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

Efficient Silver-Catalyzed Direct Sulfenylation and Selenylation of Rich Arenes

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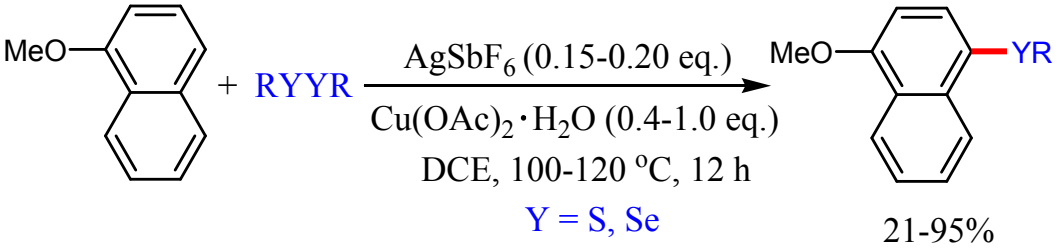
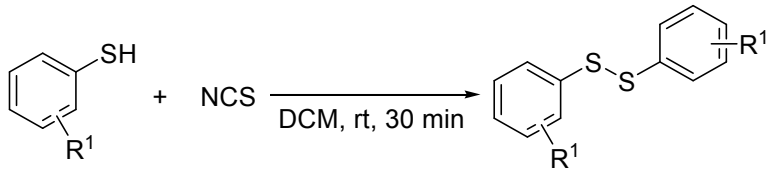


CONTENTS

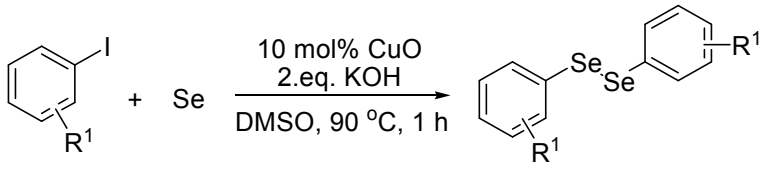
General 1-methoxynaphthalene, aryl iodides and aryl thiols were purchased from Alfa Aesar and Shaoyuan Webstore. Chloroform-*d* was purchased from Cambridge Isotope Laboratories. All solvents were distilled prior to use. All reactions with air- and moisture-sensitive components were performed under a nitrogen atmosphere in a flame-dried reaction flask. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were measure on Bruker 300 M spectrometers. $CDCl_3$ was used as solvent with tetramethylsilane (TMS) as internal standard.

General procedure for the preparation of diaryl disulfides [1]



To the stirred solution of thiols (5 mmol) in dichloromethane (10 mL), NCS (0.5 eq.) was added. The mixture was then stirred for 30 min. The progress of the reaction was monitored by TLC. After completion of the reaction, CH_2Cl_2 (10 mL) was added and the mixture was washed successively with water (2×20mL). The organic layer was separated and dried by adding anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure gave almost pure product. Further purification was achieved by column chromatography on silica gel (ethyl acetate: hexane (1:30)) to give pure product in good to excellent yield.

General procedure for the preparation of diaryl diselenides [2]



To a stirred solution of Se (0) metal (4.0 mmol) and aryl iodides (2.0 mmol) in dry DMSO (3.0 mL) was added CuO (10 mol %) followed by KOH (2.0 equiv) under nitrogen atmosphere at 90 ^{o}C. The progress of the reaction was monitored by TLC. After the reaction was complete, Et_2O (10 mL) was added and the mixture was washed successively with water (2×20mL). The organic layer was separated and dried by adding anhydrous Na_2SO_4. Evaporation of the solvent under reduced pressure gave

almost pure product. Further purification was achieved by column chromatography on silica gel (ethylacetate: hexane (1:50)) to give pure product in good to excellent yield.

Typical procedure for sulfenylation of sp^2 C-H bonds

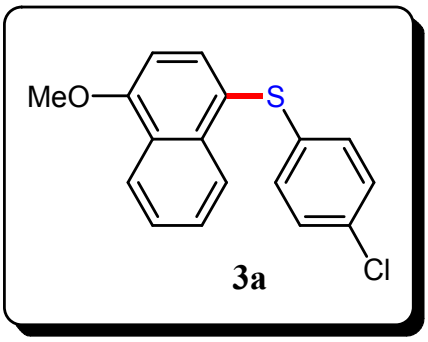
Under air atmosphere, 1-methoxynaphthalene(47.4 mg, 0.3 mmol), diaryl disulfides (0.3 mmol), $AgSbF_6$ (15.4 mg, 15 mol%), $Cu(OAc)_2 \cdot H_2O$ (24 mg, 0.4 eq.) were added to a screw-capped vial, followed by addition of a stir bar and DCE (2 mL). The reaction vial was placed in a temperature-controlled aluminum-heating block set at 100 ^oC. After 12 h of stirring, the vial was removed from the heating block and was left to cool to the ambient temperature. The solvents were removed under reduced pressure and the crude reaction mixture was purified by silica gel column chromatography with Petroleum ether/EtOAc as an eluent to give the desired product.

Typical procedure for selenylation of sp^2 C-H bonds

Under air atmosphere, 1-methoxynaphthalene(47.4 mg, 0.3 mmol), diaryl diselenides (0.3 mmol), $AgSbF_6$ (20.6 mg, 20 mol%), $Cu(OAc)_2 \cdot H_2O$ (60 mg, 1.0 eq.) were added to a screw-capped vial, followed by addition of a stir bar and DCE (2 mL). The reaction vial was placed in a temperature-controlled aluminum-heating block set at 120 ^oC. After 12 h of stirring, the vial was removed from the heating block and was left to cool to ambient temperature. The solvents were removed under reduced pressure and the crude reaction mixture was purified by silica gel column chromatography with Petroleum ether/EtOAc as an eluent to give the desired product.

Spectral data for the products

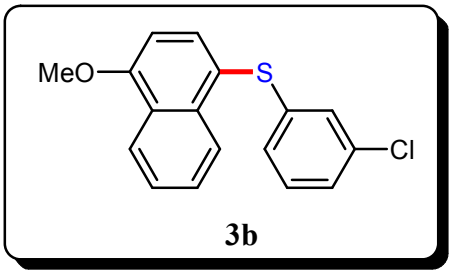
(4-chlorophenyl)(1-methoxynaphthalen-4-yl)sulfane (3a)



3a

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.37-8.31 (m, 2H), 7.84(d, *J* = 8.0 Hz, 1H), 7.60-7.53 (m, 2H), 7.18-7.13 (m, 2H), 7.01-6.98 (m, 2H), 6.84 (d, *J* = 8.0 Hz, 1H), 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.4, 137.8, 136.1, 135.1, 130.9, 129.0, 127.9, 127.9, 126.7, 125.9, 125.9, 122.8, 119.6, 104.1, 55.8. MS(EI): 300(100), 285(7), 257(4), 220(12). HRMS calcd for $C_{17}H_{13}ClOS$ [M $^{+}$]: 300.0376, found: 300.0374.

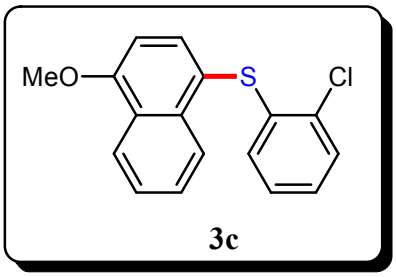
(3-chlorophenyl)(1-methoxynaphthalen-4-yl)sulfane (3b)



3b

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.41-8.32(m, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 4.0 Hz, 2H), 7.07 (t, *J* = 6.8 Hz, 3H); 6.92 (d, *J* = 7.8 Hz, 1H), 6.87(d, *J* = 8.0 Hz, 1H), 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.6, 141.6, 136.5, 135.2, 134.8, 129.9, 128.0, 126.8, 126.0, 126.0, 125.8, 125.2, 124.5, 122.8, 104.2, 55.8. MS(EI): 300(60), 221(50), 145(100), 114(70), 63(55). HRMS calcd for $C_{17}H_{13}ClOS$ [M $^{+}$]: 300.0376, found: 300.0375.

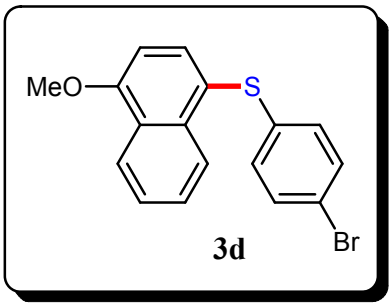
(2-chlorophenyl)(1-methoxynaphthalen-4-yl)sulfane (3c)



3c

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.39-8.27(m, 2H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.59-7.53 (m, 2H), 7.40-7.38(m, 1H), 7.03-6.98(m, 1H), 6.92-6.87(m, 2H); 6.42-6.39(m, 1H), 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.7, 138.6, 136.9, 135.4, 130.4, 129.4, 128.0, 127.0, 126.9, 126.8, 126.0, 125.9, 125.6, 122.8, 118.3, 104.3, 55.8. MS(EI): 300(60), 145(100), 113(1.5). HRMS calcd for $C_{17}H_{13}ClOS$ [M^+]: 300.0376, found: 300.0373.

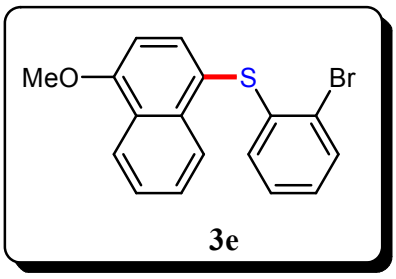
(4-bromophenyl)(1-methoxynaphthalen-4-yl)sulfane (3d)



3d

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.38-8.27(m, 2H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.58-7.53(m, 2H), 7.30-7.25(m, 2H), 6.94-6.85(m, 3H), 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.5, 138.5, 136.2, 135.1, 131.8, 128.1, 127.9, 126.7, 125.9, 125.8, 122.7, 118.6, 104.1, 55.8. MS(EI): 344(2.5), 145(100), 113(48), 63(18). HRMS calcd for $C_{17}H_{13}BrOS$ [M^+]: 343.9871, found: 343.9873.

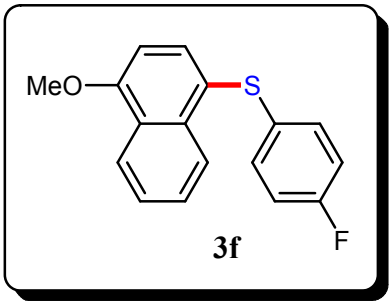
(2-bromophenyl)(1-methoxynaphthalen-4-yl)sulfane (3e)



3e

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.39-8.24(m, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.58-7.53(m, 3H), 6.94-6.88(m, 3H), 6.39-6.36(m, 1H), 4.09 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.7, 140.5, 136.8, 135.3, 132.7, 128.0, 127.6, 126.8, 126.0, 125.9, 125.8, 122.7, 120.0, 118.8, 104.3, 55.8. MS(EI): 344(2.5), 210(30), 145(100), 113(33). HRMS calcd for $C_{17}H_{13}BrOS$ [M $^{+}$]: 343.9871, found: 343.9874.

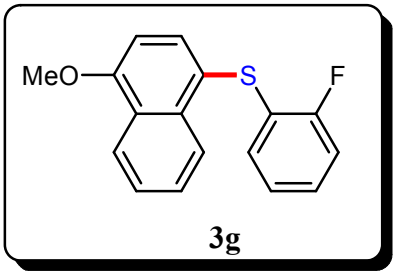
(4-fluorophenyl)(1-methoxynaphthalen-4-yl)sulfane (3f)



3f

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.37-8.33(m, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.57-7.53(m, 2H), 7.10-7.05(m, 2H), 6.93-6.83(m, 3H), 4.06 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 162.8, 159.5, 157.2, 135.4, 135.0, 133.9, 133.8, 129.0, 129.0, 127.8, 126.7, 125.9, 125.8, 122.7, 120.8, 116.2, 115.9, 104.1, 55.7. MS(EI): 284(100), 269(53), 239(28), 144(25), 113(27), 102(18), 63(24). HRMS calcd for $C_{17}H_{13}FOS$ [M $^{+}$]: 284.0671, found: 284.0668.

(2-fluorophenyl)(1-methoxynaphthalen-4-yl)sulfane (3g)

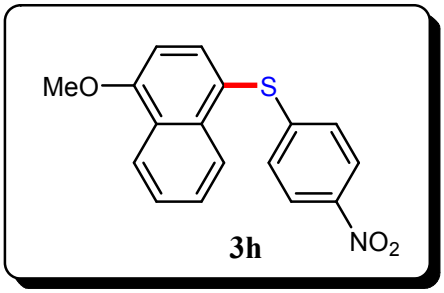


3g

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.39-8.37(m, 2H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.60-7.53(m, 2H), 7.10-7.06(m, 2H), 6.90-6.82(m, 2H), 6.66-6.63(m, 1H), 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 160.8, 157.5, 236.3, 135.3, 128.8, 127.9, 126.7, 126.6, 125.9, 125.8, 124.5, 124.5, 122.7, 118.2, 115.4, 115.2, 104.2, 55.8.

MS(EI): 284(45), 269(50), 241(100), 221(55), 145(50), 113(55), 102(55), 75(55), 63(55). HRMS calcd for $C_{17}H_{13}FOS$ [M $^{+}$]: 284.0671, found: 284.0669.

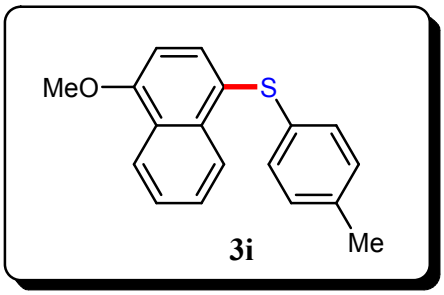
(1-methoxynaphthalen-4-yl)(4-nitrophenyl)sulfane (3h)



3h

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.41-8.17(m, 2H), 7.99 (d, *J* = 8.9 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.58-7.55(m, 2H), 7.03 (d, *J* = 8.9 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 1H), 4.11 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 158.2, 149.7, 137.0, 135.1, 128.3, 126.8, 126.5, 126.2, 125.4, 124.5, 124.0, 123.0, 104.2, 55.9. MS(EI): 311(5), 145(90), 115(100), 102(90), 63(80). HRMS calcd for $C_{17}H_{13}NO_3S$ [M $^{+}$]: 311.0616, found: 311.0615

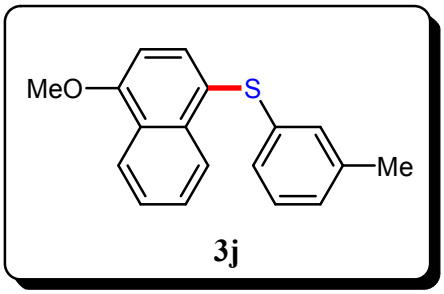
(1-methoxynaphthalen-4-yl)(p-tolyl)sulfane (3i)



3i

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.41-8.35 (m, 2H), 7.80(d, *J* = 8.0 Hz, 1H), 7.57-7.53 (m, 2H), 7.03 (s, 4H), 6.84 (d, *J* = 8.0 Hz, 1H), 4.06 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 156.9, 135.2, 135.2, 135.1, 129.7, 127.6, 127.4, 126.6, 126.0, 125.7, 122.6, 121.1, 104.1, 55.7, 21.0. MS(EI): 280(100), 265(25), 220(25), 145(13), 113(10), 89(15), 63(15). HRMS calcd for $C_{18}H_{16}OS$ [M^{+}]: 280.0922, found: 280.0919.

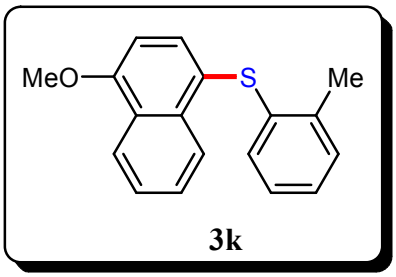
(1-methoxynaphthalen-4-yl)(m-tolyl)sulfane (3j)



3j

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.40-8.30 (m, 2H), 7.75(d, *J* = 8.0 Hz, 1H), 7.59-7.55 (m, 2H), 7.22 (d, *J* = 7.3 Hz, 1H), 7.08-7.03 (m, 1H), 6.95-6.90(m, 1H), 6.87(d, *J* = 8.0 Hz, 1H), 6.62 (d, *J* = 7.5 Hz, 1H), 4.07 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.0,137.9, 135.3, 135.2, 135.2, 130.1, 127.7, 126.8, 126.7, 126.5, 125.9, 125.8, 125.1, 122.7, 120.1, 104.3, 55.7, 20.2. MS(EI): 280(100), 265(23), 220(25), 115(4), 92(2), 65(4). HRMS calcd for $C_{18}H_{16}OS$ [M^+]: 280.0922, found: 280.0920.

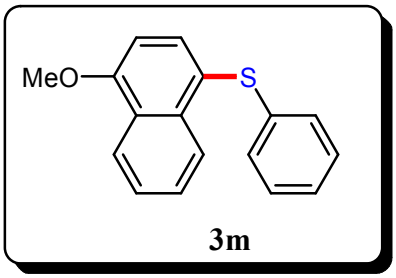
(1-methoxynaphthalen-4-yl)(o-tolyl)sulfane (3k)



3k

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.33-8.29 (m, 2H), 7.75(d, *J* = 8.0 Hz, 1H), 7.59-7.51 (m, 2H), 7.22(d, *J* = 7.2 Hz, 1H), 7.07-7.02(m, 1H), 6.95-6.90 (m, 1H), 6.86 (d, *J* = 8.0 Hz, 1H); 6.61 (d, *J* = 7.8 Hz, 1H), 4.07 (s, 3H), 2.55 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.0, 137.9, 135.3, 135.2, 135.2, 130.1, 127.7, 126.8, 126.7, 126.5, 125.9, 125.8, 125.1, 122.7, 120.1, 104.3, 55.7, 20.2. MS(EI): 280(100), 265(16), 189(65), 220(10), 147(13), 121(9), 92(9), 65(4). HRMS calcd for $C_{18}H_{16}OS$ [M^+]: 280.0922, found: 280.0920.

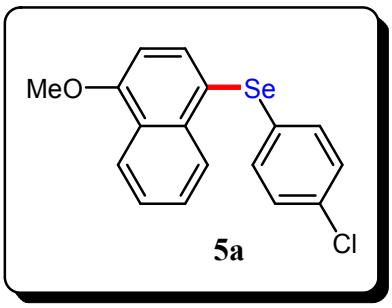
(1-methoxynaphthalen-4-yl)(phenyl)sulfane (3m)



3m

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.44-8.40 (m, 2H), 7.87(d, *J* = 8.0 Hz, 1H), 7.60-7.56 (m, 2H), 7.24-7.19 (m, 2H), 7.14-7.11 (m, 3H), 6.87 (d, *J* = 8.0 Hz, 1H); 4.07 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.2, 139.2, 135.9, 135.3, 128.9, 127.8, 126.8, 126.7, 126.1, 125.8, 125.2, 122.7, 120.2, 104.2, 55.7. MS(EI): 266(60), 221(28), 189(65), 145(100), 114(67), 63(52). HRMS calcd for $C_{17}H_{14}OS$ [M^+]: 266.0765, found: 266.0763.

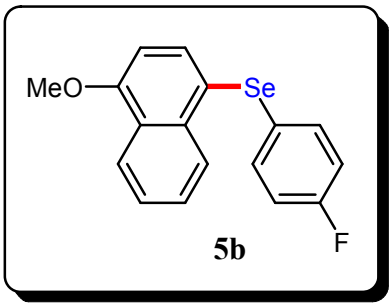
(4-chlorophenyl)(1-methoxynaphthalen-4-yl)selane (5a)



5a

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.40-8.33 (m, 2H), 7.94(d, *J* = 8.0 Hz, 1H), 7.60-7.56 (m, 2H), 7.19-7.12 (m, 4H), 6.80 (d, *J* = 8.0 Hz, 1H); 4.05 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.3, 136.9, 135.4, 132.0, 131.9, 130.9, 129.3, 128.1, 127.9, 126.7, 125.9, 122.7, 118.2, 104.4, 55.7. MS(EI): 348(12), 127(100), 114(80), 103(39), 87(40), 63(55). HRMS calcd for $C_{17}H_{13}ClOSe$ [M^+]: 347.9820, found: 347.9818.

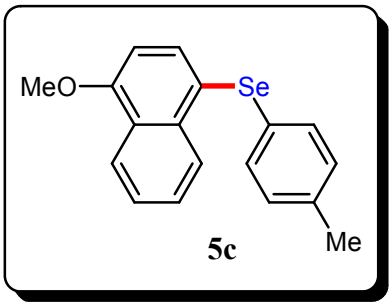
(4-fluorophenyl)(1-methoxynaphthalen-4-yl)selane (5b)



5b

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.36-8.33 (m, 2H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.59-7.53 (m, 2H), 7.28-7.23 (m, 2H), 6.92-6.86 (m, 2H), 6.80 (d, *J* = 8.0 Hz, 1H); 4.05 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 163.4, 160.2, 157.0, 136.2, 135.3, 132.1, 132.0, 128.0, 127.7, 126.6, 125.8, 122.6, 119.1, 116.4, 116.2, 104.3, 55.7. MS(EI): 332(19), 143(18), 114(55), 102(45), 75(40), 62(100). HRMS calcd for $C_{17}H_{13}FOSe$ [M^+]: 332.0116, found: 332.0118.

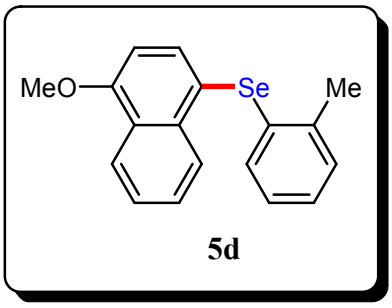
(1-methoxynaphthalen-4-yl)(p-tolyl)selane (5c)



5c

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.43-8.36 (m, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.60-7.52 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 8.0 Hz, 1H), 4.05 (s, 3H); 2.31 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 156.8, 136.1, 136.0, 135.4, 130.4, 130.0, 129.4, 128.2, 127.6, 126.6, 125.7, 122.6, 119.3, 104.4, 55.7, 21.1. MS(EI): 328(2.5), 142(8), 128(26), 113(100), 89(30), 65(48). HRMS calcd for $C_{18}H_{16}OSe$ [M^+]: 328.0366, found: 328.0363.

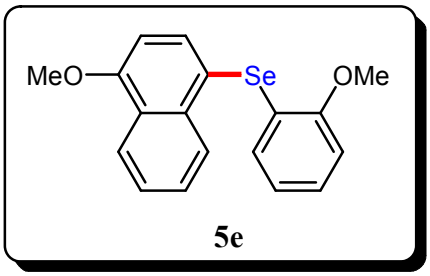
(1-methoxynaphthalen-4-yl)(o-tolyl)selane (5d)



5d

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.37-8.31 (m, 2H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.59-7.53 (m, 2H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.12-7.07 (m, 1H), 6.92-6.77 (m, 3H), 4.07 (s, 3H), 2.53 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.1, 137.0, 136.6, 135.7, 134.2, 130.0, 129.4, 128.2, 127.7, 126.7, 126.6, 125.9, 125.8, 122.6, 117.9, 104.5, 55.7, 21.7. MS(EI): 328(1.5), 113(100), 91(65), 65(35). HRMS calcd for $C_{18}H_{16}OSe$ [M $^{+}$]: 328.0366, found: 328.0364.

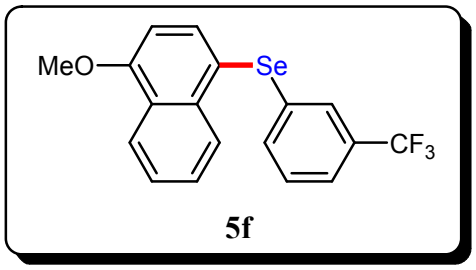
(1-methoxynaphthalen-4-yl)(2-methoxyphenyl)selane (5e)



5e

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.37-8.36 (m, 2H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.58-7.53 (m, 2H), 7.15-7.10 (m, 1H), 6.90-6.84 (m, 2H), 6.67-6.52 (m, 1H), 6.49 (d, *J* = 1.5 Hz, 1H), 4.07 (s, 3H), 4.00 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.4, 138.0, 136.2, 128.7, 128.5, 127.8, 126.6, 126.5, 125.8, 123.3, 122.6, 121.7, 121.6, 110.1, 104.5, 56.0, 55.7. MS(EI): 344(10), 146(45), 114(100), 64(46). HRMS calcd for $C_{18}H_{16}O_2Se$ [M $^{+}$]: 344.0316, found: 344.0313.

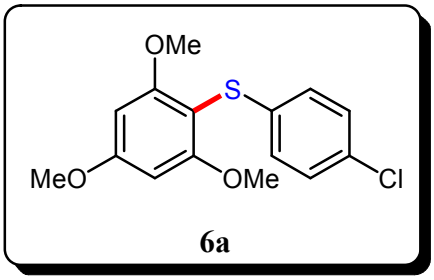
(3-(trifluoromethyl)phenyl)(1-methoxynaphthalen-4-yl)selane (5f)



5f

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 8.38-8.30 (m, 2H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.57-7.52 (m, 2H), 7.38 (d, *J* = 6.8 Hz, 1H), 7.28-7.18 (m, 2H), 6.84 (d, *J* = 8.0 Hz, 1H), 4.07 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 157.5, 137.3, 135.5, 135.1, 132.5, 129.4, 128.0, 127.9, 126.7, 125.9, 125.9, 125.8, 125.2, 122.7, 122.6, 122.6, 117.3, 104.4, 55.7. MS(EI): 382(3), 145(4), 125(8), 113(100), 89(3). HRMS calcd for $C_{18}H_{13}F_3OSe$ [M^+]: 382.0084, found: 382.0086.

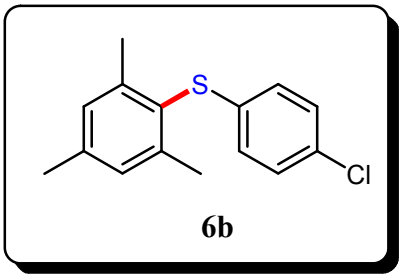
(4-chlorophenyl)(2,4,6-trimethoxyphenyl)sulfane (6a)



6a

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 7.13 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 6.23(s, 2H), 3.88 (s, 3H), 3.82(s, 6H). ^{3}C NMR (75 MHz, $CDCl_3$) δ ppm: 163.2, 162.5, 137.5, 130.1, 128.6, 127.0, 91.3, 56.3, 55.5. MS(EI): 310(20), 155(38), 141(50), 125(75), 109(100), 97(57), 81(35), 69(30). HRMS calcd for $C_{15}H_{15}ClO_3S$ [M^+]: 310.0430, found: 310.0427.

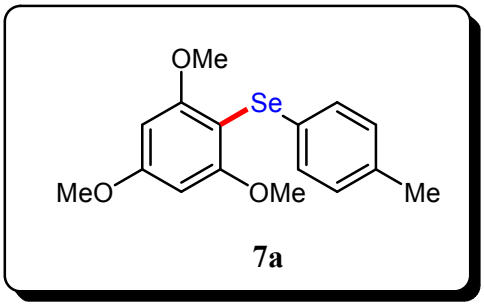
(4-chlorophenyl)(mesityl)sulfane (6b)



6b

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 7.16 (d, *J* = 8.5 Hz, 2H), 7.05 (s, 2H), 6.87 (d, *J* = 8.5 Hz, 1H), 2.41 (s, 6H), 2.36 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 143.7, 139.7, 137.1, 130.3, 129.5, 129.4, 129.0, 126.7, 21.7, 21.2. MS(EI): 262(40), 194(20)50(100), 13491(55), 76(30). HRMS calcd for $C_{15}H_{15}ClS$ [M^+]: 262.0583, found: 262.0580.

(2,4,6-trimethoxyphenyl)(p-tolyl)selane (7a)



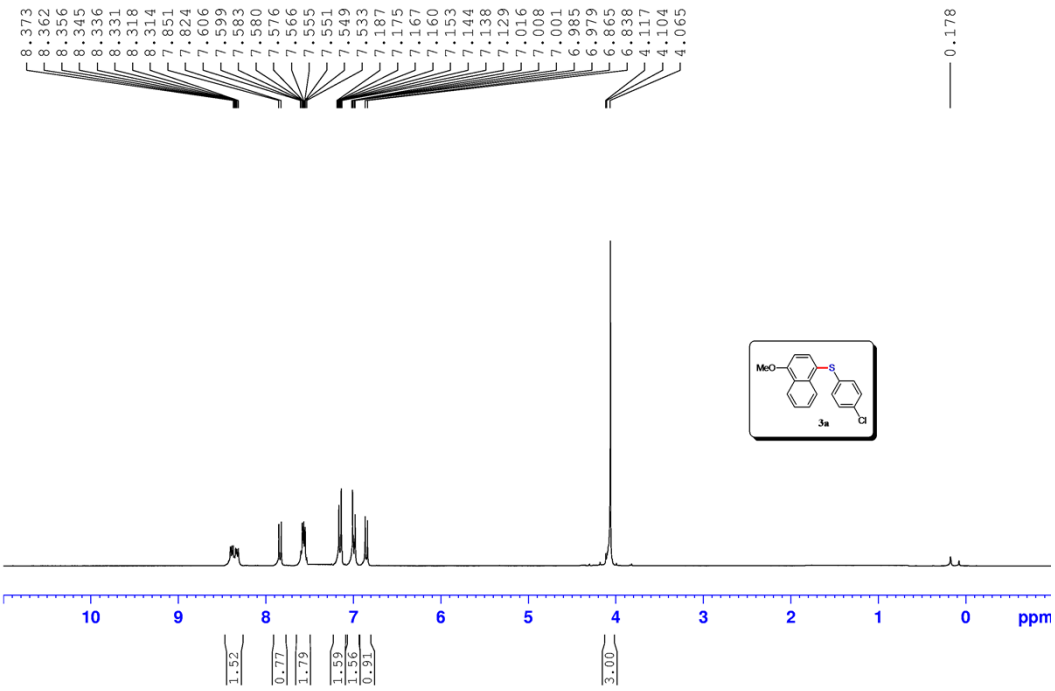
7a

^{1}H NMR (300 MHz, $CDCl_3$) δ ppm: 7.14 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.22(s, 2H), 3.88(s, 3H), 3.81 (s, 6H), 2.27(s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ ppm: 162.9, 161.9, 135.1, 129.7, 129.7, 129.6, 91.3, 56.4, 55.5, 21.0. MS(EI): 338(75), 181(40), 138(50), 125(55), 109(55), 103(60), 90(100), 65(25). HRMS calcd for $C_{16}H_{18}O_3Se$ [M^+]: 338.0421, found: 338.0419.

References:

1. Hashemi, M. M; Ghafuri, H.; Karimo-Jaberi, Z. *J. Sulfur. Chem.* **2006**, *27*, 165.

2. Singh, D.; Deobald, A. M.; Camargo, L. R. S.; Tabarelli, G.; Rodrigues,O. E. D.; Braga, A. L. *Org. Lett.* **2010**, *12*, 3288.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8.314
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7.606
7.599
7.583
7.580
7.576
7.566
7.555
7.551
7.549
7.533
7.187
7.175
7.167
7.160
7.153
7.144
7.138
7.129
7.016
7.008
7.001
6.985
6.979
6.865
6.838
4.117
4.104
4.065
0.178
MeO
S
Cl
3a
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.79
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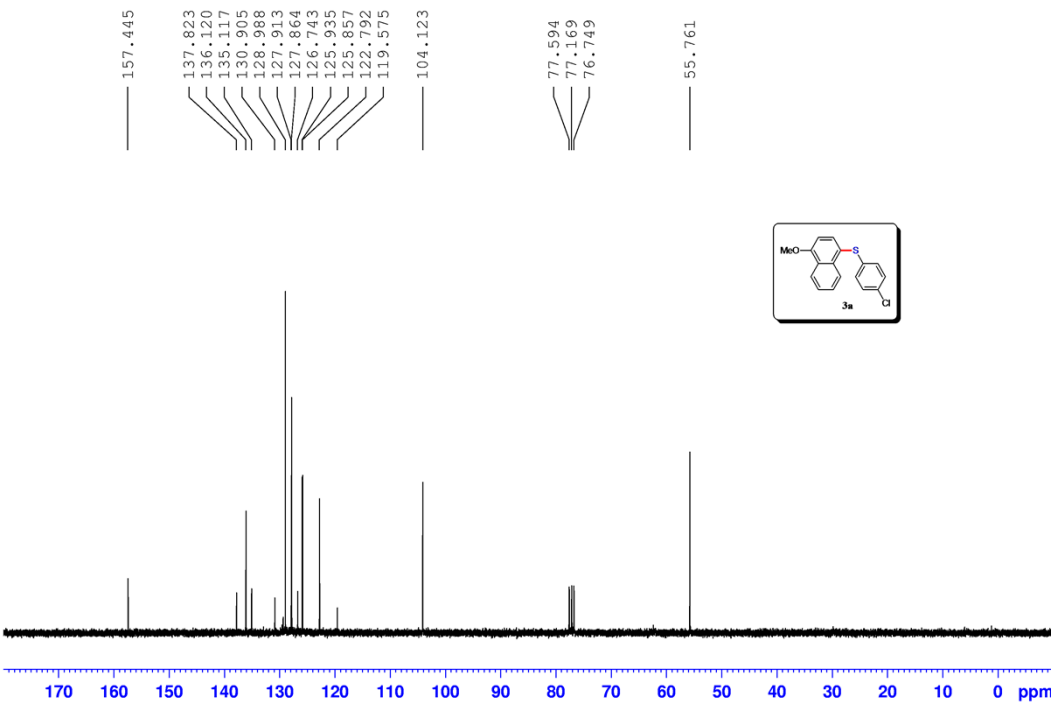
0.91
3.00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136.120
135.117
130.905
128.988
127.913
127.864
126.743
125.935
125.857
122.792
119.575
104.123
77.594
77.169
76.749
55.761
MeO
S
Cl
3a
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150
140
130
120
110
100
90
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60
50
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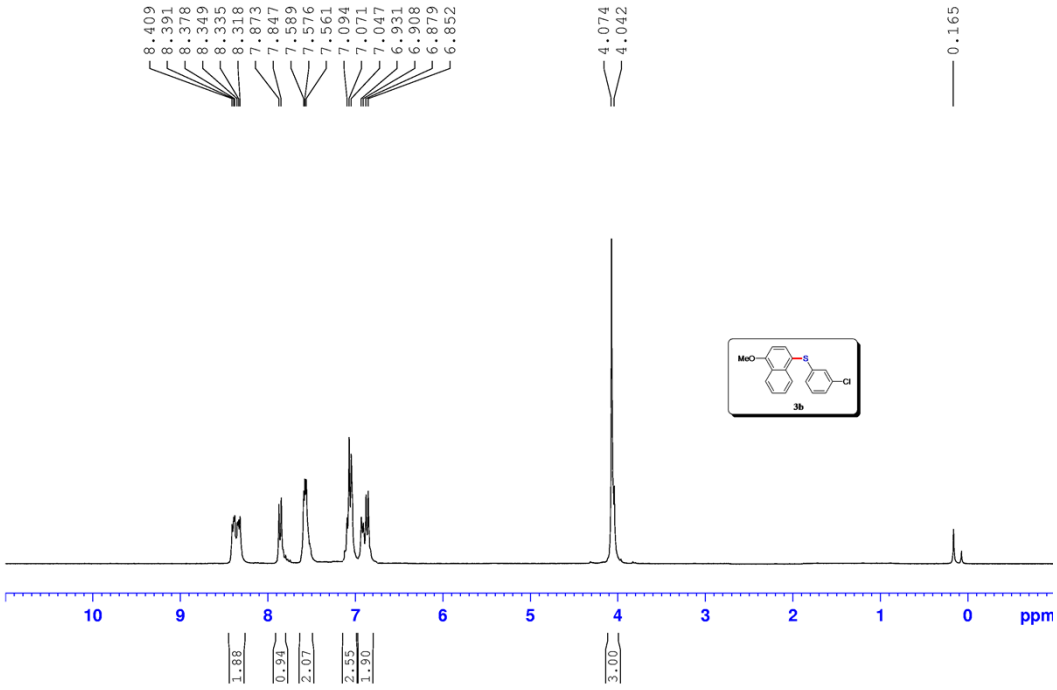
30
20
10
0
ppm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8.318
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7.847
7.589
7.576
7.561
7.094
7.071
7.047
6.931
6.908
6.879
6.852
4.074
4.042
0.165
MeO
S
Cl
3b
10
9
8
7
6
5
4
3
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1
0
ppm
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0.94
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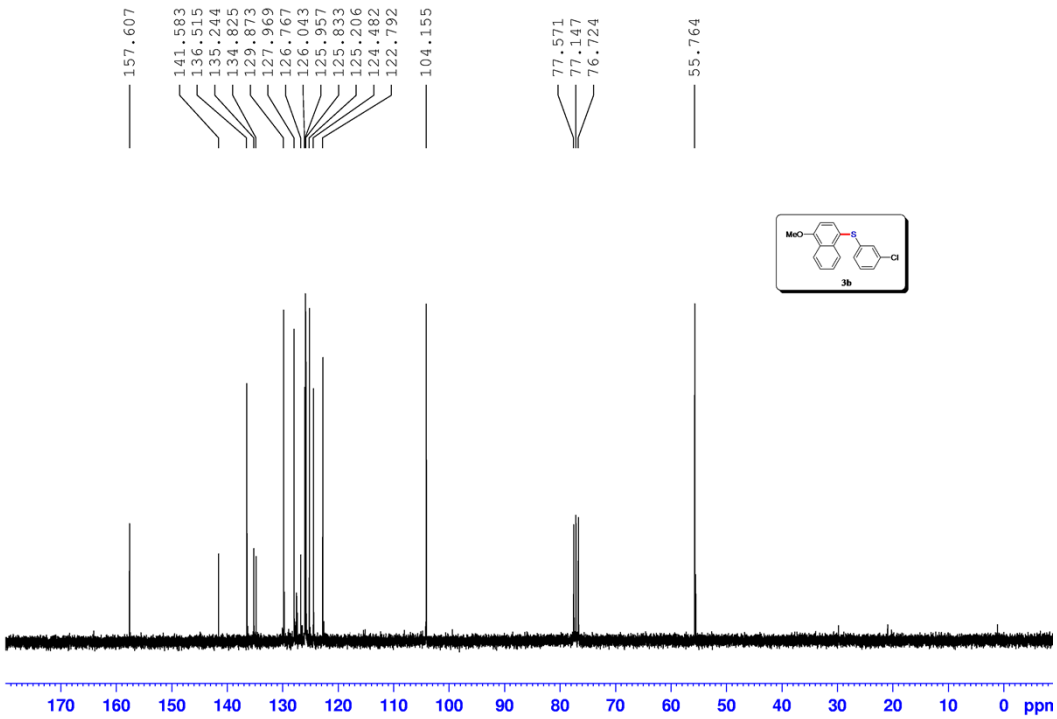
2.55
1.90
3.00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126.767
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125.957
125.833
125.206
124.482
122.792
104.155
77.571
77.147
76.724
55.764
MeO
S
Cl
3b
170
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150
140
130
120
110
100
90
80
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60
50
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30
20
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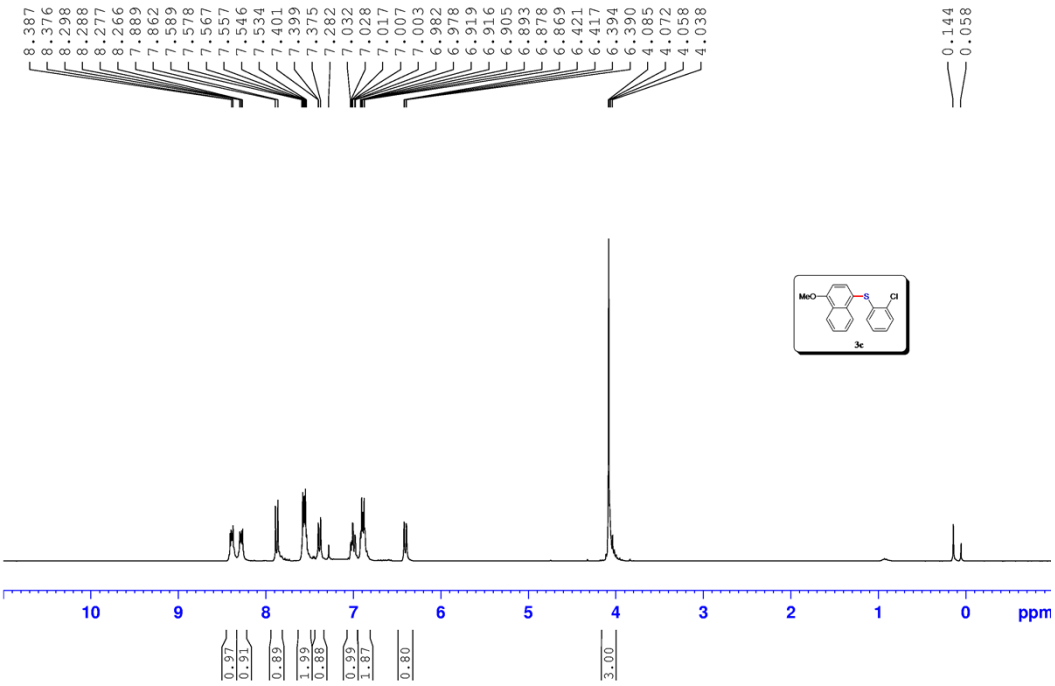
0
ppm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7.862
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7.578
7.567
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7.546
7.534
7.401
7.399
7.375
7.282
7.032
7.028
7.017
7.007
7.003
6.982
6.978
6.919
6.916
6.905
6.893
6.878
6.869
6.421
6.417
6.394
6.390
4.085
4.072
4.058
4.038
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0.058
MeO
S
Cl
3c
10
9
8
7
6
5
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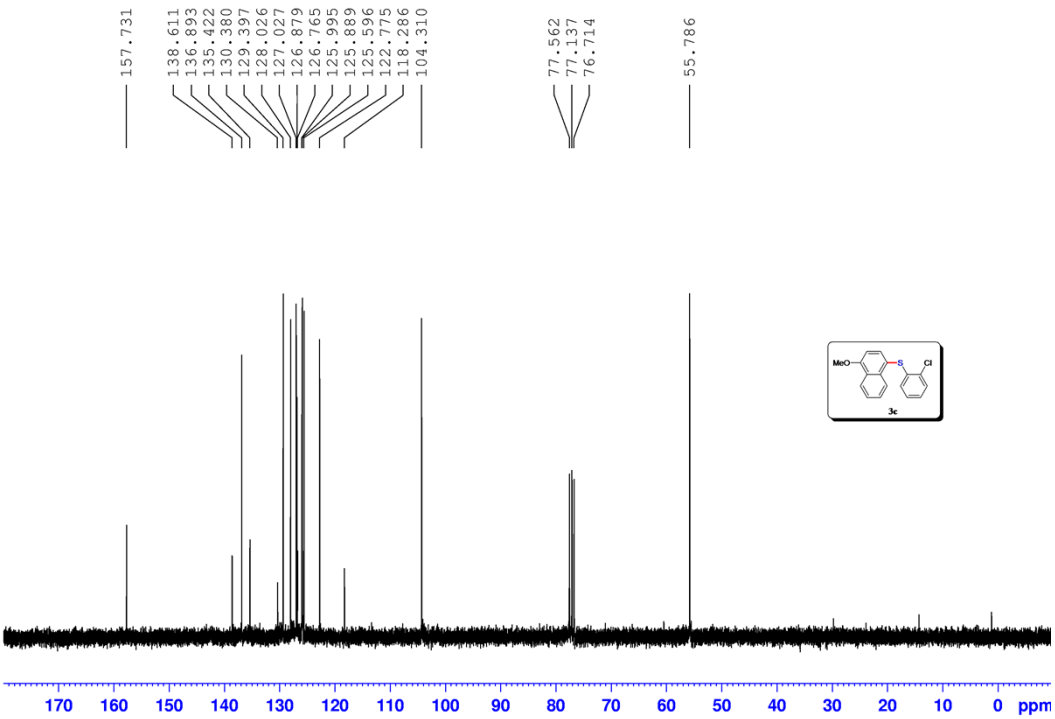
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125.995
125.889
125.596
122.775
118.286
104.310
77.562
77.137
76.714
55.786
MeO
S
Cl
3c
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150
140
130
120
110
100
90
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60
50
40
30
20
10
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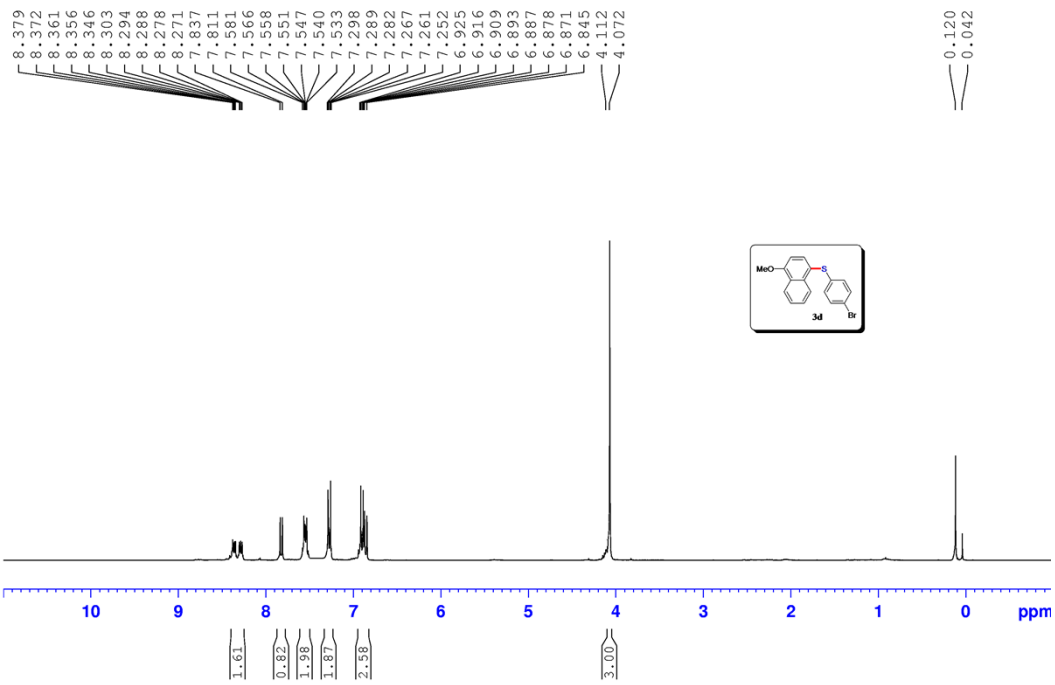
ppm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7.811
7.581
7.566
7.558
7.551
7.547
7.540
7.533
7.298
7.289
7.282
7.267
7.261
7.252
6.925
6.916
6.909
6.893
6.887
6.878
6.871
6.845
4.112
4.072
0.120
0.042
MeO
S
Br
3d
10
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7
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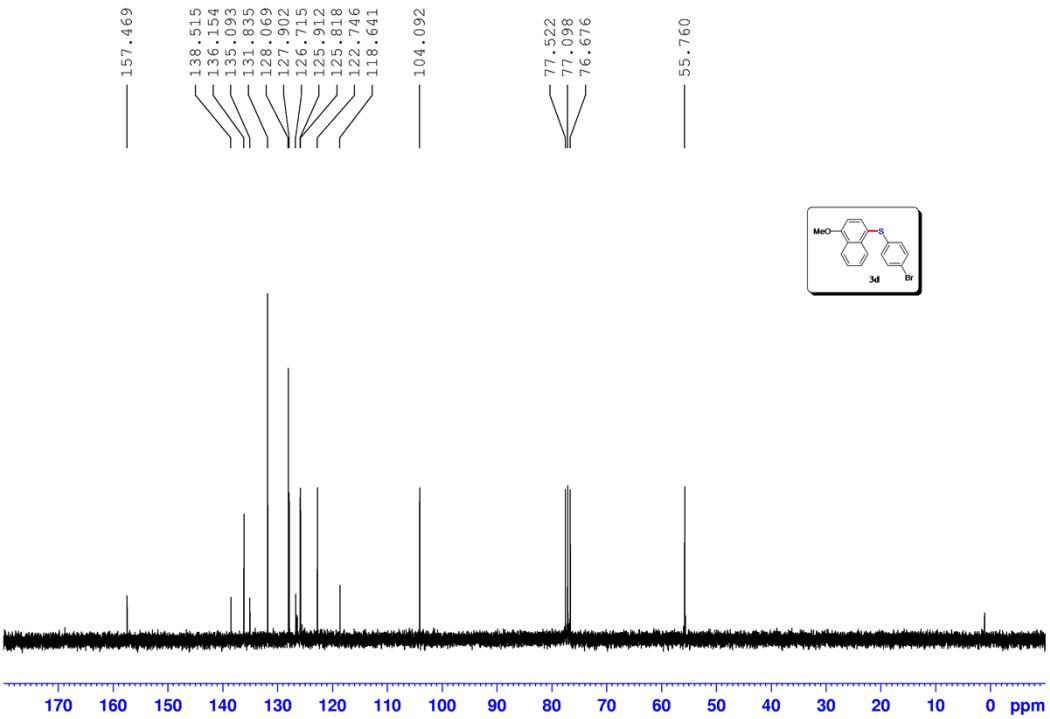
3.00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125.818
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77.522
77.098
76.676
55.760
MeO
S
Br
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140
130
120
110
100
90
80
70
60
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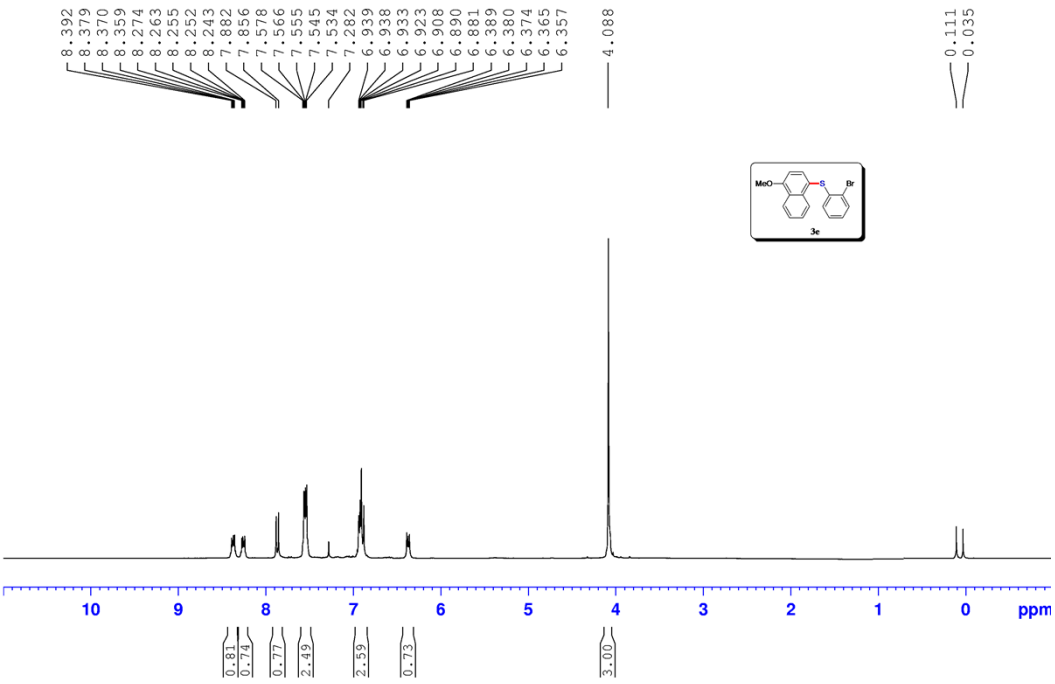
40
30
20
10
0
ppm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7.545
7.534
7.282
6.939
6.938
6.933
6.923
6.908
6.890
6.881
6.389
6.380
6.374
6.365
6.357
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0.035
MeO
Br
3e
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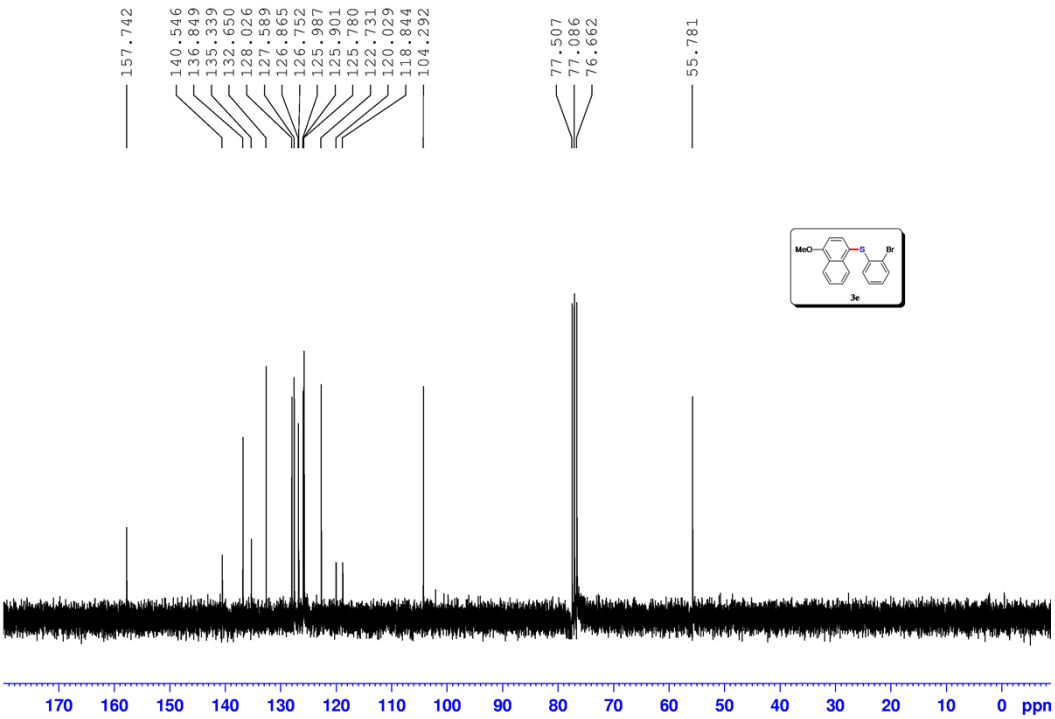
3.00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122.731
120.029
118.844
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MeO
Br
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140
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60
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20
10
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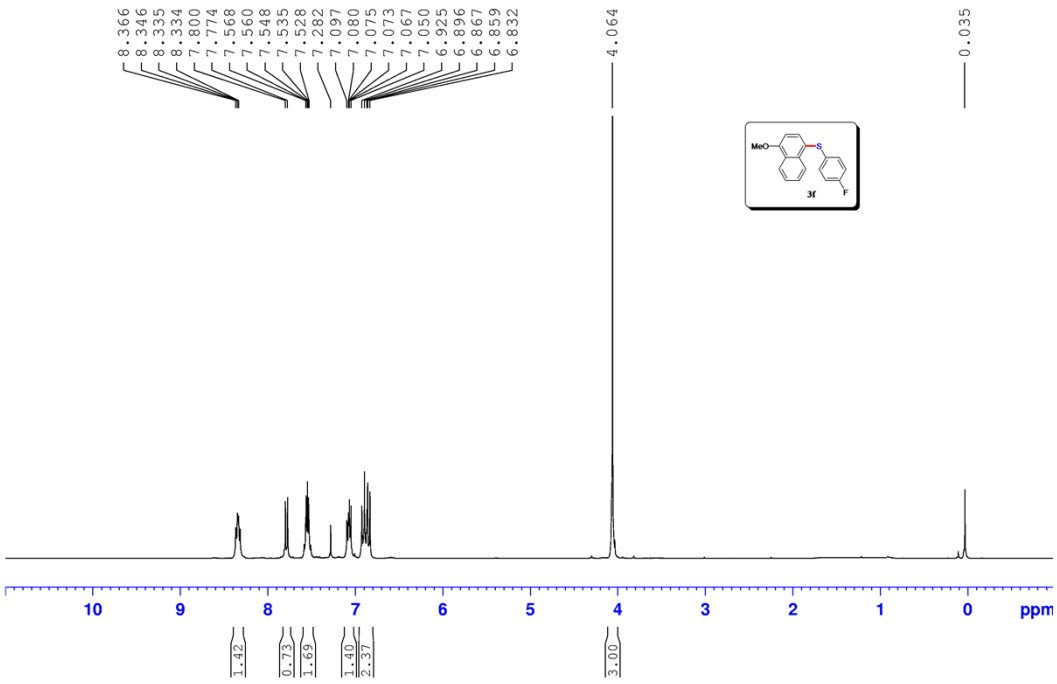
ppm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7.097
7.080
7.075
7.073
7.067
7.050
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6.896
6.867
6.859
6.832
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0.035
MeO
S
F
3f
10
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4
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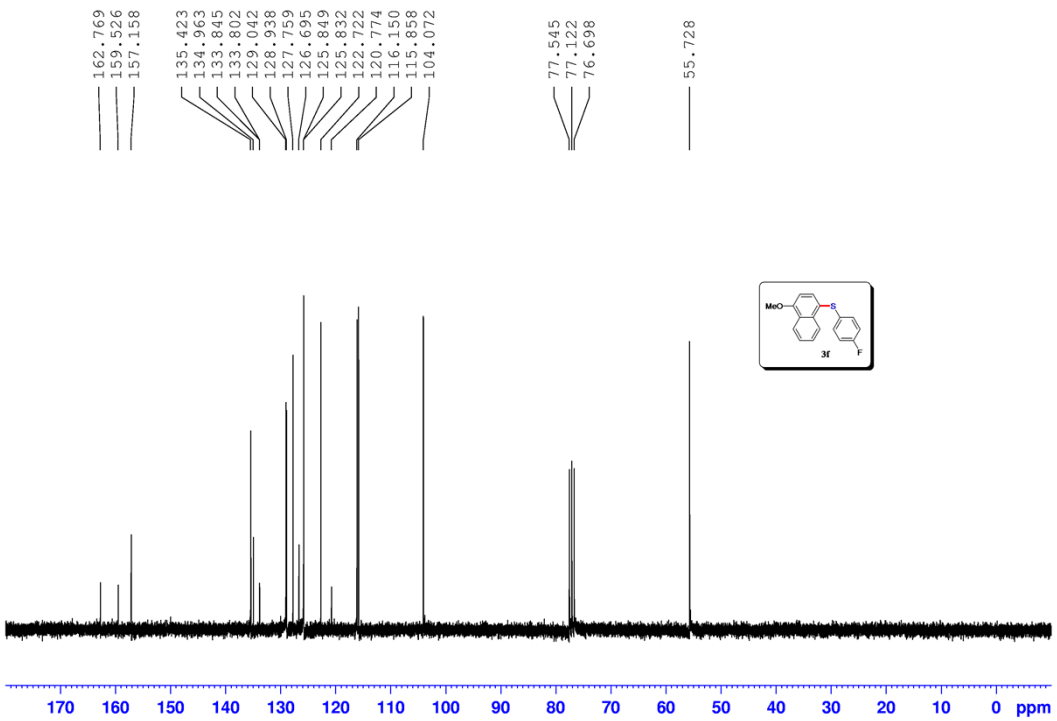
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122.722
120.774
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104.072
77.545
77.122
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MeO
S
F
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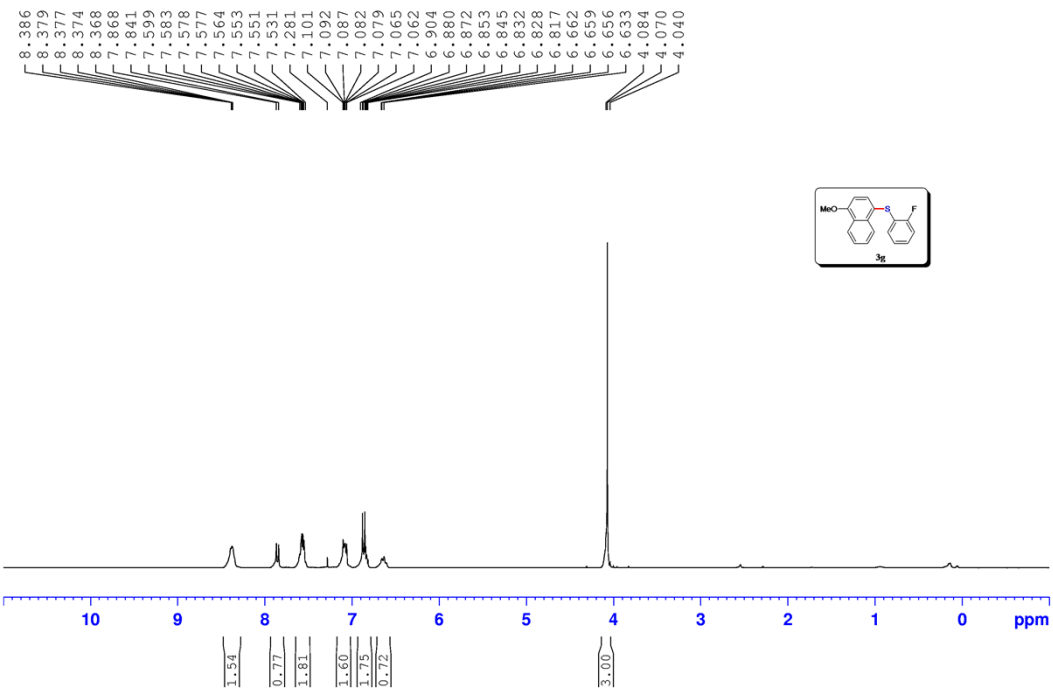
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S
F
3g
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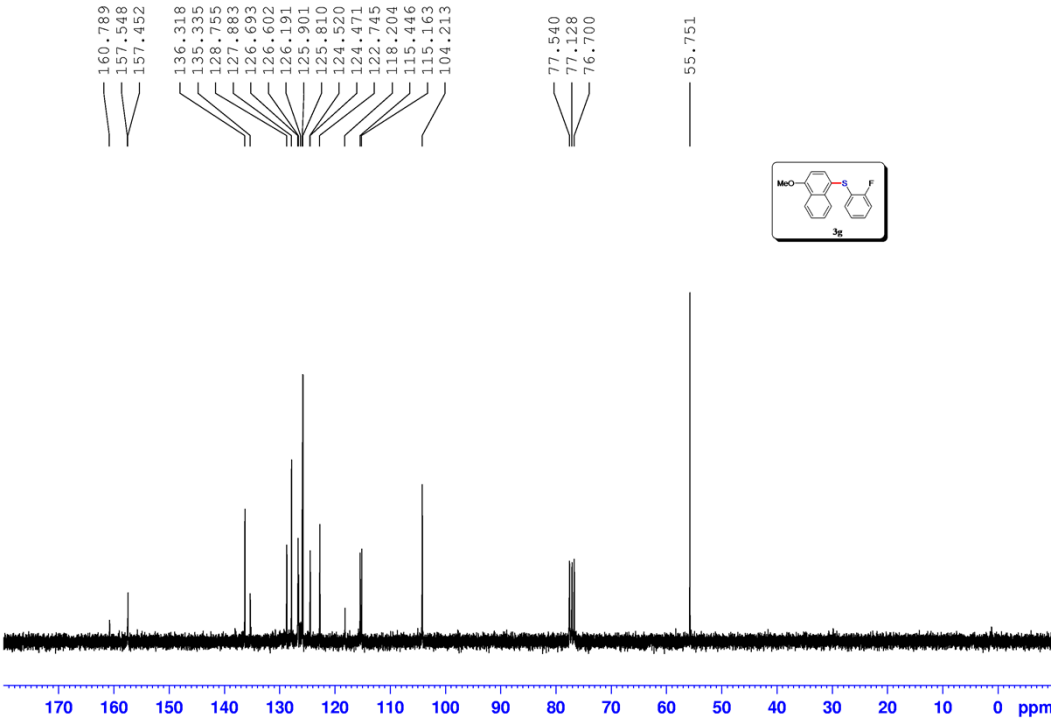
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MeO
S
F
3g
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60
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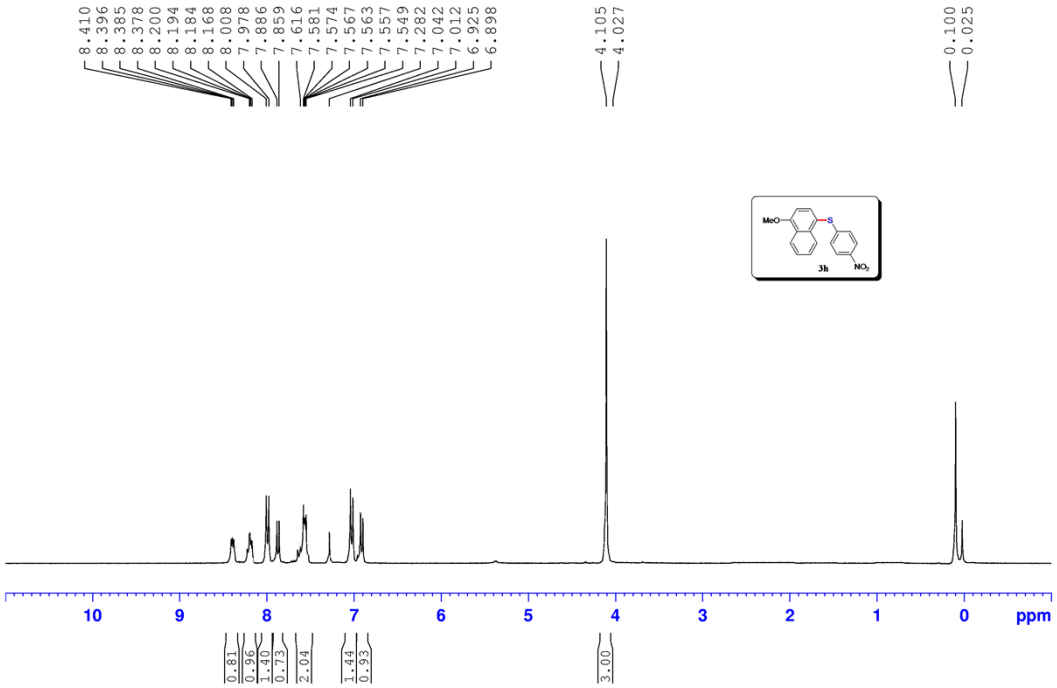
ppm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7.574
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7.557
7.549
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6.925
6.898
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0.025
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S
NO2
3h
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8
7
6
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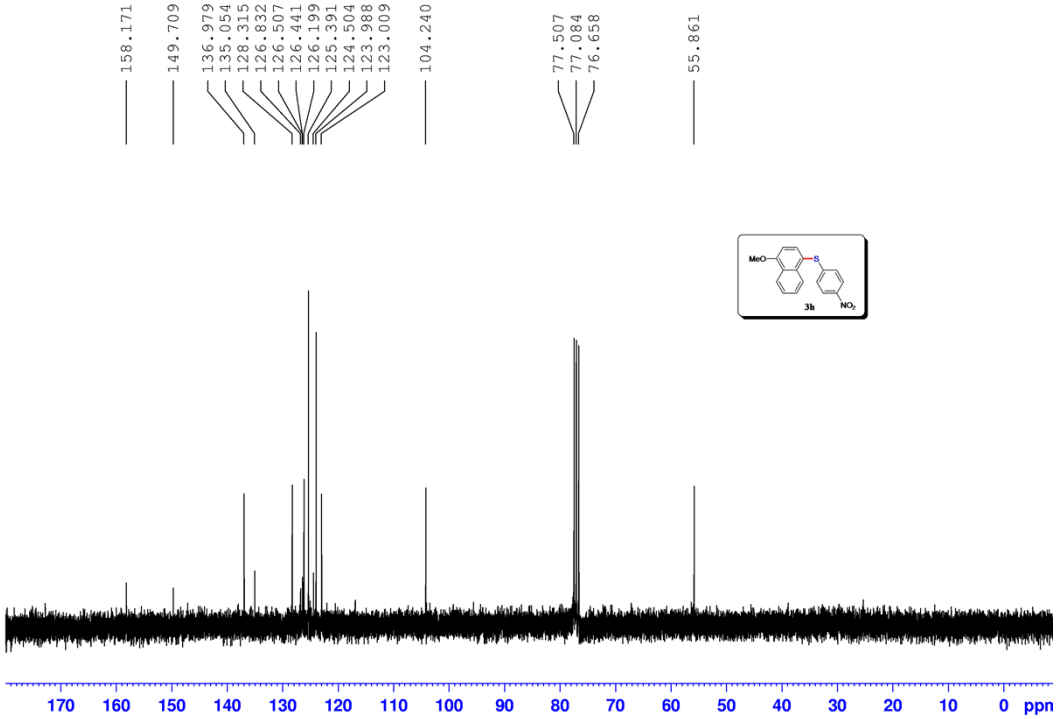
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123.009
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77.507
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76.658
55.861
MeO
S
NO2
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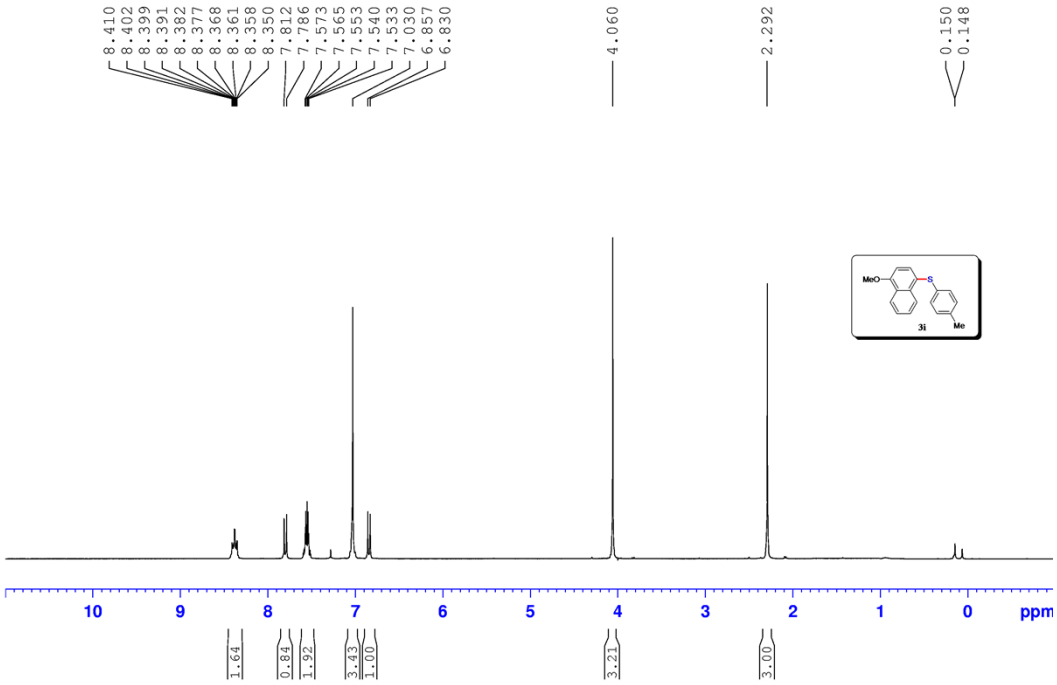
ppm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7.540
7.533
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6.830
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S
3i
Me
10
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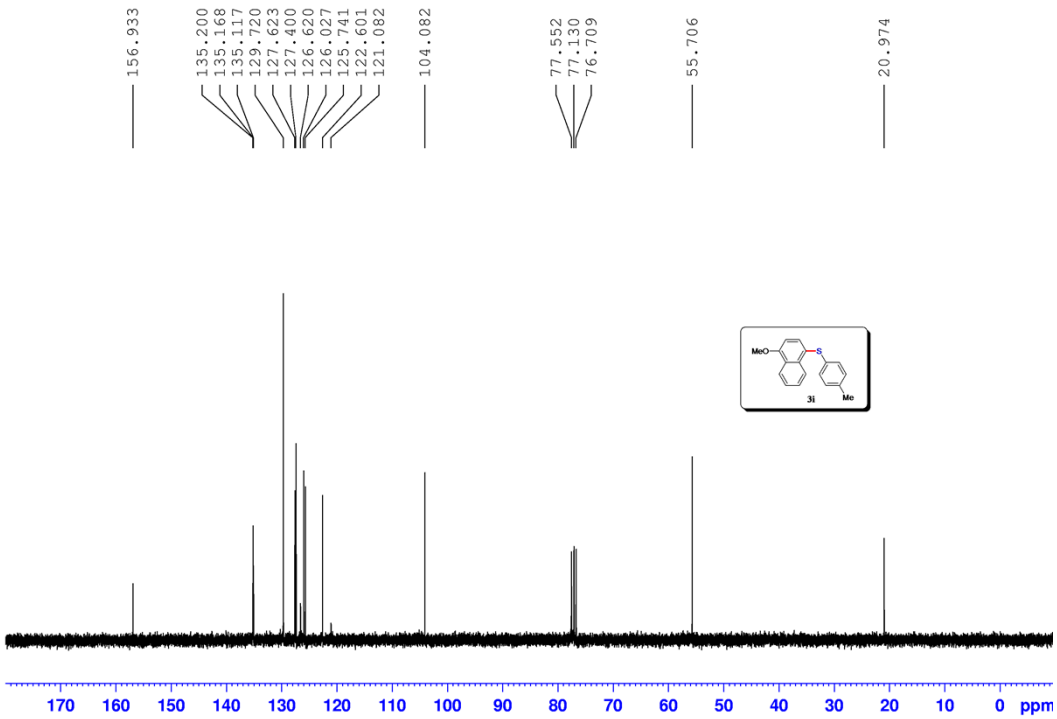
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77.130
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MeO
S
3i
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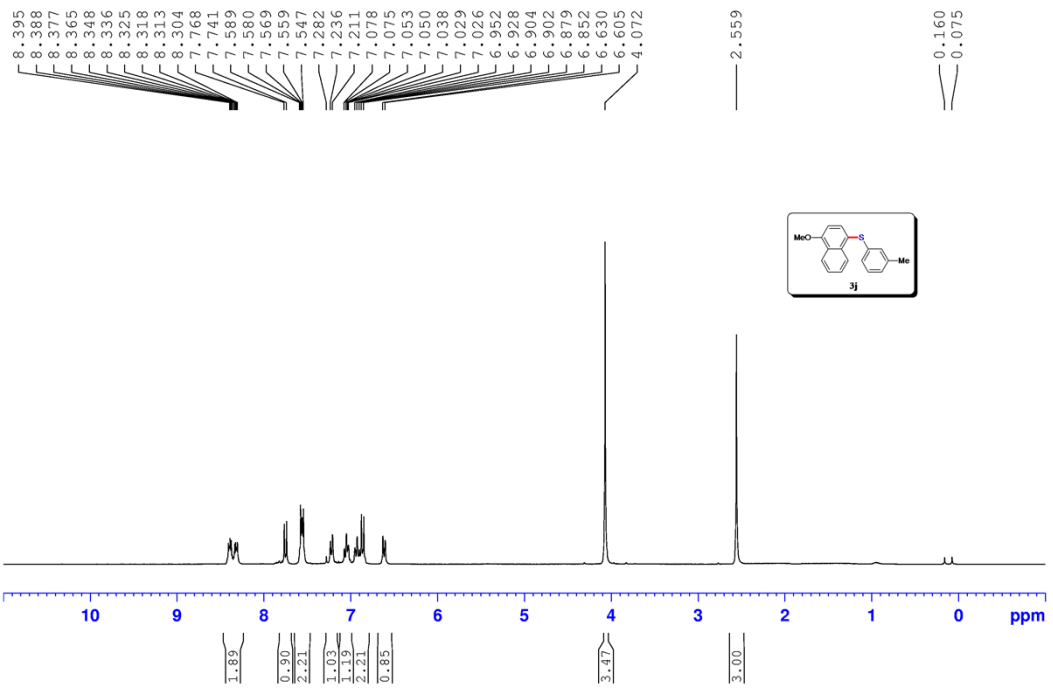
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7.580
7.569
7.559
7.547
7.282
7.236
7.211
7.078
7.075
7.053
7.050
7.038
7.029
7.026
6.952
6.928
6.904
6.902
6.879
6.852
6.630
6.605
4.072
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0.075
MeO
S
Me
3j
10
9
8
7
6
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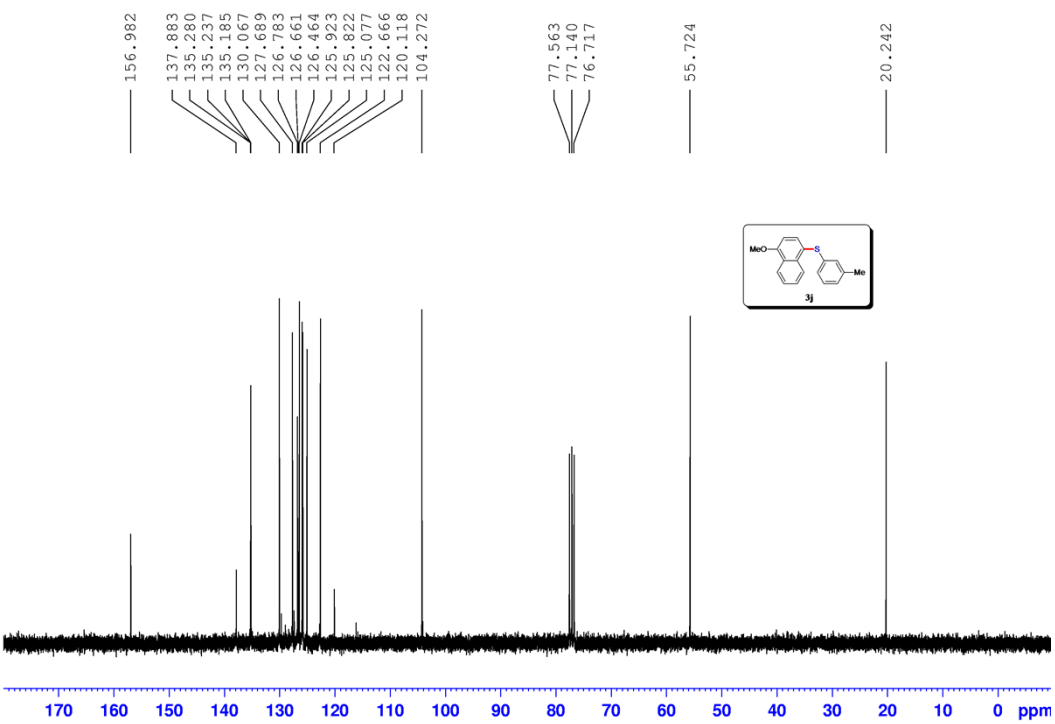
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120.118
104.272
77.563
77.140
76.717
55.724
20.242
MeO
S
Me
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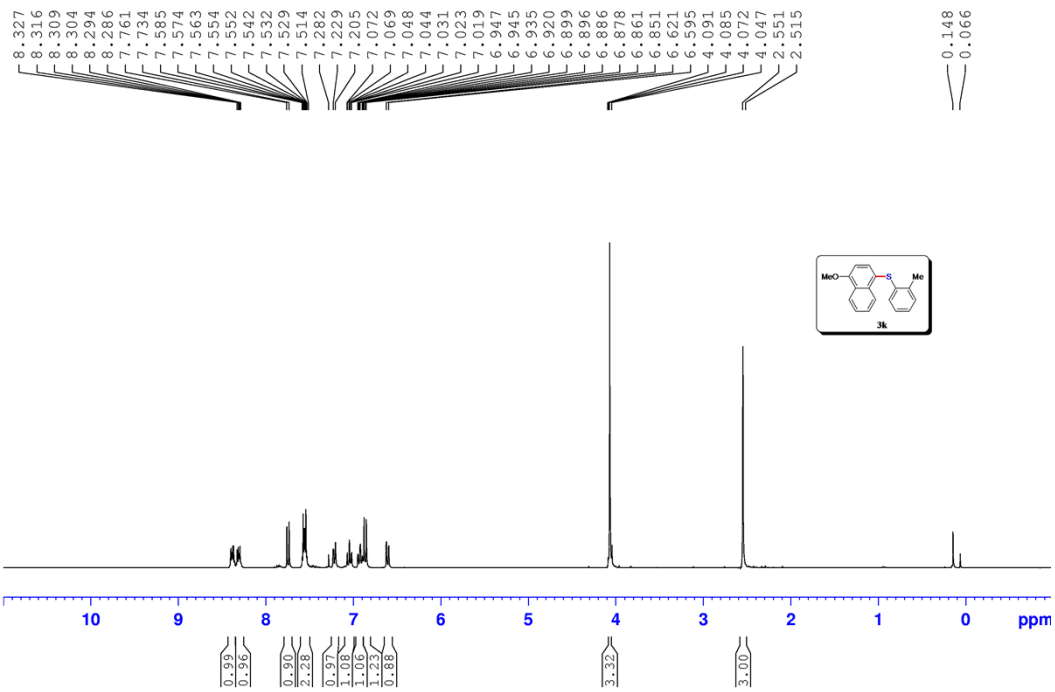
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7.542
7.532
7.529
7.514
7.282
7.229
7.205
7.072
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7.048
7.044
7.031
7.023
7.019
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6.878
6.861
6.851
6.621
6.595
4.091
4.085
4.072
4.047
2.551
2.515
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S
Me
3k
10
9
8
7
6
5
4
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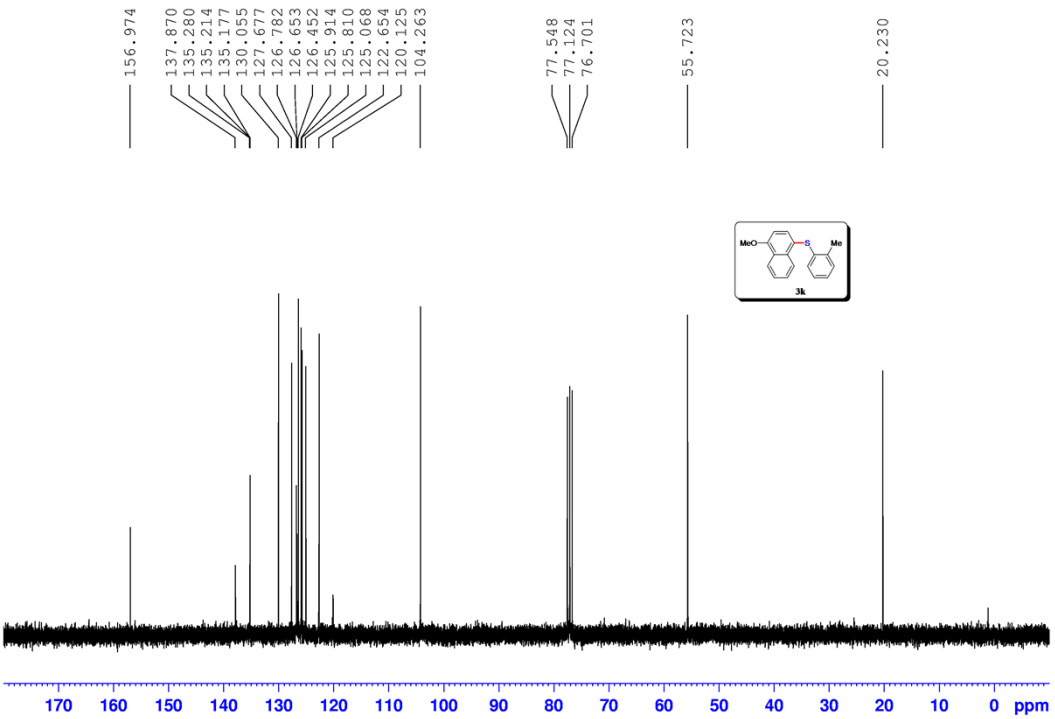
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77.124
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55.723
20.230
MeO
S
Me
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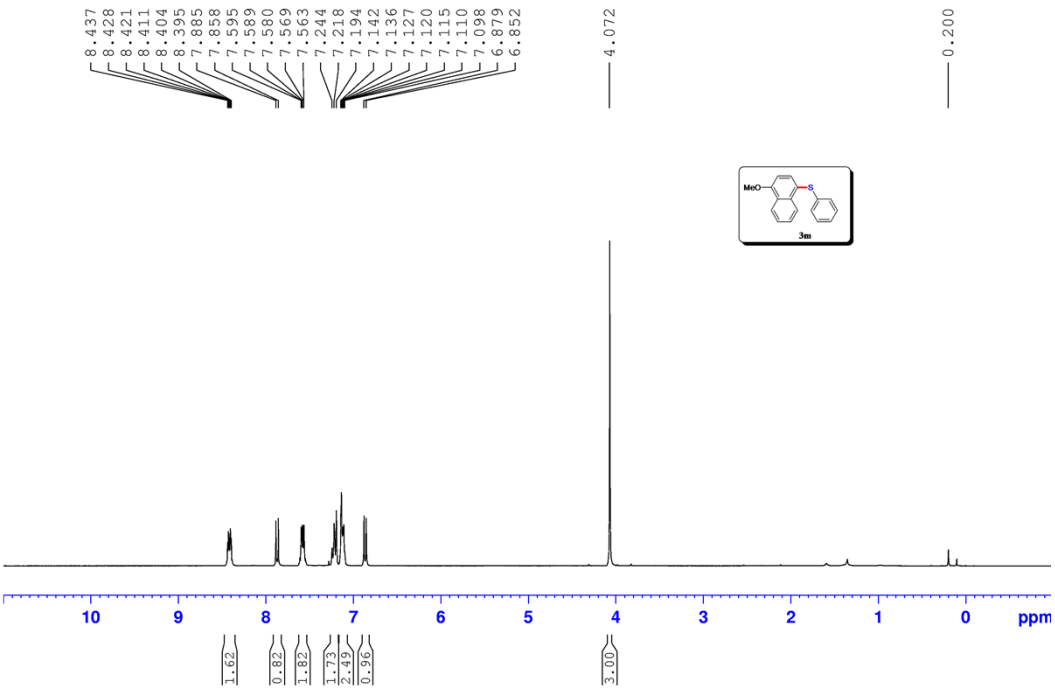
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7.580
7.569
7.563
7.244
7.218
7.194
7.142
7.136
7.127
7.120
7.115
7.110
7.098
6.879
6.852
4.072
0.200
MeO
S
3m
10
9
8
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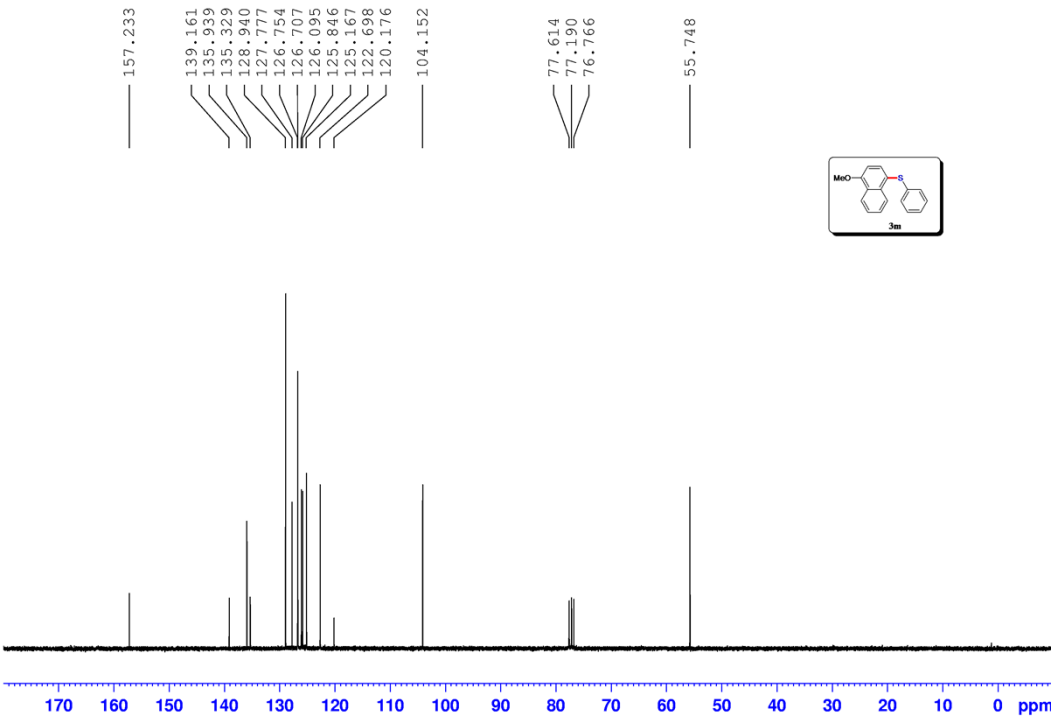
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122.698
120.176
104.152
77.614
77.190
76.766
55.748
MeO
S
3m
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140
130
120
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60
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40
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20
10
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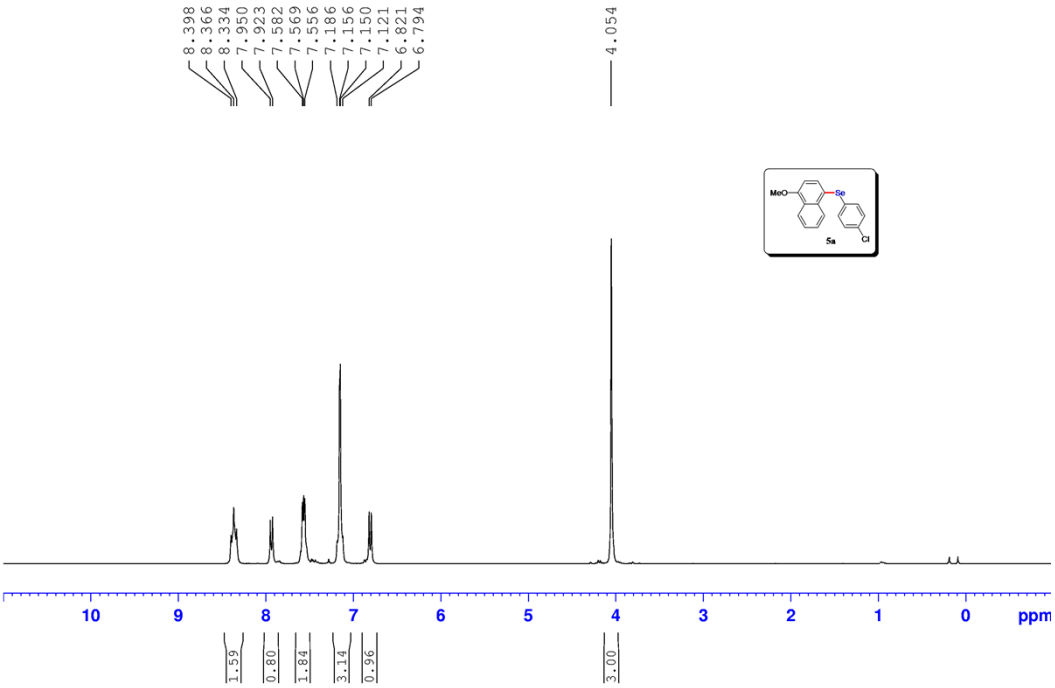
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7.582
7.569
7.556
7.186
7.156
7.150
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6.821
6.794
4.054
MeO
Se
Cl
5a
10
9
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4
3
2
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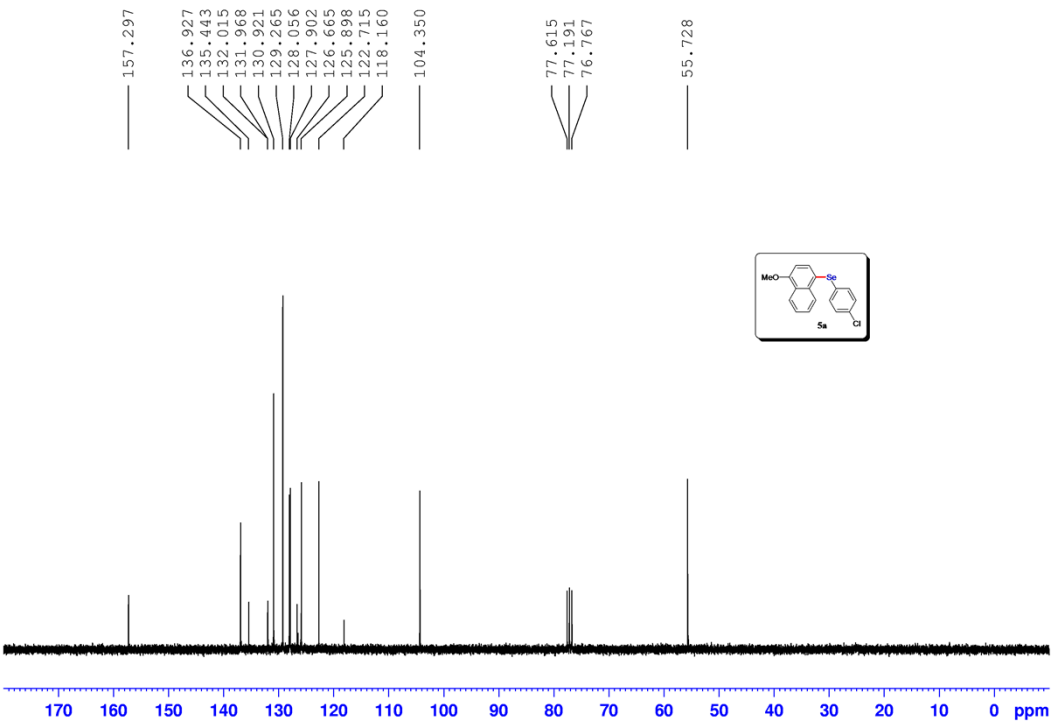
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127.902
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125.898
122.715
118.160
104.350
77.615
77.191
76.767
55.728
MeO
Se
Cl
5a
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140
130
120
110
100
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80
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60
50
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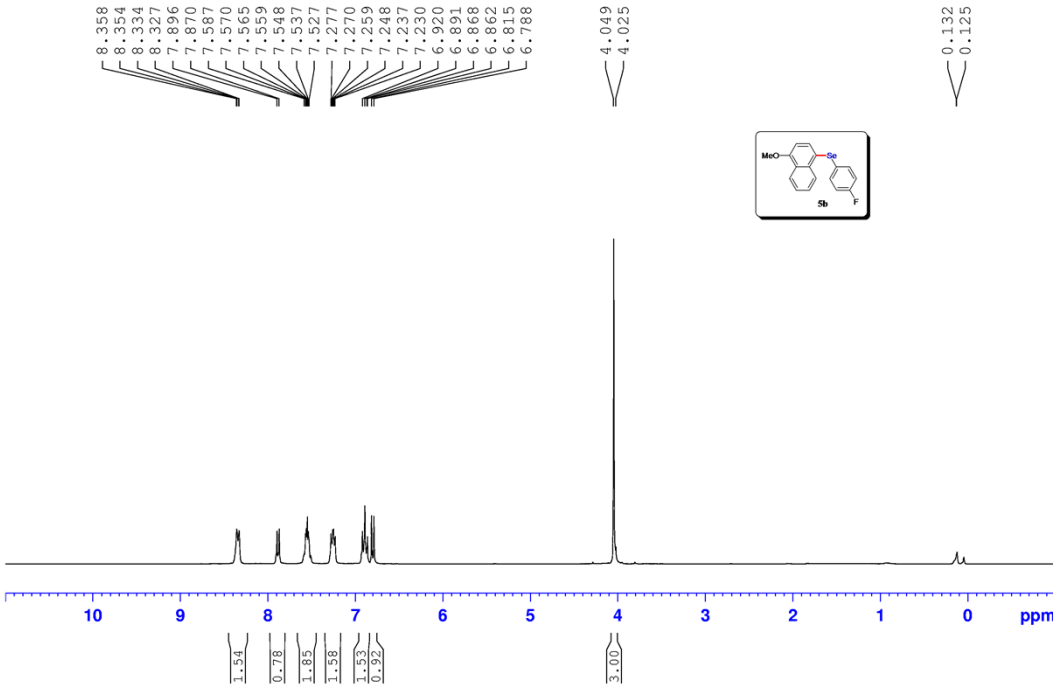
20
10
0
ppm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7.548
7.537
7.527
7.277
7.270
7.259
7.248
7.237
7.230
6.920
6.891
6.868
6.862
6.815
6.788
4.049
4.025
0.132
0.125
MeO
Se
F
5b
10
9
8
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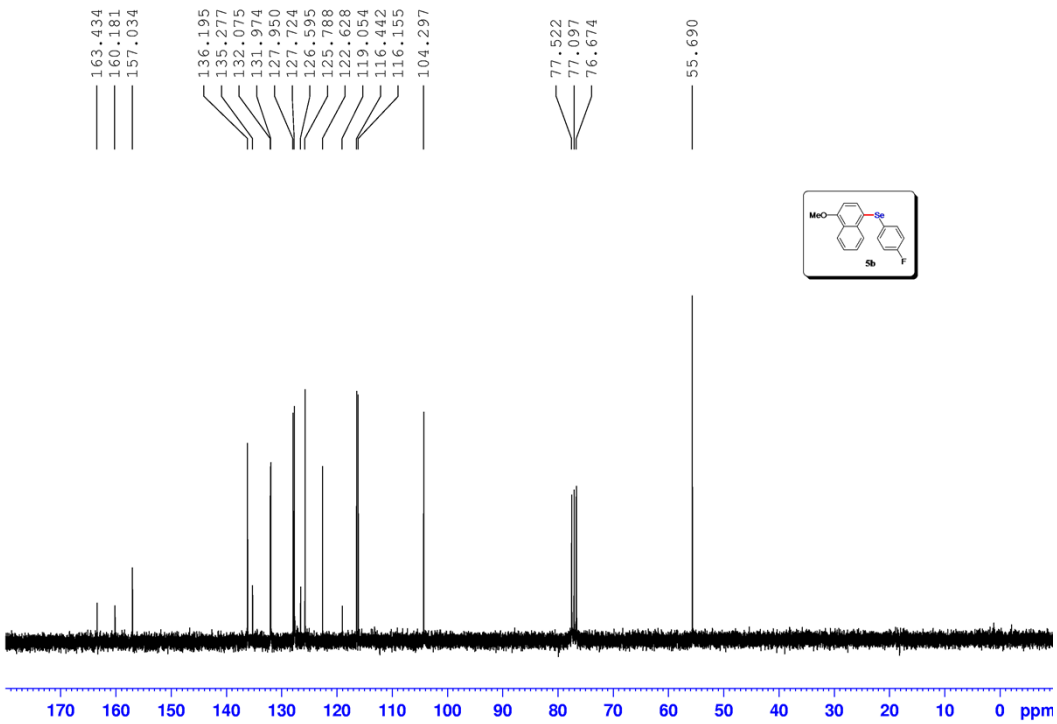
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122.628
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116.442
116.155
104.297
77.522
77.097
76.674
55.690
MeO
Se
F
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140
130
120
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100
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50
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0
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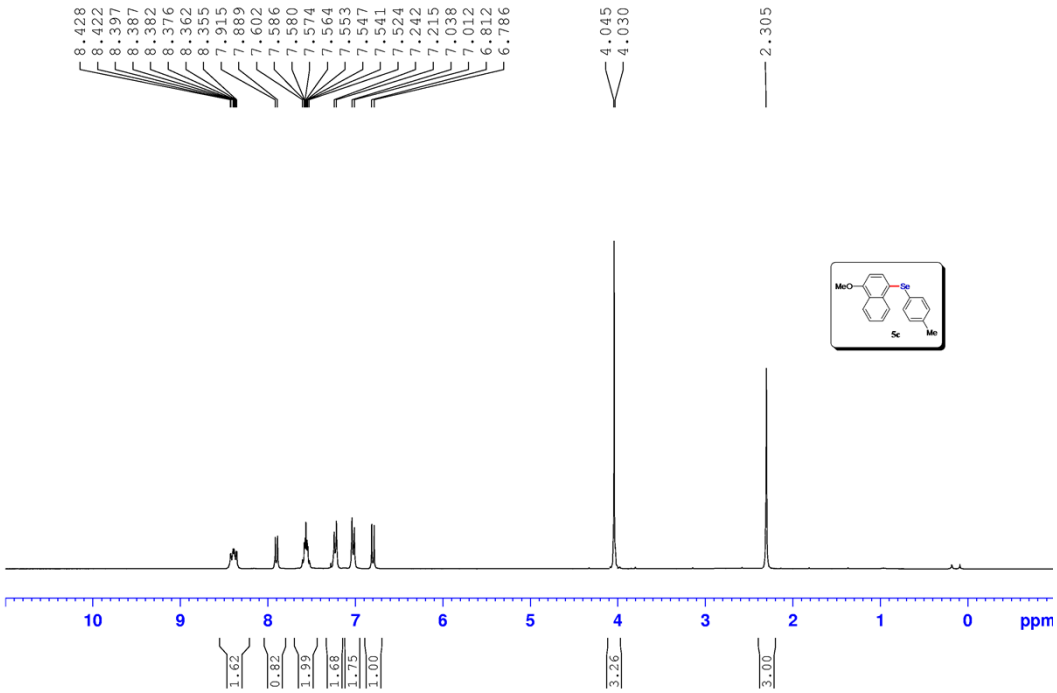
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7.580
7.574
7.564
7.553
7.547
7.541
7.524
7.242
7.215
7.038
7.012
6.812
6.786
4.045
4.030
2.305
MeO
Se
5c
Me
10
9
8
7
6
5
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1
0
ppm
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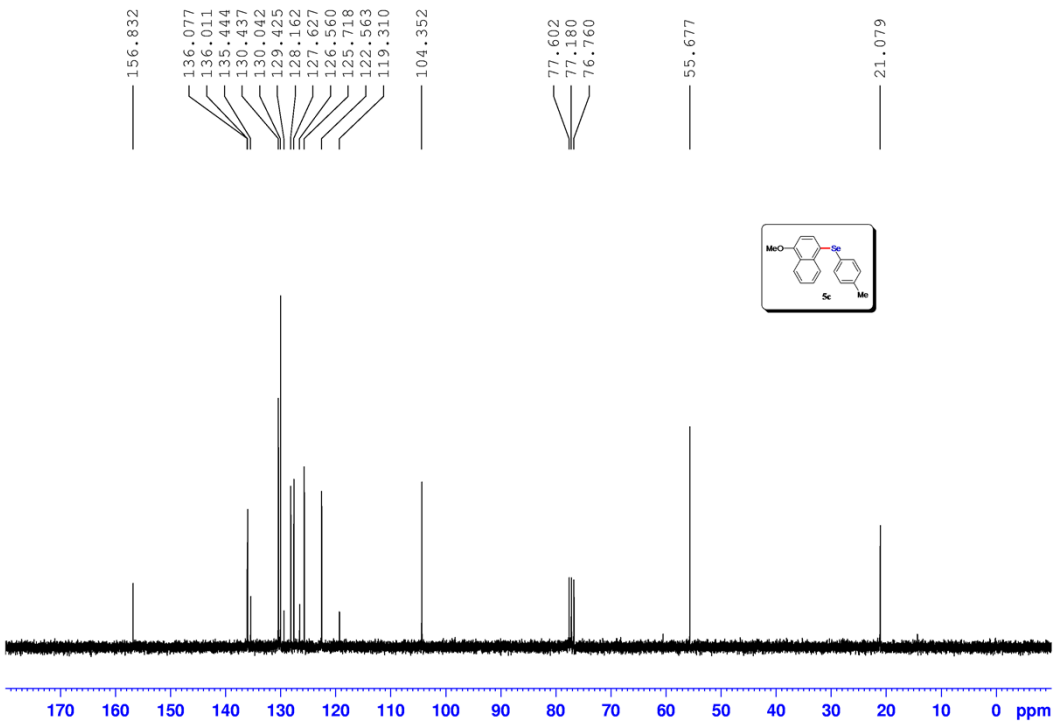
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126.560
125.718
122.563
119.310
104.352
77.602
77.180
76.760
55.677
21.079
MeO
Se
5c
Me
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140
130
120
110
100
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60
50
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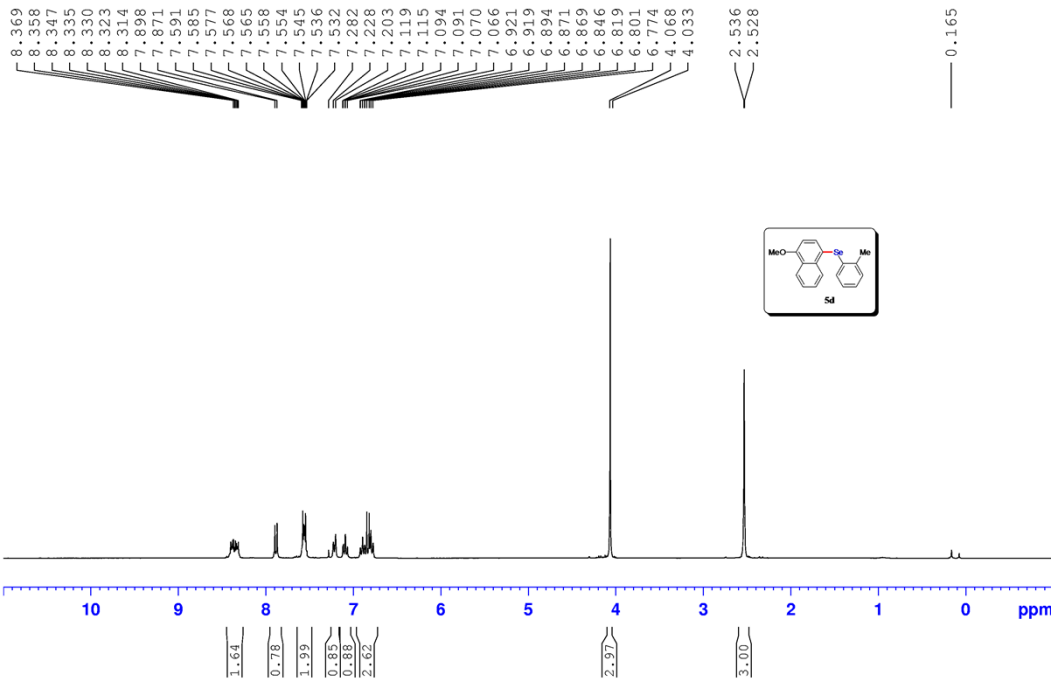
0
ppm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7.568
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7.554
7.545
7.536
7.532
7.282
7.228
7.203
7.119
7.115
7.094
7.091
7.070
7.066
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6.846
6.819
6.801
6.774
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4.033
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2.528
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Se
Me
5d
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9
8
7
6
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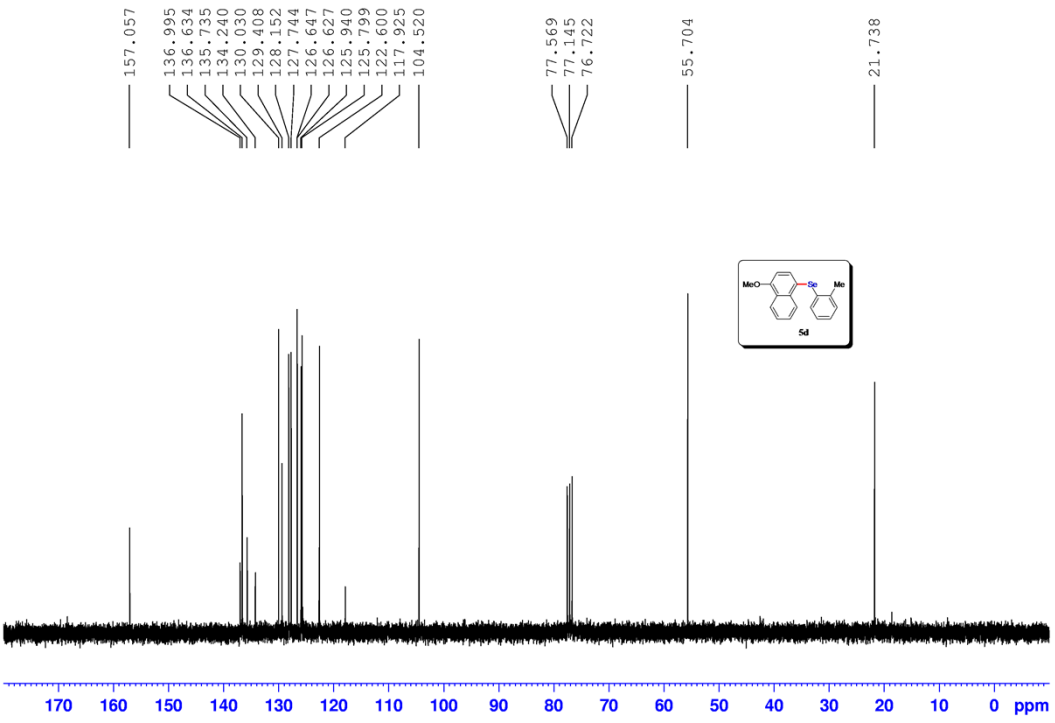
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122.600
117.925
104.520
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77.145
76.722
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21.738
MeO
Se
Me
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20
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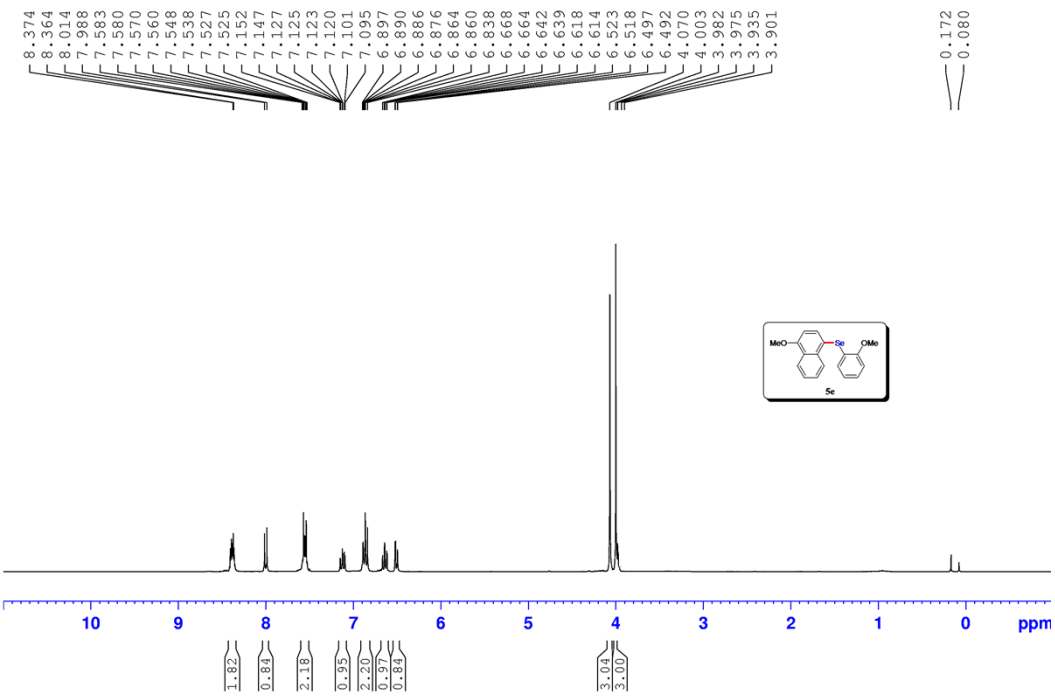
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7.123
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6.864
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6.838
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6.642
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6.618
6.614
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6.518
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3.975
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Se
OMe
5e
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9
8
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6
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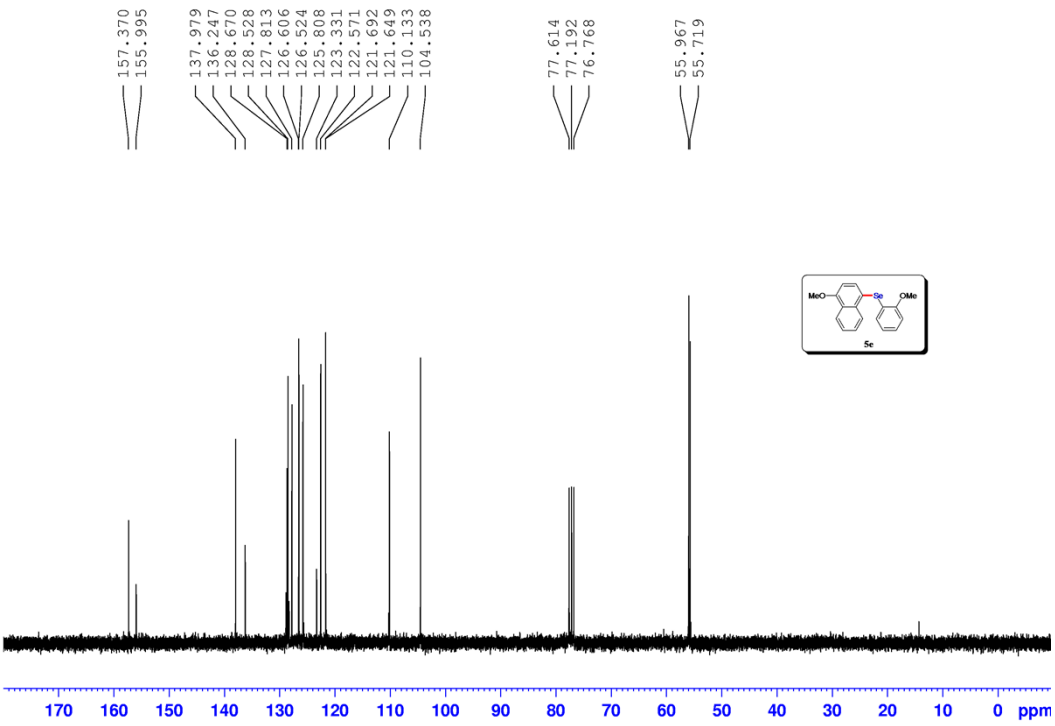
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121.692
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77.614
77.192
76.768
55.967
55.719
MeO
Se
OMe
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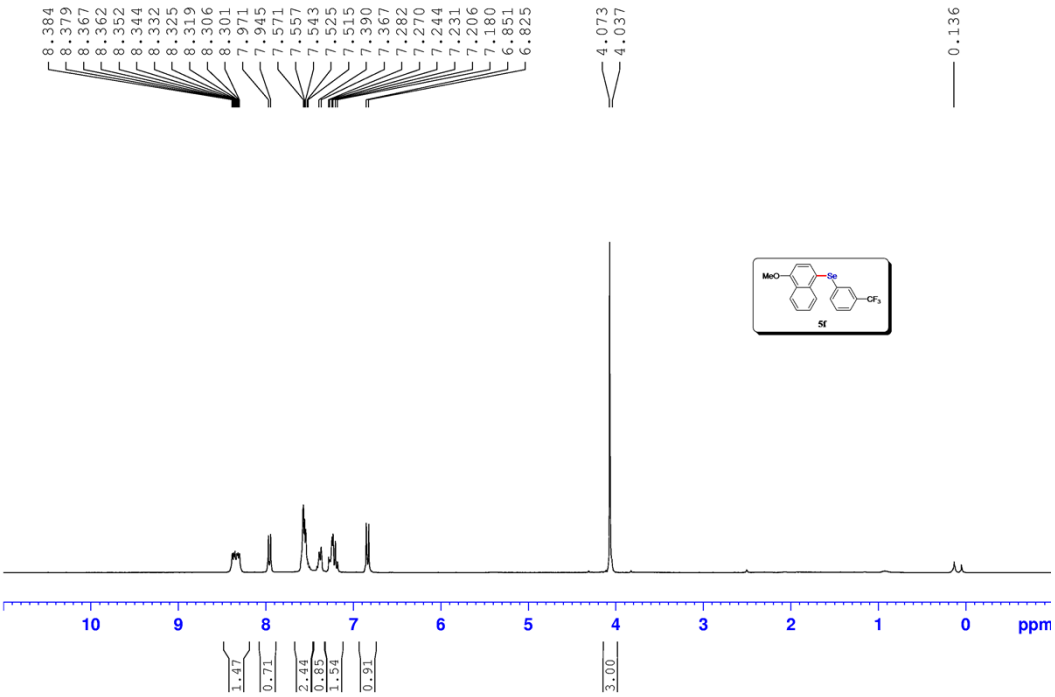
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7.557
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7.231
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6.825
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Se
CF3
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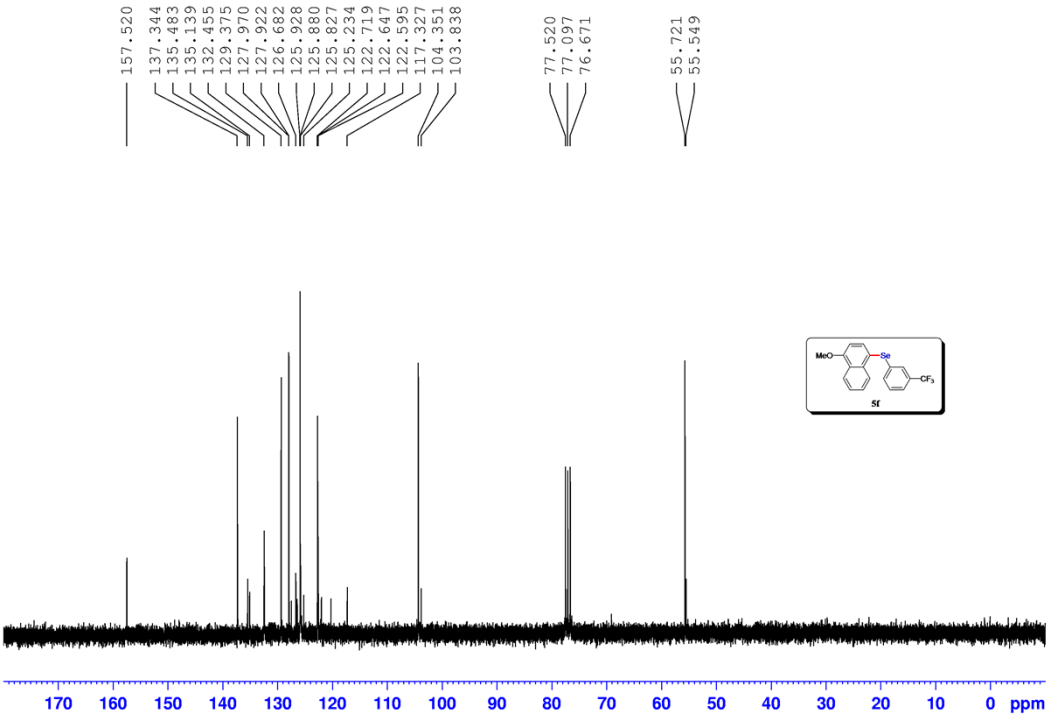
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122.647
122.595
117.327
104.351
103.838
77.520
77.097
76.671
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55.549
MeO
Se
CF3
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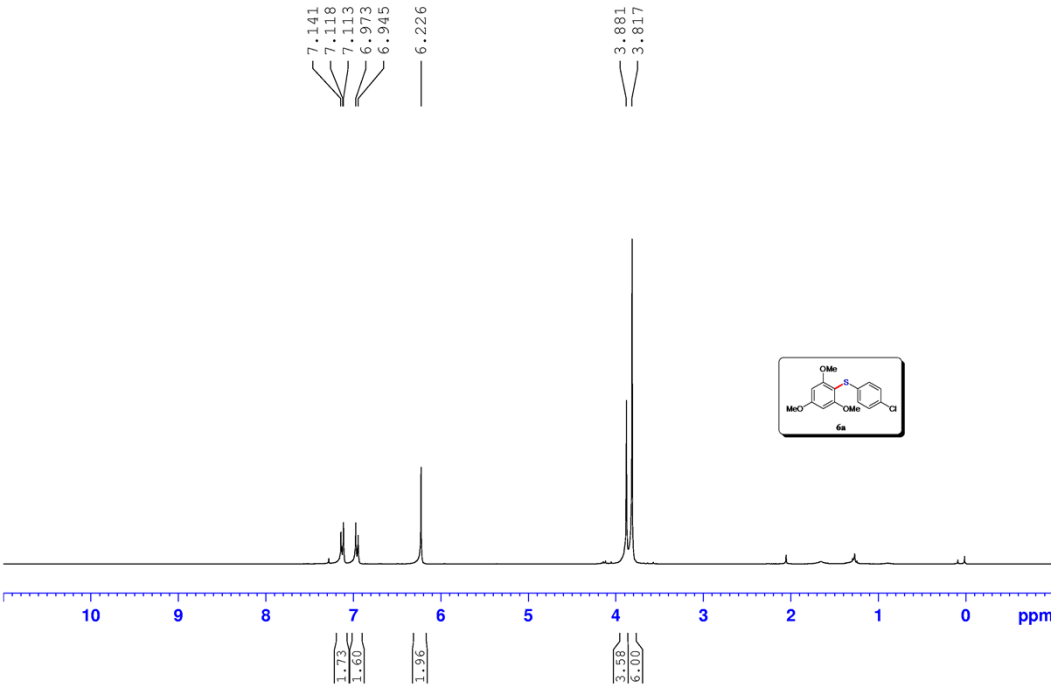
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MeO
OMe
Cl
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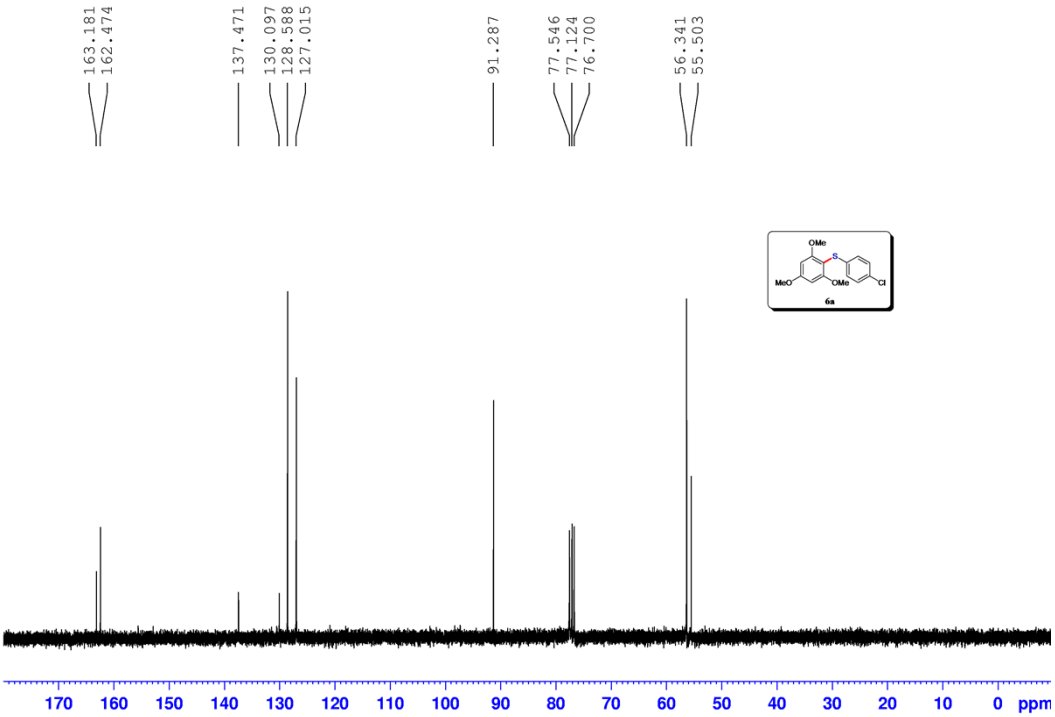
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56.341
55.503
OMe
MeO
OMe
Cl
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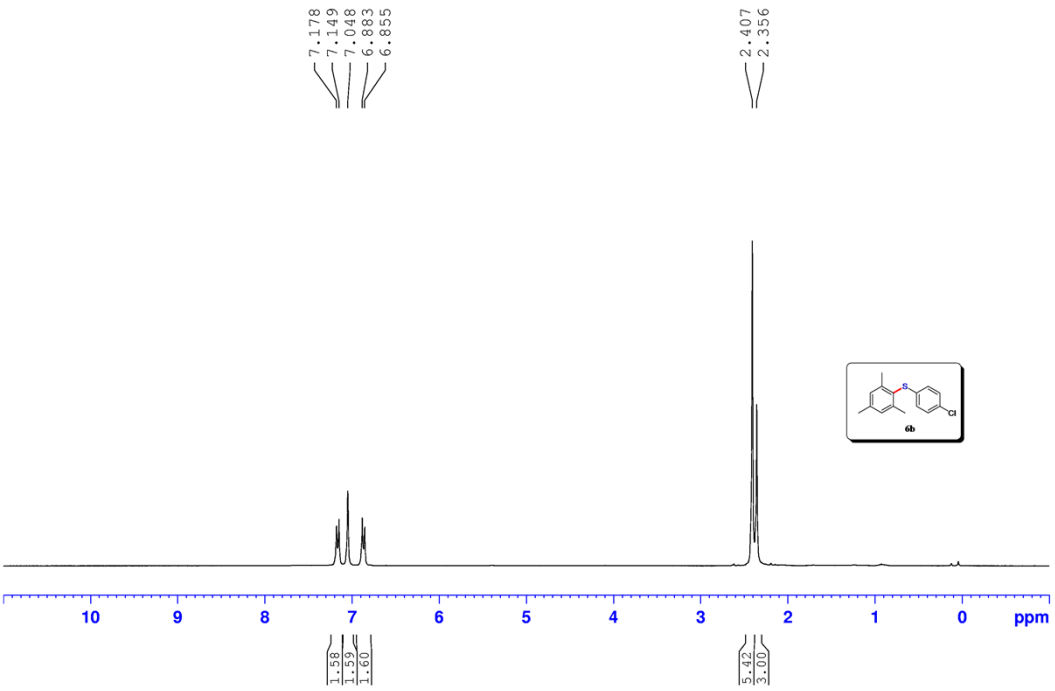
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6b
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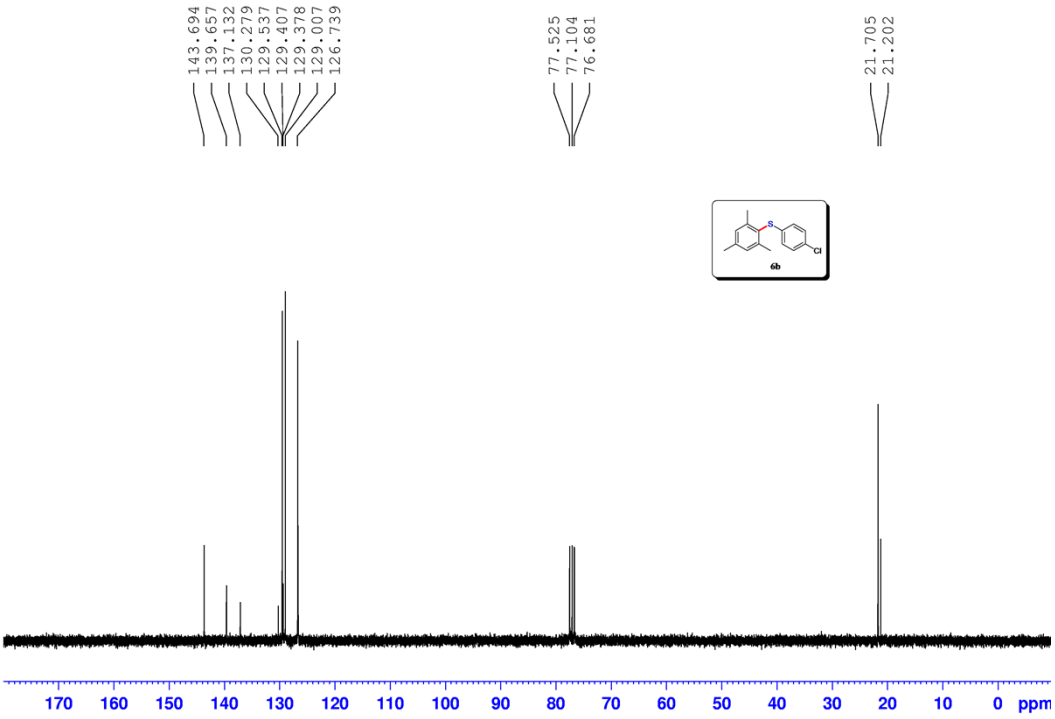
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77.104
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21.202
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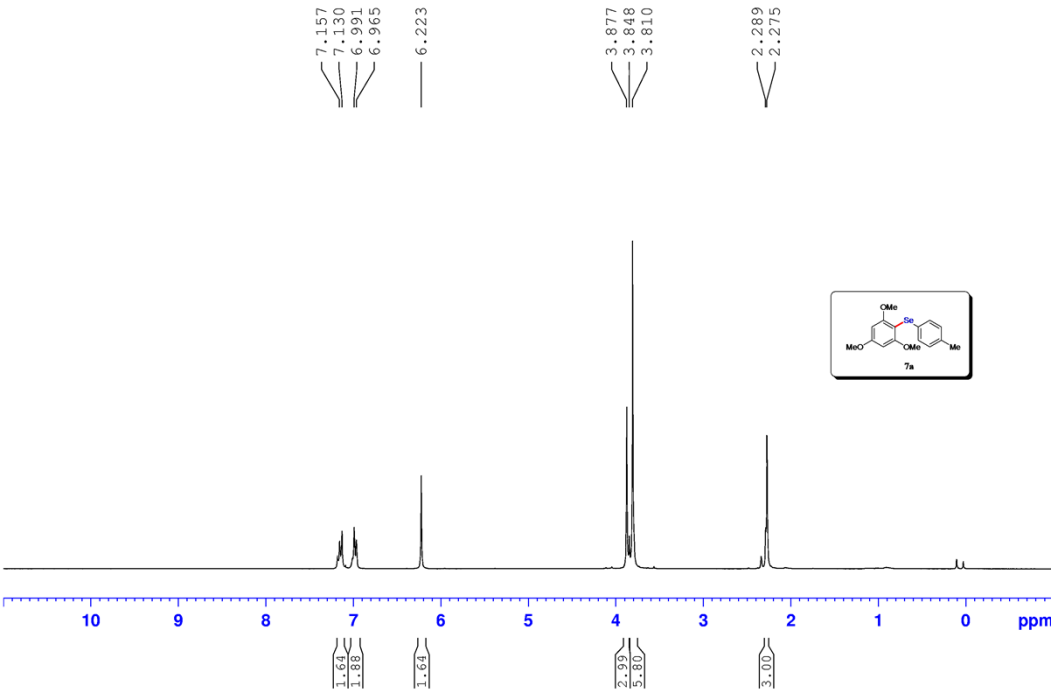
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2.289
2.275
OMe
Se
MeO
OMe
Me
7a
10
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8
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6
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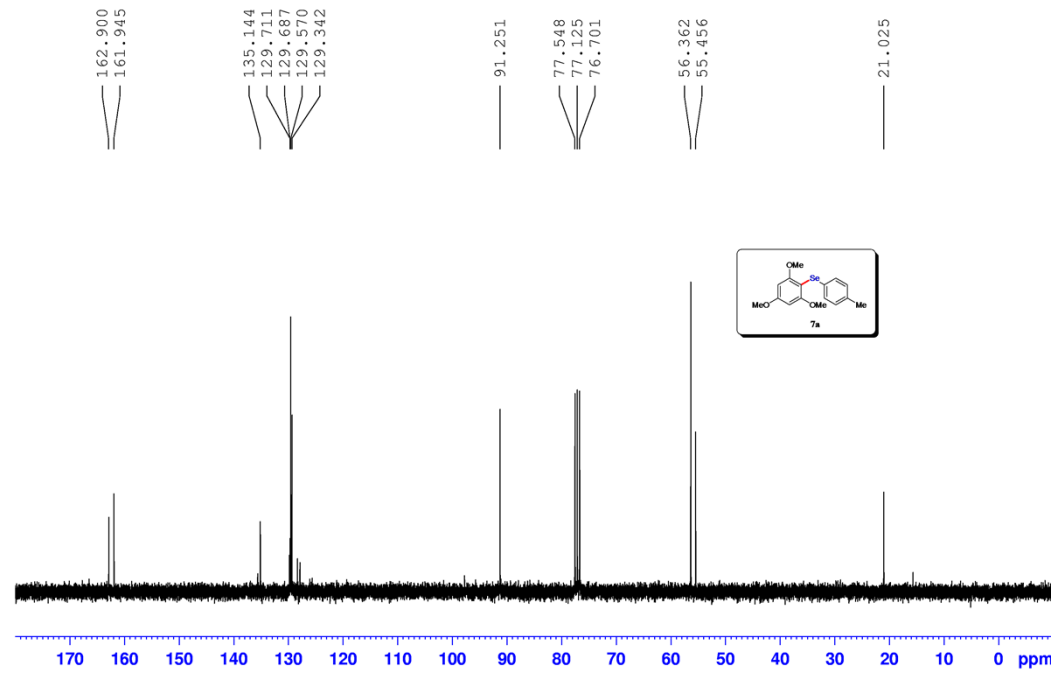
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55.456
21.025
OMe
Se
MeO
OMe
Me
7a
170
160
150
140
130
120
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100
90
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70
60
50
40
30
20
10
0
ppm