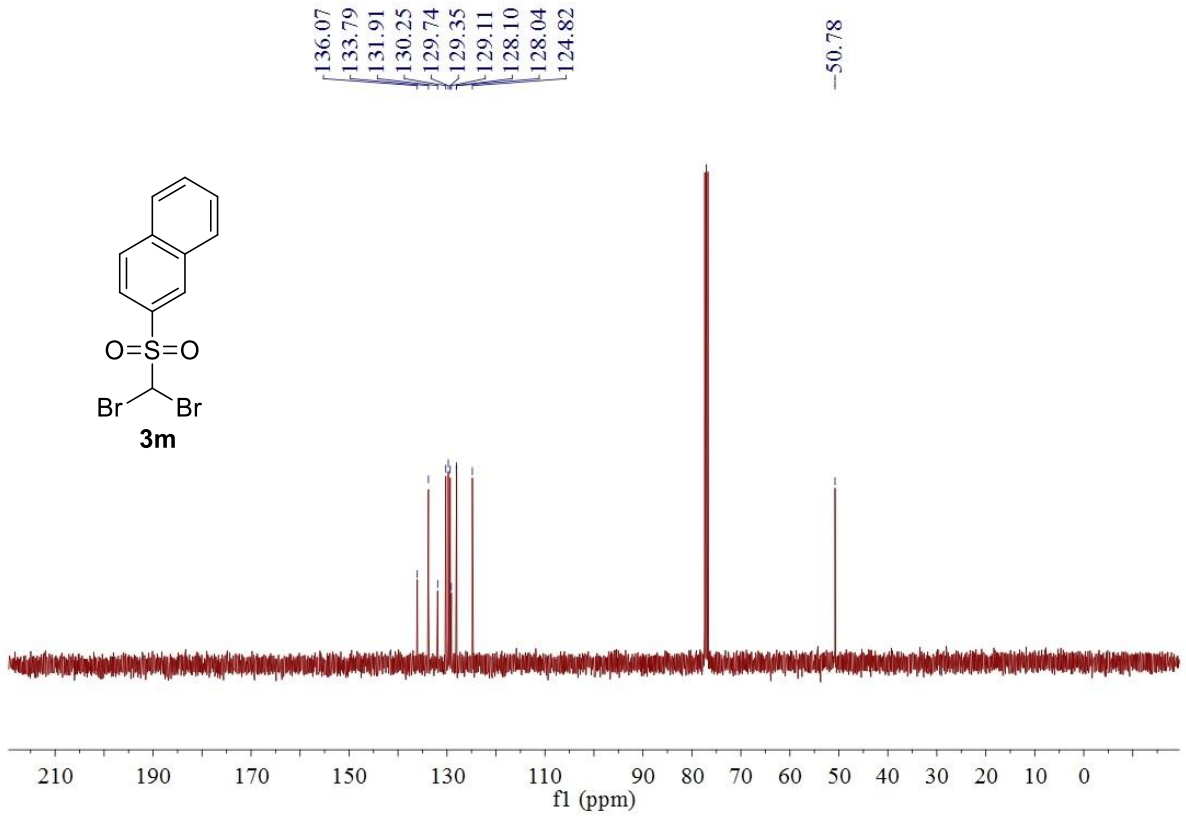

7.87
7.85
7.78
7.76
7.66
7.64
7.62
7.60
7.50
7.48
7.46
6.26
F
O=S=O
Br
Br
3k
1.02
1.00
1.01
1.02
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

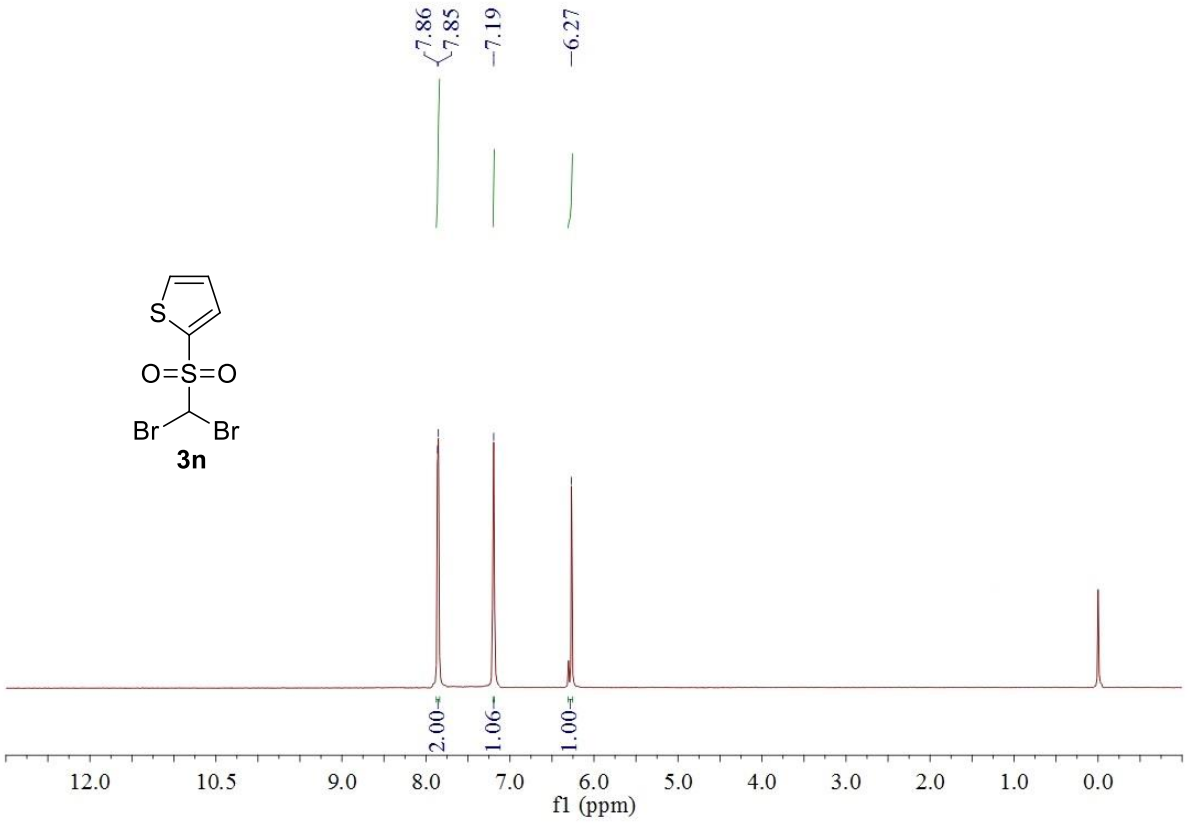

163.50
160.98
134.16
131.06
130.98
127.08
127.04
122.93
122.72
118.58
118.34
49.99
F
O=S=O
Br
Br
3k
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

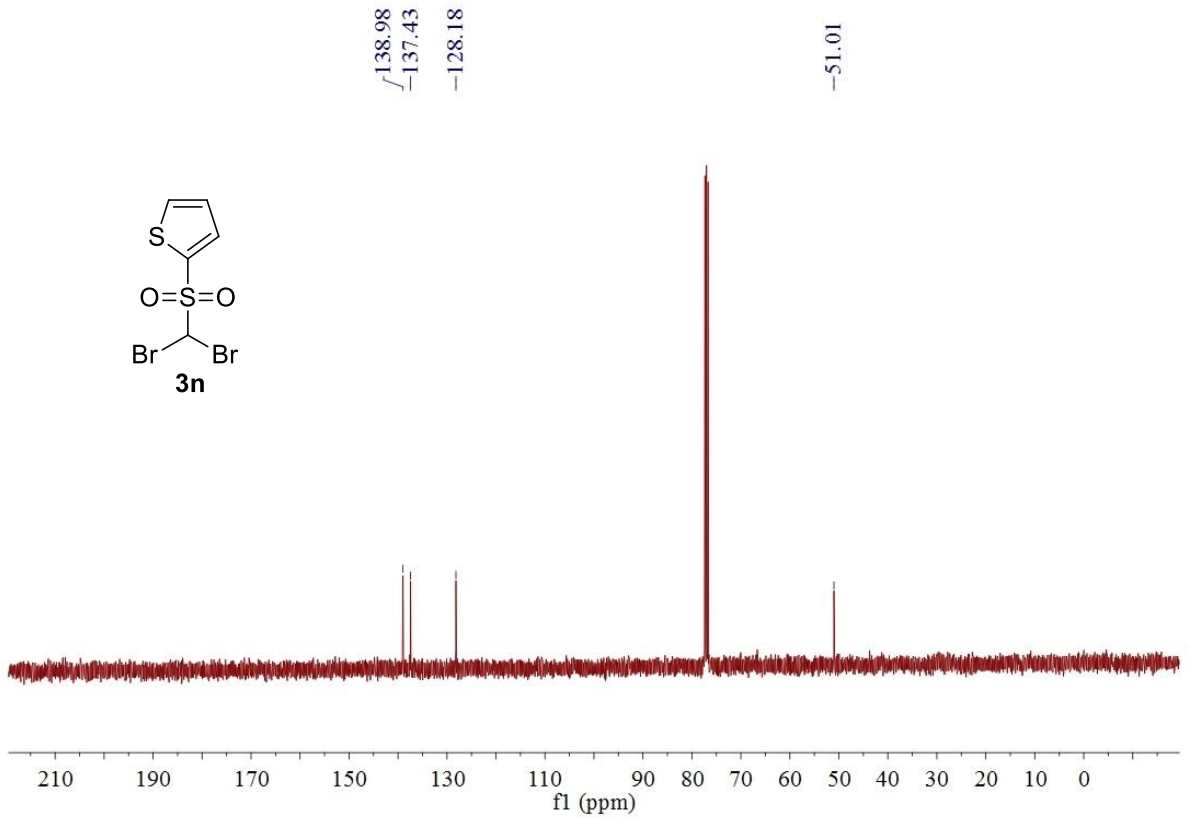

7.91
7.89
7.01
6.99
6.16
3.85
O
O=S=O
Br
Br
3l
2.02
2.04
1.00
3.01
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


165.23
133.53
123.00
114.49
55.86
51.11
O
O=S=O
Br
Br
3l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.65
8.03
7.74
7.69
7.66
6.33
O=S=O
Br
Br
3m
1.01
4.03
2.03
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


136.07
133.79
131.91
130.25
129.74
129.35
129.11
128.10
128.04
124.82
50.78
O=S=O
Br
Br
3m
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.86
7.85
7.19
6.27
S
O=S=O
Br
Br
3n
2.00
1.06
1.00
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


138.98
137.43
128.18
51.01
S
O=S=O
Br
Br
3n
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)