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Supporting Information

DDQ-Mediated Regioselective C-S Bond Formation: Efficient Access to Allylic Sulfides

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General information

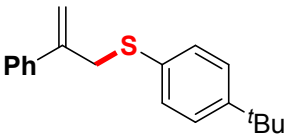
Melting points were measured using a melting point instrument and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. The chemical shifts are referenced to signals at 7.24 and 77.0 ppm, respectively, and chloroform was used as a solvent with TMS as the internal standard. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC-MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100−400 mesh silica gel plates (GF254). Unless otherwise noted, purchased chemicals were used without further purification.

General methods for the preparation of α-methylstyrene

In an oven dried flask, methyl triphenylphosphonium bromide (1.2 equiv) was taken and to this abs. THF (1.6 mL/mmol) was added. The suspension was cooled to 0 ^{o}C, KO^{t}Bu (1.2 equiv) was added and the resulting yellow suspension was stirred at 0 ^{o}C for 45 min. To this suspension, a solution of ketone (1.0 equiv.) in THF (0.7 mL/mmol) was added dropwise and the resulting mixture was warmed gradually to r.t. and stirred at r.t. for 16 h. Reaction mixture was concentrated under reduced pressure and filtered over Celite®. The filtrate was concentrated under reduced pressure to yield a yellow oil. Purification by column chromatography over silica gel (230-400 mesh) using petroleum ether as eluent afforded α-methylstyrene as a colorless oil.

Characterization data for all products

(2-Phenylallyl)(*p*-tolyl)sulfane (**3a**) : Yield: 89% (21.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 - 7.43 (m, 2H), 7.36 - 7.29 (m, 3H), 7.25 - 7.23 (m, 2H), 7.08 (d, J = 8.0 Hz, 1H), 5.36 (s, 1H), 5.12 (s, 1H), 3.92 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 139.6, 136.6, 132.3, 131.2, 129.6, 128.3, 127.8, 126.3, 115.5, 40.2, 21.0; ν_{max}(KBr)/cm^{-1} 3734, 3657, 3595, 3236, 2921, 1629, 1261, 755; HRMS-ESI (m/z): calcd for $C_{16}H_{17}S$, [M+H]+: 241.1045, found 241.1047.



(4-(*tert*-Butyl)phenyl)(2-phenylallyl)sulfane (**3b**) : Yield: 80% (22.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 8.0 Hz, 2H), 7.36 - 7.28 (m, 7H), 5.39 (s, 1H), 5.20 (s, 1H), 3.95 (s, 2H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 143.4, 139.7, 132.7, 130.4, 128.4, 127.8, 126.3, 125.8, 115.5, 39.8, 34.5, 31.3; ν_{max}(KBr)/cm^{-1} 3726, 3677, 3586, 2928, 2857, 1584, 1435, 1050; HRMS-ESI (m/z): calcd for $C_{19}H_{22}NaS$, [M+Na]+: 305.1334, found 305.1336.

(4-Methoxyphenyl)(2-phenylallyl)sulfane (**3c**) : Yield: 78% (19.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 - 7.43 (m, 2H), 7.36 - 7.29 (m, 5H), 6.82 - 6.80 (m, 2H), 5.31 (s, 1H), 4.98 (s, 1H), 3.85 (s, 2H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 143.4, 139.5, 134.4, 128.3, 127.7, 126.3, 126.0, 115.4, 114.4, 55.2, 41.5; ν_{max}(KBr)/cm^{-1} 3893, 3732, 3069, 2929, 2836, 1583, 1447, 1235; HRMS-ESI (m/z): calcd for $C_{16}H_{17}OS$, [M+H]+: 257.0995 found 257.0996.

(4-Fluorophenyl)(2-phenylallyl)sulfane (**3d**) : Yield: 83% (20.3 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 - 7.42 (m, 1H), 7.36 - 7.29 (m, 2H), 6.96 (t, J = 8.0 Hz, 1H), 5.33 (s, 1H), 5.03 (s, 1H), 3.89 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1 (d, J = 246.9 Hz), 143.1, 139.3, 133.9 (d, J = 8.1 Hz), 130.7, 128.4, 127.9, 126.3, 115.8 (d, J = 21.8 Hz,), 115.6, 40.8; ν_{max}(KBr)/cm^{-1} 3738, 3582, 2926, 2855, 1588, 1484, 1223, 759; HRMS-ESI (m/z): calcd for $C_{15}H_{14}FS$, [M+H]+: 245.0795, found 245.0792.

4-((2-Phenylallyl)thio)phenol (**3e**) : Yield: 75% (18.2 mg) as a brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 - 7.43 (m, 2H), 7.36 - 7.31 (m, 3H), 7.27 - 7.24 (m, 2H), 6.77 - 6.73 (m, 2H), 5.31 (s, 1H), 4.98 (s, 1H), 3.85 (s, 2H), 1.65 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 143.4, 139.5, 134.7, 128.3, 127.8, 126.3, 126.1, 115.9, 115.4, 41.6; ν_{max}(KBr)/cm^{-1} 3799, 3729, 3499, 2923, 1584, 1486, 1428, 1235; HRMS-ESI (m/z): calcd for $C_{15}H_{15}OS$, [M+H]+: 243.0838, found 243.0837.

(4-Nitrophenyl)(2-phenylallyl)sulfane (**3f**) : Yield: 70% (19.0 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 7.36 (dd, J = 15.2, 7.2 Hz, 5H), 5.52 (s, 1H), 5.40 (s, 1H), 4.10 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 145.4, 141.9, 139.0, 128.5, 128.2, 127.1, 126.1, 123.8, 116.4; ν_{max}(KBr)/cm^{-1} 3890, 3588, 2921, 2850, 1698, 1424, 946, 806; HRMS-ESI (m/z): calcd for $C_{15}H_{14}O_2NS$, [M+H]+: 272.0740, found 272.0741.

(2-Fluorophenyl)(2-phenylallyl)sulfane (**3g**): Yield: 77% (18.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.41 (m, 1H), 7.35 - 7.26 (m, 2H), 7.23 - 7.19 (m, 1H), 7.06 - 7.01 (m, 2H), 5.32 (s, 1H), 5.11 (s, 1H), 3.95 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.9 (d, J = 245.7 Hz), 143.1, 139.3, 133.8 (d, J = 1.7 Hz), 129.0 (d, J = 7.9 Hz), 128.3, 127.8, 126.3, 124.3 (d, J = 3.7 Hz), 122.4 (d, J = 17.9 Hz), 115.7 (d, J = 5.0 Hz), 115.5, 38.7; ν_{max}(KBr)/cm^{-1} 3897, 3785, 3604, 2923, 1631, 1230, 755, 461; HRMS-ESI (m/z): calcd for $C_{15}H_{14}FS$, [M+H]+: 245.0795, found 245.0789.

(2-Bromophenyl)(2-phenylallyl)sulfane (**3h**): Yield: 81% (24.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz), 7.47 - 7.45 (m, 1H), 7.36 - 7.29 (m, 3H), 7.23 - 7.19 (m, 2H), 7.05 - 7.01 (m, 1H), 5.44 (s, 1H), 5.28 (s, 1H), 3.99 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 139.4, 137.4, 132.9, 129.9, 128.4, 127.9, 127.6, 127.2, 126.2, 124.6, 116.1, 38.2; ν_{max}(KBr)/cm^{-1} 3893, 3588, 3054, 2925, 1435, 1261, 1020, 751; HRMS-ESI (m/z): calcd for $C_{15}H_{14}BrS$, [M+H]+: 304.9994, found 304.9992.

(3-Fluorophenyl)(2-phenylallyl)sulfane (**3i**) : Yield: 83% (20.3 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 - 7.42 (m, 1H), 7.36 - 7.29 (m, 3H), 7.22 - 7.17 (m, 1H), 7.08 - 7.05 (m, 1H), 7.03 - 7.00 (m, 1H), 6.88 - 6.83 (m, 1H), 5.41 (s, 1H), 5.23 (s, 1H), 3.97 (s, 2H); ^{13}C NMR (100

MHz, $CDCl_3$) δ 162.8 (d, J = 247.9 Hz), 142.8, 139.4, 138.8 (d, J = 7.8 Hz), 130.1 (d, J = 8.5 Hz), 128.5, 128.0, 126.3, 125.3 (d, J = 3.0 Hz), 116.4 (d, J = 22.9 Hz), 115.9, 113.2 (d, J = 21.2 Hz), 39.0; ν_{max}(KBr)/cm^{-1} 3874, 3058, 2928, 1688, 1585, 1466, 877, 769; HRMS-ESI (m/z): calcd for $C_{15}H_{14}FS$, [M+H]+: 245.0795, found 245.0792.

(3-Chlorophenyl)(2-phenylallyl)sulfane (**3j**) : Yield: 85% (22.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 7.1 Hz, 1H), 7.40 - 7.33 (m, 4H), 7.21 - 7.18 (m, 3H), 5.45 (s, 1H), 5.25 (s, 1H), 4.00 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 139.3, 138.4, 134.5, 129.7, 129.5, 128.4, 127.9, 127.9, 126.4, 126.2, 115.9, 39.1; ν_{max}(KBr)/cm^{-1} 3881, 3059, 2927, 2850, 1570, 1458, 770, 688; HRMS-ESI (m/z): calcd for $C_{15}H_{14}ClS$, [M+H]+: 261.0499, found 261.0492.

(3-Nitrophenyl)(2-phenylallyl)sulfane (**3k**) : Yield: 65% (17.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (t, J = 1.8 Hz, 1H), 8.02 (dd, J = 8.0, 2.0 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.42 - 7.32 (m, 6H), 5.44 (s, 1H), 5.27 (s, 1H), 4.06 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 142.5, 139.1, 139.0, 135.3, 129.4, 128.5, 128.1, 126.3, 123.9, 120.9, 116.4, 38.8; ν_{max}(KBr)/cm^{-1} 3674, 3497, 2921, 1712, 1513, 1338, 887, 746; HRMS-ESI (m/z): calcd for $C_{15}H_{14}O_2NS$, [M+H]+: 272.0740, found 272.0738.

(3,5-Dimethylphenyl)(2-phenylallyl)sulfane (**3l**): Yield: 85% (21.6 mg) as a yellow oil;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 4.0 Hz, 2H), 7.31 (dt, J = 20.4, 7.2 Hz, 3H), 6.95 (s, 2H), 6.81 (s, 1H), 5.40 (s, 1H), 5.22 (s, 1H), 3.96 (s, 2H), 2.26 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 139.6, 138.3, 135.8, 128.3, 128.2, 127.8, 127.6, 126.2, 115.5, 39.2, 21.2; ν_{max}(KBr)/cm^{-1} 3886, 3039, 2922, 2855, 1718, 1584, 1446, 690; HRMS-ESI (m/z): calcd for $C_{17}H_{19}S$, [M+H]+: 255.1202, found 255.1201.

(3,4-Difluorophenyl)(2-phenylallyl)sulfane (**3m**) : Yield: 77% (20.2 mg) as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 - 7.42 (dd, J = 8.1, 1.4 Hz, 2H), 7.39 - 7.32 (m, 3H), 7.19 - 7.14 (m, 1H), 7.09 - 7.05 (m, 2H), 5.39 (s, 1H), 5.13 (s, 1H), 3.94 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0 (dd, J = 51.6, 12.9 Hz,), 148.6 (dd, J = 49.5, 12.9 Hz,), 142.9, 139.1, 132.11 (dd, J = 5.8, 4.0 Hz, 2H), 128.43 (s, 17H), 128.0, 127.6 (dd, J = 6.1, 3.6 Hz), 126.2, 120.2 (d, J = 17.8 Hz), 117.5 (d, J = 17.4 Hz), 115.9, 40.4; ν_{max}(KBr)/cm^{-1} 3892, 3495, 3053, 2926, 1597, 1495, 1419, 1270 HRMS-ESI (m/z):

calcd for $C_{15}H_{13}F_2S$, [M+H]+: 263.0701, found 263.0698.

2-Methyl-3-((2-phenylallyl)thio)furan (**3n**) : Yield: 73% (16.8 mg) as a brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 - 7.44 (m, 2H), 7.36 - 7.29 (m, 3H), 7.25 - 7.24 (m, 1H), 6.30 (d, J = 4.0 Hz, 1H), 5.30 (s, 1H), 4.94 (s, 1H), 3.67 (s, 2H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 143.6, 140.4, 139.2, 128.3, 127.7, 126.3, 115.3, 115.1, 109.8, 40.9, 11.7; ν_{max}(KBr)/cm^{-1} 3891, 3578, 2926, 1749, 1697, 921, 757, 687; HRMS-ESI (m/z): calcd for $C_{14}H_{15}OS$, [M+H]+: 231.0838, found 231.0840.

Benzyl(2-phenylallyl)sulfane (**3o**) : Yield: 53% (12.7 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.41 (m, 2H), 7.35 - 7.30 (m, 7H), 7.25 - 7.22 (m, 1H), 5.46 (s, 1H), 5.19 (s, 1H), 3.67 (s, 2H), 3.49 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 139.5, 138.1), 129.0, 128.4, 128.3, 127.8, 126.9, 126.3, 115.2, 35.8, 35.6; ν_{max}(KBr)/cm^{-1} 3891, 3676, 2924, 2855 1451, 1303, 1144 905; HRMS-ESI (m/z): calcd for $C_{16}H_{17}O_2NS$, [M+H]+: 241.1045, found 241.1047.

p-Tolyl(2-(*p*-tolyl)allyl)sulfane (**4a**) : Yield: 88% (22.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 5.33 (s, 1H), 5.07 (s, 1H), 3.90 (s, 2H), 2.35 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 137.6, 136.6, 136.6, 132.4, 131.1, 129.5, 129.1, 126.1, 114.7, 40.2, 21.1, 21.0; ν_{max}(KBr)/cm^{-1} 3890, 3733, 3500, 2921, 2854, 1696, 1499, 806; HRMS-ESI (m/z): calcd for $C_{17}H_{19}S$, [M+H]+: 255.1202, found 255.1201.

(2-(4-*iso*Propylphenyl)allyl)(*p*-tolyl)sulfane (**4b**) : Yield: 81% (22.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, J = 8.0 Hz, 2H), 7.25 - 7.23 (m, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 5.35 (s, 1H), 5.09 (s, 1H), 3.91 (s, 2H), 2.91 (dt, J = 13.8, 6.8 Hz, 1H), 2.31 (s, 3H), 1.26 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 143.0, 136.9, 136.5, 132.5, 131.1, 129.5, 126.4, 126.1, 114.7, 40.2, 33.8, 23.9, 21.0; ν_{max}(KBr)/cm^{-1} 3886, 3732, 3580, 2944, 1686, 1599, 1489, 890; HRMS-ESI (m/z): calcd for $C_{19}H_{23}S$, [M+H]+: 283.1515, found 283.1516.

(2-(4-*iso*Butylphenyl)allyl)(*p*-tolyl)sulfane (**4c**) : Yield: 85% (25.2 mg) as a yellow oil; ^{1}H NMR

(400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 7.09 (dd, J = 16.0, 8.0 Hz, 4H), 5.35 (s, 1H), 5.09 (s,1H), 3.91 (s, 2H), 2.47 (d, J = 8.0 Hz, 2H), 2.31 (s, 3H), 1.87 (dp, J = 13.5, 6.8 Hz, 1H), 0.92 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 141.5, 136.9, 136.6, 132.6, 129.6, 129.1, 125.9, 114.7, 45.2, 40.2, 30.2, 22.4, 21.1; ν_{max}(KBr)/cm^{-1} 3890, 3597, 2925, 2855, 1701, 1504, 1231, 755; HRMS-ESI (m/z): calcd for $C_{20}H_{25}S$, [M+H]+: 297.1671, found 297.1670.

(2-(4-Fluorophenyl)allyl)(p-tolyl)sulfane (**4d**) : Yield: 79% (20.4 mg) as yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 - 7.38 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.08 (d, J = 8.0 Hz, 2H), 7.01 (t, J = 8.6 Hz, 2H), 5.28 (s, 1H), 5.08 (s, 1H), 3.88 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5 (d, J = 246.9 Hz), 142.4, 136.8, 135.6 (d, J = 3.2 Hz), 132.1, 131.4, 129.6, 127.9 (d, J = 8.0 Hz), 115.4 (d, J = 1.0 Hz), 115.2 (d, J = 21.4 Hz), 40.4, 21.0; ν_{max}(KBr)/cm^{-1} 3889, 3671, 3495, 2927, 1597, 1500, 1304, 823; HRMS-ESI (m/z): calcd for $C_{16}H_{16}FS$, [M+H]+: 259.0951, found 259.0949.

(2-(4-Bromophenyl)allyl)(p-tolyl)sulfane (**4e**) : Yield: 75% (23.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 5.34 (s, 1H), 5.11 (s, 1H), 3.89 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.4, 138.4, 136.9, 131.9, 131.5, 131.5, 129.6, 127.9, 121.8, 116.0, 40.2, 21.0; ν_{max}(KBr)/cm^{-1} 3901, 3673, 2921, 2853, 1587, 1483, 1080, 754; HRMS-ESI (m/z): calcd for $C_{16}H_{15}BrNaS$, [M+Na]+: 340.9970, found 340.9968.

(2-(2-Chlorophenyl)allyl)(p-tolyl)sulfane (**4f**) : Yield: 83% (22.7 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (dd, J = 6.0, 3.2 Hz, 1H), 7.24 (s, 1H), 7.23 - 7.21 (m, 3H), 7.16 (dd, J = 6.0, 3.2 Hz, 1H), 7.07 (d, J = 8.0 Hz, 2H), 5.32 (s, 1H), 5.06 (s, 1H), 3.93 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 139.9, 136.4, 132.3, 132.1, 131.3, 130.7, 129.5, 129.5, 128.7, 126.5, 40.7, 21.0; ν_{max}(KBr)/cm^{-1} 3848, 3676, 3343, 2921, 2852, 1660, 1478, 1237; HRMS-ESI (m/z): calcd for $C_{16}H_{16}ClS$, [M+H]+: 276.0656, found 276.0648.

(2-(2-Bromophenyl)allyl)(p-tolyl)sulfane (**4g**): Yield: 78% (24.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz, 1H), 7.25 - 7.23 (m, 3H), 7.17 - 7.12 (m, 2H), 7.08 (d, J = 8.0 Hz, 2H), 5.32 (s, 1H), 5.03 (s, 1H), 3.92 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0,

141.9, 136.4, 132.6, 132.3, 131.3, 130.7, 129.6, 128.9), 127.1, 121.9, 118.4, 40.8, 21.0; ν_{max}(KBr)/cm^{-1} 3728, 3676, 3343, 2921, 2852, 1660, 1478, 1237; HRMS-ESI (m/z): calcd for $C_{16}H_{16}BrS$, [M+H]+: 319.0151, found 319.0149.

p-Tolyl(2-(*m*-Tolyl)allyl)sulfane (**4h**): Yield: 87% (22.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (dd, J = 7.2, 3.6 Hz, 5H), 7.11 - 7.09 (m, 2H), 7.07 (s, 1H), 5.34 (s, 1H), 5.11 (s, 1H), 3.91 (s, 2H), 2.35 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 139.6, 137.9, 136.6, 132.5, 131.1, 129.5, 128.6, 128.2, 127.0, 123.4, 115.2, 40.2, 21.5, 21.0; ν_{max}(KBr)/cm^{-1} 3896, 3673, 2920, 1704, 1480, 896, 778, 686; HRMS-ESI (m/z): calcd for $C_{17}H_{19}S$, [M+H]+: 255.1202, found 255.1201.

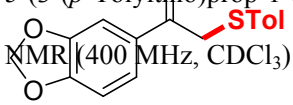
(2-(3-Methoxyphenyl)allyl)(*p*-tolyl)sulfane (**4i**) : Yield: 83% (22.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, CDCl3) δ 7.24 (d, J = 8.0 Hz, 3H), 7.09 - 7.03 (m, 3H), 6.99 - 6.98 (m, 1H), 6.84 (dd, J = 8.2, 2.4 Hz, 1H), 5.35 (s, 1H), 5.11 (s, 1H), 3.90 (s, 3H), 3.80 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 143.3, 141.2, 136.7, 132.3, 131.2, 129.6, 129.3, 118.8, 115.6, 113.1, 112.3, 55.2, 40.3, 21.0; ν_{max}(KBr)/cm^{-1} 3818, 3577, 3492, 2982, 1592 1489, 1039, 755; HRMS-ESI (m/z): calcd for $C_{17}H_{19}OS$, [M+H]+: 271.1151, found 271.1152.

(2-(3-Fluorophenyl)allyl)(*p*-tolyl)sulfane (**4j**): Yield: 82% (21.2 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 - 7.21 (m, 5H), 7.16 - 7.12 (m, 1H), 7.09 (d, J = 8.0 Hz, 2H), 6.99 (td, J = 8.4, 2.4 Hz, 1H), 5.36 (s, 1H), 5.12 (s, 1H), 3.88 (s, 2H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, J = 245.3 Hz), 142.4 (d, J = 2.1 Hz), 141.9 (d, J = 7.6 Hz), 136.9, 131.9, 131.5), 129.8 (d, J = 8.4 Hz), 129.6, 121.9 (d, J = 2.8 Hz), 116.4, 114.6 (d, J = 21.2 Hz), 113.3 (d, J = 22.1 Hz), 40.2, 21.1; ν_{max}(KBr)/cm^{-1} 3892, 3584, 3044, 2924, 1712, 1588, 1479, 798; HRMS-ESI (m/z): calcd for $C_{16}H_{16}FS$, [M+H]+: 259.0951, found 259.0945.

(2-(3,4-Dichlorophenyl)allyl)(p-tolyl)sulfane (**4k**): Yield: 80% (24.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1H NMR (400 MHz, CDCl3) δ 7.49 (d, J = 1.6 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.27 - 7.21 (m, 3H), 7.08 (d, J = 8.0 Hz, 2H), 5.32 (s, 1H), 5.11 (s, 1H), 3.84 (s, 2H), 2.32 (s, 34H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 139.5, 137.2, 132.4, 131.8, 131.7, 131.5, 130.2, 129.7, 128.3, 125.8, 116.9, 40.2, 21.1; ν_{max}(KBr)/cm^{-1} 3901, 3585, 2921, 2853, 1647, 1483, 814, 754;

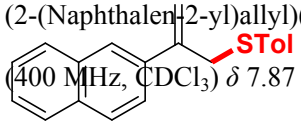
HRMS-ESI (m/z): calcd for $C_{16}H_{15}Cl_2S$, [M+H]+: 309.0266, found 309.0267.

5-(3-(*p*-Tolylthio)prop-1-en-2-yl)benzo[d][1,3]dioxole (**4l**): Yield: 75% (21.3 mg) as a yellow oil;



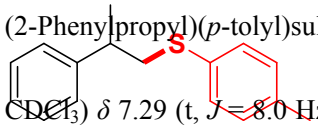
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.0 Hz, 2H), 7.08 (d, J = 8.0 Hz, 2H), 6.97 (s, 1H), 6.93 (dd, J = 8.0, 1.2 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 5.92 (s, 2H), 5.24 (s, 1H), 4.98 (s, 1H), 2.30 (s, 2H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 146.9, 142.7, 137.4, 135.6, 133.9, 129.8, 128.6, 119.1, 111.3, 107.8, 106.0, 100.9, 22.0, 20.9; ν_{max}(KBr)/cm^{-1} 3889, 3581, 2925, 2854, 1581, 1483, 1243, 1036; HRMS-ESI (m/z): calcd for $C_{17}H_{17}O_2S$, [M+H]+: 285.0944, found 285.0936.

(2-(Naphthalen-2-yl)allyl)(p-tolyl)sulfane (**4m**): Yield: 85% (24.7 mg) as a yellow oil; ^{1}H NMR



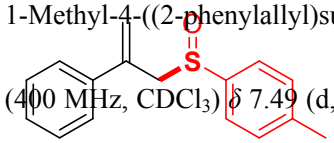
(400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.82 - 7.78 (m, 3H), 7.59 (dd, J = 8.4, 1.6 Hz, 1H), 7.48 - 7.43 (m, 2H), 7.26 (d, J = 8.0 Hz, 1H), 7.08 (d, J = 8.0 Hz, 1H), 5.50 (s, 1H), 5.22 (s, 1H), 4.03 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 136.7, 133.3, 132.9, 132.4, 131.3, 129.6, 128.3, 127.9, 127.5, 126.2, 126.0, 125.2, 124.5, 115.9, 40.3, 21.0; ν_{max}(KBr)/cm^{-1} 3901, 3673, 3148, 2921, 2853, 1587, 1483, 1243, 1036; HRMS-ESI (m/z): calcd for $C_{20}H_{19}S$, [M+H]+: 291.1202, found 291.1203.

(2-Phenylpropyl)(*p*-tolyl)sulfane (**5**): Yield: 93% (45.0 mg) as a light yellow oil; ^{1}H NMR (400 MHz,



$CDCl_3$) δ 7.29 (t, J = 8.0 Hz, 2H), 7.23 - 7.17 (m, 5H), 7.07 (d, J = 8.0 Hz, 2H), 3.17 (dd, J = 12.0, 6.0 Hz, 1H), 3.03 - 2.91 (m, 2H), 2.30 (s, 3H), 1.37 (d, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 136.0, 133.0, 130.0, 129.6, 128.5, 126.9, 126.5, 42.8, 39.4, 20.9, 20.9; ν_{max}(KBr)/cm^{-1} 3739, 3591, 3031, 2924, 1688, 1487, 1089, 699; HRMS-ESI (m/z): calcd for $C_{16}H_{18}NaS$, [M+Na]+: 265.1021, found 265.1019.

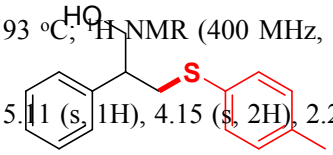
1-Methyl-4-((2-phenylallyl)sulfinyl)benzene (**6**): Yield: 90% (46.0 mg) as a yellow oil; ^{1}H NMR



(400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.0 Hz, 2H), 7.42 - 7.39 (m, 2H), 7.36 - 7.32 (m, 3H), 7.27 (d, J = 8.0 Hz, 2H), 5.55 (s, 1H), 5.12 (s, 1H), 4.09 (d, J = 12.0 Hz, 1H), 3.84 (d, J = 12.0 Hz, 1H), 2.40 (s,

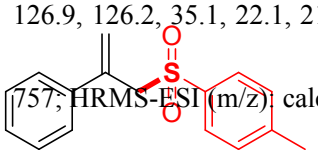
3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 140.2, 138.9, 137.5, 129.6, 128.5, 128.1, 126.0, 124.5, 119.8, 64.8, 21.3 ppm; ν_{max}(KBr)/cm^{-1} 3893, 3734, 3041, 2925, 2862, 1695, 1489, 1078; HRMS-ESI (m/z): calcd for $C_{16}H_{17}OS$, [M+H]+: 257.0995, found 257.0991.

1-Methyl-4-((2-phenylallyl)sulfonyl)benzene (**7**): Yield: 88% (47.8 mg) as a white solid; mp = 91 - 93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.0 Hz, 1H), 7.19 - 7.09 (m, 7H), 5.48 (s, 1H), 5.11 (s, 1H), 4.15 (s, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.5), 138.7, 136.5, 135.4, 129.4, 128.5, 128.2, 127.8, 126.1, 121.6, 62.0, 21.40 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2929, 1598, 1407, 1127, 778, 697, 523; HRMS-ESI (m/z): calcd for $C_{16}H_{17}O_2S$, [M+H]+: 273.0944, found 273.0943.

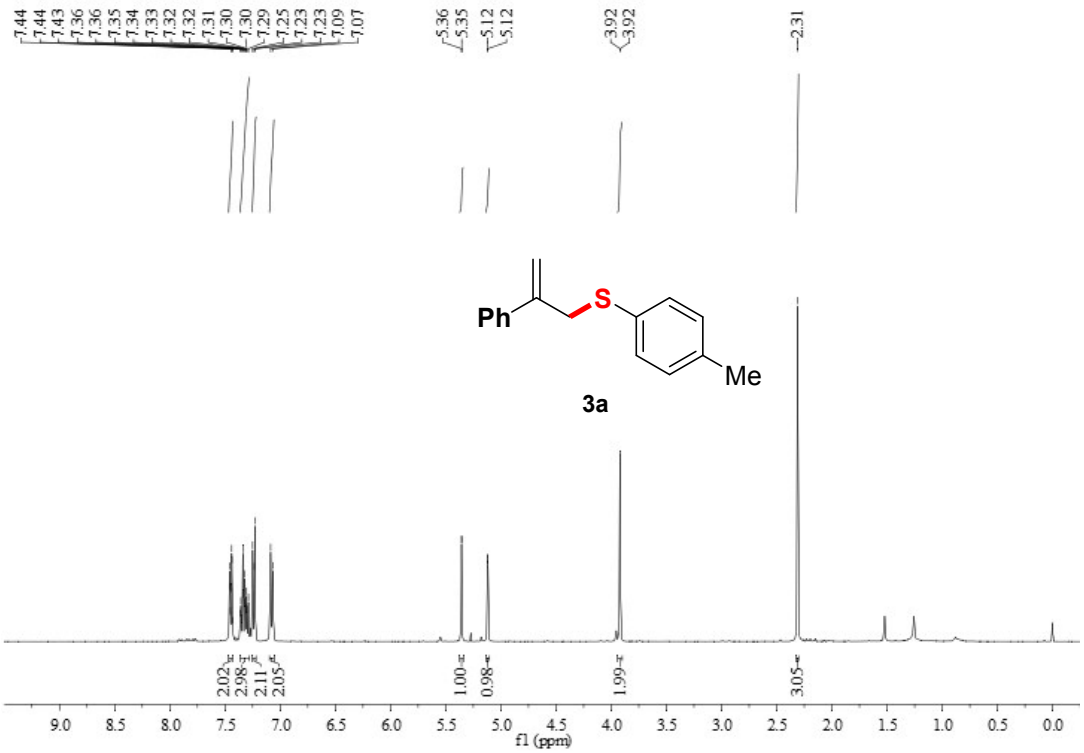


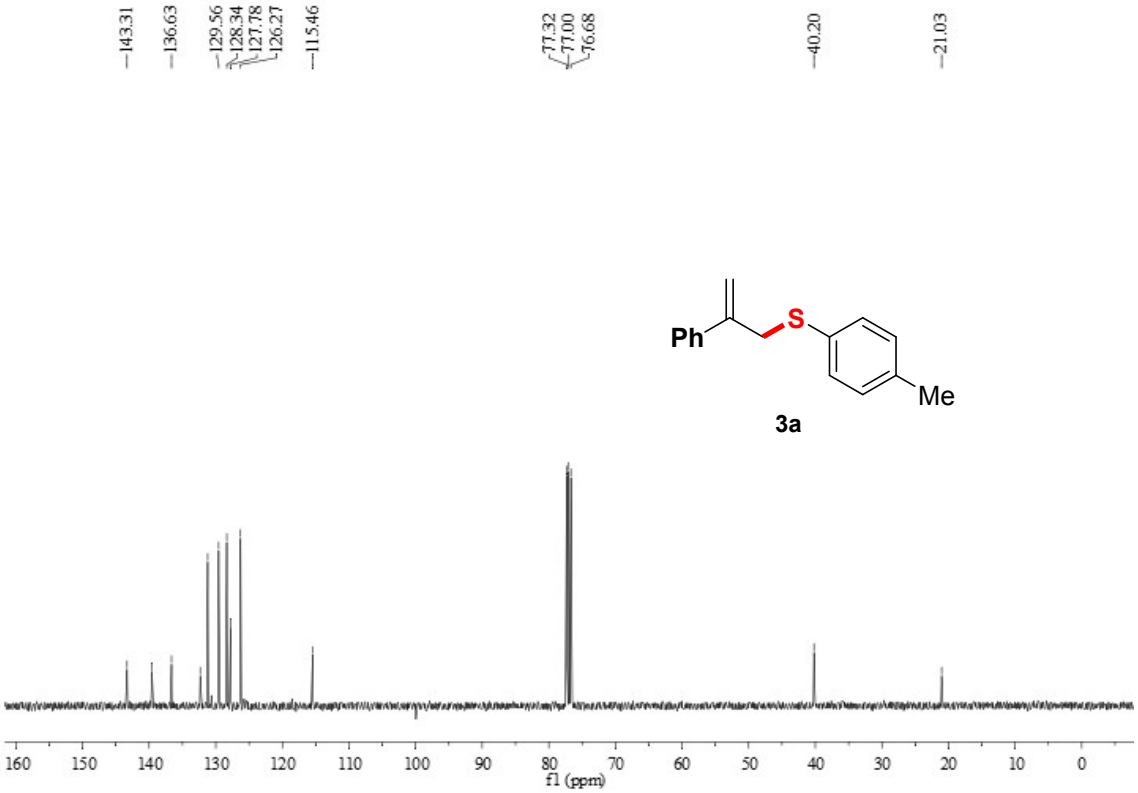
2-Phenyl-3-(*p*-tolylthio)propan-1-ol (**8**): Yield: 85% (43.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, J = 8.0 Hz, 2H), 7.27 - 7.23 (m, 3H), 7.21 - 7.19 (m, 2H), 7.08 (d, J = 8.1 Hz, 1H), 3.92 - 3.84 (m, 2H), 3.29 - 3.14 (m, 2H), 3.05 - 2.98 (m, 1H), 2.31 (s, 3H), 1.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 136.3, 132.3, 130.2, 129.7, 128.7, 127.9, 127.2, 66.0, 47.4, 37.0, 21.0 ppm; ν_{max}(KBr)/cm^{-1} 3885, 3674, 3232, 2921, 1690, 1440 1038, 758; HRMS-ESI (m/z): calcd for $C_{16}H_{19}OS$, [M+H]+: 259.1151, found 259.1150.

(*E*)-(4-Phenylpent-3-en-1-yl)(*p*-tolyl)sulfane (**9**): Yield: 67% (17.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 - 7.42 (m, 2H), 7.33 - 7.28 (m, 3H), 7.26 - 7.20 (m, 2H), 7.08 (d, J = 8.0 Hz, 2H), 5.82 (t, J = 8.0 Hz, 1H), 3.94 (s, 2H), 2.32 (s, 3H), 2.11 (p, J = 7.5 Hz, 1H), 0.97 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 136.6, 134.8, 134.0, 132.9, 131.3, 129.5, 128.3, 126.9, 126.2, 35.1, 22.1, 21.0, 14.1 ppm; ν_{max}(KBr)/cm^{-1} 3675, 3591, 2927, 2861, 1719, 1473, 938, 757; HRMS-ESI (m/z): calcd for $C_{18}H_{21}S$, [M+H]+: 269.1358, found 269.1355.



NMR spectra for all the compounds

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126.27
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77.32
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Ph
S
Me
3a
160
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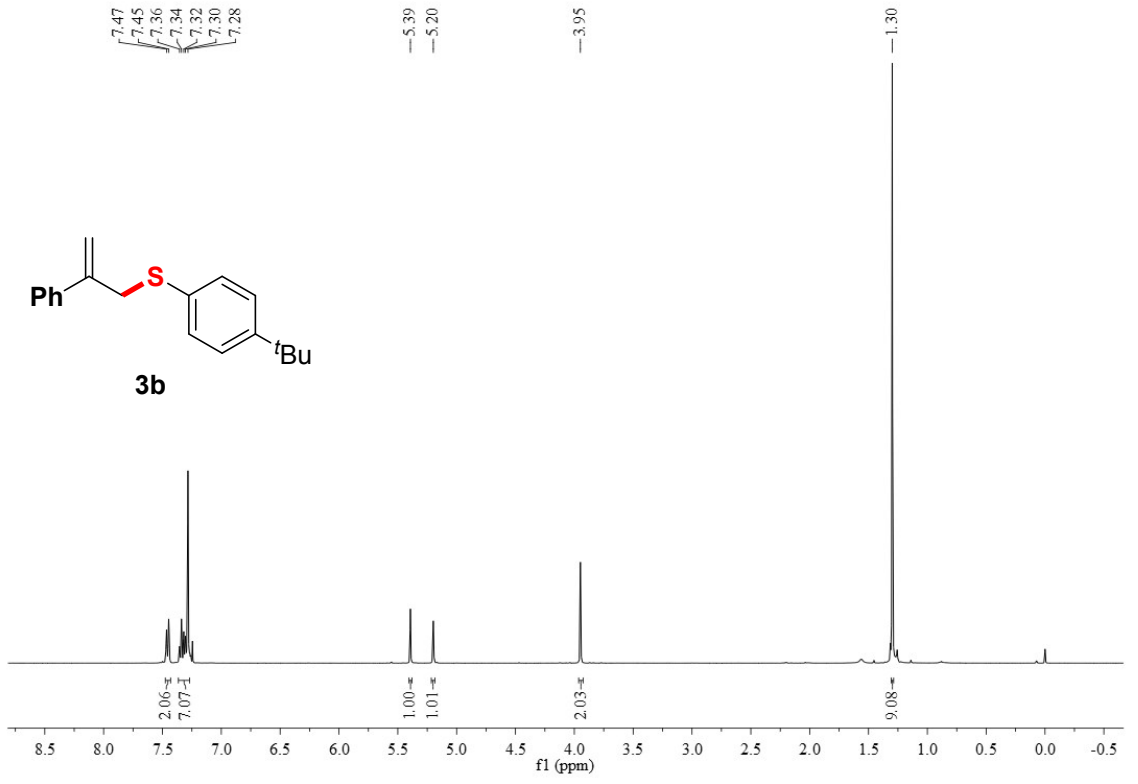
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.95
1.30
Ph
S
tBu
3b
2.06
7.07
1.00
1.01
2.03
9.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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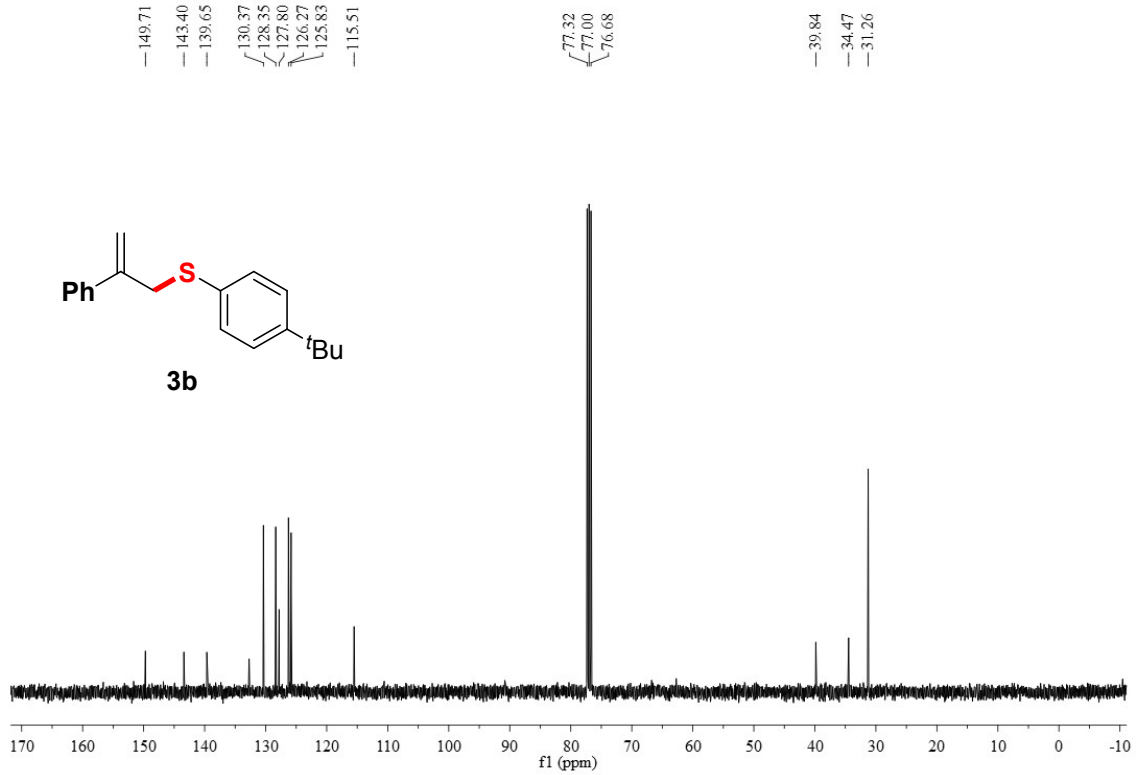
0.5
0.0
-0.5
f1 (ppm)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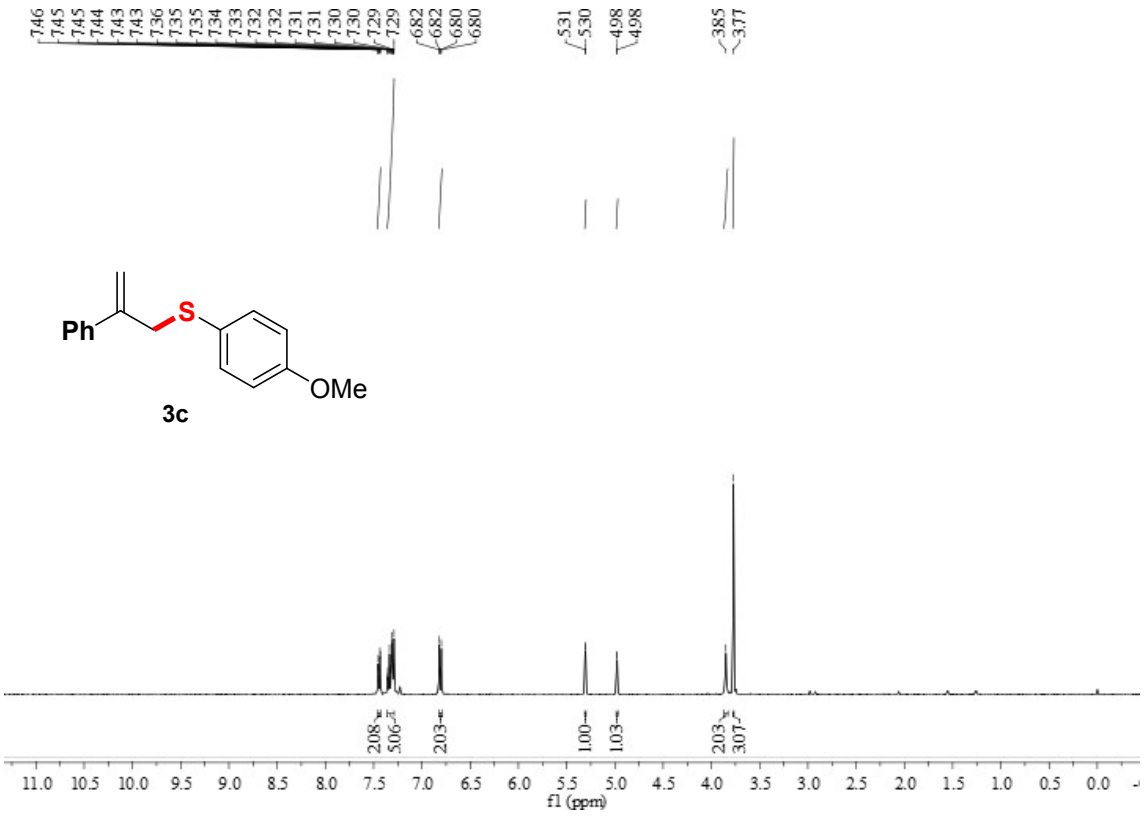
31.26
Ph
S
tBu
3b
f1 (ppm)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733
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729
729
682
682
680
680
531
530
498
498
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377
Ph
S
OMe
3c
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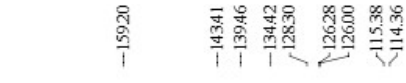
1.00
1.03
2.03
3.07
f1 (ppm)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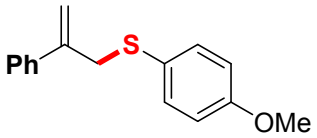
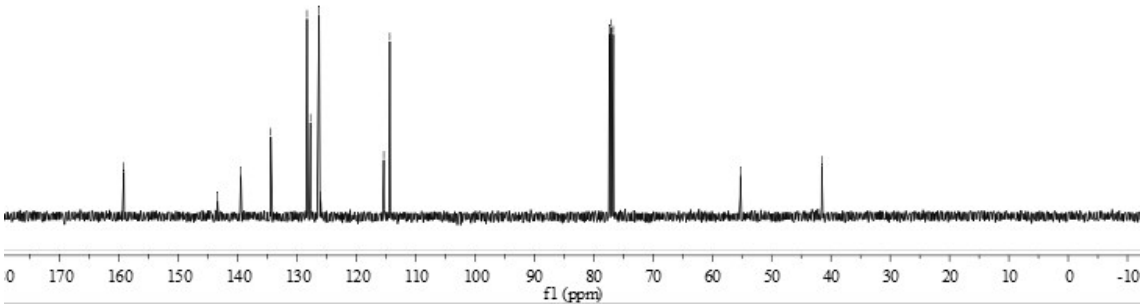
41.53


Ph
S
OMe

3c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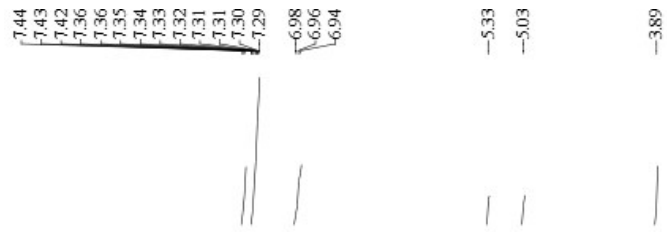
f1 (ppm)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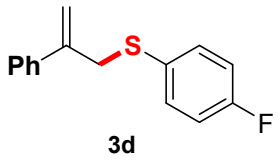
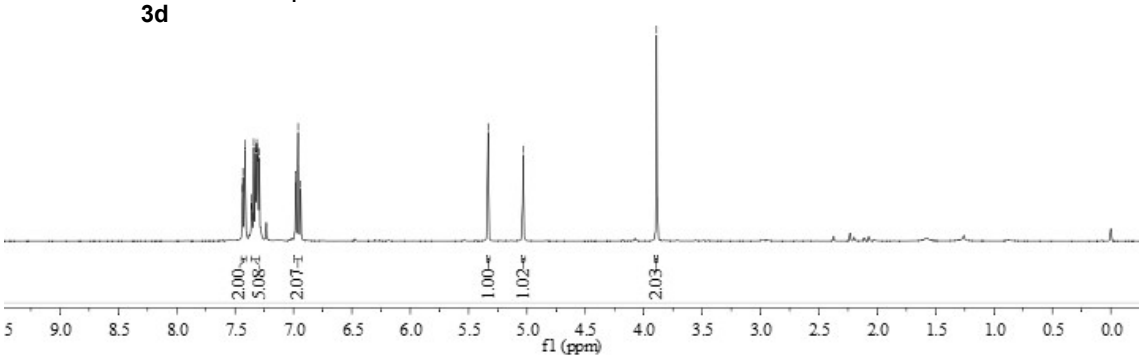
5.03
3.89


Ph
S
F

3d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1.00
1.02
2.03
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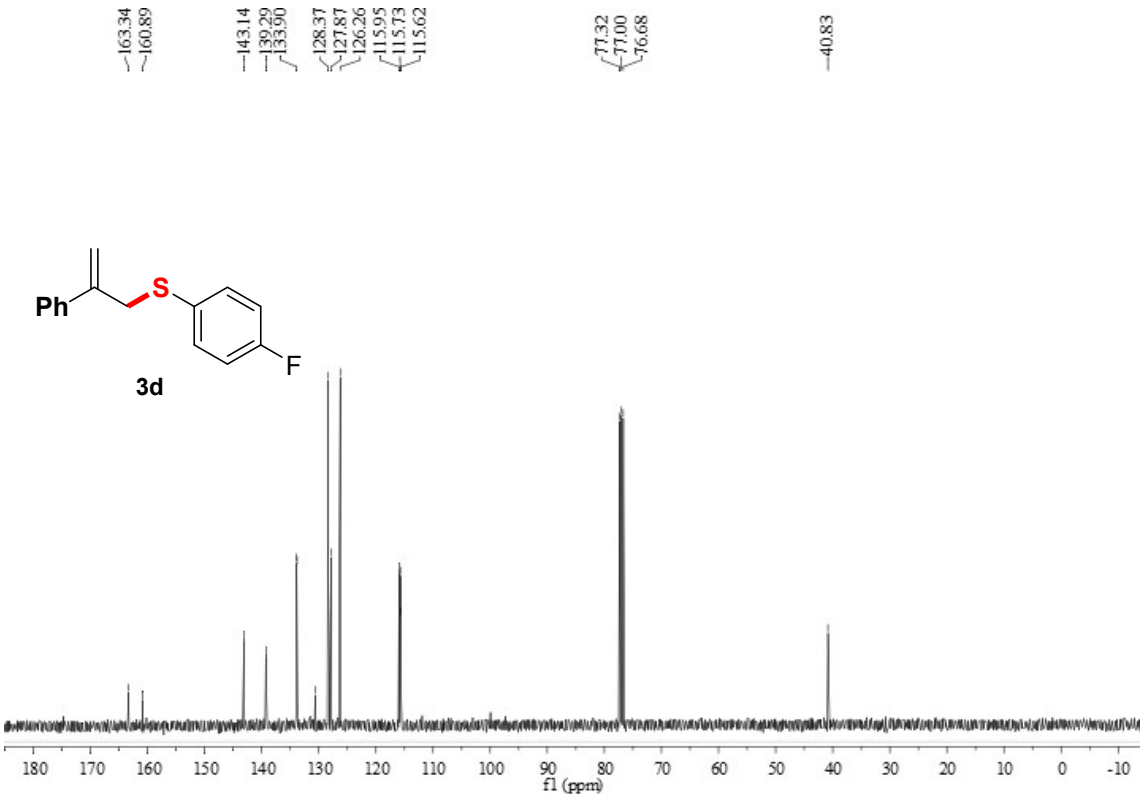
f1 (ppm)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126.26
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115.62
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Ph
S
F
3d
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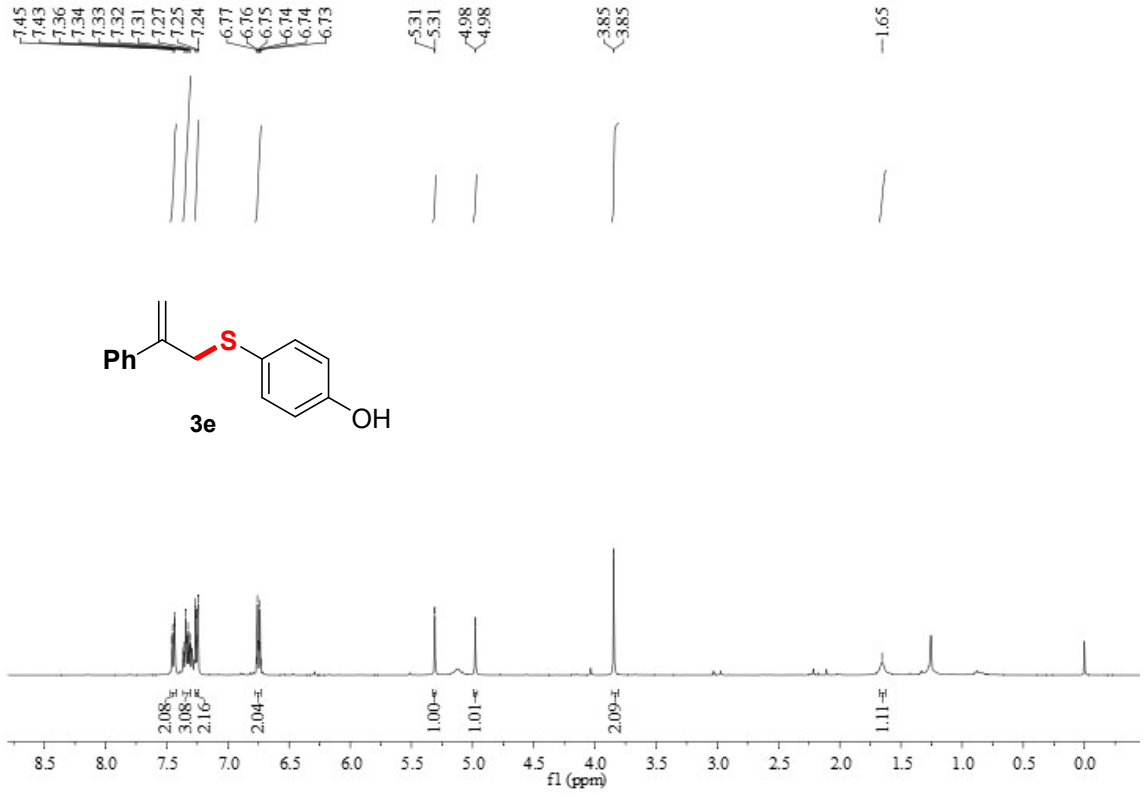
f1 (ppm)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7.25
7.24
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6.76
6.75
6.74
6.74
6.73
5.31
5.31
4.98
4.98
3.85
3.85
1.65
Ph
S
OH
3e
2.08
3.08
2.16
2.04
1.00
1.01
2.09
1.11
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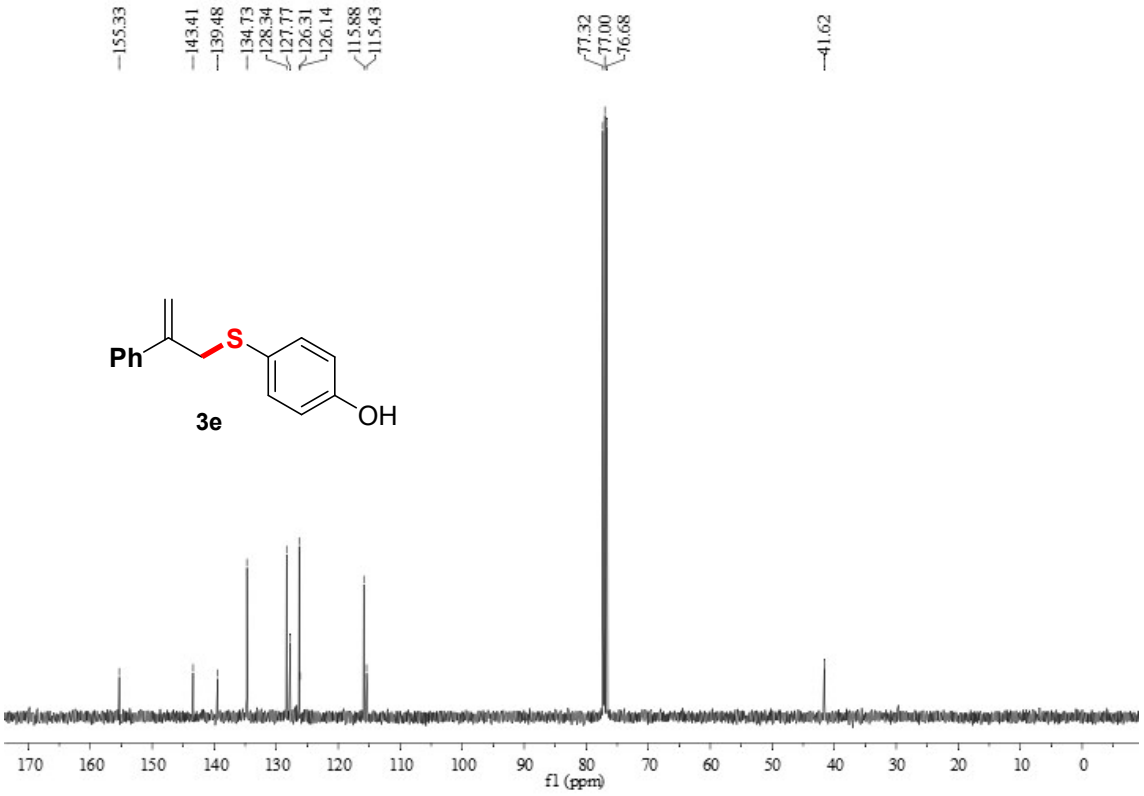
f1 (ppm)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S
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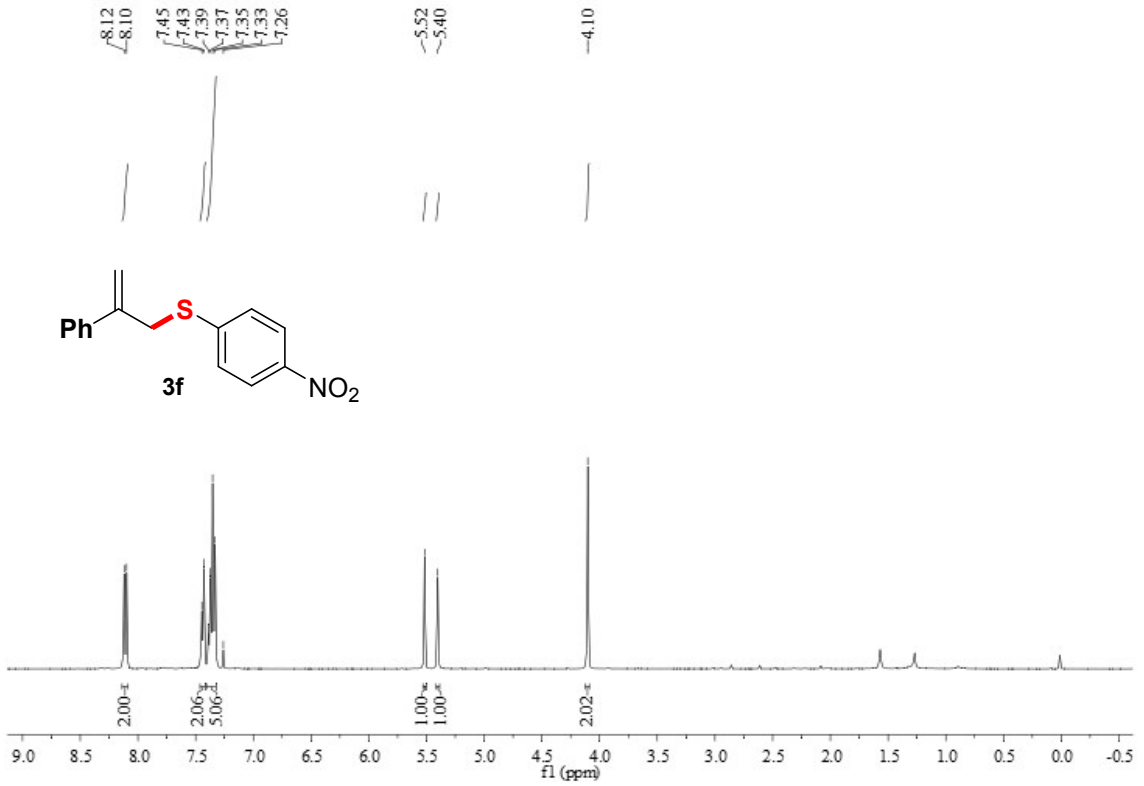
f1 (ppm)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7.33
7.26
5.52
5.40
4.10
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NO2
3f
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2.06
5.06
1.00
1.00
2.02
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


146.98
145.35
141.96
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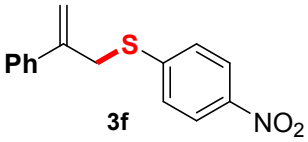
Ph
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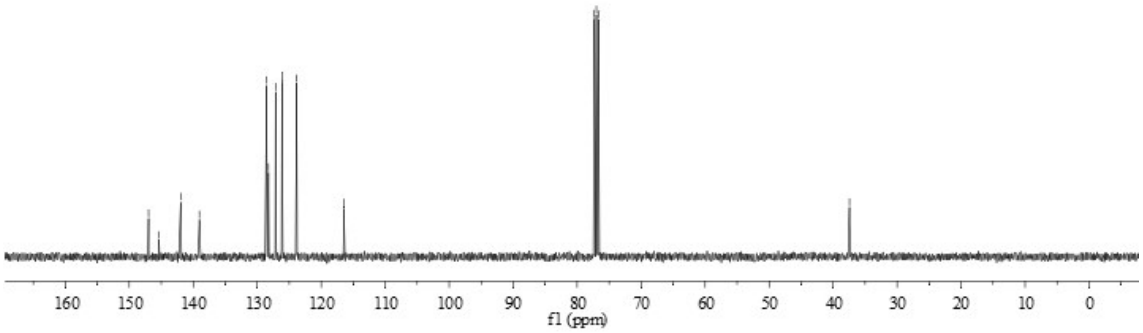
NO2

3f


160
150
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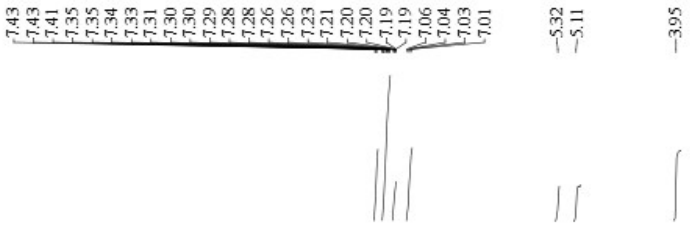
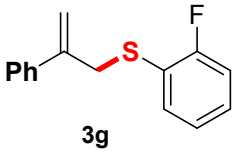
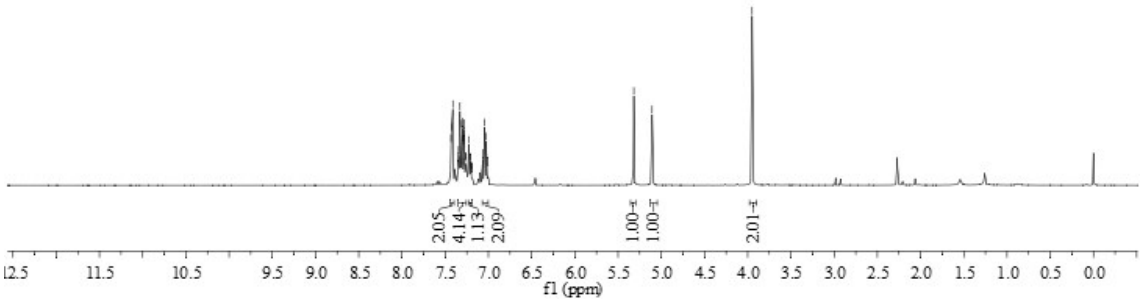
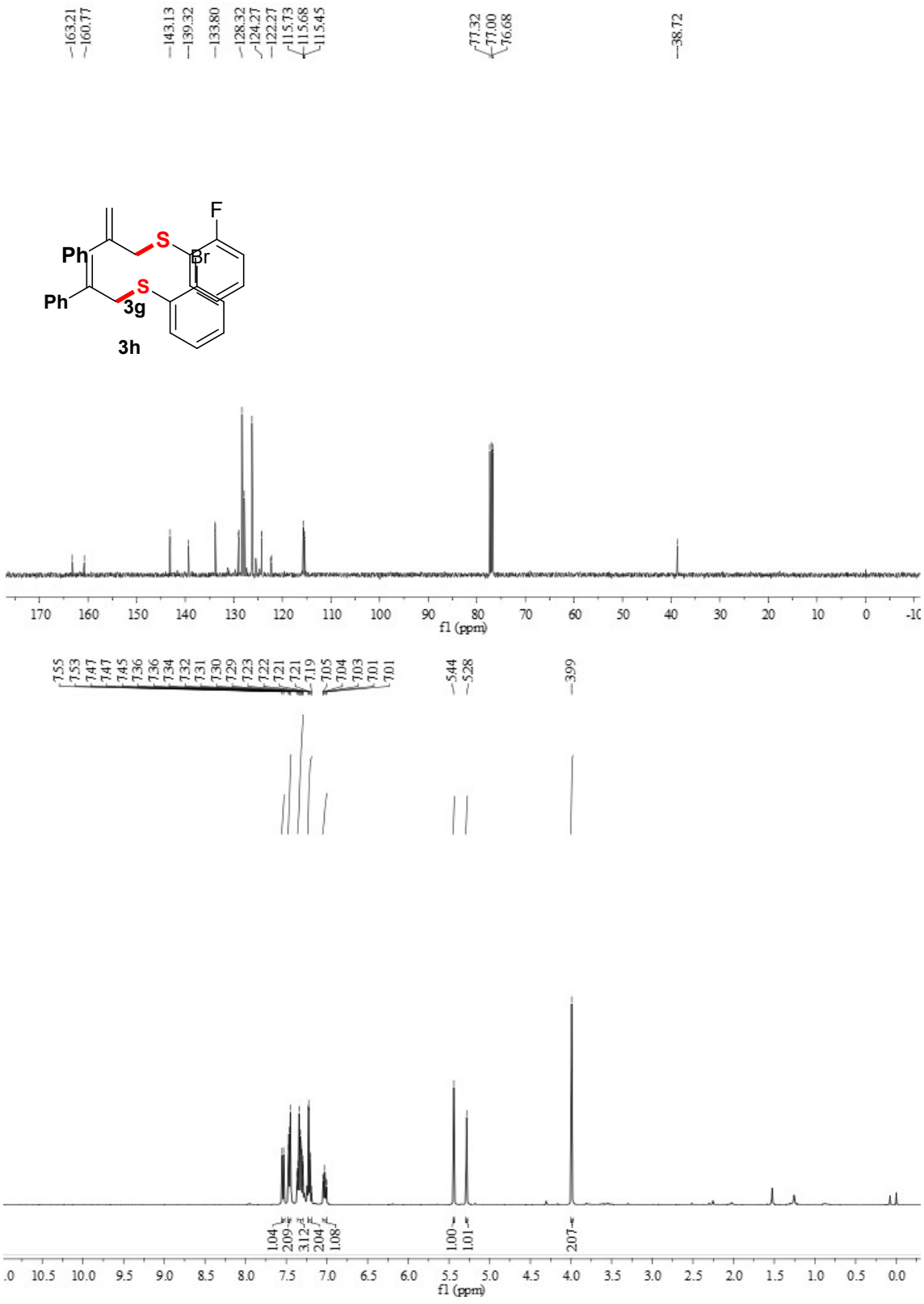
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.43
7.43
7.41
7.35
7.35
7.34
7.33
7.31
7.30
7.30
7.29
7.28
7.28
7.26
7.26
7.23
7.21
7.20
7.20
7.19
7.19
7.06
7.04
7.03
7.01
5.32
5.11
3.95


F
Ph
S

3g


2.05
4.14
1.13
2.09
1.00
1.00
2.01
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


163.21
160.77
143.13
139.32
133.80
128.32
124.27
122.27
115.73
115.68
115.45
77.32
77.00
76.68
38.72
F
Ph
S
Br
Ph
S
3g
3h
f1 (ppm)
7.55
7.53
7.47
7.47
7.45
7.36
7.36
7.34
7.32
7.31
7.30
7.29
7.23
7.22
7.21
7.21
7.19
7.05
7.04
7.03
7.01
7.01
5.44
5.28
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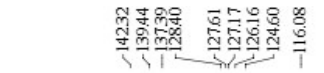
1.04
2.09
3.12
2.04
1.08
1.00
1.01
2.07
f1 (ppm)


142.32
139.44
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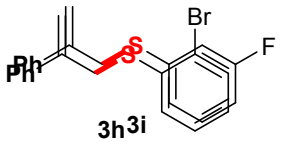
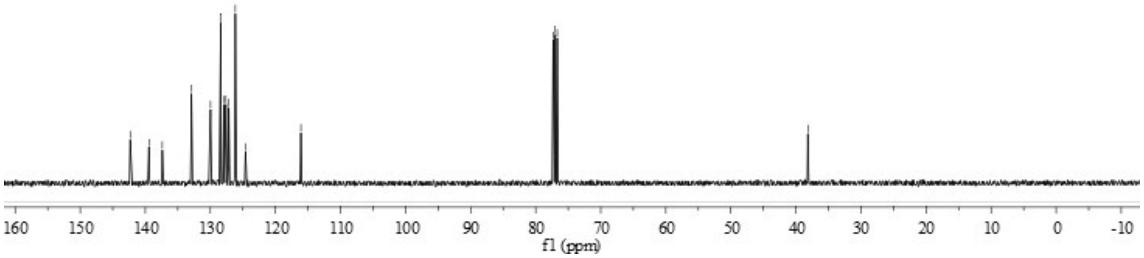
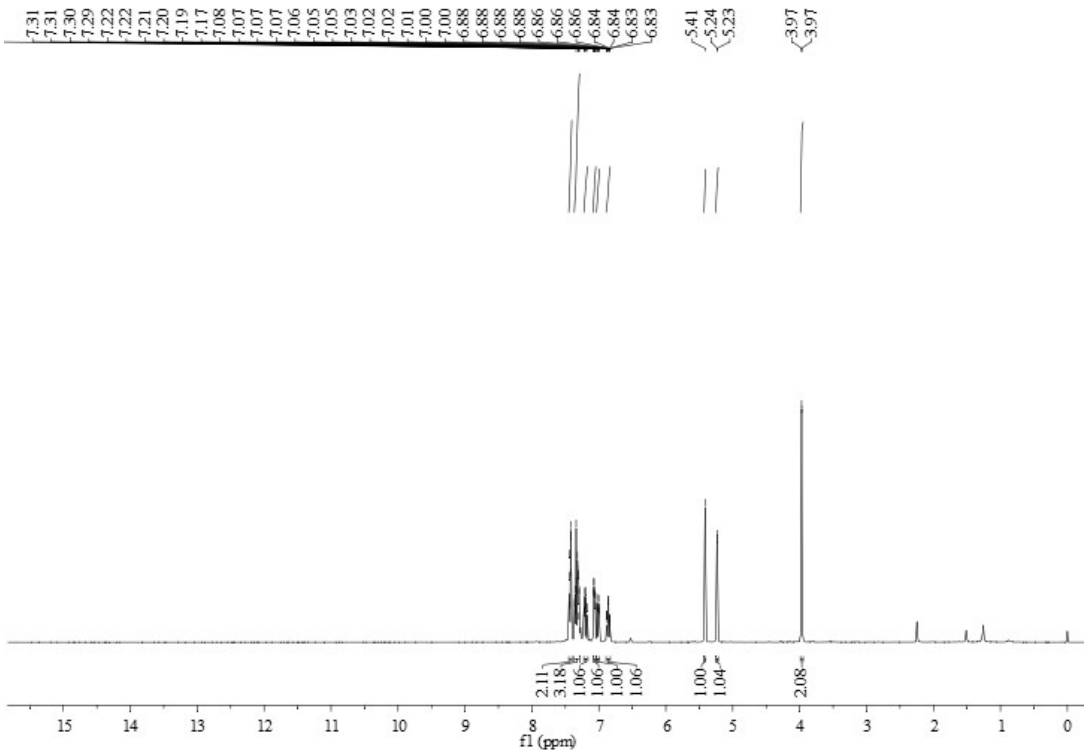
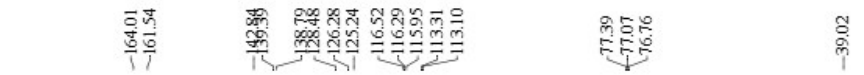
128.40
127.61
127.17
126.16
124.60
116.08
77.32
77.00
76.68
38.17

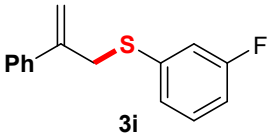

Br
F
S
Ph
Ph

3h 3i

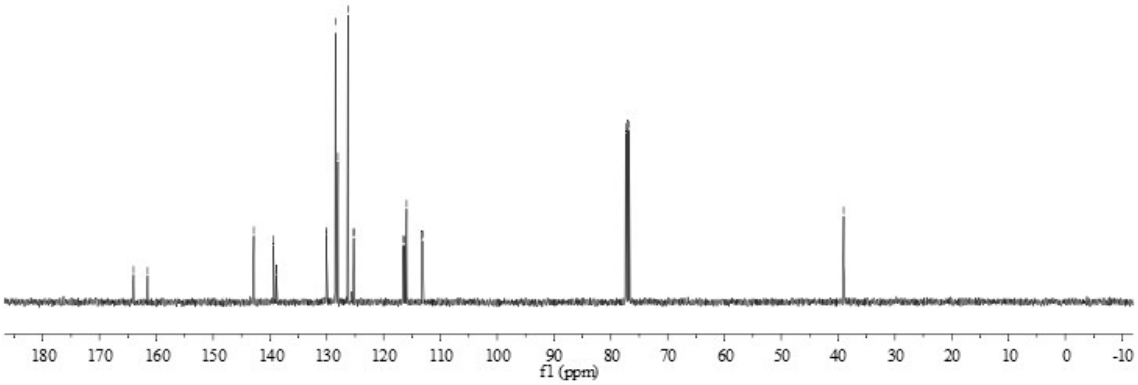

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

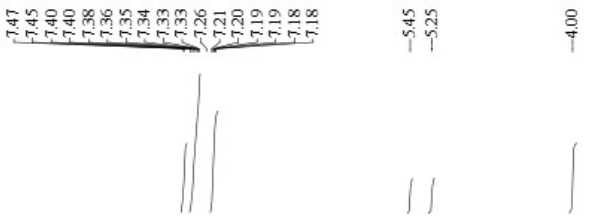

7.31
7.31
7.30
7.29
7.22
7.22
7.21
7.20
7.19
7.17
7.08
7.07
7.07
7.07
7.06
7.05
7.05
7.03
7.02
7.02
7.01
7.00
7.00
6.88
6.88
6.88
6.86
6.86
6.86
6.84
6.84
6.83
6.83
5.41
5.24
5.23
3.97
3.97
2.11
3.18
1.06
1.06
1.00
1.06
1.00
1.04
2.08
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

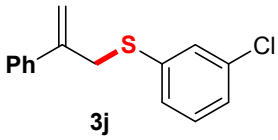

164.01
161.54
142.84
142.80
138.79
128.48
126.28
125.24
116.52
116.29
115.95
113.31
113.10
77.39
77.07
76.76
39.02


Ph
S
F

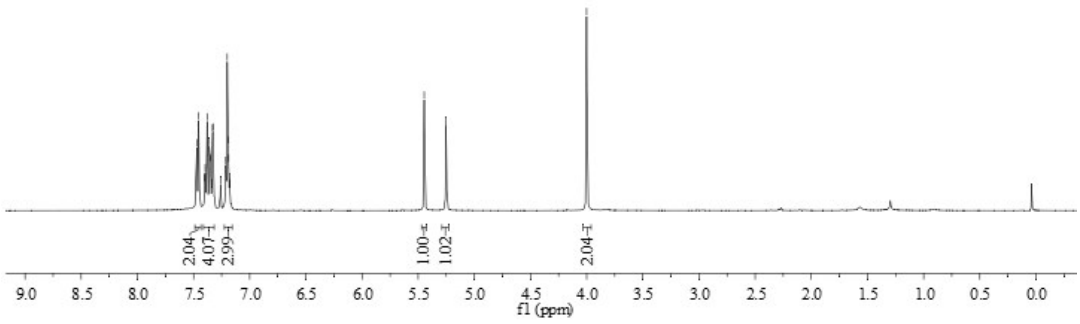
3i

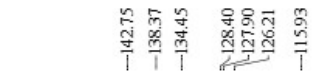

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

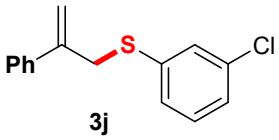

7.47
7.45
7.40
7.40
7.38
7.36
7.35
7.34
7.33
7.33
7.26
7.21
7.20
7.19
7.19
7.18
7.18
5.45
5.25
4.00


Ph
S
Cl

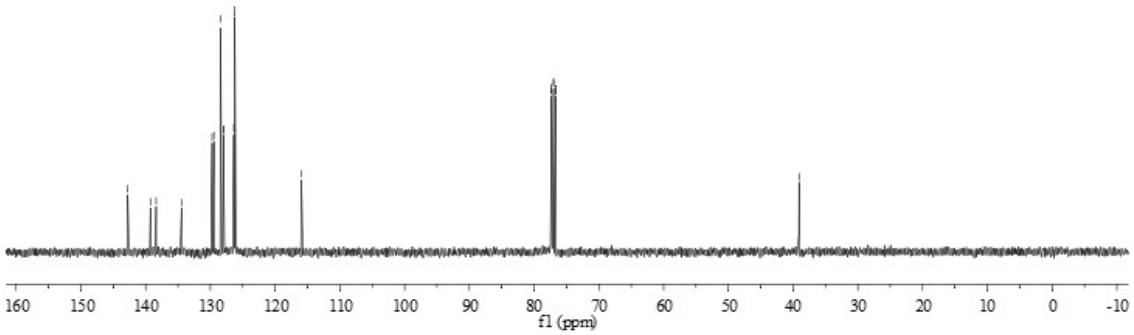
3j

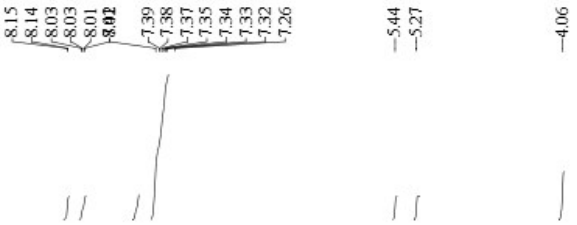

2.04
4.07
2.99
1.00
1.02
2.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

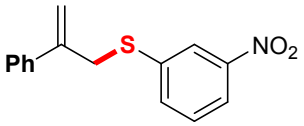

142.75
138.37
134.45
128.40
127.90
126.21
115.93
77.32
77.32
77.00
77.00
76.68
76.68
39.09


Ph
S
Cl

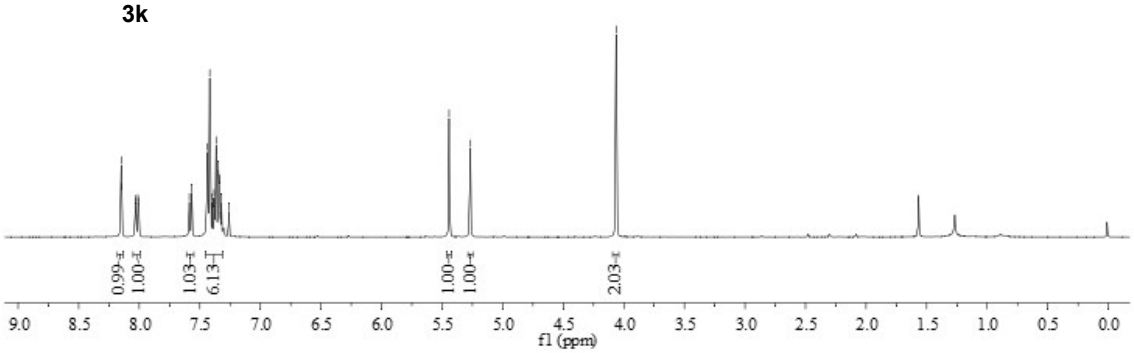
3j

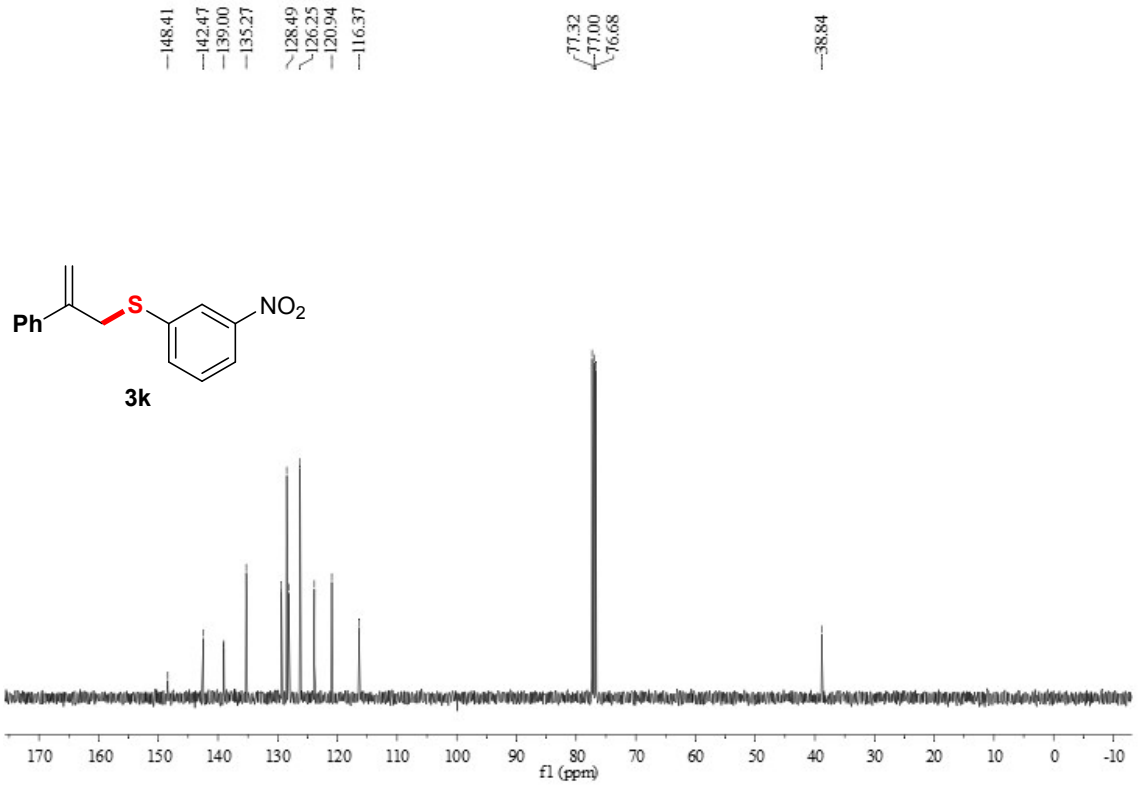

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

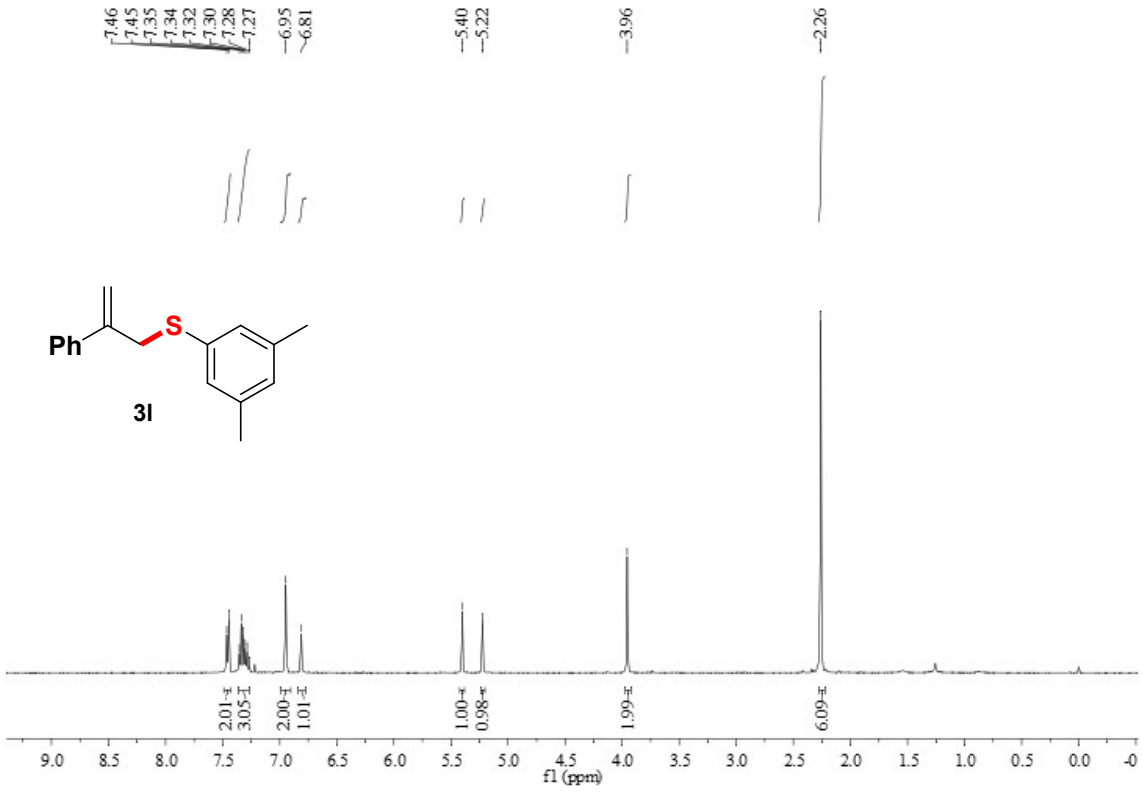

8.15
8.14
8.03
8.03
8.01
7.39
7.38
7.37
7.35
7.34
7.33
7.32
7.26
5.44
5.27
4.06

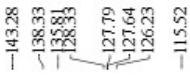

Ph
S
NO2

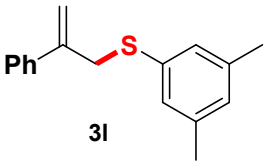
3k


0.99
1.00
1.03
6.13
1.00
1.00
2.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

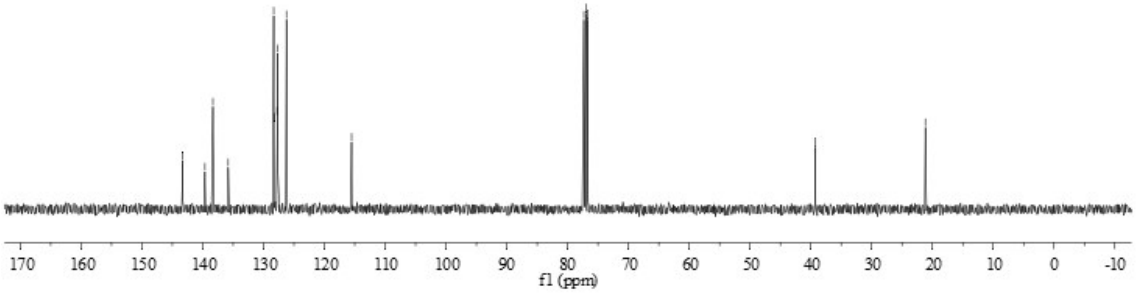

148.41
142.47
139.00
135.27
128.49
126.25
120.94
116.37
77.32
77.00
76.68
38.84
Ph
S
NO2
3k
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

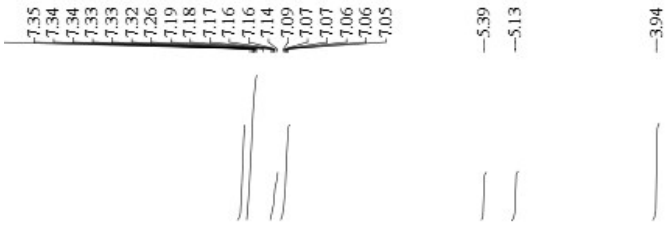

7.46
7.45
7.35
7.34
7.32
7.30
7.28
7.27
6.95
6.81
5.40
5.22
3.96
2.26
Ph
S
3l
2.01
3.05
2.00
1.01
1.00
0.98
1.99
6.09
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

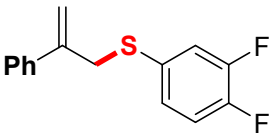

143.28
138.33
135.81
128.33
127.79
127.64
126.23
115.52
77.32
77.00
76.68
39.24
21.16


Ph
S

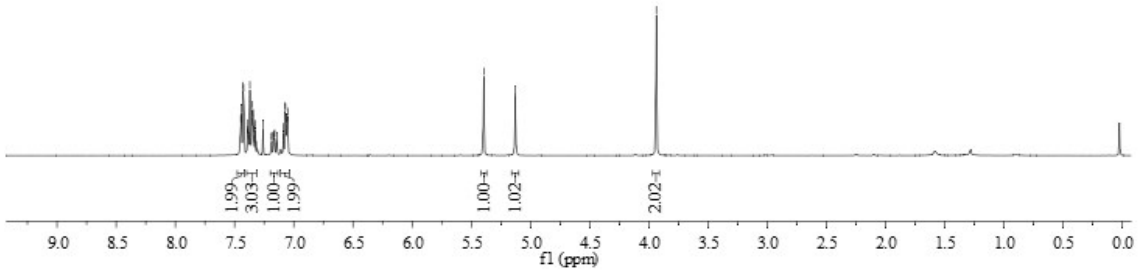
3l

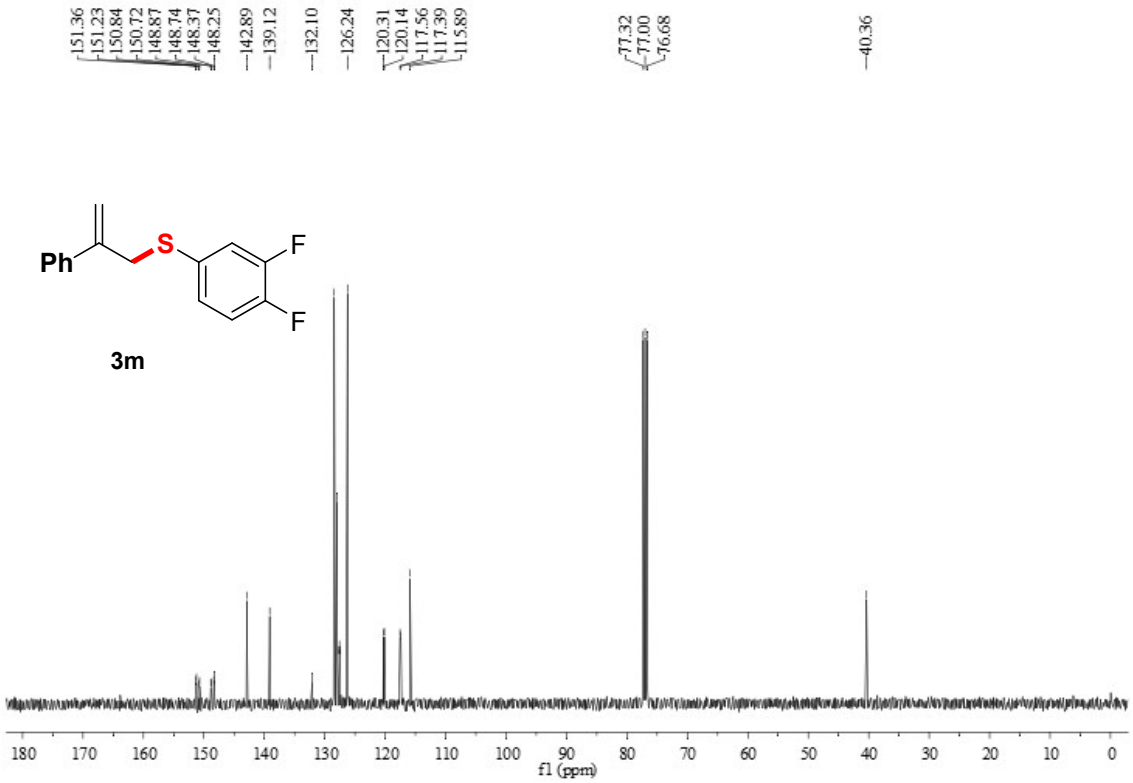

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

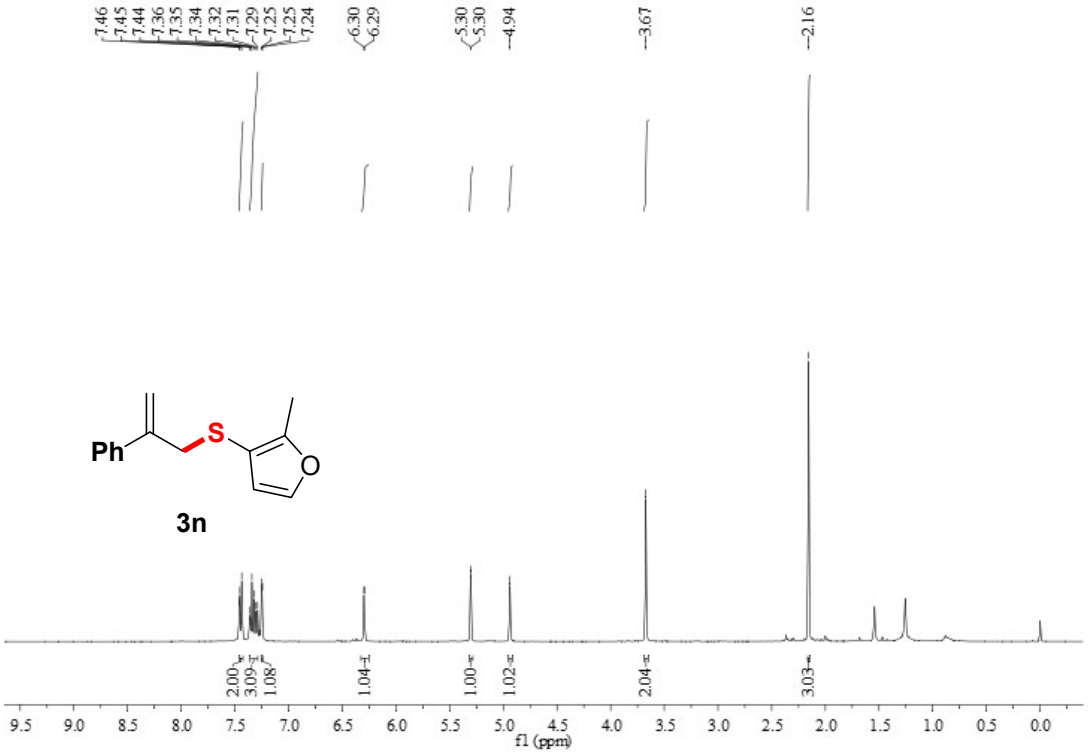

7.35
7.34
7.34
7.33
7.33
7.32
7.26
7.19
7.18
7.17
7.16
7.16
7.14
7.09
7.07
7.07
7.06
7.06
7.05
5.39
5.13
3.94

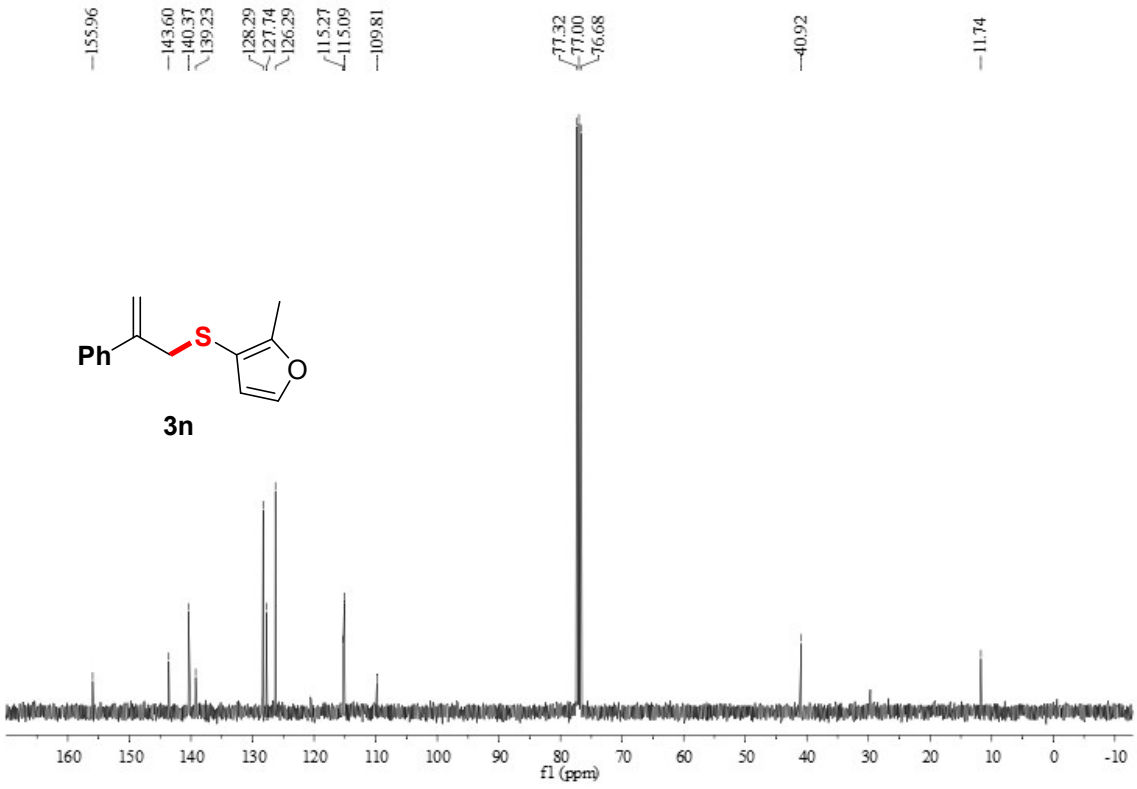

Ph
S
F
F

3m

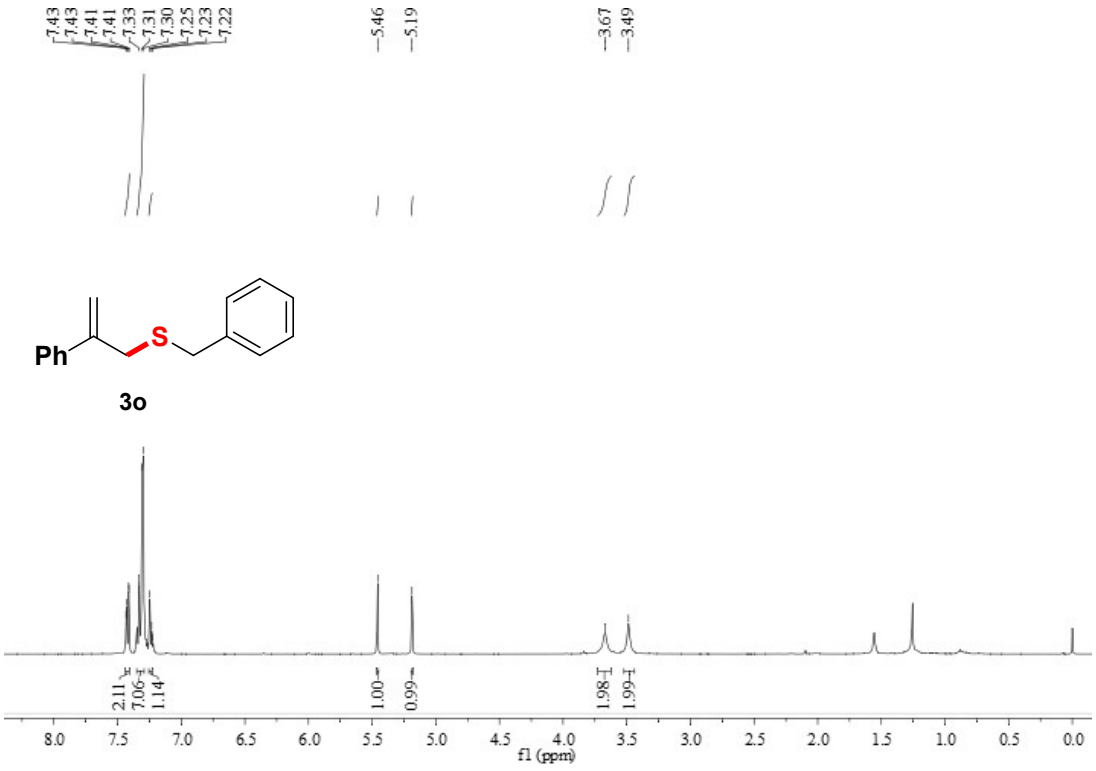

1.99
3.03
1.00
1.99
1.00
1.02
2.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


151.36
151.23
150.84
150.72
148.87
148.74
148.37
148.25
142.89
139.12
132.10
126.24
120.31
120.14
117.56
117.39
115.89
77.32
77.00
76.68
40.36
Ph
S
F
F
3m
f1 (ppm)

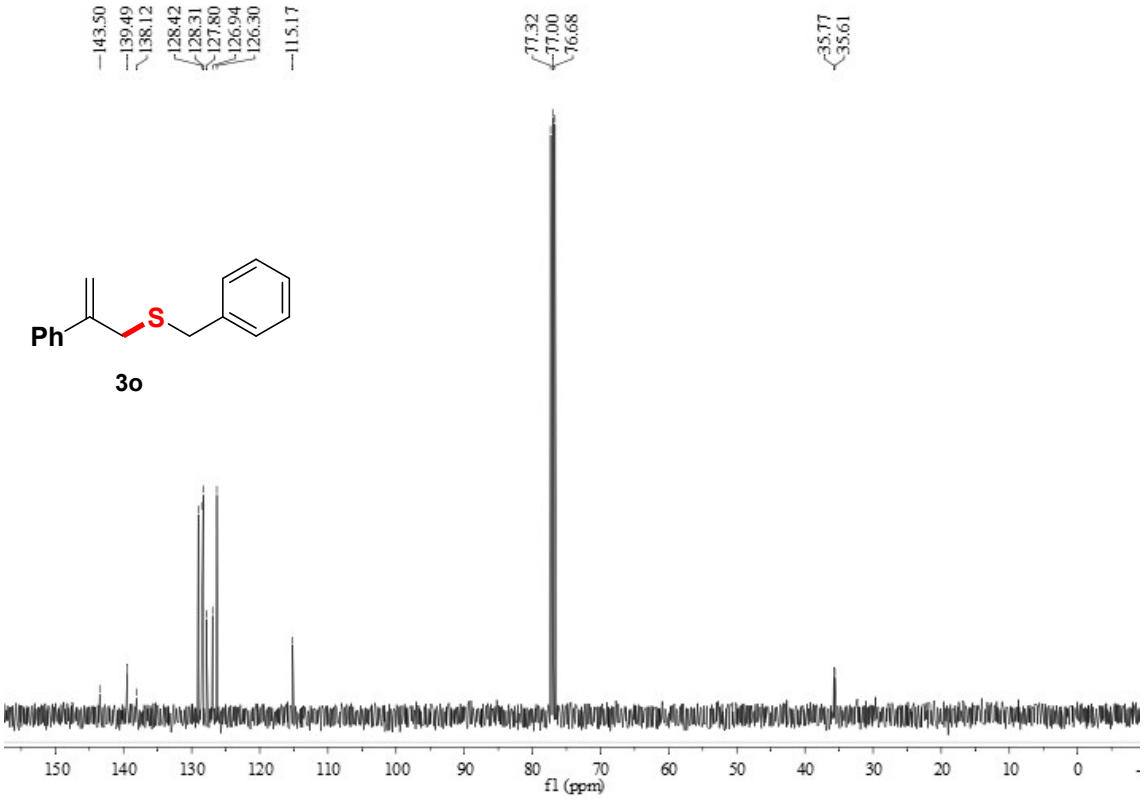

7.46
7.45
7.44
7.36
7.35
7.34
7.32
7.31
7.29
7.25
7.25
7.24
6.30
6.29
5.30
5.30
4.94
3.67
2.16
Ph
S
O
3n
2.00
3.09
1.08
1.04
1.00
1.02
2.04
3.03
f1 (ppm)

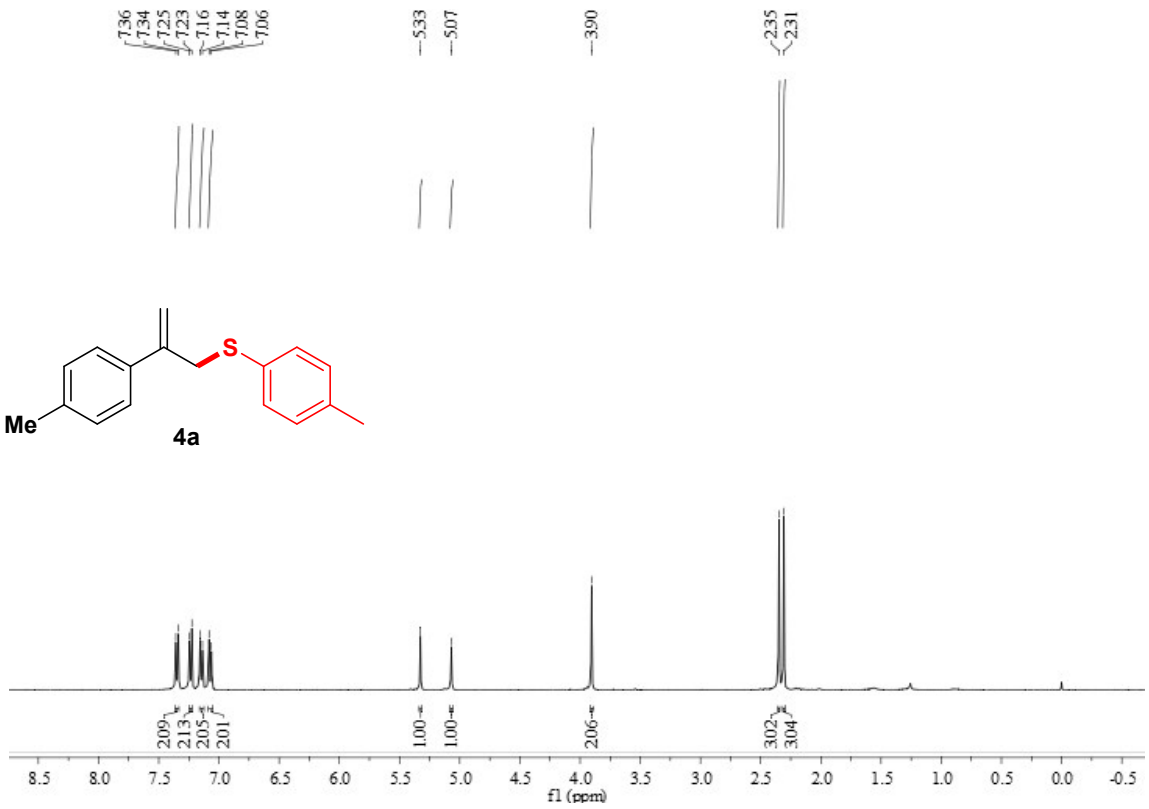

155.96
143.60
140.37
139.23
128.29
127.74
126.29
115.27
115.09
109.81
77.32
77.00
76.68
40.92
11.74
Ph
S
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

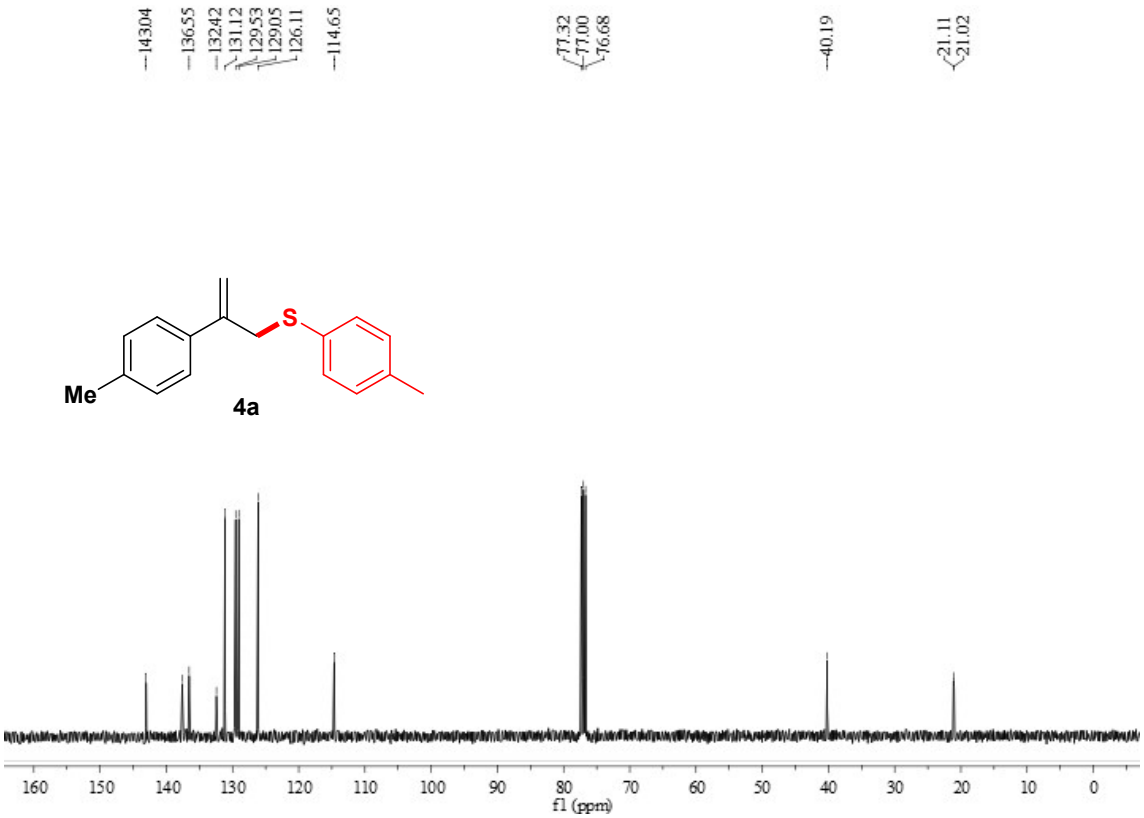
3n


7.43
7.43
7.41
7.41
7.33
7.31
7.30
7.25
7.23
7.22
5.46
5.19
3.67
3.49
Ph
S
2.11
7.06
1.14
1.00
0.99
1.98
1.99
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3o


143.50
139.49
138.12
128.42
128.31
127.80
126.94
126.30
115.17
77.32
77.00
76.68
35.77
35.61
Ph
S
3o
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.36
7.34
7.25
7.23
7.16
7.14
7.08
7.06
5.33
5.07
3.90
2.35
2.31
Me
S
4a
2.09
2.13
2.05
2.01
1.00
1.00
2.06
3.02
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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136.55
132.42
131.12
129.53
129.05
126.11
114.65
77.32
77.00
76.68
40.19
21.11
21.02
S
Me
4a
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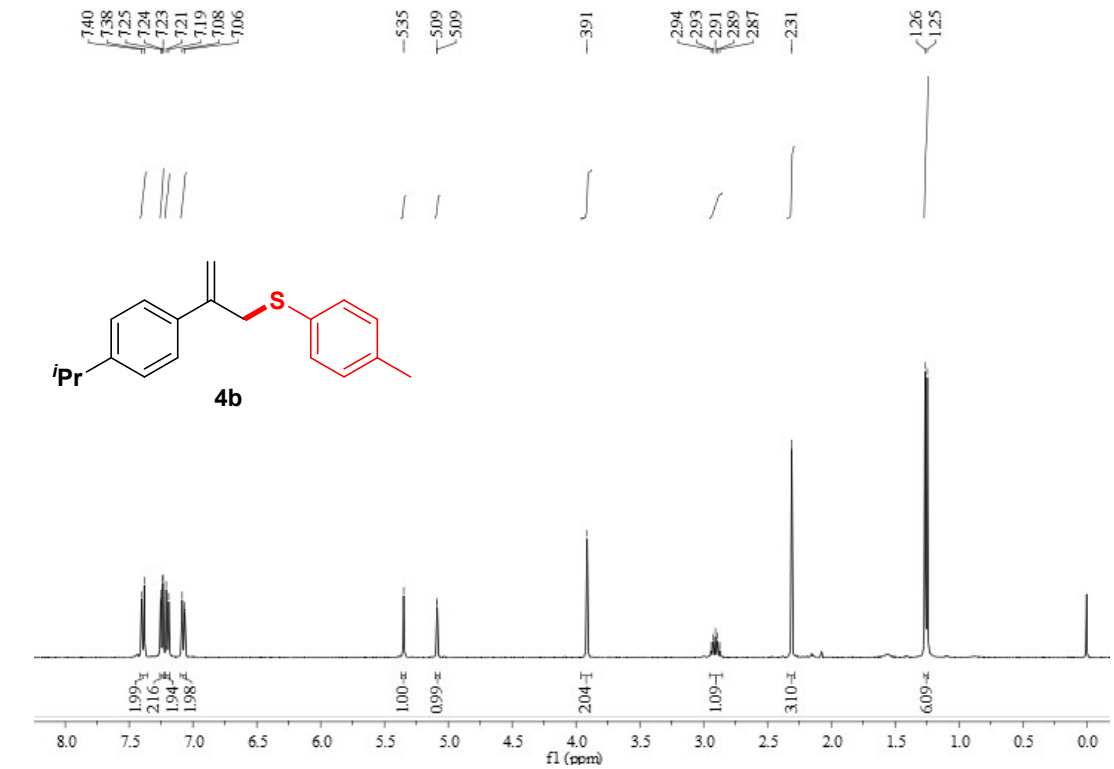
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.24
7.23
7.21
7.19
7.08
7.06
5.35
5.09
5.09
3.91
2.94
2.93
2.91
2.89
2.87
2.31
1.26
1.25
S
iPr
4b
1.99
2.16
1.94
1.98
1.00
0.99
2.04
1.09
3.10
6.09
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
3.0
2.5
2.0
1.5
1.0
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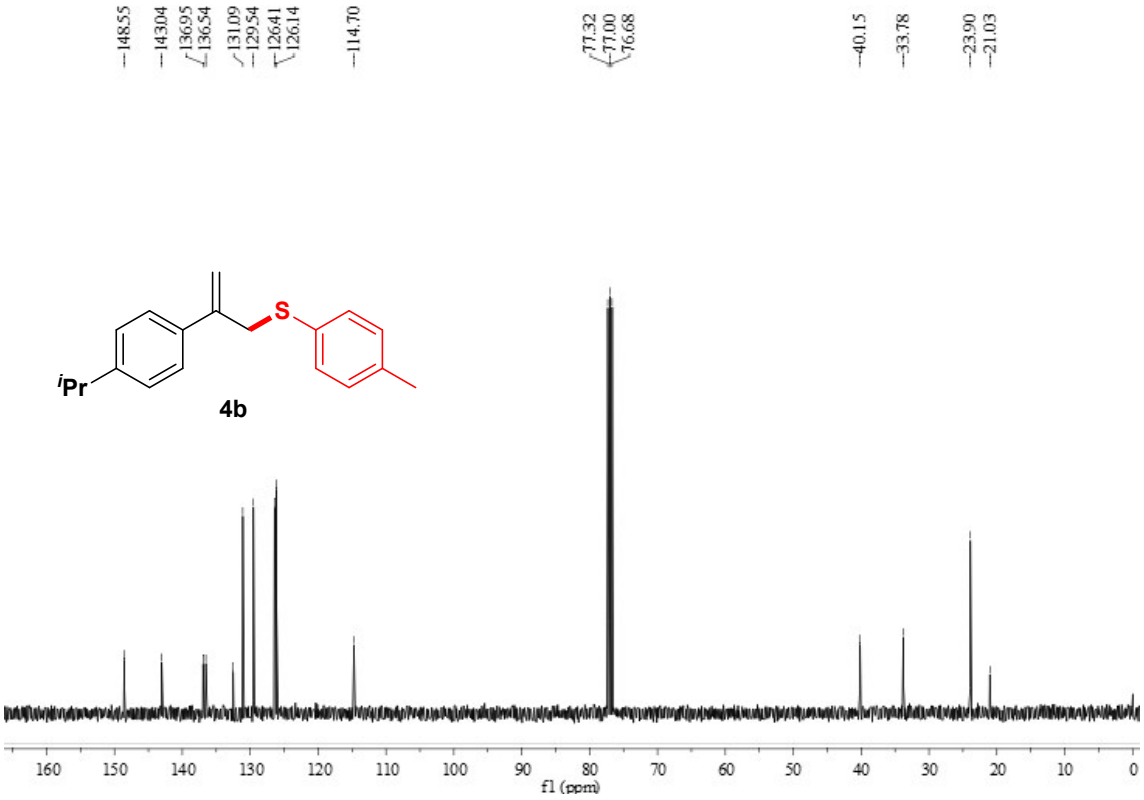
0.0
f1 (ppm)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129.54
126.41
126.14
114.70
77.32
77.00
76.68
40.15
33.78
23.90
21.03
S
iPr
4b
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110
100
90
80
70
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50
40
30
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10
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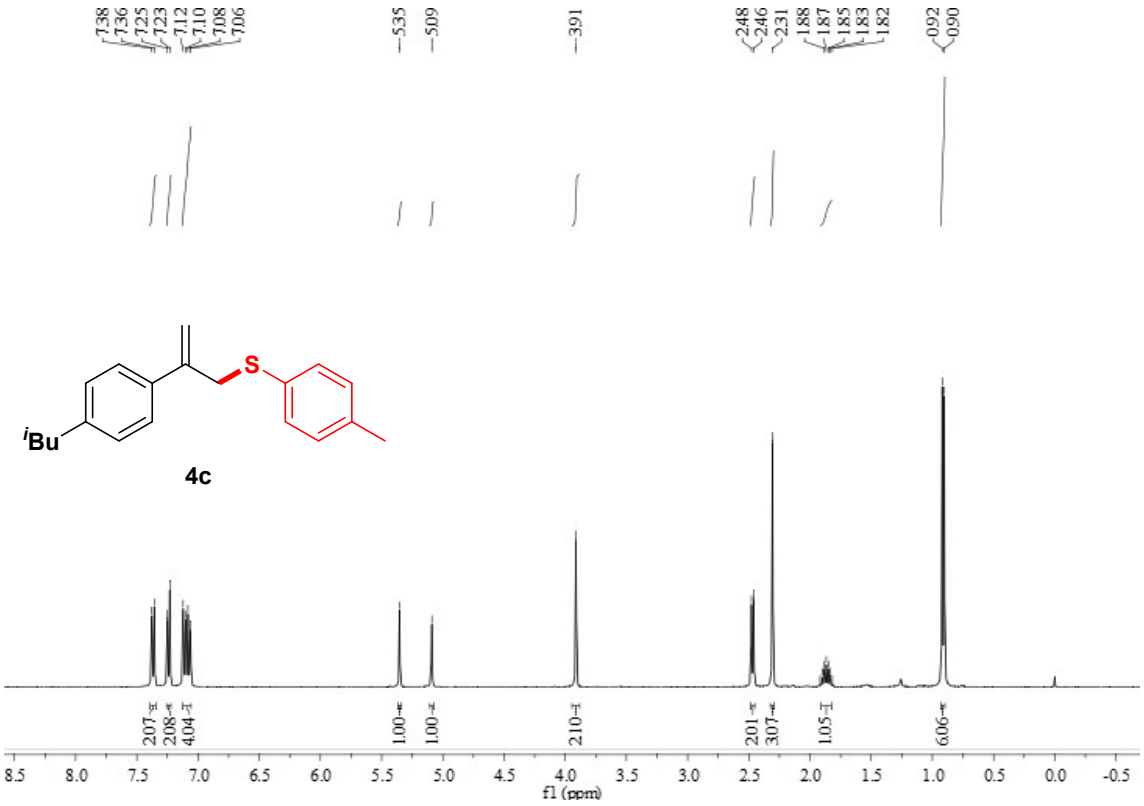
f1 (ppm)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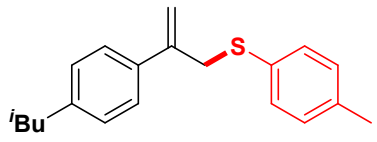
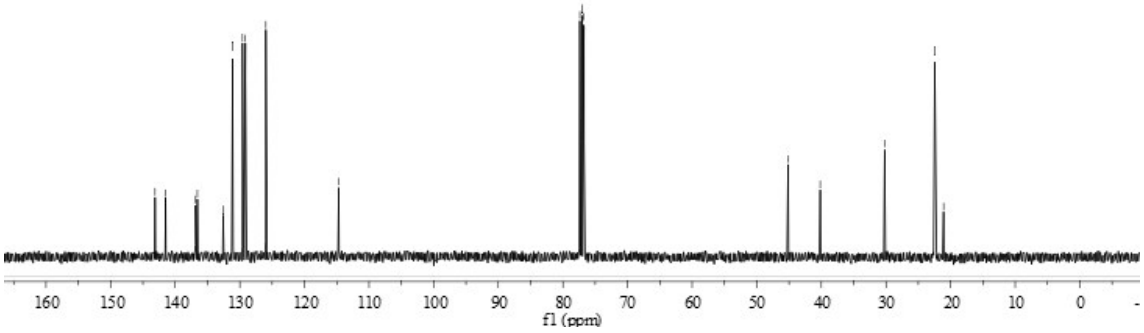
7.12
7.10
7.08
7.06
5.35
5.09
3.91
2.48
2.46
2.31
1.88
1.87
1.85
1.83
1.82
0.92
0.90
S
iBu
4c
2.07
2.08
4.04
1.00
1.00
2.10
2.01
3.07
1.05
6.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


143.12
141.48
136.57
131.12
129.14
125.97
114.69
77.37
77.06
76.74
45.15
40.18
30.20
22.44
21.08


S
iBu

4c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90
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50
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30
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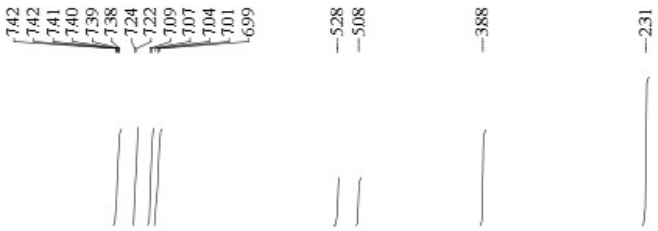
10
0
f1 (ppm)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7.22
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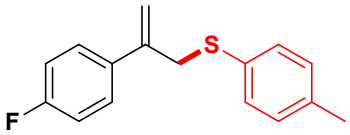
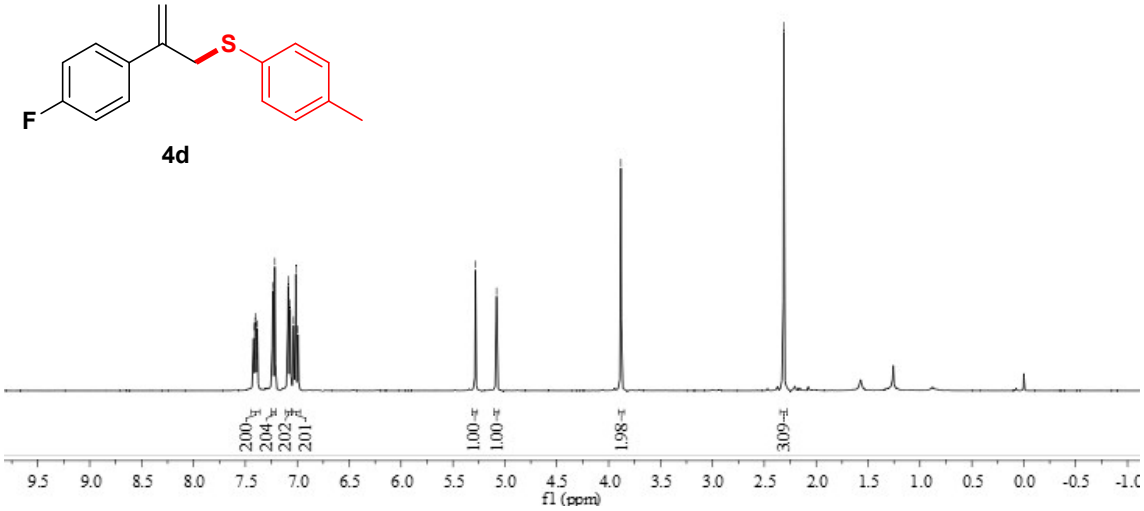
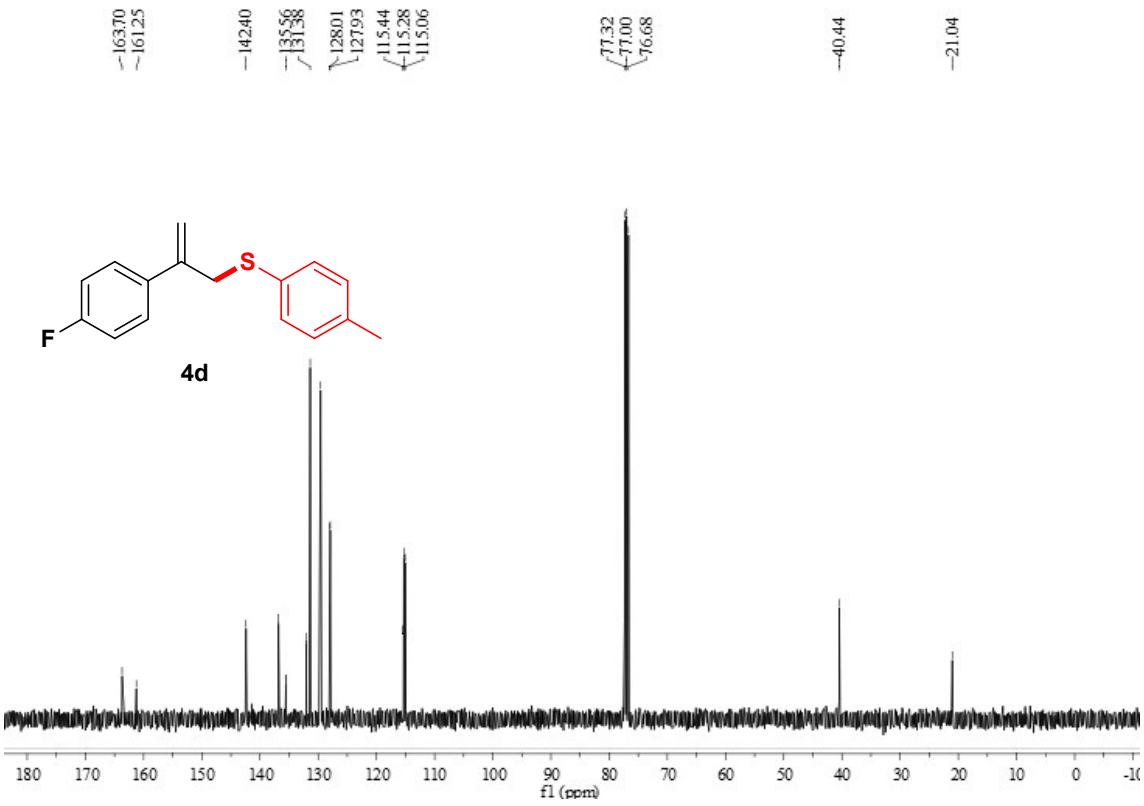
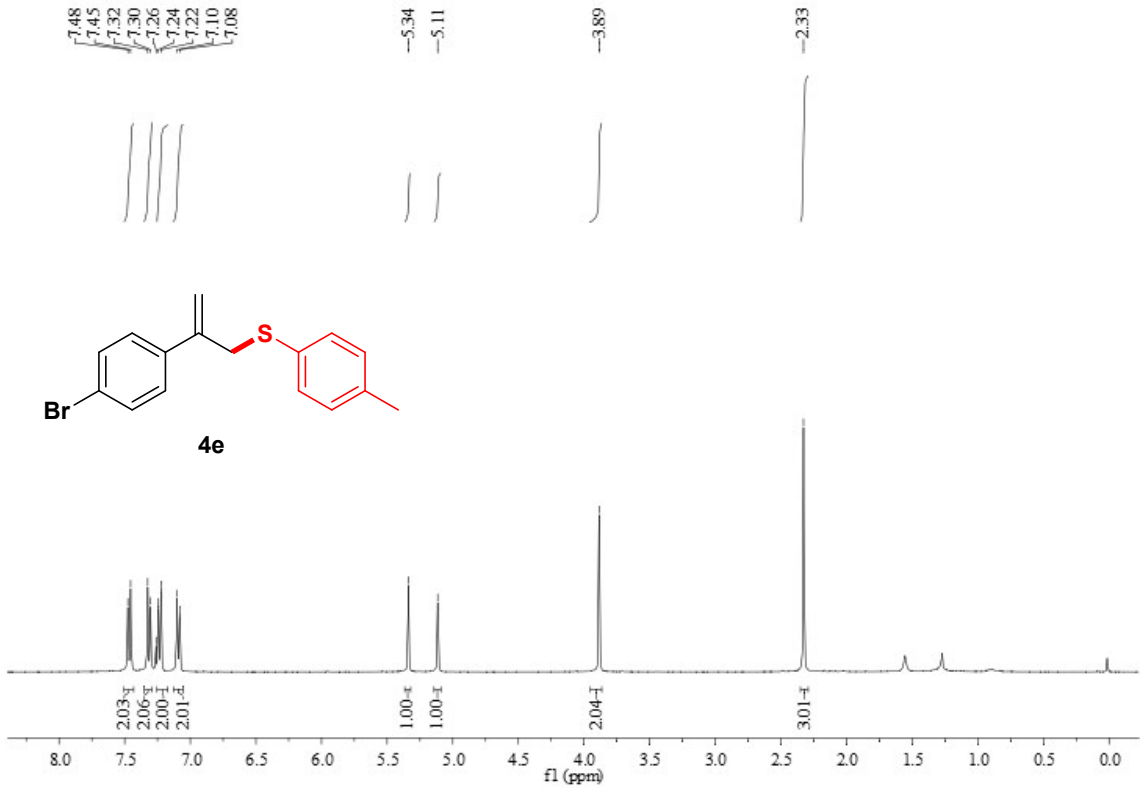
7.07
7.04
7.01
6.99
5.28
5.08
3.88
2.31


S
F

4d


2.00
2.04
2.02
2.01
1.00
1.00
1.98
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.70
161.25
142.40
135.56
131.38
128.01
127.93
115.44
115.28
115.06
77.32
77.00
76.68
40.44
21.04
S
F
4d
f1 (ppm)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7.45
7.32
7.30
7.26
7.24
7.22
7.10
7.08
5.34
5.11
3.89
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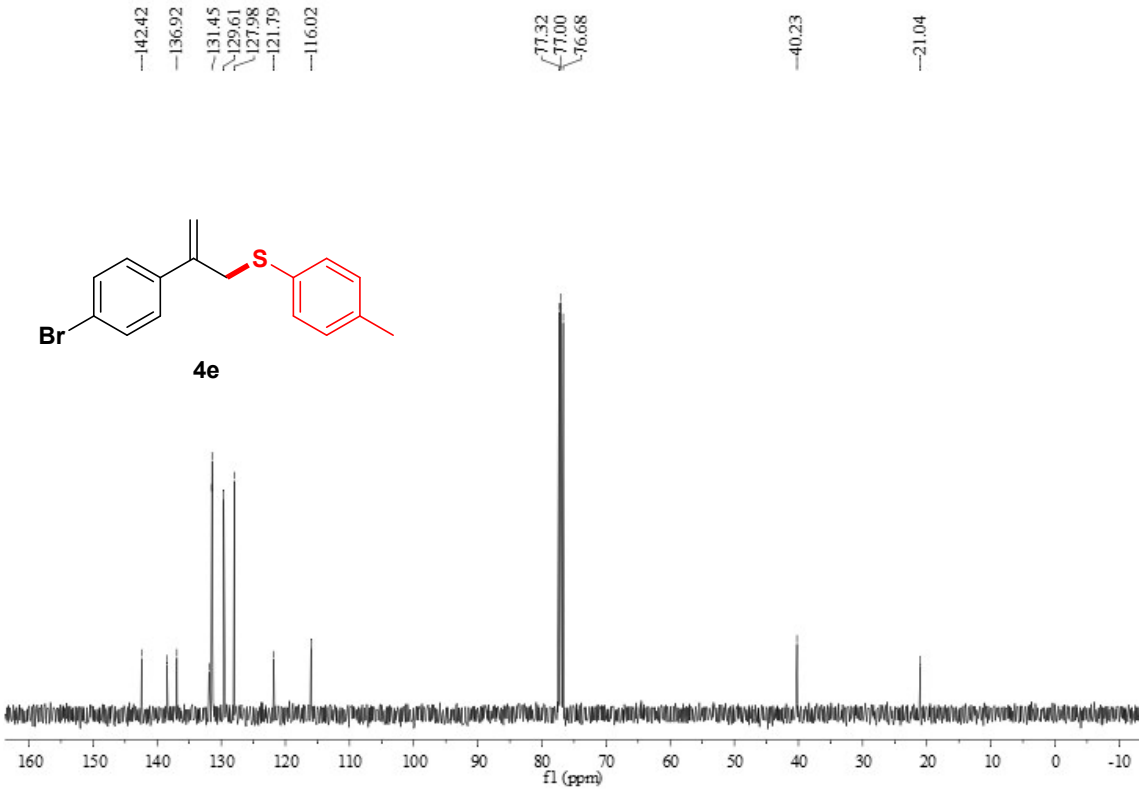
S
Br
4e
2.03
2.06
2.00
2.01
1.00
1.00
2.04
3.01
f1 (ppm)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136.92
131.45
129.61
127.98
121.79
116.02
77.32
77.00
76.68
40.23
21.04
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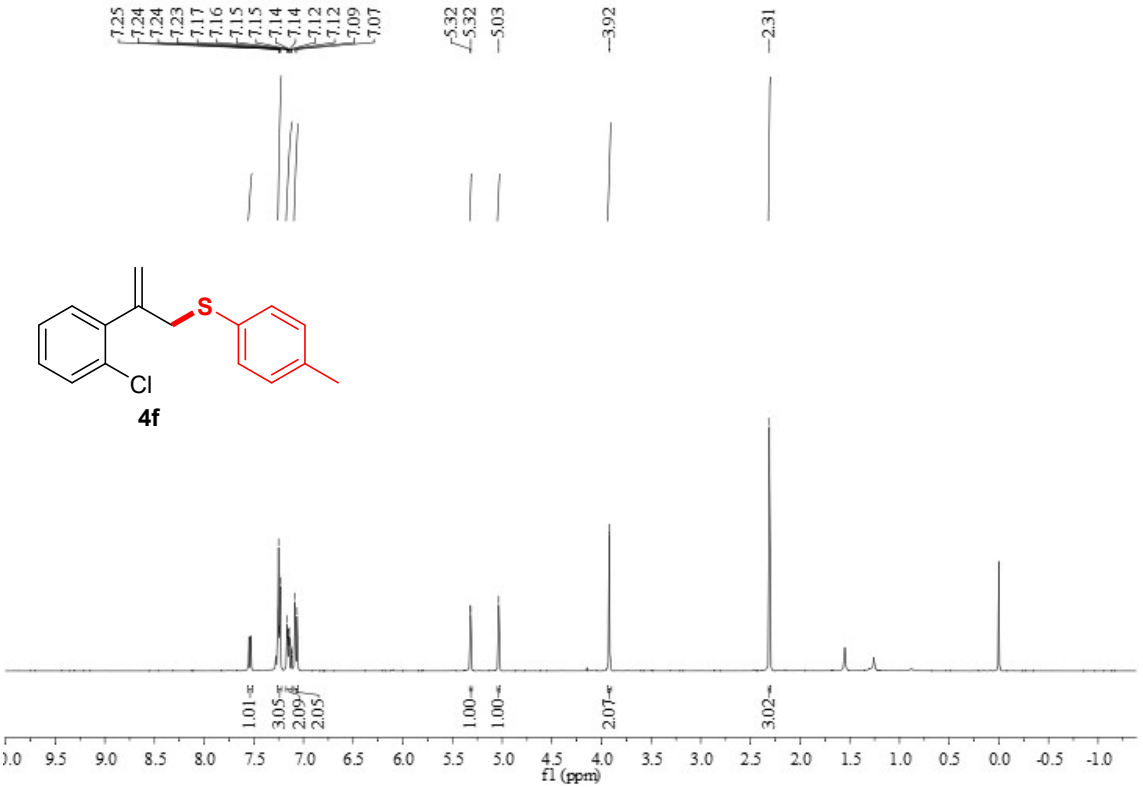
S
4e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.24
7.24
7.23
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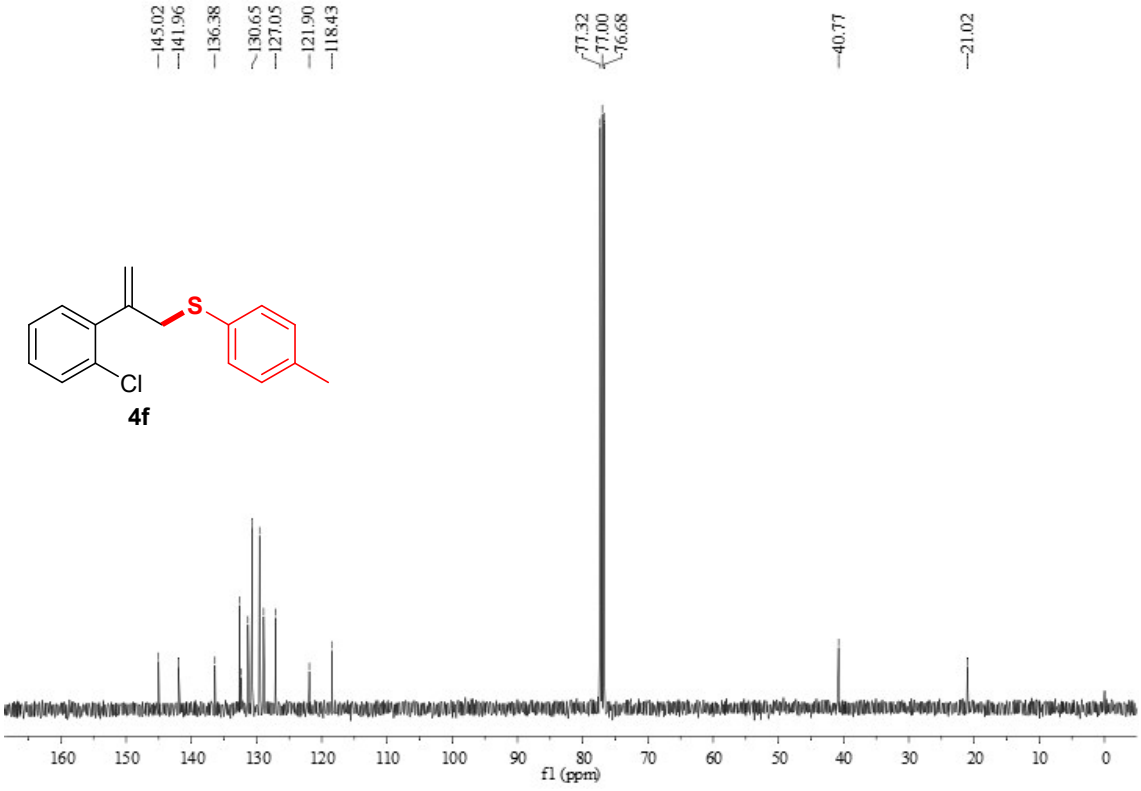
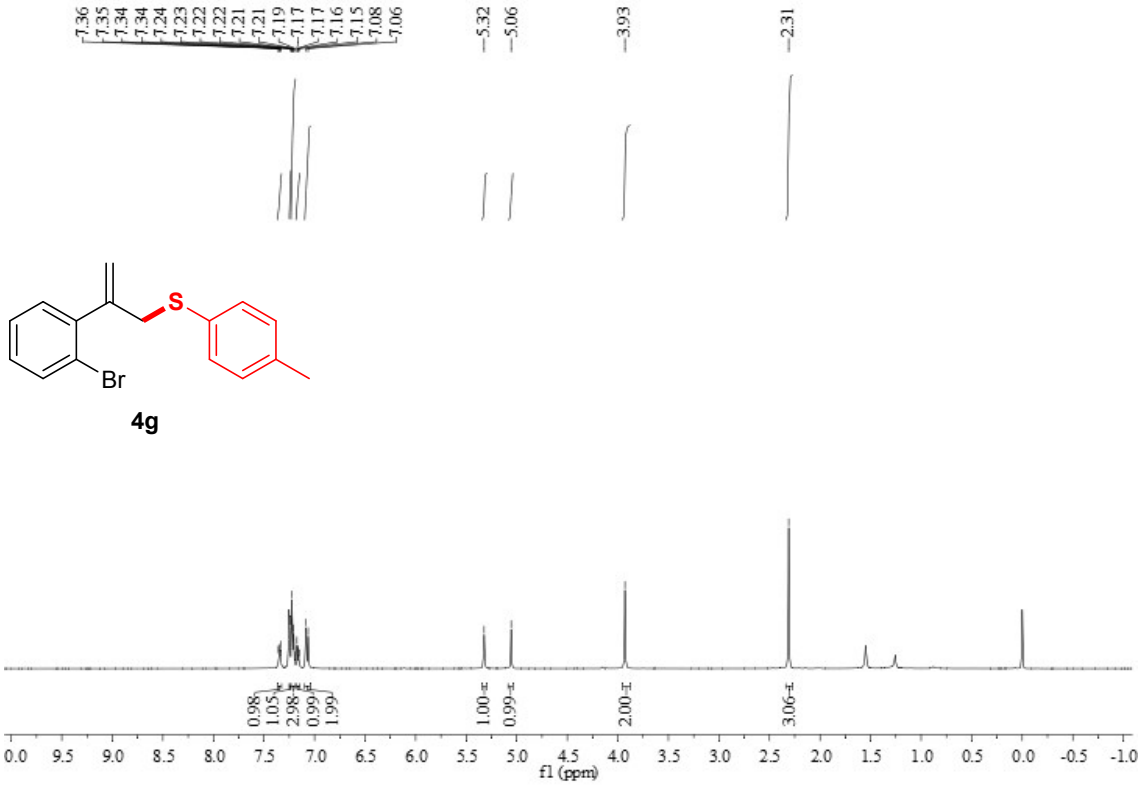
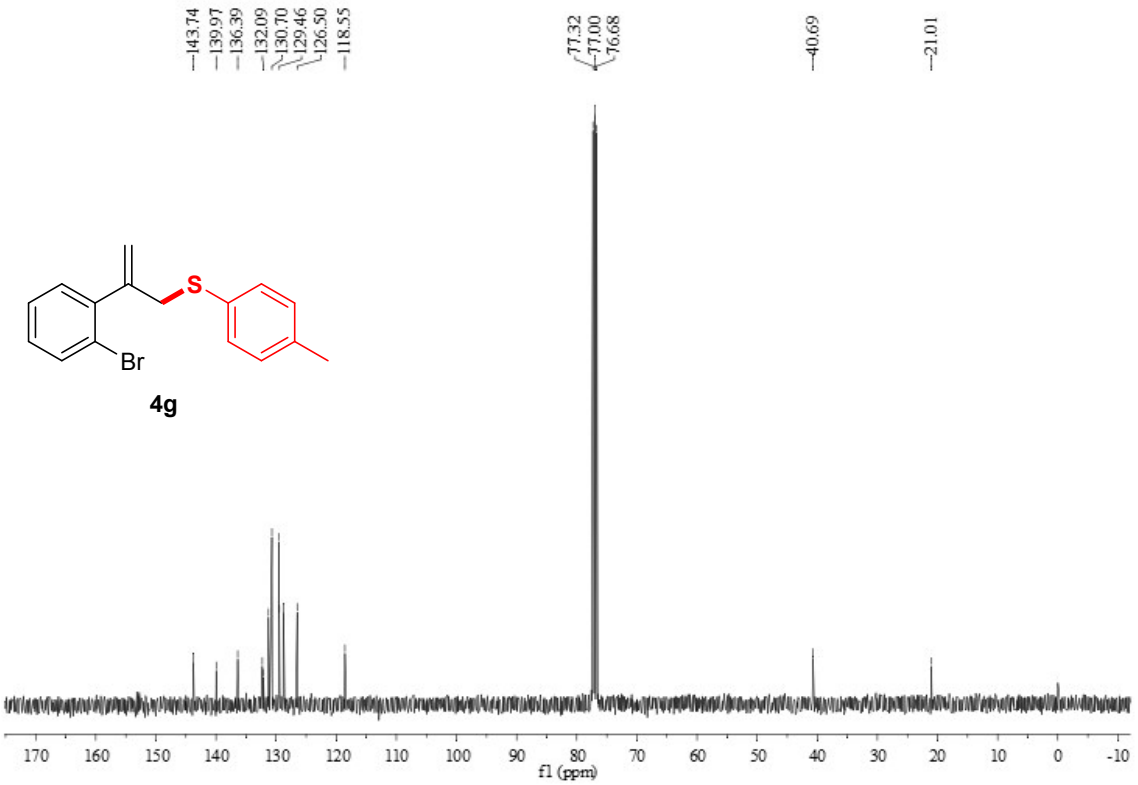
7.15
7.14
7.14
7.12
7.12
7.09
7.07
5.32
5.32
5.03
3.92
2.31
Cl
S
4f
1.01
3.05
2.09
2.05
1.00
1.00
2.07
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


145.02
141.96
136.38
130.65
127.05
121.90
118.43
77.32
77.00
76.68
40.77
21.02
S
Cl
f1 (ppm)

4f


7.36
7.35
7.34
7.34
7.24
7.23
7.22
7.22
7.21
7.21
7.19
7.17
7.17
7.16
7.15
7.08
7.06
5.32
5.06
3.93
2.31
S
Br
0.98
1.05
2.98
0.99
1.99
1.00
0.99
2.00
3.06
f1 (ppm)

4g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132.09
130.70
129.46
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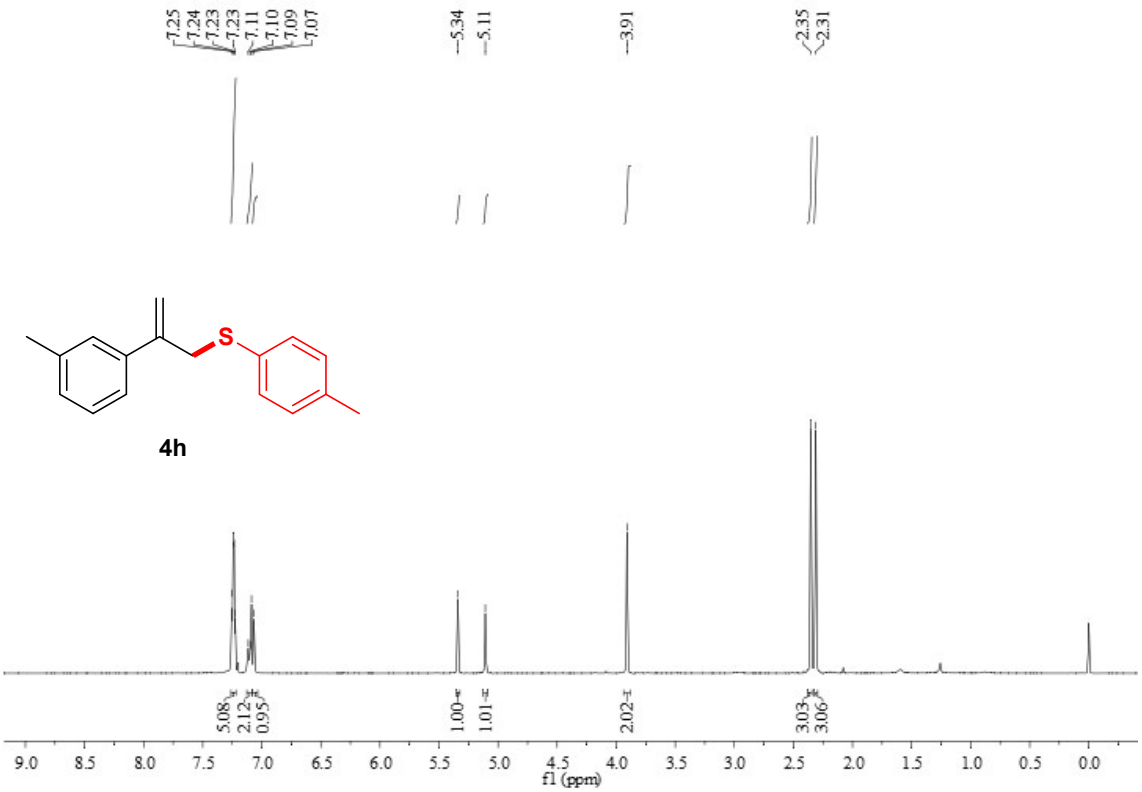
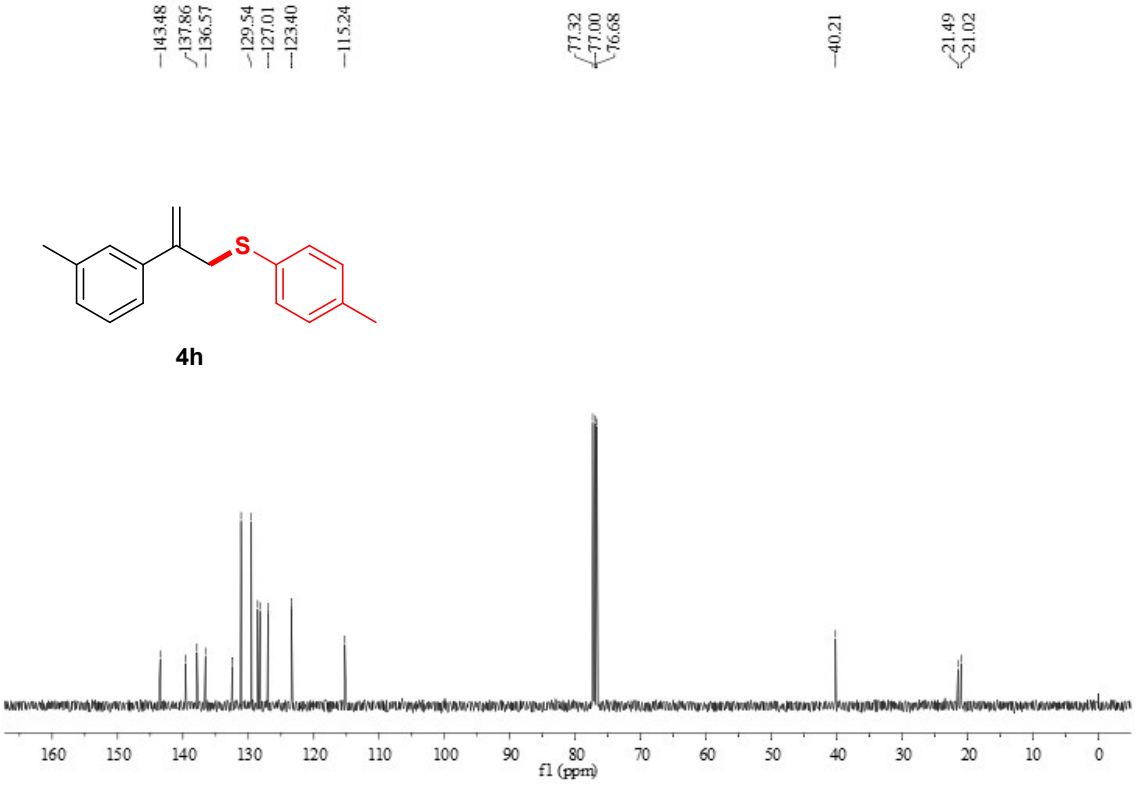
118.55
77.32
77.00
76.68
40.69
21.01
S
Br
4g
f1 (ppm)


7.25
7.24
7.23
7.23
7.11
7.10
7.09
7.07
5.34
5.11
3.91
2.35
2.31
S
4h
5.08
2.12
0.95
1.00
1.01
2.02
3.03
3.06
f1 (ppm)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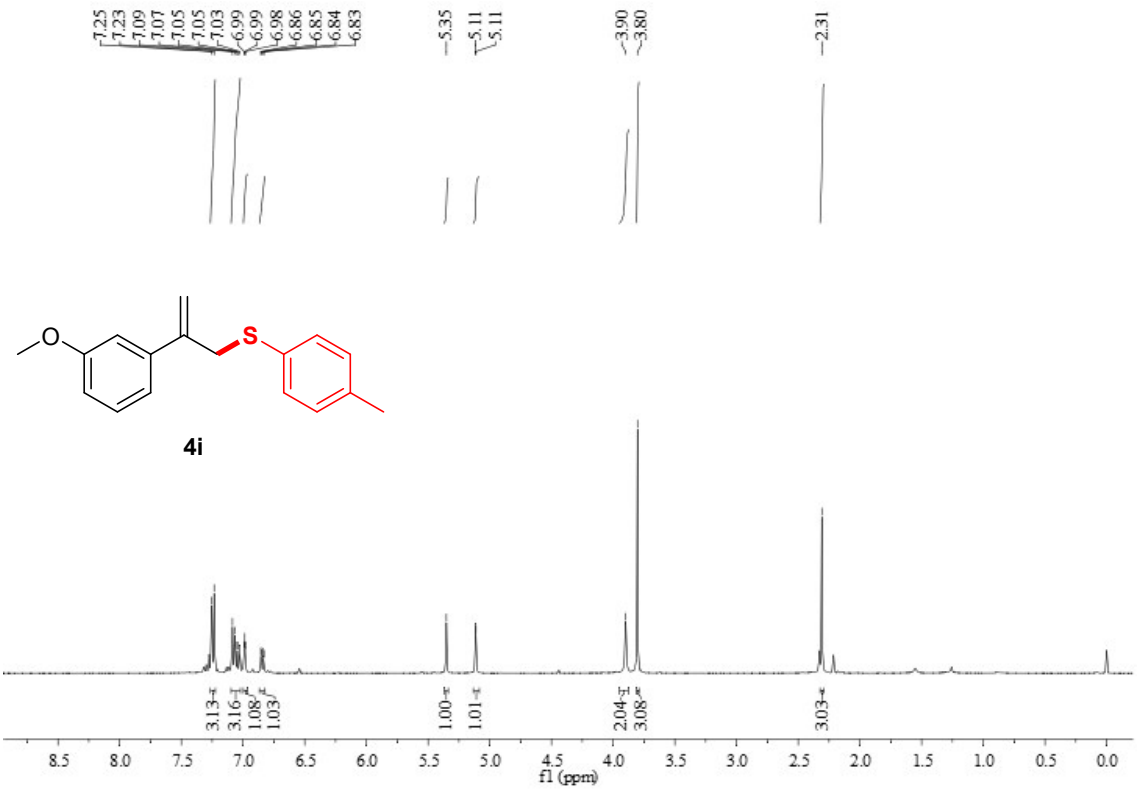
136.57
129.54
127.01
123.40
115.24
77.32
77.00
76.68
40.21
21.49
21.02
S
4h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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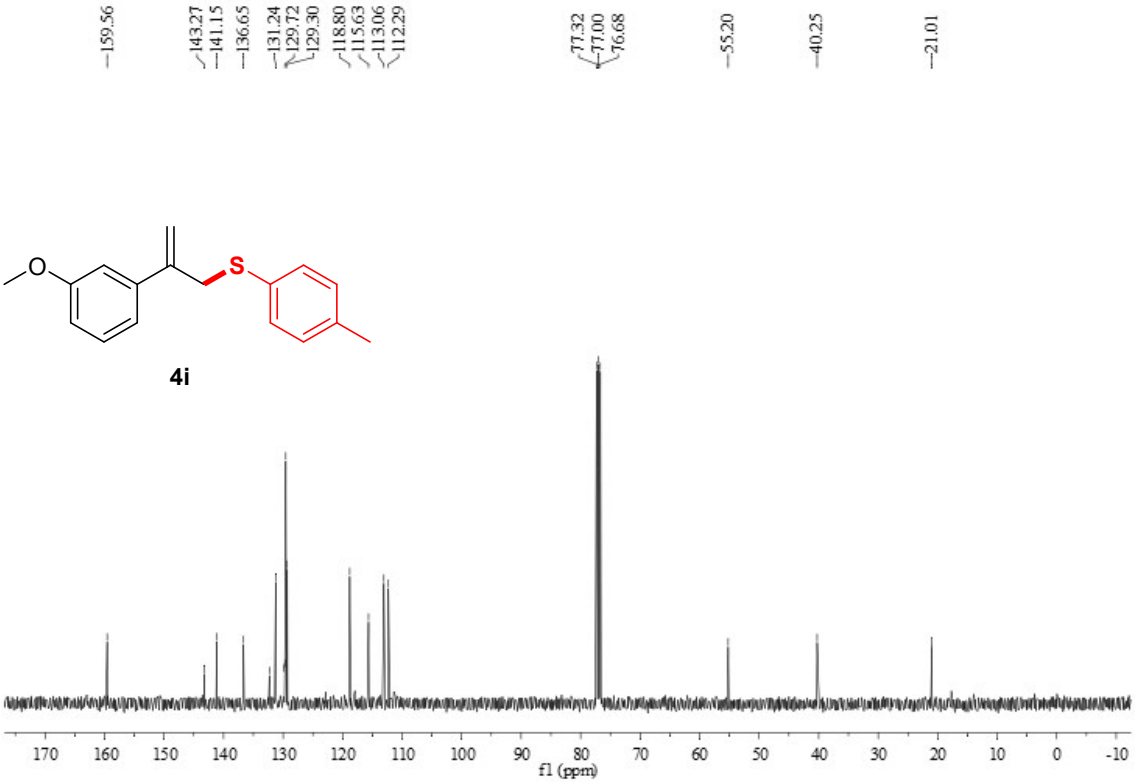
7.23
7.09
7.07
7.05
7.05
7.03
6.99
6.99
6.98
6.86
6.85
6.84
6.83
5.35
5.11
5.11
3.90
3.80
2.31
O
S
4i
3.13
3.16
1.08
1.03
1.00
1.01
2.04
3.08
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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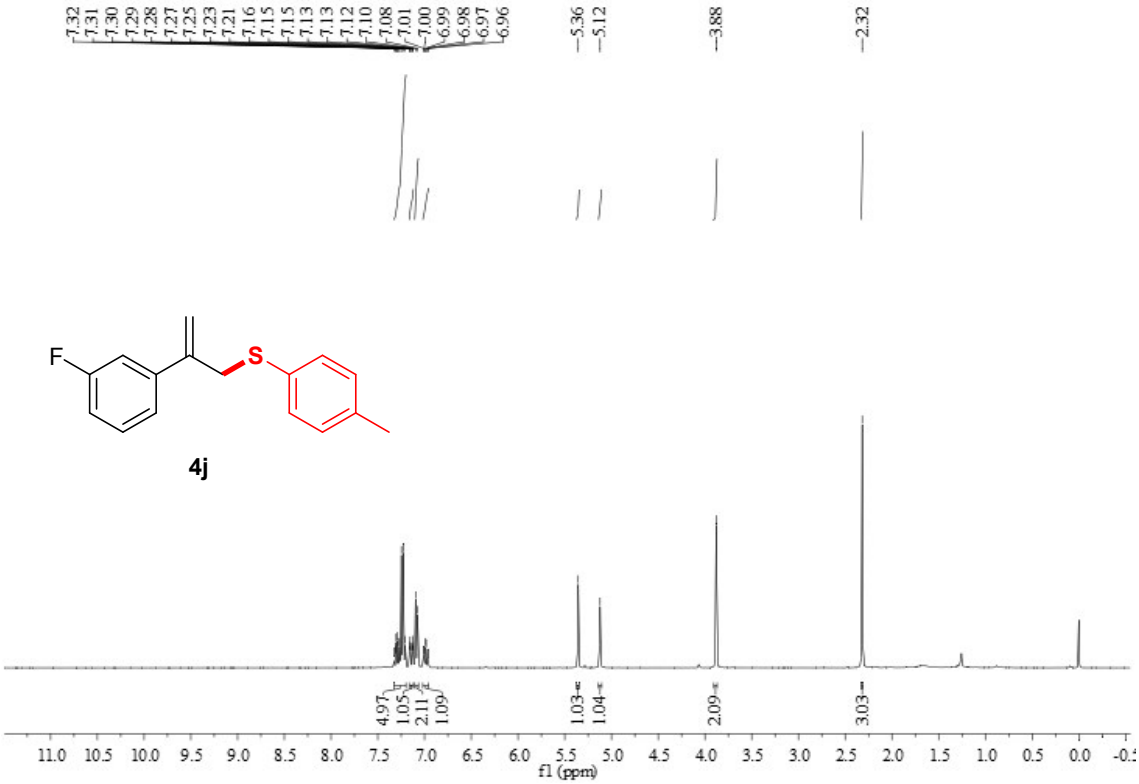
129.72
129.30
118.80
115.63
113.06
112.29
77.32
77.00
76.68
55.20
40.25
21.01
O
S
4i
f1 (ppm)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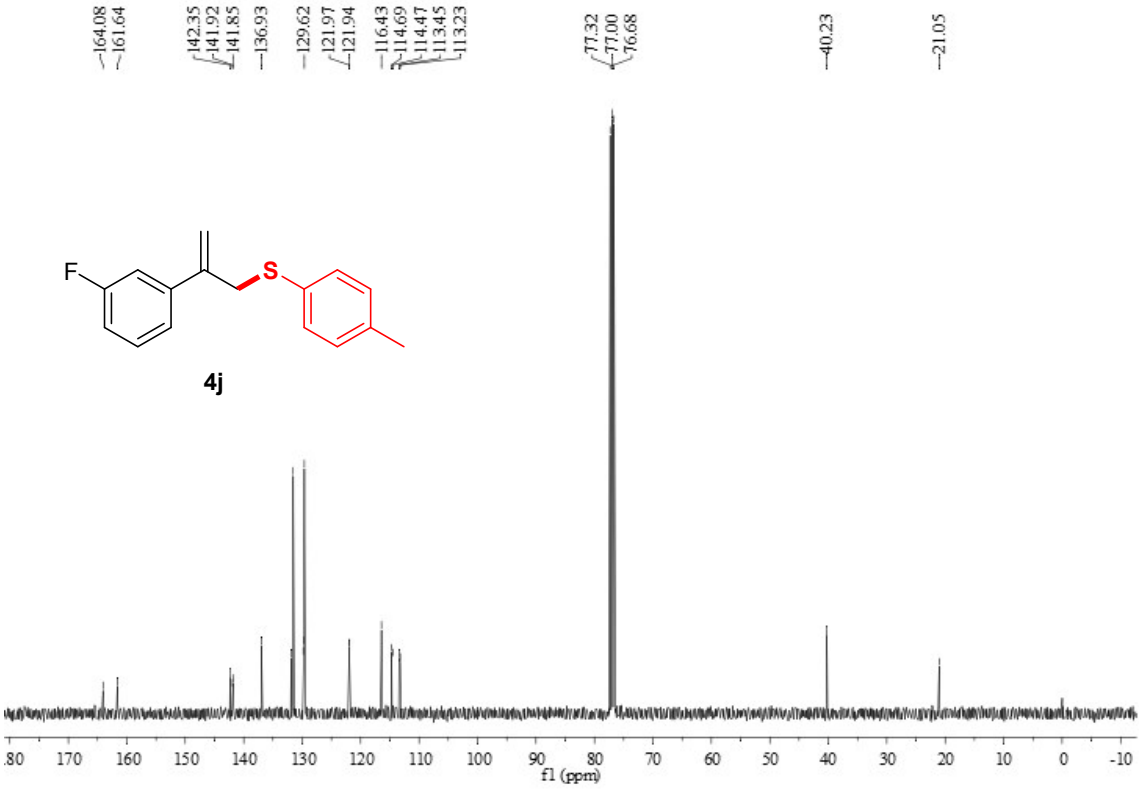
7.23
7.21
7.16
7.15
7.15
7.13
7.13
7.12
7.10
7.08
7.01
7.00
6.99
6.98
6.97
6.96
5.36
5.12
3.88
2.32
F
S
4j
4.97
1.05
2.11
1.09
1.03
1.04
2.09
3.03
f1 (ppm)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136.93
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121.97
121.94
116.43
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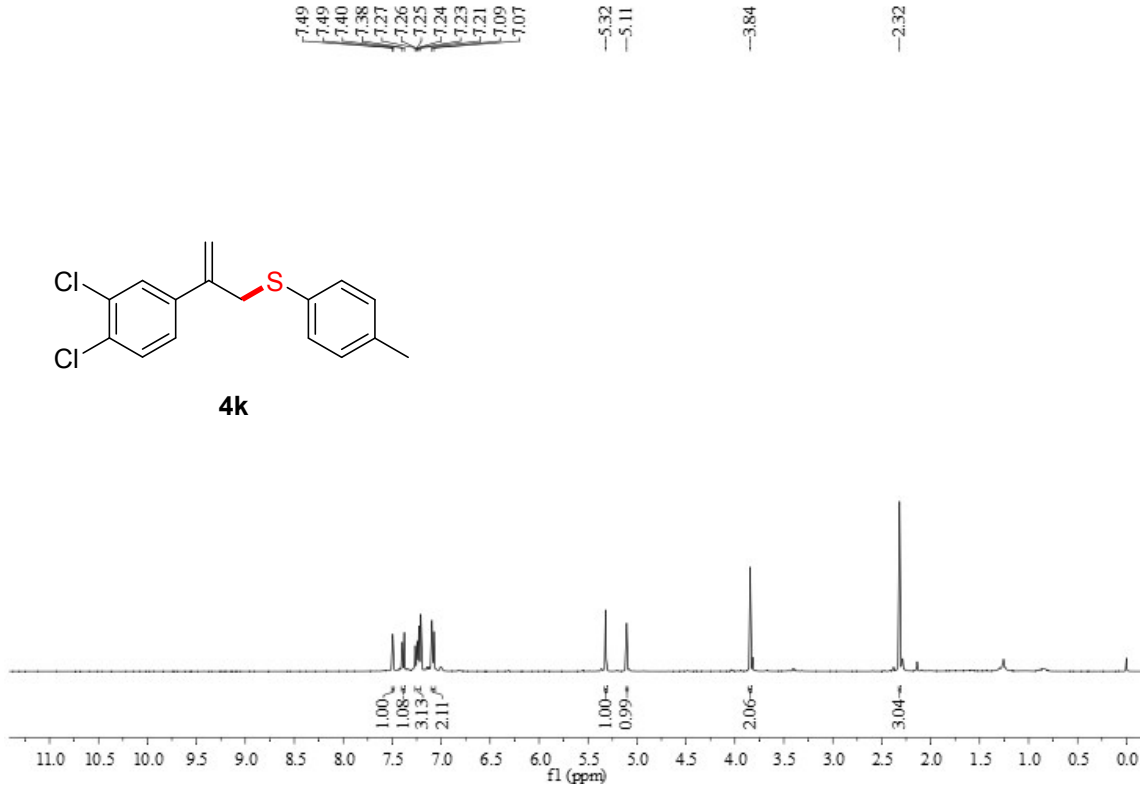
113.45
113.23
77.32
77.00
76.68
40.23
21.05
F
S
f1 (ppm)

4j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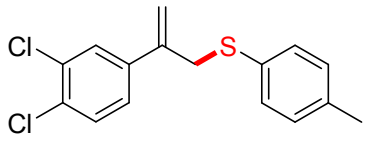
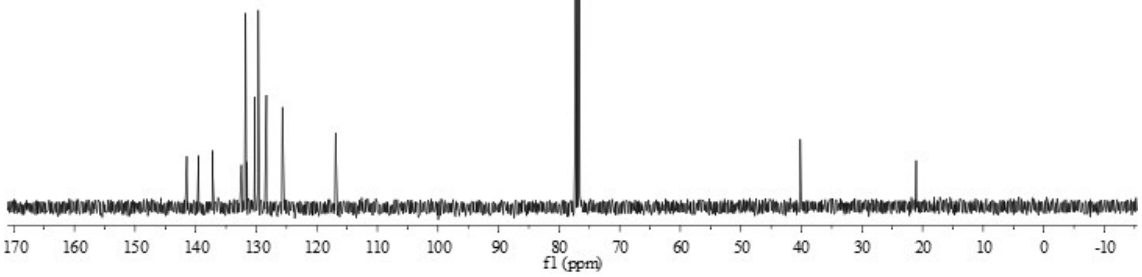
7.27
7.26
7.25
7.24
7.23
7.21
7.09
7.07
5.32
5.11
3.84
2.32
Cl
Cl
S
1.00
1.08
3.13
2.11
1.00
0.99
2.06
3.04
f1 (ppm)

4k


141.46
139.53
137.16
131.75
131.50
129.66
125.67
116.89
77.32
77.00
76.68
40.19
21.06


Cl
Cl
S

4k


170
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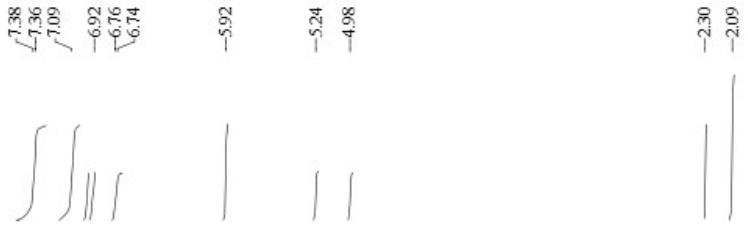
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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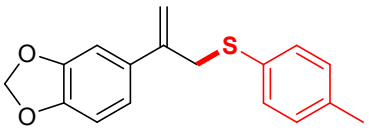
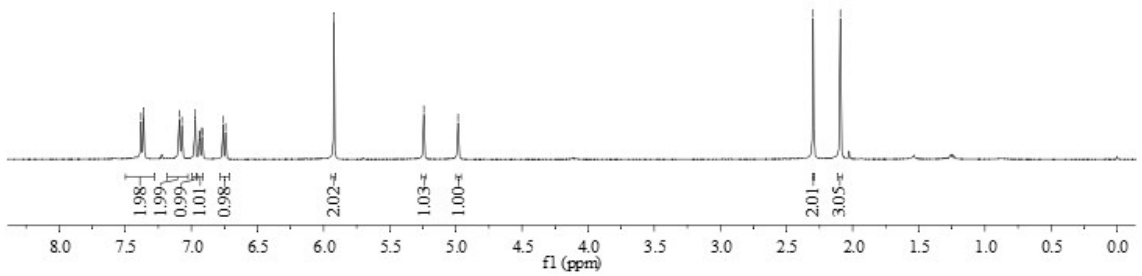
7.09
6.92
6.76
6.74
5.92
5.24
4.98
2.30
2.09


O
O
S

4l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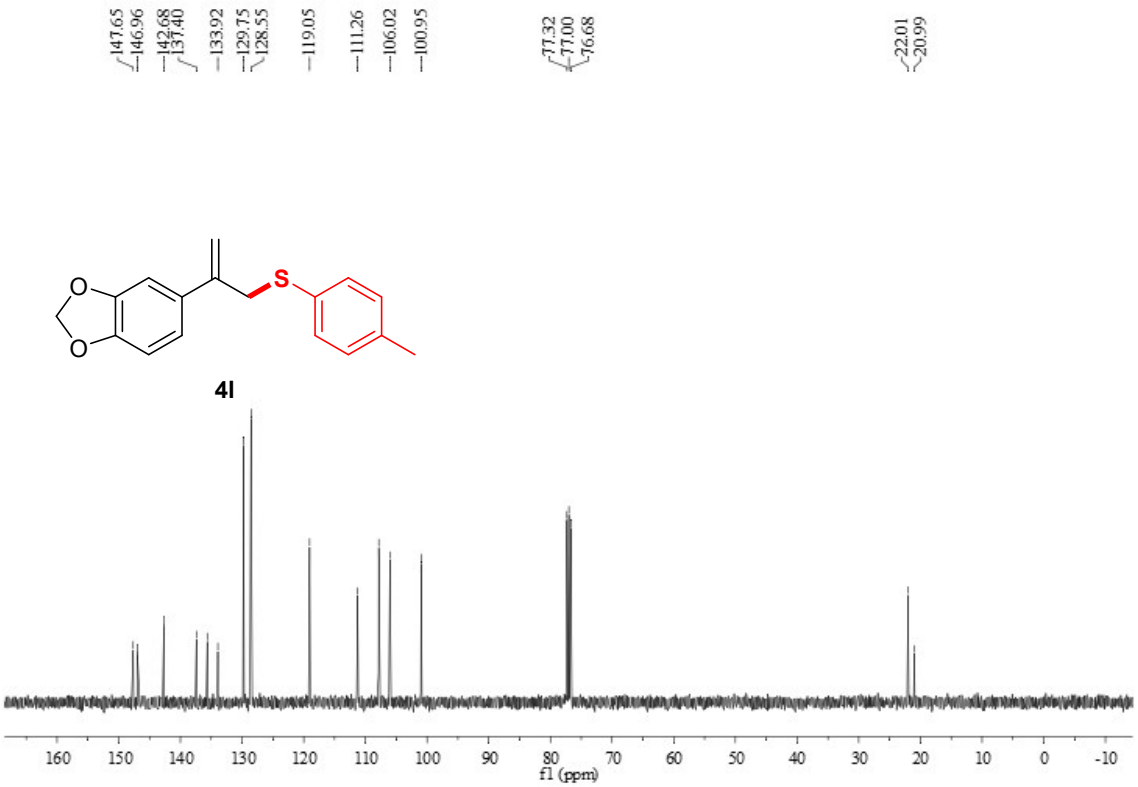
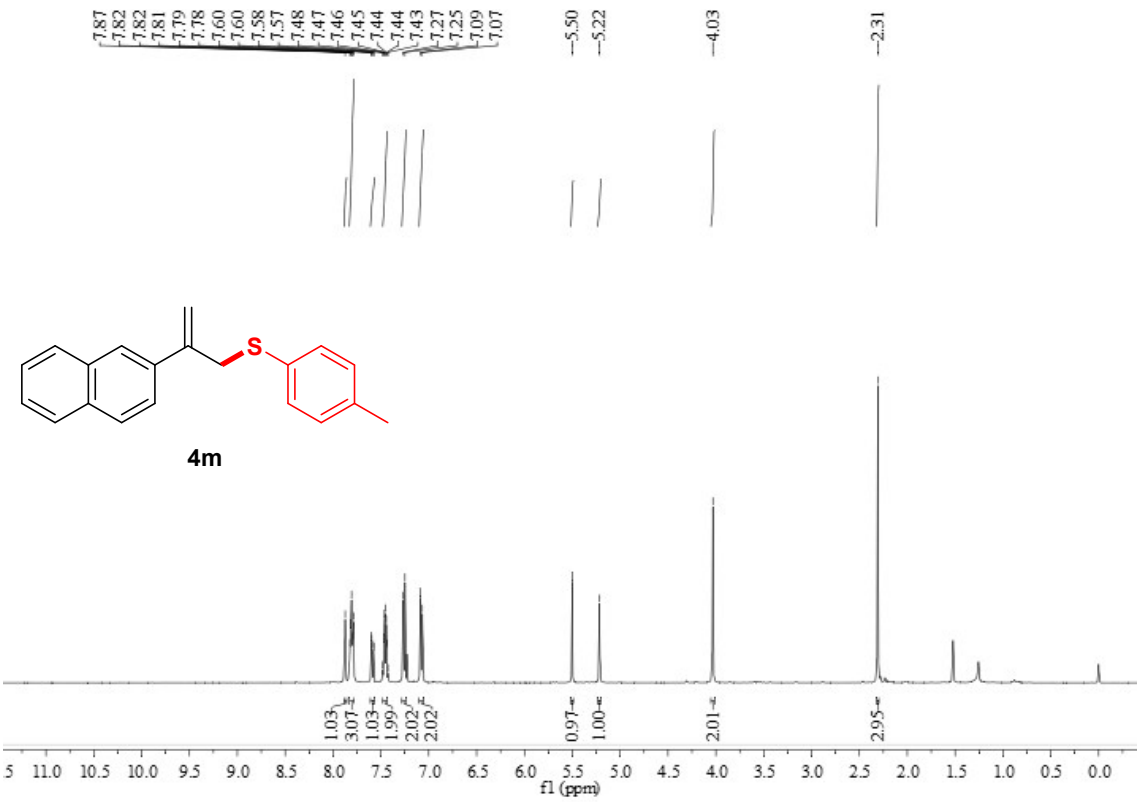
1.01
0.98
2.02
1.03
1.00
2.01
3.05
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


147.65
146.96
142.68
137.40
133.92
129.75
128.55
119.05
111.26
106.02
100.95
77.32
77.00
76.68
22.01
20.99
O
O
S
4l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.82
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7.60
7.58
7.57
7.48
7.47
7.46
7.45
7.44
7.44
7.43
7.27
7.25
7.09
7.07
5.50
5.22
4.03
2.31
S
4m
1.03
3.07
1.03
1.99
2.02
2.02
0.97
1.00
2.01
2.95
5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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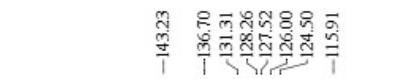
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


143.23
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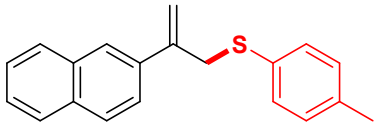
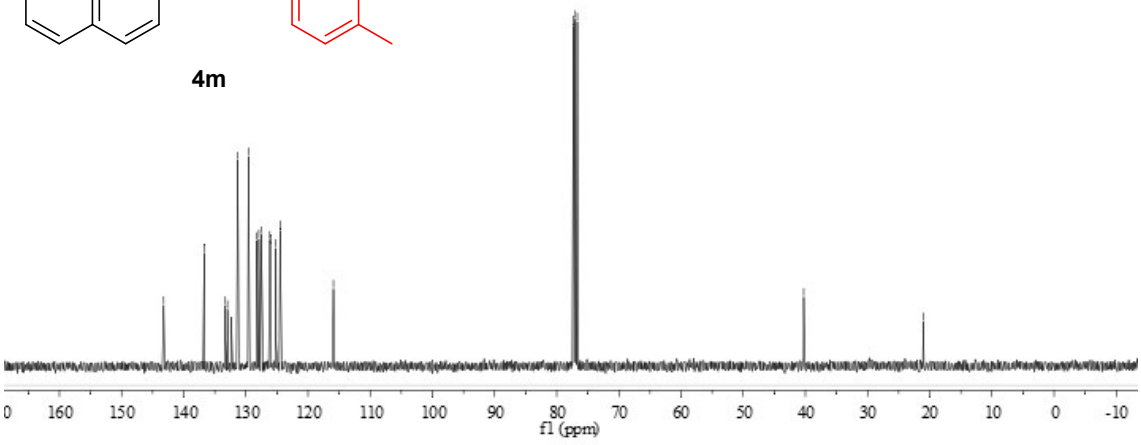
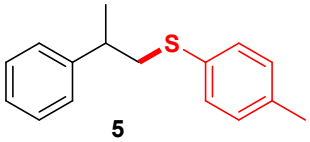
128.26
127.52
126.00
124.50
115.91
77.32
77.00
76.68
40.27
21.03


S

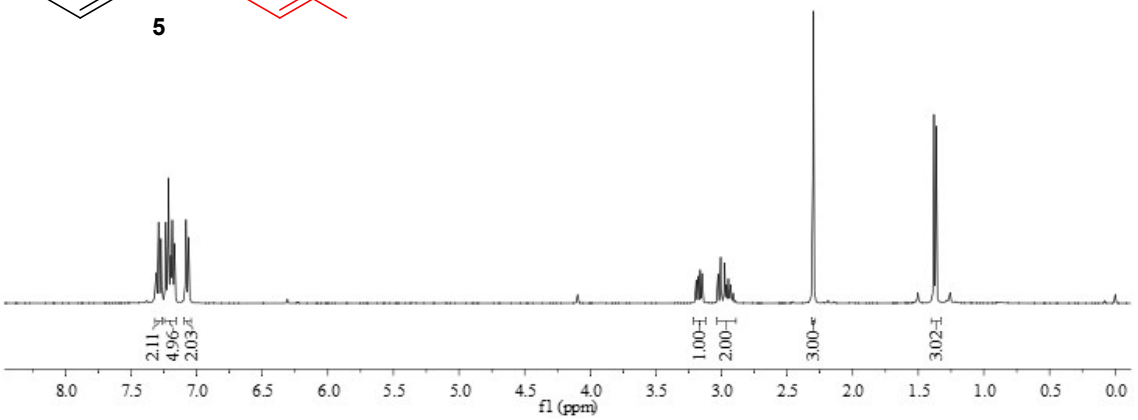
4m

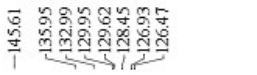

0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

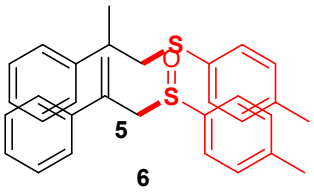

7.31
7.29
7.27
7.23
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.08
7.06
3.19
3.18
3.16
3.15
3.03
3.01
3.00
2.98
2.96
2.95
2.93
2.91
2.30
1.38
1.36

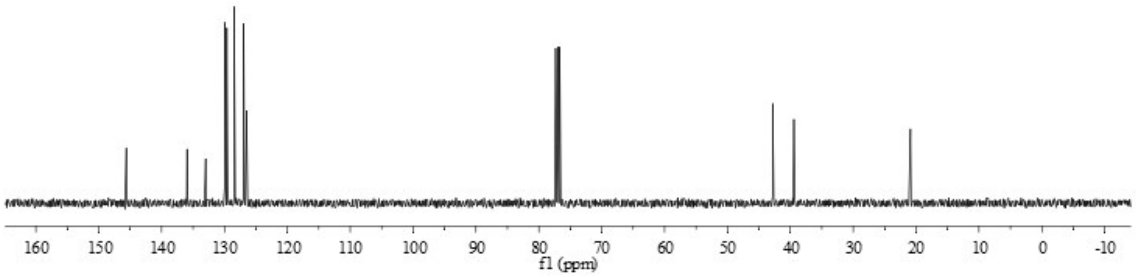

S

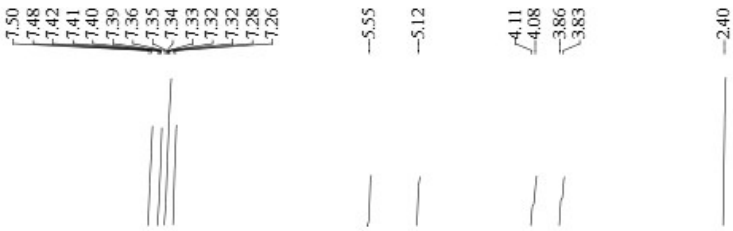
5

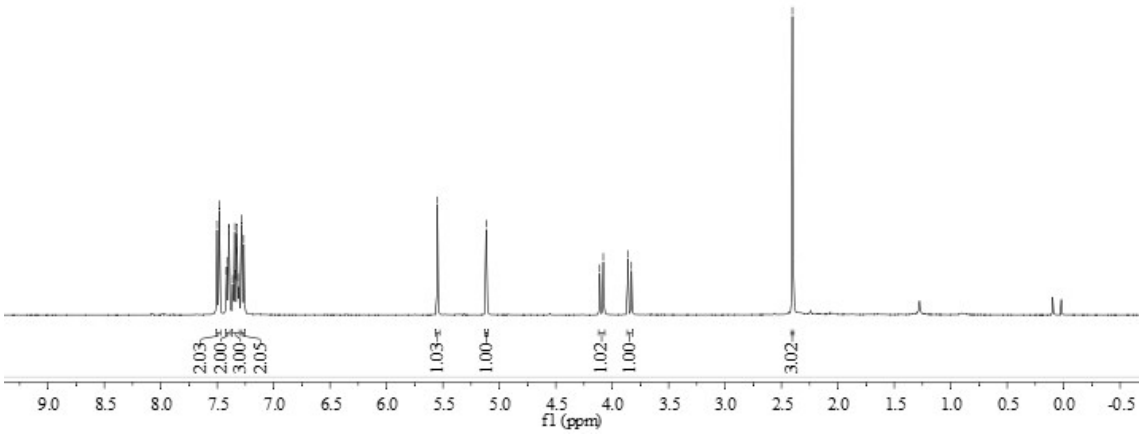

2.11
4.96
2.03
1.00
2.00
3.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

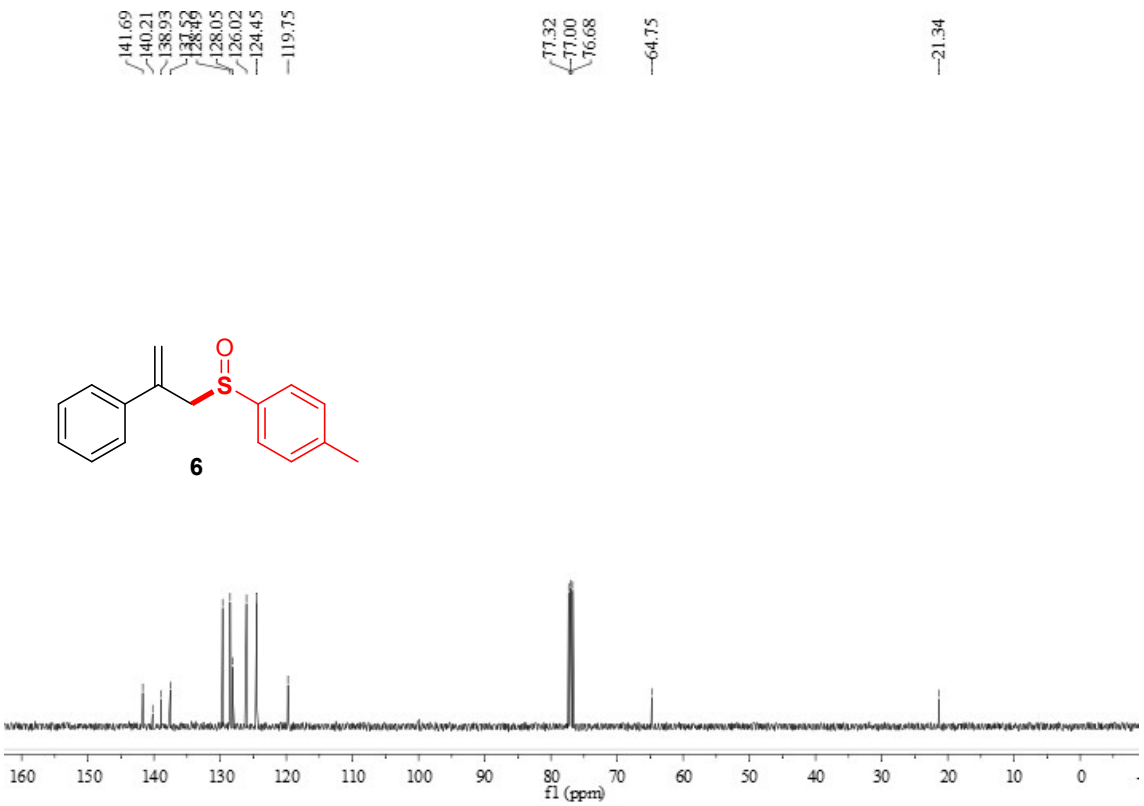

145.61
135.95
132.99
129.95
129.62
128.45
126.93
126.47
77.32
77.00
76.68
42.79
39.43
20.90

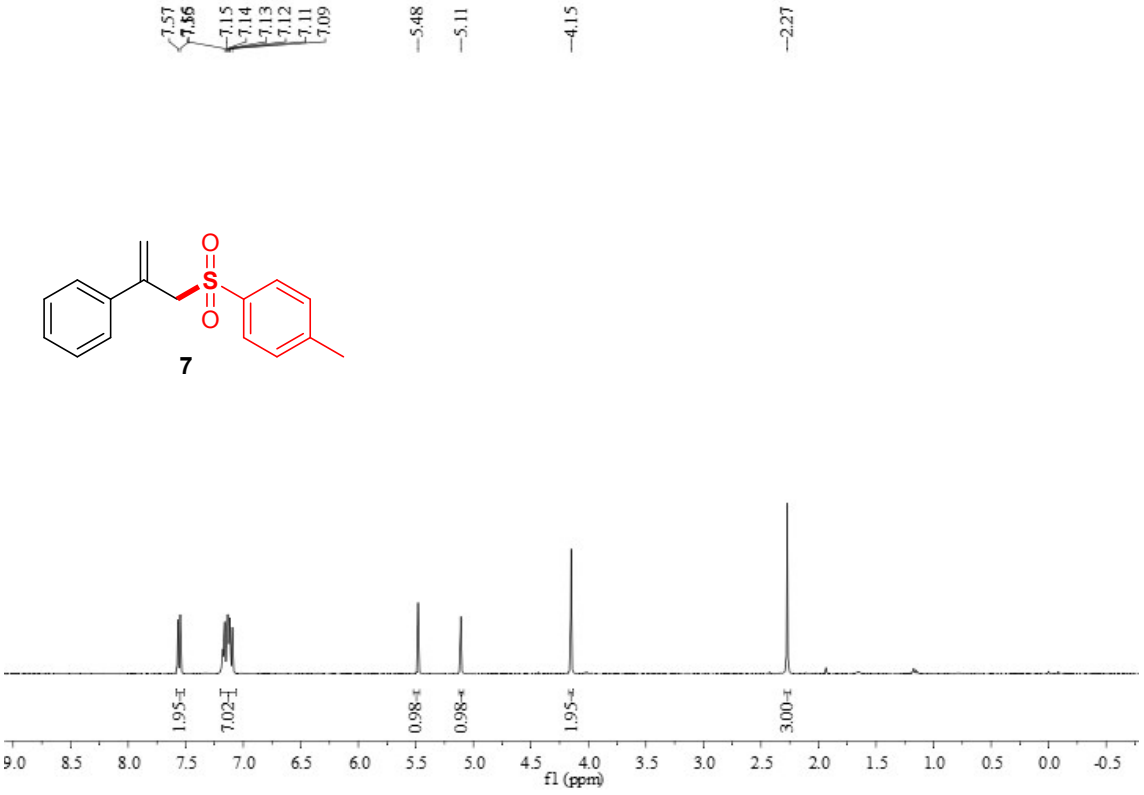

S
O
S
5
6

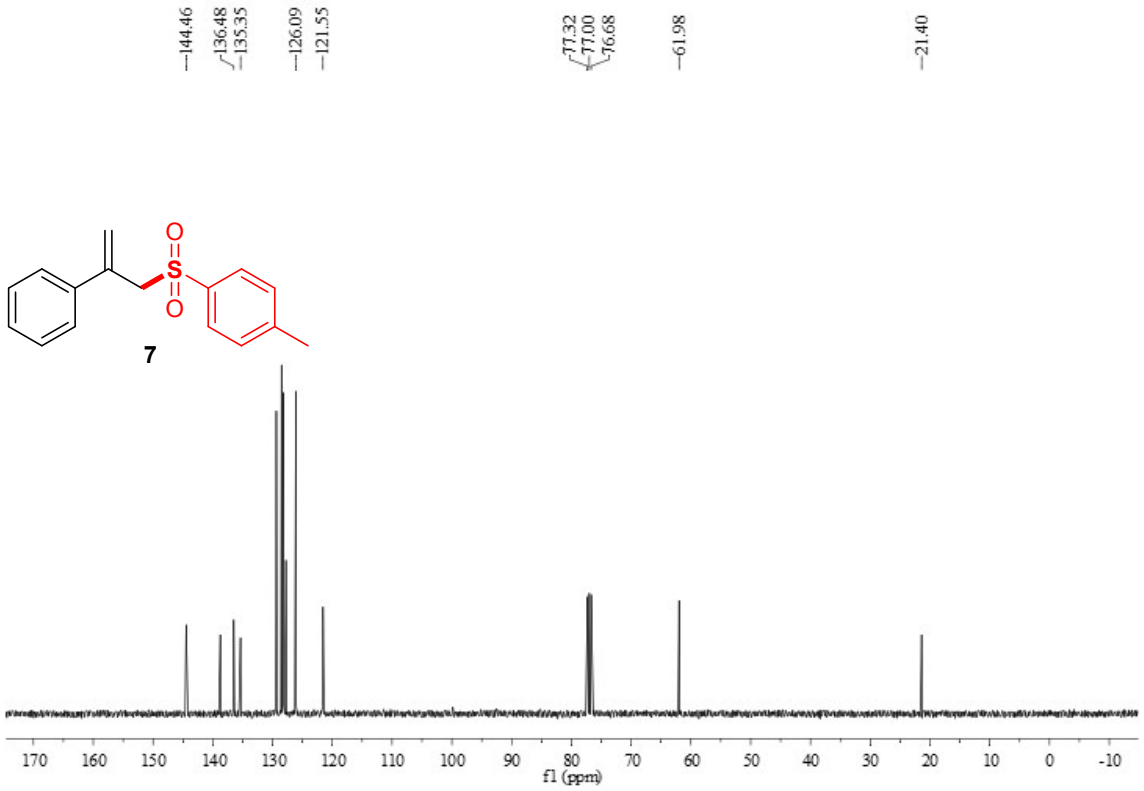

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

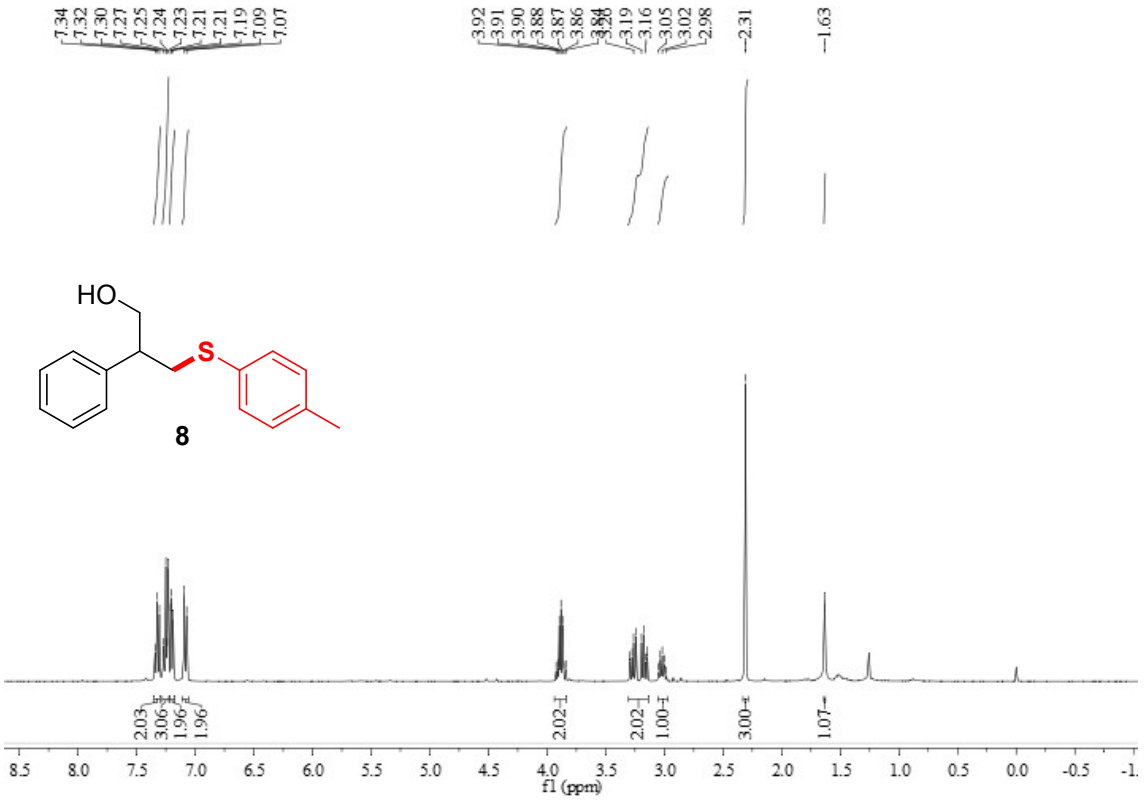

7.50
7.48
7.42
7.41
7.40
7.39
7.36
7.35
7.34
7.33
7.32
7.32
7.28
7.26
5.55
5.12
4.11
4.08
3.86
3.83
2.40


2.03
2.00
3.00
2.05
1.03
1.00
1.02
1.00
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

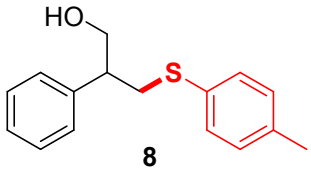

141.69
140.21
138.93
128.05
126.02
124.45
119.75
77.32
77.00
76.68
64.75
21.34
6
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.57
7.56
7.15
7.14
7.13
7.12
7.11
7.09
5.48
5.11
4.15
2.27
7
1.95
7.02
0.98
0.98
1.95
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

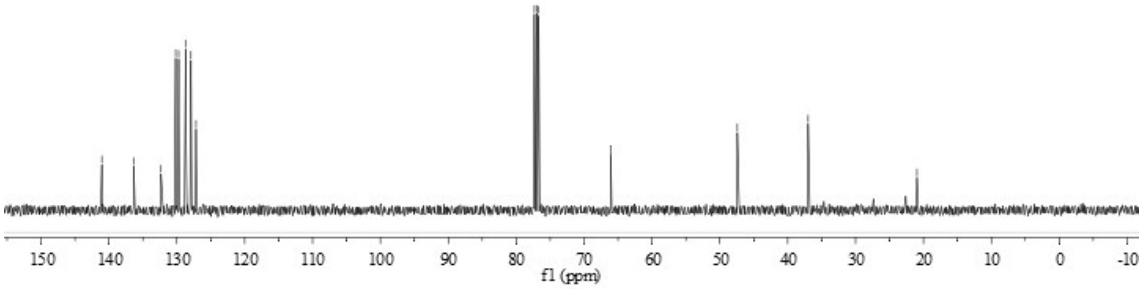

144.46
136.48
135.35
126.09
121.55
77.32
77.00
76.68
61.98
21.40
7
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

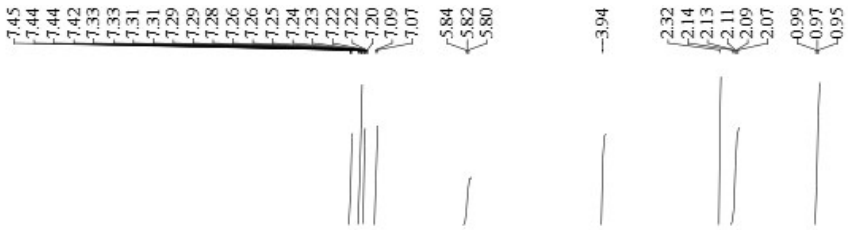

7.34
7.32
7.30
7.27
7.25
7.24
7.23
7.21
7.21
7.19
7.09
7.07
3.92
3.91
3.90
3.88
3.87
3.86
3.84
3.84
3.19
3.16
3.05
3.02
2.98
2.31
1.63
HO
S
8
2.03
3.06
1.96
1.96
2.02
2.02
1.00
3.00
1.07
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

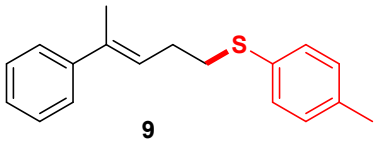

141.05
136.31
132.32
130.17
129.71
128.71
127.91
127.17
77.32
77.00
76.68
66.04
47.42
36.98
20.96


HO
S

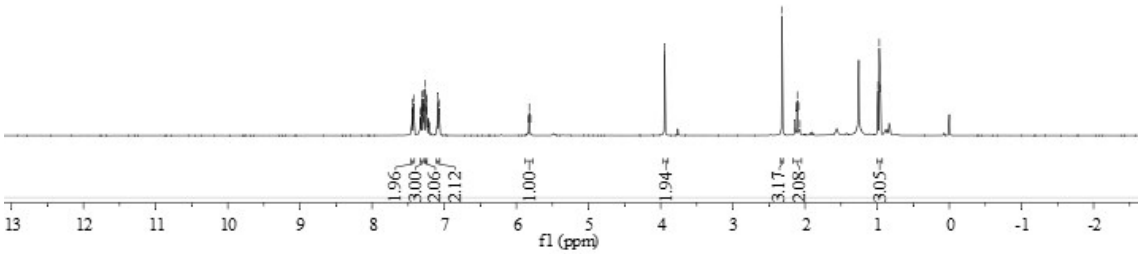
8

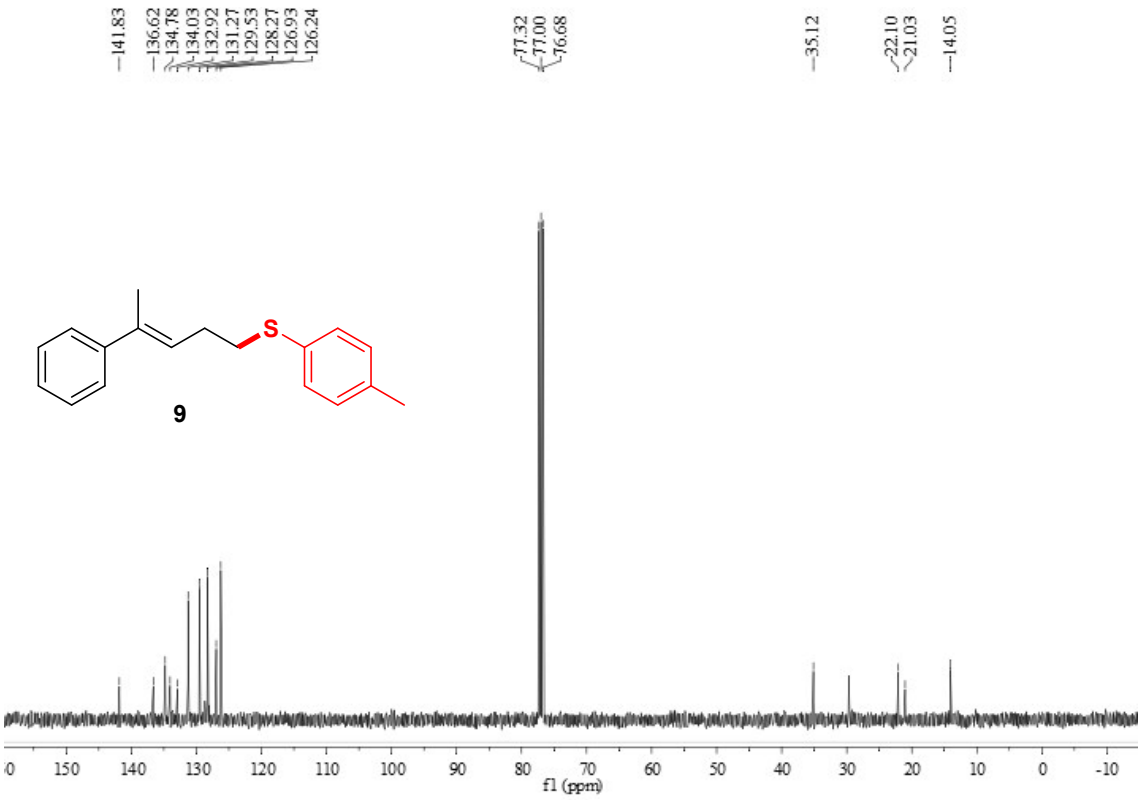

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.45
7.44
7.44
7.42
7.33
7.33
7.31
7.31
7.29
7.29
7.28
7.26
7.26
7.25
7.24
7.23
7.22
7.22
7.20
7.09
7.07
5.84
5.82
5.80
3.94
2.32
2.14
2.13
2.11
2.09
2.07
0.99
0.97
0.95


S

9


1.96
3.00
2.06
2.12
1.00
1.94
3.17
2.08
3.05
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


141.83
136.62
134.78
134.03
132.92
131.27
129.53
128.27
126.93
126.24
77.32
77.00
76.68
35.12
22.10
21.03
14.05
S
9
0
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)